



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:02 AM GMT

PDB ID : 3GPT
Title : Crystal structure of the yeast 20S proteasome in complex with Salinosporamide derivatives: slow substrate ligand
Authors : Groll, M.; Macherla, V.R.; Manam, R.R.; Arthur, K.A.M.; Potts, C.B.
Deposited on : 2009-03-23
Resolution : 2.41 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

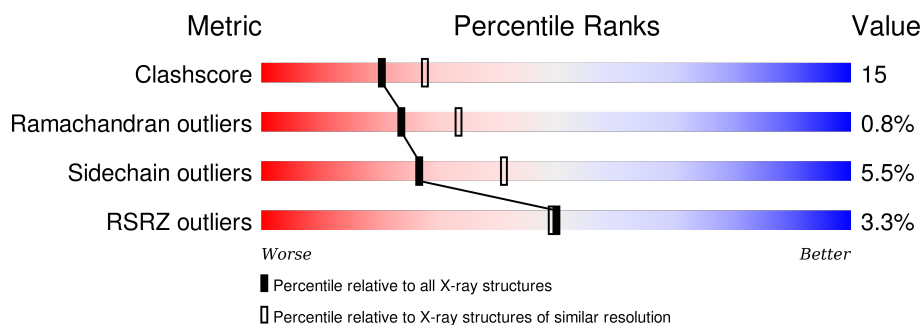
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (2.44-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	<div> <div></div> <div>78% 21% .</div> </div>
1	O	250	<div> <div></div> <div>78% 21% .</div> </div>
2	B	244	<div> <div></div> <div>65% 30% 5%</div> </div>
2	P	244	<div> <div></div> <div>66% 28% 5%</div> </div>
3	C	241	<div> <div></div> <div>62% 34% .</div> </div>
3	Q	241	<div> <div></div> <div>60% 36% .</div> </div>
4	D	242	<div> <div></div> <div>72% 24% .</div> </div>

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Mol	Chain	Length	Quality of chain
4	R	242	
5	E	233	
5	S	233	
6	F	244	
6	T	244	
7	G	243	
7	U	243	
8	H	222	
8	V	222	
9	I	204	
9	W	204	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	1	233	
13	M	233	
14	2	196	
14	N	196	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	GPT	H	224	-	-	-	X

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 51018 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome component Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome component Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1905	1201	321	380	3			
2	P	244	Total	C	N	O	S	0	0	0
			1905	1201	321	380	3			

- Molecule 3 is a protein called Proteasome component PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			

- Molecule 4 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			
4	R	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			

- Molecule 5 is a protein called Proteasome component PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			
5	S	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

- Molecule 6 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			
6	T	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			

- Molecule 7 is a protein called Proteasome component C7-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
7	U	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			

- Molecule 8 is a protein called Proteasome component PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			
8	V	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			

- Molecule 9 is a protein called Proteasome component PUP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called Proteasome component C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

- Molecule 11 is a protein called Proteasome component PRE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1643	1045	280	311	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1643	1045	280	311	7			

- Molecule 12 is a protein called Proteasome component C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

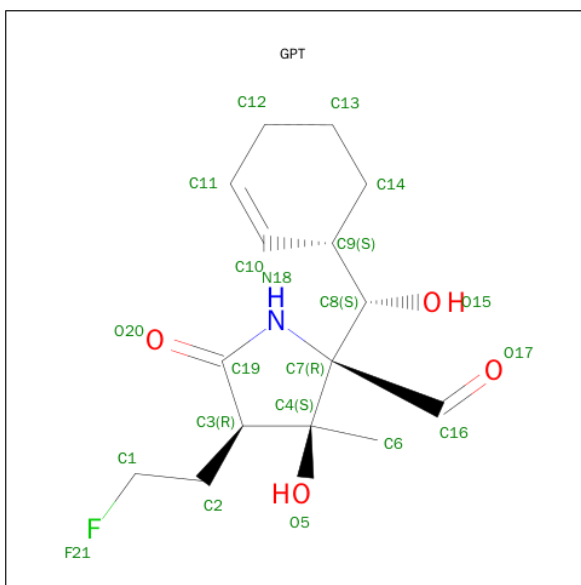
- Molecule 13 is a protein called Proteasome component PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	1	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called Proteasome component PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	2	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is (2R,3S,4R)-2-[(S)-(1S)-CYCLOHEX-2-EN-1-YL(HYDROXY)METHYL]-4-(2-FLUOROETHYL)-3-HYDROXY-3-METHYL-5-OXOPYRROLIDINE-2-CARBALDEHYDE (three-letter code: GPT) (formula: C₁₅H₂₂FNO₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	H	1	Total	C	F	N	O	0	0
			21	15	1	1	4		
15	K	1	Total	C	F	N	O	0	0
			21	15	1	1	4		
15	N	1	Total	C	F	N	O	0	0
			21	15	1	1	4		
15	V	1	Total	C	F	N	O	0	0
			21	15	1	1	4		
15	Y	1	Total	C	F	N	O	0	0
			21	15	1	1	4		
15	2	1	Total	C	F	N	O	0	0
			21	15	1	1	4		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	58	Total	O	0	0
			58	58		
16	B	38	Total	O	0	0
			38	38		
16	C	44	Total	O	0	0
			44	44		
16	D	39	Total	O	0	0
			39	39		
16	E	23	Total	O	0	0
			23	23		
16	F	47	Total	O	0	0
			47	47		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	58	Total O 58 58	0	0
16	H	54	Total O 54 54	0	0
16	I	69	Total O 69 69	0	0
16	J	51	Total O 51 51	0	0
16	K	49	Total O 49 49	0	0
16	L	58	Total O 58 58	0	0
16	M	73	Total O 73 73	0	0
16	N	56	Total O 56 56	0	0
16	O	34	Total O 34 34	0	0
16	P	29	Total O 29 29	0	0
16	Q	27	Total O 27 27	0	0
16	R	31	Total O 31 31	0	0
16	S	19	Total O 19 19	0	0
16	T	39	Total O 39 39	0	0
16	U	62	Total O 62 62	0	0
16	V	49	Total O 49 49	0	0
16	W	62	Total O 62 62	0	0
16	X	45	Total O 45 45	0	0
16	Y	48	Total O 48 48	0	0
16	Z	53	Total O 53 53	0	0
16	1	75	Total O 75 75	0	0

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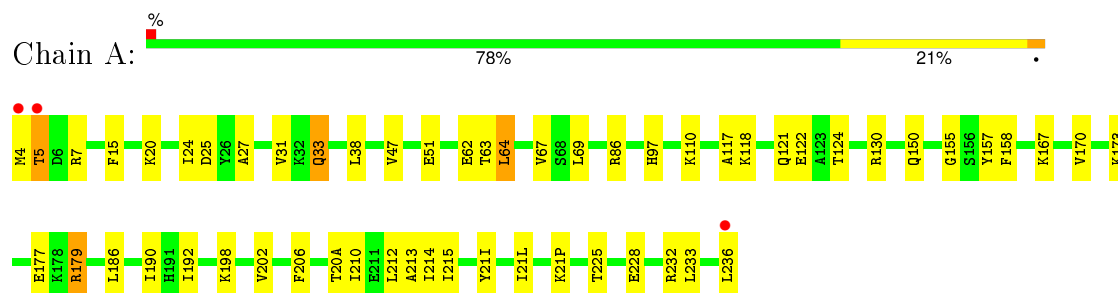
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	2	56	Total	O	0	0
			56	56		

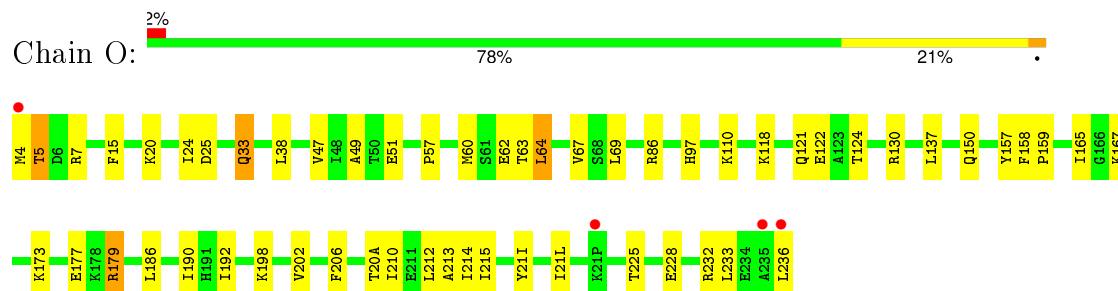
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

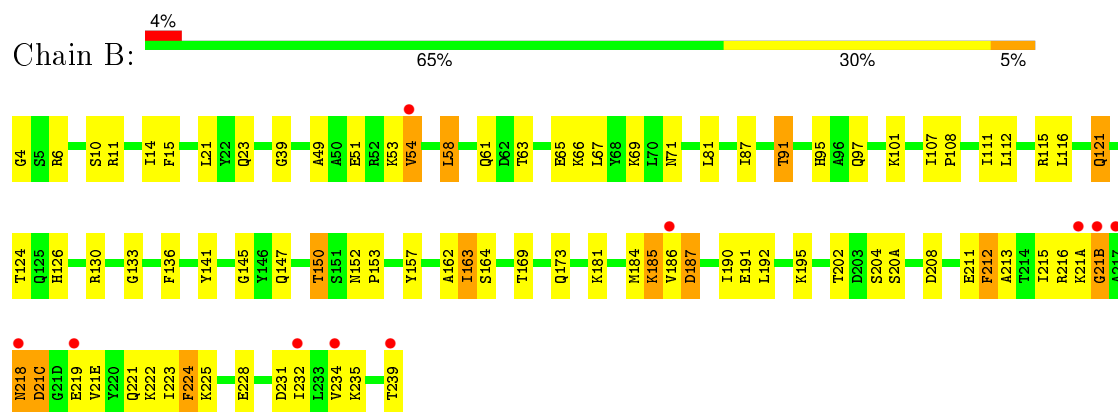
• Molecule 1: Proteasome component Y7



• Molecule 1: Proteasome component Y7

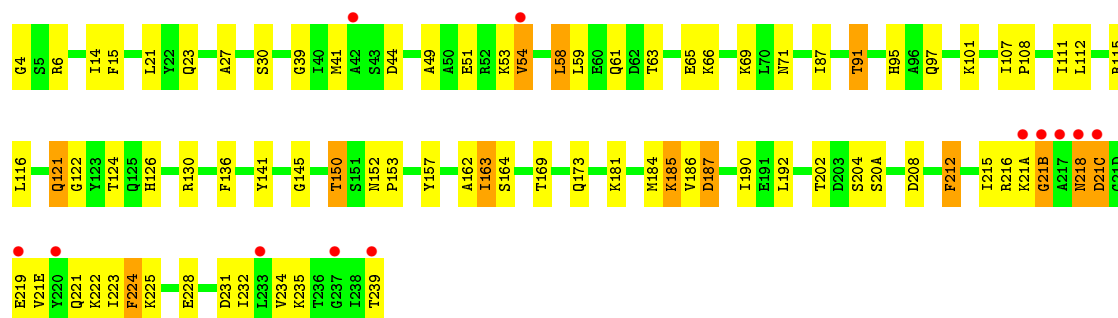


• Molecule 2: Proteasome component Y13

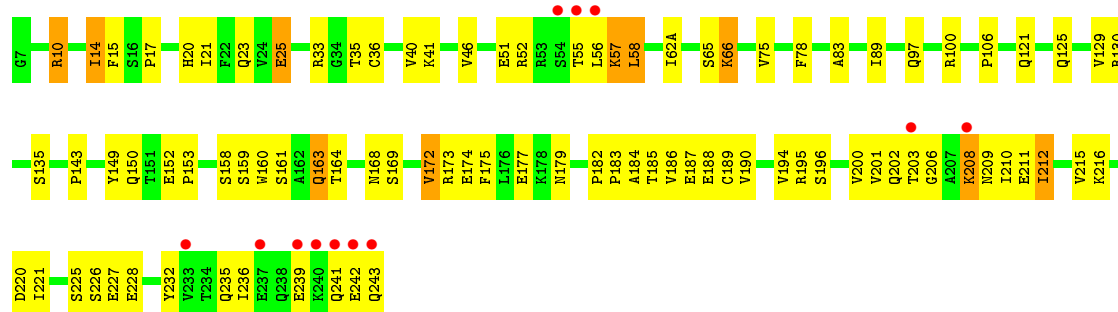


• Molecule 2: Proteasome component Y13

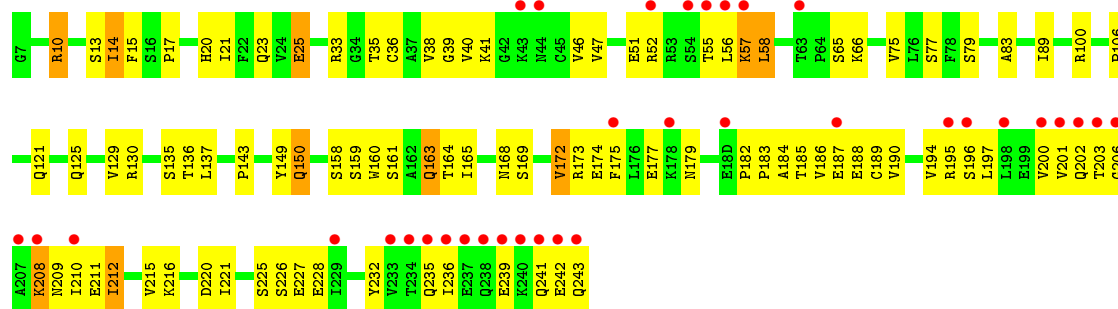




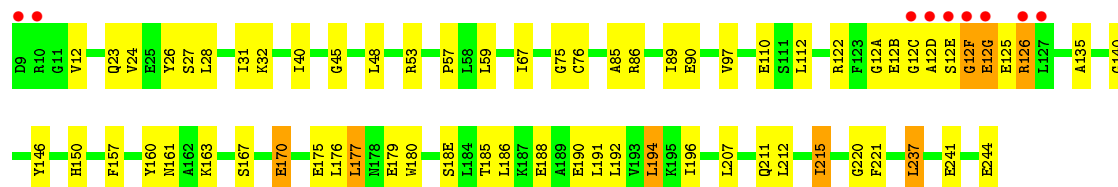
• Molecule 3: Proteasome component PRE6



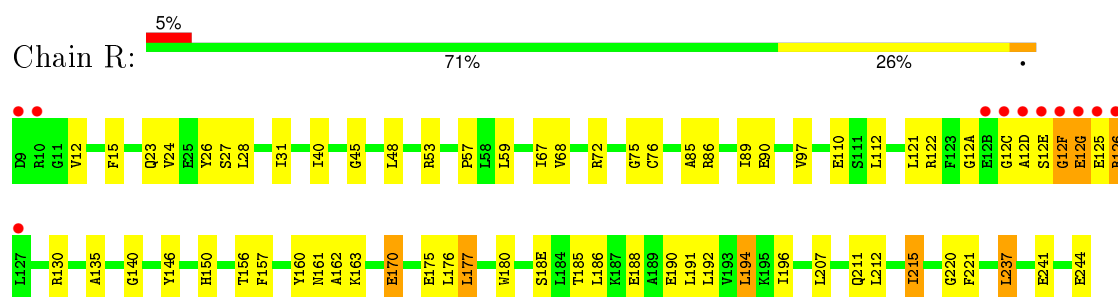
• Molecule 3: Proteasome component PRE6



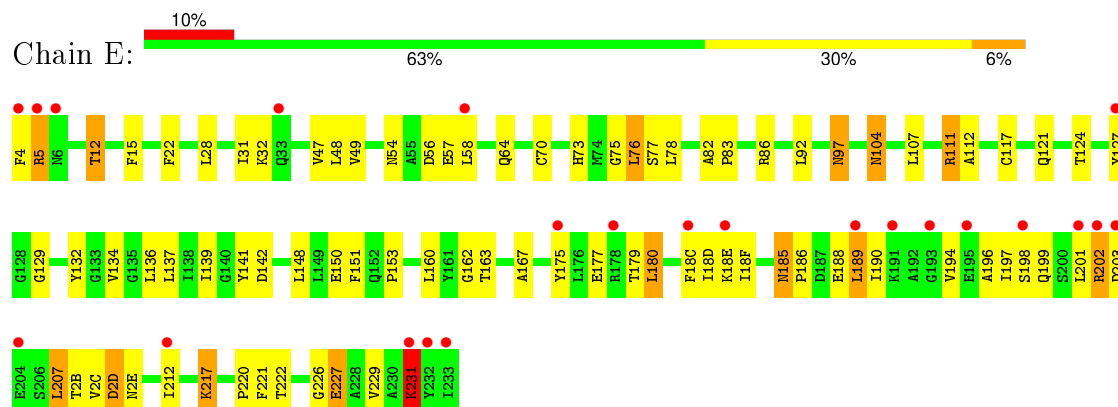
• Molecule 4: Proteasome component PUP2



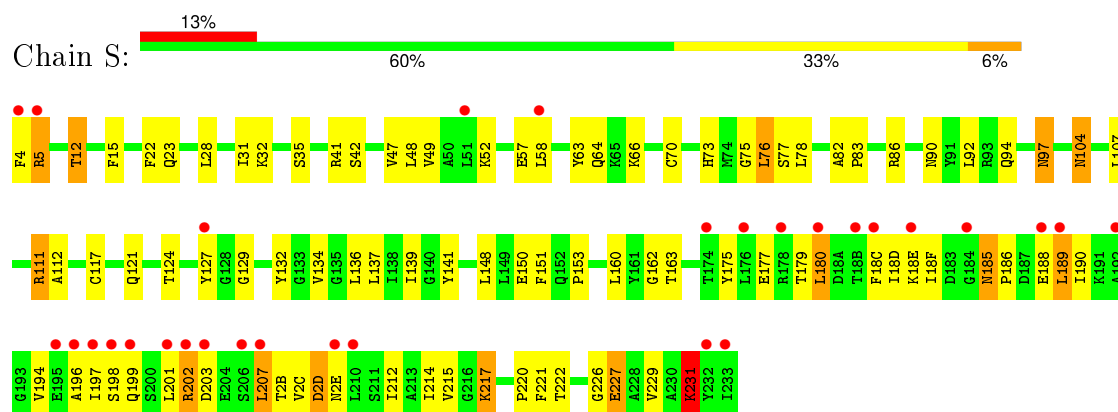
• Molecule 4: Proteasome component PUP2



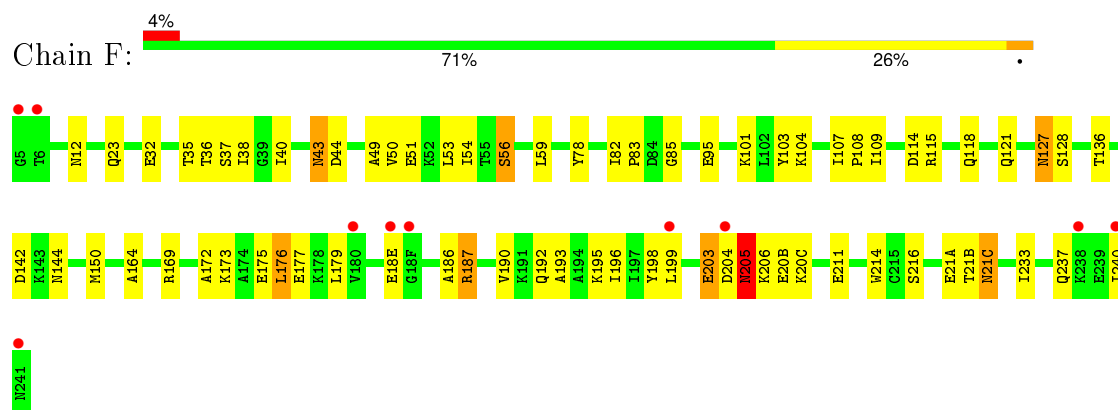
• Molecule 5: Proteasome component PRE5



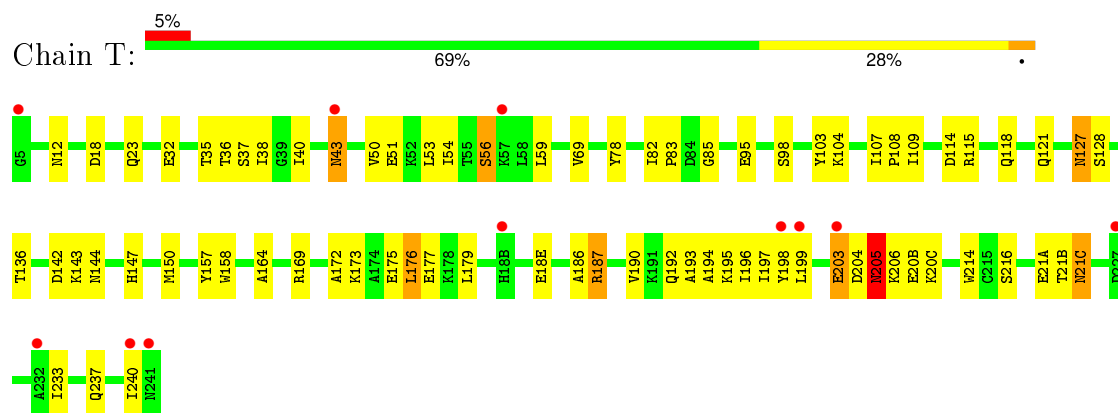
• Molecule 5: Proteasome component PRE5



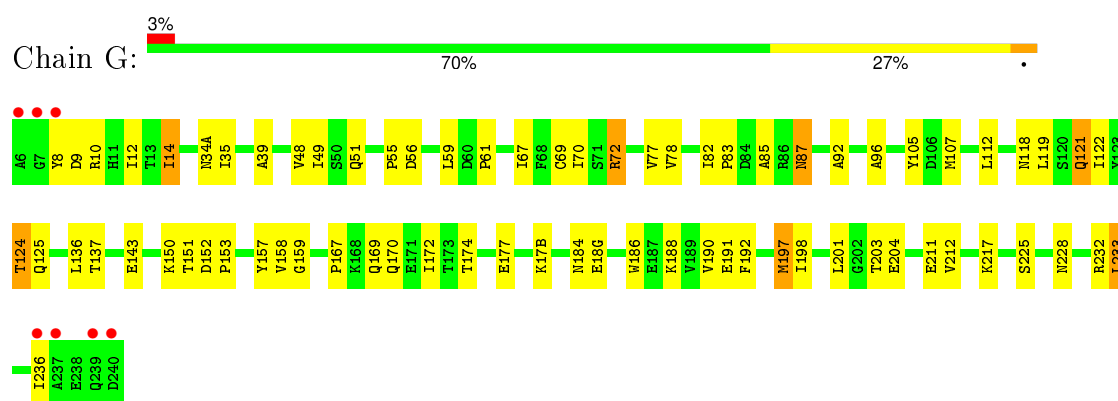
• Molecule 6: Proteasome component C1



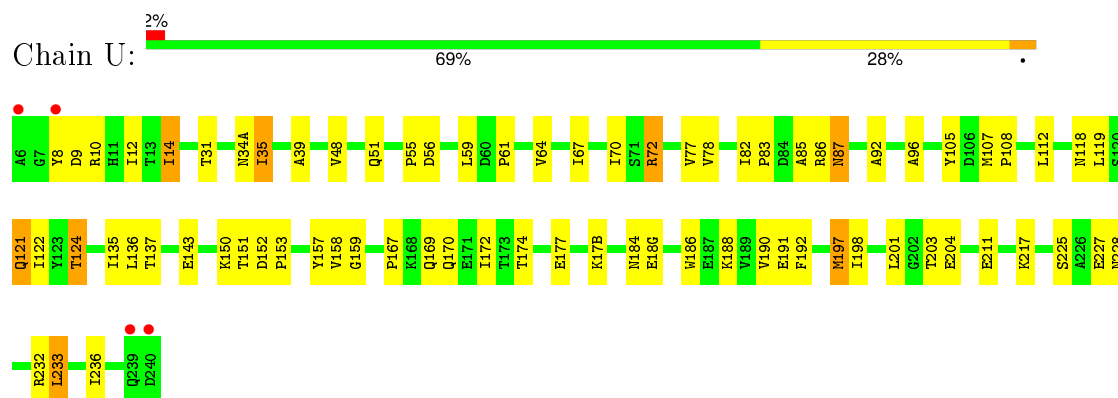
- Molecule 6: Proteasome component C1



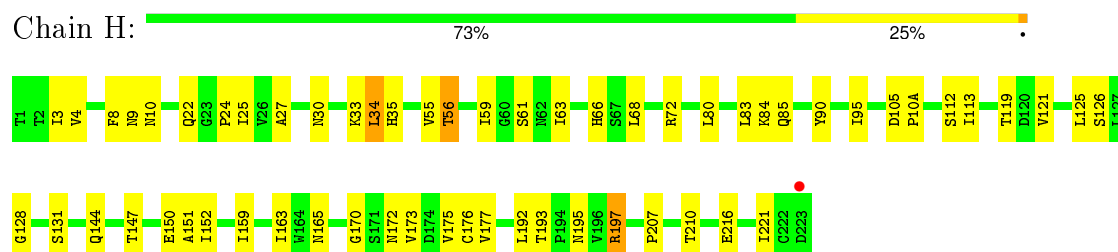
- Molecule 7: Proteasome component C7-alpha



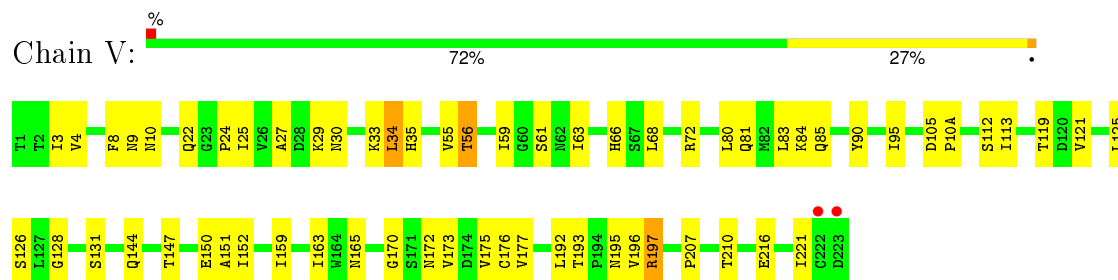
- Molecule 7: Proteasome component C7-alpha



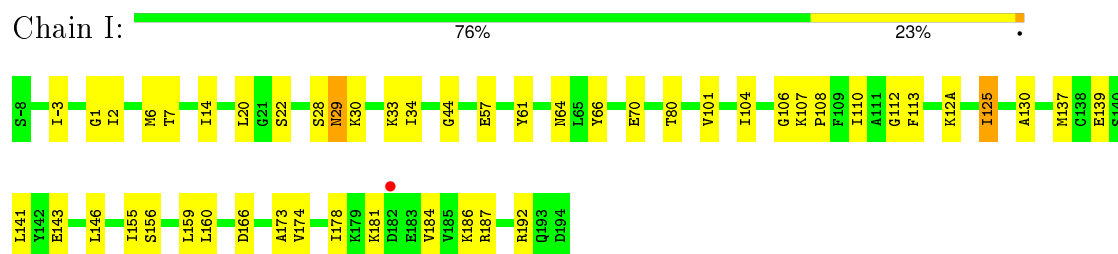
- Molecule 8: Proteasome component PUP1



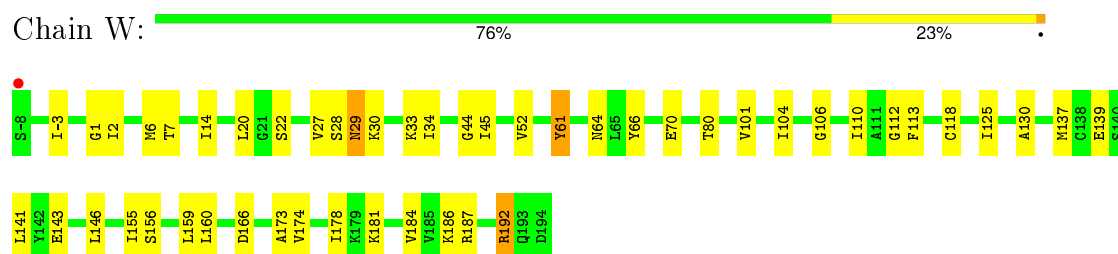
- Molecule 8: Proteasome component PUP1



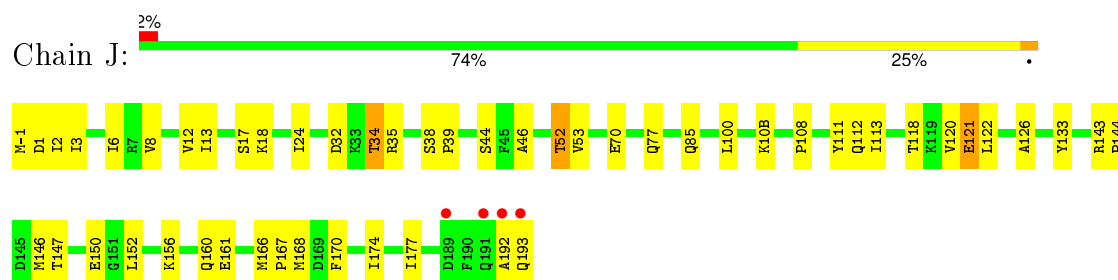
- Molecule 9: Proteasome component PUP3



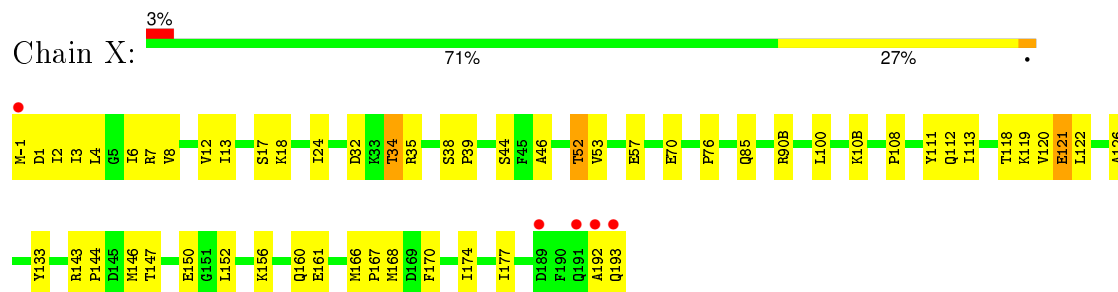
- Molecule 9: Proteasome component PUP3



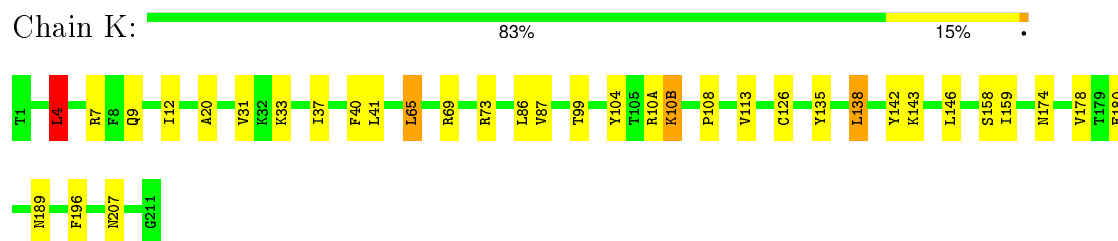
- Molecule 10: Proteasome component C11



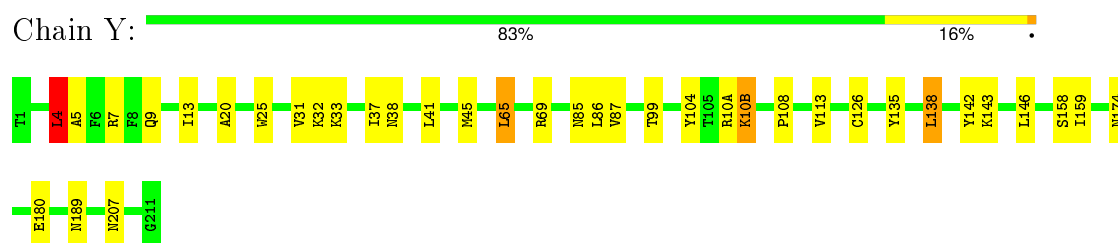
- Molecule 10: Proteasome component C11



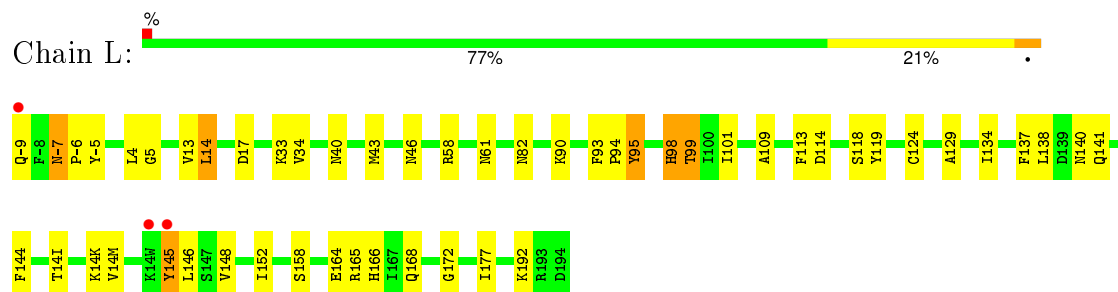
- Molecule 11: Proteasome component PRE2



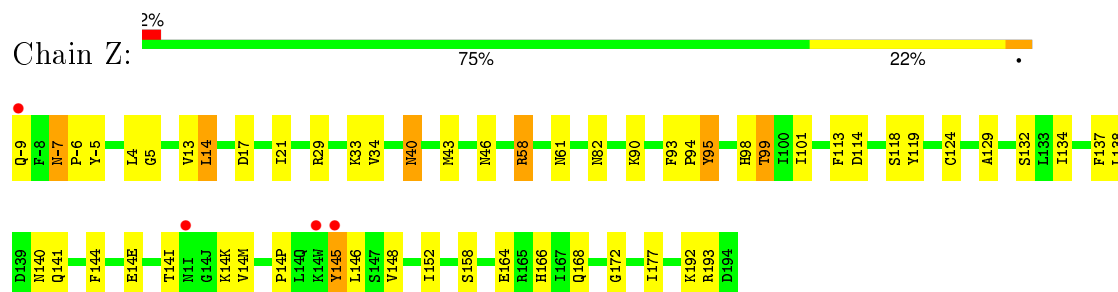
- Molecule 11: Proteasome component PRE2



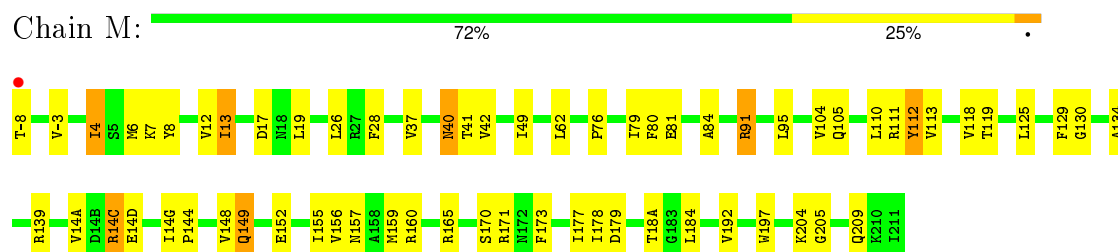
- Molecule 12: Proteasome component C5



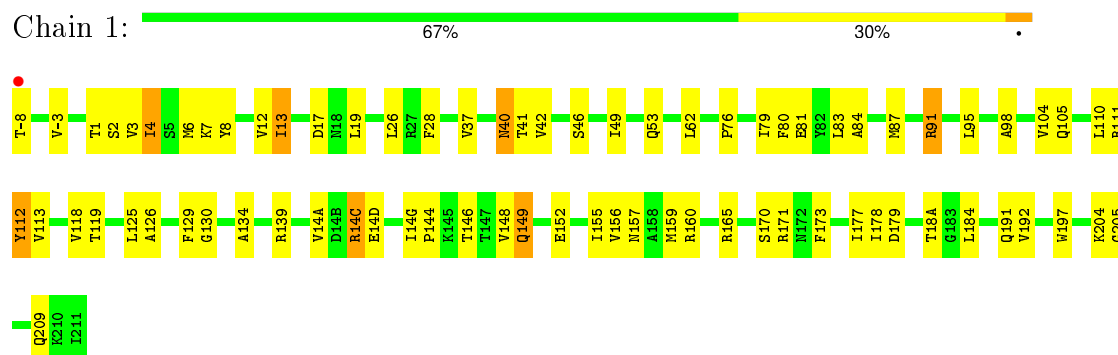
- Molecule 12: Proteasome component C5



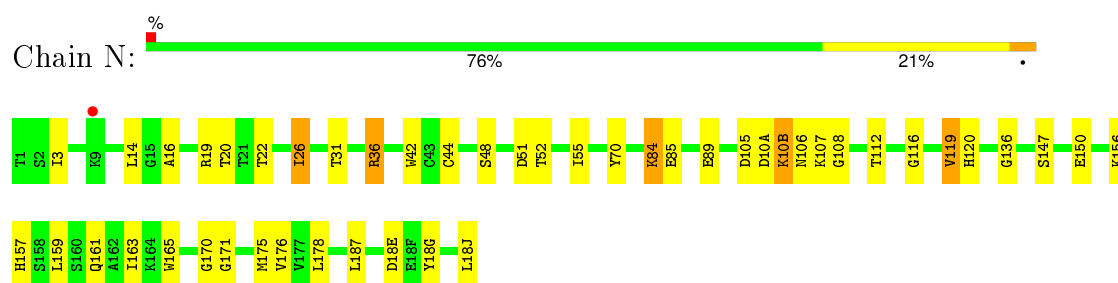
- Molecule 13: Proteasome component PRE4



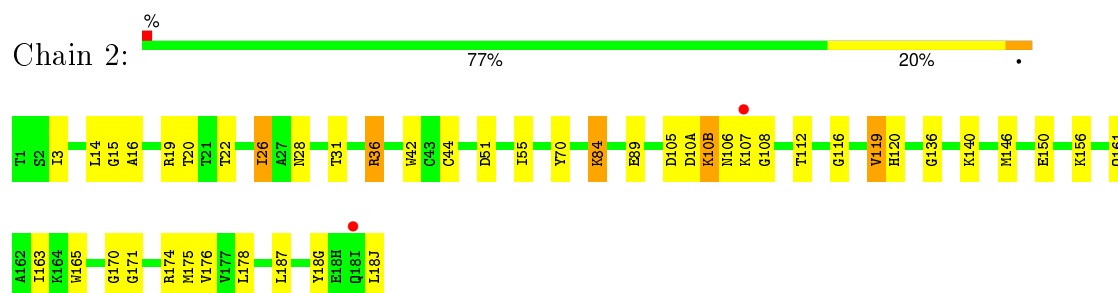
- Molecule 13: Proteasome component PRE4



- Molecule 14: Proteasome component PRE3



- Molecule 14: Proteasome component PRE3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	134.00Å 301.26Å 143.81Å 90.00° 112.56° 90.00°	Depositor
Resolution (Å)	15.00 – 2.41 49.31 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.3 (15.00-2.41) 99.4 (49.31-2.41)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.245 0.216 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.912	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 401845 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	51018	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GPT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.37	0/1952	0.64	1/2642 (0.0%)
1	O	0.37	0/1952	0.64	1/2642 (0.0%)
2	B	0.35	0/1935	0.62	0/2618
2	P	0.37	0/1935	0.63	0/2618
3	C	0.35	0/1920	0.61	0/2598
3	Q	0.35	0/1920	0.61	0/2598
4	D	0.35	0/1887	0.62	0/2541
4	R	0.35	0/1887	0.62	0/2541
5	E	0.35	0/1823	0.59	0/2463
5	S	0.37	0/1823	0.59	0/2463
6	F	0.36	0/1937	0.61	0/2614
6	T	0.37	0/1937	0.62	0/2614
7	G	0.41	0/1959	0.64	0/2652
7	U	0.40	0/1959	0.64	0/2652
8	H	0.38	0/1716	0.66	0/2326
8	V	0.36	0/1716	0.66	0/2326
9	I	0.39	0/1611	0.66	0/2174
9	W	0.40	0/1611	0.67	0/2174
10	J	0.36	0/1613	0.65	0/2173
10	X	0.38	0/1613	0.66	0/2173
11	K	0.39	0/1680	0.65	1/2274 (0.0%)
11	Y	0.39	0/1680	0.65	1/2274 (0.0%)
12	L	0.37	0/1795	0.66	1/2420 (0.0%)
12	Z	0.38	0/1795	0.66	1/2420 (0.0%)
13	1	0.41	0/1855	0.66	1/2514 (0.0%)
13	M	0.39	0/1855	0.66	1/2514 (0.0%)
14	2	0.39	0/1541	0.65	1/2087 (0.0%)
14	N	0.41	0/1541	0.65	1/2087 (0.0%)
All	All	0.38	0/50448	0.64	10/68192 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Z	95	TYR	N-CA-C	-5.62	95.81	111.00
12	L	95	TYR	N-CA-C	-5.59	95.90	111.00
11	K	4	LEU	CA-CB-CG	5.53	128.02	115.30
11	Y	4	LEU	CA-CB-CG	5.46	127.86	115.30
14	2	22	THR	N-CA-C	-5.27	96.77	111.00
13	1	95	LEU	N-CA-C	-5.23	96.89	111.00
14	N	22	THR	N-CA-C	-5.21	96.94	111.00
1	O	215	ILE	N-CA-C	-5.13	97.14	111.00
13	M	95	LEU	N-CA-C	-5.04	97.38	111.00
1	A	215	ILE	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1926	53	0
1	O	1915	0	1926	51	0
2	B	1905	0	1901	79	0
2	P	1905	0	1901	74	0
3	C	1891	0	1900	91	0
3	Q	1891	0	1900	92	0
4	D	1862	0	1836	50	0
4	R	1862	0	1836	55	0
5	E	1795	0	1797	80	0
5	S	1795	0	1797	87	0
6	F	1897	0	1886	65	0
6	T	1897	0	1886	67	0
7	G	1921	0	1910	72	0
7	U	1921	0	1910	79	0
8	H	1685	0	1687	45	0
8	V	1685	0	1687	46	0
9	I	1581	0	1574	37	0
9	W	1581	0	1574	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	1585	0	1590	53	0
10	X	1585	0	1590	57	0
11	K	1643	0	1594	30	0
11	Y	1643	0	1594	31	0
12	L	1757	0	1711	43	0
12	Z	1757	0	1711	45	0
13	1	1824	0	1832	64	0
13	M	1824	0	1832	54	0
14	2	1512	0	1480	38	0
14	N	1512	0	1480	40	0
15	2	21	0	21	2	0
15	H	21	0	21	1	0
15	K	21	0	21	2	0
15	N	21	0	21	2	0
15	V	21	0	21	1	0
15	Y	21	0	21	2	0
16	1	75	0	0	2	0
16	2	56	0	0	1	0
16	A	58	0	0	4	0
16	B	38	0	0	1	0
16	C	44	0	0	2	0
16	D	39	0	0	0	0
16	E	23	0	0	2	0
16	F	47	0	0	0	0
16	G	58	0	0	2	0
16	H	54	0	0	1	0
16	I	69	0	0	1	0
16	J	51	0	0	1	0
16	K	49	0	0	1	0
16	L	58	0	0	3	0
16	M	73	0	0	1	0
16	N	56	0	0	2	0
16	O	34	0	0	1	0
16	P	29	0	0	1	0
16	Q	27	0	0	1	0
16	R	31	0	0	2	0
16	S	19	0	0	0	0
16	T	39	0	0	2	0
16	U	62	0	0	4	0
16	V	49	0	0	2	0
16	W	62	0	0	0	0
16	X	45	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	Y	48	0	0	2	0
16	Z	53	0	0	4	0
All	All	51018	0	49374	1446	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (1446) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:96:ALA:HA	7:U:107:MET:HE2	1.29	1.11
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.14	1.11
11:Y:10(B):LYS:HD2	11:Y:10(B):LYS:H	1.14	1.10
7:G:96:ALA:HA	7:G:107:MET:HE2	1.29	1.09
11:K:10(B):LYS:H	11:K:10(B):LYS:HD2	1.14	1.07
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.13	1.06
7:U:9:ASP:HA	7:U:14:ILE:HD11	1.34	1.04
7:G:9:ASP:HA	7:G:14:ILE:HD11	1.34	1.04
2:P:202:THR:HG22	2:P:204:SER:H	1.25	0.99
2:B:202:THR:HG22	2:B:204:SER:H	1.27	0.98
2:B:15:PHE:H	3:C:23:GLN:HE22	1.02	0.97
1:O:15:PHE:H	2:P:23:GLN:HE22	1.15	0.93
2:B:108:PRO:HB2	2:B:111:ILE:HD13	1.51	0.93
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.34	0.92
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.52	0.92
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.49	0.92
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.13	0.91
3:C:15:PHE:H	4:D:23:GLN:HE22	1.17	0.91
14:N:161:GLN:NE2	14:2:136:GLY:HA2	1.86	0.91
13:M:157:ASN:HD22	13:M:160:ARG:HH11	0.97	0.91
14:N:136:GLY:HA2	14:2:161:GLN:NE2	1.87	0.90
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.20	0.89
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.19	0.89
5:E:207:LEU:HD23	5:E:207:LEU:H	1.38	0.88
13:1:157:ASN:HD22	13:1:160:ARG:HH11	0.96	0.88
5:S:207:LEU:HD23	5:S:207:LEU:H	1.36	0.88
5:S:15:PHE:H	6:T:23:GLN:HE22	1.22	0.87
2:P:108:PRO:HB2	2:P:111:ILE:HD13	1.54	0.86
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.40	0.86
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.88	0.86
1:A:15:PHE:H	2:B:23:GLN:HE22	1.20	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.74	0.86
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.24	0.86
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.39	0.85
11:Y:99:THR:HG22	11:Y:113:VAL:O	1.77	0.85
13:1:157:ASN:HD22	13:1:160:ARG:NH1	1.74	0.85
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.75	0.85
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.39	0.84
13:1:157:ASN:ND2	13:1:160:ARG:HH11	1.75	0.84
6:F:109:ILE:H	6:F:109:ILE:HD12	1.42	0.84
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.43	0.84
3:Q:163:GLN:HE21	3:Q:164:THR:H	1.23	0.83
14:2:84:LYS:HG3	14:2:119:VAL:HG22	1.60	0.83
6:F:36:THR:HG22	6:F:51:GLU:OE2	1.78	0.83
6:T:109:ILE:H	6:T:109:ILE:HD12	1.44	0.83
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.26	0.83
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.42	0.83
5:E:15:PHE:H	6:F:23:GLN:HE22	1.27	0.83
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.44	0.82
14:N:107:LYS:HG2	14:N:108:GLY:H	1.43	0.82
14:2:107:LYS:HG2	14:2:108:GLY:H	1.44	0.82
8:H:165:ASN:HD22	13:1:139:ARG:HH11	1.27	0.82
6:T:36:THR:HG22	6:T:51:GLU:OE2	1.77	0.82
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.62	0.82
6:T:35:THR:HG21	6:T:51:GLU:O	1.80	0.81
11:K:99:THR:HG22	11:K:113:VAL:O	1.79	0.81
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.63	0.81
3:C:185:THR:HG22	3:C:187:GLU:H	1.44	0.81
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.27	0.81
5:S:18(C):PHE:HA	5:S:18(F):ILE:HG13	1.61	0.81
6:F:35:THR:HG21	6:F:51:GLU:O	1.80	0.81
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.62	0.81
3:C:163:GLN:HE21	3:C:164:THR:H	1.24	0.81
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.63	0.80
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.94	0.80
5:E:18(C):PHE:HA	5:E:18(F):ILE:HG13	1.62	0.80
13:1:42:VAL:HG23	13:1:178:ILE:HD11	1.64	0.79
3:C:185:THR:HB	3:C:188:GLU:HG2	1.63	0.79
14:N:84:LYS:HG3	14:N:119:VAL:HG22	1.62	0.79
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.64	0.79
1:A:177:GLU:HG2	2:B:58:LEU:HD22	1.63	0.79
3:C:163:GLN:NE2	3:C:164:THR:H	1.81	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.65	0.78
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.81	0.78
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.64	0.78
16:B:565:HOH:O	3:C:33:ARG:HD2	1.83	0.78
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.29	0.78
13:1:6:MET:HG2	13:1:155:ILE:HD11	1.66	0.77
8:H:22:GLN:HG3	8:H:27:ALA:HB2	1.65	0.77
14:2:84:LYS:HG3	14:2:119:VAL:CG2	2.14	0.77
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.65	0.77
8:V:22:GLN:HG3	8:V:27:ALA:HB2	1.66	0.76
1:O:20:LYS:HE3	1:O:25:ASP:OD1	1.85	0.76
13:M:42:VAL:HG23	13:M:178:ILE:HD11	1.66	0.76
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.66	0.76
13:M:6:MET:HG2	13:M:155:ILE:HD11	1.68	0.76
4:D:192:LEU:O	4:D:196:ILE:HG12	1.86	0.76
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.32	0.76
7:G:18(G):GLU:HG2	7:G:188:LYS:HB2	1.67	0.76
14:N:84:LYS:HG3	14:N:119:VAL:CG2	2.16	0.75
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.33	0.75
7:U:18(G):GLU:HG2	7:U:188:LYS:HB2	1.67	0.75
3:C:232:TYR:O	3:C:236:ILE:HG13	1.86	0.75
12:L:33:LYS:HD2	12:L:46:ASN:HD22	1.52	0.74
5:E:201:LEU:HD11	5:E:207:LEU:HD22	1.69	0.74
3:C:195:ARG:HG3	3:C:236:ILE:HD13	1.67	0.74
7:U:217:LYS:HE3	7:U:217:LYS:HA	1.69	0.74
13:1:7:LYS:HG3	13:1:14(G):ILE:HD12	1.70	0.74
3:Q:33:ARG:HB2	3:Q:33:ARG:NH1	2.03	0.74
1:A:20:LYS:HE3	1:A:25:ASP:OD1	1.87	0.74
5:S:201:LEU:HD11	5:S:207:LEU:HD22	1.69	0.74
9:W:6:MET:HE3	9:W:155:ILE:HD12	1.69	0.74
4:R:192:LEU:O	4:R:196:ILE:HG12	1.86	0.74
12:Z:134:ILE:HD13	12:Z:158:SER:HB3	1.69	0.74
2:B:124:THR:CG2	3:C:130:ARG:HH21	2.01	0.73
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.53	0.73
3:Q:65:SER:HB2	16:Q:303:HOH:O	1.89	0.73
2:B:61:GLN:OE1	2:B:208:ASP:HA	1.88	0.73
11:Y:142:TYR:O	11:Y:143:LYS:HD2	1.88	0.73
3:C:41:LYS:HG2	3:C:161:SER:O	1.88	0.73
11:Y:10(B):LYS:CD	11:Y:10(B):LYS:H	1.92	0.73
7:G:18(G):GLU:HG2	7:G:188:LYS:CB	2.19	0.73
7:G:217:LYS:HA	7:G:217:LYS:HE3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:61:GLN:OE1	2:P:208:ASP:HA	1.89	0.72
3:Q:195:ARG:HG3	3:Q:236:ILE:HD13	1.70	0.72
5:S:207:LEU:H	5:S:207:LEU:CD2	2.01	0.72
7:U:170:GLN:HE21	7:U:174:THR:HG23	1.54	0.72
12:L:134:ILE:HD13	12:L:158:SER:HB3	1.72	0.72
5:E:207:LEU:CD2	5:E:207:LEU:H	2.03	0.72
12:L:166:HIS:HD2	12:L:168:GLN:H	1.37	0.72
7:U:18(G):GLU:HG2	7:U:188:LYS:CB	2.20	0.72
3:Q:232:TYR:O	3:Q:236:ILE:HG13	1.87	0.72
1:O:179:ARG:HH11	1:O:179:ARG:HB3	1.54	0.72
6:F:20(B):GLU:HG3	6:F:20(C):LYS:HG3	1.71	0.72
12:Z:33:LYS:HD2	12:Z:46:ASN:HD22	1.53	0.72
9:I:1:GLY:HA3	9:I:33:LYS:HE2	1.72	0.72
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.36	0.72
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.20	0.71
12:Z:114:ASP:HB2	12:Z:118:SER:HB3	1.72	0.71
6:T:20(B):GLU:HG3	6:T:20(C):LYS:HG3	1.72	0.71
7:G:96:ALA:HA	7:G:107:MET:CE	2.16	0.71
6:T:192:GLN:O	6:T:196:ILE:HG12	1.90	0.71
1:O:124:THR:CG2	2:P:130:ARG:HH21	2.03	0.71
12:L:114:ASP:HB2	12:L:118:SER:HB3	1.73	0.71
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.03	0.71
11:K:142:TYR:O	11:K:143:LYS:HD2	1.89	0.71
13:M:7:LYS:HG3	13:M:14(G):ILE:HD12	1.73	0.71
5:E:12:THR:HG21	5:E:124:THR:HA	1.72	0.71
7:U:96:ALA:CA	7:U:107:MET:HE2	2.15	0.71
11:K:10(B):LYS:N	11:K:10(B):LYS:HD2	1.99	0.71
3:C:33:ARG:HB2	3:C:33:ARG:NH1	2.05	0.71
1:A:179:ARG:HB3	1:A:179:ARG:HH11	1.56	0.70
7:U:59:LEU:O	7:U:61:PRO:HD3	1.89	0.70
3:Q:41:LYS:HG2	3:Q:161:SER:O	1.91	0.70
9:I:6:MET:HE3	9:I:155:ILE:HD12	1.72	0.70
1:O:86:ARG:HE	7:U:118:ASN:ND2	1.88	0.70
2:B:219:GLU:HG2	2:B:21(E):VAL:H	1.57	0.70
4:R:177:LEU:HD22	5:S:58:LEU:HD13	1.71	0.70
5:S:12:THR:HG21	5:S:124:THR:HA	1.71	0.70
5:E:207:LEU:HA	5:E:2(E):ASN:ND2	2.07	0.70
4:D:177:LEU:HD22	5:E:58:LEU:HD13	1.74	0.70
6:F:192:GLN:O	6:F:196:ILE:HG12	1.91	0.70
11:Y:10(B):LYS:N	11:Y:10(B):LYS:HD2	1.99	0.70
5:E:207:LEU:HA	5:E:2(E):ASN:HD22	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:106:PRO:HG2	3:C:143:PRO:HG3	1.73	0.70
7:G:96:ALA:CA	7:G:107:MET:HE2	2.17	0.69
6:F:109:ILE:HD12	6:F:109:ILE:N	2.06	0.69
6:T:109:ILE:HD12	6:T:109:ILE:N	2.07	0.69
7:U:96:ALA:HA	7:U:107:MET:CE	2.16	0.69
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.06	0.69
13:1:40:ASN:HD22	13:1:40:ASN:H	1.39	0.69
5:S:207:LEU:HA	5:S:2(E):ASN:ND2	2.07	0.69
3:C:163:GLN:HE21	3:C:164:THR:N	1.91	0.69
10:J:3:ILE:HD13	10:J:46:ALA:HB2	1.75	0.69
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.27	0.69
7:G:59:LEU:O	7:G:61:PRO:HD3	1.93	0.69
8:H:35:HIS:CB	8:H:56:THR:HG21	2.23	0.68
6:F:175:GLU:HB3	6:F:196:ILE:HD12	1.75	0.68
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	1.75	0.68
3:Q:100:ARG:NH1	3:Q:106:PRO:HB3	2.08	0.68
2:P:219:GLU:HG2	2:P:21(E):VAL:H	1.58	0.68
7:U:227:GLU:HG2	16:U:1255:HOH:O	1.93	0.68
3:Q:106:PRO:HG2	3:Q:143:PRO:HG3	1.76	0.68
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.29	0.68
3:Q:33:ARG:HH11	3:Q:33:ARG:CB	2.06	0.68
3:Q:106:PRO:HG2	3:Q:143:PRO:CG	2.22	0.68
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.42	0.68
11:K:10(B):LYS:H	11:K:10(B):LYS:CD	1.91	0.68
13:M:40:ASN:H	13:M:40:ASN:HD22	1.40	0.68
8:V:35:HIS:CB	8:V:56:THR:HG21	2.24	0.68
2:B:219:GLU:HG2	2:B:21(E):VAL:N	2.09	0.68
7:U:86:ARG:HD2	16:U:248:HOH:O	1.91	0.68
5:S:31:ILE:HD11	5:S:153:PRO:HG2	1.74	0.68
5:S:207:LEU:HA	5:S:2(E):ASN:HD22	1.57	0.67
3:Q:163:GLN:HE21	3:Q:164:THR:N	1.90	0.67
6:T:237:GLN:O	6:T:240:ILE:HG22	1.95	0.67
2:B:163:ILE:HD13	2:B:164:SER:N	2.09	0.67
5:S:207:LEU:N	5:S:207:LEU:HD23	2.09	0.67
3:Q:57:LYS:O	3:Q:58:LEU:HB2	1.94	0.67
3:C:57:LYS:O	3:C:58:LEU:HB2	1.94	0.67
2:B:186:VAL:HG21	2:B:216:ARG:HD3	1.75	0.67
9:W:1:GLY:HA3	9:W:33:LYS:HE2	1.75	0.67
13:1:14(C):ARG:HG3	13:1:14(C):ARG:HH11	1.60	0.67
11:Y:143:LYS:HB2	11:Y:146:LEU:HD13	1.77	0.67
3:C:52:ARG:HB2	3:C:209:ASN:HA	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:148:VAL:O	12:Z:152:ILE:HG12	1.95	0.67
3:Q:168:ASN:HB2	3:Q:200:VAL:HG11	1.76	0.67
5:E:31:ILE:HD11	5:E:153:PRO:HG2	1.77	0.67
14:2:20:THR:HG23	14:2:31:THR:OG1	1.95	0.67
4:R:12(D):ALA:HB3	4:R:126:ARG:HD3	1.77	0.66
7:U:121:GLN:O	7:U:124:THR:HB	1.95	0.66
5:E:207:LEU:HD23	5:E:207:LEU:N	2.10	0.66
6:T:175:GLU:HB3	6:T:196:ILE:HD12	1.76	0.66
10:J:-1:MET:HG2	10:J:1:ASP:H	1.60	0.66
1:A:86:ARG:HE	7:G:118:ASN:ND2	1.94	0.66
6:T:186:ALA:O	6:T:190:VAL:HG23	1.96	0.66
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.43	0.66
5:E:97:ASN:HD21	12:L:61:ASN:HD21	1.43	0.66
10:X:3:ILE:HD13	10:X:46:ALA:HB2	1.76	0.66
5:S:49:VAL:HG22	5:S:212:ILE:HD13	1.77	0.66
3:C:46:VAL:O	3:C:215:VAL:HG12	1.95	0.66
14:N:20:THR:HG23	14:N:31:THR:OG1	1.96	0.66
12:L:4:LEU:HD11	12:L:138:LEU:HD21	1.78	0.66
1:A:121:GLN:O	1:A:124:THR:HB	1.96	0.65
1:O:121:GLN:O	1:O:124:THR:HB	1.95	0.65
7:G:233:LEU:O	7:G:236:ILE:HG13	1.96	0.65
6:F:237:GLN:O	6:F:240:ILE:HG22	1.97	0.65
3:C:33:ARG:CB	3:C:33:ARG:HH11	2.08	0.65
7:G:121:GLN:O	7:G:124:THR:HB	1.97	0.65
7:U:233:LEU:O	7:U:236:ILE:HG13	1.96	0.65
3:Q:186:VAL:O	3:Q:190:VAL:HG23	1.97	0.65
2:P:186:VAL:HG21	2:P:216:ARG:HD3	1.76	0.65
8:H:33:LYS:HG2	15:H:224:GPT:H12	1.78	0.65
11:K:143:LYS:HB2	11:K:146:LEU:HD13	1.77	0.65
3:Q:46:VAL:O	3:Q:215:VAL:HG12	1.96	0.65
12:L:148:VAL:O	12:L:152:ILE:HG12	1.96	0.65
12:Z:4:LEU:HD11	12:Z:138:LEU:HD21	1.78	0.65
2:P:219:GLU:HG2	2:P:21(E):VAL:N	2.10	0.65
7:U:77:VAL:HG12	7:U:137:THR:HB	1.79	0.65
3:C:186:VAL:HG21	3:C:216:LYS:HE2	1.79	0.65
13:M:14(C):ARG:HH11	13:M:14(C):ARG:HG3	1.62	0.65
4:R:175:GLU:HG2	4:R:196:ILE:HD12	1.79	0.65
3:Q:186:VAL:HG21	3:Q:216:LYS:HE2	1.78	0.64
2:P:163:ILE:HD13	2:P:164:SER:N	2.11	0.64
14:N:107:LYS:HG2	14:N:108:GLY:N	2.13	0.64
5:E:226:GLY:O	5:E:229:VAL:HG22	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:12(D):ALA:HB3	4:D:126:ARG:HD3	1.78	0.64
3:C:186:VAL:O	3:C:190:VAL:HG23	1.98	0.64
8:V:33:LYS:HG2	15:V:224:GPT:H12	1.78	0.64
3:C:100:ARG:NH1	3:C:106:PRO:HB3	2.10	0.64
5:S:28:LEU:HA	5:S:31:ILE:HD12	1.77	0.64
3:C:168:ASN:HB2	3:C:200:VAL:HG11	1.78	0.64
11:Y:33:LYS:HG2	15:Y:224:GPT:H12	1.79	0.64
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.30	0.64
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.79	0.64
1:O:225:THR:OG1	1:O:228:GLU:HG3	1.97	0.64
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.45	0.64
10:X:-1:MET:HG2	10:X:1:ASP:H	1.63	0.64
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.32	0.64
7:G:77:VAL:HG12	7:G:137:THR:HB	1.79	0.64
11:Y:143:LYS:HB2	11:Y:146:LEU:CD1	2.28	0.64
6:F:186:ALA:O	6:F:190:VAL:HG23	1.97	0.64
5:S:226:GLY:O	5:S:229:VAL:HG22	1.98	0.64
2:P:101:LYS:HZ2	10:X:85:GLN:NE2	1.96	0.63
12:Z:90:LYS:HD3	12:Z:95:TYR:CE1	2.33	0.63
5:S:97:ASN:HD21	12:Z:61:ASN:HD21	1.44	0.63
13:1:-3:VAL:HG12	13:1:49:ILE:HG13	1.80	0.63
5:E:28:LEU:HA	5:E:31:ILE:HD12	1.79	0.63
1:A:33:GLN:HA	1:A:33:GLN:HE21	1.63	0.63
13:M:-3:VAL:HG12	13:M:49:ILE:HG13	1.81	0.63
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.81	0.63
12:L:14:LEU:HD13	12:L:34:VAL:HG13	1.79	0.63
5:S:220:PRO:O	5:S:222:THR:HG23	1.98	0.63
2:B:121:GLN:O	2:B:124:THR:HB	1.99	0.63
4:D:175:GLU:HG2	4:D:196:ILE:HD12	1.79	0.63
7:U:56:ASP:HB3	7:U:59:LEU:HG	1.81	0.63
2:P:185:LYS:HD3	2:P:186:VAL:N	2.14	0.63
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.79	0.63
4:D:12(D):ALA:HA	5:E:129:GLY:HA2	1.80	0.63
9:I:112:GLY:N	9:I:125:ILE:HD12	2.14	0.63
2:B:181:LYS:O	2:B:184:MET:HG3	1.99	0.63
5:E:220:PRO:O	5:E:222:THR:HG23	1.99	0.63
7:U:198:ILE:HG23	7:U:203:THR:O	1.99	0.62
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	1.80	0.62
2:B:15:PHE:H	3:C:23:GLN:NE2	1.86	0.62
1:A:225:THR:OG1	1:A:228:GLU:HG3	1.99	0.62
6:F:198:TYR:HE2	6:F:237:GLN:HE21	1.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:65:SER:HB2	16:C:274:HOH:O	1.99	0.62
14:2:107:LYS:HG2	14:2:108:GLY:N	2.13	0.62
7:G:14:ILE:HD13	7:G:14:ILE:H	1.65	0.62
7:G:56:ASP:HB3	7:G:59:LEU:HG	1.81	0.62
1:O:4:MET:SD	1:O:5:THR:N	2.67	0.62
11:K:33:LYS:HG2	15:K:224:GPT:H12	1.82	0.62
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.81	0.62
10:J:156:LYS:O	10:J:160:GLN:HG3	2.00	0.62
1:O:86:ARG:HH21	7:U:118:ASN:ND2	1.98	0.62
11:K:7:ARG:HG2	11:K:108:PRO:HB2	1.82	0.62
11:K:143:LYS:HB2	11:K:146:LEU:CD1	2.28	0.62
10:X:156:LYS:O	10:X:160:GLN:HG3	2.00	0.62
8:H:24:PRO:HG2	8:H:25:ILE:HD12	1.81	0.62
9:I:29:ASN:ND2	9:I:30:LYS:HG3	2.15	0.62
2:B:185:LYS:HD3	2:B:186:VAL:N	2.15	0.61
8:H:159:ILE:HG22	8:H:163:ILE:CD1	2.29	0.61
5:S:18(D):ILE:O	5:S:18(D):ILE:HG12	2.01	0.61
14:N:26:ILE:HG13	13:1:165:ARG:C	2.21	0.61
1:O:33:GLN:HA	1:O:33:GLN:HE21	1.64	0.61
1:O:179:ARG:NH1	1:O:179:ARG:HB3	2.15	0.61
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.64	0.61
12:L:43:MET:HB2	12:L:101:ILE:HG22	1.82	0.61
1:A:4:MET:SD	1:A:5:THR:N	2.65	0.61
8:V:172:ASN:HD22	8:V:193:THR:HA	1.66	0.61
1:A:86:ARG:HH21	7:G:118:ASN:ND2	1.97	0.61
2:P:112:LEU:HD23	2:P:112:LEU:C	2.21	0.61
5:S:48:LEU:HG	5:S:139:ILE:HD13	1.81	0.61
13:1:42:VAL:CG2	13:1:178:ILE:HD11	2.31	0.61
6:T:198:TYR:HE2	6:T:237:GLN:HE21	1.47	0.61
2:P:181:LYS:O	2:P:184:MET:HG3	2.00	0.61
7:U:72:ARG:HB2	7:U:72:ARG:NH1	2.15	0.61
13:1:37:VAL:HG11	13:1:79:ILE:HD13	1.82	0.61
11:Y:7:ARG:HG2	11:Y:108:PRO:HB2	1.81	0.61
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.66	0.61
5:S:227:GLU:CD	5:S:227:GLU:H	2.03	0.61
5:E:86:ARG:HH11	5:E:86:ARG:HG3	1.65	0.61
5:S:132:TYR:O	5:S:153:PRO:HB3	2.01	0.61
6:T:38:ILE:HG22	6:T:164:ALA:CB	2.31	0.61
3:C:35:THR:HB	3:C:51:GLU:HG3	1.82	0.61
5:S:86:ARG:HH11	5:S:86:ARG:HG3	1.65	0.61
5:E:18(D):ILE:O	5:E:18(D):ILE:HG12	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:201:LEU:HD11	5:S:207:LEU:CD2	2.30	0.60
5:E:48:LEU:HG	5:E:139:ILE:HD13	1.82	0.60
5:E:201:LEU:HD11	5:E:207:LEU:CD2	2.31	0.60
13:1:152:GLU:O	13:1:156:VAL:HG23	2.01	0.60
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.81	0.60
4:R:162:ALA:HB3	5:S:58:LEU:HD23	1.83	0.60
1:A:97:HIS:HD2	8:H:61:SER:OG	1.85	0.60
5:E:49:VAL:HG22	5:E:212:ILE:HD13	1.83	0.60
12:Z:43:MET:HB2	12:Z:101:ILE:HG22	1.84	0.60
5:E:227:GLU:CD	5:E:227:GLU:H	2.03	0.60
13:M:165:ARG:C	14:2:26:ILE:HG13	2.22	0.60
7:U:14:ILE:H	7:U:14:ILE:HD13	1.67	0.60
8:V:159:ILE:HG22	8:V:163:ILE:CD1	2.32	0.60
2:P:121:GLN:O	2:P:124:THR:HB	1.99	0.60
3:Q:241:GLN:C	3:Q:243:GLN:H	2.05	0.60
7:U:8:TYR:C	7:U:10:ARG:H	2.05	0.59
7:G:198:ILE:HG23	7:G:203:THR:O	2.00	0.59
8:V:24:PRO:HG2	8:V:25:ILE:HD12	1.83	0.59
5:S:47:VAL:HG23	5:S:189:LEU:HD13	1.84	0.59
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.84	0.59
13:M:139:ARG:HH11	8:V:165:ASN:ND2	1.99	0.59
13:M:42:VAL:CG2	13:M:178:ILE:HD11	2.33	0.59
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.37	0.59
2:P:231:ASP:O	2:P:235:LYS:HG2	2.03	0.59
2:B:112:LEU:C	2:B:112:LEU:HD23	2.22	0.59
5:S:73:HIS:HE1	5:S:107:LEU:O	1.85	0.59
3:Q:173:ARG:O	3:Q:177:GLU:HG3	2.03	0.59
12:Z:-7:ASN:ND2	12:Z:-5:TYR:H	2.01	0.59
10:J:133:TYR:HD1	16:Y:593:HOH:O	1.85	0.59
13:M:37:VAL:HG11	13:M:79:ILE:CD1	2.33	0.59
7:G:72:ARG:NH1	7:G:72:ARG:HB2	2.18	0.59
3:Q:33:ARG:HH11	3:Q:33:ARG:HB2	1.66	0.59
2:P:6:ARG:HG2	3:Q:10:ARG:HH21	1.68	0.59
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.84	0.59
3:C:241:GLN:C	3:C:243:GLN:H	2.05	0.59
12:L:-7:ASN:ND2	12:L:-5:TYR:H	2.01	0.59
5:S:97:ASN:ND2	12:Z:61:ASN:HD21	2.01	0.59
13:M:37:VAL:HG11	13:M:79:ILE:HD13	1.83	0.59
4:R:156:THR:HG22	5:S:83:PRO:HD3	1.84	0.59
13:1:41:THR:OG1	13:1:76:PRO:HG3	2.02	0.59
5:E:73:HIS:HE1	5:E:107:LEU:O	1.86	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:185:LYS:HE2	2:P:187:ASP:OD1	2.03	0.59
10:J:2:ILE:C	10:J:3:ILE:HD12	2.23	0.59
5:S:31:ILE:HD11	5:S:153:PRO:CG	2.33	0.59
6:F:38:ILE:HG22	6:F:164:ALA:CB	2.33	0.59
4:R:185:THR:OG1	4:R:188:GLU:HG3	2.03	0.59
5:E:82:ALA:HB3	5:E:83:PRO:HD3	1.85	0.59
4:R:121:LEU:HB2	16:R:853:HOH:O	2.02	0.59
3:C:173:ARG:O	3:C:177:GLU:HG3	2.03	0.58
6:T:173:LYS:O	6:T:177:GLU:HG3	2.03	0.58
7:G:8:TYR:C	7:G:10:ARG:H	2.04	0.58
13:M:84:ALA:HA	13:M:113:VAL:HG21	1.85	0.58
10:X:10(B):LYS:NZ	10:X:10(B):LYS:HB2	2.18	0.58
2:B:224:PHE:HD2	2:B:224:PHE:H	1.51	0.58
1:A:179:ARG:HB3	1:A:179:ARG:NH1	2.17	0.58
8:H:165:ASN:ND2	13:1:139:ARG:HH11	1.98	0.58
4:D:177:LEU:HD22	5:E:58:LEU:CD1	2.33	0.58
10:X:2:ILE:O	10:X:3:ILE:HD12	2.02	0.58
5:S:82:ALA:HB3	5:S:83:PRO:HD3	1.86	0.58
6:T:69:VAL:HG12	16:T:811:HOH:O	2.03	0.58
8:H:159:ILE:HG22	8:H:163:ILE:HD12	1.85	0.58
11:K:31:VAL:HG11	15:K:224:GPT:H11	1.86	0.58
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.32	0.58
1:A:177:GLU:HG2	2:B:58:LEU:CD2	2.33	0.58
5:E:97:ASN:HD21	12:L:61:ASN:ND2	2.02	0.58
8:V:159:ILE:HG22	8:V:163:ILE:HD12	1.84	0.58
2:B:231:ASP:O	2:B:235:LYS:HG2	2.03	0.58
5:E:97:ASN:ND2	12:L:61:ASN:HD21	2.01	0.58
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.86	0.58
8:H:172:ASN:HD22	8:H:193:THR:HA	1.68	0.58
2:P:101:LYS:HZ2	10:X:85:GLN:HE21	1.50	0.58
5:E:132:TYR:O	5:E:153:PRO:HB3	2.03	0.58
5:E:31:ILE:HD11	5:E:153:PRO:CG	2.34	0.58
2:P:224:PHE:H	2:P:224:PHE:HD2	1.49	0.58
10:J:10(B):LYS:HB2	10:J:10(B):LYS:NZ	2.18	0.58
10:X:2:ILE:C	10:X:3:ILE:HD12	2.24	0.58
9:W:29:ASN:ND2	9:W:30:LYS:HG3	2.18	0.57
5:E:167:ALA:HB3	16:E:1131:HOH:O	2.03	0.57
6:F:109:ILE:H	6:F:109:ILE:CD1	2.16	0.57
5:S:97:ASN:HD21	12:Z:61:ASN:ND2	2.01	0.57
13:1:37:VAL:HG11	13:1:79:ILE:CD1	2.33	0.57
13:M:41:THR:OG1	13:M:76:PRO:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:LEU:HD13	2:B:124:THR:HG23	1.86	0.57
10:J:2:ILE:O	10:J:3:ILE:HD12	2.03	0.57
13:M:152:GLU:O	13:M:156:VAL:HG23	2.04	0.57
10:J:52:THR:CG2	10:J:53:VAL:N	2.68	0.57
10:X:32:ASP:OD2	10:X:34:THR:HG22	2.04	0.57
5:E:47:VAL:HG23	5:E:189:LEU:HD13	1.85	0.57
14:N:51:ASP:O	14:N:55:ILE:HG12	2.04	0.57
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.86	0.57
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	1.87	0.57
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.86	0.57
4:D:185:THR:OG1	4:D:188:GLU:HG3	2.04	0.57
6:T:109:ILE:CD1	6:T:109:ILE:H	2.17	0.57
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.69	0.57
3:C:195:ARG:CG	3:C:236:ILE:HD13	2.35	0.56
3:Q:100:ARG:HH11	3:Q:106:PRO:HB3	1.68	0.56
13:1:84:ALA:HA	13:1:113:VAL:HG21	1.86	0.56
2:B:202:THR:HG22	2:B:204:SER:N	2.10	0.56
9:I:7:THR:HG23	9:I:110:ILE:HD13	1.87	0.56
1:O:177:GLU:HG2	2:P:58:LEU:HD22	1.86	0.56
6:F:173:LYS:O	6:F:177:GLU:HG3	2.04	0.56
14:2:51:ASP:O	14:2:55:ILE:HG12	2.06	0.56
8:V:172:ASN:ND2	8:V:193:THR:HA	2.20	0.56
10:X:38:SER:HB2	10:X:39:PRO:HD2	1.87	0.56
11:K:138:LEU:HD13	11:K:158:SER:OG	2.05	0.56
9:W:27:VAL:HG13	16:X:622:HOH:O	2.04	0.56
11:Y:138:LEU:HD13	11:Y:158:SER:OG	2.05	0.56
8:H:34:LEU:HB2	16:H:540:HOH:O	2.04	0.56
10:X:133:TYR:CE2	10:X:166:MET:HG3	2.40	0.56
1:O:69:LEU:HD23	1:O:69:LEU:C	2.26	0.56
7:U:172:ILE:HD11	7:U:201:LEU:HD21	1.87	0.56
3:C:20:HIS:HB3	3:C:25:GLU:OE1	2.06	0.56
10:J:168:MET:HE1	10:X:167:PRO:HB2	1.88	0.56
7:G:228:ASN:HB3	16:G:255:HOH:O	2.06	0.56
2:B:185:LYS:HE2	2:B:187:ASP:OD1	2.05	0.56
10:J:167:PRO:HB2	10:X:168:MET:HE1	1.88	0.56
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.88	0.56
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.88	0.56
10:J:10(B):LYS:HB2	10:J:10(B):LYS:HZ3	1.71	0.56
13:1:76:PRO:HD2	13:1:105:GLN:OE1	2.06	0.56
1:A:69:LEU:HD23	1:A:69:LEU:C	2.26	0.56
9:W:6:MET:HE3	9:W:155:ILE:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:195:ARG:CG	3:Q:236:ILE:HD13	2.35	0.56
13:1:40:ASN:HD22	13:1:40:ASN:N	1.99	0.56
1:O:60:MET:HE1	16:U:400:HOH:O	2.06	0.55
7:G:172:ILE:HD11	7:G:201:LEU:HD21	1.88	0.55
1:A:206:PHE:CD1	1:A:210:ILE:HD11	2.41	0.55
1:A:170:VAL:HB	16:A:402:HOH:O	2.05	0.55
9:I:6:MET:CE	9:I:155:ILE:HA	2.36	0.55
11:Y:31:VAL:HG11	15:Y:224:GPT:H11	1.89	0.55
10:J:3:ILE:CD1	10:J:46:ALA:HB2	2.35	0.55
10:J:133:TYR:CE2	10:J:166:MET:HG3	2.42	0.55
9:W:7:THR:HG23	9:W:110:ILE:HD13	1.88	0.55
2:P:121:GLN:HG3	3:Q:83:ALA:HB1	1.89	0.55
10:X:3:ILE:CD1	10:X:46:ALA:HB2	2.37	0.55
6:T:38:ILE:HG22	6:T:164:ALA:HB2	1.88	0.55
6:F:21(B):THR:O	6:F:21(C):ASN:HB2	2.06	0.55
3:C:55:THR:HG22	3:C:56:LEU:HD22	1.88	0.55
4:R:31:ILE:HD13	4:R:135:ALA:HB2	1.87	0.55
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.42	0.55
3:C:14:ILE:HD12	3:C:14:ILE:H	1.72	0.55
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.37	0.55
1:O:206:PHE:CD1	1:O:210:ILE:HD11	2.42	0.55
3:C:185:THR:HG22	3:C:187:GLU:N	2.18	0.55
3:C:33:ARG:HB2	3:C:33:ARG:HH11	1.69	0.55
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.42	0.55
4:R:85:ALA:O	4:R:89:ILE:HG12	2.06	0.55
13:M:149:GLN:NE2	13:M:149:GLN:H	2.05	0.55
6:F:192:GLN:HE21	6:F:195:LYS:HE3	1.72	0.55
3:Q:20:HIS:HB3	3:Q:25:GLU:OE1	2.07	0.55
10:X:52:THR:CG2	10:X:53:VAL:N	2.69	0.55
10:J:38:SER:HB2	10:J:39:PRO:HD2	1.89	0.55
5:E:198:SER:HA	5:E:201:LEU:HG	1.88	0.55
5:S:198:SER:HA	5:S:201:LEU:HG	1.88	0.55
1:O:97:HIS:HD2	8:V:61:SER:OG	1.89	0.55
4:R:75:GLY:HA3	4:R:221:PHE:CD2	2.42	0.55
3:C:100:ARG:HH11	3:C:106:PRO:HB3	1.70	0.54
4:D:237:LEU:O	4:D:241:GLU:HG3	2.08	0.54
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.89	0.54
8:H:172:ASN:ND2	8:H:193:THR:HA	2.22	0.54
4:D:186:LEU:O	4:D:190:GLU:HG3	2.07	0.54
8:H:147:THR:OG1	8:H:150:GLU:HG3	2.07	0.54
1:A:21(P):LYS:N	16:A:1147:HOH:O	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:190:ILE:HG23	5:S:212:ILE:HD12	1.89	0.54
6:F:38:ILE:HG22	6:F:164:ALA:HB2	1.89	0.54
2:P:202:THR:HG22	2:P:204:SER:N	2.08	0.54
3:C:163:GLN:HA	3:C:163:GLN:HE21	1.72	0.54
7:U:228:ASN:HB3	16:U:242:HOH:O	2.07	0.54
6:T:37:SER:HB3	6:T:50:VAL:HG23	1.89	0.54
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.43	0.54
6:F:175:GLU:CB	6:F:196:ILE:HD12	2.38	0.54
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.42	0.54
1:A:198:LYS:HE3	1:A:236:LEU:HD11	1.89	0.54
8:V:216:GLU:HG3	9:W:187:ARG:HG2	1.88	0.54
8:V:90:TYR:CG	8:V:95:ILE:HD12	2.42	0.54
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.42	0.54
7:G:77:VAL:CG1	7:G:137:THR:HB	2.37	0.54
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.38	0.54
13:1:149:GLN:H	13:1:149:GLN:NE2	2.06	0.54
6:T:203:GLU:O	6:T:206:LYS:HD2	2.08	0.54
3:C:41:LYS:HD3	3:C:161:SER:HA	1.90	0.54
5:S:227:GLU:N	5:S:227:GLU:CD	2.61	0.54
1:O:198:LYS:HE3	1:O:236:LEU:HD11	1.90	0.54
2:P:239:THR:HG22	2:P:239:THR:OXT	2.06	0.54
6:T:192:GLN:HE21	6:T:195:LYS:HE3	1.73	0.54
11:K:7:ARG:HD2	11:K:108:PRO:O	2.08	0.54
3:Q:163:GLN:HA	3:Q:163:GLN:HE21	1.72	0.53
3:Q:41:LYS:HD3	3:Q:161:SER:HA	1.90	0.53
2:B:239:THR:OXT	2:B:239:THR:HG22	2.07	0.53
4:R:186:LEU:O	4:R:190:GLU:HG3	2.08	0.53
7:U:151:THR:HG22	7:U:157:TYR:HB2	1.90	0.53
4:D:85:ALA:O	4:D:89:ILE:HG12	2.08	0.53
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.89	0.53
9:W:6:MET:CE	9:W:155:ILE:HA	2.38	0.53
2:B:6:ARG:HB2	5:E:127:TYR:OH	2.07	0.53
5:E:148:LEU:CD2	5:E:162:GLY:HA2	2.38	0.53
13:1:19:LEU:HD21	13:1:26:LEU:HD22	1.90	0.53
3:Q:149:TYR:CE1	3:Q:159:SER:HB3	2.43	0.53
4:D:31:ILE:HD13	4:D:135:ALA:HB2	1.88	0.53
5:E:227:GLU:CD	5:E:227:GLU:N	2.61	0.53
8:H:90:TYR:CG	8:H:95:ILE:HD12	2.43	0.53
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.38	0.53
5:S:141:TYR:CE2	5:S:217:LYS:HA	2.43	0.53
11:K:86:LEU:HD13	11:K:86:LEU:C	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.89	0.53
7:U:35:ILE:HG23	7:U:51:GLN:HB2	1.89	0.53
6:F:127:ASN:HD22	6:F:127:ASN:C	2.12	0.53
11:Y:7:ARG:HD2	11:Y:108:PRO:O	2.09	0.53
3:Q:15:PHE:N	4:R:23:GLN:HE22	1.95	0.53
2:P:87:ILE:O	2:P:91:THR:HG23	2.09	0.53
5:S:15:PHE:H	6:T:23:GLN:NE2	2.01	0.53
1:O:33:GLN:CA	1:O:33:GLN:HE21	2.21	0.53
6:T:216:SER:HB3	6:T:21(A):GLU:HB2	1.90	0.53
14:2:36:ARG:HG3	14:2:42:TRP:CE2	2.43	0.53
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.91	0.53
4:R:237:LEU:O	4:R:241:GLU:HG3	2.09	0.53
2:B:107:ILE:HD11	2:B:111:ILE:HG22	1.91	0.53
2:B:49:ALA:HB2	2:B:212:PHE:CE1	2.44	0.52
5:S:148:LEU:CD2	5:S:162:GLY:HA2	2.39	0.52
4:D:194:LEU:HD22	4:D:212:LEU:HD11	1.91	0.52
1:O:150:GLN:O	1:O:157:TYR:HA	2.09	0.52
10:J:147:THR:OG1	10:J:150:GLU:HG3	2.09	0.52
1:O:232:ARG:HH11	1:O:232:ARG:HG3	1.74	0.52
3:Q:185:THR:HG22	3:Q:187:GLU:N	2.18	0.52
7:U:77:VAL:CG1	7:U:137:THR:HB	2.39	0.52
3:Q:211:GLU:C	3:Q:212:ILE:HD13	2.29	0.52
8:H:8:PHE:HB3	8:H:151:ALA:HB2	1.91	0.52
6:T:172:ALA:O	6:T:176:LEU:HD22	2.08	0.52
6:T:21(B):THR:O	6:T:21(C):ASN:HB2	2.09	0.52
10:J:24:ILE:HG12	10:J:24:ILE:O	2.09	0.52
2:B:169:THR:O	2:B:173:GLN:HB2	2.09	0.52
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.39	0.52
4:R:194:LEU:HD22	4:R:212:LEU:HD11	1.90	0.52
7:G:9:ASP:HA	7:G:14:ILE:CD1	2.24	0.52
5:S:201:LEU:O	5:S:202:ARG:HB2	2.09	0.52
2:P:224:PHE:N	2:P:224:PHE:CD2	2.78	0.52
2:B:51:GLU:OE2	2:B:202:THR:HG23	2.10	0.52
5:E:201:LEU:O	5:E:202:ARG:HB2	2.10	0.52
7:G:18(G):GLU:HG2	7:G:188:LYS:HB3	1.91	0.52
1:A:33:GLN:HE21	1:A:33:GLN:CA	2.21	0.52
6:T:175:GLU:CB	6:T:196:ILE:HD12	2.39	0.52
2:B:224:PHE:N	2:B:224:PHE:CD2	2.78	0.52
6:F:136:THR:O	6:F:150:MET:HA	2.10	0.52
6:F:35:THR:HG23	6:F:51:GLU:HB3	1.92	0.52
1:O:159:PRO:O	2:P:59:LEU:HD12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:175:GLU:OE1	6:T:199:LEU:HD23	2.09	0.52
6:F:175:GLU:OE1	6:F:199:LEU:HD23	2.10	0.52
13:M:40:ASN:HD22	13:M:40:ASN:N	2.00	0.52
2:P:224:PHE:N	2:P:224:PHE:HD2	2.08	0.52
13:M:76:PRO:HD2	13:M:105:GLN:OE1	2.10	0.52
5:S:70:CYS:SG	5:S:92:LEU:HD23	2.50	0.52
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.92	0.52
6:F:216:SER:HB3	6:F:21(A):GLU:HB2	1.90	0.52
2:P:107:ILE:HD11	2:P:111:ILE:HG22	1.91	0.51
2:B:141:TYR:CD1	2:B:21(E):VAL:HG21	2.45	0.51
6:T:136:THR:O	6:T:150:MET:HA	2.10	0.51
3:C:227:GLU:OE1	3:C:227:GLU:N	2.42	0.51
8:H:165:ASN:HD22	13:1:139:ARG:NH1	2.04	0.51
1:A:150:GLN:O	1:A:157:TYR:HA	2.09	0.51
11:Y:10(A):ARG:HH11	11:Y:10(A):ARG:HG2	1.75	0.51
13:M:19:LEU:HD21	13:M:26:LEU:HD22	1.91	0.51
9:I:28:SER:HB2	10:J:120:VAL:HG21	1.91	0.51
10:X:111:TYR:CE1	10:X:121:GLU:HG3	2.45	0.51
8:V:147:THR:OG1	8:V:150:GLU:HG3	2.10	0.51
9:I:34:ILE:HB	16:I:955:HOH:O	2.09	0.51
1:O:130:ARG:NH2	7:U:124:THR:HG22	2.15	0.51
3:C:15:PHE:CD1	3:C:21:ILE:HD11	2.46	0.51
5:S:134:VAL:O	5:S:153:PRO:HG3	2.10	0.51
4:D:24:VAL:O	4:D:27:SER:HB3	2.11	0.51
3:Q:227:GLU:N	3:Q:227:GLU:OE1	2.41	0.51
9:W:28:SER:HB2	10:X:120:VAL:HG21	1.92	0.51
2:P:169:THR:O	2:P:173:GLN:HB2	2.10	0.51
7:U:18(G):GLU:HG2	7:U:188:LYS:HB3	1.93	0.51
12:L:129:ALA:HB1	12:L:166:HIS:CE1	2.46	0.51
14:N:20:THR:HG22	15:N:224:GPT:H10	1.92	0.51
2:B:215:ILE:HG13	2:B:221:GLN:HG2	1.93	0.51
5:S:160:LEU:HD13	5:S:163:THR:HB	1.92	0.51
2:B:87:ILE:O	2:B:91:THR:HG23	2.11	0.51
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.46	0.51
10:J:111:TYR:CE1	10:J:121:GLU:HG3	2.46	0.51
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.31	0.51
4:R:112:LEU:C	4:R:112:LEU:HD13	2.31	0.51
5:E:190:ILE:HG23	5:E:212:ILE:HD12	1.92	0.51
6:F:203:GLU:O	6:F:206:LYS:HD2	2.10	0.51
13:M:7:LYS:HB3	13:M:12:VAL:HG12	1.93	0.51
10:J:-1:MET:HG2	10:J:1:ASP:N	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:72:ARG:HB2	7:U:72:ARG:HH11	1.74	0.51
4:D:40:ILE:HD11	4:D:176:LEU:HD22	1.93	0.51
8:V:8:PHE:HB3	8:V:151:ALA:HB2	1.92	0.51
7:G:35:ILE:HG23	7:G:51:GLN:HB2	1.91	0.51
5:E:141:TYR:CE2	5:E:217:LYS:HA	2.46	0.51
6:F:187:ARG:HG3	6:F:187:ARG:HH11	1.76	0.51
6:T:187:ARG:HG3	6:T:187:ARG:HH11	1.76	0.51
5:E:15:PHE:H	6:F:23:GLN:NE2	2.04	0.51
8:V:4:VAL:HG12	8:V:126:SER:HB3	1.93	0.51
10:X:113:ILE:HA	10:X:118:THR:O	2.10	0.51
2:P:49:ALA:HB2	2:P:212:PHE:CE1	2.45	0.51
4:R:72:ARG:HG3	16:R:1302:HOH:O	2.11	0.51
1:A:62:GLU:H	1:A:62:GLU:CD	2.14	0.51
2:P:6:ARG:HG2	3:Q:10:ARG:NH2	2.26	0.51
2:B:224:PHE:HD2	2:B:224:PHE:N	2.08	0.51
8:H:216:GLU:HG3	9:I:187:ARG:HG2	1.92	0.51
14:N:3:ILE:HG22	14:N:16:ALA:CB	2.41	0.51
13:M:14(D):GLU:O	13:M:14(G):ILE:HG12	2.11	0.51
12:Z:-7:ASN:HD22	12:Z:-7:ASN:C	2.15	0.51
13:M:19:LEU:HB2	13:M:170:SER:HB2	1.93	0.51
12:L:109:ALA:HA	16:L:975:HOH:O	2.11	0.51
10:X:133:TYR:CZ	10:X:166:MET:HG3	2.46	0.50
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.93	0.50
2:P:222:LYS:NZ	2:P:228:GLU:OE2	2.44	0.50
12:Z:129:ALA:HB1	12:Z:166:HIS:CE1	2.46	0.50
4:D:177:LEU:CD2	5:E:58:LEU:HD13	2.41	0.50
6:F:192:GLN:HE21	6:F:195:LYS:CE	2.24	0.50
14:2:3:ILE:HG22	14:2:16:ALA:CB	2.42	0.50
10:X:147:THR:OG1	10:X:150:GLU:HG3	2.11	0.50
7:U:9:ASP:HA	7:U:14:ILE:CD1	2.24	0.50
5:S:15:PHE:HB2	6:T:23:GLN:HE22	1.76	0.50
4:R:12(D):ALA:HB3	4:R:126:ARG:CD	2.41	0.50
8:H:4:VAL:HG12	8:H:126:SER:HB3	1.94	0.50
8:V:152:ILE:HD11	8:V:177:VAL:HG21	1.93	0.50
7:G:87:ASN:HD22	7:G:87:ASN:C	2.15	0.50
4:D:112:LEU:C	4:D:112:LEU:HD13	2.31	0.50
7:U:107:MET:HE1	7:U:112:LEU:HD13	1.93	0.50
14:2:20:THR:HG22	15:2:224:GPT:H10	1.94	0.50
13:1:19:LEU:HB2	13:1:170:SER:HB2	1.93	0.50
8:V:196:VAL:HG23	16:V:652:HOH:O	2.11	0.50
8:H:128:GLY:O	8:H:131:SER:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:172:ALA:O	6:F:176:LEU:HD22	2.12	0.50
6:T:53:LEU:HD11	6:T:205:ASN:OD1	2.11	0.50
1:A:173:LYS:O	1:A:177:GLU:HG3	2.11	0.50
13:M:13:ILE:HB	13:M:155:ILE:HD13	1.92	0.50
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.93	0.50
13:M:179:ASP:HB3	13:M:18(A):THR:OG1	2.11	0.50
2:P:63:THR:HG22	2:P:63:THR:O	2.12	0.50
6:F:53:LEU:HD11	6:F:205:ASN:OD1	2.12	0.50
10:J:24:ILE:HG12	10:X:133:TYR:OH	2.12	0.50
3:Q:215:VAL:HG23	3:Q:221:ILE:HG12	1.93	0.50
10:J:143:ARG:O	10:J:146:MET:HG3	2.11	0.50
8:H:221:ILE:HD11	9:I:184:VAL:HG21	1.92	0.50
14:2:175:MET:HB2	14:2:187:LEU:HB2	1.93	0.50
5:E:134:VAL:O	5:E:153:PRO:HG3	2.12	0.50
3:C:215:VAL:HG23	3:C:221:ILE:HG12	1.94	0.50
10:X:-1:MET:HG2	10:X:1:ASP:N	2.27	0.50
1:O:173:LYS:O	1:O:177:GLU:HG3	2.12	0.50
1:O:62:GLU:CD	1:O:62:GLU:H	2.15	0.50
6:T:82:ILE:HB	6:T:83:PRO:HD3	1.93	0.50
2:P:215:ILE:HG13	2:P:221:GLN:HG2	1.93	0.50
8:V:173:VAL:HB	8:V:192:LEU:HB2	1.93	0.50
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.75	0.50
3:Q:15:PHE:CD1	3:Q:21:ILE:HD11	2.46	0.50
10:X:24:ILE:HG12	10:X:24:ILE:O	2.11	0.50
5:E:70:CYS:SG	5:E:92:LEU:HD23	2.52	0.50
16:L:200:HOH:O	9:W:192:ARG:HG3	2.10	0.50
13:1:4:ILE:HD13	13:1:4:ILE:H	1.77	0.50
10:J:32:ASP:OD2	10:J:34:THR:HG22	2.12	0.50
6:T:127:ASN:HD22	6:T:127:ASN:C	2.14	0.49
3:C:149:TYR:CE1	3:C:159:SER:HB3	2.47	0.49
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.47	0.49
3:C:15:PHE:CE1	3:C:21:ILE:HD11	2.47	0.49
2:B:11:ARG:HD2	3:C:10:ARG:NH1	2.27	0.49
8:H:84:LYS:HG3	8:H:85:GLN:N	2.27	0.49
2:P:4:GLY:HA3	5:S:127:TYR:CE1	2.47	0.49
12:Z:145:TYR:CD1	12:Z:146:LEU:N	2.80	0.49
12:L:145:TYR:CD1	12:L:146:LEU:N	2.80	0.49
10:J:112:GLN:NE2	10:J:126:ALA:H	2.09	0.49
7:U:70:ILE:HD12	7:U:92:ALA:HB3	1.94	0.49
7:G:49:ILE:HD12	7:G:212:VAL:HG22	1.93	0.49
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:122:ARG:HG2	4:D:122:ARG:HH11	1.76	0.49
14:N:10(B):LYS:HD3	14:N:10(B):LYS:C	2.33	0.49
2:P:51:GLU:OE2	2:P:202:THR:HG23	2.12	0.49
3:Q:15:PHE:CE1	3:Q:21:ILE:HD11	2.47	0.49
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.27	0.49
3:C:33:ARG:CB	3:C:33:ARG:NH1	2.70	0.49
6:F:179:LEU:HD11	6:F:192:GLN:HG3	1.93	0.49
1:O:62:GLU:C	1:O:64:LEU:H	2.16	0.49
2:B:222:LYS:NZ	2:B:228:GLU:OE2	2.43	0.49
14:2:116:GLY:HA3	16:2:191:HOH:O	2.12	0.49
7:G:105:TYR:OH	8:H:66:HIS:HE1	1.95	0.49
2:B:63:THR:HG22	2:B:63:THR:O	2.12	0.49
4:D:207:LEU:HD23	4:D:207:LEU:C	2.33	0.49
4:R:207:LEU:C	4:R:207:LEU:HD23	2.32	0.49
3:C:15:PHE:N	4:D:23:GLN:HE22	1.98	0.49
5:E:4:PHE:CG	5:E:5:ARG:N	2.79	0.49
11:K:10(A):ARG:HG2	11:K:10(A):ARG:HH11	1.76	0.49
9:W:143:GLU:HG3	9:W:146:LEU:HD21	1.94	0.49
11:K:207:ASN:HD21	10:X:144:PRO:CG	2.25	0.49
4:D:170:GLU:N	4:D:170:GLU:OE1	2.45	0.49
7:U:192:PHE:C	7:U:192:PHE:CD1	2.86	0.49
13:1:104:VAL:HG23	13:1:178:ILE:HG22	1.95	0.49
13:1:14(D):GLU:O	13:1:14(G):ILE:HG12	2.12	0.49
7:U:170:GLN:NE2	7:U:174:THR:HG23	2.25	0.49
4:D:12(D):ALA:HB3	4:D:126:ARG:CD	2.43	0.49
11:K:207:ASN:ND2	10:X:144:PRO:CG	2.75	0.49
10:X:143:ARG:O	10:X:146:MET:HG3	2.11	0.49
13:1:7:LYS:HB3	13:1:12:VAL:HG12	1.95	0.49
5:E:31:ILE:HD11	5:E:153:PRO:CD	2.42	0.49
14:N:26:ILE:HB	13:1:165:ARG:HA	1.94	0.49
3:C:211:GLU:C	3:C:212:ILE:HD13	2.33	0.49
6:F:40:ILE:HD12	6:F:193:ALA:HB2	1.95	0.49
2:B:15:PHE:N	3:C:23:GLN:HE22	1.87	0.49
7:G:70:ILE:HD12	7:G:92:ALA:HB3	1.94	0.49
10:J:113:ILE:HA	10:J:118:THR:O	2.12	0.49
8:V:84:LYS:HG3	8:V:85:GLN:N	2.27	0.49
7:U:39:ALA:HB2	7:U:48:VAL:HG12	1.94	0.49
5:E:2(B):THR:H	5:E:2(E):ASN:HD22	1.60	0.49
2:B:181:LYS:HG3	2:B:184:MET:HG3	1.95	0.49
7:G:34(A):ASN:HA	7:G:167:PRO:HG2	1.94	0.49
5:S:107:LEU:HD11	5:S:111:ARG:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.28	0.49
4:R:24:VAL:O	4:R:27:SER:HB3	2.12	0.49
8:V:128:GLY:O	8:V:131:SER:HB2	2.12	0.49
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.94	0.49
14:2:10(B):LYS:C	14:2:10(B):LYS:HD3	2.33	0.49
3:C:163:GLN:CA	3:C:163:GLN:HE21	2.26	0.49
3:Q:52:ARG:HD2	3:Q:208:LYS:O	2.13	0.49
3:C:52:ARG:HD2	3:C:208:LYS:O	2.13	0.49
9:W:112:GLY:N	9:W:125:ILE:HD12	2.28	0.49
2:P:150:THR:O	2:P:157:TYR:HA	2.12	0.49
10:X:112:GLN:NE2	10:X:126:ALA:H	2.11	0.49
7:U:107:MET:CE	7:U:112:LEU:HD13	2.42	0.49
5:S:2(B):THR:H	5:S:2(E):ASN:HD22	1.59	0.49
6:T:192:GLN:HE21	6:T:195:LYS:CE	2.25	0.49
13:1:40:ASN:ND2	13:1:40:ASN:N	2.61	0.49
3:C:57:LYS:HD2	3:C:58:LEU:N	2.28	0.49
13:M:165:ARG:HA	14:2:26:ILE:HB	1.95	0.49
10:J:133:TYR:OH	10:X:24:ILE:HG12	2.13	0.49
12:L:98:HIS:HD2	16:L:199:HOH:O	1.96	0.49
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.94	0.49
3:C:182:PRO:O	3:C:184:ALA:N	2.46	0.49
6:T:179:LEU:HD11	6:T:192:GLN:HG3	1.94	0.48
7:G:72:ARG:HB2	7:G:72:ARG:HH11	1.78	0.48
7:G:8:TYR:C	7:G:10:ARG:N	2.66	0.48
1:O:20(A):THR:C	1:O:210:ILE:HD12	2.34	0.48
4:R:12(F):GLY:O	4:R:12(G):GLU:HB2	2.13	0.48
3:Q:40:VAL:HG23	3:Q:189:CYS:SG	2.52	0.48
4:D:12(F):GLY:O	4:D:12(G):GLU:HB2	2.13	0.48
5:E:78:LEU:HD12	5:E:78:LEU:C	2.33	0.48
6:T:109:ILE:CD1	6:T:142:ASP:HB3	2.43	0.48
3:Q:33:ARG:NH1	3:Q:33:ARG:CB	2.67	0.48
13:1:40:ASN:ND2	13:1:40:ASN:H	2.10	0.48
3:Q:55:THR:C	3:Q:56:LEU:HD22	2.33	0.48
9:W:178:ILE:HG23	9:W:184:VAL:HG22	1.94	0.48
9:I:137:MET:HE3	9:I:141:LEU:HD11	1.95	0.48
1:O:57:PRO:HG2	7:U:177:GLU:HG2	1.94	0.48
3:Q:163:GLN:HE21	3:Q:163:GLN:CA	2.26	0.48
5:S:180:LEU:HA	5:S:18(C):PHE:CE2	2.48	0.48
10:J:133:TYR:CZ	10:J:166:MET:HG3	2.48	0.48
2:P:41:MET:HE2	16:P:254:HOH:O	2.12	0.48
3:Q:182:PRO:O	3:Q:184:ALA:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:160:LEU:HD13	5:E:163:THR:HB	1.94	0.48
8:H:152:ILE:HD11	8:H:177:VAL:HG21	1.95	0.48
4:R:40:ILE:HD11	4:R:176:LEU:HD22	1.93	0.48
13:1:179:ASP:HB3	13:1:18(A):THR:OG1	2.12	0.48
2:B:163:ILE:HD13	2:B:164:SER:H	1.79	0.48
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.94	0.48
7:G:107:MET:CE	7:G:112:LEU:HD13	2.44	0.48
5:S:111:ARG:HG2	5:S:111:ARG:HH11	1.78	0.48
1:A:20(A):THR:C	1:A:210:ILE:HD12	2.34	0.48
7:G:192:PHE:CD1	7:G:192:PHE:C	2.86	0.48
12:L:129:ALA:HB1	12:L:166:HIS:NE2	2.28	0.48
12:L:166:HIS:CD2	12:L:168:GLN:H	2.24	0.48
12:Z:166:HIS:CD2	12:Z:168:GLN:H	2.25	0.48
3:C:190:VAL:O	3:C:194:VAL:HG23	2.14	0.48
11:Y:4:LEU:HD11	11:Y:159:ILE:HG12	1.96	0.48
4:R:175:GLU:CG	4:R:196:ILE:HD12	2.43	0.48
7:U:203:THR:HG22	7:U:204:GLU:N	2.29	0.48
9:I:130:ALA:HB2	9:I:166:ASP:HB2	1.96	0.48
7:U:82:ILE:HG22	7:U:83:PRO:HD3	1.95	0.48
8:H:173:VAL:HB	8:H:192:LEU:HB2	1.95	0.48
13:M:139:ARG:NH1	8:V:165:ASN:HD22	2.05	0.48
2:P:141:TYR:CD1	2:P:21(E):VAL:HG21	2.49	0.48
5:S:4:PHE:CG	5:S:5:ARG:N	2.80	0.48
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.96	0.48
6:T:35:THR:HG23	6:T:51:GLU:HB3	1.94	0.48
5:E:180:LEU:HA	5:E:18(C):PHE:CE2	2.49	0.48
4:D:175:GLU:CG	4:D:196:ILE:HD12	2.44	0.48
10:J:133:TYR:HE1	16:X:876:HOH:O	1.97	0.48
2:B:101:LYS:NZ	10:J:85:GLN:NE2	2.61	0.48
10:J:6:ILE:CG2	10:J:13:ILE:HB	2.44	0.48
3:C:40:VAL:HG23	3:C:189:CYS:SG	2.54	0.48
4:R:122:ARG:HH11	4:R:122:ARG:HG2	1.79	0.48
12:L:-7:ASN:C	12:L:-7:ASN:HD22	2.15	0.47
2:B:4:GLY:HA3	5:E:127:TYR:CE1	2.48	0.47
10:X:119:LYS:HE2	16:X:705:HOH:O	2.14	0.47
10:X:6:ILE:CG2	10:X:13:ILE:HB	2.44	0.47
13:M:4:ILE:HD13	13:M:4:ILE:H	1.79	0.47
2:B:150:THR:O	2:B:157:TYR:HA	2.14	0.47
3:Q:190:VAL:O	3:Q:194:VAL:HG23	2.14	0.47
10:X:120:VAL:HG13	10:X:122:LEU:HG	1.96	0.47
8:V:128:GLY:O	8:V:131:SER:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:177:GLU:OE1	6:F:56:SER:HB2	2.13	0.47
11:K:174:ASN:HD21	11:K:189:ASN:HD22	1.62	0.47
12:Z:14(I):THR:O	12:Z:14(K):LYS:HB2	2.14	0.47
6:F:109:ILE:CD1	6:F:142:ASP:HB3	2.44	0.47
13:1:13:ILE:HB	13:1:155:ILE:HD13	1.96	0.47
9:I:33:LYS:O	9:I:44:GLY:HA2	2.14	0.47
5:E:107:LEU:HD11	5:E:111:ARG:HG2	1.95	0.47
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.49	0.47
7:G:186:TRP:O	7:G:190:VAL:HG23	2.13	0.47
4:R:53:ARG:HG2	4:R:53:ARG:O	2.14	0.47
5:S:186:PRO:O	5:S:190:ILE:HD12	2.15	0.47
2:B:121:GLN:HG3	3:C:83:ALA:HB1	1.96	0.47
5:S:31:ILE:HD11	5:S:153:PRO:CD	2.44	0.47
4:R:59:LEU:HD13	4:R:59:LEU:C	2.35	0.47
9:I:178:ILE:HG23	9:I:184:VAL:HG22	1.96	0.47
1:O:118:LYS:HE2	1:O:122:GLU:OE1	2.14	0.47
9:I:143:GLU:HG3	9:I:146:LEU:HD21	1.96	0.47
8:H:197:ARG:NH2	9:I:139:GLU:O	2.47	0.47
7:G:12:ILE:HG13	7:G:14:ILE:HD12	1.97	0.47
13:M:104:VAL:HG23	13:M:178:ILE:HG22	1.96	0.47
9:I:6:MET:HE1	9:I:155:ILE:HA	1.96	0.47
10:X:44:SER:OG	10:X:100:LEU:HB2	2.14	0.47
5:S:179:THR:HG22	5:S:179:THR:O	2.14	0.47
1:A:24:ILE:HD11	1:A:124:THR:OG1	2.14	0.47
3:C:177:GLU:OE2	4:D:57:PRO:HD2	2.15	0.47
14:2:112:THR:HG22	14:2:120:HIS:HB2	1.96	0.47
14:2:161:GLN:HE22	14:2:165:TRP:HE1	1.61	0.47
1:O:24:ILE:HD11	1:O:124:THR:OG1	2.15	0.47
10:J:167:PRO:CB	10:X:168:MET:HE1	2.45	0.47
10:J:52:THR:HG23	10:J:53:VAL:N	2.30	0.47
1:A:233:LEU:O	1:A:236:LEU:HB2	2.15	0.47
8:H:128:GLY:O	8:H:131:SER:CB	2.63	0.47
10:J:144:PRO:CG	11:Y:207:ASN:HD21	2.27	0.47
5:S:78:LEU:HD12	5:S:78:LEU:C	2.35	0.47
2:P:181:LYS:HG3	2:P:184:MET:HG3	1.96	0.47
3:C:55:THR:C	3:C:56:LEU:HD22	2.35	0.47
9:I:66:TYR:CZ	9:I:70:GLU:HG3	2.50	0.47
5:E:179:THR:O	5:E:179:THR:HG22	2.15	0.47
6:F:203:GLU:HA	6:F:203:GLU:OE1	2.15	0.47
8:V:80:LEU:HD12	8:V:113:ILE:CD1	2.40	0.47
2:P:141:TYR:CE2	2:P:145:GLY:HA2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:130:ALA:HB2	9:W:166:ASP:HB2	1.95	0.47
6:F:127:ASN:HD22	6:F:128:SER:N	2.13	0.47
10:J:120:VAL:HG13	10:J:122:LEU:HG	1.97	0.47
6:T:127:ASN:HD22	6:T:128:SER:N	2.13	0.47
13:M:17:ASP:HA	13:M:173:PHE:CB	2.45	0.47
7:G:82:ILE:HG22	7:G:83:PRO:HD3	1.96	0.47
5:S:77:SER:OG	5:S:137:LEU:HB2	2.15	0.47
10:J:17:SER:HB2	10:J:170:PHE:HB2	1.97	0.47
7:U:87:ASN:HD22	7:U:87:ASN:C	2.18	0.47
9:W:14:ILE:HG12	9:W:34:ILE:HD12	1.97	0.47
1:A:177:GLU:CG	2:B:58:LEU:HD22	2.42	0.47
2:P:97:GLN:NE2	9:W:64:ASN:HD22	2.11	0.47
5:E:111:ARG:HG2	5:E:111:ARG:HH11	1.80	0.47
6:T:147:HIS:HD2	16:T:242:HOH:O	1.98	0.47
14:2:163:ILE:HG23	14:2:170:GLY:HA2	1.97	0.47
10:X:152:LEU:HD13	10:X:193:GLN:HE22	1.80	0.47
4:R:170:GLU:OE1	4:R:170:GLU:N	2.46	0.47
3:C:163:GLN:HA	3:C:163:GLN:NE2	2.30	0.46
3:Q:36:CYS:N	3:Q:51:GLU:HG2	2.30	0.46
10:J:166:MET:HA	10:J:167:PRO:HD3	1.77	0.46
9:W:29:ASN:C	9:W:29:ASN:HD22	2.18	0.46
2:B:228:GLU:O	2:B:232:ILE:HG22	2.15	0.46
4:R:12(G):GLU:HG2	4:R:125:GLU:H	1.80	0.46
10:J:144:PRO:CG	11:Y:207:ASN:ND2	2.77	0.46
13:1:205:GLY:HA3	13:1:209:GLN:HB3	1.97	0.46
6:F:101:LYS:NZ	14:N:85:GLU:OE1	2.46	0.46
7:U:186:TRP:O	7:U:190:VAL:HG23	2.15	0.46
12:Z:33:LYS:HD2	12:Z:46:ASN:ND2	2.25	0.46
4:R:177:LEU:HD22	5:S:58:LEU:CD1	2.40	0.46
3:Q:57:LYS:HD2	3:Q:58:LEU:N	2.29	0.46
3:C:158:SER:HB2	4:D:59:LEU:HD21	1.97	0.46
10:J:168:MET:HG2	10:X:168:MET:CE	2.46	0.46
1:O:233:LEU:O	1:O:236:LEU:HB2	2.15	0.46
12:L:14(I):THR:O	12:L:14(K):LYS:HB2	2.15	0.46
7:U:67:ILE:CD1	7:U:211:GLU:HG2	2.45	0.46
8:V:9:ASN:OD1	8:V:10:ASN:N	2.48	0.46
4:R:90:GLU:OE2	11:Y:69:ARG:NH1	2.48	0.46
8:V:221:ILE:HD11	9:W:184:VAL:HG21	1.97	0.46
4:D:140:GLY:HA2	4:D:215:ILE:HD12	1.97	0.46
3:Q:235:GLN:O	3:Q:239:GLU:HG2	2.16	0.46
10:J:18:LYS:HG2	10:J:174:ILE:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:8:TYR:C	7:U:10:ARG:N	2.67	0.46
7:G:203:THR:HG22	7:G:204:GLU:N	2.31	0.46
9:W:174:VAL:HG21	9:W:186:LYS:HE3	1.97	0.46
6:T:32:GLU:HB3	6:T:169:ARG:NH2	2.30	0.46
6:F:103:TYR:O	6:F:104:LYS:HB3	2.16	0.46
13:M:197:TRP:CH2	14:2:171:GLY:HA2	2.51	0.46
8:V:175:VAL:HG12	8:V:176:CYS:N	2.31	0.46
7:G:228:ASN:HD22	7:G:228:ASN:N	2.14	0.46
7:G:151:THR:HG22	7:G:157:TYR:CB	2.46	0.46
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.49	0.46
12:L:140:ASN:O	12:L:144:PHE:HA	2.15	0.46
5:S:194:VAL:HG13	5:S:207:LEU:HD11	1.97	0.46
5:S:15:PHE:HB2	6:T:23:GLN:NE2	2.31	0.46
2:P:121:GLN:CG	3:Q:83:ALA:HB1	2.46	0.46
3:Q:206:GLY:HA3	3:Q:209:ASN:HB2	1.98	0.46
9:I:29:ASN:HD22	9:I:29:ASN:C	2.19	0.46
12:L:164:GLU:CD	8:V:197:ARG:HG3	2.36	0.46
11:K:37:ILE:HB	11:K:41:LEU:HB2	1.97	0.46
1:A:51:GLU:OE1	1:A:202:VAL:HG22	2.16	0.46
13:M:14(A):VAL:O	13:M:14(A):VAL:HG23	2.16	0.46
14:N:161:GLN:HE21	14:2:136:GLY:CA	2.04	0.46
6:F:192:GLN:NE2	6:F:195:LYS:CE	2.79	0.46
9:I:29:ASN:HD22	9:I:30:LYS:HG3	1.79	0.46
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.80	0.46
4:R:67:ILE:HD12	4:R:211:GLN:HE21	1.80	0.46
2:B:6:ARG:NH1	4:D:12(B):GLU:OE2	2.49	0.46
7:G:177:GLU:O	7:G:17(B):LYS:HG3	2.16	0.46
13:M:171:ARG:HG3	13:M:192:VAL:HB	1.97	0.46
11:K:4:LEU:HD11	11:K:159:ILE:HG12	1.97	0.46
3:Q:163:GLN:HA	3:Q:163:GLN:NE2	2.30	0.46
2:B:101:LYS:HZ2	10:J:85:GLN:NE2	2.14	0.46
12:Z:140:ASN:O	12:Z:144:PHE:HA	2.15	0.46
7:G:158:VAL:HG22	7:G:159:GLY:N	2.31	0.46
7:G:39:ALA:HB2	7:G:48:VAL:HG12	1.96	0.46
4:D:86:ARG:HD3	4:D:86:ARG:HA	1.86	0.46
4:R:86:ARG:HD3	4:R:86:ARG:HA	1.84	0.46
6:T:175:GLU:HB3	6:T:196:ILE:CD1	2.45	0.46
7:U:34(A):ASN:HA	7:U:167:PRO:HG2	1.97	0.46
10:J:168:MET:CE	10:X:168:MET:HG2	2.45	0.46
1:A:62:GLU:C	1:A:64:LEU:H	2.18	0.46
8:H:207:PRO:HG2	8:H:210:THR:OG1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:137:MET:HE3	9:W:141:LEU:HD11	1.97	0.46
10:X:161:GLU:OE2	10:X:161:GLU:HA	2.15	0.46
11:Y:85:ASN:ND2	16:Y:215:HOH:O	2.49	0.46
2:B:141:TYR:CE2	2:B:145:GLY:HA2	2.51	0.46
2:P:101:LYS:HZ1	10:X:85:GLN:NE2	2.13	0.46
3:C:36:CYS:N	3:C:51:GLU:HG2	2.31	0.46
8:V:4:VAL:HG12	8:V:126:SER:CB	2.46	0.46
1:O:110:LYS:HG2	16:O:376:HOH:O	2.15	0.46
8:H:9:ASN:OD1	8:H:10:ASN:N	2.49	0.46
7:U:105:TYR:OH	8:V:66:HIS:HE1	1.98	0.46
6:T:203:GLU:OE1	6:T:203:GLU:HA	2.15	0.45
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.98	0.45
3:C:206:GLY:HA3	3:C:209:ASN:HB2	1.98	0.45
5:S:18(D):ILE:HG23	5:S:18(E):LYS:HG3	1.97	0.45
10:J:168:MET:HE1	10:X:167:PRO:CB	2.46	0.45
2:B:234:VAL:HA	2:B:239:THR:HA	1.98	0.45
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.98	0.45
12:L:33:LYS:HD2	12:L:46:ASN:ND2	2.25	0.45
2:B:6:ARG:HG2	3:C:10:ARG:HH21	1.81	0.45
2:B:147:GLN:HG2	3:C:62(A):ILE:HG21	1.99	0.45
14:N:18(G):TYR:HA	14:N:18(J):LEU:HG	1.98	0.45
12:Z:17:ASP:HA	12:Z:172:GLY:O	2.17	0.45
14:N:14:LEU:O	14:N:175:MET:HA	2.17	0.45
8:V:197:ARG:NH2	9:W:139:GLU:O	2.50	0.45
7:G:67:ILE:CD1	7:G:211:GLU:HG2	2.46	0.45
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.17	0.45
8:V:207:PRO:HG2	8:V:210:THR:OG1	2.15	0.45
5:S:175:TYR:CD2	5:S:196:ALA:HA	2.51	0.45
3:C:175:PHE:O	3:C:179:ASN:HB2	2.17	0.45
5:E:231:LYS:HD2	5:E:231:LYS:H	1.81	0.45
9:W:33:LYS:O	9:W:44:GLY:HA2	2.15	0.45
2:P:186:VAL:O	2:P:190:ILE:HG13	2.17	0.45
1:A:97:HIS:CD2	8:H:61:SER:OG	2.68	0.45
2:P:228:GLU:O	2:P:232:ILE:HG22	2.15	0.45
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.98	0.45
6:T:40:ILE:HD12	6:T:193:ALA:HB2	1.99	0.45
4:R:140:GLY:HA2	4:R:215:ILE:HD12	1.99	0.45
12:L:93:PHE:N	12:L:94:PRO:HD3	2.30	0.45
5:S:49:VAL:HG12	5:S:197:ILE:HD13	1.97	0.45
7:G:170:GLN:NE2	7:G:174:THR:HG23	2.26	0.45
2:P:163:ILE:HD13	2:P:164:SER:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:203:THR:HG22	7:U:204:GLU:O	2.17	0.45
5:E:18(D):ILE:HG23	5:E:18(E):LYS:HG3	1.97	0.45
4:D:59:LEU:C	4:D:59:LEU:HD13	2.36	0.45
5:S:64:GLN:NE2	5:S:82:ALA:HB2	2.32	0.45
1:A:210:ILE:HD12	1:A:210:ILE:N	2.32	0.45
12:L:-9:GLN:HE21	13:M:-8:THR:HG21	1.81	0.45
10:X:18:LYS:HG2	10:X:174:ILE:HG13	1.98	0.45
7:U:78:VAL:HG11	7:U:85:ALA:CB	2.47	0.45
14:N:18(E):ASP:OD2	16:N:232:HOH:O	2.21	0.45
9:W:66:TYR:CZ	9:W:70:GLU:HG3	2.52	0.45
9:I:174:VAL:HG21	9:I:186:LYS:HE3	1.98	0.45
6:F:35:THR:CG2	6:F:51:GLU:O	2.59	0.45
3:Q:241:GLN:O	3:Q:243:GLN:N	2.47	0.45
9:W:101:VAL:O	9:W:110:ILE:HA	2.16	0.45
8:V:3:ILE:O	8:V:126:SER:HA	2.17	0.45
5:E:175:TYR:CD2	5:E:196:ALA:HA	2.52	0.45
10:X:17:SER:HB2	10:X:170:PHE:HB2	1.97	0.45
2:B:39:GLY:O	2:B:162:ALA:HA	2.16	0.45
5:S:2(C):VAL:HG13	5:S:2(D):ASP:N	2.32	0.45
13:1:17:ASP:HA	13:1:173:PHE:CB	2.46	0.45
10:X:90(B):ARG:NH1	16:X:266:HOH:O	2.42	0.45
1:A:110:LYS:HG2	16:A:285:HOH:O	2.16	0.45
5:E:136:LEU:HB2	5:E:151:PHE:HB3	1.99	0.45
6:T:95:GLU:HG3	6:T:115:ARG:HH11	1.82	0.45
6:T:35:THR:CG2	6:T:36:THR:N	2.80	0.45
12:Z:129:ALA:HB1	12:Z:166:HIS:NE2	2.31	0.45
8:H:3:ILE:O	8:H:126:SER:HA	2.17	0.45
8:H:197:ARG:HG3	12:Z:164:GLU:CD	2.37	0.45
9:W:106:GLY:HA2	9:W:181:LYS:HD3	1.99	0.45
11:Y:37:ILE:HB	11:Y:41:LEU:HB2	1.99	0.45
8:H:175:VAL:HG12	8:H:176:CYS:N	2.31	0.45
1:A:38:LEU:HD12	1:A:38:LEU:C	2.37	0.45
5:E:160:LEU:HD23	6:F:59:LEU:HA	1.98	0.45
9:I:66:TYR:CE1	9:I:70:GLU:HG3	2.52	0.45
10:J:152:LEU:HD13	10:J:193:GLN:HE22	1.82	0.45
1:O:186:LEU:O	1:O:190:ILE:HG13	2.17	0.45
6:T:203:GLU:C	6:T:205:ASN:H	2.20	0.45
9:I:101:VAL:O	9:I:110:ILE:HA	2.17	0.45
8:H:4:VAL:HG12	8:H:126:SER:CB	2.47	0.45
7:U:78:VAL:HG11	7:U:85:ALA:HB2	1.99	0.45
6:F:114:ASP:O	6:F:118:GLN:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:12:VAL:CG2	4:D:12(A):GLY:HA2	2.47	0.45
7:G:217:LYS:CE	7:G:217:LYS:HA	2.45	0.45
3:Q:58:LEU:HD12	3:Q:58:LEU:HA	1.85	0.45
7:G:136:LEU:O	7:G:150:LYS:HA	2.17	0.45
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.98	0.45
3:C:225:SER:OG	3:C:228:GLU:HG3	2.17	0.45
14:2:18(G):TYR:HA	14:2:18(J):LEU:HG	1.98	0.45
5:E:194:VAL:HG13	5:E:207:LEU:HD11	1.97	0.44
13:1:157:ASN:HB3	16:1:558:HOH:O	2.16	0.44
3:Q:177:GLU:OE2	4:R:57:PRO:HD2	2.17	0.44
6:F:175:GLU:HB3	6:F:196:ILE:CD1	2.45	0.44
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.99	0.44
1:O:210:ILE:N	1:O:210:ILE:HD12	2.32	0.44
14:N:3:ILE:HB	14:N:44:CYS:HB3	1.99	0.44
14:2:3:ILE:HB	14:2:44:CYS:HB3	2.00	0.44
13:1:4:ILE:CD1	13:1:159:MET:SD	3.05	0.44
13:1:130:GLY:O	13:1:134:ALA:HB3	2.17	0.44
3:Q:201:VAL:HG21	3:Q:210:ILE:HD11	1.98	0.44
3:Q:17:PRO:HA	4:R:26:TYR:CD1	2.52	0.44
7:U:158:VAL:HG22	7:U:159:GLY:N	2.32	0.44
12:L:5:GLY:O	12:L:124:CYS:HA	2.16	0.44
12:Z:5:GLY:O	12:Z:124:CYS:HA	2.18	0.44
13:M:40:ASN:ND2	13:M:40:ASN:N	2.61	0.44
9:W:29:ASN:H	9:W:29:ASN:ND2	2.15	0.44
2:P:234:VAL:HA	2:P:239:THR:HA	1.98	0.44
7:U:151:THR:HG22	7:U:157:TYR:CB	2.48	0.44
1:O:67:VAL:HG11	1:O:213:ALA:CB	2.47	0.44
5:E:54:ASN:ND2	5:E:56:ASP:O	2.51	0.44
1:A:118:LYS:HE2	1:A:122:GLU:OE1	2.17	0.44
5:S:52:LYS:O	5:S:63:TYR:HD2	2.00	0.44
5:E:186:PRO:O	5:E:190:ILE:HD12	2.17	0.44
5:S:148:LEU:HD23	5:S:162:GLY:HA2	1.99	0.44
7:G:87:ASN:ND2	7:G:87:ASN:C	2.71	0.44
14:2:14:LEU:O	14:2:175:MET:HA	2.17	0.44
12:Z:99:THR:CG2	16:Z:231:HOH:O	2.64	0.44
2:P:39:GLY:O	2:P:162:ALA:HA	2.16	0.44
9:W:20:LEU:C	9:W:20:LEU:HD13	2.38	0.44
5:S:194:VAL:O	5:S:197:ILE:HG22	2.17	0.44
6:T:192:GLN:NE2	6:T:195:LYS:CE	2.80	0.44
4:R:45:GLY:HA2	4:R:146:TYR:CD1	2.52	0.44
6:F:203:GLU:C	6:F:205:ASN:H	2.19	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:LEU:HA	3:C:58:LEU:HD12	1.84	0.44
10:J:168:MET:HE2	10:X:168:MET:HE2	1.99	0.44
3:C:241:GLN:O	3:C:243:GLN:N	2.47	0.44
4:R:194:LEU:HA	4:R:194:LEU:HD12	1.88	0.44
4:D:12(G):GLU:HG2	4:D:125:GLU:H	1.82	0.44
9:W:66:TYR:CE1	9:W:70:GLU:HG3	2.53	0.44
13:1:184:LEU:C	13:1:184:LEU:HD23	2.38	0.44
6:F:95:GLU:HG3	6:F:115:ARG:HH11	1.81	0.44
13:M:40:ASN:ND2	13:M:40:ASN:H	2.10	0.44
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.83	0.44
3:C:226:SER:HB2	3:C:227:GLU:OE1	2.18	0.44
4:D:45:GLY:HA2	4:D:146:TYR:CD1	2.53	0.44
12:Z:14(I):THR:HG21	12:Z:14(M):VAL:HB	2.00	0.44
3:Q:175:PHE:O	3:Q:179:ASN:HB2	2.18	0.44
4:R:12:VAL:CG2	4:R:12(A):GLY:HA2	2.48	0.44
5:S:177:GLU:OE1	6:T:56:SER:HB2	2.17	0.44
14:2:106:ASN:O	14:2:107:LYS:HB3	2.18	0.44
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.83	0.44
5:S:5:ARG:HG3	5:S:22:PHE:CZ	2.53	0.44
1:O:47:VAL:HG23	1:O:212:LEU:HD21	1.99	0.44
12:L:17:ASP:HA	12:L:172:GLY:O	2.18	0.44
6:T:114:ASP:O	6:T:118:GLN:HG2	2.17	0.44
5:E:142:ASP:HB2	16:M:885:HOH:O	2.17	0.44
6:T:103:TYR:O	6:T:104:LYS:HB3	2.16	0.44
9:I:29:ASN:H	9:I:29:ASN:ND2	2.15	0.44
4:D:67:ILE:HD12	4:D:211:GLN:HE21	1.83	0.44
10:X:52:THR:HG23	10:X:53:VAL:N	2.32	0.44
3:Q:158:SER:HB2	4:R:59:LEU:HD21	1.99	0.44
10:X:12:VAL:CG2	10:X:108:PRO:HB2	2.48	0.44
16:E:574:HOH:O	6:F:12:ASN:HB2	2.17	0.44
6:F:43:ASN:N	6:F:43:ASN:HD22	2.16	0.44
3:C:235:GLN:O	3:C:239:GLU:HG2	2.17	0.44
8:H:195:ASN:HB3	12:Z:192:LYS:HE3	1.99	0.44
13:M:205:GLY:HA3	13:M:209:GLN:HB3	1.99	0.44
14:N:106:ASN:O	14:N:107:LYS:HB3	2.18	0.44
6:T:35:THR:CG2	6:T:51:GLU:O	2.59	0.44
4:D:179:GLU:HG3	4:D:192:LEU:HD11	2.00	0.44
3:Q:33:ARG:HH11	3:Q:33:ARG:HB3	1.81	0.44
13:1:14(C):ARG:CG	13:1:14(C):ARG:HH11	2.30	0.44
4:R:68:VAL:HG21	4:R:89:ILE:HD12	2.00	0.44
7:G:82:ILE:CG2	7:G:83:PRO:HD3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:192:LYS:HE3	8:V:195:ASN:HB3	2.00	0.44
11:Y:174:ASN:HD21	11:Y:189:ASN:HD22	1.66	0.44
1:A:186:LEU:O	1:A:190:ILE:HG13	2.17	0.44
10:X:76:PRO:HD2	16:X:275:HOH:O	2.17	0.44
13:M:14(G):ILE:HB	13:M:144:PRO:CD	2.48	0.43
14:2:19:ARG:NE	14:2:26:ILE:HD13	2.32	0.43
13:1:113:VAL:HA	13:1:118:VAL:O	2.18	0.43
7:G:172:ILE:HD11	7:G:201:LEU:CD2	2.48	0.43
7:G:152:ASP:HB2	7:G:153:PRO:HD2	2.00	0.43
3:Q:226:SER:HB2	3:Q:227:GLU:OE1	2.18	0.43
4:R:160:TYR:CE2	4:R:163:LYS:HD3	2.53	0.43
12:L:177:ILE:HD12	12:L:177:ILE:N	2.33	0.43
5:E:2(C):VAL:HG13	5:E:2(D):ASP:N	2.32	0.43
1:O:137:LEU:HG	1:O:165:ILE:HD13	2.00	0.43
8:V:105:ASP:HB2	8:V:10(A):PRO:CD	2.48	0.43
5:S:231:LYS:HD2	5:S:231:LYS:H	1.83	0.43
8:H:105:ASP:HB2	8:H:10(A):PRO:CD	2.47	0.43
6:F:50:VAL:HG22	6:F:51:GLU:N	2.33	0.43
1:O:5:THR:O	1:O:7:ARG:HG3	2.18	0.43
7:G:203:THR:HG22	7:G:204:GLU:O	2.18	0.43
9:W:29:ASN:HD22	9:W:30:LYS:HG3	1.82	0.43
10:J:18:LYS:HD3	10:J:174:ILE:HG13	2.00	0.43
4:R:15:PHE:HB2	5:S:23:GLN:OE1	2.18	0.43
10:X:35:ARG:NH1	10:X:57:GLU:OE2	2.51	0.43
1:O:21(I):TYR:HE2	1:O:21(L):ILE:HD12	1.83	0.43
13:M:184:LEU:C	13:M:184:LEU:HD23	2.39	0.43
13:1:14(A):VAL:O	13:1:14(A):VAL:HG23	2.18	0.43
2:P:112:LEU:HD23	2:P:112:LEU:O	2.18	0.43
13:1:4:ILE:HD12	13:1:159:MET:SD	2.59	0.43
7:U:82:ILE:CG2	7:U:83:PRO:HD3	2.47	0.43
9:I:106:GLY:HA2	9:I:181:LYS:HD3	1.99	0.43
13:1:8:TYR:CE2	13:1:148:VAL:HG22	2.53	0.43
10:J:44:SER:OG	10:J:100:LEU:HB2	2.17	0.43
12:Z:13:VAL:HG12	12:Z:177:ILE:HG13	2.01	0.43
3:Q:79:SER:OG	3:Q:165:ILE:HG13	2.18	0.43
3:Q:14:ILE:C	3:Q:14:ILE:CD1	2.85	0.43
5:S:76:LEU:O	5:S:76:LEU:HD23	2.18	0.43
3:Q:241:GLN:C	3:Q:243:GLN:N	2.71	0.43
10:J:52:THR:HG22	10:J:53:VAL:H	1.84	0.43
5:E:148:LEU:HD23	5:E:162:GLY:HA2	2.00	0.43
13:1:19:LEU:HD12	13:1:28:PHE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:169:SER:HA	3:Q:172:VAL:HG13	2.01	0.43
10:J:18:LYS:CG	10:J:174:ILE:HG13	2.48	0.43
1:O:212:LEU:HD23	1:O:213:ALA:N	2.33	0.43
1:A:67:VAL:HG11	1:A:213:ALA:CB	2.49	0.43
9:I:159:LEU:HD21	9:I:173:ALA:HB1	2.00	0.43
5:E:194:VAL:O	5:E:197:ILE:HG22	2.19	0.43
3:Q:36:CYS:H	3:Q:51:GLU:HG2	1.83	0.43
3:C:14:ILE:CD1	3:C:14:ILE:C	2.87	0.43
9:W:113:PHE:HA	9:W:118:CYS:O	2.19	0.43
4:D:90:GLU:OE2	11:K:69:ARG:NH1	2.52	0.43
3:Q:225:SER:OG	3:Q:228:GLU:HG3	2.17	0.43
10:J:12:VAL:CG2	10:J:108:PRO:HB2	2.48	0.43
1:O:38:LEU:HD12	1:O:38:LEU:C	2.39	0.43
13:1:171:ARG:HG3	13:1:192:VAL:HB	2.00	0.43
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	2.00	0.43
1:A:5:THR:O	1:A:7:ARG:HG3	2.18	0.43
2:B:112:LEU:HD23	2:B:112:LEU:O	2.19	0.43
7:G:225:SER:OG	7:G:228:ASN:ND2	2.51	0.43
2:B:11:ARG:HD2	3:C:10:ARG:CZ	2.48	0.43
3:C:97:GLN:NE2	16:C:6:HOH:O	2.46	0.43
13:1:14(G):ILE:HB	13:1:144:PRO:CD	2.48	0.43
11:Y:142:TYR:C	11:Y:143:LYS:HD2	2.39	0.43
4:R:12(D):ALA:HA	5:S:129:GLY:HA2	2.01	0.43
5:S:160:LEU:CD2	6:T:59:LEU:HD12	2.49	0.43
3:Q:47:VAL:HG23	3:Q:189:CYS:SG	2.59	0.43
12:L:13:VAL:HG12	12:L:177:ILE:HG13	2.00	0.43
7:U:136:LEU:O	7:U:150:LYS:HA	2.17	0.43
9:I:20:LEU:C	9:I:20:LEU:HD13	2.39	0.43
13:M:13:ILE:HD13	13:M:177:ILE:HG12	2.00	0.43
7:U:217:LYS:HA	7:U:217:LYS:CE	2.44	0.43
3:C:168:ASN:CB	3:C:200:VAL:HG11	2.46	0.43
7:U:172:ILE:HD11	7:U:201:LEU:CD2	2.48	0.43
2:B:232:ILE:O	2:B:232:ILE:HG13	2.19	0.43
1:O:15:PHE:N	2:P:23:GLN:HE22	1.98	0.43
11:K:142:TYR:C	11:K:143:LYS:HD2	2.39	0.43
3:Q:168:ASN:CB	3:Q:200:VAL:HG11	2.45	0.43
4:D:67:ILE:HG22	4:D:221:PHE:HZ	1.83	0.43
12:Z:-9:GLN:HE21	13:1:-8:THR:HG21	1.83	0.43
6:T:158:TRP:CZ3	7:U:64:VAL:HA	2.54	0.43
5:E:77:SER:OG	5:E:137:LEU:HB2	2.17	0.43
3:C:21:ILE:N	3:C:21:ILE:HD13	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:51:GLU:OE1	6:T:53:LEU:HD21	2.18	0.43
7:G:18(G):GLU:CG	7:G:188:LYS:HB2	2.44	0.43
9:W:155:ILE:HG23	9:W:156:SER:N	2.34	0.43
3:C:36:CYS:H	3:C:51:GLU:HG2	1.84	0.43
3:C:241:GLN:C	3:C:243:GLN:N	2.71	0.43
10:X:52:THR:HG22	10:X:53:VAL:H	1.84	0.43
9:I:14:ILE:HG12	9:I:34:ILE:HD12	2.00	0.43
10:X:18:LYS:CG	10:X:174:ILE:HG13	2.49	0.43
1:A:212:LEU:HD23	1:A:213:ALA:N	2.33	0.43
1:O:51:GLU:OE1	1:O:202:VAL:HG22	2.19	0.43
13:1:13:ILE:HD13	13:1:177:ILE:HG12	2.01	0.42
7:G:67:ILE:HD13	7:G:211:GLU:HG2	2.00	0.42
10:X:18:LYS:HD3	10:X:174:ILE:HG13	2.00	0.42
12:Z:99:THR:HG22	16:Z:231:HOH:O	2.18	0.42
8:V:59:ILE:HG12	8:V:83:LEU:HD23	2.00	0.42
1:A:21(I):TYR:HE2	1:A:21(L):ILE:HD12	1.83	0.42
12:L:99:THR:HG23	12:L:113:PHE:HB2	2.01	0.42
14:N:171:GLY:HA2	13:1:197:TRP:CH2	2.54	0.42
1:A:130:ARG:NH2	7:G:124:THR:HG22	2.21	0.42
6:T:50:VAL:HG22	6:T:51:GLU:N	2.34	0.42
10:X:166:MET:CE	10:X:168:MET:HB2	2.49	0.42
13:M:113:VAL:HA	13:M:118:VAL:O	2.19	0.42
2:P:232:ILE:HG13	2:P:232:ILE:O	2.19	0.42
3:Q:169:SER:HA	3:Q:172:VAL:CG1	2.49	0.42
11:K:10(A):ARG:HG2	11:K:10(A):ARG:NH1	2.34	0.42
2:B:101:LYS:HG3	9:I:57:GLU:HB3	2.00	0.42
5:S:104:ASN:HB2	13:1:81:GLU:HG2	2.01	0.42
4:D:53:ARG:HG2	4:D:53:ARG:O	2.18	0.42
3:Q:125:GLN:HG3	3:Q:125:GLN:O	2.18	0.42
6:T:43:ASN:HD22	6:T:43:ASN:N	2.16	0.42
14:N:107:LYS:CG	14:N:108:GLY:H	2.16	0.42
8:V:81:GLN:O	8:V:85:GLN:HG3	2.19	0.42
3:Q:14:ILE:H	3:Q:14:ILE:HD12	1.85	0.42
12:L:113:PHE:CD1	12:L:113:PHE:N	2.86	0.42
9:W:159:LEU:HD21	9:W:173:ALA:HB1	2.01	0.42
9:W:61:TYR:C	9:W:61:TYR:CD1	2.92	0.42
14:2:161:GLN:NE2	14:2:165:TRP:HE1	2.17	0.42
14:N:161:GLN:HE22	14:N:165:TRP:HE1	1.66	0.42
5:E:49:VAL:HG12	5:E:197:ILE:HD13	2.01	0.42
6:F:51:GLU:OE1	6:F:53:LEU:HD21	2.20	0.42
8:V:113:ILE:HG12	8:V:119:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:188:LYS:HD3	7:G:191:GLU:OE2	2.19	0.42
6:T:194:ALA:O	6:T:198:TYR:HD1	2.03	0.42
10:J:166:MET:CE	10:J:168:MET:HB2	2.49	0.42
5:E:64:GLN:NE2	5:E:82:ALA:HB2	2.35	0.42
2:P:69:LYS:HG3	2:P:221:GLN:OE1	2.19	0.42
5:S:137:LEU:CD2	5:S:150:GLU:HG3	2.48	0.42
7:U:67:ILE:HD13	7:U:211:GLU:HG2	2.02	0.42
13:1:112:TYR:O	13:1:119:THR:HA	2.19	0.42
14:N:116:GLY:HA3	16:N:195:HOH:O	2.18	0.42
6:T:107:ILE:HA	6:T:108:PRO:HD3	1.84	0.42
13:M:14(G):ILE:N	13:M:144:PRO:HD2	2.35	0.42
3:C:75:VAL:HG13	3:C:221:ILE:HD13	2.02	0.42
10:X:113:ILE:HG12	10:X:119:LYS:HG3	2.01	0.42
14:N:159:LEU:O	14:N:163:ILE:HG13	2.19	0.42
5:S:35:SER:HB3	5:S:66:LYS:NZ	2.35	0.42
3:Q:13:SER:O	4:R:130:ARG:HD3	2.19	0.42
8:H:59:ILE:HG12	8:H:83:LEU:HD23	2.02	0.42
10:J:161:GLU:HA	10:J:161:GLU:OE2	2.19	0.42
7:G:143:GLU:HA	7:G:217:LYS:NZ	2.35	0.42
9:I:155:ILE:HG23	9:I:156:SER:N	2.35	0.42
7:G:172:ILE:HD12	7:G:197:MET:CE	2.49	0.42
7:U:228:ASN:HD22	7:U:228:ASN:N	2.16	0.42
2:B:69:LYS:HG3	2:B:221:GLN:OE1	2.19	0.42
2:P:225:LYS:HG3	2:P:228:GLU:OE1	2.19	0.42
2:P:136:PHE:O	2:P:150:THR:HA	2.20	0.42
13:1:112:TYR:CD2	13:1:112:TYR:C	2.92	0.42
6:T:78:TYR:CE1	6:T:85:GLY:HA3	2.54	0.42
12:L:137:PHE:CE1	12:L:141:GLN:HG3	2.55	0.42
3:C:66:LYS:HE2	3:C:78:PHE:CZ	2.54	0.42
5:S:41:ARG:NH1	5:S:42:SER:O	2.51	0.42
8:H:72:ARG:HH11	8:H:72:ARG:HG3	1.83	0.42
4:R:150:HIS:O	4:R:157:PHE:HA	2.19	0.42
6:F:53:LEU:HD13	6:F:20(C):LYS:HD2	2.02	0.42
14:N:105:ASP:HB3	14:N:106:ASN:HB2	2.01	0.42
14:2:105:ASP:HB3	14:2:106:ASN:HB2	2.01	0.42
13:1:14(G):ILE:N	13:1:144:PRO:HD2	2.33	0.42
6:F:192:GLN:NE2	6:F:195:LYS:HE3	2.33	0.42
10:X:10(B):LYS:HB2	10:X:10(B):LYS:HZ3	1.84	0.42
1:O:49:ALA:HB2	1:O:212:LEU:HG	2.00	0.42
5:E:137:LEU:CD2	5:E:150:GLU:HG3	2.50	0.42
9:I:107:LYS:HA	9:I:108:PRO:HD3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:1:THR:OG1	13:1:2:SER:N	2.52	0.42
12:Z:137:PHE:CE1	12:Z:141:GLN:HG3	2.55	0.42
12:Z:40:ASN:ND2	16:Z:799:HOH:O	2.49	0.42
13:M:112:TYR:O	13:M:119:THR:HA	2.20	0.42
13:M:130:GLY:O	13:M:134:ALA:HB3	2.19	0.42
2:P:44:ASP:N	2:P:44:ASP:OD2	2.52	0.42
9:I:12(A):LYS:HB2	9:I:12(A):LYS:HE3	1.88	0.42
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.32	0.42
13:M:112:TYR:C	13:M:112:TYR:CD2	2.93	0.42
4:D:150:HIS:O	4:D:157:PHE:HA	2.19	0.42
2:P:27:ALA:O	2:P:30:SER:HB3	2.20	0.42
2:B:95:HIS:CD2	2:B:115:ARG:HG2	2.54	0.42
7:U:121:GLN:NE2	7:U:122:ILE:HD13	2.35	0.42
6:F:20(B):GLU:HG3	6:F:20(C):LYS:N	2.35	0.42
13:1:49:ILE:O	13:1:53:GLN:HG3	2.20	0.42
3:Q:35:THR:HB	3:Q:51:GLU:CG	2.49	0.42
8:H:163:ILE:HG23	8:H:170:GLY:HA2	2.01	0.42
10:X:52:THR:CG2	10:X:53:VAL:H	2.33	0.42
14:N:3:ILE:HG22	14:N:16:ALA:HB2	2.02	0.42
14:N:156:LYS:HG2	14:N:18(J):LEU:HD11	2.02	0.42
2:B:218:ASN:O	2:B:21(C):ASP:HB2	2.19	0.42
3:C:201:VAL:HG21	3:C:210:ILE:HD11	2.01	0.42
11:K:196:PHE:HB3	16:K:214:HOH:O	2.18	0.42
2:P:218:ASN:O	2:P:21(C):ASP:HB2	2.20	0.42
8:V:34:LEU:HB2	16:V:578:HOH:O	2.19	0.42
5:E:76:LEU:O	5:E:76:LEU:HD23	2.20	0.42
7:G:121:GLN:NE2	7:G:122:ILE:HD13	2.35	0.42
7:U:143:GLU:HA	7:U:217:LYS:NZ	2.35	0.42
1:O:179:ARG:HB3	1:O:192:ILE:HD13	2.02	0.42
14:N:20:THR:HG22	15:N:224:GPT:C10	2.49	0.42
7:U:87:ASN:ND2	7:U:87:ASN:C	2.72	0.42
12:L:14(I):THR:HG21	12:L:14(M):VAL:HB	2.02	0.42
2:P:95:HIS:CD2	2:P:115:ARG:HG2	2.54	0.42
4:D:160:TYR:CE2	4:D:163:LYS:HD3	2.55	0.42
5:E:18(C):PHE:CA	5:E:18(F):ILE:HG13	2.43	0.41
4:D:75:GLY:HA3	4:D:221:PHE:CE2	2.56	0.41
13:M:19:LEU:HD12	13:M:28:PHE:O	2.21	0.41
5:E:5:ARG:HG3	5:E:22:PHE:CZ	2.55	0.41
6:F:43:ASN:HD22	6:F:44:ASP:N	2.18	0.41
8:V:105:ASP:HB2	8:V:10(A):PRO:HD2	2.02	0.41
13:1:3:VAL:O	13:1:126:ALA:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:31:THR:HG21	7:U:135:ILE:HG13	2.02	0.41
11:Y:32:LYS:O	11:Y:45:MET:CE	2.68	0.41
13:M:80:PHE:CE1	13:M:111:ARG:HD3	2.55	0.41
7:U:152:ASP:HB2	7:U:153:PRO:HD2	2.01	0.41
5:S:160:LEU:HD23	6:T:59:LEU:HA	2.01	0.41
12:Z:177:ILE:HD12	12:Z:177:ILE:N	2.34	0.41
3:Q:38:VAL:HG22	3:Q:39:GLY:N	2.35	0.41
7:G:78:VAL:HG11	7:G:85:ALA:CB	2.50	0.41
1:A:117:ALA:HB1	1:A:155:GLY:O	2.20	0.41
11:K:40:PHE:HB3	11:K:73:ARG:NH2	2.35	0.41
3:C:152:GLU:HB2	3:C:153:PRO:HD2	2.03	0.41
6:F:78:TYR:CE1	6:F:85:GLY:HA3	2.54	0.41
2:B:191:GLU:O	2:B:195:LYS:HG2	2.20	0.41
6:F:35:THR:CG2	6:F:36:THR:N	2.81	0.41
3:Q:75:VAL:HG13	3:Q:221:ILE:HD13	2.01	0.41
12:L:-7:ASN:HD22	12:L:-6:PRO:N	2.18	0.41
7:U:172:ILE:HD12	7:U:197:MET:CE	2.49	0.41
6:F:127:ASN:ND2	6:F:127:ASN:C	2.73	0.41
11:K:12:ILE:HB	11:K:178:VAL:HB	2.03	0.41
5:E:185:ASN:OD1	5:E:188:GLU:HG2	2.21	0.41
16:A:245:HOH:O	2:B:10:SER:HB2	2.20	0.41
2:P:21(A):LYS:O	2:P:21(B):GLY:C	2.59	0.41
3:C:125:GLN:HG3	3:C:125:GLN:O	2.20	0.41
6:T:18:ASP:N	6:T:18:ASP:OD2	2.40	0.41
4:D:32:LYS:O	4:D:167:SER:HA	2.21	0.41
7:U:12:ILE:HG13	7:U:14:ILE:HD12	2.01	0.41
3:C:20:HIS:C	3:C:21:ILE:HD13	2.41	0.41
6:T:192:GLN:NE2	6:T:195:LYS:HE3	2.34	0.41
4:R:177:LEU:HA	5:S:58:LEU:HD11	2.02	0.41
14:2:20:THR:OG1	14:2:28:ASN:HB3	2.21	0.41
2:B:225:LYS:HG3	2:B:228:GLU:OE1	2.20	0.41
11:K:126:CYS:HB2	11:K:135:TYR:CE1	2.55	0.41
8:V:72:ARG:HH11	8:V:72:ARG:HG3	1.86	0.41
10:J:35:ARG:NH2	16:J:875:HOH:O	2.52	0.41
6:T:20(B):GLU:HG3	6:T:20(C):LYS:N	2.35	0.41
7:U:18(G):GLU:CG	7:U:188:LYS:HB2	2.46	0.41
1:A:179:ARG:HB3	1:A:192:ILE:HD13	2.02	0.41
8:H:159:ILE:O	8:H:163:ILE:HD12	2.21	0.41
12:L:165:ARG:NH2	8:V:29:LYS:HE2	2.34	0.41
2:P:122:GLY:C	2:P:124:THR:H	2.23	0.41
2:B:186:VAL:O	2:B:190:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:225:SER:OG	7:U:228:ASN:ND2	2.54	0.41
2:B:136:PHE:O	2:B:150:THR:HA	2.21	0.41
9:W:45:ILE:HB	9:W:52:VAL:HG13	2.02	0.41
12:Z:58:ARG:NH2	16:Z:1275:HOH:O	2.52	0.41
6:T:157:TYR:C	6:T:157:TYR:CD1	2.93	0.41
11:Y:38:ASN:OD1	11:Y:38:ASN:C	2.59	0.41
6:T:53:LEU:HD13	6:T:20(C):LYS:HD2	2.02	0.41
5:S:18(C):PHE:CA	5:S:18(F):ILE:HG13	2.42	0.41
4:R:175:GLU:OE1	4:R:175:GLU:HA	2.20	0.41
11:Y:10(A):ARG:HG2	11:Y:10(A):ARG:NH1	2.33	0.41
2:B:213:ALA:HA	2:B:222:LYS:O	2.20	0.41
5:S:5:ARG:HG3	5:S:22:PHE:CE1	2.56	0.41
12:Z:113:PHE:CD1	12:Z:113:PHE:N	2.88	0.41
13:1:83:LEU:O	13:1:87:MET:HG2	2.20	0.41
14:2:15:GLY:HA2	14:2:174:ARG:O	2.21	0.41
4:D:177:LEU:HD13	5:E:58:LEU:HD11	2.03	0.41
14:2:20:THR:HG22	15:2:224:GPT:C10	2.51	0.41
2:B:97:GLN:NE2	9:I:64:ASN:HD22	2.16	0.41
1:A:232:ARG:HG3	1:A:232:ARG:NH1	2.36	0.41
11:K:174:ASN:ND2	11:K:189:ASN:HD22	2.19	0.41
14:2:156:LYS:HG2	14:2:18(J):LEU:HD11	2.02	0.41
5:S:35:SER:HB3	5:S:66:LYS:HZ3	1.85	0.41
3:C:17:PRO:HA	4:D:26:TYR:CD1	2.56	0.41
7:G:69:CYS:HB3	16:G:840:HOH:O	2.19	0.41
13:1:191:GLN:HB3	13:1:191:GLN:HE21	1.60	0.41
7:U:14:ILE:N	7:U:14:ILE:HD13	2.35	0.41
3:C:33:ARG:HH11	3:C:33:ARG:HB3	1.83	0.41
7:U:188:LYS:HD3	7:U:191:GLU:OE2	2.21	0.41
12:Z:33:LYS:HE2	12:Z:33:LYS:HB3	1.87	0.41
9:I:6:MET:HE3	9:I:155:ILE:HA	2.03	0.41
11:K:20:ALA:HB2	11:K:31:VAL:HG21	2.03	0.41
10:J:52:THR:CG2	10:J:53:VAL:H	2.33	0.41
11:Y:10(A):ARG:HD3	11:Y:180:GLU:OE1	2.21	0.41
6:T:127:ASN:ND2	6:T:127:ASN:C	2.74	0.41
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.21	0.41
1:A:67:VAL:HG11	1:A:213:ALA:HB3	2.02	0.41
1:A:47:VAL:HG23	1:A:212:LEU:HD21	2.02	0.41
5:E:76:LEU:C	5:E:76:LEU:HD23	2.41	0.41
5:S:185:ASN:OD1	5:S:188:GLU:HG2	2.21	0.41
12:Z:29:ARG:NH1	12:Z:193:ARG:HB3	2.36	0.41
6:F:49:ALA:HA	6:F:211:GLU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:90:ASN:O	5:S:94:GLN:HG3	2.20	0.41
5:S:136:LEU:HB2	5:S:151:PHE:HB3	2.02	0.41
11:Y:126:CYS:HB2	11:Y:135:TYR:CE1	2.56	0.41
3:Q:136:THR:O	3:Q:150:GLN:HA	2.21	0.41
13:1:46:SER:OG	13:1:98:ALA:HB3	2.21	0.41
3:Q:46:VAL:HB	3:Q:215:VAL:CG1	2.50	0.41
4:R:75:GLY:HA3	4:R:221:PHE:CE2	2.56	0.41
7:U:177:GLU:O	7:U:17(B):LYS:HG3	2.21	0.41
5:S:76:LEU:HD23	5:S:76:LEU:C	2.41	0.41
7:G:78:VAL:HG11	7:G:85:ALA:HB2	2.03	0.41
6:F:95:GLU:CG	6:F:115:ARG:HB3	2.37	0.40
9:W:130:ALA:HB2	9:W:166:ASP:CB	2.51	0.40
1:O:232:ARG:HG3	1:O:232:ARG:NH1	2.35	0.40
2:B:101:LYS:HZ2	10:J:85:GLN:HE21	1.68	0.40
13:1:146:THR:HA	16:1:323:HOH:O	2.22	0.40
6:F:107:ILE:HA	6:F:108:PRO:HD3	1.82	0.40
2:B:21(A):LYS:O	2:B:21(B):GLY:C	2.58	0.40
1:A:130:ARG:HG2	7:G:125:GLN:HG3	2.03	0.40
7:G:55:PRO:HG2	7:G:56:ASP:H	1.86	0.40
3:Q:212:ILE:HD13	3:Q:212:ILE:N	2.37	0.40
10:X:4:LEU:HD23	10:X:126:ALA:HB2	2.02	0.40
4:D:215:ILE:HA	4:D:220:GLY:O	2.20	0.40
4:R:215:ILE:HA	4:R:220:GLY:O	2.22	0.40
6:F:32:GLU:HB3	6:F:169:ARG:NH2	2.35	0.40
10:X:7:ARG:NE	16:X:194:HOH:O	2.40	0.40
1:A:27:ALA:O	1:A:31:VAL:HG23	2.21	0.40
5:E:104:ASN:HB2	13:M:81:GLU:HG2	2.03	0.40
2:B:67:LEU:HD22	2:B:211:GLU:HB3	2.03	0.40
7:U:107:MET:HA	7:U:108:PRO:HD3	1.90	0.40
12:L:114:ASP:CB	12:L:118:SER:HB3	2.46	0.40
7:U:72:ARG:CB	7:U:72:ARG:HH11	2.34	0.40
5:S:52:LYS:CB	5:S:63:TYR:HB3	2.52	0.40
6:F:12:ASN:OD1	6:F:12:ASN:O	2.39	0.40
9:W:80:THR:HG23	9:W:113:PHE:CZ	2.56	0.40
14:N:147:SER:OG	14:N:150:GLU:HG3	2.22	0.40
3:Q:77:SER:OG	3:Q:137:LEU:HB2	2.22	0.40
2:B:53:LYS:HG2	2:B:54:VAL:HG23	2.03	0.40
1:O:124:THR:HG22	2:P:130:ARG:NH2	2.20	0.40
14:2:107:LYS:CG	14:2:108:GLY:H	2.17	0.40
8:H:22:GLN:CG	8:H:27:ALA:HB2	2.44	0.40
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:169:SER:HA	3:C:172:VAL:HG13	2.02	0.40
13:M:4:ILE:CD1	13:M:159:MET:SD	3.09	0.40
8:H:105:ASP:HB2	8:H:10(A):PRO:HD2	2.02	0.40
2:P:53:LYS:HG2	2:P:54:VAL:HG23	2.03	0.40
14:N:157:HIS:HD2	14:2:140:LYS:NZ	2.19	0.40
14:2:146:MET:CE	14:2:150:GLU:HB3	2.51	0.40
14:N:48:SER:O	14:N:52:THR:HG23	2.21	0.40
6:T:12:ASN:OD1	6:T:12:ASN:O	2.39	0.40
7:U:55:PRO:HG2	7:U:56:ASP:H	1.87	0.40
14:N:19:ARG:NE	14:N:26:ILE:HD13	2.36	0.40
11:K:10(A):ARG:HD3	11:K:180:GLU:OE1	2.22	0.40
7:U:39:ALA:CB	7:U:48:VAL:HG12	2.51	0.40
3:C:169:SER:HA	3:C:172:VAL:CG1	2.52	0.40
12:L:113:PHE:CD2	12:L:119:TYR:HB3	2.57	0.40
12:Z:113:PHE:CD2	12:Z:119:TYR:HB3	2.56	0.40
11:Y:25:TRP:CH2	12:Z:132:SER:HA	2.56	0.40
2:B:81:LEU:HD23	2:B:133:GLY:HA3	2.04	0.40
13:1:80:PHE:CE1	13:1:111:ARG:HD3	2.57	0.40
9:I:80:THR:HG23	9:I:113:PHE:CZ	2.57	0.40
12:Z:14(E):GLU:OE2	12:Z:14(P):PRO:HD2	2.22	0.40
5:S:214:ILE:HG12	5:S:215:VAL:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	234 (94%)	11 (4%)	3 (1%)	16	22
1	O	248/250 (99%)	235 (95%)	10 (4%)	3 (1%)	16	22
2	B	242/244 (99%)	219 (90%)	19 (8%)	4 (2%)	11	14
2	P	242/244 (99%)	219 (90%)	19 (8%)	4 (2%)	11	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	239/241 (99%)	226 (95%)	8 (3%)	5 (2%)	9	9
3	Q	239/241 (99%)	225 (94%)	9 (4%)	5 (2%)	9	9
4	D	240/242 (99%)	232 (97%)	4 (2%)	4 (2%)	11	14
4	R	240/242 (99%)	232 (97%)	4 (2%)	4 (2%)	11	14
5	E	231/233 (99%)	209 (90%)	16 (7%)	6 (3%)	7	6
5	S	231/233 (99%)	209 (90%)	16 (7%)	6 (3%)	7	6
6	F	242/244 (99%)	229 (95%)	12 (5%)	1 (0%)	39	54
6	T	242/244 (99%)	228 (94%)	12 (5%)	2 (1%)	24	33
7	G	241/243 (99%)	230 (95%)	11 (5%)	0	100	100
7	U	241/243 (99%)	231 (96%)	10 (4%)	0	100	100
8	H	220/222 (99%)	211 (96%)	9 (4%)	0	100	100
8	V	220/222 (99%)	211 (96%)	9 (4%)	0	100	100
9	I	202/204 (99%)	197 (98%)	5 (2%)	0	100	100
9	W	202/204 (99%)	197 (98%)	5 (2%)	0	100	100
10	J	196/198 (99%)	189 (96%)	5 (3%)	2 (1%)	19	27
10	X	196/198 (99%)	190 (97%)	4 (2%)	2 (1%)	19	27
11	K	210/212 (99%)	208 (99%)	2 (1%)	0	100	100
11	Y	210/212 (99%)	208 (99%)	2 (1%)	0	100	100
12	L	220/222 (99%)	212 (96%)	8 (4%)	0	100	100
12	Z	220/222 (99%)	210 (96%)	10 (4%)	0	100	100
13	1	231/233 (99%)	219 (95%)	12 (5%)	0	100	100
13	M	231/233 (99%)	218 (94%)	13 (6%)	0	100	100
14	2	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
14	N	194/196 (99%)	185 (95%)	9 (5%)	0	100	100
All	All	6312/6368 (99%)	5999 (95%)	262 (4%)	51 (1%)	24	33

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	58	LEU
3	C	203	THR
4	D	12(G)	GLU
3	Q	58	LEU
4	R	12(G)	GLU

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Mol	Chain	Res	Type
5	S	217	LYS
1	A	5	THR
2	B	54	VAL
2	B	21(B)	GLY
2	B	21(C)	ASP
5	E	202	ARG
5	E	217	LYS
10	J	192	ALA
1	O	5	THR
2	P	54	VAL
2	P	21(B)	GLY
2	P	21(C)	ASP
3	Q	203	THR
5	S	202	ARG
10	X	192	ALA
1	A	167	LYS
2	B	20(A)	SER
3	C	183	PRO
4	D	12(F)	GLY
5	E	5	ARG
5	E	180	LEU
1	O	63	THR
1	O	167	LYS
2	P	20(A)	SER
3	Q	183	PRO
4	R	12(F)	GLY
5	S	5	ARG
5	S	180	LEU
1	A	63	THR
3	C	242	GLU
3	Q	242	GLU
6	T	143	LYS
4	D	12(E)	SER
5	E	203	ASP
5	E	231	LYS
4	R	12(E)	SER
5	S	203	ASP
6	T	205	ASN
3	C	202	GLN
6	F	205	ASN
3	Q	202	GLN
5	S	231	LYS

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Mol	Chain	Res	Type
4	D	12(C)	GLY
4	R	12(C)	GLY
10	X	8	VAL
10	J	8	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	204 (98%)	5 (2%)	57	76
1	O	209/209 (100%)	204 (98%)	5 (2%)	57	76
2	B	203/203 (100%)	188 (93%)	15 (7%)	17	26
2	P	203/203 (100%)	188 (93%)	15 (7%)	17	26
3	C	213/213 (100%)	199 (93%)	14 (7%)	21	31
3	Q	213/213 (100%)	199 (93%)	14 (7%)	21	31
4	D	198/198 (100%)	185 (93%)	13 (7%)	21	31
4	R	198/198 (100%)	185 (93%)	13 (7%)	21	31
5	E	192/192 (100%)	176 (92%)	16 (8%)	14	20
5	S	192/192 (100%)	176 (92%)	16 (8%)	14	20
6	F	201/201 (100%)	186 (92%)	15 (8%)	17	26
6	T	201/201 (100%)	184 (92%)	17 (8%)	13	19
7	G	207/207 (100%)	196 (95%)	11 (5%)	28	44
7	U	207/207 (100%)	195 (94%)	12 (6%)	25	38
8	H	181/181 (100%)	172 (95%)	9 (5%)	30	47
8	V	181/181 (100%)	172 (95%)	9 (5%)	30	47
9	I	172/172 (100%)	164 (95%)	8 (5%)	32	49
9	W	172/172 (100%)	165 (96%)	7 (4%)	37	56
10	J	175/175 (100%)	169 (97%)	6 (3%)	44	64
10	X	175/175 (100%)	170 (97%)	5 (3%)	50	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	169/169 (100%)	162 (96%)	7 (4%)	37	56
11	Y	169/169 (100%)	162 (96%)	7 (4%)	37	56
12	L	185/185 (100%)	177 (96%)	8 (4%)	35	54
12	Z	185/185 (100%)	176 (95%)	9 (5%)	31	48
13	1	199/199 (100%)	189 (95%)	10 (5%)	30	47
13	M	199/199 (100%)	189 (95%)	10 (5%)	30	47
14	2	162/162 (100%)	154 (95%)	8 (5%)	31	48
14	N	162/162 (100%)	154 (95%)	8 (5%)	31	48
All	All	5332/5332 (100%)	5040 (94%)	292 (6%)	27	41

All (292) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	64	LEU
1	A	158	PHE
1	A	179	ARG
1	A	214	ILE
2	B	14	ILE
2	B	58	LEU
2	B	71	ASN
2	B	91	THR
2	B	116	LEU
2	B	121	GLN
2	B	150	THR
2	B	163	ILE
2	B	185	LYS
2	B	187	ASP
2	B	192	LEU
2	B	212	PHE
2	B	218	ASN
2	B	223	ILE
2	B	224	PHE
3	C	10	ARG
3	C	14	ILE
3	C	25	GLU
3	C	57	LYS
3	C	66	LYS
3	C	89	ILE

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Mol	Chain	Res	Type
3	C	121	GLN
3	C	135	SER
3	C	150	GLN
3	C	163	GLN
3	C	172	VAL
3	C	174	GLU
3	C	208	LYS
3	C	212	ILE
4	D	28	LEU
4	D	48	LEU
4	D	76	CYS
4	D	110	GLU
4	D	126	ARG
4	D	170	GLU
4	D	177	LEU
4	D	18(E)	SER
4	D	191	LEU
4	D	194	LEU
4	D	215	ILE
4	D	237	LEU
4	D	244	GLU
5	E	12	THR
5	E	32	LYS
5	E	57	GLU
5	E	76	LEU
5	E	97	ASN
5	E	104	ASN
5	E	111	ARG
5	E	117	CYS
5	E	121	GLN
5	E	185	ASN
5	E	189	LEU
5	E	199	GLN
5	E	207	LEU
5	E	2(D)	ASP
5	E	227	GLU
5	E	231	LYS
6	F	43	ASN
6	F	54	ILE
6	F	56	SER
6	F	121	GLN
6	F	127	ASN

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Mol	Chain	Res	Type
6	F	144	ASN
6	F	176	LEU
6	F	18(E)	GLU
6	F	187	ARG
6	F	203	GLU
6	F	204	ASP
6	F	205	ASN
6	F	214	TRP
6	F	21(C)	ASN
6	F	233	ILE
7	G	14	ILE
7	G	72	ARG
7	G	87	ASN
7	G	119	LEU
7	G	121	GLN
7	G	124	THR
7	G	169	GLN
7	G	184	ASN
7	G	197	MET
7	G	232	ARG
7	G	233	LEU
8	H	30	ASN
8	H	34	LEU
8	H	55	VAL
8	H	56	THR
8	H	63	ILE
8	H	68	LEU
8	H	121	VAL
8	H	144	GLN
8	H	197	ARG
9	I	-3	ILE
9	I	22	SER
9	I	29	ASN
9	I	61	TYR
9	I	104	ILE
9	I	125	ILE
9	I	160	LEU
9	I	192	ARG
10	J	34	THR
10	J	52	THR
10	J	70	GLU
10	J	77	GLN

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Mol	Chain	Res	Type
10	J	121	GLU
10	J	177	ILE
11	K	4	LEU
11	K	9	GLN
11	K	65	LEU
11	K	87	VAL
11	K	104	TYR
11	K	10(B)	LYS
11	K	138	LEU
12	L	-7	ASN
12	L	14	LEU
12	L	40	ASN
12	L	58	ARG
12	L	82	ASN
12	L	98	HIS
12	L	99	THR
12	L	145	TYR
13	M	4	ILE
13	M	13	ILE
13	M	40	ASN
13	M	62	LEU
13	M	91	ARG
13	M	112	TYR
13	M	129	PHE
13	M	14(C)	ARG
13	M	149	GLN
13	M	204	LYS
14	N	26	ILE
14	N	36	ARG
14	N	70	TYR
14	N	84	LYS
14	N	89	GLU
14	N	10(A)	ASP
14	N	10(B)	LYS
14	N	119	VAL
1	O	33	GLN
1	O	64	LEU
1	O	158	PHE
1	O	179	ARG
1	O	214	ILE
2	P	14	ILE
2	P	58	LEU

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Mol	Chain	Res	Type
2	P	71	ASN
2	P	91	THR
2	P	116	LEU
2	P	121	GLN
2	P	150	THR
2	P	163	ILE
2	P	185	LYS
2	P	187	ASP
2	P	192	LEU
2	P	212	PHE
2	P	218	ASN
2	P	223	ILE
2	P	224	PHE
3	Q	10	ARG
3	Q	14	ILE
3	Q	25	GLU
3	Q	57	LYS
3	Q	66	LYS
3	Q	89	ILE
3	Q	121	GLN
3	Q	135	SER
3	Q	150	GLN
3	Q	163	GLN
3	Q	172	VAL
3	Q	174	GLU
3	Q	208	LYS
3	Q	212	ILE
4	R	28	LEU
4	R	48	LEU
4	R	76	CYS
4	R	110	GLU
4	R	126	ARG
4	R	170	GLU
4	R	177	LEU
4	R	18(E)	SER
4	R	191	LEU
4	R	194	LEU
4	R	215	ILE
4	R	237	LEU
4	R	244	GLU
5	S	12	THR
5	S	32	LYS

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Mol	Chain	Res	Type
5	S	57	GLU
5	S	76	LEU
5	S	97	ASN
5	S	104	ASN
5	S	111	ARG
5	S	117	CYS
5	S	121	GLN
5	S	185	ASN
5	S	189	LEU
5	S	199	GLN
5	S	207	LEU
5	S	2(D)	ASP
5	S	227	GLU
5	S	231	LYS
6	T	43	ASN
6	T	54	ILE
6	T	56	SER
6	T	98	SER
6	T	121	GLN
6	T	127	ASN
6	T	144	ASN
6	T	176	LEU
6	T	18(E)	GLU
6	T	187	ARG
6	T	197	ILE
6	T	203	GLU
6	T	204	ASP
6	T	205	ASN
6	T	214	TRP
6	T	21(C)	ASN
6	T	233	ILE
7	U	14	ILE
7	U	35	ILE
7	U	72	ARG
7	U	87	ASN
7	U	119	LEU
7	U	121	GLN
7	U	124	THR
7	U	169	GLN
7	U	184	ASN
7	U	197	MET
7	U	232	ARG

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Mol	Chain	Res	Type
7	U	233	LEU
8	V	30	ASN
8	V	34	LEU
8	V	55	VAL
8	V	56	THR
8	V	63	ILE
8	V	68	LEU
8	V	121	VAL
8	V	144	GLN
8	V	197	ARG
9	W	-3	ILE
9	W	22	SER
9	W	29	ASN
9	W	61	TYR
9	W	104	ILE
9	W	160	LEU
9	W	192	ARG
10	X	34	THR
10	X	52	THR
10	X	70	GLU
10	X	121	GLU
10	X	177	ILE
11	Y	4	LEU
11	Y	9	GLN
11	Y	65	LEU
11	Y	87	VAL
11	Y	104	TYR
11	Y	10(B)	LYS
11	Y	138	LEU
12	Z	-7	ASN
12	Z	14	LEU
12	Z	21	ILE
12	Z	40	ASN
12	Z	58	ARG
12	Z	82	ASN
12	Z	98	HIS
12	Z	99	THR
12	Z	145	TYR
13	1	4	ILE
13	1	13	ILE
13	1	40	ASN
13	1	62	LEU

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Mol	Chain	Res	Type
13	1	91	ARG
13	1	112	TYR
13	1	129	PHE
13	1	14(C)	ARG
13	1	149	GLN
13	1	204	LYS
14	2	26	ILE
14	2	36	ARG
14	2	70	TYR
14	2	84	LYS
14	2	89	GLU
14	2	10(A)	ASP
14	2	10(B)	LYS
14	2	119	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (197) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	97	HIS
2	B	23	GLN
2	B	71	ASN
2	B	95	HIS
2	B	97	GLN
2	B	121	GLN
2	B	125	GLN
2	B	156	ASN
2	B	177	GLN
2	B	218	ASN
3	C	23	GLN
3	C	82	ASN
3	C	97	GLN
3	C	121	GLN
3	C	125	GLN
3	C	150	GLN
3	C	163	GLN
3	C	209	ASN
3	C	243	GLN
4	D	23	GLN
4	D	108	ASN
4	D	114	GLN
4	D	147	GLN

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Mol	Chain	Res	Type
4	D	161	ASN
4	D	211	GLN
4	D	218	GLN
4	D	226	ASN
5	E	7	ASN
5	E	33	GLN
5	E	64	GLN
5	E	73	HIS
5	E	104	ASN
5	E	121	GLN
5	E	123	ASN
5	E	125	GLN
5	E	185	ASN
5	E	199	GLN
5	E	2(E)	ASN
6	F	23	GLN
6	F	43	ASN
6	F	90	ASN
6	F	121	GLN
6	F	127	ASN
6	F	192	GLN
7	G	34(A)	ASN
7	G	87	ASN
7	G	118	ASN
7	G	121	GLN
7	G	125	GLN
7	G	169	GLN
7	G	170	GLN
7	G	178	ASN
7	G	184	ASN
7	G	228	ASN
8	H	30	ASN
8	H	66	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	190	ASN
9	I	29	ASN
10	J	36	GLN
10	J	54	GLN
10	J	85	GLN
10	J	112	GLN

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Mol	Chain	Res	Type
10	J	141	HIS
10	J	186	GLN
11	K	85	ASN
11	K	131	GLN
11	K	174	ASN
11	K	207	ASN
12	L	-9	GLN
12	L	-7	ASN
12	L	40	ASN
12	L	46	ASN
12	L	61	ASN
12	L	70	HIS
12	L	70(A)	ASN
12	L	82	ASN
12	L	85	HIS
12	L	98	HIS
12	L	14(B)	ASN
12	L	1(I)	ASN
12	L	166	HIS
13	M	10	ASN
13	M	40	ASN
13	M	89	GLN
13	M	93	ASN
13	M	149	GLN
13	M	157	ASN
13	M	172	ASN
13	M	191	GLN
14	N	69	GLN
14	N	145	ASN
14	N	157	HIS
14	N	161	GLN
1	O	33	GLN
1	O	97	HIS
2	P	23	GLN
2	P	71	ASN
2	P	95	HIS
2	P	97	GLN
2	P	121	GLN
2	P	125	GLN
2	P	156	ASN
2	P	177	GLN
2	P	218	ASN

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Mol	Chain	Res	Type
3	Q	23	GLN
3	Q	82	ASN
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	209	ASN
3	Q	243	GLN
4	R	23	GLN
4	R	108	ASN
4	R	114	GLN
4	R	147	GLN
4	R	161	ASN
4	R	211	GLN
4	R	218	GLN
4	R	226	ASN
5	S	7	ASN
5	S	33	GLN
5	S	64	GLN
5	S	73	HIS
5	S	104	ASN
5	S	121	GLN
5	S	123	ASN
5	S	125	GLN
5	S	156	ASN
5	S	170	GLN
5	S	185	ASN
5	S	199	GLN
5	S	2(E)	ASN
6	T	23	GLN
6	T	43	ASN
6	T	90	ASN
6	T	121	GLN
6	T	127	ASN
6	T	147	HIS
6	T	192	GLN
7	U	34(A)	ASN
7	U	87	ASN
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN
7	U	169	GLN

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Mol	Chain	Res	Type
7	U	170	GLN
7	U	178	ASN
7	U	184	ASN
7	U	228	ASN
8	V	30	ASN
8	V	66	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
9	W	29	ASN
9	W	81	GLN
10	X	36	GLN
10	X	54	GLN
10	X	85	GLN
10	X	112	GLN
10	X	141	HIS
10	X	186	GLN
10	X	193	GLN
11	Y	85	ASN
11	Y	131	GLN
11	Y	174	ASN
11	Y	207	ASN
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	40	ASN
12	Z	46	ASN
12	Z	61	ASN
12	Z	70	HIS
12	Z	70(A)	ASN
12	Z	82	ASN
12	Z	85	HIS
12	Z	14(B)	ASN
12	Z	1(I)	ASN
12	Z	166	HIS
13	1	10	ASN
13	1	40	ASN
13	1	89	GLN
13	1	93	ASN
13	1	149	GLN
13	1	157	ASN
13	1	172	ASN

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Mol	Chain	Res	Type
13	1	191	GLN
14	2	69	GLN
14	2	145	ASN
14	2	157	HIS
14	2	161	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	GPT	2	224	14	16,22,22	1.81	3 (18%)	22,33,33	1.79	4 (18%)
15	GPT	H	224	8	16,22,22	2.33	5 (31%)	22,33,33	1.74	4 (18%)
15	GPT	K	224	11	16,22,22	1.73	4 (25%)	22,33,33	1.70	5 (22%)
15	GPT	N	224	14	16,22,22	2.26	4 (25%)	22,33,33	1.81	4 (18%)
15	GPT	V	224	8	16,22,22	1.71	4 (25%)	22,33,33	1.69	4 (18%)
15	GPT	Y	224	11	16,22,22	2.09	4 (25%)	22,33,33	1.70	6 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	GPT	2	224	14	-	0/6/48/48	0/2/2/2
15	GPT	H	224	8	-	0/6/48/48	0/2/2/2
15	GPT	K	224	11	-	0/6/48/48	0/2/2/2
15	GPT	N	224	14	-	0/6/48/48	0/2/2/2
15	GPT	V	224	8	-	0/6/48/48	0/2/2/2
15	GPT	Y	224	11	-	0/6/48/48	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	224	GPT	C2-C3	2.14	1.59	1.54
15	N	224	GPT	C2-C3	2.21	1.59	1.54
15	H	224	GPT	C9-C10	2.27	1.54	1.50
15	Y	224	GPT	C9-C10	2.28	1.54	1.50
15	K	224	GPT	C9-C8	2.44	1.58	1.54
15	V	224	GPT	C6-C4	2.57	1.56	1.52
15	V	224	GPT	C9-C10	2.80	1.54	1.50
15	2	224	GPT	C6-C4	2.82	1.56	1.52
15	K	224	GPT	C9-C10	2.84	1.55	1.50
15	V	224	GPT	C9-C8	2.99	1.59	1.54
15	K	224	GPT	C6-C4	3.21	1.56	1.52
15	Y	224	GPT	C9-C8	3.30	1.59	1.54
15	V	224	GPT	C14-C9	3.38	1.59	1.54
15	K	224	GPT	C14-C9	3.47	1.59	1.54
15	2	224	GPT	C9-C8	3.58	1.60	1.54
15	2	224	GPT	C14-C9	3.89	1.60	1.54
15	H	224	GPT	C9-C8	4.02	1.60	1.54
15	N	224	GPT	C9-C8	4.02	1.60	1.54
15	H	224	GPT	C6-C4	4.29	1.58	1.52
15	N	224	GPT	C6-C4	4.33	1.58	1.52
15	Y	224	GPT	C6-C4	4.37	1.58	1.52
15	Y	224	GPT	C14-C9	4.70	1.61	1.54
15	N	224	GPT	C14-C9	5.17	1.62	1.54
15	H	224	GPT	C14-C9	5.44	1.62	1.54

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	2	224	GPT	C4-C3-C19	-4.70	100.23	104.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	224	GPT	C4-C3-C19	-4.60	100.32	104.25
15	H	224	GPT	C4-C3-C19	-4.31	100.56	104.25
15	V	224	GPT	C4-C3-C19	-3.94	100.88	104.25
15	K	224	GPT	C4-C3-C19	-3.49	101.26	104.25
15	Y	224	GPT	C4-C3-C19	-3.39	101.34	104.25
15	2	224	GPT	C6-C4-C3	-3.11	109.08	114.96
15	Y	224	GPT	C6-C4-C3	-3.09	109.12	114.96
15	N	224	GPT	C6-C4-C3	-3.08	109.14	114.96
15	K	224	GPT	C6-C4-C3	-3.05	109.19	114.96
15	V	224	GPT	C6-C4-C3	-2.64	109.97	114.96
15	H	224	GPT	C6-C4-C3	-2.48	110.27	114.96
15	Y	224	GPT	O5-C4-C6	-2.23	103.40	108.52
15	N	224	GPT	O15-C8-C9	-2.14	104.98	109.95
15	2	224	GPT	C7-N18-C19	2.02	117.50	115.47
15	K	224	GPT	C2-C3-C4	2.10	118.42	115.41
15	Y	224	GPT	C2-C3-C4	2.12	118.45	115.41
15	V	224	GPT	C1-C2-C3	2.41	117.23	112.60
15	Y	224	GPT	C7-N18-C19	2.46	117.93	115.47
15	K	224	GPT	C7-N18-C19	2.56	118.03	115.47
15	Y	224	GPT	C7-C8-C9	2.78	117.57	114.09
15	H	224	GPT	C1-C2-C3	2.83	118.04	112.60
15	N	224	GPT	C7-C8-C9	3.18	118.08	114.09
15	K	224	GPT	C7-C8-C9	3.31	118.24	114.09
15	H	224	GPT	C7-C8-C9	3.39	118.34	114.09
15	2	224	GPT	C7-C8-C9	3.46	118.44	114.09
15	V	224	GPT	C7-C8-C9	4.02	119.13	114.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	2	224	GPT	2	0
15	H	224	GPT	1	0
15	K	224	GPT	2	0
15	N	224	GPT	2	0
15	V	224	GPT	1	0
15	Y	224	GPT	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	-0.19	3 (1%) 81 81	32, 43, 73, 101	0
1	O	250/250 (100%)	-0.06	4 (1%) 74 74	34, 48, 76, 101	0
2	B	244/244 (100%)	0.08	10 (4%) 41 41	32, 49, 85, 113	0
2	P	244/244 (100%)	0.13	12 (4%) 33 33	30, 49, 86, 113	0
3	C	241/241 (100%)	0.09	12 (4%) 32 32	30, 50, 104, 117	0
3	Q	241/241 (100%)	0.48	35 (14%) 3 3	36, 56, 106, 117	0
4	D	242/242 (100%)	0.10	9 (3%) 45 45	33, 52, 85, 116	0
4	R	242/242 (100%)	0.25	11 (4%) 37 37	36, 56, 86, 117	0
5	E	233/233 (100%)	0.31	23 (9%) 9 8	39, 55, 83, 106	0
5	S	233/233 (100%)	0.60	30 (12%) 5 4	39, 59, 84, 104	0
6	F	244/244 (100%)	0.02	10 (4%) 41 41	34, 50, 85, 102	0
6	T	244/244 (100%)	0.15	11 (4%) 37 37	32, 52, 87, 103	0
7	G	243/243 (100%)	-0.15	7 (2%) 55 54	31, 44, 72, 108	0
7	U	243/243 (100%)	-0.06	4 (1%) 74 74	31, 47, 73, 108	0
8	H	222/222 (100%)	-0.28	1 (0%) 91 91	26, 40, 61, 91	0
8	V	222/222 (100%)	-0.32	2 (0%) 85 85	26, 43, 61, 92	0
9	I	204/204 (100%)	-0.32	1 (0%) 91 91	27, 40, 56, 73	0
9	W	204/204 (100%)	-0.19	1 (0%) 91 91	29, 39, 58, 75	0
10	J	198/198 (100%)	-0.19	4 (2%) 68 67	28, 42, 59, 113	0
10	X	198/198 (100%)	-0.24	5 (2%) 61 60	29, 42, 60, 115	0
11	K	212/212 (100%)	-0.37	0 100 100	24, 39, 57, 64	0
11	Y	212/212 (100%)	-0.28	0 100 100	28, 43, 60, 69	0
12	L	222/222 (100%)	-0.29	3 (1%) 78 77	26, 41, 63, 82	0
12	Z	222/222 (100%)	-0.24	4 (1%) 71 70	31, 43, 65, 85	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
13	1	233/233 (100%)	-0.36	1 (0%)	93	93	28, 42, 57, 64	0
13	M	233/233 (100%)	-0.28	1 (0%)	93	93	29, 43, 58, 65	0
14	2	196/196 (100%)	-0.24	2 (1%)	84	83	27, 40, 60, 75	0
14	N	196/196 (100%)	-0.36	1 (0%)	91	91	29, 39, 59, 74	0
All	All	6368/6368 (100%)	-0.07	207 (3%)	50	49	24, 46, 78, 117	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	R	12(D)	ALA	12.3
4	R	12(F)	GLY	12.3
4	D	12(D)	ALA	11.4
3	C	55	THR	10.7
4	R	12(C)	GLY	10.6
4	D	12(C)	GLY	10.3
4	D	12(E)	SER	9.8
2	P	217	ALA	9.7
10	J	192	ALA	9.3
4	R	12(E)	SER	9.2
2	B	217	ALA	8.9
3	C	56	LEU	8.3
2	P	218	ASN	7.9
2	B	218	ASN	7.8
10	X	192	ALA	7.6
7	U	240	ASP	7.4
1	O	236	LEU	7.2
7	U	6	ALA	7.2
4	D	126	ARG	7.0
5	S	127	TYR	6.6
5	S	5	ARG	6.5
3	Q	236	ILE	6.5
3	Q	203	THR	6.1
5	E	4	PHE	6.1
7	G	6	ALA	6.1
4	D	12(F)	GLY	6.1
4	R	126	ARG	5.8
3	Q	240	LYS	5.7
1	A	4	MET	5.7
5	S	4	PHE	5.4
1	A	236	LEU	5.4
10	X	193	GLN	5.4

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Mol	Chain	Res	Type	RSRZ
5	E	203	ASP	5.2
6	F	5	GLY	5.2
5	S	203	ASP	5.1
5	S	233	ILE	5.1
4	D	127	LEU	5.0
7	G	240	ASP	5.0
1	O	4	MET	4.8
3	Q	56	LEU	4.8
5	E	233	ILE	4.7
2	P	21(B)	GLY	4.7
3	Q	241	GLN	4.7
4	R	9	ASP	4.6
3	Q	206	GLY	4.6
10	J	193	GLN	4.5
5	S	51	LEU	4.5
5	S	210	LEU	4.4
1	O	235	ALA	4.3
5	E	127	TYR	4.3
5	S	178	ARG	4.2
2	B	239	THR	4.2
12	Z	145	TYR	4.1
3	C	240	LYS	4.1
3	Q	243	GLN	4.1
4	R	12(G)	GLU	4.1
2	P	239	THR	4.1
3	Q	239	GLU	4.0
8	V	223	ASP	4.0
8	H	223	ASP	4.0
3	Q	233	VAL	4.0
10	J	191	GLN	3.9
3	Q	242	GLU	3.9
5	E	5	ARG	3.9
3	Q	238	GLN	3.9
2	B	21(B)	GLY	3.8
3	Q	235	GLN	3.8
13	M	-8	THR	3.8
2	P	21(C)	ASP	3.6
2	B	54	VAL	3.6
10	X	-1	MET	3.5
6	T	240	ILE	3.5
6	F	240	ILE	3.4
13	1	-8	THR	3.4

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Mol	Chain	Res	Type	RSRZ
3	Q	201	VAL	3.4
3	C	237	GLU	3.4
3	Q	198	LEU	3.4
5	E	189	LEU	3.4
5	S	206	SER	3.4
5	S	18(C)	PHE	3.4
12	L	145	TYR	3.3
4	D	9	ASP	3.3
4	R	127	LEU	3.3
5	S	195	GLU	3.3
5	E	193	GLY	3.2
5	E	198	SER	3.2
7	G	239	GLN	3.2
2	P	21(A)	LYS	3.2
4	D	12(G)	GLU	3.1
3	Q	200	VAL	3.1
7	G	236	ILE	3.1
5	S	197	ILE	3.1
4	R	10	ARG	3.1
5	S	201	LEU	3.1
3	Q	202	GLN	3.1
5	S	188	GLU	3.1
2	P	54	VAL	3.0
6	T	199	LEU	3.0
2	P	219	GLU	3.0
3	Q	54	SER	3.0
3	Q	187	GLU	3.0
5	E	204	GLU	3.0
3	Q	43	LYS	3.0
6	T	18(B)	HIS	3.0
7	G	7	GLY	2.9
3	Q	55	THR	2.9
10	J	189	ASP	2.9
5	S	232	TYR	2.9
12	Z	-9	GLN	2.9
6	F	238	LYS	2.9
7	G	237	ALA	2.8
3	Q	196	SER	2.8
3	C	203	THR	2.8
6	T	5	GLY	2.8
3	Q	207	ALA	2.8
5	S	189	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
4	D	10	ARG	2.8
3	Q	234	THR	2.7
12	Z	14(W)	LYS	2.7
3	Q	237	GLU	2.7
10	X	189	ASP	2.7
8	V	222	CYS	2.7
4	R	12(B)	GLU	2.6
5	S	174	THR	2.6
6	T	203	GLU	2.6
3	Q	210	ILE	2.6
3	Q	175	PHE	2.6
6	F	180	VAL	2.6
2	B	232	ILE	2.6
3	C	241	GLN	2.6
5	E	175	TYR	2.6
6	F	18(E)	GLU	2.6
5	S	198	SER	2.6
5	E	58	LEU	2.6
5	E	6	ASN	2.5
6	F	6	THR	2.5
3	C	54	SER	2.5
5	S	192	ALA	2.5
10	X	191	GLN	2.5
5	E	231	LYS	2.5
5	E	202	ARG	2.5
6	T	43	ASN	2.4
5	S	196	ALA	2.4
3	C	233	VAL	2.4
5	E	195	GLU	2.4
6	F	241	ASN	2.4
6	T	232	ALA	2.4
5	E	18(E)	LYS	2.4
1	A	5	THR	2.4
1	O	21(P)	LYS	2.4
3	C	242	GLU	2.4
2	B	234	VAL	2.4
12	L	14(W)	LYS	2.4
7	U	239	GLN	2.4
2	B	21(A)	LYS	2.4
5	S	58	LEU	2.4
3	C	243	GLN	2.4
3	Q	44	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
3	Q	52	ARG	2.3
5	E	232	TYR	2.3
6	T	198	TYR	2.3
7	G	8	TYR	2.3
3	Q	195	ARG	2.3
6	T	241	ASN	2.3
3	C	239	GLU	2.3
5	S	180	LEU	2.3
2	B	186	VAL	2.3
5	S	184	GLY	2.3
9	I	182	ASP	2.3
14	N	9	LYS	2.3
9	W	-8	SER	2.3
5	S	176	LEU	2.3
6	F	199	LEU	2.3
5	S	199	GLN	2.3
3	Q	229	ILE	2.3
5	E	18(C)	PHE	2.3
3	Q	57	LYS	2.3
14	2	107	LYS	2.3
5	E	178	ARG	2.3
4	R	125	GLU	2.2
3	Q	208	LYS	2.2
5	E	212	ILE	2.2
5	S	18(B)	THR	2.2
5	E	191	LYS	2.2
2	B	219	GLU	2.2
5	E	201	LEU	2.2
3	Q	63	THR	2.2
3	Q	178	LYS	2.2
6	F	18(F)	GLY	2.2
5	S	207	LEU	2.2
6	F	204	ASP	2.2
2	P	237	GLY	2.1
5	S	2(E)	ASN	2.1
5	E	33	GLN	2.1
5	S	18(E)	LYS	2.1
12	L	-9	GLN	2.1
2	P	220	TYR	2.1
3	Q	18(D)	GLU	2.1
5	S	202	ARG	2.1
14	2	18(I)	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
6	T	227	ASP	2.1
6	T	57	LYS	2.0
12	Z	1(I)	ASN	2.0
2	P	42	ALA	2.0
2	P	233	LEU	2.0
3	C	208	LYS	2.0
7	U	8	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
15	GPT	H	224	21/21	0.95	0.17	2.01	37,41,45,53	0
15	GPT	V	224	21/21	0.95	0.15	1.25	41,43,48,54	0
15	GPT	N	224	21/21	0.96	0.16	1.20	30,32,41,53	0
15	GPT	2	224	21/21	0.95	0.18	0.74	33,36,44,54	0
15	GPT	K	224	21/21	0.95	0.17	0.71	29,32,36,44	0
15	GPT	Y	224	21/21	0.96	0.14	-0.14	32,36,39,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.