



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:10 AM GMT

PDB ID : 3HAE  
Title : Rational development of high-affinity T-cell receptor-like antibodies  
Authors : Stewart-Jones, G.; Wadle, A.; Hombach, A.; Shenderov, E.; Held, G.; Fischer, E.  
Deposited on : 2009-05-01  
Resolution : 2.90 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](mailto: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.

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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

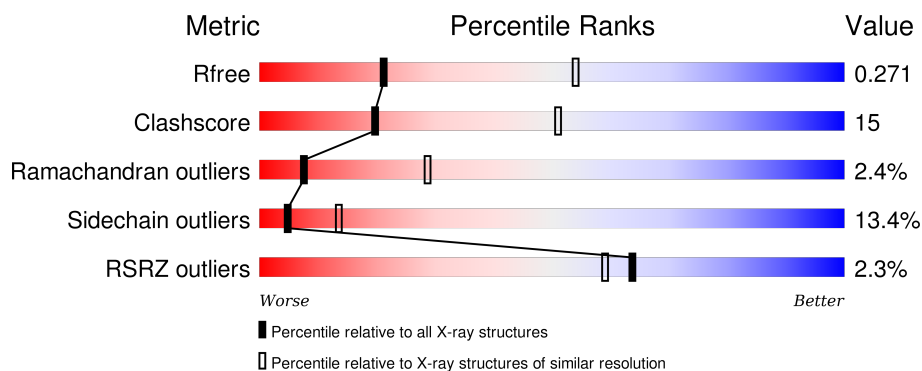
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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  $\geq 3$ , 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	276	 2% 70% 25% 6%
1	D	276	 1% 68% 26% 5%
1	J	276	 2% 72% 24% .
1	P	276	 3% 66% 30% 5%
2	B	100	 1% 59% 36% 5%

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Mol	Chain	Length	Quality of chain
2	E	100	
2	K	100	
2	Q	100	
3	C	9	
3	F	9	
3	M	9	
3	R	9	
4	G	212	
4	L	212	
4	N	212	
4	S	212	
5	H	220	
5	I	220	
5	O	220	
5	T	220	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25472 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 HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2253	1408	410	426	9			
1	D	276	Total	C	N	O	S	0	0	0
			2253	1408	410	426	9			
1	J	276	Total	C	N	O	S	0	0	0
			2253	1408	410	426	9			
1	P	276	Total	C	N	O	S	0	0	0
			2253	1408	410	426	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			
2	E	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			
2	K	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			
2	Q	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	EXPRESSION TAG	UNP P61769
E	0	MET	-	EXPRESSION TAG	UNP P61769
K	0	MET	-	EXPRESSION TAG	UNP P61769
Q	0	MET	-	EXPRESSION TAG	UNP P61769

- Molecule 3 is a protein called NYESO-1 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			75	51	11	12	1			
3	F	9	Total	C	N	O	S	0	0	0
			75	51	11	12	1			
3	M	9	Total	C	N	O	S	0	0	0
			75	51	11	12	1			
3	R	9	Total	C	N	O	S	0	0	0
			75	51	11	12	1			

- Molecule 4 is a protein called Antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	211	Total	C	N	O	S	0	0	0
			1595	1002	270	319	4			
4	G	211	Total	C	N	O	S	0	0	0
			1595	1002	270	319	4			
4	N	211	Total	C	N	O	S	0	0	0
			1595	1002	270	319	4			
4	S	211	Total	C	N	O	S	0	0	0
			1595	1002	270	319	4			

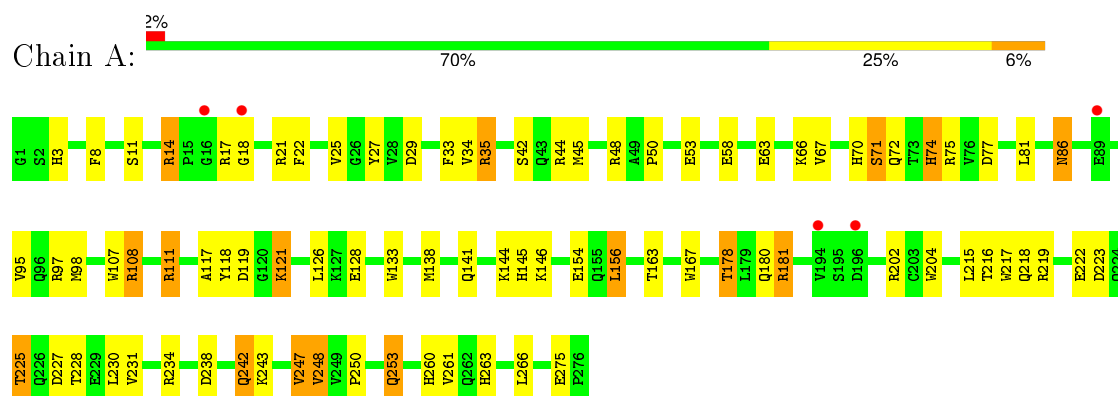
- Molecule 5 is a protein called Antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	220	Total	C	N	O	S	0	0	0
			1609	1012	268	322	7			
5	I	220	Total	C	N	O	S	0	0	0
			1609	1012	268	322	7			
5	O	220	Total	C	N	O	S	0	0	0
			1609	1012	268	322	7			
5	T	220	Total	C	N	O	S	0	0	0
			1609	1012	268	322	7			

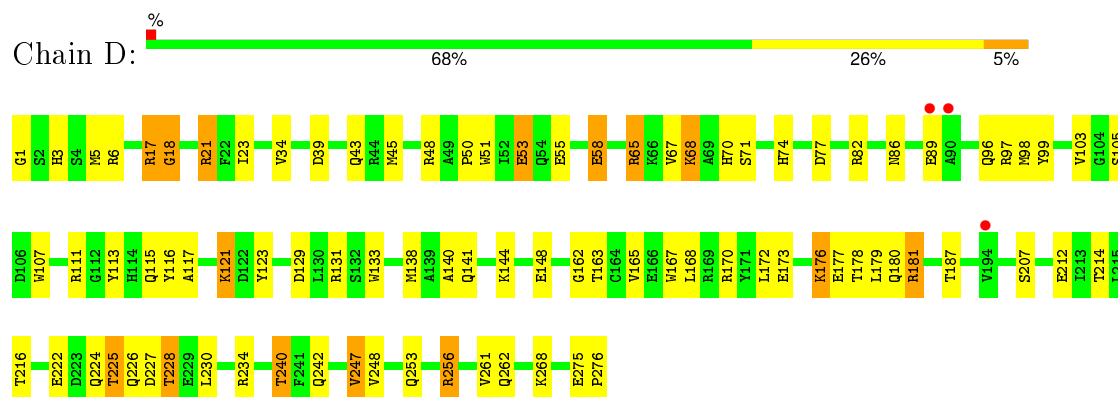
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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.

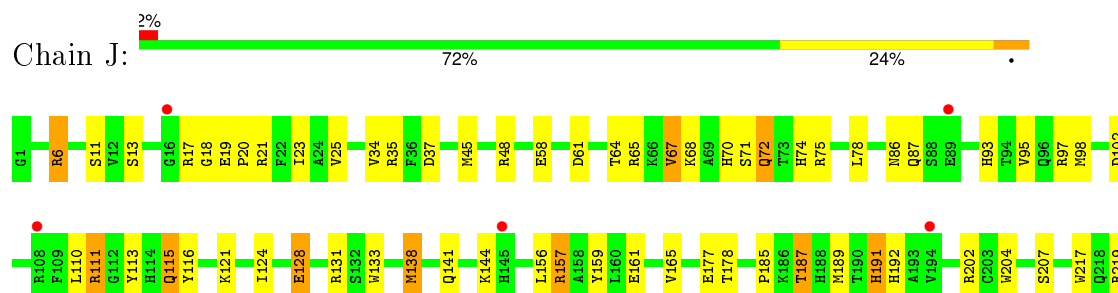
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



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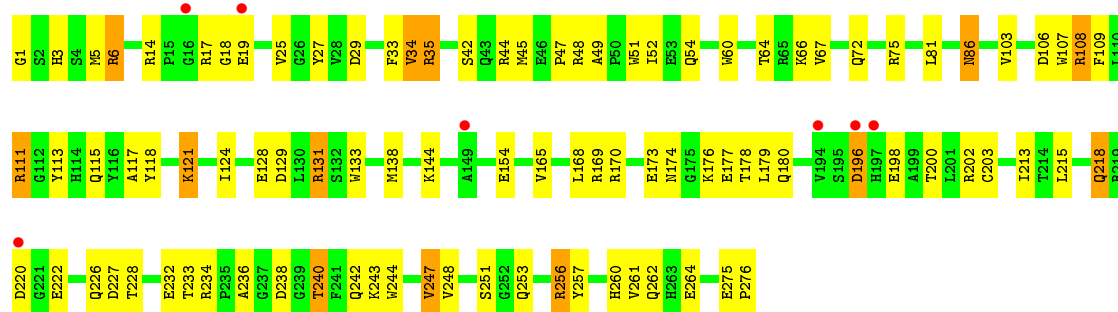


- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

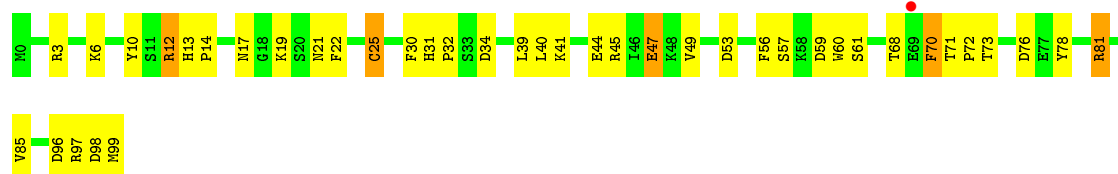




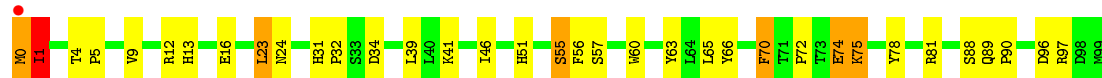
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



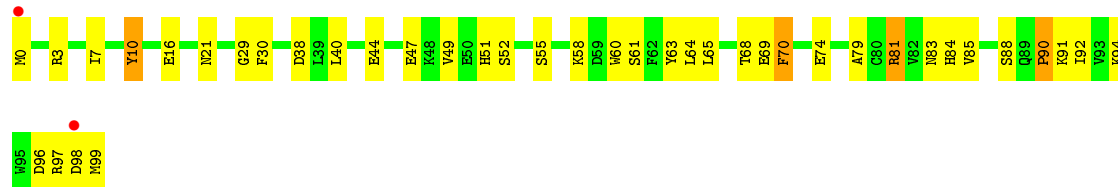
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin

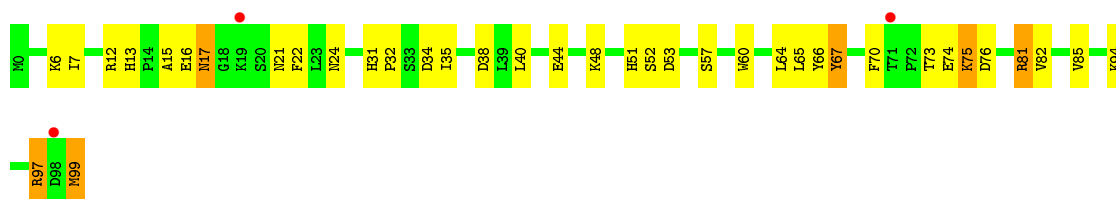


- Molecule 2: Beta-2-microglobulin

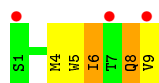
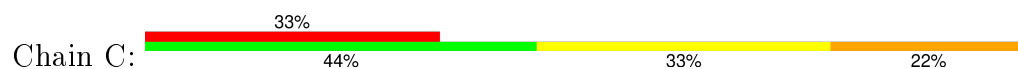


- Molecule 2: Beta-2-microglobulin

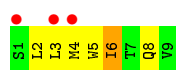




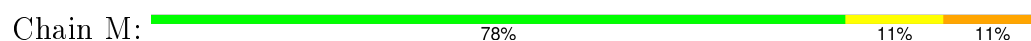
- Molecule 3: NYESO-1 peptide



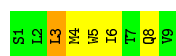
- Molecule 3: NYESO-1 peptide



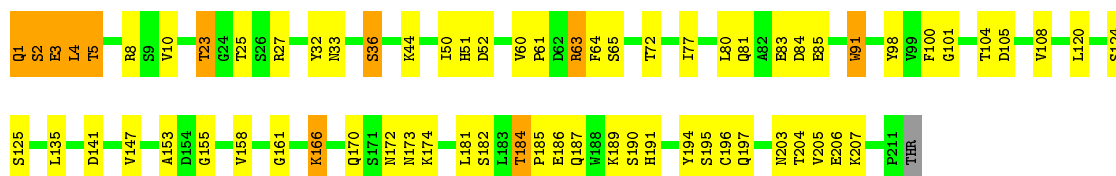
- Molecule 3: NYESO-1 peptide



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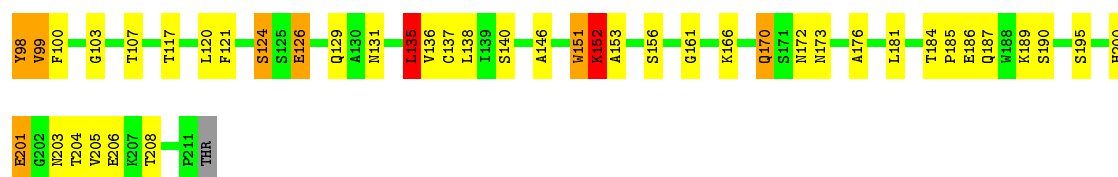
- Molecule 4: Antibody light chain



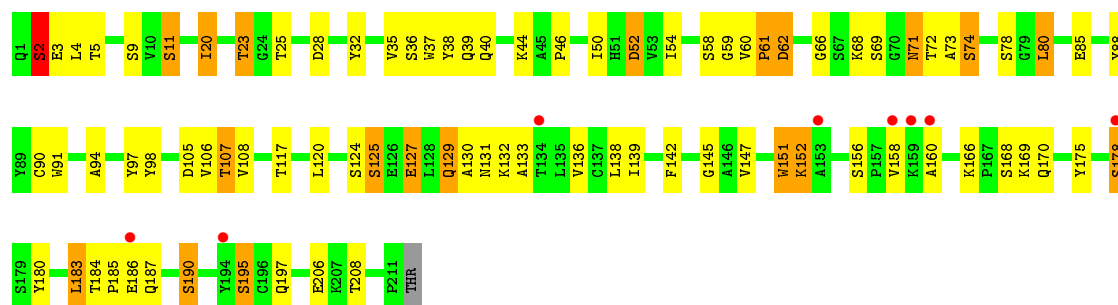
- Molecule 4: Antibody light chain



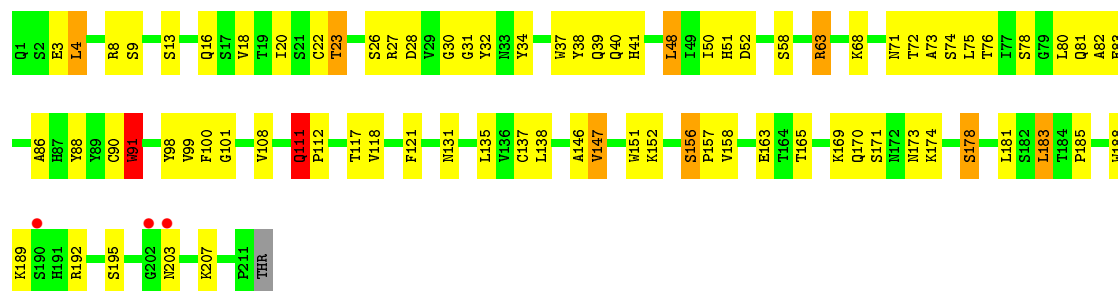




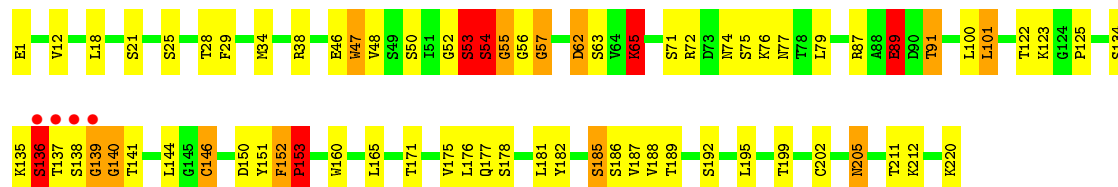
• Molecule 4: Antibody light chain



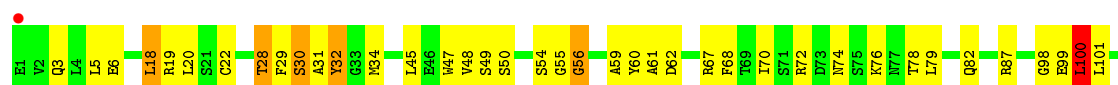
• Molecule 4: Antibody light chain

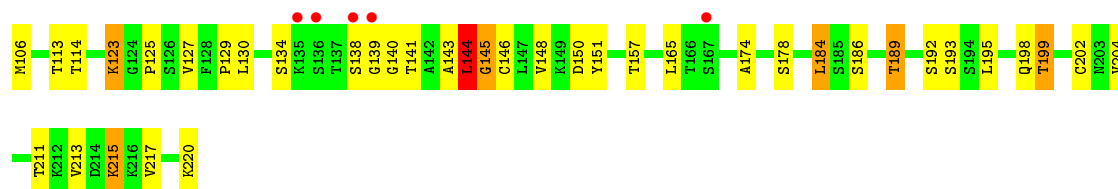


• Molecule 5: Antibody heavy chain

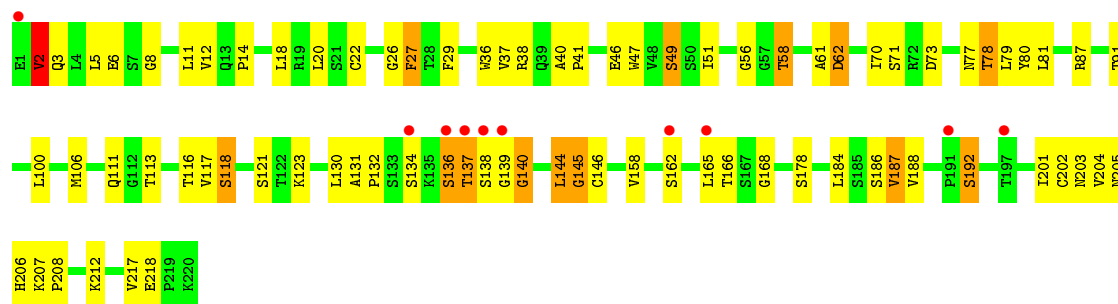


• Molecule 5: Antibody heavy chain

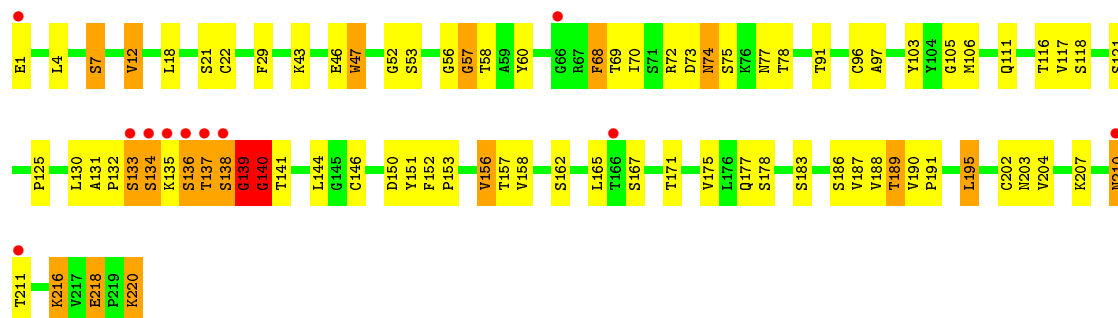




• Molecule 5: Antibody heavy chain



• Molecule 5: Antibody heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.79 Å 105.60 Å 256.45 Å 90.00° 92.26° 90.00°	Depositor
Resolution (Å)	25.00 – 2.90 29.74 – 2.86	Depositor EDS
% Data completeness (in resolution range)	98.4 (25.00-2.90) 96.6 (29.74-2.86)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.29 (at 2.85 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.201 , 0.283 0.194 , 0.271	Depositor DCC
$R_{free}$ test set	4104 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.9	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 20.2	EDS
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 84595 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	25472	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	2.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	0.91	1/2319 (0.0%)	0.92	2/3149 (0.1%)
1	D	0.92	1/2319 (0.0%)	0.91	2/3149 (0.1%)
1	J	0.79	2/2319 (0.1%)	0.84	1/3149 (0.0%)
1	P	0.94	5/2319 (0.2%)	0.89	2/3149 (0.1%)
2	B	0.85	0/859	0.93	2/1162 (0.2%)
2	E	0.87	0/859	0.91	0/1162
2	K	0.89	0/859	0.90	1/1162 (0.1%)
2	Q	0.94	0/859	0.85	0/1162
3	C	0.80	0/76	1.05	0/103
3	F	0.83	0/76	1.14	0/103
3	M	0.68	0/76	1.11	0/103
3	R	0.79	0/76	1.03	1/103 (1.0%)
4	G	0.83	1/1638 (0.1%)	0.91	3/2237 (0.1%)
4	L	0.86	0/1638	0.90	0/2237
4	N	0.77	0/1638	0.84	1/2237 (0.0%)
4	S	0.85	0/1638	0.84	2/2237 (0.1%)
5	H	0.85	1/1646 (0.1%)	0.96	6/2239 (0.3%)
5	I	0.92	0/1646	1.01	4/2239 (0.2%)
5	O	0.73	0/1646	0.83	1/2239 (0.0%)
5	T	0.86	1/1646 (0.1%)	0.90	4/2239 (0.2%)
All	All	0.86	12/26152 (0.0%)	0.90	32/35560 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
4	G	0	1
4	L	0	2
4	N	0	2
5	H	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	T	0	1
All	All	0	10

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	19	GLU	CG-CD	7.12	1.62	1.51
1	P	198	GLU	CG-CD	7.08	1.62	1.51
1	A	154	GLU	CG-CD	6.59	1.61	1.51
5	T	96	CYS	CB-SG	-6.22	1.71	1.82
1	J	177	GLU	CG-CD	5.94	1.60	1.51
1	P	203	CYS	CB-SG	-5.88	1.72	1.81
5	H	146	CYS	CB-SG	-5.75	1.72	1.81
4	G	126	GLU	CG-CD	5.47	1.60	1.51
1	J	275	GLU	CG-CD	5.42	1.60	1.51
1	P	177	GLU	CG-CD	5.41	1.60	1.51
1	P	173	GLU	CG-CD	5.34	1.59	1.51
1	D	177	GLU	CG-CD	5.08	1.59	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	53	SER	N-CA-C	6.88	129.57	111.00
1	A	202	ARG	NE-CZ-NH2	-6.72	116.94	120.30
4	G	91	TRP	CA-CB-CG	6.51	126.08	113.70
4	G	135	LEU	CA-CB-CG	6.38	129.99	115.30
5	H	53	SER	C-N-CA	6.19	137.18	121.70
5	H	47	TRP	N-CA-CB	6.19	121.73	110.60
1	P	247	VAL	CB-CA-C	-6.04	99.93	111.40
5	T	18	LEU	CB-CG-CD2	-6.00	100.81	111.00
1	J	48	ARG	NE-CZ-NH1	-5.90	117.35	120.30
5	H	101	LEU	CA-CB-CG	5.88	128.81	115.30
5	I	45	LEU	CB-CG-CD1	-5.67	101.35	111.00
5	T	140	GLY	N-CA-C	5.67	127.27	113.10
5	O	100	LEU	CA-CB-CG	5.62	128.23	115.30
5	I	18	LEU	CB-CG-CD1	5.57	120.47	111.00
2	B	12	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	D	18	GLY	N-CA-C	5.47	126.77	113.10
5	T	18	LEU	CA-CB-CG	5.44	127.82	115.30
5	I	100	LEU	CA-CB-CG	5.43	127.80	115.30
2	B	96	ASP	CB-CG-OD2	-5.39	113.45	118.30
4	N	183	LEU	CA-CB-CG	5.35	127.60	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	91	TRP	CA-CB-CG	5.35	123.86	113.70
5	H	139	GLY	N-CA-C	-5.27	99.92	113.10
3	R	3	LEU	CB-CG-CD2	-5.21	102.15	111.00
5	I	146	CYS	N-CA-C	5.17	124.97	111.00
5	H	146	CYS	CA-CB-SG	-5.17	104.70	114.00
1	A	108	ARG	CB-CA-C	5.16	120.72	110.40
1	D	247	VAL	CB-CA-C	-5.14	101.64	111.40
2	K	64	LEU	CB-CG-CD1	-5.13	102.27	111.00
4	S	111	GLN	N-CA-C	5.09	124.75	111.00
1	P	170	ARG	NE-CZ-NH2	-5.09	117.75	120.30
5	T	146	CYS	CA-CB-SG	-5.07	104.88	114.00
4	G	98	TYR	N-CA-C	-5.05	97.35	111.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	275	GLU	Peptide
4	G	9	SER	Peptide
5	H	140	GLY	Peptide
5	H	152	PHE	Peptide
5	H	153	PRO	Peptide
4	L	1	GLN	Peptide
4	L	2	SER	Peptide
4	N	2	SER	Peptide
4	N	61	PRO	Peptide
5	T	139	GLY	Peptide

## 5.2 Too-close contacts [i](#)

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	2253	0	2103	57	0
1	D	2253	0	2103	71	0
1	J	2253	0	2103	56	0
1	P	2253	0	2103	66	0
2	B	836	0	803	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	836	0	803	28	0
2	K	836	0	803	27	0
2	Q	836	0	803	26	0
3	C	75	0	83	15	0
3	F	75	0	83	12	0
3	M	75	0	83	3	0
3	R	75	0	83	3	0
4	G	1595	0	1537	61	0
4	L	1595	0	1537	56	0
4	N	1595	0	1537	54	0
4	S	1595	0	1537	54	0
5	H	1609	0	1577	58	0
5	I	1609	0	1577	51	0
5	O	1609	0	1577	51	0
5	T	1609	0	1577	55	0
All	All	25472	0	24412	744	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 (744) 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)
4:N:11:SER:HB3	4:N:107:THR:HG22	1.31	1.11
1:P:256:ARG:HH11	1:P:256:ARG:HG3	1.17	1.06
1:J:138:MET:HE2	1:J:138:MET:HA	1.39	1.03
1:J:6:ARG:HH22	1:J:113:TYR:HE1	1.08	1.00
1:P:111:ARG:HH12	1:P:128:GLU:HB3	1.26	0.99
4:S:63:ARG:HH21	4:S:63:ARG:HG3	1.29	0.97
5:H:53:SER:HB3	5:H:54:SER:CB	1.98	0.94
4:S:63:ARG:HB2	4:S:78:SER:O	1.67	0.94
1:P:72:GLN:NE2	1:P:75:ARG:HH21	1.67	0.92
2:E:0:MET:SD	2:E:32:PRO:HG3	2.10	0.91
4:S:13:SER:O	4:S:16:GLN:HB2	1.71	0.91
5:I:139:GLY:O	5:I:141:THR:HG22	1.70	0.90
4:G:187:GLN:HA	4:G:190:SER:OG	1.71	0.90
5:I:49:SER:HB2	5:I:59:ALA:O	1.72	0.89
1:P:6:ARG:NH2	1:P:113:TYR:CD1	2.40	0.89
5:T:97:ALA:HB1	5:T:106:MET:HG3	1.55	0.88
1:P:215:LEU:HD22	1:P:261:VAL:HG22	1.55	0.87
1:A:178:THR:O	1:A:181:ARG:HG2	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:72:GLN:HE22	1:P:75:ARG:HH21	1.19	0.85
4:G:1:GLN:N	4:G:2:SER:HA	1.90	0.85
5:O:130:LEU:HB2	5:O:145:GLY:CA	2.07	0.85
4:N:54:ILE:HG22	4:N:66:GLY:O	1.76	0.85
1:J:6:ARG:NH2	1:J:113:TYR:CE1	2.45	0.85
1:D:253:GLN:NE2	1:D:256:ARG:HH11	1.74	0.84
1:D:65:ARG:HG2	1:D:65:ARG:HH11	1.40	0.84
1:J:111:ARG:HG2	1:J:111:ARG:HH11	1.42	0.84
5:T:136:SER:C	5:T:138:SER:H	1.81	0.84
2:Q:81:ARG:HH11	2:Q:81:ARG:HG2	1.40	0.84
1:P:215:LEU:CD2	1:P:261:VAL:HG22	2.08	0.84
4:G:187:GLN:HA	4:G:190:SER:HG	1.42	0.82
3:C:8:GLN:NE2	4:L:27:ARG:HD2	1.94	0.82
1:J:138:MET:CE	1:J:138:MET:HA	2.10	0.82
4:N:151:TRP:HA	4:N:152:LYS:HB2	1.61	0.82
3:C:8:GLN:NE2	4:L:27:ARG:CD	2.43	0.82
2:E:89:GLN:HE21	2:E:90:PRO:HD2	1.44	0.82
1:P:256:ARG:HG3	1:P:256:ARG:NH1	1.93	0.81
5:H:53:SER:HB3	5:H:54:SER:HB3	1.63	0.81
4:N:62:ASP:HB2	5:H:178:SER:HB2	1.62	0.80
4:N:32:TYR:O	4:N:68:LYS:NZ	2.14	0.80
4:S:63:ARG:NH2	4:S:63:ARG:HG3	1.94	0.80
4:L:3:GLU:HG2	4:L:4:LEU:N	1.96	0.80
1:P:6:ARG:NH2	1:P:113:TYR:CE1	2.48	0.80
4:G:170:GLN:NE2	4:G:172:ASN:OD1	2.14	0.80
1:J:204:TRP:HZ2	2:K:99:MET:C	1.87	0.79
4:G:1:GLN:H2	4:G:2:SER:HA	1.44	0.78
1:P:165:VAL:O	1:P:169:ARG:HG3	1.81	0.78
4:L:63:ARG:NH2	4:L:84:ASP:OD2	2.16	0.77
5:T:132:PRO:O	5:T:220:LYS:NZ	2.16	0.77
5:O:37:VAL:HG22	5:O:47:TRP:HA	1.67	0.77
1:A:181:ARG:HH11	1:A:181:ARG:HG2	1.51	0.76
1:A:74:HIS:HE1	1:A:97:ARG:HE	1.30	0.76
1:D:58:GLU:CD	1:D:58:GLU:H	1.89	0.75
3:C:4:MET:HB2	5:H:56:GLY:HA3	1.69	0.75
2:B:81:ARG:HG2	2:B:81:ARG:HH11	1.51	0.75
1:D:163:THR:CG2	5:I:55:GLY:HA3	2.17	0.75
1:D:111:ARG:HD3	1:D:113:TYR:CZ	2.21	0.74
4:L:91:TRP:CH2	4:L:98:TYR:CD1	2.75	0.74
4:S:63:ARG:CB	4:S:78:SER:O	2.35	0.73
5:H:152:PHE:CD2	5:H:153:PRO:HD3	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:130:LEU:HB2	5:O:145:GLY:C	2.07	0.73
5:H:53:SER:HB3	5:H:54:SER:OG	1.89	0.72
5:I:100:LEU:HD12	5:I:101:LEU:HG	1.70	0.72
3:C:8:GLN:HE22	4:L:27:ARG:CD	2.03	0.72
1:D:163:THR:HG21	5:I:55:GLY:CA	2.19	0.72
1:J:235:PRO:HG2	2:K:65:LEU:HD13	1.72	0.72
4:N:25:THR:HA	4:N:71:ASN:OD1	1.89	0.71
1:A:231:VAL:O	1:A:243:LYS:HE3	1.91	0.71
1:J:6:ARG:NH2	1:J:113:TYR:HE1	1.85	0.71
1:P:17:ARG:HG3	1:P:17:ARG:HH11	1.56	0.71
1:P:51:TRP:CZ2	1:P:179:LEU:HD11	2.26	0.70
1:A:250:PRO:HB2	1:A:253:GLN:HG3	1.73	0.70
4:G:65:SER:O	4:G:75:LEU:HD12	1.92	0.70
1:P:51:TRP:CE2	1:P:179:LEU:HD11	2.25	0.70
1:J:234:ARG:HE	1:J:242:GLN:HE21	1.37	0.70
1:J:115:GLN:HB2	2:K:60:TRP:HH2	1.56	0.70
4:G:1:GLN:HG3	5:I:62:ASP:HB2	1.74	0.69
4:G:151:TRP:HA	4:G:152:LYS:HB2	1.74	0.69
5:H:171:THR:HA	5:H:186:SER:HA	1.74	0.69
5:O:130:LEU:HB2	5:O:145:GLY:HA2	1.73	0.69
1:D:111:ARG:HD3	1:D:113:TYR:OH	1.91	0.69
1:D:225:THR:O	1:D:228:THR:HB	1.92	0.69
4:N:184:THR:C	4:N:186:GLU:H	1.95	0.69
5:H:53:SER:CB	5:H:54:SER:OG	2.40	0.69
4:L:91:TRP:CH2	4:L:98:TYR:CE1	2.80	0.69
5:H:125:PRO:HD2	5:H:211:THR:HG21	1.74	0.68
2:E:41:LYS:HG3	2:E:78:TYR:CE1	2.27	0.68
1:D:68:LYS:O	1:D:71:SER:HB3	1.93	0.68
3:F:4:MET:HB2	5:I:56:GLY:HA3	1.75	0.68
4:S:81:GLN:O	4:S:108:VAL:HG21	1.93	0.67
2:K:29:GLY:HA2	2:K:61:SER:HB2	1.75	0.67
2:E:24:ASN:HB3	2:E:65:LEU:HD11	1.77	0.67
4:G:135:LEU:CD2	4:G:181:LEU:HB3	2.25	0.67
1:D:163:THR:HG21	5:I:55:GLY:HA3	1.77	0.67
4:N:129:GLN:C	4:N:131:ASN:H	1.98	0.67
1:A:63:GLU:OE2	1:A:66:LYS:NZ	2.24	0.67
4:N:184:THR:O	4:N:186:GLU:N	2.27	0.67
1:D:178:THR:O	1:D:181:ARG:HD3	1.94	0.67
1:D:21:ARG:NH1	1:D:23:ILE:HD11	2.10	0.67
5:O:26:GLY:O	5:O:27:PHE:HB3	1.95	0.66
1:D:45:MET:HE1	3:F:2:LEU:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:85:GLU:HG2	4:N:107:THR:HA	1.78	0.66
4:G:57:PRO:HD2	4:G:60:VAL:HG21	1.78	0.66
5:H:160:TRP:CZ3	5:H:202:CYS:HB3	2.31	0.66
4:L:4:LEU:O	4:L:23:THR:O	2.12	0.65
4:S:23:THR:HB	4:S:72:THR:HG23	1.78	0.65
3:C:5:TRP:HE1	5:H:57:GLY:HA2	1.61	0.65
4:L:91:TRP:HD1	4:L:100:PHE:CD1	2.15	0.65
2:E:89:GLN:HA	2:E:89:GLN:HE21	1.62	0.64
2:E:89:GLN:NE2	2:E:90:PRO:HD2	2.11	0.64
4:L:63:ARG:HH22	4:L:84:ASP:CG	2.01	0.64
1:A:72:GLN:HE21	4:L:32:TYR:HA	1.63	0.64
5:H:125:PRO:HG3	5:H:151:TYR:HB3	1.80	0.63
2:E:1:ILE:HG22	2:E:1:ILE:O	1.98	0.63
1:D:144:LYS:O	1:D:148:GLU:HG3	1.98	0.63
1:A:72:GLN:NE2	4:L:32:TYR:HA	2.13	0.63
5:H:100:LEU:HD13	5:H:101:LEU:HG	1.80	0.63
5:O:11:LEU:HD12	5:O:116:THR:HB	1.81	0.63
4:N:187:GLN:HA	4:N:190:SER:OG	1.99	0.62
4:S:165:THR:HG22	5:T:175:VAL:HB	1.80	0.62
4:L:172:ASN:O	4:L:173:ASN:HB2	1.98	0.62
4:N:124:SER:HB3	4:N:127:GLU:HB2	1.81	0.62
1:J:219:ARG:HD3	1:J:256:ARG:NH2	2.15	0.62
1:A:181:ARG:HH11	1:A:181:ARG:CG	2.13	0.61
2:K:29:GLY:HA2	2:K:61:SER:CB	2.31	0.61
1:P:227:ASP:HB3	1:P:248:VAL:HG22	1.82	0.61
2:Q:31:HIS:CD2	2:Q:32:PRO:HA	2.34	0.61
2:Q:64:LEU:HD13	2:Q:66:TYR:HE1	1.65	0.61
1:A:163:THR:HG21	5:H:55:GLY:HA2	1.82	0.61
5:O:140:GLY:O	5:O:192:SER:HB2	2.00	0.61
2:E:89:GLN:HA	2:E:89:GLN:NE2	2.15	0.61
1:J:19:GLU:CG	1:J:75:ARG:HH21	2.14	0.61
1:D:55:GLU:OE1	1:D:170:ARG:NH2	2.33	0.61
5:T:188:VAL:HG22	5:T:190:VAL:HG13	1.82	0.61
5:H:152:PHE:CD2	5:H:153:PRO:CD	2.84	0.61
5:I:198:GLN:HE21	5:I:199:THR:H	1.47	0.61
1:P:33:PHE:CE2	1:P:34:VAL:HG22	2.36	0.60
3:C:8:GLN:HE22	4:L:27:ARG:HD3	1.67	0.60
4:L:170:GLN:HB2	4:L:172:ASN:OD1	2.01	0.60
1:D:45:MET:CE	3:F:2:LEU:HD11	2.31	0.60
1:D:50:PRO:O	1:D:53:GLU:HB2	2.01	0.60
5:I:130:LEU:O	5:I:145:GLY:HA2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:85:GLU:HG2	4:L:108:VAL:HG23	1.82	0.60
2:Q:81:ARG:NH1	2:Q:81:ARG:HG2	2.10	0.60
4:N:184:THR:C	4:N:186:GLU:N	2.54	0.60
1:A:163:THR:CG2	5:H:55:GLY:HA2	2.31	0.60
3:F:8:GLN:HE22	4:G:27:ARG:HB3	1.67	0.60
5:H:74:ASN:C	5:H:76:LYS:H	2.05	0.60
1:J:115:GLN:HB2	2:K:60:TRP:CH2	2.37	0.60
4:G:124:SER:OG	5:I:129:PRO:O	2.20	0.60
1:A:133:TRP:HB2	1:A:144:LYS:HG3	1.84	0.60
2:Q:15:ALA:HB3	2:Q:97:ARG:HG3	1.83	0.60
2:Q:7:ILE:HD12	2:Q:82:VAL:HG21	1.82	0.59
5:I:148:VAL:HB	5:I:184:LEU:HD12	1.83	0.59
1:D:253:GLN:NE2	1:D:256:ARG:NH1	2.46	0.59
4:L:1:GLN:NE2	5:H:62:ASP:H	2.00	0.59
5:I:67:ARG:C	5:I:68:PHE:HD1	2.06	0.59
4:N:11:SER:CB	4:N:107:THR:HG22	2.21	0.59
4:G:68:LYS:HA	4:G:73:ALA:HA	1.85	0.59
1:P:14:ARG:HG3	1:P:17:ARG:HB2	1.83	0.59
5:I:130:LEU:HB2	5:I:145:GLY:O	2.03	0.59
1:A:50:PRO:O	1:A:53:GLU:HB2	2.03	0.59
1:P:54:GLN:OE1	1:P:174:ASN:ND2	2.36	0.59
1:A:3:HIS:HD2	1:A:29:ASP:OD2	1.85	0.59
2:B:10:TYR:N	2:B:10:TYR:CD1	2.71	0.59
4:L:80:LEU:HD21	4:L:108:VAL:HG22	1.84	0.59
4:S:39:GLN:HG3	4:S:88:TYR:CE1	2.38	0.59
5:I:127:VAL:HG21	5:I:204:VAL:HG21	1.83	0.59
1:J:61:ASP:O	1:J:65:ARG:HG3	2.03	0.59
1:J:138:MET:CE	1:J:138:MET:CA	2.77	0.58
1:J:133:TRP:HB2	1:J:144:LYS:HG3	1.84	0.58
1:D:167:TRP:CZ2	5:I:54:SER:HB2	2.38	0.58
4:G:30:GLY:HA3	4:G:71:ASN:HD22	1.66	0.58
4:N:35:VAL:HA	4:N:91:TRP:O	2.04	0.58
5:H:139:GLY:O	5:H:140:GLY:C	2.41	0.58
5:T:136:SER:C	5:T:138:SER:N	2.52	0.58
1:A:70:HIS:CE1	3:C:6:ILE:HD12	2.39	0.58
5:O:36:TRP:NE1	5:O:81:LEU:HB2	2.19	0.58
5:H:89:GLU:CD	5:H:89:GLU:H	2.07	0.58
4:L:100:PHE:HD2	5:H:46:GLU:O	1.87	0.58
4:G:61:PRO:HG2	4:G:64:PHE:HE2	1.69	0.58
5:I:125:PRO:HD2	5:I:211:THR:HG21	1.84	0.58
4:S:83:GLU:HG2	4:S:83:GLU:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:GLU:CD	1:D:58:GLU:N	2.57	0.57
4:N:59:GLY:HA2	5:H:181:LEU:HD11	1.86	0.57
2:K:96:ASP:C	2:K:96:ASP:OD1	2.43	0.57
1:A:178:THR:O	1:A:181:ARG:NH1	2.36	0.57
1:J:70:HIS:CE1	3:M:6:ILE:HD12	2.38	0.57
5:H:12:VAL:HB	5:H:18:LEU:HD13	1.86	0.57
5:H:176:LEU:HD13	5:H:182:TYR:CZ	2.39	0.57
1:D:234:ARG:HE	1:D:242:GLN:HE21	1.53	0.57
5:O:29:PHE:CB	5:O:77:ASN:HD22	2.17	0.57
1:J:204:TRP:CZ2	2:K:99:MET:C	2.73	0.57
5:H:144:LEU:HG	5:H:188:VAL:HG12	1.85	0.57
4:N:138:LEU:HD13	5:O:187:VAL:HG11	1.86	0.57
5:H:29:PHE:CB	5:H:77:ASN:HD22	2.18	0.57
5:H:56:GLY:C	5:H:57:GLY:O	2.40	0.57
5:O:29:PHE:HB3	5:O:77:ASN:ND2	2.20	0.57
1:A:22:PHE:CG	1:A:71:SER:HB2	2.40	0.57
1:P:227:ASP:HB3	1:P:248:VAL:CG2	2.35	0.57
1:A:234:ARG:HE	1:A:242:GLN:HE21	1.53	0.57
5:I:47:TRP:CZ2	5:I:49:SER:HA	2.39	0.56
1:A:215:LEU:HD22	1:A:261:VAL:HG22	1.86	0.56
5:T:188:VAL:HG22	5:T:190:VAL:CG1	2.35	0.56
4:L:91:TRP:HH2	4:L:98:TYR:CE1	2.24	0.56
4:G:30:GLY:HA3	4:G:71:ASN:ND2	2.20	0.56
5:I:72:ARG:HE	5:I:74:ASN:HD21	1.54	0.56
4:N:120:LEU:HD12	4:N:136:VAL:O	2.04	0.56
1:D:65:ARG:NH1	1:D:65:ARG:HG2	2.08	0.56
5:O:91:THR:HG23	5:O:116:THR:HA	1.87	0.56
4:L:23:THR:HB	4:L:72:THR:OG1	2.06	0.56
1:P:218:GLN:HB2	1:P:260:HIS:NE2	2.20	0.56
4:L:4:LEU:O	4:L:5:THR:CB	2.52	0.56
4:G:151:TRP:HA	4:G:152:LYS:CB	2.36	0.56
4:G:17:SER:HB2	4:G:78:SER:HB3	1.86	0.56
4:S:4:LEU:HB2	4:S:101:GLY:HA2	1.88	0.56
5:H:52:GLY:H	5:H:57:GLY:HA3	1.71	0.55
1:J:234:ARG:HE	1:J:242:GLN:NE2	2.02	0.55
5:O:29:PHE:HB3	5:O:77:ASN:HD22	1.70	0.55
2:K:40:LEU:HD11	2:K:81:ARG:HB3	1.87	0.55
1:A:111:ARG:CZ	1:A:128:GLU:HG3	2.36	0.55
5:I:48:VAL:O	5:I:49:SER:HB3	2.06	0.55
1:J:111:ARG:NH1	1:J:111:ARG:HG2	2.12	0.55
1:A:74:HIS:CE1	1:A:97:ARG:HE	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:13:HIS:O	2:Q:21:ASN:ND2	2.33	0.55
5:T:132:PRO:HG3	5:T:144:LEU:CB	2.36	0.55
1:D:74:HIS:CE1	1:D:97:ARG:HE	2.24	0.55
2:B:13:HIS:O	2:B:14:PRO:C	2.42	0.55
1:A:74:HIS:HE1	1:A:97:ARG:NE	2.02	0.55
4:S:20:ILE:HD12	4:S:75:LEU:HD23	1.88	0.55
4:N:23:THR:HG22	4:N:72:THR:HG23	1.89	0.55
2:Q:67:TYR:HD2	2:Q:67:TYR:N	2.05	0.55
1:D:172:LEU:O	1:D:180:GLN:NE2	2.40	0.55
1:J:19:GLU:HG2	1:J:75:ARG:HH21	1.71	0.55
1:P:106:ASP:O	1:P:107:TRP:HB2	2.06	0.55
4:N:142:PHE:CE2	4:N:145:GLY:HA2	2.42	0.55
4:L:91:TRP:HD1	4:L:100:PHE:CE1	2.25	0.55
1:A:238:ASP:HB3	2:B:12:ARG:HH11	1.71	0.55
1:D:96:GLN:OE1	2:E:31:HIS:HE1	1.89	0.55
2:B:40:LEU:HD23	2:B:45:ARG:HA	1.88	0.54
5:T:60:TYR:CZ	5:T:70:ILE:HG22	2.42	0.54
2:E:16:GLU:O	2:E:72:PRO:HG2	2.07	0.54
4:S:100:PHE:HD2	5:T:46:GLU:O	1.89	0.54
1:J:13:SER:HB3	1:J:78:LEU:HD13	1.89	0.54
1:P:35:ARG:HH11	1:P:48:ARG:NE	2.05	0.54
5:O:6:GLU:CB	5:O:113:THR:HG22	2.38	0.54
2:B:59:ASP:O	2:B:60:TRP:HB2	2.08	0.54
1:D:162:GLY:O	1:D:165:VAL:HG22	2.06	0.54
2:Q:67:TYR:CD2	2:Q:67:TYR:N	2.76	0.54
5:T:187:VAL:HG23	5:T:187:VAL:O	2.06	0.54
4:G:1:GLN:N	4:G:2:SER:CA	2.67	0.54
4:N:151:TRP:N	4:N:151:TRP:CD1	2.76	0.54
5:T:220:LYS:HZ3	5:T:220:LYS:H	1.55	0.54
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.43	0.54
5:T:72:ARG:NE	5:T:74:ASN:OD1	2.38	0.54
5:O:205:ASN:HD21	5:O:207:LYS:HE2	1.73	0.54
2:B:39:LEU:HD12	2:B:49:VAL:HG22	1.88	0.54
5:H:205:ASN:HD21	5:H:212:LYS:HE2	1.73	0.54
4:N:62:ASP:CB	5:H:178:SER:HB2	2.35	0.53
5:T:7:SER:OG	5:T:21:SER:HB2	2.08	0.53
5:O:56:GLY:O	5:O:58:THR:HG23	2.09	0.53
1:A:238:ASP:HB3	2:B:12:ARG:NH1	2.24	0.53
3:R:8:GLN:NE2	4:S:27:ARG:HE	2.06	0.53
1:J:111:ARG:HH12	1:J:128:GLU:HA	1.73	0.53
1:J:189:MET:CE	1:J:217:TRP:CH2	2.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:132:PRO:HG3	5:T:144:LEU:HB3	1.89	0.53
1:A:14:ARG:HD2	1:A:17:ARG:HE	1.74	0.53
2:E:4:THR:OG1	2:E:5:PRO:HD2	2.09	0.53
4:G:85:GLU:OE2	4:G:107:THR:HA	2.08	0.53
5:H:53:SER:HB2	5:H:54:SER:OG	2.08	0.53
4:S:30:GLY:HA3	4:S:71:ASN:HD22	1.72	0.53
4:G:52:ASP:C	4:G:53:VAL:HG23	2.29	0.53
1:P:111:ARG:NH1	1:P:128:GLU:HB3	2.10	0.53
1:J:202:ARG:HD2	2:K:99:MET:C	2.29	0.53
2:Q:17:ASN:OD1	2:Q:73:THR:C	2.47	0.53
1:D:253:GLN:HE21	1:D:256:ARG:HH11	1.51	0.53
1:D:107:TRP:N	1:D:107:TRP:CD1	2.76	0.53
4:S:111:GLN:CB	4:S:112:PRO:HD2	2.39	0.53
4:S:63:ARG:CG	4:S:63:ARG:NH2	2.70	0.53
4:S:169:LYS:HZ2	4:S:173:ASN:HA	1.74	0.53
2:B:3:ARG:O	2:B:30:PHE:HA	2.09	0.53
5:I:47:TRP:O	5:I:61:ALA:HB2	2.08	0.52
2:K:29:GLY:CA	2:K:61:SER:HB2	2.39	0.52
5:H:125:PRO:HG3	5:H:151:TYR:CB	2.39	0.52
1:A:70:HIS:ND1	3:C:6:ILE:HD12	2.23	0.52
1:P:1:GLY:HA3	1:P:264:GLU:OE1	2.09	0.52
5:O:11:LEU:HG	5:O:12:VAL:N	2.23	0.52
1:P:60:TRP:O	1:P:64:THR:OG1	2.20	0.52
4:G:37:TRP:CZ3	4:G:90:CYS:HB3	2.44	0.52
5:I:141:THR:O	5:I:141:THR:HG23	2.10	0.52
5:T:46:GLU:O	5:T:47:TRP:CB	2.56	0.52
1:A:25:VAL:HG21	1:A:27:TYR:HE1	1.75	0.52
5:T:216:LYS:HE3	5:T:218:GLU:OE2	2.10	0.52
1:P:17:ARG:HG3	1:P:17:ARG:NH1	2.25	0.52
2:Q:16:GLU:O	2:Q:17:ASN:C	2.47	0.52
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.44	0.52
1:J:189:MET:HE2	1:J:217:TRP:CH2	2.45	0.52
1:P:129:ASP:OD2	1:P:131:ARG:HB2	2.10	0.52
1:J:189:MET:HE2	1:J:217:TRP:HH2	1.74	0.52
5:O:14:PRO:HG3	5:O:117:VAL:CG1	2.40	0.52
2:K:21:ASN:HB3	2:K:70:PHE:CE1	2.45	0.52
4:G:135:LEU:HD22	4:G:181:LEU:HB3	1.92	0.52
4:G:56:ARG:HB3	4:G:60:VAL:HB	1.91	0.52
1:J:253:GLN:NE2	1:J:256:ARG:NH1	2.58	0.52
5:H:74:ASN:C	5:H:76:LYS:N	2.64	0.52
1:J:131:ARG:HG3	1:J:157:ARG:NH1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:ARG:CZ	1:D:17:ARG:HB2	2.40	0.52
3:C:4:MET:H	5:H:56:GLY:HA2	1.76	0.51
1:D:163:THR:CG2	5:I:55:GLY:CA	2.83	0.51
4:S:91:TRP:CH2	4:S:98:TYR:CE1	2.98	0.51
1:J:189:MET:CE	1:J:217:TRP:HH2	2.23	0.51
5:I:143:ALA:HB2	5:I:189:THR:HA	1.92	0.51
2:E:55:SER:HB3	2:E:63:TYR:CZ	2.46	0.51
4:G:91:TRP:CH2	4:G:98:TYR:CE1	2.98	0.51
4:L:60:VAL:HG13	4:L:61:PRO:HD2	1.92	0.51
1:A:35:ARG:HH12	1:A:48:ARG:NH1	2.08	0.51
5:O:206:HIS:CD2	5:O:208:PRO:HD2	2.45	0.51
1:P:236:ALA:O	2:Q:12:ARG:HG3	2.11	0.51
2:B:81:ARG:HG2	2:B:81:ARG:NH1	2.21	0.51
1:P:202:ARG:HD3	1:P:244:TRP:CD2	2.45	0.51
4:S:37:TRP:HB2	4:S:50:ILE:HB	1.92	0.51
2:E:51:HIS:HB3	2:E:66:TYR:CD2	2.46	0.51
4:N:36:SER:HA	4:N:50:ILE:O	2.10	0.51
1:P:111:ARG:HH12	1:P:128:GLU:CB	2.13	0.51
1:D:45:MET:HE2	1:D:67:VAL:HB	1.93	0.51
5:O:14:PRO:HG3	5:O:117:VAL:HG12	1.92	0.51
4:N:20:ILE:HD11	4:N:106:VAL:CG2	2.41	0.51
4:L:104:THR:HG22	4:L:105:ASP:N	2.25	0.51
1:A:8:PHE:HD2	2:B:56:PHE:CE1	2.28	0.51
5:H:1:GLU:HA	5:H:1:GLU:OE2	2.11	0.51
4:S:165:THR:HG22	5:T:175:VAL:CB	2.41	0.50
1:P:117:ALA:HB2	2:Q:60:TRP:CE2	2.46	0.50
1:D:214:THR:HB	1:D:262:GLN:HB2	1.93	0.50
5:T:187:VAL:CG2	5:T:187:VAL:O	2.59	0.50
4:L:104:THR:CG2	4:L:105:ASP:N	2.75	0.50
2:E:81:ARG:HG2	2:E:81:ARG:HH11	1.77	0.50
1:A:126:LEU:HD13	1:A:133:TRP:CH2	2.46	0.50
1:A:128:GLU:HG2	1:A:128:GLU:O	2.10	0.50
1:D:123:TYR:CZ	1:D:140:ALA:HA	2.47	0.50
5:H:91:THR:O	5:H:91:THR:HG22	2.11	0.50
5:T:133:SER:OG	5:T:134:SER:N	2.45	0.50
5:O:2:VAL:O	5:O:2:VAL:HG12	2.11	0.50
1:P:3:HIS:HD2	1:P:29:ASP:OD2	1.94	0.50
5:H:52:GLY:O	5:H:72:ARG:NH1	2.44	0.50
5:I:19:ARG:HD2	5:I:82:GLN:OE1	2.12	0.50
5:I:22:CYS:O	5:I:78:THR:HG23	2.11	0.50
1:D:212:GLU:HA	1:D:212:GLU:OE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:146:ALA:O	4:S:147:VAL:HG13	2.11	0.50
1:J:65:ARG:NH2	4:N:52:ASP:OD1	2.44	0.50
2:K:7:ILE:HD12	2:K:91:LYS:HD3	1.94	0.50
1:J:74:HIS:CD2	1:J:97:ARG:HH21	2.30	0.50
5:O:138:SER:O	5:O:140:GLY:N	2.46	0.49
1:D:5:MET:HB2	1:D:168:LEU:HD13	1.94	0.49
1:P:72:GLN:HG2	4:S:32:TYR:HA	1.93	0.49
1:D:253:GLN:HE22	1:D:256:ARG:NH1	2.09	0.49
5:I:130:LEU:CB	5:I:145:GLY:O	2.59	0.49
2:E:74:GLU:HG3	2:E:75:LYS:N	2.27	0.49
5:I:34:MET:HB3	5:I:79:LEU:HD22	1.94	0.49
4:L:166:LYS:N	4:L:166:LYS:HD3	2.28	0.49
2:E:1:ILE:CG2	2:E:1:ILE:O	2.61	0.49
4:N:142:PHE:HE2	4:N:145:GLY:HA2	1.76	0.49
2:Q:40:LEU:HA	2:Q:44:GLU:O	2.12	0.49
3:C:4:MET:HB2	5:H:56:GLY:CA	2.42	0.49
4:L:91:TRP:CD1	4:L:100:PHE:CE1	3.00	0.49
1:D:133:TRP:HB2	1:D:144:LYS:HG3	1.94	0.49
4:G:121:PHE:CD1	5:I:130:LEU:HB3	2.47	0.49
4:S:41:HIS:CD2	4:S:86:ALA:HB2	2.47	0.49
1:D:65:ARG:CG	1:D:65:ARG:HH11	2.19	0.49
4:S:37:TRP:CZ3	4:S:90:CYS:HB3	2.48	0.49
4:S:138:LEU:HD23	4:S:178:SER:HB3	1.95	0.49
1:J:21:ARG:NH2	1:J:37:ASP:OD2	2.44	0.49
4:G:37:TRP:HB2	4:G:50:ILE:HB	1.94	0.49
1:P:176:LYS:HB3	1:P:180:GLN:NE2	2.28	0.49
2:K:47:GLU:N	2:K:47:GLU:OE2	2.46	0.49
4:G:184:THR:OG1	4:G:187:GLN:HG2	2.12	0.49
2:K:40:LEU:HD12	2:K:79:ALA:HB3	1.95	0.49
1:A:35:ARG:NH1	1:A:48:ARG:NH1	2.61	0.49
4:N:4:LEU:HD23	4:N:90:CYS:SG	2.53	0.49
1:D:70:HIS:CE1	3:F:6:ILE:HD12	2.48	0.49
5:H:175:VAL:HG22	5:H:176:LEU:N	2.28	0.49
4:G:126:GLU:O	4:G:129:GLN:HB2	2.13	0.49
4:G:1:GLN:CG	5:I:62:ASP:HB2	2.42	0.48
5:I:32:TYR:HA	5:I:99:GLU:O	2.13	0.48
1:D:253:GLN:O	1:D:256:ARG:HG2	2.13	0.48
5:I:198:GLN:NE2	5:I:199:THR:H	2.11	0.48
2:E:23:LEU:HD21	2:E:39:LEU:HD22	1.94	0.48
4:S:121:PHE:CD1	5:T:130:LEU:HB3	2.48	0.48
2:Q:24:ASN:HB3	2:Q:65:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:133:ALA:HB3	4:N:183:LEU:O	2.13	0.48
2:Q:7:ILE:N	2:Q:7:ILE:HD13	2.28	0.48
5:H:38:ARG:HG2	5:H:48:VAL:HG22	1.95	0.48
1:A:225:THR:O	1:A:228:THR:HB	2.13	0.48
5:T:132:PRO:O	5:T:220:LYS:CE	2.62	0.48
2:E:41:LYS:HG3	2:E:78:TYR:CZ	2.48	0.48
4:G:135:LEU:HD21	4:G:181:LEU:HD23	1.94	0.48
5:T:56:GLY:O	5:T:57:GLY:C	2.51	0.48
4:L:25:THR:C	4:L:27:ARG:H	2.15	0.48
5:O:136:SER:C	5:O:138:SER:H	2.16	0.48
5:I:125:PRO:HB3	5:I:151:TYR:HB3	1.94	0.48
1:J:6:ARG:NH2	1:J:113:TYR:CD1	2.82	0.48
2:E:89:GLN:CA	2:E:89:GLN:HE21	2.26	0.48
5:T:29:PHE:CD2	5:T:77:ASN:HA	2.48	0.48
4:N:85:GLU:OE1	4:N:169:LYS:HE3	2.14	0.48
5:I:127:VAL:HB	5:I:213:VAL:HG11	1.96	0.48
1:D:187:THR:HG21	1:D:261:VAL:HG21	1.96	0.48
4:L:4:LEU:HB2	4:L:101:GLY:HA2	1.96	0.47
2:Q:73:THR:OG1	2:Q:76:ASP:HB2	2.13	0.47
2:Q:51:HIS:HD2	2:Q:52:SER:O	1.97	0.47
4:S:80:LEU:HG	4:S:108:VAL:HG22	1.95	0.47
5:H:62:ASP:HA	5:H:65:LYS:HD3	1.96	0.47
2:Q:17:ASN:OD1	2:Q:73:THR:O	2.32	0.47
4:N:178:SER:HB2	4:N:180:TYR:CE1	2.49	0.47
4:G:60:VAL:HA	4:G:61:PRO:HD2	1.72	0.47
4:S:135:LEU:HD11	4:S:183:LEU:HD11	1.95	0.47
1:J:110:LEU:HD12	1:J:110:LEU:HA	1.77	0.47
5:O:11:LEU:HD11	5:O:118:SER:HB2	1.96	0.47
4:N:91:TRP:CH2	4:N:98:TYR:CE1	3.02	0.47
1:D:77:ASP:OD2	1:D:116:TYR:OH	2.28	0.47
1:D:167:TRP:CH2	5:I:54:SER:HB2	2.50	0.47
1:A:234:ARG:HE	1:A:242:GLN:NE2	2.12	0.47
1:P:108:ARG:HB2	4:G:17:SER:CB	2.45	0.47
3:F:4:MET:HB2	5:I:56:GLY:CA	2.42	0.47
1:J:19:GLU:HB3	1:J:20:PRO:HD2	1.96	0.47
1:P:33:PHE:CD2	1:P:34:VAL:HG22	2.50	0.47
5:O:6:GLU:HB3	5:O:113:THR:CG2	2.45	0.47
5:O:6:GLU:HB3	5:O:113:THR:HG22	1.97	0.47
1:A:217:TRP:CE2	1:A:247:VAL:HG22	2.50	0.47
1:P:234:ARG:HE	1:P:242:GLN:HE21	1.62	0.47
2:B:31:HIS:CD2	2:B:32:PRO:HA	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:9:SER:HB3	4:N:105:ASP:HB3	1.97	0.47
4:L:189:LYS:HE3	5:O:166:THR:HG23	1.97	0.47
4:L:64:PHE:CE1	4:L:77:ILE:HG12	2.49	0.47
2:K:58:LYS:O	2:K:58:LYS:HG2	2.15	0.47
1:P:72:GLN:HG2	4:S:31:GLY:O	2.14	0.47
5:T:46:GLU:O	5:T:47:TRP:HB3	2.15	0.47
2:B:39:LEU:HD13	2:B:68:THR:HG22	1.96	0.47
1:P:42:SER:O	1:P:44:ARG:HG2	2.15	0.47
1:P:234:ARG:HE	1:P:242:GLN:NE2	2.13	0.47
1:J:45:MET:CE	1:J:67:VAL:HB	2.45	0.47
5:O:144:LEU:O	5:O:188:VAL:N	2.39	0.47
1:A:138:MET:HG3	1:D:138:MET:HG3	1.97	0.47
2:B:39:LEU:HD12	2:B:49:VAL:CG2	2.44	0.47
4:N:152:LYS:HB2	4:N:195:SER:O	2.15	0.46
1:A:42:SER:O	1:A:44:ARG:HG2	2.16	0.46
1:A:77:ASP:OD1	3:C:9:VAL:HG22	2.15	0.46
5:O:37:VAL:HG13	5:O:47:TRP:H	1.79	0.46
4:N:129:GLN:C	4:N:131:ASN:N	2.67	0.46
4:N:139:ILE:HG22	4:N:142:PHE:CE1	2.51	0.46
5:T:12:VAL:O	5:T:117:VAL:HA	2.15	0.46
1:J:6:ARG:HE	1:J:6:ARG:HB3	1.56	0.46
1:P:238:ASP:HB3	2:Q:12:ARG:HD3	1.98	0.46
1:D:212:GLU:OE1	1:D:212:GLU:CA	2.63	0.46
2:K:3:ARG:O	2:K:30:PHE:HA	2.15	0.46
4:G:63:ARG:H	4:G:63:ARG:HG2	1.38	0.46
5:T:97:ALA:HB1	5:T:106:MET:CG	2.38	0.46
1:J:64:THR:O	1:J:68:LYS:HG2	2.16	0.46
1:J:68:LYS:O	1:J:72:GLN:OE1	2.34	0.46
2:B:70:PHE:CZ	2:B:72:PRO:HG3	2.50	0.46
1:D:48:ARG:HA	1:D:48:ARG:HD2	1.63	0.46
4:L:36:SER:HB3	4:L:50:ILE:O	2.15	0.46
4:N:39:GLN:HG3	4:N:88:TYR:CE1	2.51	0.46
5:I:184:LEU:C	5:I:184:LEU:HD12	2.36	0.46
1:J:189:MET:HE1	1:J:217:TRP:CH2	2.51	0.46
5:I:19:ARG:HH11	5:I:19:ARG:HG3	1.81	0.46
1:D:98:MET:SD	1:D:98:MET:C	2.94	0.46
4:L:81:GLN:O	4:L:84:ASP:HB2	2.16	0.46
4:S:91:TRP:CZ2	4:S:98:TYR:CD1	3.03	0.46
4:L:185:PRO:O	4:L:189:LYS:HG3	2.15	0.46
5:H:146:CYS:O	5:H:185:SER:HA	2.15	0.46
1:A:263:HIS:HB3	1:A:266:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:187:THR:HG21	1:J:261:VAL:HG21	1.98	0.46
5:O:137:THR:HG22	5:O:137:THR:O	2.16	0.46
2:K:38:ASP:OD2	2:K:81:ARG:NH1	2.49	0.46
1:P:238:ASP:OD1	1:P:240:THR:OG1	2.33	0.46
4:S:181:LEU:HG	4:S:183:LEU:HD21	1.98	0.46
1:P:66:LYS:HD2	3:R:4:MET:HA	1.97	0.46
1:J:192:HIS:NE2	2:K:98:ASP:O	2.49	0.46
4:N:40:GLN:HB2	4:N:46:PRO:HA	1.97	0.46
5:H:144:LEU:HG	5:H:188:VAL:CG1	2.45	0.46
2:B:40:LEU:HA	2:B:44:GLU:O	2.16	0.46
5:H:53:SER:CB	5:H:54:SER:CB	2.82	0.45
2:E:23:LEU:HB2	2:E:70:PHE:CE1	2.51	0.45
4:N:60:VAL:HG13	4:N:61:PRO:HD2	1.98	0.45
1:P:118:TYR:O	1:P:121:LYS:HD2	2.15	0.45
2:K:49:VAL:HG22	2:K:68:THR:HB	1.96	0.45
1:J:68:LYS:O	1:J:71:SER:HB3	2.16	0.45
4:G:91:TRP:HA	4:G:99:VAL:O	2.17	0.45
4:L:141:ASP:O	4:L:174:LYS:HD3	2.16	0.45
1:P:176:LYS:HB3	1:P:180:GLN:HE21	1.82	0.45
4:N:94:ALA:HB3	4:N:97:TYR:CE1	2.52	0.45
4:S:38:TYR:CE1	4:S:48:LEU:HD12	2.52	0.45
4:N:151:TRP:HA	4:N:152:LYS:CB	2.41	0.45
1:P:218:GLN:HB2	1:P:260:HIS:CD2	2.52	0.45
4:N:142:PHE:CE2	4:N:175:TYR:HB2	2.52	0.45
4:S:91:TRP:HD1	4:S:100:PHE:CZ	2.34	0.45
5:I:144:LEU:HD13	5:I:217:VAL:CG1	2.46	0.45
5:I:144:LEU:HD13	5:I:217:VAL:HG11	1.99	0.45
1:P:133:TRP:HB2	1:P:144:LYS:HG3	1.98	0.45
4:L:4:LEU:CB	4:L:101:GLY:HA2	2.46	0.45
4:S:40:GLN:O	4:S:86:ALA:HB1	2.17	0.45
5:O:132:PRO:HG3	5:O:144:LEU:HD22	1.96	0.45
4:N:80:LEU:HD21	4:N:108:VAL:HG22	1.99	0.45
4:G:146:ALA:O	4:G:200:HIS:HD2	1.98	0.45
1:D:121:LYS:HE3	1:D:121:LYS:HB2	1.59	0.45
4:N:131:ASN:O	4:N:132:LYS:HG2	2.17	0.45
3:R:5:TRP:NE1	5:T:57:GLY:O	2.50	0.45
1:J:95:VAL:HG13	1:J:116:TYR:CE1	2.52	0.45
2:B:41:LYS:HD3	2:B:78:TYR:OH	2.16	0.45
1:D:96:GLN:NE2	2:E:56:PHE:CD2	2.84	0.45
1:A:204:TRP:HZ2	2:B:99:MET:C	2.20	0.45
5:O:51:ILE:HG23	5:O:51:ILE:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:185:PRO:HD3	1:J:263:HIS:ND1	2.32	0.45
1:P:196:ASP:N	1:P:196:ASP:OD1	2.49	0.45
5:I:6:GLU:HB3	5:I:113:THR:CG2	2.46	0.45
1:P:5:MET:HB2	1:P:168:LEU:HD13	1.98	0.45
3:F:3:LEU:HG	3:F:5:TRP:O	2.17	0.45
1:P:233:THR:OG1	1:P:243:LYS:HD2	2.17	0.45
1:A:118:TYR:O	1:A:121:LYS:HG3	2.17	0.45
1:J:17:ARG:HE	1:J:17:ARG:HB2	1.59	0.45
4:L:3:GLU:HG2	4:L:4:LEU:CA	2.46	0.44
1:P:275:GLU:HA	1:P:276:PRO:HD2	1.59	0.44
2:B:13:HIS:HB2	2:B:21:ASN:ND2	2.31	0.44
5:O:205:ASN:ND2	5:O:207:LYS:HE2	2.32	0.44
4:G:91:TRP:CH2	4:G:98:TYR:CD1	3.05	0.44
4:G:120:LEU:HD12	4:G:136:VAL:O	2.17	0.44
1:P:6:ARG:HB3	1:P:6:ARG:HE	1.64	0.44
4:N:68:LYS:HB2	4:N:73:ALA:HA	1.99	0.44
5:H:152:PHE:CE2	5:H:153:PRO:HD3	2.51	0.44
1:P:47:PRO:O	1:P:48:ARG:HG2	2.18	0.44
2:B:25:CYS:HB3	2:B:39:LEU:HD21	1.99	0.44
5:I:143:ALA:HA	5:I:144:LEU:HB3	1.99	0.44
1:P:176:LYS:CB	1:P:180:GLN:HE21	2.30	0.44
4:S:170:GLN:NE2	4:S:174:LYS:HB2	2.32	0.44
4:L:191:HIS:HB2	4:L:194:TYR:CE1	2.52	0.44
4:G:20:ILE:O	4:G:74:SER:HA	2.17	0.44
2:Q:15:ALA:CB	2:Q:97:ARG:HG3	2.47	0.44
1:A:70:HIS:CE1	3:C:6:ILE:CD1	3.01	0.44
1:P:176:LYS:HA	1:P:180:GLN:HE21	1.82	0.44
1:D:70:HIS:CG	3:F:6:ILE:HD12	2.53	0.44
4:L:184:THR:OG1	4:L:187:GLN:OE1	2.27	0.44
5:T:136:SER:O	5:T:138:SER:N	2.49	0.44
5:T:131:ALA:HA	5:T:132:PRO:HD3	1.69	0.44
1:A:215:LEU:CD2	1:A:261:VAL:HG22	2.47	0.44
2:Q:21:ASN:OD1	2:Q:22:PHE:N	2.43	0.44
1:A:35:ARG:NH1	1:A:48:ARG:CZ	2.80	0.44
4:G:200:HIS:O	4:G:201:GLU:C	2.55	0.44
1:J:6:ARG:NH2	1:J:102:ASP:OD1	2.51	0.44
4:L:135:LEU:HB2	4:L:181:LEU:HB3	1.99	0.44
5:T:210:ASN:HD22	5:T:210:ASN:C	2.20	0.44
1:D:43:GLN:O	1:D:68:LYS:HE3	2.18	0.44
5:T:195:LEU:HD12	5:T:195:LEU:HA	1.78	0.44
5:T:138:SER:O	5:T:140:GLY:HA2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:138:SER:O	5:T:139:GLY:C	2.55	0.44
4:G:17:SER:CB	4:G:78:SER:HB3	2.48	0.44
4:L:153:ALA:HB2	4:L:194:TYR:CE2	2.53	0.44
4:S:152:LYS:HD3	4:S:157:PRO:HA	2.00	0.44
4:G:137:CYS:C	4:G:138:LEU:HG	2.38	0.44
1:P:256:ARG:NH1	1:P:256:ARG:CG	2.69	0.44
1:P:81:LEU:HD13	1:P:118:TYR:CD1	2.53	0.44
4:S:48:LEU:HD21	4:S:51:HIS:HB3	1.99	0.44
1:A:167:TRP:HZ2	5:H:54:SER:HA	1.82	0.43
5:O:87:ARG:O	5:O:117:VAL:HG21	2.18	0.43
5:T:150:ASP:H	5:T:183:SER:HB3	1.83	0.43
1:D:275:GLU:O	1:D:276:PRO:C	2.56	0.43
3:C:8:GLN:HE21	4:L:27:ARG:HD2	1.80	0.43
1:J:70:HIS:ND1	3:M:6:ILE:HD12	2.34	0.43
1:J:58:GLU:CD	1:J:58:GLU:H	2.22	0.43
1:D:82:ARG:HH11	1:D:82:ARG:HG2	1.83	0.43
5:I:184:LEU:HD12	5:I:184:LEU:O	2.18	0.43
2:B:12:ARG:O	2:B:12:ARG:HG2	2.18	0.43
1:J:21:ARG:CZ	1:J:23:ILE:HD11	2.48	0.43
5:T:68:PHE:CD1	5:T:68:PHE:N	2.86	0.43
4:N:91:TRP:CH2	4:N:98:TYR:CD1	3.07	0.43
5:H:29:PHE:HB3	5:H:77:ASN:ND2	2.33	0.43
1:D:6:ARG:HH11	1:D:6:ARG:HG3	1.83	0.43
5:O:204:VAL:HG12	5:O:205:ASN:N	2.33	0.43
1:P:44:ARG:HA	1:P:64:THR:HG23	2.00	0.43
5:O:158:VAL:HG21	5:O:186:SER:HB2	2.00	0.43
1:J:191:HIS:C	1:J:191:HIS:CD2	2.91	0.43
5:T:144:LEU:C	5:T:144:LEU:HD12	2.39	0.43
5:H:176:LEU:HD13	5:H:182:TYR:CE1	2.53	0.43
2:K:40:LEU:HA	2:K:44:GLU:O	2.18	0.43
5:T:52:GLY:N	5:T:57:GLY:HA3	2.32	0.43
5:T:150:ASP:OD1	5:T:177:GLN:OE1	2.35	0.43
5:O:70:ILE:HD11	5:O:79:LEU:HD11	2.01	0.43
5:H:135:LYS:C	5:H:137:THR:N	2.71	0.43
5:T:156:VAL:HG13	5:T:157:THR:N	2.33	0.43
1:D:207:SER:HA	1:D:240:THR:HB	2.00	0.43
4:G:151:TRP:N	4:G:151:TRP:CD1	2.87	0.43
5:I:174:ALA:HA	5:I:184:LEU:HB3	1.99	0.43
1:J:78:LEU:HA	1:J:78:LEU:HD23	1.82	0.43
5:O:22:CYS:O	5:O:78:THR:HG22	2.19	0.43
2:E:12:ARG:HG2	2:E:13:HIS:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:61:ALA:O	5:O:62:ASP:C	2.55	0.43
1:D:163:THR:HG21	5:I:55:GLY:HA2	1.97	0.43
1:D:21:ARG:NE	1:D:39:ASP:HB2	2.34	0.43
1:D:99:TYR:OH	3:F:3:LEU:HB2	2.19	0.43
5:T:125:PRO:HB3	5:T:151:TYR:HB3	2.00	0.43
2:K:51:HIS:HD2	2:K:52:SER:O	2.01	0.43
4:S:163:GLU:OE1	4:S:163:GLU:HA	2.18	0.43
4:S:91:TRP:CH2	5:T:105:GLY:HA2	2.54	0.43
4:L:191:HIS:HB2	4:L:194:TYR:HE1	1.84	0.43
5:H:135:LYS:O	5:H:136:SER:C	2.56	0.43
4:S:68:LYS:HA	4:S:73:ALA:HA	2.00	0.43
3:C:8:GLN:NE2	4:L:27:ARG:HD3	2.24	0.43
4:L:91:TRP:CZ2	4:L:98:TYR:CD1	3.07	0.43
4:G:151:TRP:HB3	4:G:195:SER:O	2.19	0.43
4:S:23:THR:CB	4:S:72:THR:HG23	2.48	0.43
1:P:202:ARG:NH1	2:Q:99:MET:O	2.50	0.43
4:N:37:TRP:CZ3	4:N:90:CYS:HB3	2.53	0.43
5:T:4:LEU:HD22	5:T:22:CYS:SG	2.59	0.43
4:G:23:THR:HG22	4:G:72:THR:HG23	2.01	0.43
1:A:227:ASP:HB3	1:A:248:VAL:HG13	2.01	0.43
5:H:152:PHE:CG	5:H:153:PRO:CD	3.02	0.42
4:S:81:GLN:HB3	4:S:82:ALA:H	1.64	0.42
5:T:189:THR:C	5:T:190:VAL:HG13	2.40	0.42
4:S:156:SER:HA	4:S:157:PRO:HD2	1.80	0.42
1:D:129:ASP:OD1	1:D:131:ARG:N	2.52	0.42
4:N:197:GLN:HB3	4:N:206:GLU:HG3	2.00	0.42
2:E:96:ASP:O	2:E:97:ARG:C	2.57	0.42
5:T:68:PHE:N	5:T:68:PHE:HD1	2.16	0.42
5:T:73:ASP:O	5:T:75:SER:N	2.51	0.42
5:I:184:LEU:C	5:I:184:LEU:CD1	2.87	0.42
1:D:103:VAL:CG2	1:D:107:TRP:HA	2.49	0.42
5:O:168:GLY:O	5:O:188:VAL:HA	2.19	0.42
5:T:171:THR:HA	5:T:186:SER:HA	2.01	0.42
4:L:83:GLU:HG2	4:L:83:GLU:O	2.18	0.42
1:D:111:ARG:HD3	1:D:113:TYR:CE2	2.55	0.42
1:P:17:ARG:CG	1:P:17:ARG:NH1	2.82	0.42
1:A:72:GLN:HE22	4:L:33:ASN:H	1.67	0.42
2:B:39:LEU:CD1	2:B:68:THR:HG22	2.48	0.42
1:D:70:HIS:CE1	3:F:6:ILE:CD1	3.02	0.42
4:L:189:LYS:HE2	4:L:189:LYS:HB2	1.90	0.42
4:S:34:TYR:CD1	5:T:103:TYR:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:195:SER:OG	4:N:208:THR:HA	2.20	0.42
1:D:70:HIS:HE1	3:F:3:LEU:O	2.03	0.42
5:O:71:SER:OG	5:O:80:TYR:HB2	2.19	0.42
1:D:227:ASP:HB3	1:D:248:VAL:HG12	2.02	0.42
5:T:132:PRO:HG3	5:T:144:LEU:HB2	2.00	0.42
2:K:55:SER:HB3	2:K:63:TYR:CZ	2.55	0.42
1:J:87:GLN:NE2	1:J:93:HIS:CE1	2.88	0.42
5:H:87:ARG:HH11	5:H:87:ARG:HD2	1.66	0.42
4:S:91:TRP:HA	4:S:99:VAL:O	2.19	0.42
1:A:33:PHE:CD2	1:A:34:VAL:HG13	2.55	0.42
2:K:83:ASN:ND2	2:K:84:HIS:H	2.18	0.42
4:S:118:VAL:O	4:S:207:LYS:HE2	2.20	0.42
5:O:73:ASP:OD2	5:O:73:ASP:C	2.58	0.42
1:A:107:TRP:CD1	1:A:107:TRP:N	2.86	0.42
1:A:218:GLN:HG3	1:A:260:HIS:CD2	2.55	0.42
4:N:152:LYS:HA	4:N:152:LYS:HD3	1.75	0.42
5:H:100:LEU:O	5:H:100:LEU:HD22	2.19	0.42
5:H:29:PHE:CB	5:H:77:ASN:ND2	2.83	0.42
5:I:98:GLY:O	5:I:106:MET:HA	2.19	0.42
4:N:170:GLN:HB2	4:N:170:GLN:HE21	1.72	0.42
2:E:23:LEU:HB2	2:E:70:PHE:CZ	2.55	0.42
4:L:195:SER:HA	4:L:207:LYS:O	2.20	0.42
4:S:185:PRO:O	4:S:188:TRP:HB3	2.20	0.42
1:P:25:VAL:HG21	1:P:27:TYR:HE1	1.85	0.42
1:J:98:MET:SD	1:J:98:MET:C	2.99	0.42
5:O:46:GLU:O	5:O:47:TRP:HB3	2.20	0.41
4:G:57:PRO:HG2	4:G:60:VAL:CG2	2.49	0.41
2:Q:97:ARG:HB3	2:Q:97:ARG:HE	1.75	0.41
4:N:124:SER:OG	4:N:125:SER:N	2.52	0.41
4:S:39:GLN:HG3	4:S:88:TYR:CZ	2.55	0.41
5:T:70:ILE:O	5:T:70:ILE:HG23	2.20	0.41
5:H:134:SER:O	5:H:137:THR:HB	2.20	0.41
1:D:51:TRP:CZ2	1:D:179:LEU:HD11	2.55	0.41
5:I:28:THR:O	5:I:29:PHE:C	2.57	0.41
4:G:161:GLY:O	4:G:181:LEU:HA	2.20	0.41
5:O:132:PRO:HG3	5:O:144:LEU:HB3	2.02	0.41
2:K:83:ASN:HB2	2:K:90:PRO:HB3	2.02	0.41
5:T:137:THR:O	5:T:137:THR:HG22	2.20	0.41
1:D:21:ARG:HE	1:D:39:ASP:HB2	1.85	0.41
4:N:94:ALA:CB	4:N:97:TYR:CE1	3.04	0.41
1:D:173:GLU:O	1:D:176:LYS:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:103:VAL:HG12	1:P:109:PHE:HA	2.02	0.41
5:T:152:PHE:HA	5:T:153:PRO:HA	1.70	0.41
4:G:16:GLN:O	4:G:80:LEU:HB2	2.20	0.41
5:O:40:ALA:O	5:O:41:PRO:C	2.58	0.41
4:G:151:TRP:CA	4:G:152:LYS:HB2	2.48	0.41
4:G:56:ARG:CZ	4:G:62:ASP:HB2	2.50	0.41
4:G:26:SER:HA	4:G:71:ASN:HD21	1.84	0.41
4:S:4:LEU:HB2	4:S:101:GLY:CA	2.50	0.41
4:S:51:HIS:O	4:S:52:ASP:HB2	2.21	0.41
1:D:1:GLY:O	1:D:3:HIS:CE1	2.73	0.41
2:B:61:SER:H	2:B:61:SER:HG	1.57	0.41
4:G:89:TYR:CE1	4:G:103:GLY:HA3	2.56	0.41
1:D:226:GLN:HB3	1:D:226:GLN:HE21	1.51	0.41
4:N:38:TYR:OH	5:O:106:MET:N	2.53	0.41
4:L:3:GLU:HG2	4:L:4:LEU:C	2.41	0.41
1:A:111:ARG:NH1	1:A:128:GLU:HG3	2.36	0.41
4:N:20:ILE:O	4:N:74:SER:HA	2.20	0.41
2:E:74:GLU:HG3	2:E:75:LYS:HB2	2.01	0.41
4:S:18:VAL:O	4:S:76:THR:HA	2.21	0.41
4:L:204:THR:CG2	4:L:205:VAL:N	2.83	0.41
2:Q:75:LYS:HB2	2:Q:75:LYS:NZ	2.34	0.41
5:H:160:TRP:CE3	5:H:202:CYS:HB3	2.54	0.41
3:F:8:GLN:NE2	4:G:27:ARG:HE	2.17	0.41
3:C:6:ILE:H	3:C:6:ILE:HG12	1.71	0.41
5:O:131:ALA:HA	5:O:132:PRO:HD3	1.93	0.41
1:A:219:ARG:O	1:A:222:GLU:HG2	2.21	0.41
5:H:34:MET:CB	5:H:79:LEU:HD13	2.51	0.41
2:B:73:THR:OG1	2:B:76:ASP:OD2	2.39	0.41
4:G:152:LYS:CG	4:G:195:SER:HB2	2.50	0.41
4:G:61:PRO:HG2	4:G:64:PHE:CE2	2.53	0.41
4:G:37:TRP:CE3	4:G:90:CYS:HB3	2.56	0.41
4:G:99:VAL:CG2	4:G:100:PHE:N	2.83	0.41
5:O:49:SER:HB3	5:O:70:ILE:HD12	2.03	0.41
1:J:159:TYR:CG	3:M:3:LEU:HD13	2.56	0.41
1:A:98:MET:C	1:A:98:MET:SD	2.99	0.41
2:K:97:ARG:HB2	2:K:97:ARG:HE	1.58	0.41
4:G:1:GLN:HB2	4:G:97:TYR:CE1	2.56	0.41
5:O:37:VAL:CG1	5:O:38:ARG:N	2.84	0.41
4:G:152:LYS:HA	4:G:152:LYS:HD3	1.77	0.41
1:D:55:GLU:CD	1:D:170:ARG:HH21	2.23	0.41
5:O:207:LYS:N	5:O:208:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:123:LYS:HE2	5:I:150:ASP:O	2.21	0.41
2:B:47:GLU:N	2:B:47:GLU:OE2	2.53	0.41
4:L:51:HIS:O	4:L:52:ASP:HB2	2.21	0.41
5:I:215:LYS:HA	5:I:215:LYS:HE3	2.03	0.41
4:G:131:ASN:ND2	4:G:185:PRO:HG2	2.35	0.41
1:P:72:GLN:CD	1:P:75:ARG:HH21	2.23	0.41
4:G:57:PRO:HG2	4:G:60:VAL:HG23	2.03	0.41
4:L:80:LEU:CD2	4:L:108:VAL:HG22	2.50	0.41
4:S:111:GLN:HB2	4:S:112:PRO:HD2	2.02	0.41
5:T:158:VAL:HG22	5:T:204:VAL:HG22	2.02	0.41
4:L:124:SER:O	4:L:125:SER:C	2.60	0.41
2:K:10:TYR:CD1	2:K:10:TYR:N	2.88	0.41
1:A:156:LEU:HA	1:A:156:LEU:HD13	1.89	0.41
5:O:8:GLY:O	5:O:20:LEU:HD23	2.21	0.41
1:P:49:ALA:O	1:P:52:ILE:HG22	2.21	0.41
2:E:41:LYS:HE3	2:E:78:TYR:OH	2.21	0.40
5:T:220:LYS:NZ	5:T:220:LYS:H	2.18	0.40
4:S:137:CYS:HB2	4:S:151:TRP:CH2	2.56	0.40
1:P:213:ILE:HG13	1:P:262:GLN:O	2.21	0.40
2:E:1:ILE:HA	2:E:1:ILE:HD12	1.93	0.40
4:L:161:GLY:O	4:L:181:LEU:HA	2.22	0.40
5:T:73:ASP:C	5:T:75:SER:H	2.24	0.40
1:A:81:LEU:HA	1:A:81:LEU:HD23	1.86	0.40
2:B:21:ASN:OD1	2:B:22:PHE:N	2.51	0.40
1:A:35:ARG:HD3	2:B:53:ASP:OD2	2.22	0.40
5:H:34:MET:HB3	5:H:79:LEU:HD13	2.04	0.40
5:I:60:TYR:OH	5:I:70:ILE:HG22	2.22	0.40
1:P:257:TYR:CD1	1:P:257:TYR:N	2.88	0.40
1:P:35:ARG:HD3	2:Q:53:ASP:OD2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	274/276 (99%)	261 (95%)	10 (4%)	3 (1%)	17	51
1	D	274/276 (99%)	258 (94%)	15 (6%)	1 (0%)	39	74
1	J	274/276 (99%)	260 (95%)	12 (4%)	2 (1%)	26	63
1	P	274/276 (99%)	260 (95%)	11 (4%)	3 (1%)	17	51
2	B	98/100 (98%)	88 (90%)	9 (9%)	1 (1%)	19	54
2	E	98/100 (98%)	86 (88%)	10 (10%)	2 (2%)	9	33
2	K	98/100 (98%)	90 (92%)	8 (8%)	0	100	100
2	Q	98/100 (98%)	86 (88%)	9 (9%)	3 (3%)	5	21
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	F	7/9 (78%)	7 (100%)	0	0	100	100
3	M	7/9 (78%)	7 (100%)	0	0	100	100
3	R	7/9 (78%)	7 (100%)	0	0	100	100
4	G	209/212 (99%)	182 (87%)	23 (11%)	4 (2%)	10	35
4	L	209/212 (99%)	186 (89%)	17 (8%)	6 (3%)	6	23
4	N	209/212 (99%)	183 (88%)	19 (9%)	7 (3%)	5	20
4	S	209/212 (99%)	186 (89%)	20 (10%)	3 (1%)	14	44
5	H	218/220 (99%)	197 (90%)	10 (5%)	11 (5%)	3	9
5	I	218/220 (99%)	189 (87%)	21 (10%)	8 (4%)	4	17
5	O	218/220 (99%)	189 (87%)	19 (9%)	10 (5%)	3	11
5	T	218/220 (99%)	188 (86%)	18 (8%)	12 (6%)	2	7
All	All	3224/3268 (99%)	2917 (90%)	231 (7%)	76 (2%)	7	29

All (76) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	GLY
1	D	18	GLY
1	J	18	GLY
1	P	18	GLY
4	L	2	SER
4	L	3	GLU
4	G	152	LYS
4	N	62	ASP
4	N	152	LYS
4	S	111	GLN
5	H	136	SER

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Mol	Chain	Res	Type
5	H	153	PRO
5	I	31	ALA
5	O	27	PHE
5	T	53	SER
5	T	133	SER
5	T	136	SER
5	T	137	THR
5	T	162	SER
1	J	86	ASN
4	L	5	THR
4	N	80	LEU
4	N	130	ALA
4	N	160	ALA
5	H	47	TRP
5	H	53	SER
5	H	57	GLY
5	H	65	LYS
5	I	30	SER
5	I	56	GLY
5	I	140	GLY
5	O	137	THR
5	O	139	GLY
5	O	140	GLY
5	O	145	GLY
5	O	192	SER
5	T	47	TRP
5	T	58	THR
5	T	74	ASN
5	T	140	GLY
1	A	86	ASN
2	B	17	ASN
2	E	74	GLU
2	Q	17	ASN
2	Q	74	GLU
4	G	153	ALA
4	G	201	GLU
4	N	185	PRO
5	H	54	SER
5	I	32	TYR
5	I	145	GLY
5	I	178	SER
5	O	178	SER

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Mol	Chain	Res	Type
5	T	139	GLY
2	E	1	ILE
1	P	220	ASP
4	L	4	LEU
4	L	91	TRP
4	L	155	GLY
4	G	176	ALA
4	N	2	SER
4	S	3	GLU
5	H	89	GLU
5	T	57	GLY
1	P	86	ASN
4	S	26	SER
5	H	75	SER
5	H	150	ASP
5	O	2	VAL
5	O	62	ASP
5	O	162	SER
1	A	119	ASP
5	I	144	LEU
5	T	191	PRO
2	Q	35	ILE
5	H	55	GLY

### 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	232/232 (100%)	202 (87%)	30 (13%)	5	16
1	D	232/232 (100%)	207 (89%)	25 (11%)	8	24
1	J	232/232 (100%)	205 (88%)	27 (12%)	7	20
1	P	232/232 (100%)	205 (88%)	27 (12%)	7	20
2	B	95/95 (100%)	83 (87%)	12 (13%)	5	16
2	E	95/95 (100%)	84 (88%)	11 (12%)	7	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	95/95 (100%)	83 (87%)	12 (13%)	5	16
2	Q	95/95 (100%)	82 (86%)	13 (14%)	4	13
3	C	9/9 (100%)	7 (78%)	2 (22%)	1	3
3	F	9/9 (100%)	8 (89%)	1 (11%)	8	22
3	M	9/9 (100%)	8 (89%)	1 (11%)	8	22
3	R	9/9 (100%)	7 (78%)	2 (22%)	1	3
4	G	178/179 (99%)	148 (83%)	30 (17%)	2	8
4	L	178/179 (99%)	159 (89%)	19 (11%)	8	24
4	N	178/179 (99%)	150 (84%)	28 (16%)	3	9
4	S	178/179 (99%)	155 (87%)	23 (13%)	5	16
5	H	178/178 (100%)	152 (85%)	26 (15%)	4	12
5	I	178/178 (100%)	151 (85%)	27 (15%)	3	10
5	O	178/178 (100%)	154 (86%)	24 (14%)	5	13
5	T	178/178 (100%)	148 (83%)	30 (17%)	2	8
All	All	2768/2772 (100%)	2398 (87%)	370 (13%)	5	13

All (370) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	14	ARG
1	A	21	ARG
1	A	35	ARG
1	A	45	MET
1	A	58	GLU
1	A	67	VAL
1	A	71	SER
1	A	74	HIS
1	A	75	ARG
1	A	86	ASN
1	A	95	VAL
1	A	108	ARG
1	A	111	ARG
1	A	121	LYS
1	A	141	GLN
1	A	145	HIS
1	A	146	LYS

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Mol	Chain	Res	Type
1	A	156	LEU
1	A	178	THR
1	A	180	GLN
1	A	181	ARG
1	A	216	THR
1	A	223	ASP
1	A	225	THR
1	A	230	LEU
1	A	242	GLN
1	A	247	VAL
1	A	248	VAL
1	A	253	GLN
2	B	6	LYS
2	B	19	LYS
2	B	25	CYS
2	B	34	ASP
2	B	47	GLU
2	B	57	SER
2	B	70	PHE
2	B	71	THR
2	B	81	ARG
2	B	85	VAL
2	B	97	ARG
2	B	98	ASP
1	D	17	ARG
1	D	21	ARG
1	D	34	VAL
1	D	53	GLU
1	D	58	GLU
1	D	65	ARG
1	D	68	LYS
1	D	86	ASN
1	D	89	GLU
1	D	105	SER
1	D	115	GLN
1	D	121	LYS
1	D	141	GLN
1	D	176	LYS
1	D	181	ARG
1	D	216	THR
1	D	222	GLU
1	D	224	GLN

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Mol	Chain	Res	Type
1	D	225	THR
1	D	228	THR
1	D	230	LEU
1	D	240	THR
1	D	247	VAL
1	D	256	ARG
1	D	268	LYS
2	E	0	MET
2	E	1	ILE
2	E	9	VAL
2	E	23	LEU
2	E	34	ASP
2	E	46	ILE
2	E	55	SER
2	E	57	SER
2	E	70	PHE
2	E	75	LYS
2	E	88	SER
1	J	6	ARG
1	J	11	SER
1	J	25	VAL
1	J	34	VAL
1	J	35	ARG
1	J	67	VAL
1	J	72	GLN
1	J	111	ARG
1	J	115	GLN
1	J	121	LYS
1	J	124	ILE
1	J	128	GLU
1	J	138	MET
1	J	141	GLN
1	J	156	LEU
1	J	157	ARG
1	J	161	GLU
1	J	165	VAL
1	J	178	THR
1	J	187	THR
1	J	191	HIS
1	J	207	SER
1	J	225	THR
1	J	228	THR

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Mol	Chain	Res	Type
1	J	230	LEU
1	J	247	VAL
1	J	272	LEU
2	K	0	MET
2	K	10	TYR
2	K	16	GLU
2	K	69	GLU
2	K	70	PHE
2	K	74	GLU
2	K	81	ARG
2	K	85	VAL
2	K	88	SER
2	K	90	PRO
2	K	92	ILE
2	K	94	LYS
1	P	6	ARG
1	P	34	VAL
1	P	35	ARG
1	P	45	MET
1	P	67	VAL
1	P	86	ASN
1	P	108	ARG
1	P	111	ARG
1	P	115	GLN
1	P	121	LYS
1	P	124	ILE
1	P	131	ARG
1	P	138	MET
1	P	154	GLU
1	P	178	THR
1	P	196	ASP
1	P	200	THR
1	P	218	GLN
1	P	222	GLU
1	P	226	GLN
1	P	228	THR
1	P	232	GLU
1	P	240	THR
1	P	247	VAL
1	P	251	SER
1	P	253	GLN
1	P	256	ARG

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Mol	Chain	Res	Type
2	Q	6	LYS
2	Q	34	ASP
2	Q	38	ASP
2	Q	48	LYS
2	Q	57	SER
2	Q	67	TYR
2	Q	70	PHE
2	Q	75	LYS
2	Q	81	ARG
2	Q	85	VAL
2	Q	94	LYS
2	Q	97	ARG
2	Q	99	MET
3	C	6	ILE
3	C	8	GLN
3	F	6	ILE
3	M	6	ILE
3	R	3	LEU
3	R	6	ILE
4	L	8	ARG
4	L	10	VAL
4	L	23	THR
4	L	36	SER
4	L	44	LYS
4	L	63	ARG
4	L	65	SER
4	L	120	LEU
4	L	147	VAL
4	L	158	VAL
4	L	166	LYS
4	L	182	SER
4	L	184	THR
4	L	186	GLU
4	L	190	SER
4	L	196	CYS
4	L	197	GLN
4	L	203	ASN
4	L	206	GLU
4	G	1	GLN
4	G	19	THR
4	G	23	THR
4	G	25	THR

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Mol	Chain	Res	Type
4	G	28	ASP
4	G	53	VAL
4	G	63	ARG
4	G	69	SER
4	G	74	SER
4	G	78	SER
4	G	81	GLN
4	G	83	GLU
4	G	99	VAL
4	G	117	THR
4	G	124	SER
4	G	135	LEU
4	G	140	SER
4	G	151	TRP
4	G	152	LYS
4	G	156	SER
4	G	166	LYS
4	G	170	GLN
4	G	173	ASN
4	G	186	GLU
4	G	189	LYS
4	G	203	ASN
4	G	204	THR
4	G	205	VAL
4	G	206	GLU
4	G	208	THR
4	N	2	SER
4	N	3	GLU
4	N	5	THR
4	N	11	SER
4	N	20	ILE
4	N	23	THR
4	N	28	ASP
4	N	44	LYS
4	N	52	ASP
4	N	58	SER
4	N	69	SER
4	N	71	ASN
4	N	74	SER
4	N	78	SER
4	N	107	THR
4	N	117	THR

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Mol	Chain	Res	Type
4	N	125	SER
4	N	127	GLU
4	N	129	GLN
4	N	147	VAL
4	N	151	TRP
4	N	156	SER
4	N	158	VAL
4	N	166	LYS
4	N	168	SER
4	N	178	SER
4	N	190	SER
4	N	195	SER
4	S	4	LEU
4	S	8	ARG
4	S	9	SER
4	S	22	CYS
4	S	23	THR
4	S	28	ASP
4	S	48	LEU
4	S	58	SER
4	S	63	ARG
4	S	74	SER
4	S	91	TRP
4	S	117	THR
4	S	131	ASN
4	S	147	VAL
4	S	156	SER
4	S	158	VAL
4	S	171	SER
4	S	178	SER
4	S	183	LEU
4	S	189	LYS
4	S	192	ARG
4	S	195	SER
4	S	203	ASN
5	H	21	SER
5	H	25	SER
5	H	28	THR
5	H	50	SER
5	H	54	SER
5	H	62	ASP
5	H	63	SER

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Mol	Chain	Res	Type
5	H	65	LYS
5	H	71	SER
5	H	89	GLU
5	H	91	THR
5	H	122	THR
5	H	123	LYS
5	H	136	SER
5	H	138	SER
5	H	141	THR
5	H	165	LEU
5	H	177	GLN
5	H	185	SER
5	H	187	VAL
5	H	189	THR
5	H	192	SER
5	H	195	LEU
5	H	199	THR
5	H	205	ASN
5	H	220	LYS
5	I	3	GLN
5	I	5	LEU
5	I	18	LEU
5	I	20	LEU
5	I	28	THR
5	I	30	SER
5	I	50	SER
5	I	76	LYS
5	I	87	ARG
5	I	100	LEU
5	I	114	THR
5	I	123	LYS
5	I	134	SER
5	I	138	SER
5	I	144	LEU
5	I	157	THR
5	I	165	LEU
5	I	184	LEU
5	I	186	SER
5	I	189	THR
5	I	192	SER
5	I	193	SER
5	I	195	LEU

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Mol	Chain	Res	Type
5	I	199	THR
5	I	202	CYS
5	I	215	LYS
5	I	220	LYS
5	O	2	VAL
5	O	3	GLN
5	O	5	LEU
5	O	18	LEU
5	O	49	SER
5	O	58	THR
5	O	78	THR
5	O	111	GLN
5	O	118	SER
5	O	121	SER
5	O	123	LYS
5	O	134	SER
5	O	136	SER
5	O	144	LEU
5	O	146	CYS
5	O	165	LEU
5	O	184	LEU
5	O	187	VAL
5	O	201	ILE
5	O	202	CYS
5	O	203	ASN
5	O	212	LYS
5	O	217	VAL
5	O	218	GLU
5	T	1	GLU
5	T	7	SER
5	T	12	VAL
5	T	43	LYS
5	T	68	PHE
5	T	69	THR
5	T	78	THR
5	T	91	THR
5	T	111	GLN
5	T	116	THR
5	T	118	SER
5	T	121	SER
5	T	134	SER
5	T	135	LYS

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Mol	Chain	Res	Type
5	T	138	SER
5	T	141	THR
5	T	156	VAL
5	T	165	LEU
5	T	167	SER
5	T	178	SER
5	T	189	THR
5	T	195	LEU
5	T	202	CYS
5	T	203	ASN
5	T	207	LYS
5	T	210	ASN
5	T	211	THR
5	T	216	LYS
5	T	218	GLU
5	T	220	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	72	GLN
1	A	74	HIS
1	A	141	GLN
1	A	174	ASN
1	A	224	GLN
1	A	242	GLN
1	A	253	GLN
2	B	2	GLN
2	B	31	HIS
2	B	83	ASN
1	D	74	HIS
1	D	141	GLN
1	D	174	ASN
1	D	191	HIS
1	D	224	GLN
1	D	226	GLN
1	D	242	GLN
1	D	253	GLN
2	E	2	GLN
2	E	31	HIS
2	E	83	ASN

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Mol	Chain	Res	Type
2	E	89	GLN
1	J	3	HIS
1	J	43	GLN
1	J	115	GLN
1	J	141	GLN
1	J	155	GLN
1	J	174	ASN
1	J	191	HIS
1	J	224	GLN
1	J	242	GLN
1	J	253	GLN
2	K	31	HIS
2	K	51	HIS
2	K	83	ASN
1	P	3	HIS
1	P	54	GLN
1	P	72	GLN
1	P	115	GLN
1	P	151	HIS
1	P	174	ASN
1	P	180	GLN
1	P	191	HIS
1	P	226	GLN
1	P	242	GLN
1	P	253	GLN
1	P	262	GLN
2	Q	2	GLN
2	Q	31	HIS
2	Q	51	HIS
2	Q	89	GLN
3	C	8	GLN
3	F	8	GLN
3	R	8	GLN
4	L	1	GLN
4	L	71	ASN
4	L	111	GLN
4	L	129	GLN
4	L	173	ASN
4	G	71	ASN
4	G	111	GLN
4	G	115	ASN
4	G	131	ASN

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Mol	Chain	Res	Type
4	G	173	ASN
4	G	187	GLN
4	N	81	GLN
4	N	129	GLN
4	N	131	ASN
4	N	173	ASN
4	N	200	HIS
4	N	203	ASN
4	S	71	ASN
4	S	111	GLN
4	S	170	GLN
4	S	172	ASN
4	S	191	HIS
5	H	13	GLN
5	H	77	ASN
5	H	205	ASN
5	I	74	ASN
5	I	77	ASN
5	I	198	GLN
5	O	3	GLN
5	O	77	ASN
5	O	210	ASN
5	T	77	ASN
5	T	111	GLN
5	T	177	GLN
5	T	198	GLN
5	T	210	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 5.6 Ligand geometry

There are no ligands in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	276/276 (100%)	0.13	5 (1%) 71 68	2, 2, 2, 2	0
1	D	276/276 (100%)	0.14	3 (1%) 82 80	2, 2, 2, 2	0
1	J	276/276 (100%)	0.22	6 (2%) 65 60	2, 2, 2, 2	0
1	P	276/276 (100%)	0.08	7 (2%) 61 55	2, 2, 2, 2	0
2	B	100/100 (100%)	0.21	1 (1%) 84 82	2, 2, 2, 2	0
2	E	100/100 (100%)	0.19	1 (1%) 84 82	2, 2, 2, 2	0
2	K	100/100 (100%)	0.08	2 (2%) 68 64	2, 2, 2, 2	0
2	Q	100/100 (100%)	0.00	3 (3%) 54 47	2, 2, 2, 2	0
3	C	9/9 (100%)	2.08	3 (33%) 0 0	2, 2, 2, 2	0
3	F	9/9 (100%)	1.66	3 (33%) 0 0	2, 2, 2, 2	0
3	M	9/9 (100%)	1.04	0 100 100	2, 2, 2, 2	0
3	R	9/9 (100%)	-0.55	0 100 100	2, 2, 2, 2	0
4	G	211/212 (99%)	0.16	0 100 100	2, 2, 2, 2	0
4	L	211/212 (99%)	0.02	0 100 100	2, 2, 2, 2	0
4	N	211/212 (99%)	0.34	8 (3%) 44 37	2, 2, 2, 2	0
4	S	211/212 (99%)	-0.18	3 (1%) 78 76	2, 2, 2, 2	0
5	H	220/220 (100%)	0.12	4 (1%) 71 68	2, 2, 2, 2	0
5	I	220/220 (100%)	0.24	6 (2%) 58 52	2, 2, 2, 2	0
5	O	220/220 (100%)	0.38	10 (4%) 37 31	2, 2, 2, 2	0
5	T	220/220 (100%)	-0.10	11 (5%) 32 26	2, 2, 2, 2	0
All	All	3264/3268 (99%)	0.14	76 (2%) 64 59	2, 2, 2, 2	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	I	136	SER	6.0
5	O	136	SER	4.3
5	O	137	THR	3.9
5	O	165	LEU	3.9
4	N	194	TYR	3.7
1	P	197	HIS	3.7
5	T	136	SER	3.6
4	N	153	ALA	3.6
5	I	138	SER	3.5
5	O	1	GLU	3.4
5	T	210	ASN	3.3
5	O	138	SER	3.3
2	K	98	ASP	3.3
5	H	136	SER	3.2
5	T	135	LYS	3.2
5	I	139	GLY	3.2
1	J	145	HIS	3.2
5	O	134	SER	3.1
4	N	160	ALA	3.1
1	P	194	VAL	3.0
1	A	196	ASP	3.0
4	S	203	ASN	3.0
3	C	7	THR	3.0
5	I	135	LYS	3.0
3	C	9	VAL	2.8
5	T	138	SER	2.8
4	N	186	GLU	2.8
5	O	139	GLY	2.8
1	D	194	VAL	2.7
1	P	196	ASP	2.7
5	H	138	SER	2.6
5	O	197	THR	2.6
4	N	159	LYS	2.6
3	C	1	SER	2.6
2	Q	19	LYS	2.6
3	F	1	SER	2.6
1	J	276	PRO	2.6
5	T	66	GLY	2.5
5	T	137	THR	2.5
5	H	137	THR	2.5
4	N	158	VAL	2.5
2	Q	71	THR	2.5
5	T	134	SER	2.4

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Mol	Chain	Res	Type	RSRZ
5	T	211	THR	2.4
1	P	16	GLY	2.4
2	Q	98	ASP	2.4
1	A	89	GLU	2.4
3	F	4	MET	2.4
1	A	16	GLY	2.3
5	I	167	SER	2.3
5	T	133	SER	2.3
5	T	1	GLU	2.2
4	N	178	SER	2.2
1	A	194	VAL	2.2
5	O	191	PRO	2.2
2	B	69	GLU	2.2
1	J	194	VAL	2.2
4	S	202	GLY	2.2
1	A	18	GLY	2.2
1	P	149	ALA	2.2
5	I	1	GLU	2.2
2	K	0	MET	2.2
3	F	3	LEU	2.2
1	J	16	GLY	2.1
1	P	19	GLU	2.1
4	N	134	THR	2.1
5	H	139	GLY	2.1
5	O	162	SER	2.1
1	D	90	ALA	2.1
2	E	0	MET	2.1
1	P	220	ASP	2.1
1	D	89	GLU	2.1
4	S	190	SER	2.1
1	J	89	GLU	2.0
5	T	166	THR	2.0
1	J	108	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.