



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2024 – 12:11 PM EDT

PDB ID : 8EO8
Title : Cross-reactive 3180 TCR recognition of HLA-B*35:01-NP8 epitope from 2005 H1N1 influenza strain
Authors : Littler, D.R.; Rossjohn, J.
Deposited on : 2022-10-02
Resolution : 2.30 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

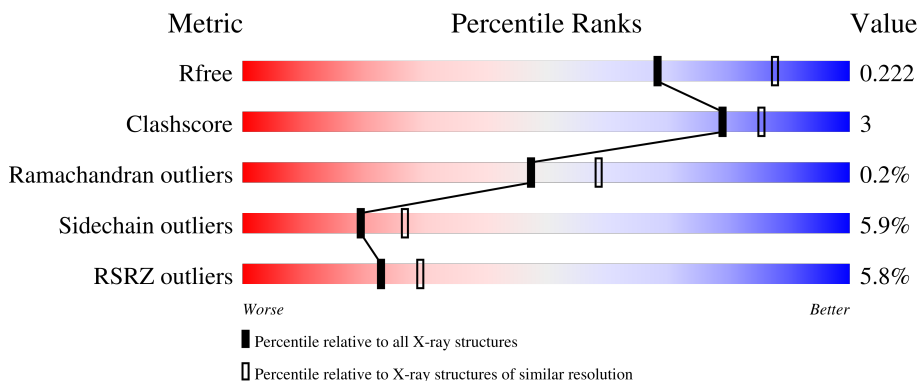
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	 9% 90% 9%
1	F	276	 6% 91% 9%
1	K	276	 8% 82% 9% 8%
1	P	276	 12% 89% 11%
2	B	100	 % 90% 8%

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Mol	Chain	Length	Quality of chain
2	G	100	 88% 11%
2	L	100	 91% 9%
2	Q	100	 88% 10%
3	C	9	 89% 11%
3	H	9	 100%
3	M	9	 100%
3	R	9	 100%
4	D	206	 92% 7%
4	I	206	 91% 8%
4	N	206	 87% 9%
4	S	206	 87% 9%
5	E	246	 78% 19%
5	J	246	 88% 10%
5	O	246	 88% 10%
5	T	246	 87% 9%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 28288 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	275	Total	C	N	O	S	0	1	0
			2258	1408	411	431	8			
1	F	275	Total	C	N	O	S	0	1	0
			2261	1409	414	431	7			
1	K	253	Total	C	N	O	S	0	0	0
			2073	1302	377	387	7			
1	P	275	Total	C	N	O	S	0	0	0
			2250	1403	410	430	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	G	99	Total	C	N	O	S	0	2	0
			848	540	145	160	3			
2	L	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	Q	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
G	0	MET	-	initiating methionine	UNP P61769
L	0	MET	-	initiating methionine	UNP P61769
Q	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Nucleoprotein NP8 epitope.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			72	48	10	13	1			
3	H	9	Total	C	N	O	S	0	0	0
			72	48	10	13	1			
3	M	9	Total	C	N	O	S	0	0	0
			72	48	10	13	1			
3	R	9	Total	C	N	O	S	0	0	0
			72	48	10	13	1			

- Molecule 4 is a protein called 3180 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	206	Total	C	N	O	S	0	0	0
			1597	995	267	328	7			
4	I	206	Total	C	N	O	S	0	0	0
			1597	995	267	328	7			
4	N	199	Total	C	N	O	S	0	0	0
			1539	956	260	316	7			
4	S	199	Total	C	N	O	S	0	0	0
			1539	956	260	316	7			

- Molecule 5 is a protein called 3180 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	246	Total	C	N	O	S	0	0	0
			1942	1222	335	376	9			
5	J	246	Total	C	N	O	S	0	2	0
			1961	1233	340	378	10			
5	O	246	Total	C	N	O	S	0	0	0
			1942	1222	335	376	9			
5	T	244	Total	C	N	O	S	0	0	0
			1928	1215	333	371	9			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	151	Total	O	0	0
			151	151		
6	B	77	Total	O	0	0
			77	77		
6	C	6	Total	O	0	0
			6	6		

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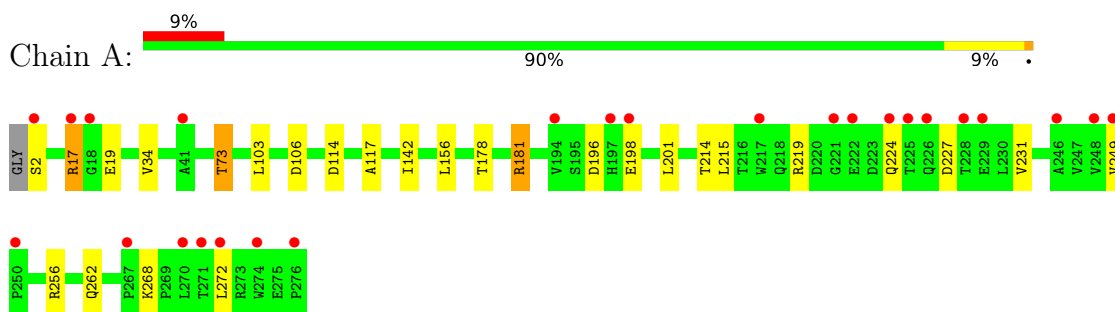
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	70	Total 70	O 70	0	0
6	E	89	Total 89	O 89	0	0
6	F	190	Total 190	O 190	0	0
6	G	86	Total 86	O 86	0	0
6	H	7	Total 7	O 7	0	0
6	I	95	Total 95	O 95	0	0
6	J	104	Total 104	O 104	0	0
6	K	189	Total 189	O 189	0	0
6	L	84	Total 84	O 84	0	0
6	M	8	Total 8	O 8	0	0
6	N	96	Total 96	O 96	0	0
6	O	114	Total 114	O 114	0	0
6	P	162	Total 162	O 162	0	0
6	Q	67	Total 67	O 67	0	0
6	R	9	Total 9	O 9	0	0
6	S	81	Total 81	O 81	0	0
6	T	85	Total 85	O 85	0	0

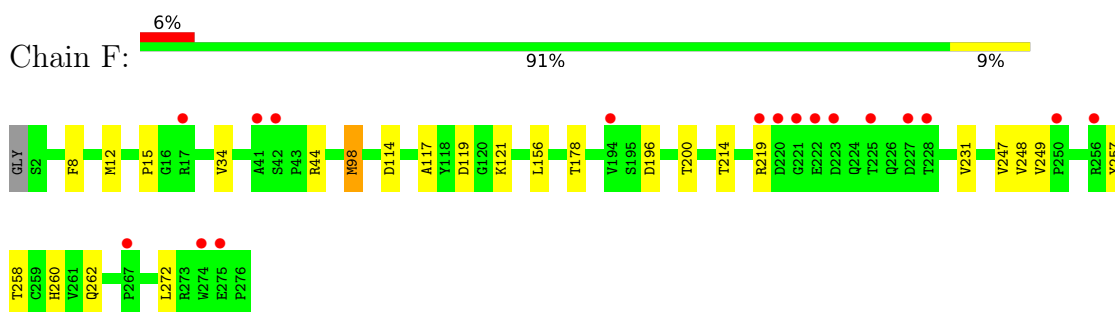
3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

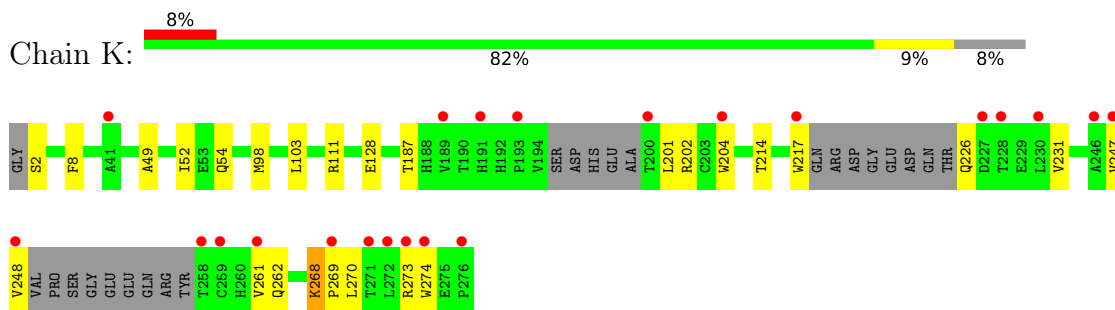
- Molecule 1: MHC class I antigen



- Molecule 1: MHC class I antigen

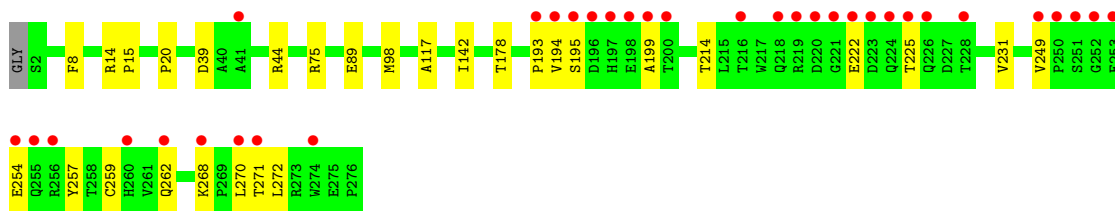


- Molecule 1: MHC class I antigen

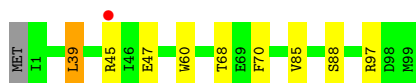
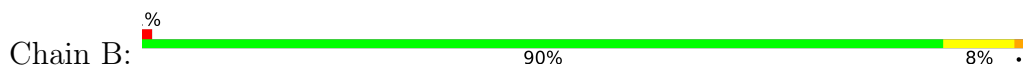


- Molecule 1: MHC class I antigen

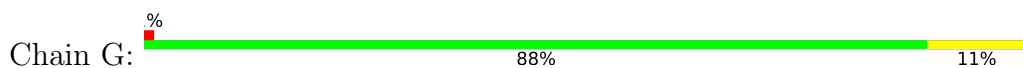




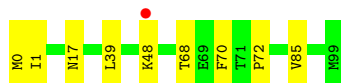
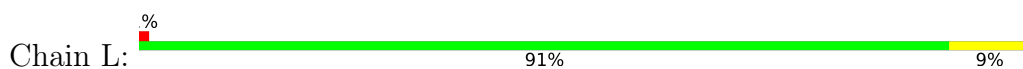
- Molecule 2: Beta-2-microglobulin



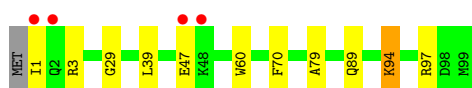
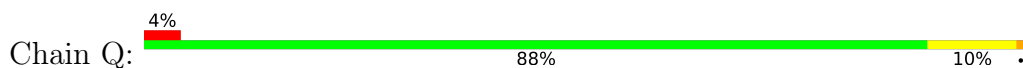
- Molecule 2: Beta-2-microglobulin



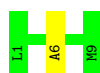
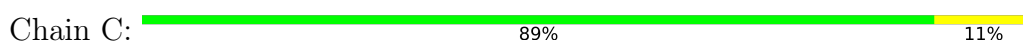
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 3: Nucleoprotein NP8 epitope



- Molecule 3: Nucleoprotein NP8 epitope



There are no outlier residues recorded for this chain.

- Molecule 3: Nucleoprotein NP8 epitope

Chain M:  100%

There are no outlier residues recorded for this chain.

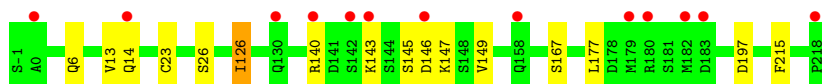
- Molecule 3: Nucleoprotein NP8 epitope

Chain R:  100%


There are no outlier residues recorded for this chain.

- Molecule 4: 3180 alpha chain

Chain D:  6% 92% 7%




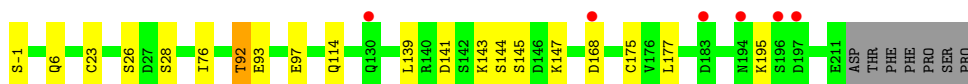
- Molecule 4: 3180 alpha chain

Chain I:  3% 91% 8%




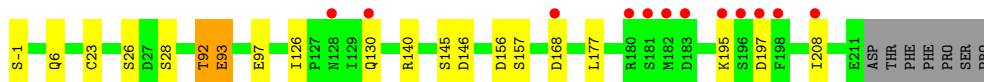
- Molecule 4: 3180 alpha chain

Chain N:  3% 87% 9%




- Molecule 4: 3180 alpha chain

Chain S:  6% 87% 9%

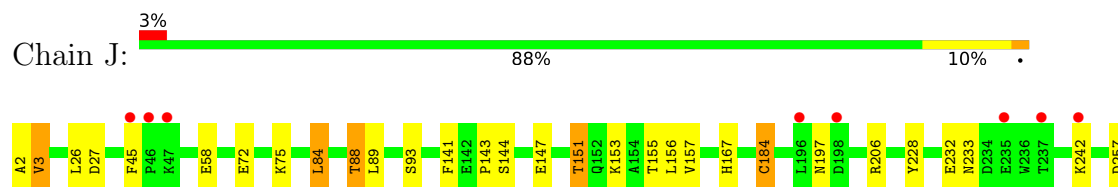


- Molecule 5: 3180 beta chain

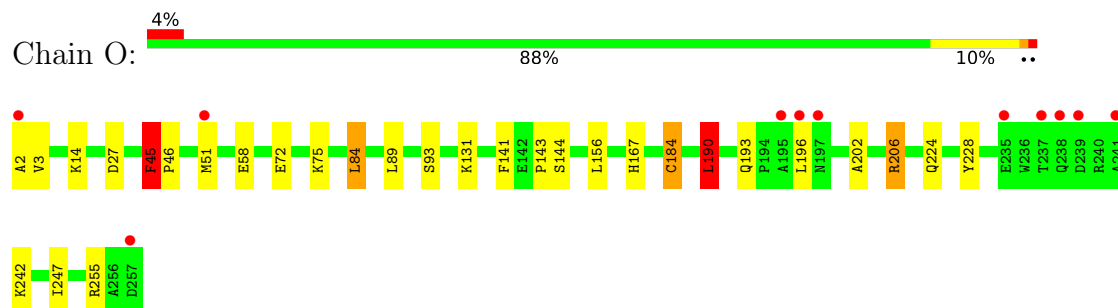
Chain E:  9% 78% 19%



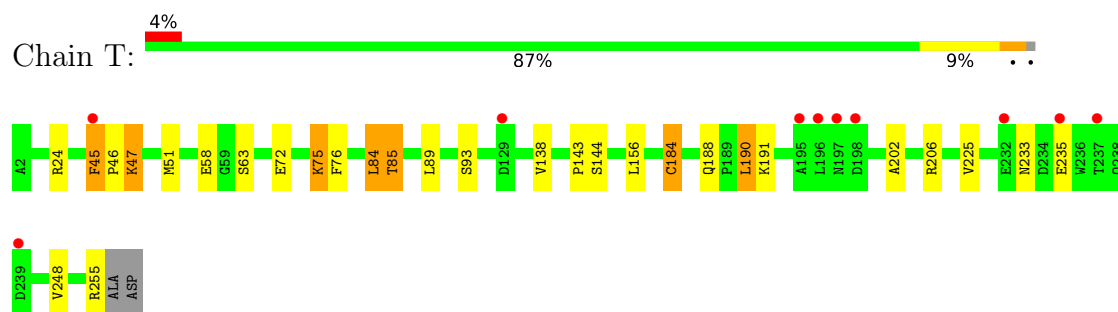
- Molecule 5: 3180 beta chain



- Molecule 5: 3180 beta chain



- Molecule 5: 3180 beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	168.09Å 79.47Å 172.17Å 90.00° 95.53° 90.00°	Depositor
Resolution (Å)	48.95 – 2.30 48.95 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.95-2.30) 100.0 (48.95-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.29Å)	Xtrriage
Refinement program	BUSTER, PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.181 , 0.219 0.186 , 0.222	Depositor DCC
R_{free} test set	10122 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtrriage
Anisotropy	0.165	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.000 for l,-k,h	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28288	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.21 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.0722e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.53	0/2321	0.67	0/3155
1	F	0.53	0/2324	0.66	0/3159
1	K	0.51	0/2130	0.66	0/2893
1	P	0.49	0/2313	0.65	0/3145
2	B	0.52	0/852	0.69	0/1152
2	G	0.55	0/871	0.69	0/1177
2	L	0.51	0/860	0.68	0/1162
2	Q	0.51	0/852	0.67	0/1152
3	C	0.62	0/73	0.65	0/96
3	H	0.62	0/73	0.65	0/96
3	M	0.66	0/73	0.69	0/96
3	R	0.68	0/73	0.65	0/96
4	D	0.48	0/1631	0.68	0/2210
4	I	0.50	0/1631	0.69	0/2210
4	N	0.50	0/1569	0.69	0/2125
4	S	0.50	0/1569	0.70	0/2125
5	E	0.52	0/1993	0.73	0/2712
5	J	0.54	0/2012	0.69	0/2736
5	O	0.53	0/1993	0.72	1/2712 (0.0%)
5	T	0.54	0/1979	0.73	1/2694 (0.0%)
All	All	0.52	0/27192	0.69	2/36903 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	190	LEU	CA-CB-CG	6.93	131.24	115.30
5	T	188	GLN	C-N-CD	5.10	139.12	128.40

There are no chirality outliers.

There are no planarity outliers.

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	2258	0	2119	12	0
1	F	2261	0	2123	10	0
1	K	2073	0	1962	14	0
1	P	2250	0	2111	11	0
2	B	829	0	794	3	0
2	G	848	0	818	6	0
2	L	837	0	803	2	0
2	Q	829	0	794	3	0
3	C	72	0	78	1	0
3	H	72	0	78	0	0
3	M	72	0	78	0	0
3	R	72	0	78	0	0
4	D	1597	0	1522	9	0
4	I	1597	0	1522	7	0
4	N	1539	0	1474	8	0
4	S	1539	0	1474	5	0
5	E	1942	0	1861	29	0
5	J	1961	0	1881	16	0
5	O	1942	0	1861	12	0
5	T	1928	0	1852	18	0
6	A	151	0	0	1	0
6	B	77	0	0	0	0
6	C	6	0	0	0	0
6	D	70	0	0	0	0
6	E	89	0	0	1	0
6	F	190	0	0	1	0
6	G	86	0	0	0	0
6	H	7	0	0	0	0
6	I	95	0	0	0	0
6	J	104	0	0	2	0
6	K	189	0	0	1	0
6	L	84	0	0	0	0
6	M	8	0	0	0	0
6	N	96	0	0	0	0
6	O	114	0	0	0	0
6	P	162	0	0	1	0
6	Q	67	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	R	9	0	0	0	0
6	S	81	0	0	0	0
6	T	85	0	0	0	0
All	All	28288	0	25283	147	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 3.

All (147) 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:D:13:VAL:O	4:D:126:ILE:HG12	1.73	0.88
4:D:14:GLN:HA	4:D:126:ILE:HG13	1.58	0.83
2:L:48:LYS:O	2:L:68:THR:HG22	1.81	0.80
5:E:236:TRP:HZ2	5:E:243:PRO:HD3	1.46	0.79
5:J:3:VAL:CG1	5:J:26:LEU:HD12	2.15	0.76
5:E:3:VAL:CG1	5:E:26:LEU:HD12	2.16	0.76
4:I:149:VAL:HG21	5:J:157:VAL:HG21	1.68	0.75
4:D:6:GLN:HG3	4:D:23:CYS:SG	2.29	0.73
4:D:143:LYS:HE3	5:E:250:ALA:HA	1.72	0.72
5:T:24:ARG:HH11	5:T:85:THR:CG2	2.02	0.72
1:K:247:VAL:O	1:K:248:VAL:HG12	1.90	0.71
5:E:236:TRP:CZ2	5:E:243:PRO:HD3	2.26	0.71
5:T:138:VAL:HG12	5:T:248:VAL:HG12	1.75	0.69
5:E:2:ALA:HA	5:E:27:ASP:OD1	1.94	0.67
5:E:141:PHE:HB2	5:E:157:VAL:HG22	1.77	0.66
5:T:190:LEU:C	5:T:190:LEU:HD23	2.16	0.65
5:E:45:PHE:HB3	5:E:46:PRO:HD2	1.79	0.65
5:J:141:PHE:HB2	5:J:157:VAL:HG22	1.78	0.64
5:E:169:GLU:HG3	5:E:226:GLN:HB3	1.79	0.64
1:F:121:LYS:HG3	2:G:1[B]:ILE:HG21	1.80	0.64
1:F:119:ASP:O	2:G:1[B]:ILE:HG23	1.98	0.64
5:O:45:PHE:CG	5:O:46:PRO:HD2	2.33	0.62
5:E:157:VAL:HG12	5:E:206:ARG:HG2	1.81	0.62
1:A:73:THR:HG21	3:C:6:ALA:HB1	1.83	0.61
5:E:58:GLU:HG3	5:E:84:LEU:HD13	1.83	0.61
5:T:190:LEU:CD2	5:T:202:ALA:HB3	2.31	0.60
1:K:8:PHE:CE1	1:K:98:MET:HG3	2.38	0.59
5:T:190:LEU:HD23	5:T:190:LEU:O	2.02	0.59
4:I:6:GLN:HG3	4:I:23:CYS:SG	2.43	0.58
5:O:58:GLU:HG3	5:O:84:LEU:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ILE:HD11	5:T:24:ARG:HD2	1.86	0.57
5:J:147:GLU:OE2	5:J:155:THR:HG23	2.04	0.57
4:I:166:ASP:HB3	4:I:169:VAL:HG22	1.87	0.57
5:O:190:LEU:HD22	5:O:202:ALA:HB3	1.88	0.56
5:J:141:PHE:HB2	5:J:157:VAL:CG2	2.34	0.56
4:N:-1:SER:HB2	4:N:114:GLN:HG2	1.88	0.56
4:N:92:THR:HG23	4:N:93:GLU:HG3	1.87	0.55
1:K:111:ARG:CZ	1:K:128:GLU:HG2	2.36	0.55
5:E:141:PHE:HB2	5:E:157:VAL:CG2	2.37	0.55
4:N:177:LEU:HB3	5:O:184:CYS:HB3	1.87	0.55
4:N:6:GLN:HG3	4:N:23:CYS:SG	2.47	0.54
5:J:58:GLU:HG3	5:J:84:LEU:HD13	1.90	0.53
1:F:8:PHE:CE2	1:F:98:MET:HG3	2.44	0.52
5:O:224:GLN:HG3	5:O:247:ILE:HG23	1.91	0.52
5:J:167:HIS:HB3	5:J:228:TYR:HB2	1.90	0.52
4:D:14:GLN:HA	4:D:126:ILE:CG1	2.36	0.52
4:D:149:VAL:HG21	5:E:157:VAL:HG21	1.92	0.51
5:E:167:HIS:HB3	5:E:228:TYR:HB2	1.91	0.51
5:T:24:ARG:CD	5:T:85:THR:HG23	2.41	0.51
4:I:92:THR:HG23	4:I:93:GLU:HG3	1.93	0.51
1:F:214:THR:HB	1:F:262:GLN:HB2	1.93	0.51
5:J:151:THR:HG23	5:J:153:LYS:HB2	1.92	0.51
1:P:249:VAL:HG21	1:P:254:GLU:HA	1.93	0.51
4:N:141:ASP:HB3	4:N:144:SER:O	2.11	0.50
1:A:214:THR:HB	1:A:262:GLN:HB2	1.93	0.50
2:G:49:VAL:HG22	2:G:68:THR:HG23	1.93	0.50
1:A:219:ARG:HD3	1:A:256:ARG:HE	1.75	0.50
4:D:177:LEU:HB3	5:E:184:CYS:HB3	1.92	0.50
4:I:149:VAL:CG2	5:J:157:VAL:HG21	2.39	0.50
5:E:3:VAL:HG12	5:E:26:LEU:HD12	1.93	0.49
4:I:177:LEU:HB3	5:J:184:CYS:HB3	1.93	0.49
4:I:141:ASP:HB3	4:I:144:SER:O	2.12	0.49
2:L:17:ASN:HA	2:L:72:PRO:O	2.11	0.49
5:E:72:GLU:HB3	5:E:75:LYS:HB3	1.94	0.49
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.48	0.49
5:T:46:PRO:HD2	5:T:47:LYS:HE3	1.93	0.49
1:F:249:VAL:HG23	1:F:257:TYR:CE1	2.48	0.48
1:P:270:LEU:HD13	1:P:272:LEU:HD13	1.94	0.48
1:A:17:ARG:HB2	6:A:406:HOH:O	2.12	0.48
5:E:236:TRP:CZ2	5:E:242:LYS:HA	2.49	0.48
5:E:236:TRP:HZ2	5:E:242:LYS:HA	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:49:VAL:HG22	2:G:68:THR:CG2	2.43	0.48
1:A:2:SER:HB3	1:A:103:LEU:O	2.12	0.48
1:K:214:THR:HB	1:K:262:GLN:HB2	1.94	0.48
5:O:2:ALA:HA	5:O:27:ASP:OD1	2.13	0.48
1:P:214:THR:HB	1:P:262:GLN:HB2	1.94	0.48
1:K:261:VAL:HG22	1:K:270:LEU:HB2	1.96	0.48
5:J:88:THR:HG22	6:J:310:HOH:O	2.14	0.48
5:E:230:LEU:HD12	5:E:243:PRO:HD2	1.95	0.48
5:E:24:ARG:HD2	1:P:142:ILE:HD11	1.96	0.48
4:S:177:LEU:HB3	5:T:184:CYS:HB3	1.96	0.47
5:E:10:ARG:HD3	5:E:228:TYR:CG	2.49	0.47
5:E:20:LYS:HE2	5:E:88:THR:HG21	1.96	0.47
5:E:143:PRO:HD3	5:E:156:LEU:HG	1.97	0.47
5:T:143:PRO:HD3	5:T:156:LEU:HG	1.97	0.47
5:J:2:ALA:HA	5:J:27:ASP:OD1	2.15	0.47
1:A:224:GLN:HG3	1:A:227:ASP:HB2	1.97	0.46
1:P:8:PHE:CE2	1:P:98:MET:HG3	2.49	0.46
5:T:24:ARG:HD2	5:T:85:THR:HG23	1.97	0.46
4:N:139:LEU:HB3	5:O:141:PHE:HB3	1.98	0.46
1:A:201:LEU:HD12	1:A:249:VAL:HG21	1.96	0.46
2:B:39:LEU:HD23	2:B:68:THR:HG22	1.98	0.46
1:P:89:GLU:H	1:P:89:GLU:CD	2.19	0.46
5:E:137:GLU:HG3	6:E:307:HOH:O	2.15	0.46
5:T:58:GLU:HG3	5:T:84:LEU:HD13	1.98	0.45
1:K:201:LEU:HD11	1:K:274:TRP:HB2	1.98	0.45
1:K:268:LYS:HG3	1:K:269:PRO:HD2	1.97	0.45
1:P:117:ALA:HB2	2:Q:60:TRP:CE2	2.51	0.45
5:O:143:PRO:HD3	5:O:156:LEU:HG	1.98	0.45
1:P:20:PRO:HG3	1:P:75:ARG:HA	1.99	0.45
1:F:200:THR:HG22	1:F:248:VAL:HG22	1.98	0.45
5:J:3:VAL:HG13	5:J:26:LEU:HD12	1.95	0.45
4:S:6:GLN:HG2	4:S:23:CYS:SG	2.57	0.45
1:K:49:ALA:O	1:K:52:ILE:HG22	2.17	0.45
5:J:147:GLU:O	5:J:151:THR:HG22	2.17	0.45
1:K:187:THR:HG21	1:K:261:VAL:HG21	1.99	0.44
1:K:247:VAL:HG13	1:K:248:VAL:N	2.32	0.44
1:P:193:PRO:HA	1:P:199:ALA:HA	1.98	0.44
5:J:143:PRO:HD3	5:J:156:LEU:HG	1.98	0.44
4:S:126:ILE:CG2	4:S:157:SER:HB3	2.48	0.44
5:J:88:THR:CG2	6:J:310:HOH:O	2.66	0.44
1:P:178:THR:HG22	6:P:439:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:168:ASP:HB3	4:S:195:LYS:HD2	2.00	0.43
1:F:117:ALA:HB2	2:G:60:TRP:CE2	2.53	0.43
2:G:69:GLU:H	2:G:69:GLU:CD	2.21	0.43
4:N:-1:SER:HB2	4:N:114:GLN:CG	2.49	0.43
5:T:190:LEU:HD21	5:T:202:ALA:HB3	1.99	0.43
4:S:92:THR:HG23	4:S:93:GLU:HG2	2.01	0.42
1:A:114:ASP:OD2	1:A:156:LEU:HD11	2.19	0.42
5:O:167:HIS:HB3	5:O:228:TYR:HB2	1.99	0.42
1:K:54:GLN:HG3	6:K:335:HOH:O	2.19	0.42
2:Q:79:ALA:HB2	2:Q:94:LYS:HE3	2.00	0.42
1:A:117:ALA:HB2	2:B:60:TRP:CD2	2.54	0.42
1:K:217:TRP:CG	1:K:247:VAL:HB	2.54	0.42
5:T:75:LYS:HG2	5:T:76:PHE:CE2	2.55	0.42
5:T:24:ARG:HH11	5:T:85:THR:HG23	1.84	0.42
5:T:190:LEU:C	5:T:190:LEU:CD2	2.85	0.42
5:E:8:PRO:HG2	5:E:11:VAL:CG2	2.50	0.41
5:E:170:LEU:HA	5:E:224:GLN:O	2.20	0.41
1:P:249:VAL:HG23	1:P:257:TYR:CE1	2.54	0.41
1:F:114:ASP:OD2	1:F:156:LEU:HD11	2.20	0.41
1:F:178:THR:HG22	6:F:461:HOH:O	2.20	0.41
1:F:258:THR:HG23	1:F:260:HIS:NE2	2.35	0.41
4:D:14:GLN:OE1	4:D:126:ILE:HD12	2.21	0.41
5:E:129:ASP:OD2	5:E:131:LYS:HB2	2.20	0.41
5:E:196:LEU:HD23	5:E:197:ASN:H	1.85	0.41
5:E:217:PRO:HA	5:E:254:GLY:HA3	2.03	0.41
4:N:175:CYS:HB3	5:O:206:ARG:NH1	2.35	0.41
5:T:190:LEU:HD22	5:T:202:ALA:HB3	2.02	0.41
1:A:178:THR:HA	1:A:181:ARG:HD2	2.03	0.41
4:D:145:SER:C	4:D:147:LYS:HG2	2.42	0.40
5:O:193:GLN:HB3	5:O:196:LEU:HD13	2.03	0.40
1:K:2:SER:HB2	1:K:103:LEU:O	2.22	0.40
1:K:202:ARG:HG2	1:K:204:TRP:NE1	2.37	0.40
5:O:45:PHE:CD2	5:O:46:PRO:HD2	2.56	0.40
2:Q:3:ARG:HB3	2:Q:29:GLY:O	2.21	0.40
5:T:24:ARG:HD3	5:T:85:THR:HG23	2.02	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%)	13 (5%)	0	100	100
1	F	274/276 (99%)	263 (96%)	11 (4%)	0	100	100
1	K	245/276 (89%)	238 (97%)	7 (3%)	0	100	100
1	P	273/276 (99%)	264 (97%)	8 (3%)	1 (0%)	34	42
2	B	97/100 (97%)	97 (100%)	0	0	100	100
2	G	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	L	98/100 (98%)	98 (100%)	0	0	100	100
2	Q	97/100 (97%)	97 (100%)	0	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	H	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	D	204/206 (99%)	198 (97%)	6 (3%)	0	100	100
4	I	204/206 (99%)	198 (97%)	6 (3%)	0	100	100
4	N	197/206 (96%)	188 (95%)	9 (5%)	0	100	100
4	S	197/206 (96%)	189 (96%)	7 (4%)	1 (0%)	29	35
5	E	244/246 (99%)	231 (95%)	11 (4%)	2 (1%)	19	23
5	J	246/246 (100%)	236 (96%)	10 (4%)	0	100	100
5	O	244/246 (99%)	237 (97%)	6 (2%)	1 (0%)	34	42
5	T	242/246 (98%)	233 (96%)	7 (3%)	2 (1%)	19	23
All	All	3262/3348 (97%)	3152 (97%)	103 (3%)	7 (0%)	47	58

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	48	GLN

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Mol	Chain	Res	Type
4	S	145	SER
5	T	63	SER
5	T	45	PHE
5	E	72	GLU
5	O	45	PHE
1	P	15	PRO

5.3.2 Protein sidechains [i](#)

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	235/234 (100%)	223 (95%)	12 (5%)	24	33
1	F	235/234 (100%)	225 (96%)	10 (4%)	29	40
1	K	215/234 (92%)	211 (98%)	4 (2%)	57	73
1	P	234/234 (100%)	223 (95%)	11 (5%)	26	37
2	B	94/95 (99%)	87 (93%)	7 (7%)	13	17
2	G	96/95 (101%)	90 (94%)	6 (6%)	18	24
2	L	95/95 (100%)	90 (95%)	5 (5%)	22	31
2	Q	94/95 (99%)	87 (93%)	7 (7%)	13	17
3	C	8/8 (100%)	8 (100%)	0	100	100
3	H	8/8 (100%)	8 (100%)	0	100	100
3	M	8/8 (100%)	8 (100%)	0	100	100
3	R	8/8 (100%)	8 (100%)	0	100	100
4	D	182/182 (100%)	175 (96%)	7 (4%)	33	47
4	I	182/182 (100%)	173 (95%)	9 (5%)	25	35
4	N	175/182 (96%)	165 (94%)	10 (6%)	20	28
4	S	175/182 (96%)	163 (93%)	12 (7%)	15	20
5	E	216/216 (100%)	196 (91%)	20 (9%)	9	10
5	J	218/216 (101%)	201 (92%)	17 (8%)	12	16
5	O	216/216 (100%)	200 (93%)	16 (7%)	13	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	T	215/216 (100%)	197 (92%)	18 (8%)	11	13
All	All	2909/2940 (99%)	2738 (94%)	171 (6%)	19	27

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	19	GLU
1	A	34	VAL
1	A	73	THR
1	A	106	ASP
1	A	181	ARG
1	A	196	ASP
1	A	198	GLU
1	A	215	LEU
1	A	231	VAL
1	A	268	LYS
1	A	272	LEU
2	B	39	LEU
2	B	45	ARG
2	B	47	GLU
2	B	70	PHE
2	B	85	VAL
2	B	88	SER
2	B	97	ARG
4	D	26	SER
4	D	126	ILE
4	D	140	ARG
4	D	146	ASP
4	D	167	SER
4	D	197	ASP
4	D	215	PHE
5	E	3	VAL
5	E	47	LYS
5	E	64	LYS
5	E	72	GLU
5	E	73	LYS
5	E	75	LYS
5	E	84	LEU
5	E	89	LEU
5	E	123	ARG
5	E	144	SER

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Mol	Chain	Res	Type
5	E	145	GLU
5	E	177	LYS
5	E	179	VAL
5	E	184	CYS
5	E	188	GLN
5	E	196	LEU
5	E	197	ASN
5	E	212	THR
5	E	233	ASN
5	E	239	ASP
1	F	12	MET
1	F	15	PRO
1	F	34	VAL
1	F	44	ARG
1	F	98	MET
1	F	196	ASP
1	F	219	ARG
1	F	231	VAL
1	F	247	VAL
1	F	272	LEU
2	G	39	LEU
2	G	47	GLU
2	G	48	LYS
2	G	70	PHE
2	G	85	VAL
2	G	88	SER
4	I	26	SER
4	I	92	THR
4	I	140	ARG
4	I	148	SER
4	I	156	ASP
4	I	180	ARG
4	I	194	ASN
4	I	215	PHE
4	I	217	SER
5	J	3	VAL
5	J	45	PHE
5	J	72	GLU
5	J	75	LYS
5	J	84	LEU
5	J	88	THR
5	J	89	LEU

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Mol	Chain	Res	Type
5	J	93	SER
5	J	144	SER
5	J	151	THR
5	J	184	CYS
5	J	197	ASN
5	J	206	ARG
5	J	232	GLU
5	J	233	ASN
5	J	242	LYS
5	J	257	ASP
1	K	226	GLN
1	K	231	VAL
1	K	268	LYS
1	K	273	ARG
2	L	0	MET
2	L	1	ILE
2	L	39	LEU
2	L	70	PHE
2	L	85	VAL
4	N	26	SER
4	N	28	SER
4	N	76	ILE
4	N	92	THR
4	N	97	GLU
4	N	143	LYS
4	N	145	SER
4	N	147	LYS
4	N	168	ASP
4	N	195	LYS
5	O	3	VAL
5	O	14	LYS
5	O	45	PHE
5	O	51	MET
5	O	72	GLU
5	O	75	LYS
5	O	84	LEU
5	O	89	LEU
5	O	93	SER
5	O	131	LYS
5	O	144	SER
5	O	184	CYS
5	O	190	LEU

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Mol	Chain	Res	Type
5	O	206	ARG
5	O	242	LYS
5	O	255	ARG
1	P	14	ARG
1	P	39	ASP
1	P	44	ARG
1	P	194	VAL
1	P	195	SER
1	P	222	GLU
1	P	225	THR
1	P	231	VAL
1	P	259	CYS
1	P	268	LYS
1	P	271	THR
2	Q	1	ILE
2	Q	39	LEU
2	Q	47	GLU
2	Q	70	PHE
2	Q	89	GLN
2	Q	94	LYS
2	Q	97	ARG
4	S	-1	SER
4	S	26	SER
4	S	28	SER
4	S	92	THR
4	S	93	GLU
4	S	97	GLU
4	S	130	GLN
4	S	140	ARG
4	S	146	ASP
4	S	156	ASP
4	S	197	ASP
4	S	208	ILE
5	T	45	PHE
5	T	47	LYS
5	T	51	MET
5	T	72	GLU
5	T	75	LYS
5	T	84	LEU
5	T	85	THR
5	T	89	LEU
5	T	93	SER

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Mol	Chain	Res	Type
5	T	144	SER
5	T	184	CYS
5	T	190	LEU
5	T	191	LYS
5	T	206	ARG
5	T	225	VAL
5	T	233	ASN
5	T	235	GLU
5	T	255	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 i

6.1 Protein, DNA and RNA chains i

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	275/276 (99%)	0.27	25 (9%) 9 12	21, 38, 101, 121	0
1	F	275/276 (99%)	0.19	17 (6%) 20 26	17, 31, 87, 110	1 (0%)
1	K	253/276 (91%)	0.23	22 (8%) 10 14	18, 35, 98, 119	0
1	P	275/276 (99%)	0.27	34 (12%) 4 5	18, 39, 105, 124	0
2	B	99/100 (99%)	-0.29	1 (1%) 82 86	29, 45, 68, 75	0
2	G	99/100 (99%)	-0.39	1 (1%) 82 86	23, 38, 59, 72	0
2	L	100/100 (100%)	-0.24	1 (1%) 82 86	23, 41, 64, 74	0
2	Q	99/100 (99%)	-0.00	4 (4%) 38 45	29, 49, 74, 88	0
3	C	9/9 (100%)	-0.26	0 100 100	24, 25, 31, 32	0
3	H	9/9 (100%)	0.01	0 100 100	19, 20, 25, 28	0
3	M	9/9 (100%)	0.03	0 100 100	19, 21, 24, 28	0
3	R	9/9 (100%)	-0.13	0 100 100	20, 22, 25, 32	0
4	D	206/206 (100%)	0.11	13 (6%) 20 25	25, 58, 98, 112	0
4	I	206/206 (100%)	-0.02	7 (3%) 45 52	21, 50, 86, 105	0
4	N	199/206 (96%)	-0.06	6 (3%) 50 57	21, 47, 84, 102	0
4	S	199/206 (96%)	0.07	12 (6%) 21 28	21, 53, 97, 118	0
5	E	246/246 (100%)	0.53	21 (8%) 10 14	21, 63, 109, 133	1 (0%)
5	J	246/246 (100%)	0.03	8 (3%) 46 53	19, 49, 88, 108	0
5	O	246/246 (100%)	0.01	11 (4%) 33 40	18, 45, 83, 109	2 (0%)
5	T	244/246 (99%)	-0.01	10 (4%) 37 44	18, 52, 92, 113	1 (0%)
All	All	3303/3348 (98%)	0.10	193 (5%) 23 29	17, 45, 93, 133	5 (0%)

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	238	GLN	7.2
1	K	191	HIS	6.6
1	P	197	HIS	6.4
5	E	257	ASP	6.2
4	S	198	PHE	5.9
1	P	223	ASP	5.7
1	K	274	TRP	5.6
5	T	232	GLU	5.6
5	E	2	ALA	5.6
5	E	242	LYS	5.5
4	D	146	ASP	5.4
1	P	194	VAL	5.4
5	E	253	TRP	5.2
1	P	249	VAL	5.1
4	N	197	ASP	5.1
1	F	220	ASP	4.9
4	I	218	PRO	4.8
4	D	0	ALA	4.6
5	O	2	ALA	4.5
2	Q	1	ILE	4.5
1	K	276	PRO	4.5
1	K	247	VAL	4.4
1	F	17	ARG	4.3
1	A	17	ARG	4.3
1	K	227	ASP	4.3
4	S	197	ASP	4.3
1	A	194	VAL	4.3
1	K	193	PRO	4.2
5	E	237	THR	4.2
5	O	239	ASP	4.2
1	P	252	GLY	4.1
4	I	194	ASN	4.1
1	A	222	GLU	4.1
5	J	46	PRO	4.0
1	K	259	CYS	4.0
4	D	182	MET	4.0
5	E	174	VAL	4.0
5	T	197	ASN	3.9
1	P	256	ARG	3.9
5	E	236	TRP	3.9
4	I	0	ALA	3.9
1	A	198	GLU	3.8
1	P	195	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	K	228	THR	3.8
1	P	196	ASP	3.8
1	A	267	PRO	3.8
1	K	248	VAL	3.7
1	P	198	GLU	3.7
1	K	230	LEU	3.7
1	K	200	THR	3.7
4	N	194	ASN	3.7
5	E	196	LEU	3.6
1	F	222	GLU	3.6
5	E	241	ALA	3.6
1	P	274	TRP	3.6
1	F	223	ASP	3.5
4	I	180	ARG	3.5
5	E	46	PRO	3.4
1	A	18	GLY	3.4
1	A	228	THR	3.4
5	E	138	VAL	3.4
1	P	219	ARG	3.4
1	A	197	HIS	3.4
1	P	224	GLN	3.4
5	E	48	GLN	3.3
1	F	221	GLY	3.3
5	T	237	THR	3.3
5	T	195	ALA	3.3
1	P	226	GLN	3.3
4	N	196	SER	3.3
1	A	248	VAL	3.3
1	K	258	THR	3.3
1	P	270	LEU	3.2
1	K	272	LEU	3.2
4	S	182	MET	3.2
1	K	217	TRP	3.2
4	D	130	GLN	3.2
1	P	228	THR	3.2
1	A	246	ALA	3.2
5	J	237	THR	3.1
1	K	261	VAL	3.1
4	I	181	SER	3.1
1	F	41	ALA	3.1
4	D	183	ASP	3.1
1	A	271	THR	3.1

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Mol	Chain	Res	Type	RSRZ
5	J	242	LYS	3.1
1	K	246	ALA	3.1
1	P	220	ASP	3.0
4	D	142	SER	3.0
4	S	208	ILE	3.0
1	F	256	ARG	3.0
5	J	196	LEU	3.0
1	F	274	TRP	3.0
5	O	197	ASN	3.0
5	J	198	ASP	3.0
1	A	226	GLN	3.0
1	F	250	PRO	3.0
4	S	196	SER	2.9
1	P	225	THR	2.9
5	T	239	ASP	2.9
4	D	218	PRO	2.9
1	F	227	ASP	2.9
1	P	253	GLU	2.9
1	P	193	PRO	2.9
5	T	196	LEU	2.9
5	E	239	ASP	2.9
1	A	217	TRP	2.9
1	P	216	THR	2.8
4	S	168	ASP	2.8
1	A	250	PRO	2.8
2	Q	48	LYS	2.8
1	A	221	GLY	2.7
1	P	250	PRO	2.7
1	P	222	GLU	2.7
1	P	260	HIS	2.7
1	K	41	ALA	2.7
2	L	48	LYS	2.7
1	P	254	GLU	2.7
4	D	140	ARG	2.7
5	E	198	ASP	2.7
5	E	212	THR	2.7
1	A	249	VAL	2.7
2	Q	2	GLN	2.7
4	I	146	ASP	2.6
1	A	2	SER	2.6
1	A	274	TRP	2.6
4	D	14	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	224	GLN	2.6
5	E	195	ALA	2.6
5	E	211	ALA	2.6
4	I	130	GLN	2.6
1	K	271	THR	2.6
4	D	180	ARG	2.6
1	A	276	PRO	2.6
1	P	255	GLN	2.6
5	E	256	ALA	2.6
4	S	128	ASN	2.6
1	F	225	THR	2.5
5	E	169	GLU	2.5
1	K	189	VAL	2.5
5	O	51	MET	2.5
5	O	195	ALA	2.5
1	P	271	THR	2.5
2	B	45	ARG	2.5
2	G	1[A]	ILE	2.5
1	P	221	GLY	2.5
5	T	45	PHE	2.5
4	S	130	GLN	2.5
1	P	251	SER	2.4
1	F	194	VAL	2.4
4	S	195	LYS	2.4
1	F	219	ARG	2.4
4	S	181	SER	2.4
4	N	183	ASP	2.4
4	D	158	GLN	2.4
1	A	41	ALA	2.4
5	O	196	LEU	2.4
1	P	218	GLN	2.4
2	Q	47	GLU	2.4
5	T	235	GLU	2.4
4	S	180	ARG	2.3
1	F	267	PRO	2.3
5	J	45	PHE	2.3
5	E	240	ARG	2.3
1	P	199	ALA	2.3
1	A	225	THR	2.3
1	K	269	PRO	2.3
5	O	235	GLU	2.2
4	N	168	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	229	GLU	2.2
1	P	41	ALA	2.2
5	O	237	THR	2.2
5	T	198	ASP	2.2
5	J	235	GLU	2.2
5	O	257	ASP	2.2
1	F	228	THR	2.2
4	N	130	GLN	2.2
1	A	270	LEU	2.2
5	O	241	ALA	2.1
1	P	268	LYS	2.1
1	P	262	GLN	2.1
4	D	179	MET	2.1
4	S	183	ASP	2.1
1	F	275	GLU	2.1
4	D	143	LYS	2.1
5	T	129	ASP	2.1
5	J	47	LYS	2.0
1	P	200	THR	2.0
5	O	238	GLN	2.0
1	K	273	ARG	2.0
1	K	204	TRP	2.0
1	A	272	LEU	2.0
1	F	42	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.