Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2024 – 04:10 PM JST

PDB ID	:	8WFM
Title	:	Crystal structure of Omicron BA.1 in complex with a neutralizing antibody scFv T11
Authors	:	Zhang, M.; Zhang, N.; Gabibov, A.; Guo, Y.
Deposited on	:	2023-09-19
Resolution	:	2.99 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:

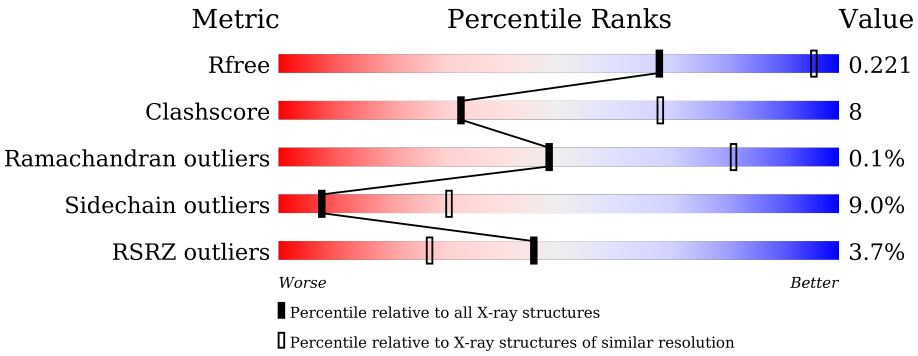
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (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 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 <=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	255	3% 65% 26% 9%
1	C	255	2% 73% 16% • 9%
1	E	255	5% 69% 21% • 9%
1	G	255	8% 64% 26% • 9%
2	B	223	% 66% 16% 18%
2	D	223	62% 20% 18%

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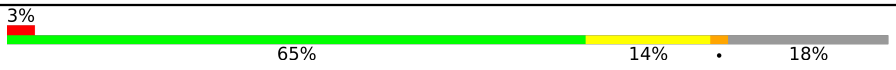
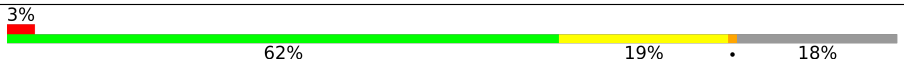
Mol	Chain	Length	Quality of chain
2	F	223	
2	H	223	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12900 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 T11 scFv.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	0
			1741	1100	287	346	8			
1	C	233	Total	C	N	O	S	0	0	0
			1741	1100	287	346	8			
1	E	233	Total	C	N	O	S	0	0	0
			1741	1100	287	346	8			
1	G	233	Total	C	N	O	S	0	0	0
			1741	1100	287	346	8			

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	183	Total	C	N	O	S	0	0	0
			1484	957	250	270	7			
2	D	183	Total	C	N	O	S	0	0	0
			1484	957	250	270	7			
2	F	183	Total	C	N	O	S	0	0	0
			1484	957	250	270	7			
2	H	183	Total	C	N	O	S	0	0	0
			1484	957	250	270	7			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	21	ASP	GLY	variant	UNP P0DTC2
B	53	LEU	SER	variant	UNP P0DTC2
B	55	PRO	SER	variant	UNP P0DTC2
B	57	PHE	SER	variant	UNP P0DTC2
B	99	ASN	LYS	variant	UNP P0DTC2
B	122	LYS	ASN	variant	UNP P0DTC2
B	128	SER	GLY	variant	UNP P0DTC2
B	159	ASN	SER	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	160	LYS	THR	variant	UNP P0DTC2
B	166	ALA	GLU	variant	UNP P0DTC2
B	175	ARG	GLN	variant	UNP P0DTC2
B	178	SER	GLY	variant	UNP P0DTC2
B	180	ARG	GLN	variant	UNP P0DTC2
B	183	TYR	ASN	variant	UNP P0DTC2
B	187	HIS	TYR	variant	UNP P0DTC2
D	21	ASP	GLY	variant	UNP P0DTC2
D	53	LEU	SER	variant	UNP P0DTC2
D	55	PRO	SER	variant	UNP P0DTC2
D	57	PHE	SER	variant	UNP P0DTC2
D	99	ASN	LYS	variant	UNP P0DTC2
D	122	LYS	ASN	variant	UNP P0DTC2
D	128	SER	GLY	variant	UNP P0DTC2
D	159	ASN	SER	variant	UNP P0DTC2
D	160	LYS	THR	variant	UNP P0DTC2
D	166	ALA	GLU	variant	UNP P0DTC2
D	175	ARG	GLN	variant	UNP P0DTC2
D	178	SER	GLY	variant	UNP P0DTC2
D	180	ARG	GLN	variant	UNP P0DTC2
D	183	TYR	ASN	variant	UNP P0DTC2
D	187	HIS	TYR	variant	UNP P0DTC2
F	21	ASP	GLY	variant	UNP P0DTC2
F	53	LEU	SER	variant	UNP P0DTC2
F	55	PRO	SER	variant	UNP P0DTC2
F	57	PHE	SER	variant	UNP P0DTC2
F	99	ASN	LYS	variant	UNP P0DTC2
F	122	LYS	ASN	variant	UNP P0DTC2
F	128	SER	GLY	variant	UNP P0DTC2
F	159	ASN	SER	variant	UNP P0DTC2
F	160	LYS	THR	variant	UNP P0DTC2
F	166	ALA	GLU	variant	UNP P0DTC2
F	175	ARG	GLN	variant	UNP P0DTC2
F	178	SER	GLY	variant	UNP P0DTC2
F	180	ARG	GLN	variant	UNP P0DTC2
F	183	TYR	ASN	variant	UNP P0DTC2
F	187	HIS	TYR	variant	UNP P0DTC2
H	21	ASP	GLY	variant	UNP P0DTC2
H	53	LEU	SER	variant	UNP P0DTC2
H	55	PRO	SER	variant	UNP P0DTC2
H	57	PHE	SER	variant	UNP P0DTC2
H	99	ASN	LYS	variant	UNP P0DTC2

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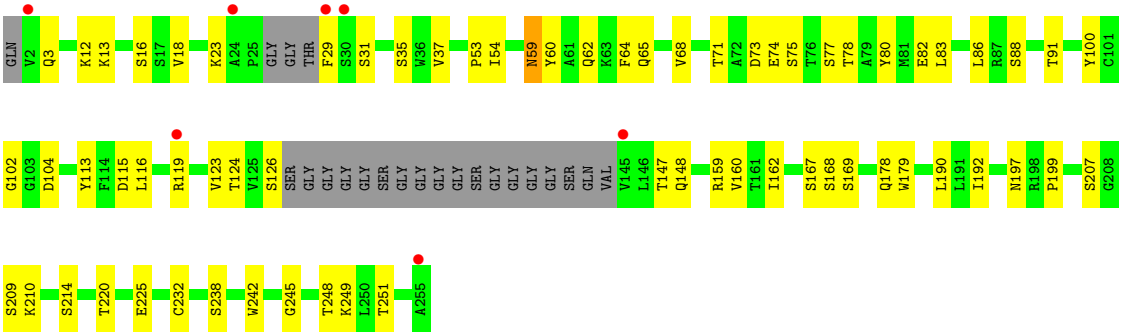
Chain	Residue	Modelled	Actual	Comment	Reference
H	122	LYS	ASN	variant	UNP P0DTC2
H	128	SER	GLY	variant	UNP P0DTC2
H	159	ASN	SER	variant	UNP P0DTC2
H	160	LYS	THR	variant	UNP P0DTC2
H	166	ALA	GLU	variant	UNP P0DTC2
H	175	ARG	GLN	variant	UNP P0DTC2
H	178	SER	GLY	variant	UNP P0DTC2
H	180	ARG	GLN	variant	UNP P0DTC2
H	183	TYR	ASN	variant	UNP P0DTC2
H	187	HIS	TYR	variant	UNP P0DTC2

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.

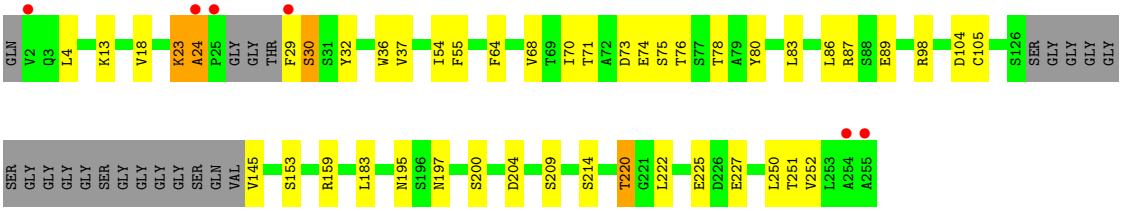
• Molecule 1: T11 scFv

Chain A:



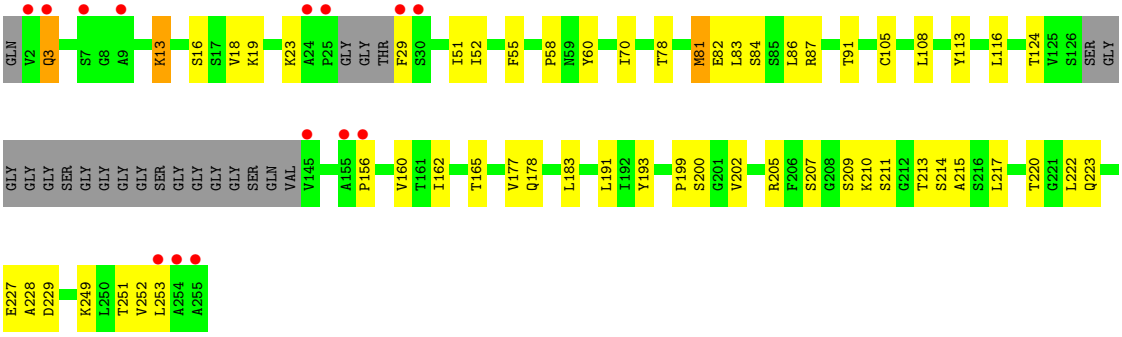
• Molecule 1: T11 scFv

Chain C:



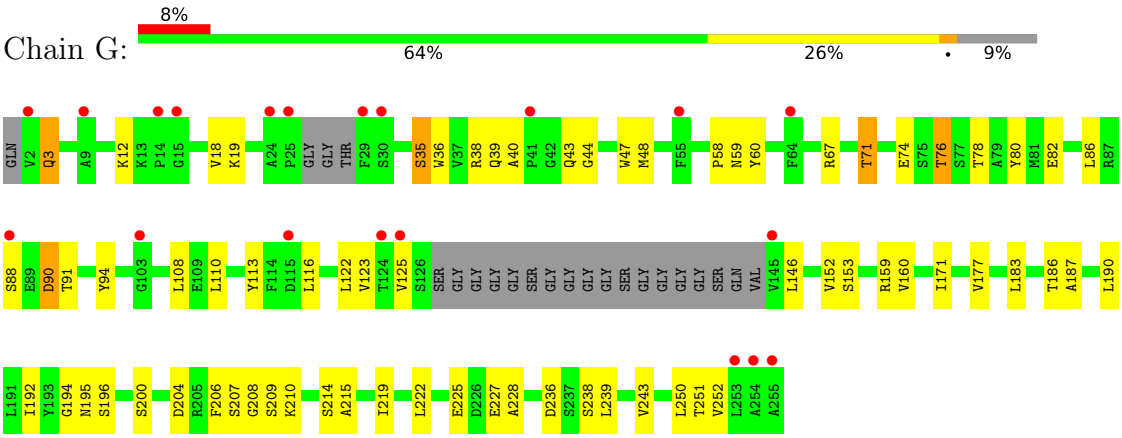
• Molecule 1: T11 scFv

Chain E:



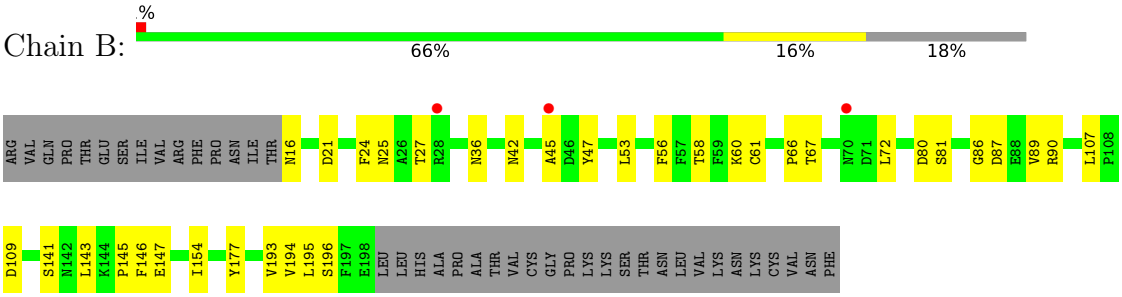
• Molecule 1: T11 scFv

Chain G:



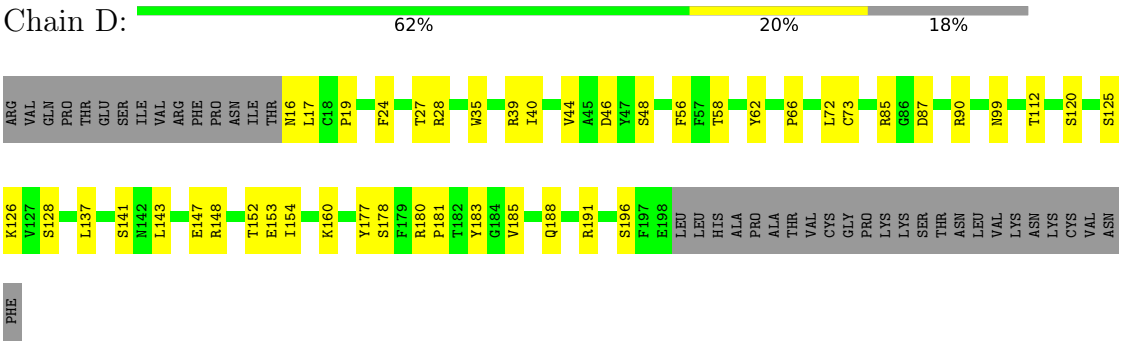
• Molecule 2: Spike protein S1

Chain B:



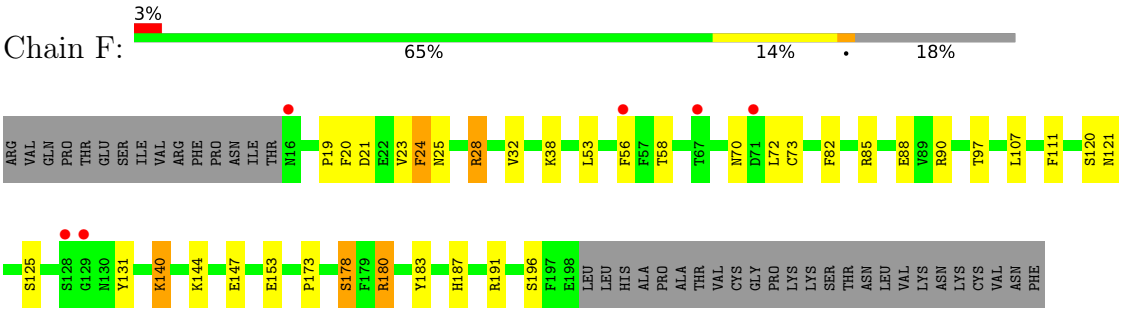
• Molecule 2: Spike protein S1

Chain D:



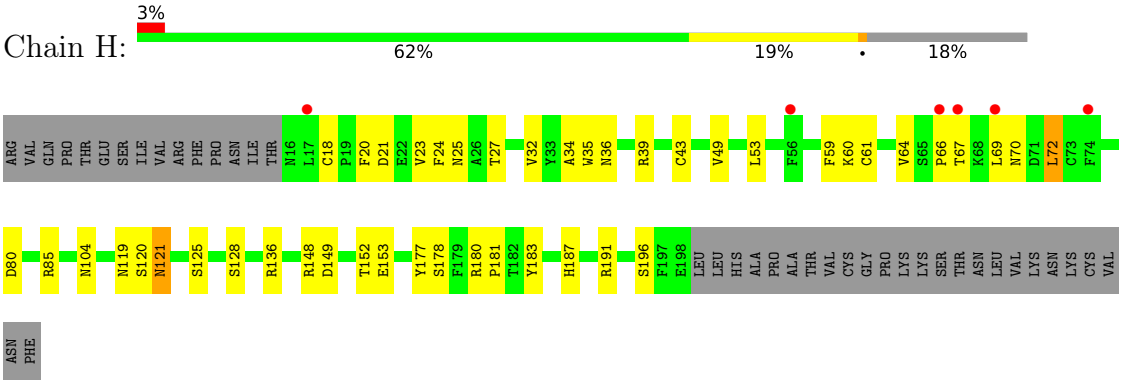
• Molecule 2: Spike protein S1

Chain F:



• Molecule 2: Spike protein S1

Chain H:


3%
62%
19%
18%
ARG VAL GLN PRO THR GLU SER ILE VAL ARG PHE PRO ASN ILE THR N16 L17 C18 P19 F20 D21 E22 V23 F24 N25 A26 T27 V32 Y33 A34 W35 N36 R39 C43 V49 L53 F56 F59 K60 C61 V64 S65 P66 T67 K68 L69 N70 D71 L72 C73 F74
D80 R85 N104 N119 S120 N121 S125 S128 R136 R148 D149 T152 E153 Y177 S178 F179 R180 P181 T182 Y183 H187 R191 S196 F197 E198 LEU LEU HIS ALA PRO ALA THR VAL CYS GLY PRO LYS LYS SER THR ASN LEU VAL LYS ASN LYS CYS VAL
ASN PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	55.41Å 172.49Å 487.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.61 – 2.99 64.61 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.9 (64.61-2.99) 90.7 (64.61-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.215 , 0.265 0.217 , 0.221	Depositor DCC
R_{free} test set	2478 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	51.9	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 32.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	12900	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.55	0/1782	0.71	0/2424
1	C	0.53	0/1782	0.72	0/2424
1	E	0.47	0/1782	0.64	0/2424
1	G	0.44	0/1782	0.64	0/2424
2	B	0.51	0/1528	0.70	0/2077
2	D	0.50	0/1528	0.67	0/2077
2	F	0.47	0/1528	0.65	0/2077
2	H	0.48	0/1528	0.65	0/2077
All	All	0.49	0/13240	0.67	0/18004

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1741	0	1670	36	0
1	C	1741	0	1670	22	0
1	E	1741	0	1670	28	0
1	G	1741	0	1670	38	0
2	B	1484	0	1412	16	0
2	D	1484	0	1412	18	0
2	F	1484	0	1412	21	0
2	H	1484	0	1412	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12900	0	12328	196	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 8.

All (196) 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:A:54:ILE:HD11	1:A:74:GLU:HB2	1.52	0.90
2:B:60:LYS:HG2	2:H:60:LYS:HG2	1.54	0.88
1:G:35:SER:HG	1:G:47:TRP:HE1	1.17	0.87
2:B:66:PRO:HB2	2:H:66:PRO:HB2	1.60	0.83
1:C:71:THR:HG22	1:C:80:TYR:HB2	1.64	0.80
1:E:183:LEU:HD23	1:E:228:ALA:HB2	1.66	0.78
1:E:91:THR:HG23	1:E:124:THR:HA	1.66	0.78
1:G:67:ARG:NH2	1:G:90:ASP:OD2	2.18	0.76
1:C:4:LEU:HD23	1:C:24:ALA:HB3	1.69	0.74
1:A:148:GLN:NE2	1:A:245:GLY:HA3	2.03	0.74
2:H:23:VAL:HG23	2:H:24:PHE:H	1.53	0.74
1:E:18:VAL:HG23	1:E:86:LEU:HD11	1.70	0.73
1:E:3:GLN:HA	1:E:116:LEU:HD11	1.70	0.72
1:A:148:GLN:NE2	1:A:232:CYS:SG	2.63	0.71
2:H:180:ARG:HB2	2:H:183:TYR:CE1	2.26	0.69
1:C:36:TRP:CD1	1:C:70:ILE:HD13	2.29	0.68
2:H:32:VAL:HG22	2:H:104:ASN:HB3	1.75	0.68
1:E:19:LYS:HD3	1:E:82:GLU:HB2	1.77	0.67
2:D:185:VAL:HA	2:D:188:GLN:HG3	1.77	0.67
2:F:131:TYR:OH	2:F:180:ARG:NH2	2.29	0.66
1:A:64:PHE:HB3	1:A:68:VAL:CG2	2.25	0.65
1:C:23:LYS:HB2	1:C:78:THR:HG22	1.77	0.65
1:C:64:PHE:HB3	1:C:68:VAL:HG23	1.79	0.65
2:D:46:ASP:OD1	2:D:48:SER:OG	2.15	0.64
1:A:159:ARG:HG3	1:A:220:THR:HG22	1.80	0.63
2:H:136:ARG:NH2	2:H:149:ASP:O	2.30	0.63
2:F:140:LYS:HD3	2:F:140:LYS:H	1.61	0.63
2:D:19:PRO:HD2	2:D:40:ILE:HD12	1.80	0.63
2:D:126:LYS:O	2:D:181:PRO:HD3	1.98	0.62
2:H:49:VAL:HG22	2:H:53:LEU:CD2	2.29	0.62
1:G:108:LEU:H	1:G:108:LEU:HD12	1.63	0.62
2:D:143:LEU:HG	2:D:147:GLU:HB3	1.82	0.62
1:A:64:PHE:HB3	1:A:68:VAL:HG21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ARG:CZ	1:A:119:ARG:HA	2.32	0.59
1:C:36:TRP:HD1	1:C:70:ILE:HD13	1.66	0.59
1:E:162:ILE:HD12	1:E:217:LEU:HD23	1.85	0.59
1:C:64:PHE:HB3	1:C:68:VAL:CG2	2.33	0.59
2:B:67:THR:HG22	2:H:70:ASN:HB2	1.85	0.58
1:A:59:ASN:HD22	1:A:60:TYR:N	2.01	0.58
2:F:25:ASN:HB2	2:F:53:LEU:HD21	1.85	0.58
2:H:18:CYS:SG	2:H:72:LEU:HD11	2.42	0.58
1:A:100:TYR:CZ	1:A:102:GLY:HA2	2.39	0.58
1:G:71:THR:HG23	1:G:80:TYR:HB2	1.84	0.58
1:G:177:VAL:HG21	1:G:215:ALA:HB2	1.85	0.57
2:H:121:ASN:HD21	2:H:181:PRO:HA	1.69	0.57
1:E:23:LYS:HB2	1:E:78:THR:HG22	1.86	0.57
1:A:162:ILE:HD13	1:A:248:THR:HG21	1.86	0.57
2:D:16:ASN:CG	2:D:17:LEU:H	2.08	0.57
1:E:227:GLU:HB2	1:E:252:VAL:HG23	1.86	0.56
1:A:73:ASP:OD1	1:A:75:SER:OG	2.19	0.56
2:D:17:LEU:HD23	2:D:44:VAL:O	2.04	0.56
1:A:91:THR:HG23	1:A:124:THR:HA	1.87	0.56
1:G:18:VAL:O	1:G:82:GLU:HA	2.05	0.56
1:C:89:GLU:OE1	1:C:89:GLU:N	2.31	0.56
1:A:18:VAL:HG23	1:A:86:LEU:HD11	1.88	0.55
1:G:3:GLN:HA	1:G:116:LEU:HD11	1.88	0.55
1:G:36:TRP:O	1:G:48:MET:HB2	2.06	0.55
2:H:66:PRO:O	2:H:69:LEU:HB2	2.07	0.55
1:C:197:ASN:OD1	2:D:154:ILE:HG12	2.06	0.55
1:G:222:LEU:HD21	1:G:250:LEU:HD21	1.89	0.55
1:C:30:SER:HB3	1:C:54:ILE:HD12	1.89	0.54
2:D:16:ASN:OD1	2:D:17:LEU:N	2.40	0.54
2:B:61:CYS:SG	2:B:66:PRO:HG3	2.47	0.54
2:B:143:LEU:HG	2:B:147:GLU:HB3	1.89	0.54
1:E:165:THR:HG23	1:E:214:SER:OG	2.08	0.54
2:F:19:PRO:HG2	2:F:38:LYS:HZ1	1.73	0.54
2:F:32:VAL:HG23	2:F:82:PHE:CD1	2.43	0.54
1:C:222:LEU:HD11	1:C:250:LEU:HD21	1.88	0.54
1:A:29:PHE:CZ	1:A:77:SER:HA	2.43	0.53
1:G:194:GLY:HA2	2:H:152:THR:HG23	1.89	0.53
2:H:119:ASN:HD21	2:H:121:ASN:HB2	1.73	0.53
1:A:62:GLN:HA	1:A:65:GLN:HG2	1.90	0.53
1:A:113:TYR:CD1	1:A:115:ASP:HB3	2.43	0.53
1:E:60:TYR:HE1	1:E:70:ILE:HD12	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:159:ARG:HA	1:G:219:ILE:O	2.08	0.53
1:A:12:LYS:HG3	1:A:18:VAL:HG22	1.89	0.52
1:A:64:PHE:HB3	1:A:68:VAL:HG23	1.90	0.52
1:G:19:LYS:HE3	1:G:80:TYR:CG	2.45	0.52
1:G:227:GLU:HG3	1:G:252:VAL:HG23	1.92	0.52
2:H:39:ARG:HG2	2:H:39:ARG:HH11	1.75	0.52
1:A:23:LYS:HG3	1:A:78:THR:HG22	1.91	0.51
2:F:121:ASN:O	2:F:125:SER:HB2	2.10	0.51
2:H:20:PHE:HD1	2:H:23:VAL:HG21	1.75	0.51
2:H:120:SER:HB3	2:H:191:ARG:HG3	1.92	0.51
2:F:85:ARG:HD3	2:F:187:HIS:HA	1.91	0.51
2:F:85:ARG:HG2	2:F:88:GLU:OE1	2.11	0.51
2:H:36:ASN:O	2:H:80:ASP:HA	2.11	0.51
1:G:195:ASN:H	2:H:153:GLU:HG3	1.76	0.50
1:A:29:PHE:CE1	1:A:77:SER:HA	2.46	0.50
1:G:227:GLU:HG3	1:G:252:VAL:H	1.75	0.50
2:B:36:ASN:O	2:B:80:ASP:HA	2.11	0.50
1:G:90:ASP:OD1	1:G:90:ASP:N	2.44	0.50
2:B:66:PRO:CB	2:H:66:PRO:HB2	2.37	0.50
1:A:18:VAL:HG21	1:A:123:VAL:HG11	1.93	0.50
1:G:192:ILE:CD1	1:G:208:GLY:HA3	2.41	0.50
2:F:178:SER:OG	2:F:183:TYR:OH	2.22	0.50
1:E:113:TYR:HD2	1:E:193:TYR:CG	2.30	0.49
1:A:119:ARG:HA	1:A:119:ARG:NH1	2.27	0.49
2:H:121:ASN:HD22	2:H:125:SER:HB2	1.76	0.49
1:G:39:GLN:HG3	1:G:44:GLY:O	2.13	0.49
2:D:120:SER:HB3	2:D:191:ARG:HG3	1.95	0.48
1:A:71:THR:OG1	1:A:80:TYR:HB2	2.13	0.48
1:E:199:PRO:HD2	1:E:202:VAL:HG21	1.96	0.47
2:F:120:SER:HB3	2:F:191:ARG:HG3	1.96	0.47
1:G:91:THR:HA	1:G:123:VAL:O	2.15	0.47
2:F:107:LEU:HD22	2:F:111:PHE:CD1	2.49	0.47
1:E:60:TYR:CE1	1:E:70:ILE:HD12	2.50	0.47
1:A:178:GLN:NE2	1:A:242:TRP:CZ3	2.82	0.47
2:F:20:PHE:HD1	2:F:23:VAL:HG21	1.80	0.47
1:G:196:SER:OG	2:H:153:GLU:OE2	2.22	0.47
1:E:205:ARG:HA	1:E:220:THR:HG22	1.96	0.47
1:E:229:ASP:OD1	1:E:249:LYS:HG2	2.15	0.46
1:A:179:TRP:HB2	1:A:192:ILE:HG13	1.97	0.46
1:E:52:ILE:HD11	1:E:108:LEU:N	2.30	0.46
2:B:86:GLY:HA2	2:B:89:VAL:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:211:SER:O	1:E:211:SER:OG	2.29	0.46
1:A:148:GLN:HE22	1:A:232:CYS:H	1.64	0.46
2:D:178:SER:O	2:D:178:SER:OG	2.33	0.46
1:E:18:VAL:O	1:E:82:GLU:HA	2.15	0.46
2:D:39:ARG:O	2:D:40:ILE:HD13	2.16	0.46
1:C:18:VAL:CG2	1:C:86:LEU:HD11	2.45	0.45
2:F:23:VAL:HG23	2:F:24:PHE:H	1.82	0.45
1:A:197:ASN:OD1	2:B:154:ILE:HG12	2.16	0.45
2:H:39:ARG:HG2	2:H:39:ARG:NH1	2.32	0.45
1:G:113:TYR:HB2	1:G:190:LEU:HD22	1.99	0.45
1:G:183:LEU:HD23	1:G:228:ALA:HB2	1.98	0.45
1:C:105:CYS:O	2:D:28:ARG:NH2	2.50	0.45
1:G:40:ALA:HB3	1:G:43:GLN:HG3	1.99	0.45
1:G:186:THR:OG1	1:G:187:ALA:N	2.50	0.45
1:C:183:LEU:HD12	1:C:183:LEU:H	1.82	0.44
2:H:61:CYS:SG	2:H:66:PRO:HG3	2.56	0.44
1:A:68:VAL:HG22	1:A:83:LEU:HD13	1.99	0.44
1:G:152:VAL:HG12	1:G:250:LEU:HD12	1.99	0.44
1:G:171:ILE:HG23	1:G:210:LYS:HD2	2.00	0.44
1:G:236:ASP:HB3	1:G:239:LEU:HG	1.98	0.44
1:C:18:VAL:HG23	1:C:86:LEU:HD11	1.99	0.44
1:A:167:SER:OG	1:A:168:SER:N	2.49	0.44
1:C:29:PHE:HZ	1:C:74:GLU:HA	1.82	0.44
2:D:35:TRP:O	2:D:148:ARG:NH1	2.49	0.44
1:E:51:ILE:HD12	1:E:58:PRO:HG3	2.00	0.44
1:A:18:VAL:O	1:A:82:GLU:HA	2.17	0.44
1:A:13:LYS:HB2	1:A:13:LYS:HE3	1.89	0.44
2:B:195:LEU:HD23	2:B:195:LEU:HA	1.88	0.44
1:E:13:LYS:HE3	1:E:16:SER:OG	2.17	0.44
1:E:191:LEU:HD12	1:E:191:LEU:HA	1.86	0.44
1:C:87:ARG:HB2	1:C:89:GLU:OE1	2.18	0.44
1:A:225:GLU:H	1:A:225:GLU:HG3	1.54	0.44
1:G:146:LEU:HD11	1:G:243:VAL:HG23	2.00	0.44
1:E:177:VAL:HG21	1:E:215:ALA:CB	2.47	0.43
2:B:25:ASN:N	2:B:53:LEU:HD21	2.32	0.43
2:D:66:PRO:HB2	2:F:70:ASN:ND2	2.34	0.43
2:F:140:LYS:HD3	2:F:140:LYS:N	2.31	0.43
1:G:110:LEU:HD21	2:H:34:ALA:HB1	2.00	0.43
1:A:190:LEU:HD23	1:A:199:PRO:HG3	2.00	0.43
1:A:148:GLN:NE2	1:A:232:CYS:H	2.16	0.43
2:D:62:TYR:O	2:D:112:THR:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:45:ALA:HB2	2:B:72:LEU:HD21	2.01	0.43
2:B:80:ASP:O	2:B:193:VAL:HA	2.18	0.43
1:G:76:THR:HB	1:G:78:THR:OG1	2.19	0.43
1:G:206:PHE:CE1	1:G:219:ILE:HG12	2.54	0.43
1:E:83:LEU:HD12	1:E:84:SER:N	2.34	0.42
2:F:20:PHE:HA	2:F:23:VAL:HG22	2.01	0.42
1:E:81:MET:HE3	1:E:81:MET:HB3	1.84	0.42
2:H:121:ASN:ND2	2:H:125:SER:HB2	2.34	0.42
1:E:177:VAL:HG21	1:E:215:ALA:HB1	2.01	0.42
2:F:19:PRO:HG2	2:F:38:LYS:NZ	2.34	0.42
2:H:25:ASN:HB2	2:H:53:LEU:HD21	2.02	0.42
1:C:32:TYR:HB3	1:C:98:ARG:HG2	2.02	0.42
2:D:180:ARG:HB2	2:D:183:TYR:CZ	2.54	0.42
1:E:156:PRO:HA	1:E:222:LEU:HB3	2.02	0.42
2:B:107:LEU:HD21	2:B:194:VAL:HG11	2.02	0.42
2:F:140:LYS:H	2:F:140:LYS:CD	2.31	0.42
1:G:183:LEU:HD23	1:G:183:LEU:HA	1.84	0.42
2:H:23:VAL:HG23	2:H:24:PHE:N	2.28	0.42
1:G:12:LYS:HE3	1:G:12:LYS:HB3	1.84	0.42
1:G:59:ASN:ND2	1:G:108:LEU:HD13	2.35	0.42
2:F:144:LYS:HE2	2:F:147:GLU:OE1	2.20	0.42
2:H:85:ARG:HD3	2:H:187:HIS:HA	2.01	0.42
1:C:195:ASN:H	2:D:153:GLU:HG3	1.85	0.41
1:G:58:PRO:HB2	1:G:60:TYR:CZ	2.55	0.41
1:G:86:LEU:HB3	1:G:125:VAL:HG21	2.02	0.41
2:B:145:PRO:O	2:B:146:PHE:HB2	2.19	0.41
1:C:159:ARG:HG3	1:C:220:THR:HG22	2.01	0.41
1:E:105:CYS:O	2:F:28:ARG:NH2	2.52	0.41
2:H:35:TRP:O	2:H:148:ARG:NH1	2.53	0.41
1:G:195:ASN:OD1	1:G:210:LYS:HD3	2.21	0.41
1:E:113:TYR:HA	1:E:178:GLN:OE1	2.21	0.41
2:F:153:GLU:O	2:F:173:PRO:HG3	2.19	0.41
1:G:38:ARG:HB3	1:G:94:TYR:CD2	2.55	0.41
1:C:23:LYS:HB3	1:C:23:LYS:HE2	1.71	0.41
2:H:43:CYS:O	2:H:72:LEU:HD12	2.21	0.41
2:B:47:TYR:CD2	2:H:67:THR:HG21	2.56	0.41
2:H:178:SER:O	2:H:178:SER:OG	2.32	0.41
1:A:113:TYR:HD1	1:A:115:ASP:HB3	1.82	0.40
1:C:227:GLU:HB2	1:C:252:VAL:HG23	2.03	0.40
1:A:29:PHE:O	1:A:53:PRO:HG2	2.20	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	227/255 (89%)	219 (96%)	8 (4%)	0	100 100
1	C	227/255 (89%)	212 (93%)	14 (6%)	1 (0%)	30 66
1	E	227/255 (89%)	211 (93%)	15 (7%)	1 (0%)	30 66
1	G	227/255 (89%)	209 (92%)	18 (8%)	0	100 100
2	B	181/223 (81%)	172 (95%)	9 (5%)	0	100 100
2	D	181/223 (81%)	164 (91%)	17 (9%)	0	100 100
2	F	181/223 (81%)	170 (94%)	11 (6%)	0	100 100
2	H	181/223 (81%)	170 (94%)	11 (6%)	0	100 100
All	All	1632/1912 (85%)	1527 (94%)	103 (6%)	2 (0%)	48 81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	253	LEU
1	C	24	ALA

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	187/195 (96%)	167 (89%)	20 (11%)	5 22
1	C	187/195 (96%)	168 (90%)	19 (10%)	6 24
1	E	187/195 (96%)	173 (92%)	14 (8%)	11 38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	187/195 (96%)	169 (90%)	18 (10%)	7 27
2	B	161/198 (81%)	147 (91%)	14 (9%)	8 32
2	D	161/198 (81%)	143 (89%)	18 (11%)	5 21
2	F	161/198 (81%)	148 (92%)	13 (8%)	9 34
2	H	161/198 (81%)	152 (94%)	9 (6%)	17 49
All	All	1392/1572 (88%)	1267 (91%)	125 (9%)	8 30

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	16	SER
1	A	31	SER
1	A	35	SER
1	A	37	VAL
1	A	59	ASN
1	A	88	SER
1	A	104	ASP
1	A	116	LEU
1	A	126	SER
1	A	147	THR
1	A	160	VAL
1	A	169	SER
1	A	207	SER
1	A	209	SER
1	A	210	LYS
1	A	214	SER
1	A	238	SER
1	A	249	LYS
1	A	251	THR
2	B	16	ASN
2	B	21	ASP
2	B	24	PHE
2	B	27	THR
2	B	42	ASN
2	B	56	PHE
2	B	58	THR
2	B	81	SER
2	B	87	ASP
2	B	90	ARG

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Mol	Chain	Res	Type
2	B	109	ASP
2	B	141	SER
2	B	177	TYR
2	B	196	SER
1	C	13	LYS
1	C	23	LYS
1	C	30	SER
1	C	37	VAL
1	C	55	PHE
1	C	73	ASP
1	C	75	SER
1	C	76	THR
1	C	83	LEU
1	C	104	ASP
1	C	145	VAL
1	C	153	SER
1	C	200	SER
1	C	204	ASP
1	C	209	SER
1	C	214	SER
1	C	220	THR
1	C	225	GLU
1	C	251	THR
2	D	24	PHE
2	D	27	THR
2	D	56	PHE
2	D	58	THR
2	D	72	LEU
2	D	73	CYS
2	D	85	ARG
2	D	87	ASP
2	D	90	ARG
2	D	99	ASN
2	D	125	SER
2	D	128	SER
2	D	137	LEU
2	D	141	SER
2	D	152	THR
2	D	160	LYS
2	D	177	TYR
2	D	196	SER
1	E	3	GLN

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Mol	Chain	Res	Type
1	E	13	LYS
1	E	29	PHE
1	E	55	PHE
1	E	81	MET
1	E	87	ARG
1	E	160	VAL
1	E	200	SER
1	E	207	SER
1	E	209	SER
1	E	210	LYS
1	E	213	THR
1	E	223	GLN
1	E	251	THR
2	F	21	ASP
2	F	24	PHE
2	F	28	ARG
2	F	56	PHE
2	F	58	THR
2	F	72	LEU
2	F	73	CYS
2	F	90	ARG
2	F	97	THR
2	F	140	LYS
2	F	178	SER
2	F	180	ARG
2	F	196	SER
1	G	3	GLN
1	G	35	SER
1	G	71	THR
1	G	74	GLU
1	G	76	THR
1	G	88	SER
1	G	90	ASP
1	G	122	LEU
1	G	153	SER
1	G	160	VAL
1	G	200	SER
1	G	204	ASP
1	G	207	SER
1	G	209	SER
1	G	214	SER
1	G	225	GLU

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Mol	Chain	Res	Type
1	G	238	SER
1	G	251	THR
2	H	21	ASP
2	H	27	THR
2	H	59	PHE
2	H	64	VAL
2	H	72	LEU
2	H	121	ASN
2	H	128	SER
2	H	177	TYR
2	H	196	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	148	GLN
2	B	42	ASN
1	C	59	ASN
2	D	121	ASN
2	D	188	GLN
2	F	16	ASN
2	F	70	ASN
1	G	223	GLN
2	H	119	ASN
2	H	121	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides 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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	233/255 (91%)	-0.15	7 (3%) 52 31	28, 43, 74, 88	0
1	C	233/255 (91%)	-0.05	6 (2%) 57 35	32, 47, 79, 98	0
1	E	233/255 (91%)	0.50	14 (6%) 29 16	50, 66, 96, 114	0
1	G	233/255 (91%)	0.70	20 (8%) 18 10	52, 73, 98, 115	0
2	B	183/223 (82%)	-0.02	3 (1%) 70 49	28, 46, 78, 89	0
2	D	183/223 (82%)	-0.11	0 100 100	30, 45, 84, 97	0
2	F	183/223 (82%)	0.16	6 (3%) 49 29	42, 55, 82, 92	0
2	H	183/223 (82%)	0.23	6 (3%) 49 29	43, 58, 89, 104	0
All	All	1664/1912 (87%)	0.17	62 (3%) 45 27	28, 56, 87, 115	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	66	PRO	7.3
1	E	29	PHE	4.9
1	E	255	ALA	4.7
1	C	25	PRO	4.5
1	E	254	ALA	4.4
1	G	29	PHE	4.2
1	G	255	ALA	4.0
1	A	29	PHE	3.9
2	H	74	PHE	3.7
1	E	145	VAL	3.7
1	G	254	ALA	3.7
1	C	29	PHE	3.6
1	G	30	SER	3.6
1	G	2	VAL	3.6
1	E	24	ALA	3.6
1	A	24	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	24	ALA	3.2
1	G	145	VAL	3.2
1	G	25	PRO	3.2
2	H	67	THR	3.1
1	A	119	ARG	3.1
2	H	56	PHE	3.1
1	G	14	PRO	3.1
1	G	115	ASP	3.0
1	G	253	LEU	3.0
1	E	3	GLN	3.0
1	G	124	THR	3.0
1	C	254	ALA	3.0
1	C	255	ALA	2.9
2	F	129	GLY	2.8
1	E	155	ALA	2.8
1	C	24	ALA	2.7
1	E	30	SER	2.7
2	F	71	ASP	2.7
1	E	2	VAL	2.6
1	E	25	PRO	2.6
1	A	30	SER	2.6
1	A	145	VAL	2.6
1	G	64	PHE	2.5
1	G	55	PHE	2.4
1	G	41	PRO	2.4
2	F	56	PHE	2.4
1	E	253	LEU	2.3
1	A	2	VAL	2.3
1	E	156	PRO	2.3
1	G	15	GLY	2.3
1	G	125	VAL	2.3
2	F	67	THR	2.3
1	G	103	GLY	2.2
1	A	255	ALA	2.2
1	E	7	SER	2.2
2	F	128	SER	2.2
2	H	17	LEU	2.1
1	G	88	SER	2.1
2	B	28	ARG	2.1
2	B	45	ALA	2.1
2	H	69	LEU	2.1
1	E	9	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	70	ASN	2.1
1	G	9	ALA	2.1
1	C	2	VAL	2.1
2	F	16	ASN	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.