Full wwPDB X-ray Structure Validation Report ⓘ

Jan 10, 2024 – 07:18 pm GMT

PDB ID	:	8Q7S
Title	:	Crystal structure of the SARS-CoV-2 RBD (Wuhan) with neutralizing VHHs Ma6F06 and Re21H01
Authors	:	Guttler, T.; Aksu, M.; Gorlich, D.
Deposited on	:	2023-08-16
Resolution	:	2.70 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:

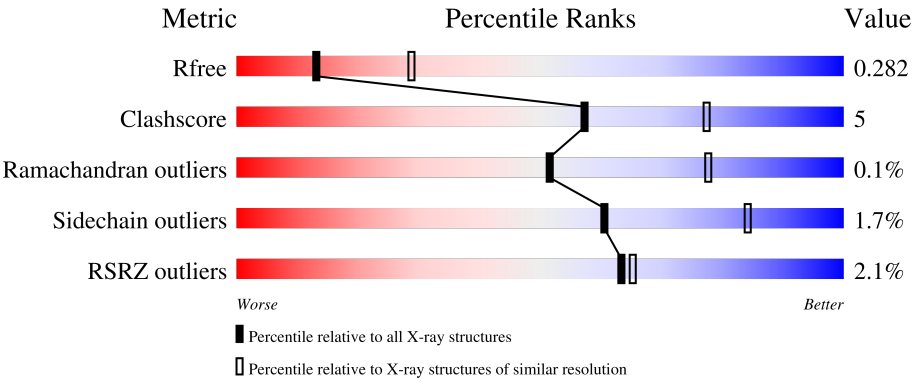
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	196	87% 9% ·
1	D	196	2% 83% 11% 6%
1	G	196	3% 83% 10% · 6%
1	J	196	85% 9% 7%
1	M	196	4% 79% 15% 7%

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Mol	Chain	Length	Quality of chain
2	B	117	2% 91% 8%
2	E	117	2% 89% 8%
2	H	117	3% 89% 9%
2	K	117	2% 84% 12%
2	N	117	5% 83% 15%
3	C	131	% 83% 12%
3	F	131	2% 83% 14%
3	I	131	% 79% 18%
3	L	131	% 78% 20%
3	O	131	2% 76% 21%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 16729 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	1	0
			1506	966	250	283	7			
1	D	185	Total	C	N	O	S	0	0	0
			1478	949	244	278	7			
1	G	184	Total	C	N	O	S	0	2	0
			1476	947	243	278	8			
1	J	183	Total	C	N	O	S	0	0	0
			1462	937	242	276	7			
1	M	183	Total	C	N	O	S	0	0	0
			1462	939	241	275	7			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	331	GLU	-	expression tag	UNP P0DTC2
A	332	GLY	-	expression tag	UNP P0DTC2
A	333	SER	-	expression tag	UNP P0DTC2
A	343	ASP	ASN	engineered mutation	UNP P0DTC2
D	331	GLU	-	expression tag	UNP P0DTC2
D	332	GLY	-	expression tag	UNP P0DTC2
D	333	SER	-	expression tag	UNP P0DTC2
D	343	ASP	ASN	engineered mutation	UNP P0DTC2
G	331	GLU	-	expression tag	UNP P0DTC2
G	332	GLY	-	expression tag	UNP P0DTC2
G	333	SER	-	expression tag	UNP P0DTC2
G	343	ASP	ASN	engineered mutation	UNP P0DTC2
J	331	GLU	-	expression tag	UNP P0DTC2
J	332	GLY	-	expression tag	UNP P0DTC2
J	333	SER	-	expression tag	UNP P0DTC2
J	343	ASP	ASN	engineered mutation	UNP P0DTC2
M	331	GLU	-	expression tag	UNP P0DTC2
M	332	GLY	-	expression tag	UNP P0DTC2
M	333	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
M	343	ASP	ASN	engineered mutation	UNP P0DTC2

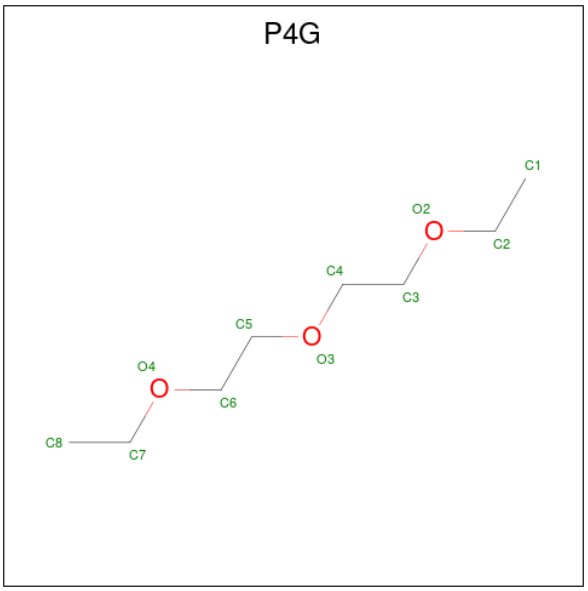
- Molecule 2 is a protein called VHH Antibody Re21H01.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	116	Total	C	N	O	S	0	0	0
			861	533	149	173	6			
2	E	114	Total	C	N	O	S	0	0	0
			848	527	147	168	6			
2	H	114	Total	C	N	O	S	0	0	0
			848	527	147	168	6			
2	K	113	Total	C	N	O	S	0	0	0
			839	522	145	166	6			
2	N	115	Total	C	N	O	S	0	0	0
			854	530	148	170	6			

- Molecule 3 is a protein called VHH Antibody Ma6F06.

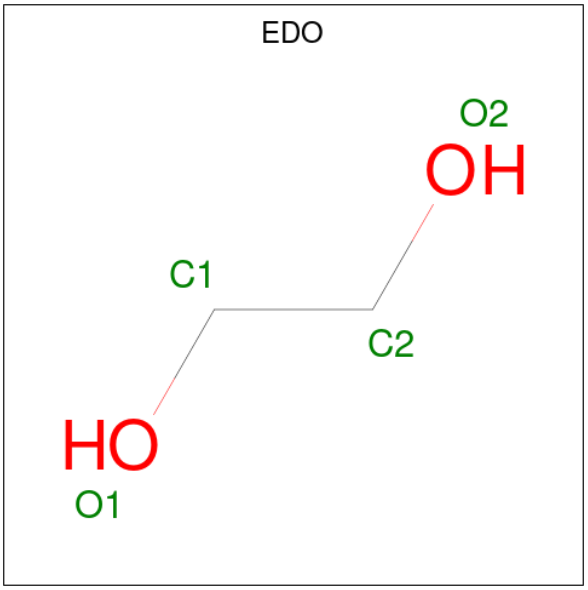
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	126	Total	C	N	O	S	0	0	0
			951	598	160	187	6			
3	F	128	Total	C	N	O	S	0	0	0
			967	606	163	192	6			
3	I	128	Total	C	N	O	S	0	0	0
			967	606	163	192	6			
3	L	128	Total	C	N	O	S	0	0	0
			967	606	163	192	6			
3	O	128	Total	C	N	O	S	0	0	0
			967	606	163	192	6			

- Molecule 4 is 1-ETHOXY-2-(2-ETHOXYETHOXY)ETHANE (three-letter code: P4G) (formula: $C_8H_{18}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 22 16 6	0	1

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0

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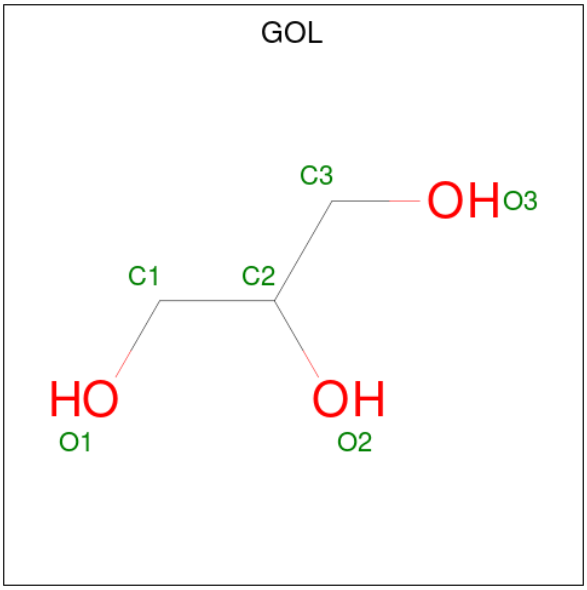
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	O	1	Total C O 4 2 2	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total C O 6 3 3	0	0
6	G	1	Total C O 6 3 3	0	0
6	M	1	Total C O 6 3 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	40	Total O 40 40	0	0
7	B	25	Total O 25 25	0	0
7	C	16	Total O 16 16	0	0
7	D	20	Total O 20 20	0	0
7	E	12	Total O 12 12	0	0

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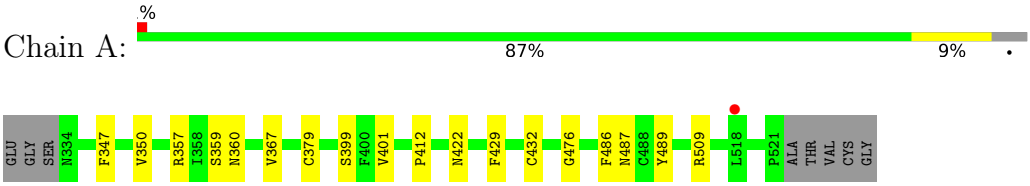
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	17	Total O 17 17	0	0
7	G	15	Total O 15 15	0	0
7	H	4	Total O 4 4	0	0
7	I	9	Total O 9 9	0	0
7	J	26	Total O 26 26	0	0
7	K	3	Total O 3 3	0	0
7	L	6	Total O 6 6	0	0
7	M	8	Total O 8 8	0	0
7	N	6	Total O 6 6	0	0
7	O	13	Total O 13 13	0	0

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.

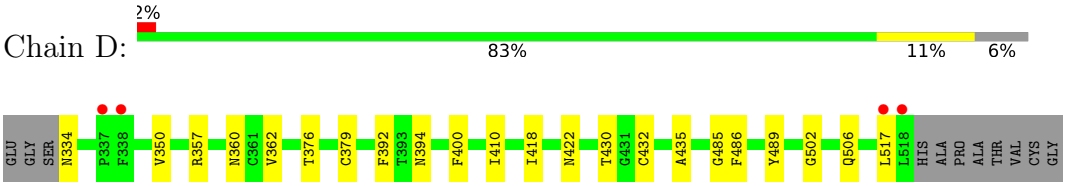
• Molecule 1: Spike protein S1

Chain A:



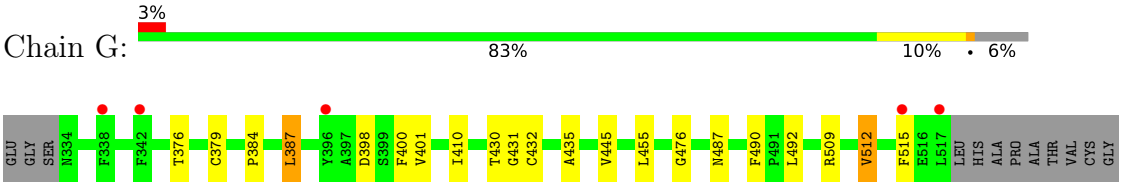
• Molecule 1: Spike protein S1

Chain D:



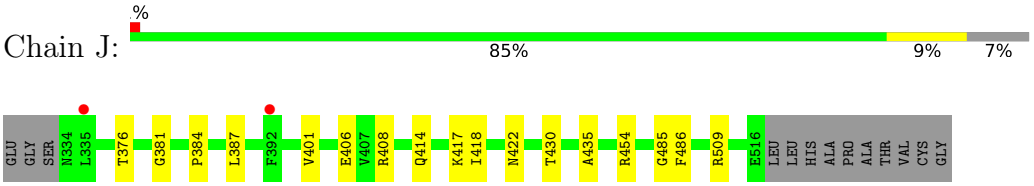
• Molecule 1: Spike protein S1

Chain G:



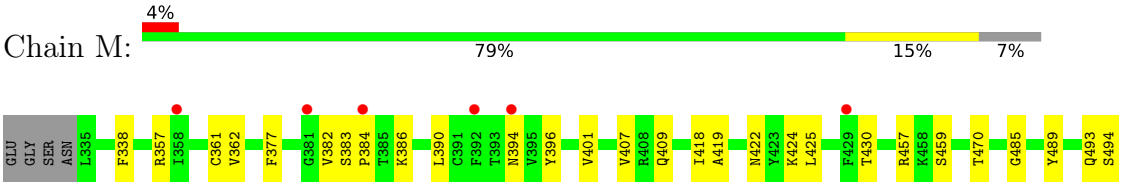
• Molecule 1: Spike protein S1

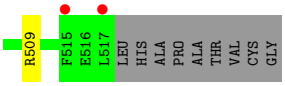
Chain J:



• Molecule 1: Spike protein S1

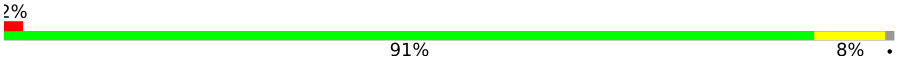
Chain M:

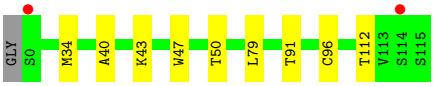




• Molecule 2: VHH Antibody Re21H01

Chain B:



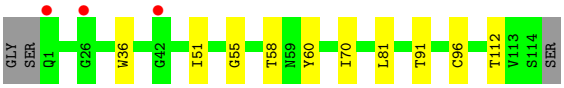


• Molecule 2: VHH Antibody Re21H01

Chain E:

• Molecule 2: VHH Antibody Re21H01

Chain H:



• Molecule 2: VHH Antibody Re21H01

Chain K:

• Molecule 2: VHH Antibody Re21H01

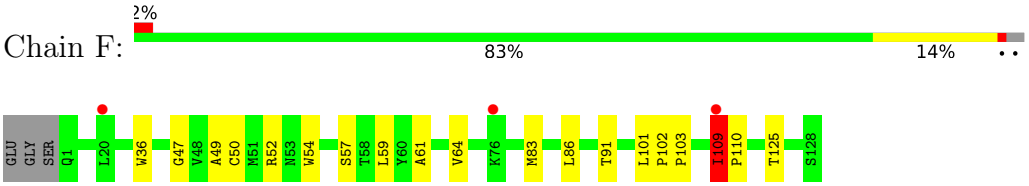
Chain N:

• Molecule 3: VHH Antibody Ma6F06

Chain C:

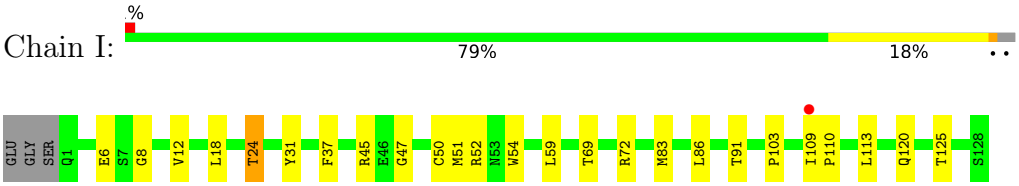
• Molecule 3: VHH Antibody Ma6F06

Chain F:



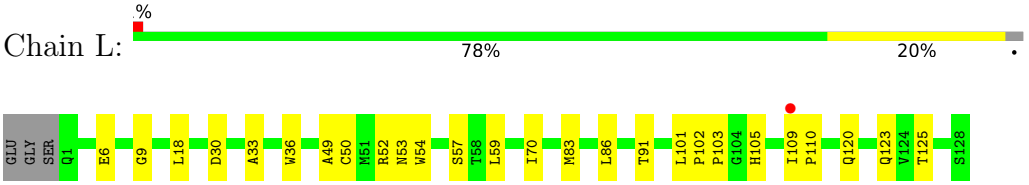
• Molecule 3: VHH Antibody Ma6F06

Chain I:



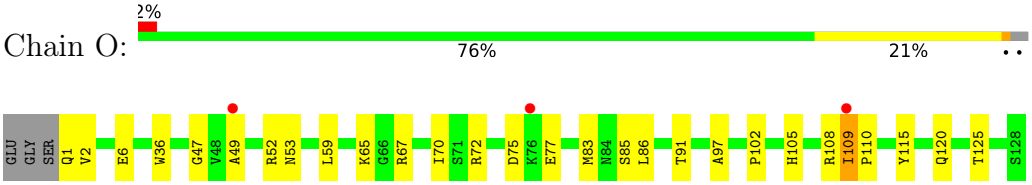
• Molecule 3: VHH Antibody Ma6F06

Chain L:



• Molecule 3: VHH Antibody Ma6F06

Chain O:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.23Å 100.84Å 192.17Å 90.00° 95.63° 90.00°	Depositor
Resolution (Å)	48.25 – 2.70 48.75 – 2.48	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.25-2.70) 86.0 (48.75-2.48)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.22 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.233 , 0.283 0.234 , 0.282	Depositor DCC
R_{free} test set	2016 reflections (2.30%)	wwPDB-VP
Wilson B-factor (Å^2)	44.9	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 26.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16729	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, EDO, P4G

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	0.25	0/1549	0.47	0/2107
1	D	0.25	0/1519	0.48	0/2065
1	G	0.25	0/1523	0.47	0/2070
1	J	0.25	0/1503	0.47	0/2043
1	M	0.25	0/1503	0.46	0/2043
2	B	0.25	0/878	0.50	0/1189
2	E	0.25	0/865	0.49	0/1173
2	H	0.25	0/865	0.49	0/1173
2	K	0.25	0/856	0.50	0/1161
2	N	0.25	0/871	0.50	0/1181
3	C	0.26	0/974	0.50	0/1325
3	F	0.26	0/990	0.51	0/1345
3	I	0.25	0/990	0.50	0/1345
3	L	0.25	0/990	0.50	0/1345
3	O	0.25	0/990	0.50	0/1345
All	All	0.25	0/16866	0.49	0/22910

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	1506	0	1421	11	0
1	D	1478	0	1398	12	0
1	G	1476	0	1397	10	0
1	J	1462	0	1376	11	0
1	M	1462	0	1381	16	0
2	B	861	0	826	4	0
2	E	848	0	816	4	0
2	H	848	0	816	6	0
2	K	839	0	805	8	0
2	N	854	0	821	11	0
3	C	951	0	911	11	0
3	F	967	0	927	15	0
3	I	967	0	927	14	0
3	L	967	0	927	20	0
3	O	967	0	927	20	0
4	A	22	0	36	2	0
5	B	8	0	12	0	0
5	F	4	0	6	0	0
5	O	4	0	6	0	0
6	G	12	0	16	0	0
6	M	6	0	8	0	0
7	A	40	0	0	0	0
7	B	25	0	0	0	0
7	C	16	0	0	0	0
7	D	20	0	0	0	0
7	E	12	0	0	0	0
7	F	17	0	0	0	0
7	G	15	0	0	0	0
7	H	4	0	0	0	0
7	I	9	0	0	0	0
7	J	26	0	0	1	0
7	K	3	0	0	1	0
7	L	6	0	0	0	0
7	M	8	0	0	0	0
7	N	6	0	0	0	0
7	O	13	0	0	1	0
All	All	16729	0	15760	157	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 5.

All (157) 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)
3:O:109:ILE:HG23	3:O:110:PRO:HD3	1.65	0.79
3:L:9:GLY:HA2	3:L:18:LEU:HD21	1.64	0.78
3:C:83:MET:HB3	3:C:86:LEU:HD21	1.70	0.72
2:B:91:THR:HG23	2:B:112:THR:HA	1.73	0.71
3:I:109:ILE:HG23	3:I:110:PRO:HD3	1.73	0.70
3:F:50:CYS:HB2	3:F:109:ILE:HG23	1.75	0.69
3:F:59:LEU:HG	3:F:109:ILE:HD11	1.76	0.67
2:N:9:GLY:HA2	2:N:18:LEU:HD21	1.76	0.66
3:L:59:LEU:HG	3:L:109:ILE:HD11	1.78	0.66
3:F:91:THR:HG23	3:F:125:THR:HA	1.78	0.66
1:D:486:PHE:HD1	3:F:109:ILE:HD12	1.62	0.64
2:N:91:THR:HG23	2:N:112:THR:HA	1.80	0.63
1:A:486:PHE:HD1	3:C:109:ILE:HD12	1.64	0.63
1:A:476:GLY:H	1:A:487:ASN:HB3	1.63	0.63
3:O:65:LYS:NZ	7:O:301:HOH:O	2.32	0.62
2:K:40:ALA:H	2:K:43:LYS:HE2	1.65	0.61
3:C:91:THR:HG23	3:C:125:THR:HA	1.81	0.61
3:O:6:GLU:H	3:O:120:GLN:HE22	1.46	0.61
2:N:23:VAL:HG22	2:N:78:THR:HG22	1.83	0.60
1:A:360:ASN:H	4:A:601[A]:P4G:H22	1.66	0.60
3:F:47:GLY:H	3:F:110:PRO:HA	1.67	0.59
2:B:47:TRP:HE1	2:B:50:THR:HG1	1.51	0.59
1:M:489:TYR:HE1	3:O:110:PRO:HD2	1.67	0.59
3:F:101:LEU:HD12	3:F:102:PRO:HD2	1.83	0.58
1:J:408:ARG:NH1	1:J:414:GLN:OE1	2.36	0.58
2:N:40:ALA:HB3	2:N:43:LYS:HB2	1.86	0.58
3:L:83:MET:HB3	3:L:86:LEU:HD21	1.84	0.58
1:G:398:ASP:HB2	1:G:512:VAL:HG13	1.85	0.58
3:I:24:THR:O	3:I:24:THR:OG1	2.19	0.56
3:I:91:THR:HG23	3:I:125:THR:HA	1.87	0.56
2:E:20:LEU:HD12	2:E:81:LEU:HD23	1.87	0.56
1:A:489:TYR:OH	3:C:110:PRO:HG2	2.05	0.56
3:C:12:VAL:HG11	3:C:18:LEU:HG	1.87	0.56
1:J:486:PHE:HD1	3:L:109:ILE:HD12	1.70	0.56
1:M:485:GLY:HA2	3:O:59:LEU:HD21	1.88	0.56
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.88	0.56
2:N:47:TRP:HE1	2:N:50:THR:HG1	1.53	0.55
3:I:83:MET:HB3	3:I:86:LEU:HD21	1.88	0.54
3:O:83:MET:HB3	3:O:86:LEU:HD21	1.90	0.54
3:C:101:LEU:HD12	3:C:102:PRO:HD2	1.88	0.54
1:D:392:PHE:HA	1:D:517:LEU:HD23	1.90	0.54
1:J:485:GLY:HA2	3:L:59:LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:36:TRP:HB2	3:O:49:ALA:HB3	1.88	0.54
3:L:50:CYS:HB2	3:L:109:ILE:HG23	1.90	0.54
1:G:384:PRO:HA	1:G:387:LEU:HD23	1.89	0.54
1:D:489:TYR:OH	3:F:110:PRO:HG2	2.08	0.53
3:F:83:MET:HB3	3:F:86:LEU:HD21	1.90	0.53
1:M:401:VAL:HG22	1:M:509:ARG:HG2	1.91	0.53
3:L:52:ARG:HE	3:L:57:SER:HB3	1.73	0.53
1:G:401:VAL:HG22	1:G:509:ARG:HG2	1.91	0.52
3:C:50:CYS:HB2	3:C:109:ILE:HG23	1.91	0.52
1:J:401:VAL:HG22	1:J:509:ARG:HG2	1.92	0.52
1:G:376:THR:HB	1:G:435:ALA:HB3	1.92	0.52
1:M:383:SER:HB3	1:M:386:LYS:HG2	1.91	0.52
3:F:52:ARG:HD2	3:F:54:TRP:CZ2	2.45	0.51
1:D:418:ILE:HA	1:D:422:ASN:HD22	1.76	0.51
3:F:36:TRP:HB2	3:F:49:ALA:HB3	1.93	0.51
2:B:40:ALA:HB3	2:B:43:LYS:HB2	1.93	0.51
3:I:37:PHE:HA	3:I:47:GLY:HA2	1.93	0.51
2:K:22:CYS:HB3	2:K:79:LEU:HB3	1.93	0.51
1:J:376:THR:HB	1:J:435:ALA:HB3	1.93	0.50
2:K:86:LEU:HB3	2:K:113:VAL:HG11	1.92	0.50
2:B:34:MET:HB3	2:B:79:LEU:HD22	1.93	0.50
3:I:51:MET:HE1	3:I:72:ARG:HB2	1.94	0.50
2:H:91:THR:HG23	2:H:112:THR:HA	1.93	0.50
3:O:36:TRP:CD1	3:O:70:ILE:HD13	2.47	0.49
3:C:59:LEU:HG	3:C:109:ILE:HD11	1.95	0.49
3:L:33:ALA:HB2	3:L:101:LEU:HD22	1.93	0.49
3:O:52:ARG:NH1	3:O:105:HIS:O	2.41	0.49
2:E:9:GLY:H	2:E:109:THR:HG21	1.79	0.48
3:F:52:ARG:HE	3:F:57:SER:HB3	1.78	0.48
1:G:379:CYS:HA	1:G:432:CYS:HA	1.94	0.48
1:A:360:ASN:H	4:A:601[B]:P4G:H22	1.78	0.48
1:A:350:VAL:HG22	1:A:422:ASN:HB3	1.96	0.47
1:A:412:PRO:HG3	1:A:429:PHE:HB3	1.95	0.47
1:D:376:THR:HB	1:D:435:ALA:HB3	1.97	0.47
3:I:6:GLU:H	3:I:120:GLN:HE22	1.63	0.46
2:N:47:TRP:NE1	2:N:50:THR:OG1	2.42	0.46
1:M:409:GLN:HB3	1:M:419:ALA:HB2	1.96	0.46
2:K:40:ALA:HB3	2:K:43:LYS:HG2	1.96	0.46
1:A:347:PHE:CE2	1:A:399:SER:HB2	2.50	0.46
2:E:3:GLN:HG3	2:E:25:SER:HB2	1.98	0.46
1:J:486:PHE:CE1	3:L:110:PRO:HG3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:75:ASP:O	3:O:77:GLU:N	2.40	0.46
3:I:52:ARG:HD2	3:I:54:TRP:CZ2	2.51	0.45
3:L:36:TRP:HB2	3:L:49:ALA:HB3	1.98	0.45
1:M:418:ILE:HA	1:M:422:ASN:HD22	1.81	0.45
1:D:357:ARG:NH1	1:D:394:ASN:OD1	2.50	0.45
3:F:52:ARG:NE	3:F:57:SER:HB3	2.31	0.45
1:M:384:PRO:HG3	2:N:53:ILE:HG21	1.98	0.45
3:L:30:ASP:O	3:L:53:ASN:ND2	2.43	0.44
1:M:382:VAL:HG23	1:M:430:THR:HG23	1.97	0.44
1:J:381:GLY:HA3	1:J:430:THR:HG22	1.99	0.44
3:L:91:THR:HG23	3:L:125:THR:HA	1.97	0.44
2:H:36:TRP:CE2	2:H:81:LEU:HB2	2.52	0.44
1:D:485:GLY:HA2	3:F:59:LEU:HD21	2.00	0.44
1:M:357:ARG:NH2	1:M:394:ASN:OD1	2.41	0.44
1:M:424:LYS:NZ	1:M:425:LEU:O	2.48	0.44
1:D:400:PHE:HZ	1:D:410:ILE:HG12	1.82	0.44
2:H:51:ILE:HG12	2:H:55:GLY:HA2	1.98	0.44
3:I:8:GLY:O	3:I:18:LEU:HD21	2.18	0.43
2:K:67:ARG:NH2	7:K:201:HOH:O	2.51	0.43
1:D:502:GLY:O	1:D:506:GLN:HG3	2.18	0.43
3:L:52:ARG:HD2	3:L:54:TRP:CZ2	2.52	0.43
1:M:357:ARG:HD2	1:M:396:TYR:CZ	2.53	0.43
1:A:379:CYS:HA	1:A:432:CYS:HA	2.00	0.43
3:C:33:ALA:HB2	3:C:101:LEU:HD22	2.00	0.43
1:D:379:CYS:HA	1:D:432:CYS:HA	1.99	0.43
3:L:123:GLN:NE2	3:L:125:THR:OG1	2.40	0.43
3:O:53:ASN:O	3:O:72:ARG:NH1	2.51	0.43
3:L:102:PRO:HB2	3:L:105:HIS:HD2	1.84	0.43
1:M:493:GLN:OE1	3:O:108:ARG:NH1	2.50	0.43
1:G:431:GLY:HA2	1:G:515:PHE:HD2	1.84	0.43
2:H:60:TYR:CE1	2:H:70:ILE:HG22	2.54	0.43
3:I:31:TYR:CG	3:I:103:PRO:HG3	2.53	0.43
3:O:47:GLY:HA3	3:O:109:ILE:O	2.18	0.43
1:M:407:VAL:HB	2:N:100:PRO:HD2	2.01	0.42
2:K:76:LYS:HB2	2:K:78:THR:HG22	2.00	0.42
2:N:4:LEU:HD13	2:N:96:CYS:O	2.18	0.42
1:J:454:ARG:NH1	7:J:601:HOH:O	2.42	0.42
3:L:102:PRO:HA	3:L:103:PRO:HD3	1.93	0.42
1:M:494:SER:HB2	3:O:102:PRO:HG3	1.99	0.42
3:O:67:ARG:NH1	3:O:85:SER:O	2.52	0.42
3:O:97:ALA:HB1	3:O:115:TYR:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:350:VAL:HG22	1:D:422:ASN:HB3	2.02	0.42
3:F:61:ALA:HB3	3:F:64:VAL:HG22	2.01	0.42
1:M:489:TYR:CE1	3:O:110:PRO:HD2	2.51	0.42
3:F:102:PRO:HA	3:F:103:PRO:HD3	1.95	0.42
3:C:72:ARG:NH2	3:C:76:LYS:O	2.53	0.42
3:I:12:VAL:HG11	3:I:86:LEU:HD13	2.02	0.42
2:K:18:LEU:HD23	2:K:19:ARG:N	2.35	0.42
3:O:75:ASP:C	3:O:77:GLU:H	2.21	0.42
1:D:334:ASN:HB3	1:D:362:VAL:HG12	2.01	0.42
1:M:457:ARG:NH1	1:M:459:SER:O	2.52	0.42
3:I:37:PHE:HB3	3:I:45:ARG:HG2	2.02	0.41
1:J:406:GLU:HB3	1:J:418:ILE:HG13	2.03	0.41
2:H:36:TRP:NE1	2:H:81:LEU:HB2	2.35	0.41
1:J:417:LYS:O	1:J:422:ASN:ND2	2.53	0.41
2:K:52:THR:O	2:K:72:ARG:NH1	2.49	0.41
3:C:52:ARG:HD2	3:C:54:TRP:CH2	2.55	0.41
3:L:102:PRO:HB2	3:L:105:HIS:CD2	2.55	0.41
1:A:357:ARG:NH1	1:A:359:SER:HB3	2.36	0.41
3:I:50:CYS:HB3	3:I:59:LEU:HB3	2.01	0.41
2:N:52:THR:HG23	2:N:55:GLY:H	1.86	0.41
2:E:61:ALA:O	2:E:65:LYS:HG3	2.21	0.41
2:H:51:ILE:HG13	2:H:58:THR:HG22	2.03	0.41
3:L:101:LEU:HD12	3:L:102:PRO:HD2	2.03	0.41
3:O:49:ALA:HB1	3:O:70:ILE:HB	2.02	0.41
1:G:490:PHE:CE2	1:G:492:LEU:HB2	2.56	0.41
1:J:384:PRO:HA	1:J:387:LEU:HD13	2.02	0.41
1:G:400:PHE:HZ	1:G:410:ILE:HG12	1.87	0.40
2:N:52:THR:OG1	2:N:53:ILE:N	2.54	0.40
1:G:476:GLY:H	1:G:487:ASN:HB3	1.86	0.40
3:L:6:GLU:H	3:L:120:GLN:HE22	1.69	0.40
3:L:49:ALA:HB1	3:L:70:ILE:HB	2.03	0.40
3:O:91:THR:HG23	3:O:125:THR:HA	2.03	0.40
1:G:455:LEU:HD21	3:I:113:LEU:HB3	2.04	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	187/196 (95%)	179 (96%)	8 (4%)	0	100	100
1	D	183/196 (93%)	171 (93%)	11 (6%)	1 (0%)	29	54
1	G	184/196 (94%)	176 (96%)	8 (4%)	0	100	100
1	J	181/196 (92%)	171 (94%)	10 (6%)	0	100	100
1	M	181/196 (92%)	172 (95%)	9 (5%)	0	100	100
2	B	114/117 (97%)	107 (94%)	7 (6%)	0	100	100
2	E	112/117 (96%)	107 (96%)	5 (4%)	0	100	100
2	H	112/117 (96%)	109 (97%)	3 (3%)	0	100	100
2	K	111/117 (95%)	104 (94%)	7 (6%)	0	100	100
2	N	113/117 (97%)	108 (96%)	5 (4%)	0	100	100
3	C	124/131 (95%)	118 (95%)	5 (4%)	1 (1%)	19	43
3	F	126/131 (96%)	121 (96%)	4 (3%)	1 (1%)	19	43
3	I	126/131 (96%)	123 (98%)	3 (2%)	0	100	100
3	L	126/131 (96%)	122 (97%)	4 (3%)	0	100	100
3	O	126/131 (96%)	117 (93%)	9 (7%)	0	100	100
All	All	2106/2220 (95%)	2005 (95%)	98 (5%)	3 (0%)	51	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	430	THR
3	C	109	ILE
3	F	109	ILE

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	164/168 (98%)	163 (99%)	1 (1%)	86 95
1	D	161/168 (96%)	160 (99%)	1 (1%)	86 95
1	G	162/168 (96%)	158 (98%)	4 (2%)	47 76
1	J	159/168 (95%)	159 (100%)	0	100 100
1	M	159/168 (95%)	153 (96%)	6 (4%)	33 62
2	B	93/93 (100%)	92 (99%)	1 (1%)	73 90
2	E	91/93 (98%)	88 (97%)	3 (3%)	38 67
2	H	91/93 (98%)	90 (99%)	1 (1%)	73 90
2	K	90/93 (97%)	87 (97%)	3 (3%)	38 67
2	N	92/93 (99%)	89 (97%)	3 (3%)	38 67
3	C	102/106 (96%)	101 (99%)	1 (1%)	76 91
3	F	104/106 (98%)	103 (99%)	1 (1%)	76 91
3	I	104/106 (98%)	102 (98%)	2 (2%)	57 82
3	L	104/106 (98%)	104 (100%)	0	100 100
3	O	104/106 (98%)	101 (97%)	3 (3%)	42 71
All	All	1780/1835 (97%)	1750 (98%)	30 (2%)	60 84

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	367	VAL
2	B	96	CYS
3	C	109	ILE
1	D	360	ASN
2	E	1	GLN
2	E	96	CYS
2	E	109	THR
3	F	109	ILE
1	G	387	LEU
1	G	430	THR

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Mol	Chain	Res	Type
1	G	445	VAL
1	G	512	VAL
2	H	96	CYS
3	I	24	THR
3	I	69	THR
2	K	48	VAL
2	K	96	CYS
2	K	113	VAL
1	M	338	PHE
1	M	361	CYS
1	M	362	VAL
1	M	377	PHE
1	M	390	LEU
1	M	470	THR
2	N	3	GLN
2	N	65	LYS
2	N	96	CYS
3	O	1	GLN
3	O	2	VAL
3	O	109	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	EDO	B	201	-	3,3,3	0.48	0	2,2,2	0.32	0
6	GOL	G	602	-	5,5,5	0.90	0	5,5,5	0.98	0
6	GOL	M	601	-	5,5,5	0.94	0	5,5,5	0.93	0
6	GOL	G	601	-	5,5,5	0.93	0	5,5,5	0.97	0
5	EDO	B	202	-	3,3,3	0.48	0	2,2,2	0.31	0
5	EDO	F	201	-	3,3,3	0.46	0	2,2,2	0.34	0
4	P4G	A	601[A]	-	10,10,10	0.37	0	9,9,9	0.18	0
4	P4G	A	601[B]	-	10,10,10	0.38	0	9,9,9	0.17	0
5	EDO	O	201	-	3,3,3	0.49	0	2,2,2	0.27	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	201	-	-	0/1/1/1	-
6	GOL	G	602	-	-	0/4/4/4	-
6	GOL	M	601	-	-	1/4/4/4	-
6	GOL	G	601	-	-	0/4/4/4	-
5	EDO	B	202	-	-	0/1/1/1	-
5	EDO	F	201	-	-	0/1/1/1	-
4	P4G	A	601[A]	-	-	2/8/8/8	-
4	P4G	A	601[B]	-	-	3/8/8/8	-
5	EDO	O	201	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601[B]	P4G	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
4	A	601[A]	P4G	O3-C5-C6-O4
4	A	601[B]	P4G	C3-C4-O3-C5
4	A	601[A]	P4G	C8-C7-O4-C6
6	M	601	GOL	O1-C1-C2-C3
4	A	601[B]	P4G	C8-C7-O4-C6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601[A]	P4G	1	0
4	A	601[B]	P4G	1	0

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	188/196 (95%)	-0.27	1 (0%)	91	92	33, 44, 78, 98	0
1	D	185/196 (94%)	-0.16	4 (2%)	62	63	42, 55, 91, 101	0
1	G	184/196 (93%)	0.01	5 (2%)	54	55	49, 64, 88, 97	0
1	J	183/196 (93%)	0.02	2 (1%)	80	82	40, 53, 94, 105	0
1	M	183/196 (93%)	0.28	8 (4%)	34	33	39, 67, 99, 113	0
2	B	116/117 (99%)	-0.26	2 (1%)	70	72	35, 47, 65, 81	0
2	E	114/117 (97%)	-0.09	2 (1%)	68	70	49, 69, 87, 97	0
2	H	114/117 (97%)	0.02	3 (2%)	56	57	55, 69, 85, 96	0
2	K	113/117 (96%)	0.11	2 (1%)	68	70	50, 73, 87, 96	0
2	N	115/117 (98%)	0.33	6 (5%)	27	25	48, 73, 88, 99	0
3	C	126/131 (96%)	-0.08	1 (0%)	86	87	36, 47, 75, 92	0
3	F	128/131 (97%)	-0.13	3 (2%)	60	62	41, 53, 77, 86	0
3	I	128/131 (97%)	-0.25	1 (0%)	86	87	45, 53, 71, 83	0
3	L	128/131 (97%)	-0.16	1 (0%)	86	87	43, 55, 78, 91	0
3	O	128/131 (97%)	0.09	3 (2%)	60	62	38, 65, 87, 106	0
All	All	2133/2220 (96%)	-0.04	44 (2%)	63	65	33, 58, 88, 113	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	515	PHE	6.9
1	D	518	LEU	5.6
1	M	392	PHE	5.4
3	O	109	ILE	4.2
1	G	517	LEU	4.1
1	M	358	ILE	3.8
2	B	0	SER	3.8

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Mol	Chain	Res	Type	RSRZ
3	C	109	ILE	3.6
1	M	384	PRO	3.5
1	G	396	TYR	3.4
2	E	0	SER	3.1
2	H	1	GLN	2.9
2	H	26	GLY	2.9
3	I	109	ILE	2.9
1	M	381	GLY	2.9
1	D	517	LEU	2.8
2	N	89	GLU	2.8
2	N	0	SER	2.8
3	L	109	ILE	2.8
2	N	41	PRO	2.7
1	G	342	PHE	2.6
2	E	88	PRO	2.6
3	O	76	LYS	2.6
1	M	429	PHE	2.6
2	K	2	VAL	2.6
1	J	335	LEU	2.5
1	M	394	ASN	2.5
1	G	338	PHE	2.4
1	D	337	PRO	2.4
1	M	517	LEU	2.4
1	D	338	PHE	2.4
2	K	107	GLN	2.3
1	J	392	PHE	2.3
3	F	76	LYS	2.3
2	N	113	VAL	2.3
2	N	91	THR	2.2
3	O	49	ALA	2.1
2	B	114	SER	2.1
3	F	109	ILE	2.1
1	G	515	PHE	2.1
3	F	20	LEU	2.1
2	N	114	SER	2.1
2	H	42	GLY	2.1
1	A	518	LEU	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)

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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
6	GOL	G	602	6/6	0.59	0.20	82,91,93,94	0
4	P4G	A	601[B]	11/11	0.83	0.28	74,76,76,77	11
6	GOL	G	601	6/6	0.83	0.21	60,64,72,72	0
4	P4G	A	601[A]	11/11	0.83	0.28	71,75,76,77	11
5	EDO	F	201	4/4	0.84	0.14	53,55,57,59	0
5	EDO	O	201	4/4	0.85	0.20	54,58,58,60	0
5	EDO	B	202	4/4	0.88	0.27	40,40,43,44	0
6	GOL	M	601	6/6	0.92	0.12	52,54,56,60	0
5	EDO	B	201	4/4	0.93	0.13	46,48,49,50	0

6.5 Other polymers (i)

There are no such residues in this entry.