



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:48 AM GMT

PDB ID : 3PVO
Title : Monoclinic form of Human C-Reactive Protein
Authors : Guillon, C.; Mavoungou Bigouagou, U.; Jeannin, P.; Delneste, Y.; Gouet, P.
Deposited on : 2010-12-07
Resolution : 3.00 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

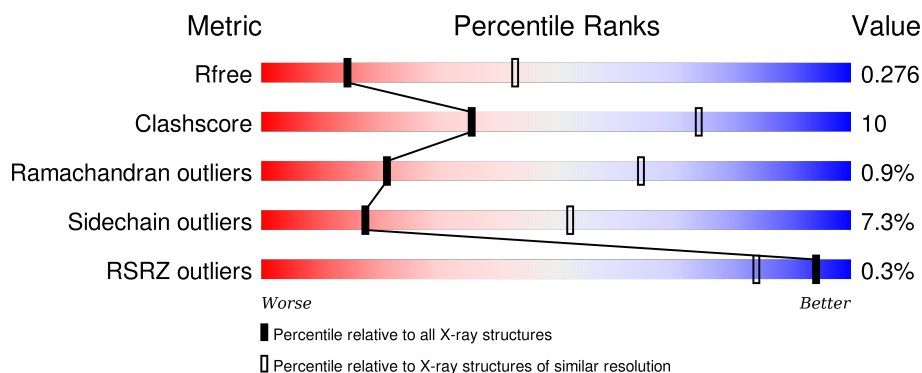
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	206	<div> <div>76%</div> <div>19%</div> <div>5%</div> </div>
1	B	206	<div> <div>67%</div> <div>27%</div> <div>• •</div> </div>
1	C	206	<div> <div>76%</div> <div>20%</div> <div>•</div> </div>
1	D	206	<div> <div>77%</div> <div>20%</div> <div>•</div> </div>
1	E	206	<div> <div>73%</div> <div>25%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	206	 76% 23% .
1	G	206	 73% 24% .
1	H	206	 74% 19% 7%
1	I	206	 80% 18% .
1	J	206	 74% 22% .
1	K	206	 69% 24% 6%
1	L	206	 68% 26% 5% .
1	M	206	 71% 22% 5% .
1	N	206	 70% 27% .
1	O	206	 78% 18% .
1	P	206	 % 74% 21% . .
1	Q	206	 69% 25% 5%
1	R	206	 % 73% 20% 7%
1	S	206	 76% 21% .
1	T	206	 % 78% 18% .

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
2	CA	A	5002	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33077 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 C-Reactive Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	B	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	C	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	D	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	E	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	F	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	G	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	H	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	I	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	J	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	K	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	L	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	M	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	N	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	O	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	P	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	206	Total 1632	C 1058	N 261	O 309	S 4	0	0	0
1	R	206	Total 1632	C 1058	N 261	O 309	S 4	0	0	0
1	S	206	Total 1632	C 1058	N 261	O 309	S 4	0	0	0
1	T	206	Total 1632	C 1058	N 261	O 309	S 4	0	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	2	Total 2	Ca 2	0	0
2	G	2	Total 2	Ca 2	0	0
2	J	2	Total 2	Ca 2	0	0
2	Q	2	Total 2	Ca 2	0	0
2	D	2	Total 2	Ca 2	0	0
2	K	2	Total 2	Ca 2	0	0
2	E	2	Total 2	Ca 2	0	0
2	H	2	Total 2	Ca 2	0	0
2	B	2	Total 2	Ca 2	0	0
2	I	2	Total 2	Ca 2	0	0
2	C	2	Total 2	Ca 2	0	0
2	A	2	Total 2	Ca 2	0	0
2	T	2	Total 2	Ca 2	0	0
2	N	2	Total 2	Ca 2	0	0
2	O	2	Total 2	Ca 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	R	2	Total 2	Ca 2	0	0
2	L	2	Total 2	Ca 2	0	0
2	S	2	Total 2	Ca 2	0	0
2	F	2	Total 2	Ca 2	0	0
2	M	2	Total 2	Ca 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total 12	O 12	0	0
3	B	20	Total 20	O 20	0	0
3	C	20	Total 20	O 20	0	0
3	D	14	Total 14	O 14	0	0
3	E	10	Total 10	O 10	0	0
3	F	20	Total 20	O 20	0	0
3	G	15	Total 15	O 15	0	0
3	H	16	Total 16	O 16	0	0
3	I	14	Total 14	O 14	0	0
3	J	30	Total 30	O 30	0	0
3	K	24	Total 24	O 24	0	0
3	L	24	Total 24	O 24	0	0
3	M	19	Total 19	O 19	0	0
3	N	19	Total 19	O 19	0	0

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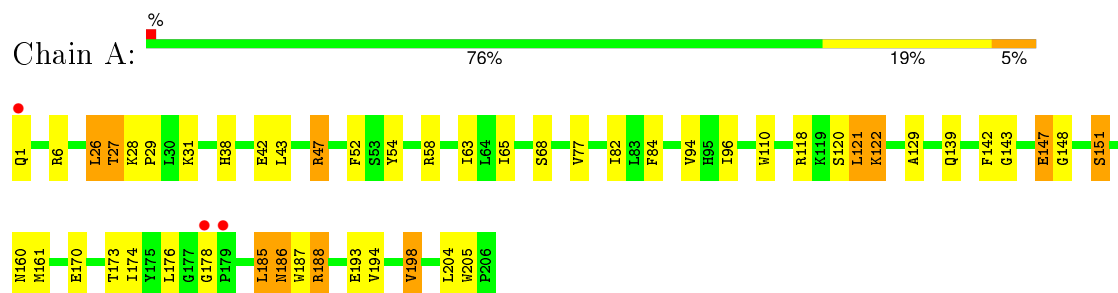
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	25	Total 25	O 25	0	0
3	P	19	Total 19	O 19	0	0
3	Q	28	Total 28	O 28	0	0
3	R	30	Total 30	O 30	0	0
3	S	21	Total 21	O 21	0	0
3	T	17	Total 17	O 17	0	0

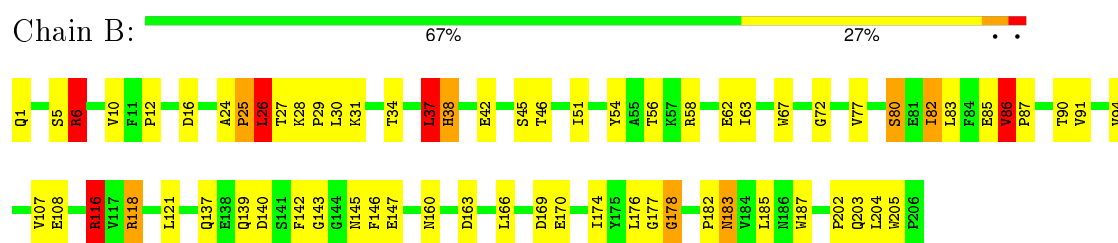
3 Residue-property plots [i](#)

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.

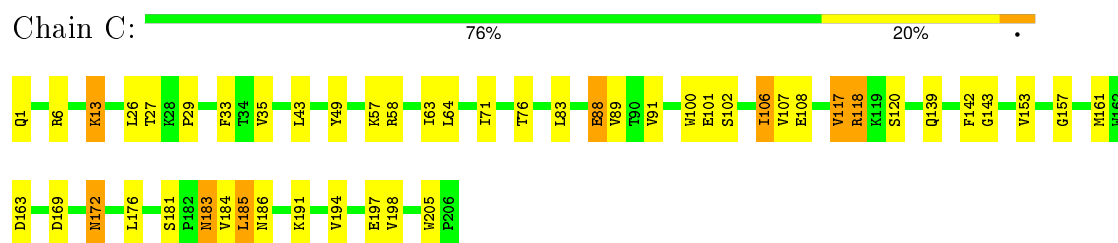
• Molecule 1: C-Reactive Protein



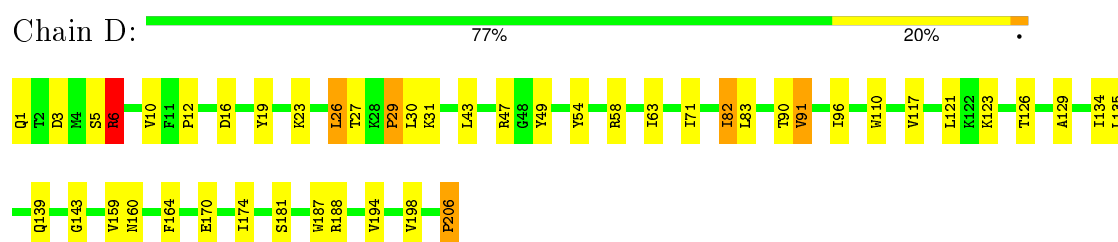
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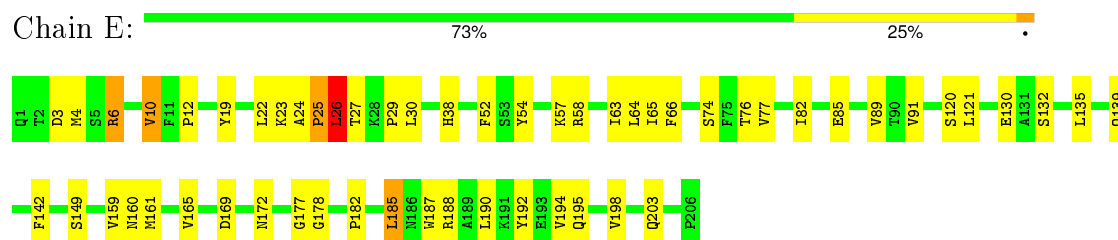
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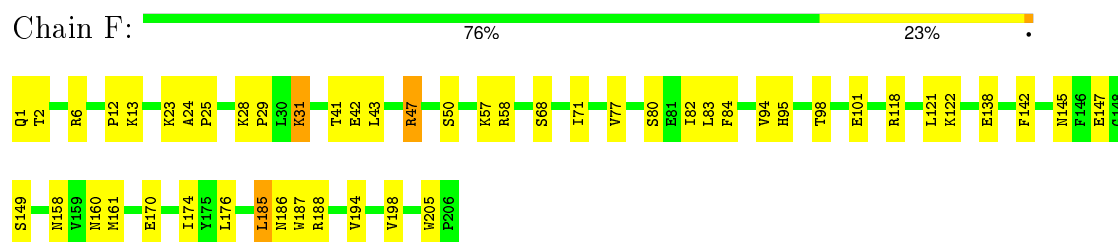
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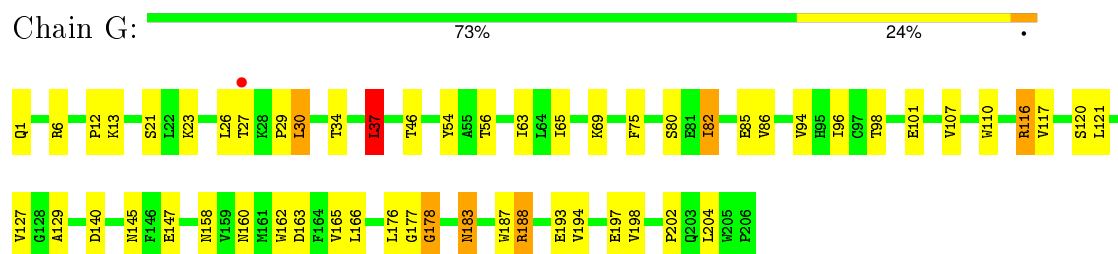
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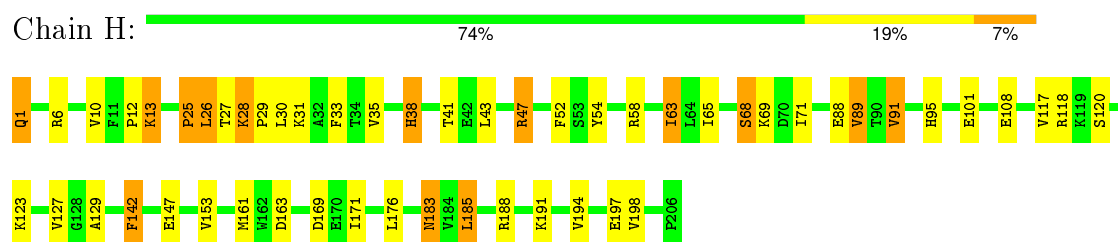
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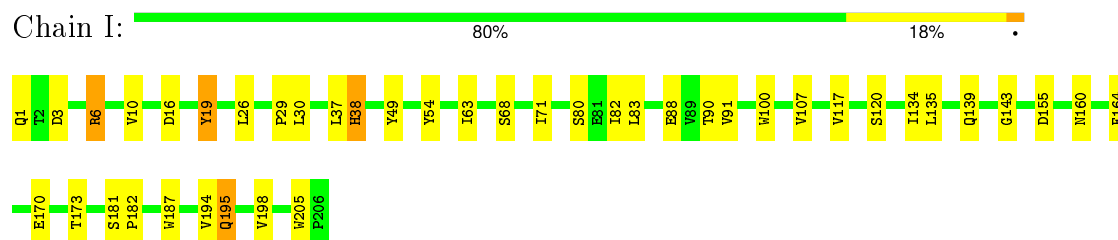
- Molecule 1: C-Reactive Protein



- Molecule 1: C-Reactive Protein

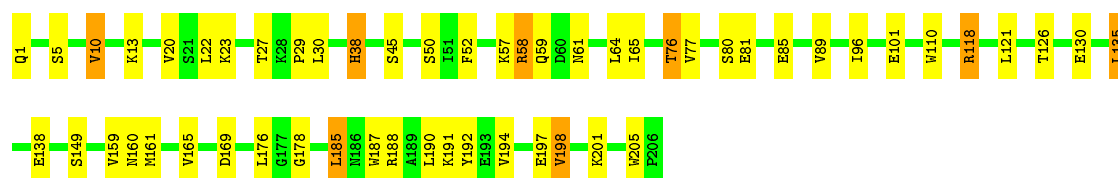


- Molecule 1: C-Reactive Protein



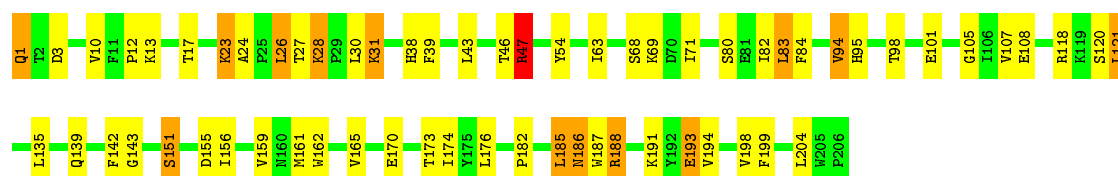
- Molecule 1: C-Reactive Protein

Chain J:  74% 22% .



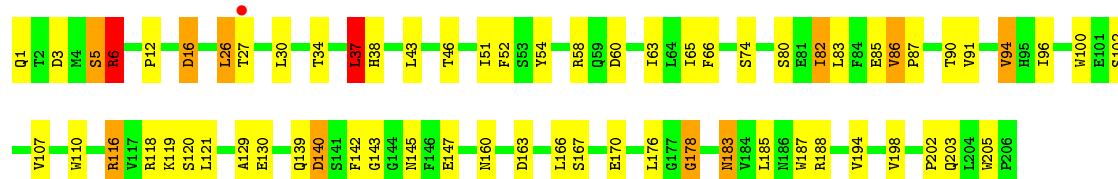
• Molecule 1: C-Reactive Protein

Chain K:  69% 24% 6%



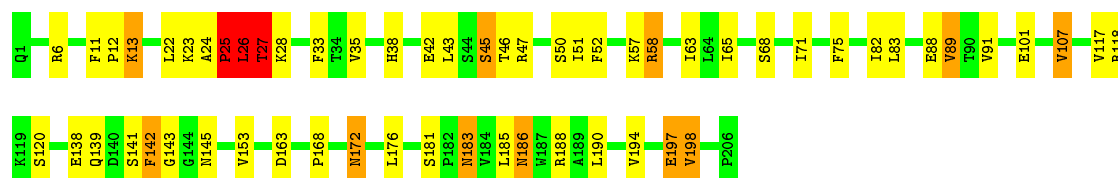
• Molecule 1: C-Reactive Protein

Chain L:  68% 26% 5% .



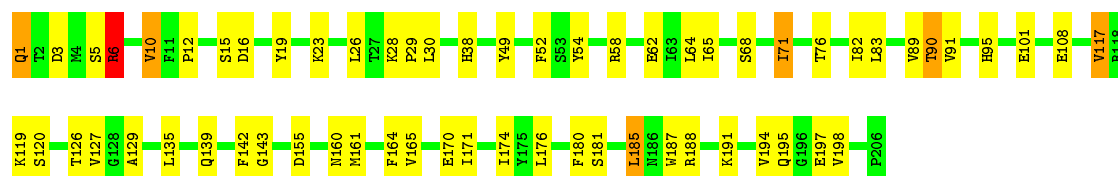
• Molecule 1: C-Reactive Protein

Chain M:  71% 22% 5% .




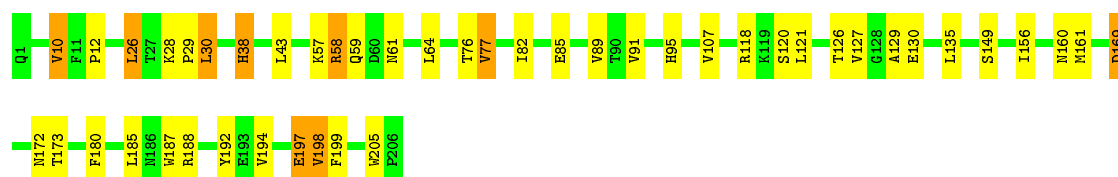
• Molecule 1: C-Reactive Protein

Chain N:  70% 27%

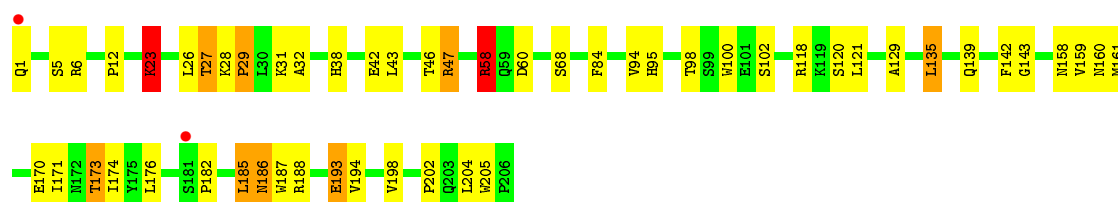
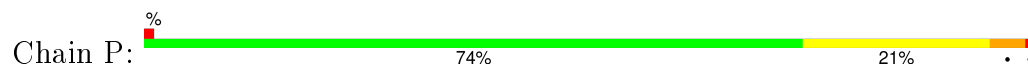


• Molecule 1: C-Reactive Protein

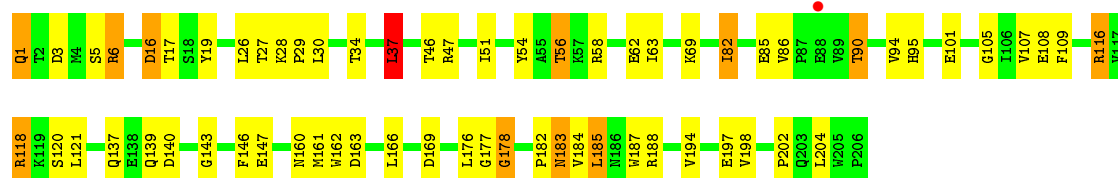
Chain O:  78% 18%



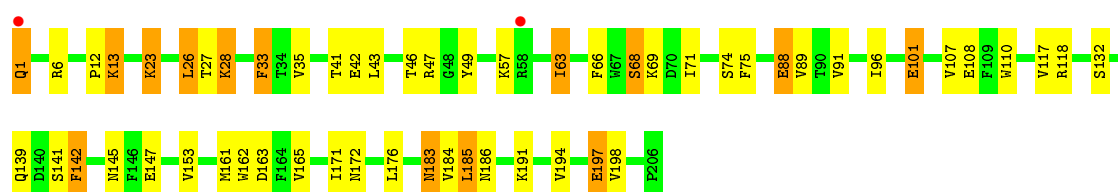
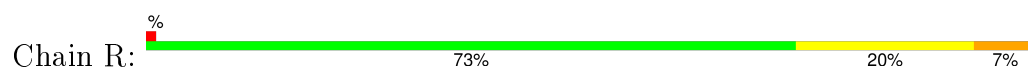
• Molecule 1: C-Reactive Protein



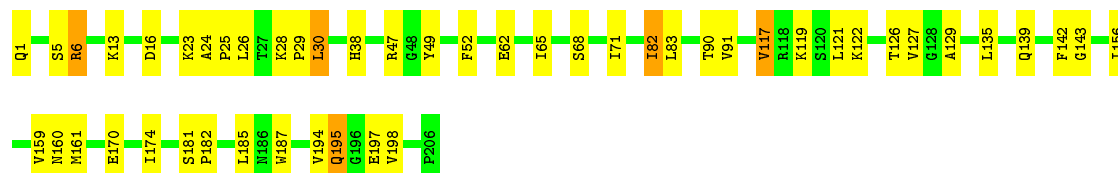
• Molecule 1: C-Reactive Protein



• Molecule 1: C-Reactive Protein

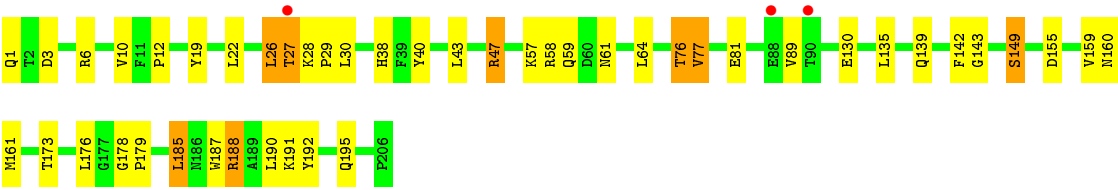


• Molecule 1: C-Reactive Protein



• Molecule 1: C-Reactive Protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.60 Å 143.20 Å 161.20 Å 90.00° 89.70° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.8 (20.00-3.00) 97.8 (20.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.98 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.227 , 0.285 0.222 , 0.276	Depositor DCC
R_{free} test set	4380 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 11.9	EDS
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 86415 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	33077	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.37% 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: CA

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	0.99	8/1678 (0.5%)	0.91	7/2279 (0.3%)
1	B	1.03	7/1678 (0.4%)	1.06	14/2279 (0.6%)
1	C	1.13	22/1678 (1.3%)	0.96	7/2279 (0.3%)
1	D	1.07	13/1678 (0.8%)	0.95	9/2279 (0.4%)
1	E	0.95	9/1678 (0.5%)	0.88	5/2279 (0.2%)
1	F	0.94	6/1678 (0.4%)	0.91	7/2279 (0.3%)
1	G	0.99	3/1678 (0.2%)	1.00	9/2279 (0.4%)
1	H	1.10	13/1678 (0.8%)	0.97	8/2279 (0.4%)
1	I	1.06	17/1678 (1.0%)	0.94	10/2279 (0.4%)
1	J	0.99	9/1678 (0.5%)	0.87	6/2279 (0.3%)
1	K	0.95	8/1678 (0.5%)	0.90	4/2279 (0.2%)
1	L	1.02	8/1678 (0.5%)	1.07	15/2279 (0.7%)
1	M	1.13	18/1678 (1.1%)	0.98	10/2279 (0.4%)
1	N	1.07	14/1678 (0.8%)	0.92	6/2279 (0.3%)
1	O	0.97	7/1678 (0.4%)	0.86	3/2279 (0.1%)
1	P	0.94	6/1678 (0.4%)	0.87	5/2279 (0.2%)
1	Q	1.04	8/1678 (0.5%)	1.05	16/2279 (0.7%)
1	R	1.13	20/1678 (1.2%)	0.96	8/2279 (0.4%)
1	S	0.99	7/1678 (0.4%)	0.95	10/2279 (0.4%)
1	T	0.96	7/1678 (0.4%)	0.86	3/2279 (0.1%)
All	All	1.02	210/33560 (0.6%)	0.95	162/45580 (0.4%)

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	H	0	1
1	M	0	1
1	R	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	3

All (210) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	23	LYS	C-N	10.72	1.58	1.34
1	M	35	VAL	CB-CG2	-8.90	1.34	1.52
1	R	198	VAL	CB-CG2	-8.09	1.35	1.52
1	M	35	VAL	CB-CG1	-7.71	1.36	1.52
1	N	117	VAL	CB-CG1	-7.68	1.36	1.52
1	D	117	VAL	CB-CG2	-7.54	1.37	1.52
1	R	35	VAL	CB-CG1	-7.49	1.37	1.52
1	H	35	VAL	CB-CG2	-7.41	1.37	1.52
1	O	85	GLU	CD-OE1	-7.40	1.17	1.25
1	J	85	GLU	CD-OE1	-7.39	1.17	1.25
1	A	29	PRO	C-N	7.36	1.50	1.34
1	T	29	PRO	C-N	7.31	1.50	1.34
1	H	198	VAL	CB-CG2	-7.26	1.37	1.52
1	O	192	TYR	CE1-CZ	-7.25	1.29	1.38
1	H	35	VAL	CB-CG1	-7.24	1.37	1.52
1	C	35	VAL	CB-CG2	-7.19	1.37	1.52
1	O	192	TYR	CE2-CZ	-7.19	1.29	1.38
1	I	117	VAL	CB-CG1	-7.18	1.37	1.52
1	R	35	VAL	CB-CG2	-7.18	1.37	1.52
1	H	117	VAL	CB-CG2	-7.12	1.38	1.52
1	E	29	PRO	C-N	6.99	1.50	1.34
1	J	23	LYS	C-N	6.85	1.49	1.34
1	S	6	ARG	CG-CD	-6.84	1.34	1.51
1	M	198	VAL	CB-CG1	-6.83	1.38	1.52
1	C	89	VAL	CB-CG1	-6.78	1.38	1.52
1	I	117	VAL	CB-CG2	-6.73	1.38	1.52
1	A	84	PHE	CE2-CZ	-6.70	1.24	1.37
1	C	198	VAL	CB-CG1	-6.66	1.38	1.52
1	D	206	PRO	C-OXT	6.62	1.35	1.23
1	S	117	VAL	CB-CG2	-6.61	1.39	1.52
1	K	84	PHE	CE2-CZ	-6.57	1.24	1.37
1	N	117	VAL	CB-CG2	-6.57	1.39	1.52
1	T	192	TYR	CE2-CZ	-6.56	1.30	1.38
1	M	198	VAL	CB-CG2	-6.55	1.39	1.52
1	C	35	VAL	CB-CG1	-6.55	1.39	1.52
1	I	49	TYR	CE1-CZ	-6.54	1.30	1.38
1	M	89	VAL	CB-CG1	-6.51	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	192	TYR	CE1-CZ	-6.48	1.30	1.38
1	B	116	ARG	CZ-NH1	-6.47	1.24	1.33
1	R	88	GLU	CB-CG	-6.44	1.40	1.52
1	D	170	GLU	CD-OE2	-6.43	1.18	1.25
1	A	84	PHE	CE1-CZ	-6.36	1.25	1.37
1	N	10	VAL	CB-CG2	-6.34	1.39	1.52
1	O	192	TYR	CG-CD1	-6.33	1.30	1.39
1	J	77	VAL	CB-CG2	-6.33	1.39	1.52
1	Q	94	VAL	CB-CG2	-6.30	1.39	1.52
1	M	117	VAL	CB-CG2	-6.27	1.39	1.52
1	J	10	VAL	CB-CG2	-6.26	1.39	1.52
1	R	101	GLU	CD-OE2	-6.26	1.18	1.25
1	R	117	VAL	CB-CG2	-6.26	1.39	1.52
1	D	170	GLU	CD-OE1	-6.22	1.18	1.25
1	L	94	VAL	CB-CG1	-6.22	1.39	1.52
1	T	192	TYR	CE1-CZ	-6.22	1.30	1.38
1	M	33	PHE	CE2-CZ	-6.20	1.25	1.37
1	C	117	VAL	CB-CG1	-6.16	1.40	1.52
1	H	117	VAL	CB-CG1	-6.15	1.40	1.52
1	G	116	ARG	CZ-NH1	-6.13	1.25	1.33
1	A	84	PHE	CG-CD2	-6.11	1.29	1.38
1	J	192	TYR	CG-CD2	-6.10	1.31	1.39
1	L	94	VAL	CB-CG2	-6.08	1.40	1.52
1	I	164	PHE	CE1-CZ	-6.08	1.25	1.37
1	M	33	PHE	CE1-CZ	-6.06	1.25	1.37
1	A	94	VAL	CB-CG1	-6.04	1.40	1.52
1	K	84	PHE	CE1-CZ	-6.03	1.25	1.37
1	B	6	ARG	NE-CZ	-6.01	1.25	1.33
1	K	94	VAL	CB-CG1	-6.00	1.40	1.52
1	P	94	VAL	CB-CG1	-5.99	1.40	1.52
1	R	198	VAL	CB-CG1	-5.97	1.40	1.52
1	I	195	GLN	CG-CD	-5.96	1.37	1.51
1	S	117	VAL	CB-CG1	-5.95	1.40	1.52
1	I	164	PHE	CG-CD2	-5.95	1.29	1.38
1	E	192	TYR	CE2-CZ	-5.94	1.30	1.38
1	J	192	TYR	CE2-CZ	-5.92	1.30	1.38
1	R	49	TYR	CE1-CZ	-5.91	1.30	1.38
1	R	33	PHE	CE1-CZ	-5.91	1.26	1.37
1	C	91	VAL	CB-CG2	-5.91	1.40	1.52
1	A	84	PHE	CG-CD1	-5.90	1.29	1.38
1	C	142	PHE	CE2-CZ	-5.88	1.26	1.37
1	P	84	PHE	CG-CD2	-5.87	1.29	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	117	VAL	CB-CG2	-5.87	1.40	1.52
1	I	164	PHE	CE2-CZ	-5.84	1.26	1.37
1	B	86	VAL	CB-CG2	-5.84	1.40	1.52
1	R	33	PHE	CE2-CZ	-5.83	1.26	1.37
1	S	49	TYR	CE2-CZ	-5.83	1.30	1.38
1	F	84	PHE	CE1-CZ	-5.82	1.26	1.37
1	F	94	VAL	CB-CG2	-5.82	1.40	1.52
1	I	49	TYR	CG-CD1	-5.82	1.31	1.39
1	O	10	VAL	CB-CG2	-5.80	1.40	1.52
1	Q	94	VAL	CB-CG1	-5.80	1.40	1.52
1	C	33	PHE	CE2-CZ	-5.78	1.26	1.37
1	Q	107	VAL	CB-CG1	-5.77	1.40	1.52
1	D	164	PHE	CE2-CZ	-5.76	1.26	1.37
1	P	84	PHE	CE1-CZ	-5.76	1.26	1.37
1	K	84	PHE	CG-CD1	-5.76	1.30	1.38
1	L	6	ARG	NE-CZ	-5.75	1.25	1.33
1	G	94	VAL	CB-CG2	-5.75	1.40	1.52
1	Q	107	VAL	CB-CG2	-5.75	1.40	1.52
1	T	89	VAL	CB-CG1	-5.73	1.40	1.52
1	O	192	TYR	CG-CD2	-5.72	1.31	1.39
1	D	164	PHE	CE1-CZ	-5.72	1.26	1.37
1	D	10	VAL	CB-CG2	-5.71	1.40	1.52
1	F	84	PHE	CE2-CZ	-5.71	1.26	1.37
1	J	10	VAL	CB-CG1	-5.69	1.40	1.52
1	C	198	VAL	CB-CG2	-5.69	1.41	1.52
1	M	142	PHE	CE1-CZ	-5.67	1.26	1.37
1	R	142	PHE	CE1-CZ	-5.66	1.26	1.37
1	H	198	VAL	CB-CG1	-5.65	1.41	1.52
1	C	33	PHE	CE1-CZ	-5.64	1.26	1.37
1	D	117	VAL	CB-CG1	-5.64	1.41	1.52
1	Q	116	ARG	CZ-NH1	-5.62	1.25	1.33
1	K	84	PHE	CG-CD2	-5.59	1.30	1.38
1	E	10	VAL	CB-CG2	-5.57	1.41	1.52
1	B	94	VAL	CB-CG2	-5.56	1.41	1.52
1	S	23	LYS	C-N	5.55	1.46	1.34
1	C	142	PHE	CG-CD1	-5.54	1.30	1.38
1	M	107	VAL	CB-CG1	-5.54	1.41	1.52
1	M	33	PHE	CG-CD2	-5.54	1.30	1.38
1	C	142	PHE	CE1-CZ	-5.54	1.26	1.37
1	M	88	GLU	CB-CG	-5.53	1.41	1.52
1	I	164	PHE	CG-CD1	-5.53	1.30	1.38
1	R	49	TYR	CG-CD1	-5.52	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	33	PHE	CG-CD1	-5.52	1.30	1.38
1	M	101	GLU	CD-OE1	-5.52	1.19	1.25
1	G	94	VAL	CB-CG1	-5.52	1.41	1.52
1	N	49	TYR	CE1-CZ	-5.52	1.31	1.38
1	I	10	VAL	CB-CG2	-5.51	1.41	1.52
1	C	118	ARG	CZ-NH1	-5.51	1.25	1.33
1	N	164	PHE	CG-CD2	-5.51	1.30	1.38
1	H	89	VAL	CB-CG2	-5.51	1.41	1.52
1	R	49	TYR	CE2-CZ	-5.51	1.31	1.38
1	C	33	PHE	CG-CD2	-5.48	1.30	1.38
1	P	84	PHE	CE2-CZ	-5.45	1.26	1.37
1	Q	19	TYR	CE2-CZ	-5.45	1.31	1.38
1	Q	19	TYR	CE1-CZ	-5.45	1.31	1.38
1	N	164	PHE	CE1-CZ	-5.44	1.27	1.37
1	C	101	GLU	CD-OE1	-5.43	1.19	1.25
1	L	107	VAL	CB-CG1	-5.43	1.41	1.52
1	D	49	TYR	CE2-CZ	-5.42	1.31	1.38
1	E	89	VAL	CB-CG1	-5.42	1.41	1.52
1	J	89	VAL	CB-CG1	-5.42	1.41	1.52
1	D	91	VAL	CB-CG2	-5.41	1.41	1.52
1	A	94	VAL	CB-CG2	-5.41	1.41	1.52
1	C	49	TYR	CE2-CZ	-5.41	1.31	1.38
1	C	49	TYR	CE1-CZ	-5.39	1.31	1.38
1	T	192	TYR	CG-CD1	-5.39	1.32	1.39
1	N	6	ARG	CG-CD	-5.38	1.38	1.51
1	I	10	VAL	CB-CG1	-5.38	1.41	1.52
1	F	84	PHE	CG-CD2	-5.37	1.30	1.38
1	R	142	PHE	CG-CD2	-5.37	1.30	1.38
1	A	193	GLU	CD-OE2	-5.37	1.19	1.25
1	R	33	PHE	CG-CD1	-5.37	1.30	1.38
1	L	86	VAL	CB-CG2	-5.36	1.41	1.52
1	M	24	ALA	CA-CB	-5.36	1.41	1.52
1	N	19	TYR	CE1-CZ	-5.36	1.31	1.38
1	M	101	GLU	CD-OE2	-5.35	1.19	1.25
1	T	10	VAL	CB-CG2	-5.35	1.41	1.52
1	L	116	ARG	CZ-NH1	-5.34	1.26	1.33
1	R	101	GLU	CD-OE1	-5.34	1.19	1.25
1	S	170	GLU	CD-OE1	-5.33	1.19	1.25
1	T	77	VAL	CB-CG2	-5.33	1.41	1.52
1	P	29	PRO	C-N	-5.33	1.21	1.34
1	N	170	GLU	CD-OE2	-5.32	1.19	1.25
1	H	33	PHE	CE1-CZ	-5.32	1.27	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	117	VAL	CB-CG1	-5.32	1.41	1.52
1	C	101	GLU	CD-OE2	-5.30	1.19	1.25
1	R	33	PHE	CG-CD2	-5.30	1.30	1.38
1	L	6	ARG	CZ-NH2	-5.30	1.26	1.33
1	I	195	GLN	CB-CG	-5.30	1.38	1.52
1	E	85	GLU	CD-OE1	-5.30	1.19	1.25
1	K	94	VAL	CB-CG2	-5.28	1.41	1.52
1	R	142	PHE	CE2-CZ	-5.28	1.27	1.37
1	F	29	PRO	C-N	-5.27	1.22	1.34
1	S	49	TYR	CE1-CZ	-5.27	1.31	1.38
1	B	107	VAL	CB-CG1	-5.26	1.41	1.52
1	E	192	TYR	CE1-CZ	-5.25	1.31	1.38
1	D	29	PRO	C-N	-5.25	1.22	1.34
1	B	94	VAL	CB-CG1	-5.25	1.41	1.52
1	N	197	GLU	CD-OE1	-5.23	1.19	1.25
1	M	142	PHE	CG-CD2	-5.22	1.30	1.38
1	N	170	GLU	CD-OE1	-5.21	1.20	1.25
1	C	107	VAL	CB-CG2	-5.21	1.42	1.52
1	R	23	LYS	C-N	-5.20	1.22	1.34
1	K	107	VAL	CB-CG1	-5.19	1.42	1.52
1	E	192	TYR	CG-CD2	-5.19	1.32	1.39
1	I	49	TYR	CE2-CZ	-5.19	1.31	1.38
1	H	91	VAL	CB-CG2	-5.18	1.42	1.52
1	I	170	GLU	CD-OE2	-5.16	1.20	1.25
1	C	33	PHE	CG-CD1	-5.14	1.31	1.38
1	C	88	GLU	CB-CG	-5.14	1.42	1.52
1	H	89	VAL	CB-CG1	-5.14	1.42	1.52
1	I	49	TYR	CG-CD2	-5.14	1.32	1.39
1	B	118	ARG	CZ-NH1	-5.14	1.26	1.33
1	H	142	PHE	CE2-CZ	-5.13	1.27	1.37
1	I	170	GLU	CD-OE1	-5.13	1.20	1.25
1	L	107	VAL	CB-CG2	-5.13	1.42	1.52
1	M	117	VAL	CB-CG1	-5.13	1.42	1.52
1	O	77	VAL	CB-CG2	-5.12	1.42	1.52
1	E	89	VAL	CB-CG2	-5.10	1.42	1.52
1	Q	6	ARG	CZ-NH2	-5.10	1.26	1.33
1	E	10	VAL	CB-CG1	-5.09	1.42	1.52
1	P	23	LYS	C-N	5.08	1.45	1.34
1	H	101	GLU	CD-OE2	-5.08	1.20	1.25
1	F	84	PHE	CG-CD1	-5.07	1.31	1.38
1	N	180	PHE	CE2-CZ	-5.07	1.27	1.37
1	H	33	PHE	CE2-CZ	-5.07	1.27	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	49	TYR	CE1-CZ	-5.06	1.31	1.38
1	D	10	VAL	CB-CG1	-5.05	1.42	1.52
1	I	19	TYR	CE1-CZ	-5.04	1.31	1.38
1	K	10	VAL	CB-CG1	-5.03	1.42	1.52
1	N	49	TYR	CG-CD2	-5.03	1.32	1.39

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	116	ARG	NE-CZ-NH2	13.32	126.96	120.30
1	Q	116	ARG	NE-CZ-NH2	12.22	126.41	120.30
1	B	116	ARG	NE-CZ-NH2	11.83	126.22	120.30
1	G	116	ARG	NE-CZ-NH1	-11.70	114.45	120.30
1	L	116	ARG	NE-CZ-NH2	11.57	126.09	120.30
1	S	6	ARG	NE-CZ-NH1	-11.39	114.60	120.30
1	L	116	ARG	NE-CZ-NH1	-10.84	114.88	120.30
1	Q	116	ARG	NE-CZ-NH1	-10.76	114.92	120.30
1	L	6	ARG	CG-CD-NE	-9.88	91.05	111.80
1	S	6	ARG	NE-CZ-NH2	9.83	125.22	120.30
1	N	6	ARG	NE-CZ-NH1	-9.73	115.43	120.30
1	G	82	ILE	CG1-CB-CG2	-9.00	91.60	111.40
1	D	16	ASP	CB-CG-OD1	8.87	126.29	118.30
1	L	82	ILE	CG1-CB-CG2	-8.86	91.92	111.40
1	B	6	ARG	CG-CD-NE	-8.79	93.34	111.80
1	B	6	ARG	NE-CZ-NH1	-8.73	115.94	120.30
1	F	58	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	O	188	ARG	NE-CZ-NH1	8.43	124.51	120.30
1	B	82	ILE	CG1-CB-CG2	-8.41	92.89	111.40
1	B	116	ARG	NE-CZ-NH1	-8.33	116.14	120.30
1	H	198	VAL	CG1-CB-CG2	-8.20	97.78	110.90
1	I	170	GLU	OE1-CD-OE2	-8.10	113.58	123.30
1	C	57	LYS	CD-CE-NZ	-7.93	93.45	111.70
1	Q	6	ARG	CG-CD-NE	-7.82	95.39	111.80
1	K	188	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	C	198	VAL	CG1-CB-CG2	-7.76	98.48	110.90
1	R	101	GLU	OE1-CD-OE2	-7.74	114.02	123.30
1	D	6	ARG	NE-CZ-NH1	-7.65	116.48	120.30
1	Q	37	LEU	CA-CB-CG	7.64	132.87	115.30
1	G	188	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	R	35	VAL	CG1-CB-CG2	-7.54	98.83	110.90
1	D	170	GLU	OE1-CD-OE2	-7.53	114.26	123.30
1	H	101	GLU	OE1-CD-OE2	-7.50	114.31	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	47	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	M	57	LYS	CD-CE-NZ	-7.44	94.59	111.70
1	A	47	ARG	NE-CZ-NH1	7.41	124.01	120.30
1	T	47	ARG	NE-CZ-NH2	7.39	123.99	120.30
1	S	170	GLU	OE1-CD-OE2	-7.30	114.55	123.30
1	R	57	LYS	CD-CE-NZ	-7.28	94.97	111.70
1	Q	82	ILE	CG1-CB-CG2	-7.26	95.44	111.40
1	F	188	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	A	58	ARG	NE-CZ-NH1	7.19	123.90	120.30
1	N	6	ARG	NE-CZ-NH2	7.19	123.89	120.30
1	Q	118	ARG	NE-CZ-NH2	7.18	123.89	120.30
1	B	118	ARG	NE-CZ-NH2	7.17	123.89	120.30
1	F	58	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	C	6	ARG	NE-CZ-NH1	-7.15	116.72	120.30
1	H	117	VAL	CG1-CB-CG2	-7.13	99.49	110.90
1	B	16	ASP	CB-CG-OD1	7.11	124.70	118.30
1	L	6	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	L	37	LEU	CA-CB-CG	7.08	131.59	115.30
1	M	58	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	Q	6	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	K	47	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	P	58	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	J	188	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	M	101	GLU	OE1-CD-OE2	-6.91	115.01	123.30
1	C	101	GLU	OE1-CD-OE2	-6.88	115.05	123.30
1	A	188	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	D	47	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	L	16	ASP	CB-CG-OD1	6.81	124.43	118.30
1	I	6	ARG	NE-CZ-NH1	-6.72	116.94	120.30
1	B	140	ASP	CB-CG-OD1	6.71	124.34	118.30
1	M	198	VAL	CG1-CB-CG2	-6.70	100.18	110.90
1	M	35	VAL	CG1-CB-CG2	-6.66	100.24	110.90
1	C	117	VAL	CG1-CB-CG2	-6.66	100.25	110.90
1	L	6	ARG	CD-NE-CZ	-6.65	114.29	123.60
1	I	3	ASP	CB-CG-OD1	6.55	124.19	118.30
1	R	6	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	B	6	ARG	CD-NE-CZ	-6.54	114.45	123.60
1	R	198	VAL	CG1-CB-CG2	-6.53	100.46	110.90
1	H	35	VAL	CG1-CB-CG2	-6.51	100.48	110.90
1	I	29	PRO	O-C-N	-6.51	112.29	122.70
1	R	47	ARG	NE-CZ-NH2	6.41	123.51	120.30
1	D	16	ASP	CB-CG-OD2	-6.39	112.55	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	37	LEU	CA-CB-CG	6.38	129.97	115.30
1	A	6	ARG	NE-CZ-NH1	-6.36	117.12	120.30
1	E	169	ASP	CB-CG-OD2	6.26	123.94	118.30
1	S	6	ARG	CB-CG-CD	-6.24	95.38	111.60
1	Q	16	ASP	CB-CG-OD1	6.23	123.91	118.30
1	B	26	LEU	CA-CB-CG	6.23	129.63	115.30
1	S	47	ARG	NE-CZ-NH2	6.22	123.41	120.30
1	Q	6	ARG	CD-NE-CZ	-6.16	114.97	123.60
1	R	191	LYS	CD-CE-NZ	-6.13	97.60	111.70
1	T	188	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	B	6	ARG	NH1-CZ-NH2	6.08	126.09	119.40
1	I	117	VAL	CG1-CB-CG2	-6.08	101.17	110.90
1	S	16	ASP	CB-CG-OD1	6.07	123.76	118.30
1	G	37	LEU	CA-CB-CG	6.07	129.25	115.30
1	A	31	LYS	CB-CG-CD	-6.06	95.84	111.60
1	P	6	ARG	NE-CZ-NH1	-6.06	117.27	120.30
1	N	3	ASP	CB-CG-OD2	6.04	123.73	118.30
1	M	26	LEU	CA-CB-CG	6.02	129.14	115.30
1	K	31	LYS	CB-CG-CD	-6.01	95.98	111.60
1	J	85	GLU	OE1-CD-OE2	-6.00	116.09	123.30
1	E	26	LEU	CA-CB-CG	6.00	129.11	115.30
1	L	140	ASP	CB-CG-OD2	5.98	123.68	118.30
1	E	23	LYS	O-C-N	-5.97	113.15	122.70
1	M	117	VAL	CG1-CB-CG2	-5.96	101.37	110.90
1	Q	169	ASP	CB-CG-OD2	5.94	123.64	118.30
1	B	169	ASP	CB-CG-OD1	5.94	123.64	118.30
1	Q	140	ASP	CB-CG-OD2	5.89	123.60	118.30
1	P	47	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	58	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	D	3	ASP	CB-CG-OD2	5.85	123.57	118.30
1	G	140	ASP	CB-CG-OD1	5.84	123.56	118.30
1	N	16	ASP	N-CA-CB	-5.84	100.08	110.60
1	F	6	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	S	117	VAL	CG1-CB-CG2	-5.79	101.63	110.90
1	L	26	LEU	CB-CG-CD2	-5.79	101.16	111.00
1	J	77	VAL	CG1-CB-CG2	-5.76	101.68	110.90
1	L	6	ARG	NH1-CZ-NH2	5.76	125.74	119.40
1	P	188	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	R	117	VAL	CG1-CB-CG2	-5.72	101.74	110.90
1	N	170	GLU	OE1-CD-OE2	-5.71	116.45	123.30
1	I	16	ASP	CB-CG-OD1	5.68	123.42	118.30
1	N	117	VAL	CG1-CB-CG2	-5.68	101.82	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	117	VAL	CG1-CB-CG2	-5.66	101.84	110.90
1	Q	188	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	S	6	ARG	CD-NE-CZ	-5.63	115.71	123.60
1	L	178	GLY	N-CA-C	5.63	127.18	113.10
1	L	6	ARG	NE-CZ-NH1	-5.61	117.49	120.30
1	S	16	ASP	N-CA-CB	-5.58	100.55	110.60
1	Q	6	ARG	CA-CB-CG	-5.55	101.18	113.40
1	M	47	ARG	NE-CZ-NH2	5.55	123.08	120.30
1	H	188	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	D	6	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	E	188	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	O	77	VAL	CG1-CB-CG2	-5.48	102.13	110.90
1	Q	47	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	I	6	ARG	NE-CZ-NH2	5.45	123.03	120.30
1	Q	6	ARG	NH1-CZ-NH2	5.44	125.38	119.40
1	G	188	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	I	3	ASP	OD1-CG-OD2	-5.42	113.01	123.30
1	P	193	GLU	OE1-CD-OE2	-5.42	116.80	123.30
1	C	118	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	G	69	LYS	CD-CE-NZ	5.41	124.15	111.70
1	M	6	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	D	23	LYS	O-C-N	5.35	131.26	122.70
1	C	35	VAL	CG1-CB-CG2	-5.33	102.38	110.90
1	F	31	LYS	CB-CG-CD	-5.29	97.83	111.60
1	I	16	ASP	N-CA-CB	-5.28	101.10	110.60
1	H	47	ARG	NE-CZ-NH2	5.23	122.92	120.30
1	L	140	ASP	OD1-CG-OD2	-5.22	113.37	123.30
1	A	147	GLU	OE1-CD-OE2	-5.21	117.04	123.30
1	L	140	ASP	CB-CG-OD1	5.16	122.94	118.30
1	E	6	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	J	89	VAL	CG1-CB-CG2	-5.15	102.67	110.90
1	H	89	VAL	CG1-CB-CG2	-5.14	102.67	110.90
1	K	193	GLU	OE1-CD-OE2	-5.14	117.13	123.30
1	M	26	LEU	N-CA-C	-5.12	97.17	111.00
1	J	118	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	O	169	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	140	ASP	OD1-CG-OD2	-5.11	113.59	123.30
1	F	147	GLU	OE1-CD-OE2	-5.09	117.19	123.30
1	I	16	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	J	169	ASP	CB-CG-OD2	5.09	122.88	118.30
1	S	30	LEU	CB-CG-CD1	-5.08	102.36	111.00
1	T	89	VAL	CG1-CB-CG2	-5.07	102.79	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	6	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	G	140	ASP	OD1-CG-OD2	-5.01	113.78	123.30
1	Q	107	VAL	CG1-CB-CG2	-5.00	102.90	110.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	26	LEU	Peptide
1	M	26	LEU	Peptide
1	R	23	LYS	Mainchain

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	1632	0	1593	27	0
1	B	1632	0	1593	52	0
1	C	1632	0	1593	23	1
1	D	1632	0	1592	24	5
1	E	1632	0	1593	30	0
1	F	1632	0	1592	22	1
1	G	1632	0	1593	38	0
1	H	1632	0	1593	44	1
1	I	1632	0	1593	17	3
1	J	1632	0	1593	31	1
1	K	1632	0	1593	43	0
1	L	1632	0	1593	47	1
1	M	1632	0	1593	46	0
1	N	1632	0	1593	39	5
1	O	1632	0	1593	27	0
1	P	1632	0	1593	29	1
1	Q	1632	0	1593	41	0
1	R	1632	0	1593	30	0
1	S	1632	0	1593	33	0
1	T	1632	0	1593	25	3
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	0	0
2	O	2	0	0	0	0
2	P	2	0	0	0	0
2	Q	2	0	0	0	0
2	R	2	0	0	0	0
2	S	2	0	0	0	0
2	T	2	0	0	0	0
3	A	12	0	0	2	0
3	B	20	0	0	8	0
3	C	20	0	0	0	0
3	D	14	0	0	5	0
3	E	10	0	0	6	0
3	F	20	0	0	4	0
3	G	15	0	0	6	0
3	H	16	0	0	8	0
3	I	14	0	0	1	0
3	J	30	0	0	4	0
3	K	24	0	0	5	0
3	L	24	0	0	8	0
3	M	19	0	0	8	0
3	N	19	0	0	10	0
3	O	25	0	0	6	0
3	P	19	0	0	5	0
3	Q	28	0	0	3	0
3	R	30	0	0	3	0
3	S	21	0	0	7	0
3	T	17	0	0	2	0
All	All	33077	0	31858	624	11

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 10.

All (624) 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)
1:D:31:LYS:HB2	3:D:208:HOH:O	1.30	1.24
1:S:30:LEU:N	1:S:30:LEU:HD12	1.57	1.18
1:J:58:ARG:HG2	1:J:58:ARG:HH11	1.07	1.15
1:F:13:LYS:HE2	3:F:221:HOH:O	1.47	1.11
1:L:130:GLU:HB3	3:L:392:HOH:O	1.49	1.09
1:G:188:ARG:HD2	3:G:209:HOH:O	1.52	1.07
1:R:26:LEU:HD11	1:R:184:VAL:HG13	1.33	1.06
1:G:82:ILE:HG23	1:G:121:LEU:HD13	1.37	1.06
1:R:26:LEU:CD1	1:R:184:VAL:HG13	1.86	1.04
1:B:28:LYS:NZ	3:B:324:HOH:O	1.94	0.99
1:J:58:ARG:HG2	1:J:58:ARG:NH1	1.63	0.97
1:D:206:PRO:HG2	3:D:215:HOH:O	1.67	0.93
1:S:30:LEU:N	1:S:30:LEU:CD1	2.29	0.93
1:F:42:GLU:OE2	1:G:116:ARG:NH1	2.01	0.92
3:M:213:HOH:O	1:N:119:LYS:HG2	1.69	0.91
1:F:57:LYS:HE3	3:F:213:HOH:O	1.69	0.91
1:B:34:THR:HG21	1:B:166:LEU:HD12	1.54	0.90
1:T:26:LEU:HB3	1:T:27:THR:HB	1.53	0.89
1:E:172:ASN:HB3	3:E:208:HOH:O	1.70	0.89
1:L:130:GLU:CB	3:L:392:HOH:O	2.10	0.89
1:H:28:LYS:C	1:H:129:ALA:HB2	1.92	0.89
1:L:6:ARG:HB2	1:L:6:ARG:NH1	1.87	0.88
1:L:26:LEU:HD12	1:L:27:THR:H	1.39	0.88
1:J:58:ARG:CG	1:J:58:ARG:HH11	1.84	0.88
1:M:71:ILE:HG21	1:M:83:LEU:HD23	1.55	0.87
1:S:91:VAL:HG23	1:S:91:VAL:O	1.74	0.87
1:H:28:LYS:O	1:H:129:ALA:CB	2.22	0.87
1:P:26:LEU:HB3	1:P:129:ALA:O	1.73	0.86
1:S:29:PRO:C	1:S:30:LEU:HD12	1.96	0.86
1:L:34:THR:HG21	1:L:166:LEU:HD12	1.56	0.86
1:H:43:LEU:HD11	1:H:153:VAL:HB	1.59	0.85
1:M:26:LEU:O	1:M:27:THR:HB	1.75	0.85
1:H:25:PRO:HG2	3:H:262:HOH:O	1.74	0.85
1:P:173:THR:HG23	3:P:401:HOH:O	1.76	0.84
1:K:13:LYS:HD2	3:K:384:HOH:O	1.76	0.83
1:B:91:VAL:HG23	3:B:214:HOH:O	1.79	0.83
1:L:26:LEU:HB3	3:L:509:HOH:O	1.77	0.82
1:F:2:THR:HA	3:F:272:HOH:O	1.79	0.82
1:K:82:ILE:HB	1:K:121:LEU:HD12	1.62	0.81
1:K:26:LEU:HG	1:K:27:THR:H	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:PRO:HD2	3:B:390:HOH:O	1.81	0.81
1:B:202:PRO:O	1:C:118:ARG:NH2	2.14	0.81
1:H:28:LYS:O	1:H:129:ALA:HB2	1.79	0.81
1:M:25:PRO:O	1:M:25:PRO:CD	2.29	0.81
1:L:147:GLU:HB2	3:L:305:HOH:O	1.80	0.80
1:P:58:ARG:HH11	1:P:58:ARG:HG2	1.44	0.80
1:I:91:VAL:HB	3:I:207:HOH:O	1.80	0.79
1:E:3:ASP:HB3	1:T:1:GLN:HE22	1.47	0.79
1:G:34:THR:HG21	1:G:166:LEU:HD12	1.63	0.79
1:D:91:VAL:HG23	1:D:91:VAL:O	1.83	0.79
1:N:58:ARG:HG3	1:N:58:ARG:HH21	1.49	0.79
1:J:13:LYS:HG2	3:J:220:HOH:O	1.82	0.78
1:M:25:PRO:O	1:M:25:PRO:CG	2.29	0.78
1:T:19:TYR:CZ	1:T:195:GLN:HG3	2.19	0.77
1:R:147:GLU:HB3	3:R:222:HOH:O	1.85	0.77
1:O:180:PHE:HB3	3:O:361:HOH:O	1.84	0.76
1:K:26:LEU:CG	1:K:27:THR:H	1.96	0.76
1:I:91:VAL:O	1:I:91:VAL:HG23	1.84	0.76
1:B:31:LYS:HE2	3:B:276:HOH:O	1.86	0.76
1:G:21:SER:OG	1:G:23:LYS:NZ	2.19	0.75
1:K:47:ARG:NH2	1:K:151:SER:O	2.17	0.75
1:B:85:GLU:O	1:B:116:ARG:NH2	2.20	0.75
1:S:82:ILE:HG12	1:S:121:LEU:HD13	1.69	0.74
1:M:58:ARG:HB2	3:M:211:HOH:O	1.87	0.74
1:L:26:LEU:HD12	1:L:27:THR:N	2.02	0.74
1:G:197:GLU:HG2	3:G:365:HOH:O	1.86	0.73
1:N:71:ILE:HG21	1:N:83:LEU:HD23	1.71	0.73
1:Q:28:LYS:HG2	1:Q:29:PRO:HD2	1.70	0.73
1:S:26:LEU:HD21	1:S:30:LEU:HD11	1.71	0.73
1:M:46:THR:HG23	3:M:207:HOH:O	1.89	0.73
1:M:91:VAL:HG23	1:M:91:VAL:O	1.89	0.72
1:L:60:ASP:OD1	3:L:510:HOH:O	2.07	0.72
1:Q:202:PRO:O	1:R:118:ARG:NH2	2.22	0.72
1:B:203:GLN:NE2	3:B:382:HOH:O	2.22	0.72
1:D:26:LEU:HD12	1:D:27:THR:H	1.55	0.72
1:L:26:LEU:HD23	1:L:129:ALA:O	1.89	0.71
1:S:5:SER:O	1:S:6:ARG:HB2	1.91	0.71
1:P:58:ARG:HG2	1:P:58:ARG:NH1	2.01	0.70
1:M:26:LEU:HD22	1:M:27:THR:HA	1.73	0.70
1:J:58:ARG:CG	1:J:58:ARG:NH1	2.40	0.70
1:C:1:GLN:OE1	1:C:191:LYS:HE3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:163:ASP:H	1:M:183:ASN:HD21	1.39	0.70
1:L:139:GLN:HE21	1:L:143:GLY:H	1.37	0.69
1:R:43:LEU:HD11	1:R:153:VAL:HB	1.72	0.69
1:M:25:PRO:HG2	1:M:25:PRO:O	1.91	0.69
1:P:120:SER:HB2	1:T:12:PRO:HB2	1.75	0.69
1:T:59:GLN:HE21	1:T:61:ASN:H	1.41	0.68
1:J:57:LYS:HE2	1:J:130:GLU:OE1	1.92	0.68
1:H:52:PHE:HB3	1:H:65:ILE:HD12	1.74	0.68
1:P:170:GLU:O	1:P:174:ILE:HG12	1.94	0.68
1:L:26:LEU:HG	1:L:129:ALA:HB1	1.75	0.68
1:H:28:LYS:C	1:H:129:ALA:CB	2.60	0.68
1:H:27:THR:HG23	3:H:261:HOH:O	1.93	0.68
1:N:26:LEU:HD21	1:N:30:LEU:HD11	1.76	0.68
1:P:27:THR:O	1:P:29:PRO:HD3	1.93	0.68
1:N:58:ARG:HG3	1:N:58:ARG:NH2	2.09	0.67
1:M:27:THR:HG23	1:M:28:LYS:N	2.10	0.67
1:K:26:LEU:HG	1:K:27:THR:N	2.09	0.67
1:C:163:ASP:H	1:C:183:ASN:HD21	1.43	0.67
1:H:25:PRO:HD3	3:H:389:HOH:O	1.96	0.66
1:S:197:GLU:HG3	3:S:209:HOH:O	1.95	0.66
1:K:135:LEU:HD21	1:K:159:VAL:HG21	1.77	0.66
1:Q:160:ASN:HD22	1:Q:182:PRO:HG2	1.61	0.66
1:G:82:ILE:CG2	1:G:121:LEU:HD13	2.21	0.66
1:G:160:ASN:ND2	1:G:187:TRP:H	1.94	0.66
1:B:177:GLY:O	1:B:178:GLY:O	2.15	0.65
1:Q:82:ILE:HG23	1:Q:121:LEU:HD13	1.77	0.65
1:B:42:GLU:HG3	1:C:117:VAL:HG21	1.79	0.65
1:Q:177:GLY:O	1:Q:178:GLY:O	2.13	0.65
1:F:194:VAL:HG13	1:F:198:VAL:HG13	1.79	0.65
1:C:108:GLU:OE2	1:C:118:ARG:NH1	2.29	0.65
1:M:25:PRO:O	1:M:25:PRO:HD2	1.98	0.64
1:B:183:ASN:H	1:B:183:ASN:HD22	1.45	0.64
1:P:42:GLU:HG3	3:P:211:HOH:O	1.96	0.64
1:B:139:GLN:HE21	1:B:143:GLY:H	1.45	0.64
1:G:6:ARG:NH2	1:H:169:ASP:OD2	2.30	0.64
1:A:147:GLU:HB3	3:A:208:HOH:O	1.96	0.64
1:E:57:LYS:HE2	1:E:130:GLU:OE1	1.96	0.64
1:J:64:LEU:HB3	1:J:76:THR:HG23	1.78	0.64
1:T:64:LEU:HB3	1:T:76:THR:HG23	1.79	0.63
1:G:85:GLU:O	1:G:116:ARG:NH2	2.31	0.63
1:O:58:ARG:HH11	1:O:58:ARG:HG2	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:26:LEU:CD1	1:K:27:THR:H	2.12	0.63
1:Q:95:HIS:HE1	3:Q:218:HOH:O	1.81	0.63
1:A:148:GLY:O	1:A:151:SER:HB3	1.98	0.63
1:L:202:PRO:O	1:M:118:ARG:NH2	2.31	0.63
1:T:58:ARG:HG2	1:T:58:ARG:NH1	2.13	0.62
1:N:29:PRO:HB2	1:N:126:THR:CG2	2.30	0.62
1:K:82:ILE:HB	1:K:121:LEU:CD1	2.29	0.62
1:F:12:PRO:HB2	1:G:120:SER:HB2	1.81	0.62
1:N:95:HIS:HE1	3:N:209:HOH:O	1.82	0.62
1:N:5:SER:O	1:N:6:ARG:HB2	2.00	0.62
1:O:58:ARG:HG2	1:O:58:ARG:NH1	2.15	0.61
1:N:15:SER:HB2	3:N:210:HOH:O	2.00	0.61
1:K:26:LEU:CD2	1:K:30:LEU:HD21	2.30	0.61
1:A:42:GLU:OE2	1:B:116:ARG:NH1	2.33	0.61
1:O:129:ALA:HB3	3:O:287:HOH:O	1.99	0.61
1:A:120:SER:HB2	1:E:12:PRO:HB2	1.82	0.61
1:R:26:LEU:HD11	1:R:184:VAL:CG1	2.22	0.61
1:Q:163:ASP:H	1:Q:183:ASN:HD21	1.46	0.61
1:B:42:GLU:HG3	1:C:117:VAL:CG2	2.31	0.61
1:M:142:PHE:HB3	3:M:373:HOH:O	2.01	0.61
1:Q:194:VAL:HG13	1:Q:198:VAL:HG13	1.84	0.60
1:H:25:PRO:CG	3:H:262:HOH:O	2.42	0.60
1:P:161:MET:HB3	1:P:185:LEU:HB2	1.83	0.60
1:L:85:GLU:O	1:L:116:ARG:NH2	2.35	0.60
1:J:27:THR:HB	3:J:216:HOH:O	2.01	0.60
1:J:194:VAL:HG13	1:J:198:VAL:HG13	1.82	0.60
1:T:135:LEU:HD21	1:T:159:VAL:HG21	1.82	0.59
1:H:12:PRO:HB2	1:I:120:SER:HB2	1.84	0.59
1:S:119:LYS:HG2	3:S:215:HOH:O	2.02	0.59
1:L:6:ARG:HB2	1:L:6:ARG:CZ	2.32	0.59
1:S:194:VAL:HG13	1:S:198:VAL:HG13	1.84	0.59
1:T:57:LYS:HE2	1:T:130:GLU:OE1	2.02	0.59
1:H:25:PRO:O	1:H:26:LEU:HG	2.02	0.59
1:G:163:ASP:H	1:G:183:ASN:HD21	1.48	0.59
1:E:64:LEU:HB3	1:E:76:THR:HG23	1.84	0.59
1:K:12:PRO:HB2	1:L:120:SER:HB2	1.85	0.59
1:M:141:SER:HB3	1:M:145:ASN:HD22	1.64	0.59
1:G:188:ARG:CD	3:G:209:HOH:O	2.26	0.59
1:G:34:THR:CG2	1:G:166:LEU:HD12	2.33	0.58
1:E:25:PRO:O	1:E:27:THR:HG23	2.03	0.58
1:L:6:ARG:CB	1:L:6:ARG:CZ	2.75	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:194:VAL:HG13	1:L:198:VAL:HG13	1.84	0.58
1:M:12:PRO:HB2	1:N:120:SER:HB2	1.85	0.58
1:B:12:PRO:HB2	1:C:120:SER:HB2	1.85	0.58
1:M:186:ASN:HD22	1:M:188:ARG:H	1.52	0.58
1:G:160:ASN:HD21	1:G:187:TRP:H	1.49	0.58
1:A:160:ASN:ND2	1:A:187:TRP:H	2.02	0.58
1:F:82:ILE:HB	1:F:121:LEU:HD12	1.86	0.57
1:K:170:GLU:O	1:K:174:ILE:HG12	2.04	0.57
1:E:172:ASN:CB	3:E:208:HOH:O	2.41	0.57
1:C:26:LEU:HD11	1:C:184:VAL:HG13	1.86	0.57
1:O:161:MET:HB3	1:O:185:LEU:HB2	1.86	0.57
1:R:46:THR:O	1:R:69:LYS:HE2	2.04	0.57
1:R:163:ASP:H	1:R:183:ASN:HD21	1.53	0.57
1:M:43:LEU:HD11	1:M:153:VAL:HB	1.86	0.57
1:I:71:ILE:HG21	1:I:83:LEU:HD23	1.86	0.57
1:M:11:PHE:CE2	1:M:198:VAL:HG22	2.39	0.57
1:G:197:GLU:OE1	1:H:123:LYS:NZ	2.37	0.57
1:Q:108:GLU:OE2	1:Q:118:ARG:NH1	2.37	0.57
1:G:13:LYS:HE3	3:G:365:HOH:O	2.05	0.57
1:B:56:THR:HG22	1:B:62:GLU:HB2	1.87	0.57
1:G:29:PRO:HA	1:G:129:ALA:HB2	1.87	0.57
1:B:6:ARG:NH1	1:B:6:ARG:HB2	2.20	0.57
1:L:6:ARG:HA	1:L:203:GLN:NE2	2.20	0.56
1:G:204:LEU:HD11	1:H:118:ARG:HG3	1.87	0.56
1:J:29:PRO:HB2	1:J:126:THR:CG2	2.34	0.56
1:J:5:SER:HB3	3:J:207:HOH:O	2.04	0.56
1:P:38:HIS:CE1	1:P:95:HIS:HB2	2.41	0.56
1:L:12:PRO:HB2	1:M:120:SER:HB2	1.86	0.56
1:B:37:LEU:HD21	1:B:51:ILE:CG2	2.35	0.56
1:O:194:VAL:HG13	1:O:198:VAL:HG13	1.86	0.56
1:K:139:GLN:HE21	1:K:143:GLY:H	1.53	0.56
1:N:95:HIS:CE1	3:N:209:HOH:O	2.55	0.56
1:Q:56:THR:HG22	1:Q:62:GLU:HB2	1.88	0.56
1:G:193:GLU:HG3	3:G:293:HOH:O	2.04	0.56
1:G:54:TYR:HB3	1:G:63:ILE:HB	1.88	0.56
1:K:135:LEU:HG	1:K:156:ILE:HD13	1.87	0.56
1:F:77:VAL:HB	1:F:121:LEU:CD2	2.36	0.56
1:G:177:GLY:O	1:G:178:GLY:O	2.23	0.56
1:R:12:PRO:HD2	3:R:223:HOH:O	2.05	0.56
1:H:28:LYS:O	1:H:129:ALA:HB1	2.06	0.56
1:G:193:GLU:CG	3:G:293:HOH:O	2.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:ARG:NE	3:D:214:HOH:O	2.38	0.55
1:E:177:GLY:HA3	3:E:347:HOH:O	2.05	0.55
1:S:28:LYS:O	1:S:129:ALA:HB2	2.06	0.55
1:G:202:PRO:O	1:H:118:ARG:NH2	2.32	0.55
1:Q:139:GLN:HE21	1:Q:143:GLY:H	1.53	0.55
1:A:147:GLU:HG2	3:A:349:HOH:O	2.06	0.55
1:H:183:ASN:C	1:H:183:ASN:HD22	2.10	0.55
1:L:130:GLU:O	3:L:242:HOH:O	2.18	0.55
1:K:26:LEU:HD12	1:K:27:THR:H	1.71	0.55
1:K:26:LEU:HD21	1:K:30:LEU:HD21	1.88	0.55
1:B:145:ASN:HA	3:B:209:HOH:O	2.05	0.55
1:B:12:PRO:HD2	3:B:211:HOH:O	2.06	0.55
1:K:24:ALA:HB2	1:K:185:LEU:CD1	2.37	0.55
1:N:90:THR:HA	3:N:348:HOH:O	2.07	0.54
1:S:195:GLN:HG2	3:S:218:HOH:O	2.06	0.54
1:O:59:GLN:HE21	1:O:61:ASN:H	1.53	0.54
1:Q:46:THR:O	1:Q:69:LYS:HD2	2.07	0.54
1:D:71:ILE:CG2	1:D:83:LEU:HD23	2.37	0.54
1:R:96:ILE:HA	1:R:110:TRP:O	2.07	0.54
1:L:6:ARG:CB	1:L:6:ARG:NH1	2.65	0.54
1:J:80:SER:HB3	1:J:121:LEU:HD11	1.89	0.54
1:N:10:VAL:HG21	1:O:118:ARG:HD3	1.89	0.54
1:A:194:VAL:HG13	1:A:198:VAL:HG13	1.90	0.54
1:L:82:ILE:CG2	1:L:121:LEU:HD13	2.38	0.54
1:K:26:LEU:CG	1:K:27:THR:N	2.67	0.54
1:D:91:VAL:HB	3:D:281:HOH:O	2.07	0.54
1:D:26:LEU:HD21	1:D:30:LEU:HD11	1.90	0.54
1:L:139:GLN:NE2	1:L:143:GLY:H	2.04	0.54
1:F:47:ARG:HH21	1:F:149:SER:C	2.11	0.54
1:L:194:VAL:HG13	1:L:198:VAL:CG1	2.38	0.54
1:N:171:ILE:HD11	3:N:309:HOH:O	2.06	0.54
1:H:27:THR:CG2	3:H:261:HOH:O	2.55	0.54
1:Q:46:THR:OG1	3:Q:211:HOH:O	2.18	0.54
1:M:52:PHE:HB3	1:M:65:ILE:HD12	1.89	0.54
1:L:34:THR:CG2	1:L:166:LEU:HD12	2.33	0.54
1:Q:183:ASN:H	1:Q:183:ASN:HD22	1.56	0.54
1:I:194:VAL:HG13	1:I:198:VAL:HG13	1.90	0.53
1:H:13:LYS:HE2	1:H:197:GLU:HG2	1.90	0.53
1:B:183:ASN:H	1:B:183:ASN:ND2	2.07	0.53
1:H:163:ASP:H	1:H:183:ASN:HD21	1.56	0.53
1:Q:28:LYS:CG	1:Q:29:PRO:HD2	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:69:LYS:HG2	3:R:217:HOH:O	2.07	0.53
1:T:40:TYR:HA	3:T:385:HOH:O	2.09	0.53
1:S:117:VAL:HG23	3:S:217:HOH:O	2.09	0.53
1:C:183:ASN:HD22	1:C:183:ASN:C	2.11	0.53
1:P:100:TRP:CH2	1:P:102:SER:HB2	2.43	0.53
1:G:194:VAL:HG13	1:G:198:VAL:HG13	1.91	0.53
1:P:139:GLN:HE21	1:P:143:GLY:H	1.56	0.53
1:J:160:ASN:ND2	1:J:187:TRP:H	2.06	0.53
1:S:29:PRO:HB2	1:S:126:THR:CG2	2.39	0.53
1:T:26:LEU:HB3	1:T:27:THR:CB	2.35	0.53
1:N:83:LEU:CD1	3:N:370:HOH:O	2.57	0.53
1:B:183:ASN:HD22	1:B:183:ASN:N	2.05	0.53
1:Q:54:TYR:HB3	1:Q:63:ILE:HB	1.90	0.53
1:Q:6:ARG:CB	1:Q:6:ARG:CZ	2.84	0.53
1:R:13:LYS:HE2	1:R:197:GLU:HG2	1.91	0.53
1:F:101:GLU:OE1	1:J:201:LYS:NZ	2.34	0.53
1:A:52:PHE:HB3	1:A:65:ILE:HD12	1.91	0.52
1:T:139:GLN:HE21	1:T:143:GLY:HA2	1.73	0.52
1:L:37:LEU:HD21	1:L:51:ILE:HG22	1.91	0.52
1:B:24:ALA:HB2	1:B:185:LEU:CD1	2.39	0.52
1:L:54:TYR:HB3	1:L:63:ILE:HB	1.91	0.52
1:M:139:GLN:HE21	1:M:143:GLY:H	1.56	0.52
1:G:82:ILE:HG23	1:G:121:LEU:CD1	2.26	0.52
1:K:204:LEU:HD11	1:L:118:ARG:HG3	1.90	0.52
1:N:6:ARG:CZ	3:O:213:HOH:O	2.58	0.52
1:M:186:ASN:ND2	1:M:188:ARG:H	2.06	0.52
1:N:26:LEU:HB3	1:N:129:ALA:HB1	1.92	0.52
1:D:139:GLN:HE21	1:D:143:GLY:H	1.57	0.52
1:R:75:PHE:CD2	1:R:107:VAL:HG11	2.45	0.52
1:B:34:THR:CG2	1:B:166:LEU:HD12	2.33	0.51
1:I:38:HIS:HB3	1:I:205:TRP:CZ2	2.46	0.51
1:E:177:GLY:CA	3:E:347:HOH:O	2.59	0.51
1:B:170:GLU:O	1:B:174:ILE:HD12	2.09	0.51
1:H:1:GLN:H1	1:H:191:LYS:HD3	1.75	0.51
1:O:26:LEU:HD22	3:O:209:HOH:O	2.10	0.51
1:D:12:PRO:HB2	1:E:120:SER:HB2	1.93	0.51
1:S:135:LEU:HD21	1:S:159:VAL:HG21	1.91	0.51
1:Q:90:THR:HA	3:Q:217:HOH:O	2.10	0.51
1:E:160:ASN:ND2	1:E:187:TRP:H	2.09	0.51
1:Q:85:GLU:O	1:Q:116:ARG:NH2	2.43	0.50
1:H:108:GLU:OE2	1:H:118:ARG:NH1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:95:HIS:HD2	3:P:207:HOH:O	1.93	0.50
1:M:71:ILE:CG2	1:M:83:LEU:HD23	2.35	0.50
1:A:139:GLN:HE21	1:A:143:GLY:H	1.59	0.50
1:L:130:GLU:HB2	3:L:392:HOH:O	1.94	0.50
1:E:64:LEU:HB3	1:E:76:THR:CG2	2.41	0.50
1:P:32:ALA:HA	1:P:100:TRP:O	2.11	0.50
1:R:91:VAL:O	1:R:91:VAL:HG23	2.11	0.50
1:C:139:GLN:HE21	1:C:143:GLY:H	1.58	0.50
1:S:71:ILE:HG21	1:S:83:LEU:HD23	1.92	0.50
1:C:100:TRP:CH2	1:C:102:SER:HB2	2.47	0.50
1:M:27:THR:CG2	1:M:28:LYS:N	2.74	0.50
1:A:186:ASN:ND2	1:A:188:ARG:H	2.10	0.50
1:C:43:LEU:HD11	1:C:153:VAL:HB	1.94	0.50
1:P:158:ASN:ND2	1:P:205:TRP:HE1	2.09	0.50
1:O:30:LEU:HB2	1:O:127:VAL:HB	1.93	0.50
1:D:160:ASN:ND2	1:D:187:TRP:H	2.10	0.49
1:L:160:ASN:ND2	1:L:187:TRP:H	2.11	0.49
1:T:58:ARG:HG2	1:T:58:ARG:HH11	1.75	0.49
1:P:60:ASP:HB3	3:P:518:HOH:O	2.12	0.49
1:M:13:LYS:HE2	1:M:197:GLU:HG2	1.94	0.49
1:A:54:TYR:HB3	1:A:63:ILE:HB	1.94	0.49
1:M:27:THR:HG23	1:M:28:LYS:H	1.73	0.49
1:D:71:ILE:HG21	1:D:83:LEU:HD23	1.94	0.49
1:J:22:LEU:HD22	1:J:190:LEU:HD11	1.94	0.49
1:K:161:MET:HB3	1:K:185:LEU:HB2	1.94	0.49
1:C:13:LYS:HE2	1:C:197:GLU:HG2	1.95	0.49
1:F:194:VAL:HG13	1:F:198:VAL:CG1	2.43	0.49
1:S:52:PHE:HB3	1:S:65:ILE:HD12	1.95	0.49
1:P:135:LEU:HD21	1:P:159:VAL:HG21	1.94	0.49
1:M:168:PRO:HD3	3:M:399:HOH:O	2.12	0.49
1:K:38:HIS:CE1	1:K:95:HIS:HB2	2.48	0.49
1:Q:204:LEU:HD11	1:R:118:ARG:HG3	1.94	0.49
1:K:120:SER:HB2	1:O:12:PRO:HB2	1.93	0.49
1:B:160:ASN:HD22	1:B:182:PRO:HG2	1.77	0.49
1:O:28:LYS:HB2	1:O:29:PRO:HD2	1.95	0.49
1:G:12:PRO:HB2	1:H:120:SER:HB2	1.93	0.49
1:H:25:PRO:CG	3:H:389:HOH:O	2.60	0.49
1:R:162:TRP:HA	1:R:183:ASN:ND2	2.27	0.49
1:M:51:ILE:HD12	1:M:65:ILE:HG22	1.95	0.49
1:B:163:ASP:H	1:B:183:ASN:HD21	1.61	0.49
1:Q:26:LEU:HD21	1:Q:183:ASN:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:VAL:HG11	1:C:106:ILE:CD1	2.42	0.49
1:S:82:ILE:CG1	1:S:121:LEU:HD13	2.39	0.48
1:E:161:MET:HB3	1:E:185:LEU:HB2	1.95	0.48
1:M:186:ASN:HD22	1:M:186:ASN:C	2.16	0.48
1:D:174:ILE:HG23	3:D:357:HOH:O	2.13	0.48
1:R:68:SER:HB3	1:R:71:ILE:HB	1.94	0.48
1:O:197:GLU:HB3	3:O:212:HOH:O	2.12	0.48
1:I:139:GLN:HE21	1:I:143:GLY:H	1.61	0.48
1:S:13:LYS:HE3	3:S:317:HOH:O	2.12	0.48
1:K:69:LYS:HD3	3:K:215:HOH:O	2.12	0.48
1:N:89:VAL:HG12	3:N:214:HOH:O	2.13	0.48
1:E:58:ARG:HG2	1:E:58:ARG:NH1	2.29	0.48
1:F:161:MET:HB3	1:F:185:LEU:HB2	1.95	0.48
1:R:27:THR:O	1:R:28:LYS:HB3	2.13	0.48
1:L:140:ASP:HB2	1:L:145:ASN:HB3	1.96	0.48
1:S:160:ASN:HD22	1:S:182:PRO:HG2	1.77	0.48
1:N:160:ASN:ND2	1:N:187:TRP:H	2.12	0.48
1:E:6:ARG:HA	1:E:203:GLN:NE2	2.29	0.48
1:N:64:LEU:HB3	1:N:76:THR:HB	1.96	0.48
1:N:58:ARG:CG	1:N:58:ARG:NH2	2.69	0.47
1:K:199:PHE:HB3	3:K:210:HOH:O	2.13	0.47
1:R:33:PHE:CE1	1:R:63:ILE:CD1	2.97	0.47
1:B:82:ILE:HG23	1:B:121:LEU:HD13	1.95	0.47
1:B:6:ARG:HH11	1:B:6:ARG:HD3	1.32	0.47
1:K:54:TYR:HB3	1:K:63:ILE:HB	1.95	0.47
1:M:26:LEU:HD22	1:M:27:THR:CA	2.44	0.47
1:J:59:GLN:HE21	1:J:61:ASN:H	1.61	0.47
1:E:22:LEU:HD22	1:E:190:LEU:HD11	1.97	0.47
1:R:101:GLU:HB2	1:R:165:VAL:HG21	1.96	0.47
1:K:162:TRP:CD1	1:K:182:PRO:HA	2.49	0.47
1:T:22:LEU:HD22	1:T:190:LEU:HD11	1.97	0.47
1:N:71:ILE:CG2	1:N:83:LEU:HD23	2.42	0.47
1:R:41:THR:OG1	1:R:43:LEU:HD12	2.14	0.47
1:P:204:LEU:HD11	1:Q:118:ARG:HG3	1.96	0.47
1:A:186:ASN:HD22	1:A:188:ARG:H	1.61	0.47
1:H:147:GLU:HG2	3:H:211:HOH:O	2.14	0.47
1:A:118:ARG:HD3	1:E:10:VAL:HG21	1.96	0.47
1:O:64:LEU:HB3	1:O:76:THR:CG2	2.44	0.47
1:R:141:SER:HB3	1:R:145:ASN:HD22	1.78	0.47
1:J:160:ASN:HD21	1:J:187:TRP:H	1.63	0.47
1:P:42:GLU:CG	3:P:211:HOH:O	2.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:41:THR:OG1	1:H:43:LEU:HD12	2.14	0.47
1:G:37:LEU:HA	1:G:158:ASN:O	2.15	0.47
1:E:52:PHE:HB3	1:E:65:ILE:HD12	1.97	0.47
1:N:1:GLN:OE1	1:N:191:LYS:HE3	2.14	0.47
1:J:1:GLN:H1	1:J:191:LYS:HG2	1.79	0.47
1:K:108:GLU:HA	3:K:207:HOH:O	2.16	0.46
1:G:30:LEU:HB2	1:G:127:VAL:HB	1.96	0.46
1:E:135:LEU:HD21	1:E:159:VAL:HG21	1.97	0.46
1:F:71:ILE:HG21	1:F:83:LEU:HD22	1.97	0.46
1:Q:101:GLU:O	1:Q:105:GLY:N	2.48	0.46
1:H:58:ARG:HD2	1:H:58:ARG:HH11	1.42	0.46
1:J:38:HIS:HB3	1:J:205:TRP:CZ2	2.51	0.46
1:A:26:LEU:HD12	1:A:27:THR:HG22	1.97	0.46
1:D:5:SER:O	1:D:6:ARG:HB2	2.14	0.46
1:R:161:MET:HB3	1:R:185:LEU:HB2	1.98	0.46
1:L:66:PHE:HB3	1:L:74:SER:HB3	1.97	0.46
1:O:135:LEU:HG	1:O:156:ILE:HD13	1.97	0.46
1:K:71:ILE:HG21	1:K:83:LEU:CD2	2.46	0.46
1:C:161:MET:HB3	1:C:185:LEU:HB2	1.98	0.46
1:L:163:ASP:H	1:L:183:ASN:HD21	1.64	0.46
1:H:1:GLN:HE21	1:H:1:GLN:HB2	1.48	0.46
1:A:161:MET:HB3	1:A:185:LEU:HB2	1.98	0.46
1:T:179:PRO:HA	3:T:404:HOH:O	2.15	0.46
1:E:172:ASN:CG	3:E:208:HOH:O	2.52	0.46
1:L:82:ILE:HD12	1:L:119:LYS:HD3	1.98	0.46
1:S:83:LEU:N	1:S:83:LEU:HD12	2.30	0.46
1:I:139:GLN:NE2	1:I:143:GLY:H	2.13	0.46
1:F:95:HIS:HE1	3:F:210:HOH:O	1.99	0.46
1:J:96:ILE:HA	1:J:110:TRP:O	2.15	0.46
1:M:50:SER:HB2	1:M:138:GLU:HB2	1.97	0.46
1:D:135:LEU:HD21	1:D:159:VAL:HG21	1.98	0.46
1:H:28:LYS:HG3	1:H:29:PRO:HD2	1.97	0.46
1:H:25:PRO:CD	3:H:389:HOH:O	2.57	0.46
1:G:75:PHE:CD2	1:G:107:VAL:HG11	2.51	0.46
1:H:91:VAL:HG23	1:H:91:VAL:O	2.16	0.46
1:F:160:ASN:ND2	1:F:187:TRP:H	2.13	0.46
1:O:95:HIS:HD2	3:O:229:HOH:O	1.98	0.46
1:D:29:PRO:HA	1:D:129:ALA:HB2	1.97	0.46
1:J:101:GLU:HB2	1:J:165:VAL:HG21	1.97	0.45
1:F:170:GLU:O	1:F:174:ILE:HG12	2.16	0.45
1:D:82:ILE:HG12	1:D:121:LEU:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:1:GLN:HB2	1:R:1:GLN:HE21	1.60	0.45
1:H:27:THR:OG1	1:H:129:ALA:O	2.34	0.45
1:L:6:ARG:HD3	1:L:6:ARG:HH11	1.43	0.45
1:C:26:LEU:HA	1:C:26:LEU:HD12	1.66	0.45
1:G:26:LEU:HD12	1:G:27:THR:H	1.82	0.45
1:M:58:ARG:CB	3:M:211:HOH:O	2.56	0.45
1:Q:37:LEU:HD21	1:Q:51:ILE:CG2	2.46	0.45
1:T:160:ASN:ND2	1:T:187:TRP:H	2.15	0.45
1:I:160:ASN:ND2	1:I:187:TRP:H	2.15	0.45
1:S:26:LEU:HG	1:S:129:ALA:HB1	1.98	0.45
1:Q:160:ASN:ND2	1:Q:187:TRP:H	2.15	0.45
1:B:183:ASN:N	1:B:183:ASN:ND2	2.65	0.45
1:E:132:SER:OG	1:E:139:GLN:NE2	2.50	0.45
1:F:24:ALA:HA	1:F:25:PRO:HD3	1.78	0.45
1:S:122:LYS:HA	3:S:307:HOH:O	2.16	0.45
1:C:64:LEU:HB3	1:C:76:THR:HB	1.99	0.45
1:N:26:LEU:CD2	1:N:30:LEU:HD11	2.46	0.45
1:B:80:SER:HB3	1:B:121:LEU:HD11	1.99	0.45
1:I:160:ASN:HD22	1:I:182:PRO:HG2	1.81	0.45
1:F:50:SER:HB2	1:F:138:GLU:HB2	1.99	0.45
1:H:29:PRO:N	1:H:129:ALA:HB2	2.31	0.45
1:N:6:ARG:HD3	1:N:6:ARG:HH11	1.42	0.45
1:N:161:MET:HB3	1:N:185:LEU:HB2	1.99	0.45
1:R:183:ASN:HD22	1:R:183:ASN:H	1.65	0.44
1:B:62:GLU:O	1:B:77:VAL:HA	2.16	0.44
1:A:170:GLU:O	1:A:174:ILE:HG12	2.17	0.44
1:M:172:ASN:HD22	1:M:172:ASN:HA	1.58	0.44
1:B:31:LYS:CE	3:B:276:HOH:O	2.56	0.44
1:B:137:GLN:HB3	1:B:146:PHE:CD1	2.52	0.44
1:O:57:LYS:HE2	1:O:130:GLU:OE1	2.17	0.44
1:M:75:PHE:CD2	1:M:107:VAL:HG11	2.52	0.44
1:H:47:ARG:HA	1:H:69:LYS:HD2	2.00	0.44
1:Q:161:MET:HB3	1:Q:185:LEU:HB2	2.00	0.44
1:E:165:VAL:HG11	3:E:218:HOH:O	2.18	0.44
1:L:167:SER:OG	1:L:170:GLU:HG3	2.18	0.44
1:O:58:ARG:HH11	1:O:58:ARG:CG	2.26	0.44
1:J:50:SER:HB2	1:J:138:GLU:HB2	1.99	0.44
1:R:132:SER:OG	1:R:139:GLN:NE2	2.48	0.44
1:S:161:MET:HB3	1:S:185:LEU:HB2	1.98	0.44
1:D:96:ILE:HA	1:D:110:TRP:O	2.17	0.44
1:E:82:ILE:HB	1:E:121:LEU:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:11:PHE:CE2	1:M:198:VAL:CG2	3.01	0.44
1:S:135:LEU:HG	1:S:156:ILE:HD13	2.00	0.44
1:O:29:PRO:HB2	1:O:126:THR:CG2	2.48	0.44
1:E:194:VAL:HG13	1:E:198:VAL:HG13	1.99	0.44
1:H:161:MET:HB3	1:H:185:LEU:HB2	2.00	0.44
1:G:145:ASN:HD22	1:G:145:ASN:N	2.16	0.44
1:J:20:VAL:HG22	1:J:194:VAL:HG22	1.99	0.44
1:T:161:MET:HB3	1:T:185:LEU:HB2	1.99	0.44
1:E:66:PHE:HB3	1:E:74:SER:HB3	2.00	0.44
1:A:38:HIS:HB3	1:A:205:TRP:CZ2	2.53	0.44
1:Q:183:ASN:ND2	1:Q:183:ASN:H	2.16	0.43
1:P:202:PRO:O	1:Q:118:ARG:NH2	2.39	0.43
1:N:52:PHE:HB3	1:N:65:ILE:HD12	2.00	0.43
1:E:54:TYR:HB3	1:E:63:ILE:HB	2.00	0.43
1:L:82:ILE:HD13	1:L:82:ILE:HG21	1.14	0.43
1:M:139:GLN:HE21	1:M:143:GLY:N	2.16	0.43
1:E:4:MET:O	1:E:187:TRP:NE1	2.51	0.43
1:H:54:TYR:CG	1:H:63:ILE:HG13	2.53	0.43
1:P:182:PRO:HG2	1:P:186:ASN:HA	2.00	0.43
1:K:39:PHE:CE1	1:K:94:VAL:HG13	2.53	0.43
1:B:54:TYR:HB3	1:B:63:ILE:HB	2.00	0.43
1:R:108:GLU:OE2	1:R:118:ARG:NH1	2.44	0.43
1:J:161:MET:HB3	1:J:185:LEU:HB2	1.99	0.43
1:P:139:GLN:NE2	1:P:143:GLY:H	2.17	0.43
1:N:194:VAL:HG13	1:N:198:VAL:HG13	1.99	0.43
1:G:65:ILE:HD11	1:G:98:THR:HG21	2.00	0.43
1:H:10:VAL:HG12	1:H:12:PRO:HD3	2.00	0.43
1:A:121:LEU:HD23	1:A:122:LYS:HG2	2.01	0.43
1:O:160:ASN:ND2	1:O:187:TRP:H	2.16	0.43
1:N:62:GLU:CG	1:N:127:VAL:HG13	2.48	0.43
1:H:26:LEU:HA	1:H:26:LEU:HD23	1.84	0.43
1:Q:6:ARG:HB2	1:Q:6:ARG:CZ	2.48	0.43
1:B:82:ILE:HG21	1:B:82:ILE:HD13	0.96	0.43
1:K:26:LEU:HD22	1:K:30:LEU:HD21	1.99	0.43
1:M:58:ARG:HG3	3:M:209:HOH:O	2.18	0.43
1:Q:82:ILE:HD13	1:Q:82:ILE:HG21	1.12	0.43
1:K:23:LYS:NZ	3:K:508:HOH:O	2.52	0.43
1:B:67:TRP:CH2	1:B:86:VAL:HG21	2.53	0.43
1:Q:162:TRP:HA	1:Q:183:ASN:ND2	2.34	0.43
1:M:194:VAL:HG22	1:M:198:VAL:HG11	2.01	0.43
1:M:139:GLN:HE21	1:M:143:GLY:CA	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1:GLN:OE1	1:H:191:LYS:CE	2.66	0.43
1:B:160:ASN:ND2	1:B:182:PRO:HG2	2.34	0.43
1:S:160:ASN:ND2	1:S:187:TRP:H	2.16	0.43
1:A:27:THR:OG1	1:A:28:LYS:N	2.51	0.43
1:B:108:GLU:HG2	1:B:118:ARG:HG2	1.99	0.43
1:F:82:ILE:HB	1:F:121:LEU:CD1	2.47	0.43
1:A:186:ASN:C	1:A:186:ASN:HD22	2.23	0.43
1:R:33:PHE:CE1	1:R:63:ILE:HD13	2.54	0.43
1:K:186:ASN:HD22	1:K:187:TRP:N	2.17	0.43
1:I:30:LEU:H	1:I:30:LEU:HD12	1.83	0.43
1:A:82:ILE:HB	1:A:121:LEU:HD12	2.00	0.43
1:C:157:GLY:HA3	1:C:205:TRP:HZ2	1.84	0.43
1:S:139:GLN:HE21	1:S:143:GLY:H	1.66	0.43
1:E:19:TYR:CZ	1:E:195:GLN:HG3	2.53	0.43
1:C:163:ASP:N	1:C:183:ASN:HD21	2.13	0.42
1:B:139:GLN:NE2	1:B:143:GLY:H	2.11	0.42
1:K:139:GLN:NE2	1:K:143:GLY:H	2.17	0.42
1:Q:1:GLN:N	1:Q:1:GLN:HE21	2.17	0.42
1:S:5:SER:O	1:S:6:ARG:CB	2.63	0.42
1:J:76:THR:HB	1:J:81:GLU:HA	2.00	0.42
1:T:139:GLN:HE21	1:T:143:GLY:CA	2.32	0.42
1:O:82:ILE:HB	1:O:121:LEU:HD13	2.01	0.42
1:S:24:ALA:HA	1:S:25:PRO:HD3	1.85	0.42
1:E:91:VAL:O	1:E:91:VAL:HG22	2.20	0.42
1:L:37:LEU:HD21	1:L:51:ILE:CG2	2.49	0.42
1:B:160:ASN:ND2	1:B:187:TRP:H	2.17	0.42
1:N:139:GLN:HE21	1:N:143:GLY:H	1.68	0.42
1:Q:34:THR:HG21	1:Q:166:LEU:HD12	2.02	0.42
1:J:135:LEU:HD21	1:J:159:VAL:HG21	2.01	0.42
1:S:13:LYS:HG2	3:S:317:HOH:O	2.18	0.42
1:O:38:HIS:CE1	1:O:95:HIS:HB2	2.55	0.42
1:B:72:GLY:HA2	1:B:86:VAL:HG23	2.01	0.42
1:K:26:LEU:HD21	1:K:30:LEU:CD2	2.50	0.42
1:P:42:GLU:OE2	1:Q:116:ARG:NH1	2.37	0.42
1:A:204:LEU:HG	1:B:118:ARG:NH2	2.35	0.42
1:I:155:ASP:OD2	1:J:118:ARG:NH1	2.53	0.42
1:P:160:ASN:ND2	1:P:187:TRP:H	2.18	0.42
1:O:38:HIS:HB3	1:O:205:TRP:CZ2	2.55	0.42
1:C:169:ASP:O	1:C:172:ASN:HB2	2.19	0.42
1:P:23:LYS:HE2	1:P:193:GLU:HB2	2.00	0.42
1:I:54:TYR:HB3	1:I:63:ILE:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:6:ARG:HB2	1:Q:6:ARG:NH1	2.35	0.42
1:M:27:THR:HG22	1:M:28:LYS:O	2.20	0.42
1:N:91:VAL:N	3:N:348:HOH:O	2.32	0.42
1:D:71:ILE:HG21	1:D:83:LEU:CD2	2.50	0.42
1:K:108:GLU:HG2	1:K:118:ARG:HG2	2.02	0.42
1:D:54:TYR:HB3	1:D:63:ILE:HB	2.02	0.42
1:Q:16:ASP:HB3	1:Q:17:THR:HG23	2.02	0.42
1:B:26:LEU:O	1:B:27:THR:CG2	2.68	0.42
1:B:204:LEU:HD11	1:C:118:ARG:HG3	2.01	0.42
1:C:197:GLU:OE1	1:D:123:LYS:NZ	2.53	0.42
1:H:38:HIS:CE1	1:H:95:HIS:HB2	2.55	0.42
1:N:101:GLU:HB2	1:N:165:VAL:HG21	2.01	0.42
1:O:91:VAL:HG22	1:O:91:VAL:O	2.20	0.42
1:B:37:LEU:HD21	1:B:51:ILE:HG21	2.00	0.42
1:D:29:PRO:HB2	1:D:126:THR:CG2	2.50	0.42
1:L:100:TRP:CH2	1:L:102:SER:HB2	2.54	0.42
1:L:91:VAL:HG22	3:L:207:HOH:O	2.19	0.42
1:S:29:PRO:HB2	1:S:126:THR:HG22	2.02	0.41
1:Q:183:ASN:HD22	1:Q:183:ASN:N	2.15	0.41
1:K:24:ALA:HB2	1:K:185:LEU:HD13	2.01	0.41
1:A:77:VAL:HB	1:A:121:LEU:HD22	2.01	0.41
1:K:194:VAL:HG13	1:K:198:VAL:HG13	2.02	0.41
1:F:41:THR:HA	1:G:117:VAL:HG11	2.02	0.41
1:H:68:SER:HB3	1:H:71:ILE:HB	2.01	0.41
1:K:27:THR:HG22	1:K:28:LYS:N	2.35	0.41
1:N:83:LEU:HD11	3:N:370:HOH:O	2.19	0.41
1:Q:26:LEU:HG	1:Q:184:VAL:HG22	2.03	0.41
1:A:26:LEU:HB3	1:A:129:ALA:O	2.19	0.41
1:J:52:PHE:HB3	1:J:65:ILE:HD12	2.02	0.41
1:T:47:ARG:HD2	1:T:149:SER:O	2.20	0.41
1:M:139:GLN:HE21	1:M:143:GLY:HA2	1.84	0.41
1:C:71:ILE:HG21	1:C:83:LEU:HD23	2.01	0.41
1:R:66:PHE:HB3	1:R:74:SER:HB3	2.02	0.41
1:Q:137:GLN:HB3	1:Q:146:PHE:CD1	2.56	0.41
1:A:96:ILE:HA	1:A:110:TRP:O	2.20	0.41
1:T:76:THR:HB	1:T:81:GLU:HA	2.02	0.41
1:B:6:ARG:CZ	1:B:6:ARG:CB	2.96	0.41
1:N:54:TYR:HD1	1:N:62:GLU:HB3	1.85	0.41
1:A:204:LEU:HD11	1:B:118:ARG:HG3	2.03	0.41
1:M:42:GLU:CD	1:N:117:VAL:HG12	2.41	0.41
1:T:1:GLN:H1	1:T:191:LYS:HG2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:52:PHE:CB	1:H:65:ILE:HD12	2.47	0.41
1:J:64:LEU:HB3	1:J:76:THR:CG2	2.47	0.41
1:B:139:GLN:HE21	1:B:143:GLY:N	2.16	0.41
1:R:42:GLU:CD	1:S:117:VAL:HG12	2.40	0.41
1:L:3:ASP:HA	1:L:188:ARG:O	2.20	0.41
1:L:52:PHE:HB3	1:L:65:ILE:HD12	2.00	0.41
1:G:96:ILE:HA	1:G:110:TRP:O	2.20	0.41
1:N:62:GLU:HG2	1:N:127:VAL:HG13	2.03	0.41
1:I:100:TRP:HB2	1:I:107:VAL:HG12	2.03	0.41
1:J:45:SER:HB2	3:J:270:HOH:O	2.20	0.41
1:T:3:ASP:HA	1:T:188:ARG:O	2.20	0.41
1:L:96:ILE:HA	1:L:110:TRP:O	2.20	0.41
1:F:118:ARG:HD3	1:J:10:VAL:HG21	2.03	0.41
1:S:62:GLU:CG	1:S:127:VAL:HG13	2.51	0.41
1:M:45:SER:HB2	3:M:207:HOH:O	2.20	0.41
1:L:82:ILE:HG23	1:L:121:LEU:HD13	2.01	0.41
1:P:139:GLN:HE21	1:P:143:GLY:N	2.18	0.41
1:T:139:GLN:HE21	1:T:143:GLY:H	1.68	0.41
1:G:26:LEU:HD21	1:G:30:LEU:HD11	2.02	0.41
1:I:19:TYR:CD1	1:I:134:ILE:HD12	2.56	0.41
1:K:101:GLU:HB2	1:K:165:VAL:HG21	2.03	0.41
1:O:169:ASP:O	1:O:172:ASN:HB2	2.21	0.41
1:O:10:VAL:CG1	1:O:199:PHE:HB2	2.51	0.41
1:P:12:PRO:HB2	1:Q:120:SER:HB2	2.03	0.41
1:I:37:LEU:HD12	1:I:37:LEU:C	2.40	0.41
1:D:194:VAL:HG13	1:D:198:VAL:HG13	2.02	0.41
1:E:24:ALA:HB2	1:E:185:LEU:CD1	2.51	0.41
1:L:3:ASP:OD1	1:L:5:SER:HB2	2.21	0.41
1:P:118:ARG:NH1	1:T:155:ASP:OD2	2.51	0.41
1:K:23:LYS:HE2	1:K:193:GLU:HB2	2.03	0.40
1:G:101:GLU:HB2	1:G:165:VAL:HG21	2.02	0.40
1:D:19:TYR:CD1	1:D:134:ILE:HD12	2.57	0.40
1:L:38:HIS:HB3	1:L:205:TRP:CZ2	2.56	0.40
1:N:108:GLU:HA	3:N:295:HOH:O	2.21	0.40
1:Q:3:ASP:OD1	1:Q:5:SER:HB2	2.20	0.40
1:N:12:PRO:HB2	1:O:120:SER:HB2	2.03	0.40
1:F:158:ASN:ND2	1:F:205:TRP:HE1	2.19	0.40
1:T:26:LEU:HA	1:T:27:THR:HA	1.95	0.40
1:M:26:LEU:HD13	1:M:26:LEU:H	1.86	0.40
1:H:63:ILE:HD11	1:H:127:VAL:HG11	2.03	0.40
1:I:30:LEU:N	1:I:30:LEU:HD12	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:1:GLN:OE1	1:K:191:LYS:HE2	2.22	0.40
1:M:22:LEU:HD22	1:M:190:LEU:HD11	2.03	0.40
1:B:24:ALA:HA	1:B:25:PRO:HD2	1.72	0.40
1:K:105:GLY:O	1:K:120:SER:HA	2.21	0.40
1:N:1:GLN:H1	1:N:191:LYS:HG2	1.86	0.40
1:K:3:ASP:HA	1:K:188:ARG:O	2.22	0.40
1:B:38:HIS:HB3	1:B:205:TRP:CZ2	2.57	0.40
1:P:194:VAL:HG13	1:P:198:VAL:HG13	2.03	0.40
1:G:162:TRP:CD2	1:G:166:LEU:HD11	2.56	0.40
1:A:139:GLN:NE2	1:A:143:GLY:H	2.19	0.40

All (11) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:58:ARG:NH1	1:T:143:GLY:CA[2_656]	1.49	0.71
1:D:123:LYS:NZ	1:I:195:GLN:OE1[2_645]	1.55	0.65
1:D:6:ARG:CD	1:N:188:ARG:NH2[2_646]	1.83	0.37
1:F:145:ASN:ND2	1:L:147:GLU:OE2[2_546]	1.98	0.22
1:D:123:LYS:CE	1:I:195:GLN:OE1[2_645]	2.06	0.14
1:C:58:ARG:NH1	1:J:58:ARG:NH2[2_645]	2.12	0.08
1:N:58:ARG:NH1	1:T:143:GLY:C[2_656]	2.12	0.08
1:D:188:ARG:NH2	1:N:6:ARG:NE[2_646]	2.14	0.06
1:H:1:GLN:NE2	1:P:5:SER:O[2_656]	2.14	0.06
1:D:123:LYS:NZ	1:I:195:GLN:CD[2_645]	2.14	0.06
1:N:58:ARG:NE	1:T:143:GLY:O[2_656]	2.18	0.02

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	204/206 (99%)	192 (94%)	10 (5%)	2 (1%)	19 61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	204/206 (99%)	191 (94%)	8 (4%)	5 (2%)	7	34
1	C	204/206 (99%)	191 (94%)	11 (5%)	2 (1%)	19	61
1	D	204/206 (99%)	192 (94%)	12 (6%)	0	100	100
1	E	204/206 (99%)	191 (94%)	9 (4%)	4 (2%)	9	41
1	F	204/206 (99%)	197 (97%)	6 (3%)	1 (0%)	34	76
1	G	204/206 (99%)	193 (95%)	10 (5%)	1 (0%)	34	76
1	H	204/206 (99%)	194 (95%)	8 (4%)	2 (1%)	19	61
1	I	204/206 (99%)	191 (94%)	13 (6%)	0	100	100
1	J	204/206 (99%)	193 (95%)	10 (5%)	1 (0%)	34	76
1	K	204/206 (99%)	192 (94%)	10 (5%)	2 (1%)	19	61
1	L	204/206 (99%)	194 (95%)	8 (4%)	2 (1%)	19	61
1	M	204/206 (99%)	193 (95%)	9 (4%)	2 (1%)	19	61
1	N	204/206 (99%)	196 (96%)	7 (3%)	1 (0%)	34	76
1	O	204/206 (99%)	193 (95%)	11 (5%)	0	100	100
1	P	204/206 (99%)	191 (94%)	10 (5%)	3 (2%)	13	50
1	Q	204/206 (99%)	191 (94%)	12 (6%)	1 (0%)	34	76
1	R	204/206 (99%)	191 (94%)	11 (5%)	2 (1%)	19	61
1	S	204/206 (99%)	193 (95%)	10 (5%)	1 (0%)	34	76
1	T	204/206 (99%)	192 (94%)	9 (4%)	3 (2%)	13	50
All	All	4080/4120 (99%)	3851 (94%)	194 (5%)	35 (1%)	21	64

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	178	GLY
1	E	26	LEU
1	G	178	GLY
1	L	178	GLY
1	Q	178	GLY
1	B	142	PHE
1	E	178	GLY
1	H	142	PHE
1	J	178	GLY
1	K	26	LEU
1	M	27	THR

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Mol	Chain	Res	Type
1	N	142	PHE
1	P	28	LYS
1	P	142	PHE
1	R	142	PHE
1	S	142	PHE
1	T	142	PHE
1	T	178	GLY
1	C	29	PRO
1	L	142	PHE
1	C	27	THR
1	E	142	PHE
1	K	142	PHE
1	R	28	LYS
1	T	28	LYS
1	A	178	GLY
1	B	26	LEU
1	E	25	PRO
1	F	142	PHE
1	H	25	PRO
1	M	25	PRO
1	A	142	PHE
1	P	27	THR
1	B	29	PRO
1	B	25	PRO

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	180/180 (100%)	166 (92%)	14 (8%)	16	49
1	B	180/180 (100%)	163 (91%)	17 (9%)	11	39
1	C	180/180 (100%)	169 (94%)	11 (6%)	23	61
1	D	180/180 (100%)	173 (96%)	7 (4%)	39	77
1	E	180/180 (100%)	173 (96%)	7 (4%)	39	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	180/180 (100%)	168 (93%)	12 (7%)	20	57
1	G	180/180 (100%)	170 (94%)	10 (6%)	26	65
1	H	180/180 (100%)	165 (92%)	15 (8%)	14	46
1	I	180/180 (100%)	168 (93%)	12 (7%)	20	57
1	J	180/180 (100%)	170 (94%)	10 (6%)	26	65
1	K	180/180 (100%)	161 (89%)	19 (11%)	8	31
1	L	180/180 (100%)	162 (90%)	18 (10%)	9	34
1	M	180/180 (100%)	162 (90%)	18 (10%)	9	34
1	N	180/180 (100%)	165 (92%)	15 (8%)	14	46
1	O	180/180 (100%)	168 (93%)	12 (7%)	20	57
1	P	180/180 (100%)	164 (91%)	16 (9%)	12	42
1	Q	180/180 (100%)	166 (92%)	14 (8%)	16	49
1	R	180/180 (100%)	165 (92%)	15 (8%)	14	46
1	S	180/180 (100%)	172 (96%)	8 (4%)	35	74
1	T	180/180 (100%)	168 (93%)	12 (7%)	20	57
All	All	3600/3600 (100%)	3338 (93%)	262 (7%)	17	52

All (262) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	26	LEU
1	A	27	THR
1	A	43	LEU
1	A	47	ARG
1	A	68	SER
1	A	121	LEU
1	A	122	LYS
1	A	151	SER
1	A	173	THR
1	A	176	LEU
1	A	185	LEU
1	A	186	ASN
1	A	198	VAL
1	B	1	GLN
1	B	5	SER
1	B	6	ARG

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Mol	Chain	Res	Type
1	B	30	LEU
1	B	37	LEU
1	B	38	HIS
1	B	45	SER
1	B	46	THR
1	B	58	ARG
1	B	80	SER
1	B	83	LEU
1	B	86	VAL
1	B	90	THR
1	B	116	ARG
1	B	147	GLU
1	B	176	LEU
1	B	183	ASN
1	C	13	LYS
1	C	63	ILE
1	C	88	GLU
1	C	106	ILE
1	C	172	ASN
1	C	176	LEU
1	C	181	SER
1	C	183	ASN
1	C	185	LEU
1	C	186	ASN
1	C	194	VAL
1	D	1	GLN
1	D	6	ARG
1	D	26	LEU
1	D	43	LEU
1	D	82	ILE
1	D	90	THR
1	D	181	SER
1	E	26	LEU
1	E	30	LEU
1	E	38	HIS
1	E	77	VAL
1	E	149	SER
1	E	182	PRO
1	E	185	LEU
1	F	1	GLN
1	F	23	LYS
1	F	28	LYS

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Mol	Chain	Res	Type
1	F	31	LYS
1	F	43	LEU
1	F	68	SER
1	F	80	SER
1	F	98	THR
1	F	122	LYS
1	F	176	LEU
1	F	185	LEU
1	F	186	ASN
1	G	1	GLN
1	G	30	LEU
1	G	37	LEU
1	G	46	THR
1	G	56	THR
1	G	80	SER
1	G	86	VAL
1	G	147	GLU
1	G	176	LEU
1	G	183	ASN
1	H	1	GLN
1	H	13	LYS
1	H	28	LYS
1	H	30	LEU
1	H	31	LYS
1	H	38	HIS
1	H	63	ILE
1	H	68	SER
1	H	88	GLU
1	H	89	VAL
1	H	171	ILE
1	H	176	LEU
1	H	183	ASN
1	H	185	LEU
1	H	194	VAL
1	I	1	GLN
1	I	6	ARG
1	I	26	LEU
1	I	38	HIS
1	I	68	SER
1	I	80	SER
1	I	82	ILE
1	I	88	GLU

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Mol	Chain	Res	Type
1	I	90	THR
1	I	135	LEU
1	I	173	THR
1	I	181	SER
1	J	30	LEU
1	J	38	HIS
1	J	58	ARG
1	J	76	THR
1	J	135	LEU
1	J	149	SER
1	J	176	LEU
1	J	185	LEU
1	J	197	GLU
1	J	198	VAL
1	K	1	GLN
1	K	17	THR
1	K	23	LYS
1	K	28	LYS
1	K	31	LYS
1	K	43	LEU
1	K	46	THR
1	K	47	ARG
1	K	68	SER
1	K	80	SER
1	K	83	LEU
1	K	98	THR
1	K	121	LEU
1	K	151	SER
1	K	155	ASP
1	K	173	THR
1	K	176	LEU
1	K	185	LEU
1	K	186	ASN
1	L	1	GLN
1	L	5	SER
1	L	6	ARG
1	L	16	ASP
1	L	30	LEU
1	L	37	LEU
1	L	43	LEU
1	L	46	THR
1	L	58	ARG

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Mol	Chain	Res	Type
1	L	80	SER
1	L	83	LEU
1	L	86	VAL
1	L	87	PRO
1	L	90	THR
1	L	94	VAL
1	L	176	LEU
1	L	183	ASN
1	L	185	LEU
1	M	13	LYS
1	M	23	LYS
1	M	25	PRO
1	M	26	LEU
1	M	27	THR
1	M	38	HIS
1	M	45	SER
1	M	63	ILE
1	M	68	SER
1	M	82	ILE
1	M	89	VAL
1	M	172	ASN
1	M	176	LEU
1	M	181	SER
1	M	183	ASN
1	M	185	LEU
1	M	186	ASN
1	M	197	GLU
1	N	1	GLN
1	N	6	ARG
1	N	28	LYS
1	N	38	HIS
1	N	68	SER
1	N	71	ILE
1	N	82	ILE
1	N	90	THR
1	N	135	LEU
1	N	155	ASP
1	N	174	ILE
1	N	176	LEU
1	N	181	SER
1	N	185	LEU
1	N	195	GLN

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Mol	Chain	Res	Type
1	O	26	LEU
1	O	30	LEU
1	O	38	HIS
1	O	43	LEU
1	O	58	ARG
1	O	77	VAL
1	O	89	VAL
1	O	107	VAL
1	O	149	SER
1	O	173	THR
1	O	197	GLU
1	O	198	VAL
1	P	1	GLN
1	P	23	LYS
1	P	31	LYS
1	P	43	LEU
1	P	46	THR
1	P	47	ARG
1	P	58	ARG
1	P	68	SER
1	P	98	THR
1	P	121	LEU
1	P	135	LEU
1	P	171	ILE
1	P	173	THR
1	P	176	LEU
1	P	185	LEU
1	P	186	ASN
1	Q	1	GLN
1	Q	27	THR
1	Q	30	LEU
1	Q	37	LEU
1	Q	56	THR
1	Q	58	ARG
1	Q	86	VAL
1	Q	90	THR
1	Q	109	PHE
1	Q	147	GLU
1	Q	176	LEU
1	Q	183	ASN
1	Q	185	LEU
1	Q	197	GLU

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Mol	Chain	Res	Type
1	R	1	GLN
1	R	13	LYS
1	R	26	LEU
1	R	63	ILE
1	R	68	SER
1	R	88	GLU
1	R	89	VAL
1	R	171	ILE
1	R	172	ASN
1	R	176	LEU
1	R	183	ASN
1	R	185	LEU
1	R	186	ASN
1	R	194	VAL
1	R	197	GLU
1	S	1	GLN
1	S	38	HIS
1	S	68	SER
1	S	82	ILE
1	S	90	THR
1	S	174	ILE
1	S	181	SER
1	S	195	GLN
1	T	6	ARG
1	T	26	LEU
1	T	27	THR
1	T	30	LEU
1	T	38	HIS
1	T	43	LEU
1	T	76	THR
1	T	77	VAL
1	T	149	SER
1	T	173	THR
1	T	176	LEU
1	T	185	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (128) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	95	HIS
1	A	137	GLN

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Mol	Chain	Res	Type
1	A	139	GLN
1	A	158	ASN
1	A	160	ASN
1	A	186	ASN
1	B	137	GLN
1	B	139	GLN
1	B	145	ASN
1	B	160	ASN
1	B	172	ASN
1	B	183	ASN
1	B	203	GLN
1	C	137	GLN
1	C	139	GLN
1	C	145	ASN
1	C	158	ASN
1	C	172	ASN
1	C	183	ASN
1	C	186	ASN
1	C	203	GLN
1	D	95	HIS
1	D	137	GLN
1	D	139	GLN
1	D	160	ASN
1	E	59	GLN
1	E	95	HIS
1	E	137	GLN
1	E	139	GLN
1	E	158	ASN
1	E	160	ASN
1	E	203	GLN
1	F	38	HIS
1	F	95	HIS
1	F	137	GLN
1	F	139	GLN
1	F	158	ASN
1	F	160	ASN
1	F	186	ASN
1	G	38	HIS
1	G	137	GLN
1	G	139	GLN
1	G	145	ASN
1	G	160	ASN

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Mol	Chain	Res	Type
1	G	172	ASN
1	G	183	ASN
1	G	203	GLN
1	H	137	GLN
1	H	139	GLN
1	H	158	ASN
1	H	172	ASN
1	H	183	ASN
1	H	186	ASN
1	H	203	GLN
1	I	95	HIS
1	I	137	GLN
1	I	139	GLN
1	I	158	ASN
1	I	160	ASN
1	J	59	GLN
1	J	137	GLN
1	J	139	GLN
1	J	160	ASN
1	J	203	GLN
1	K	38	HIS
1	K	95	HIS
1	K	137	GLN
1	K	139	GLN
1	K	160	ASN
1	K	186	ASN
1	L	38	HIS
1	L	95	HIS
1	L	137	GLN
1	L	139	GLN
1	L	160	ASN
1	L	183	ASN
1	L	203	GLN
1	M	137	GLN
1	M	139	GLN
1	M	145	ASN
1	M	158	ASN
1	M	172	ASN
1	M	183	ASN
1	M	186	ASN
1	N	95	HIS
1	N	137	GLN

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Mol	Chain	Res	Type
1	N	139	GLN
1	N	158	ASN
1	N	160	ASN
1	N	203	GLN
1	O	59	GLN
1	O	95	HIS
1	O	137	GLN
1	O	139	GLN
1	O	160	ASN
1	P	38	HIS
1	P	95	HIS
1	P	137	GLN
1	P	139	GLN
1	P	158	ASN
1	P	160	ASN
1	P	186	ASN
1	Q	1	GLN
1	Q	38	HIS
1	Q	95	HIS
1	Q	137	GLN
1	Q	139	GLN
1	Q	160	ASN
1	Q	183	ASN
1	Q	203	GLN
1	R	1	GLN
1	R	137	GLN
1	R	139	GLN
1	R	145	ASN
1	R	158	ASN
1	R	172	ASN
1	R	183	ASN
1	R	186	ASN
1	R	203	GLN
1	S	137	GLN
1	S	139	GLN
1	S	160	ASN
1	T	59	GLN
1	T	137	GLN
1	T	139	GLN
1	T	158	ASN
1	T	160	ASN

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](#)

Of 40 ligands modelled in this entry, 40 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	206/206 (100%)	-0.36	3 (1%) 76 49	6, 16, 27, 32	0
1	B	206/206 (100%)	-0.48	0 100 100	4, 14, 25, 31	0
1	C	206/206 (100%)	-0.52	0 100 100	4, 13, 22, 34	0
1	D	206/206 (100%)	-0.40	0 100 100	4, 16, 28, 33	0
1	E	206/206 (100%)	-0.38	0 100 100	7, 17, 28, 33	0
1	F	206/206 (100%)	-0.38	0 100 100	5, 16, 28, 34	0
1	G	206/206 (100%)	-0.36	1 (0%) 91 76	8, 17, 28, 32	0
1	H	206/206 (100%)	-0.34	0 100 100	9, 18, 29, 35	0
1	I	206/206 (100%)	-0.34	0 100 100	9, 17, 29, 35	0
1	J	206/206 (100%)	-0.44	0 100 100	6, 15, 25, 33	0
1	K	206/206 (100%)	-0.34	0 100 100	7, 16, 27, 36	0
1	L	206/206 (100%)	-0.42	1 (0%) 91 76	6, 15, 27, 38	0
1	M	206/206 (100%)	-0.40	0 100 100	6, 15, 27, 36	0
1	N	206/206 (100%)	-0.37	0 100 100	6, 17, 28, 34	0
1	O	206/206 (100%)	-0.33	0 100 100	7, 16, 27, 36	0
1	P	206/206 (100%)	-0.10	2 (0%) 84 60	8, 20, 32, 44	0
1	Q	206/206 (100%)	-0.38	1 (0%) 91 76	7, 15, 26, 35	0
1	R	206/206 (100%)	-0.44	2 (0%) 84 60	5, 14, 26, 35	0
1	S	206/206 (100%)	-0.37	0 100 100	7, 17, 29, 34	0
1	T	206/206 (100%)	-0.18	3 (1%) 76 49	10, 20, 32, 43	0
All	All	4120/4120 (100%)	-0.37	13 (0%) 94 84	4, 16, 29, 44	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	GLN	3.8
1	G	27	THR	3.0
1	R	1	GLN	2.5
1	A	179	PRO	2.4
1	P	181	SER	2.4
1	Q	88	GLU	2.4
1	P	1	GLN	2.3
1	A	178	GLY	2.2
1	T	88	GLU	2.1
1	T	90	THR	2.1
1	L	27	THR	2.1
1	T	27	THR	2.1
1	R	58	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 ⓘ

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
2	CA	A	5002	1/1	0.93	0.49	7.13	62,62,62,62	0
2	CA	I	5018	1/1	0.80	0.25	1.29	65,65,65,65	0
2	CA	D	5008	1/1	0.91	0.23	0.86	49,49,49,49	0
2	CA	K	5022	1/1	0.89	0.16	-0.99	40,40,40,40	0
2	CA	F	5012	1/1	0.92	0.14	-1.32	68,68,68,68	0
2	CA	M	5026	1/1	0.83	0.15	-1.62	59,59,59,59	0
2	CA	G	5014	1/1	0.92	0.09	-2.17	51,51,51,51	0
2	CA	S	5038	1/1	0.86	0.12	-2.25	29,29,29,29	0
2	CA	T	5040	1/1	0.87	0.11	-2.26	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	C	5005	1/1	0.88	0.07	-2.54	32,32,32,32	0
2	CA	S	5037	1/1	0.84	0.09	-3.17	22,22,22,22	0
2	CA	T	5039	1/1	0.93	0.07	-	45,45,45,45	0
2	CA	L	5024	1/1	0.91	0.16	-	52,52,52,52	0
2	CA	G	5013	1/1	0.83	0.11	-	48,48,48,48	0
2	CA	O	5030	1/1	0.95	0.27	-	54,54,54,54	0
2	CA	O	5029	1/1	0.81	0.09	-	40,40,40,40	0
2	CA	R	5035	1/1	0.95	0.07	-	35,35,35,35	0
2	CA	D	5007	1/1	0.92	0.16	-	25,25,25,25	0
2	CA	B	5004	1/1	0.80	0.15	-	55,55,55,55	0
2	CA	E	5009	1/1	0.96	0.07	-	23,23,23,23	0
2	CA	K	5021	1/1	0.80	0.11	-	32,32,32,32	0
2	CA	I	5017	1/1	0.92	0.10	-	35,35,35,35	0
2	CA	Q	5034	1/1	0.86	0.10	-	32,32,32,32	0
2	CA	N	5028	1/1	0.85	0.26	-	48,48,48,48	0
2	CA	C	5003	1/1	0.96	0.05	-	28,28,28,28	0
2	CA	E	5010	1/1	0.79	0.13	-	80,80,80,80	0
2	CA	B	5006	1/1	0.94	0.06	-	34,34,34,34	0
2	CA	L	5023	1/1	0.90	0.09	-	37,37,37,37	0
2	CA	J	5020	1/1	0.86	0.15	-	43,43,43,43	0
2	CA	P	5031	1/1	0.90	0.07	-	35,35,35,35	0
2	CA	H	5015	1/1	0.87	0.13	-	44,44,44,44	0
2	CA	J	5019	1/1	0.89	0.12	-	41,41,41,41	0
2	CA	M	5025	1/1	0.84	0.09	-	36,36,36,36	0
2	CA	N	5027	1/1	0.92	0.10	-	30,30,30,30	0
2	CA	H	5016	1/1	0.53	0.24	-	57,57,57,57	0
2	CA	R	5036	1/1	0.81	0.14	-	53,53,53,53	0
2	CA	F	5011	1/1	0.97	0.08	-	27,27,27,27	0
2	CA	A	5001	1/1	0.96	0.05	-	20,20,20,20	0
2	CA	Q	5033	1/1	0.95	0.11	-	36,36,36,36	0
2	CA	P	5032	1/1	0.72	0.14	-	72,72,72,72	0

6.5 Other polymers

There are no such residues in this entry.