Full wwPDB X-ray Structure Validation Report (i)

May 16, 2020 – 09:12 am BST

PDB ID	:	5NAF
Title	:	Co-crystal structure of an MeCP2 peptide with TBLR1 WD40 domain
Authors	:	Kruusvee, V.; Cook, A.G.
Deposited on	:	2017-02-27
Resolution	:	2.49 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

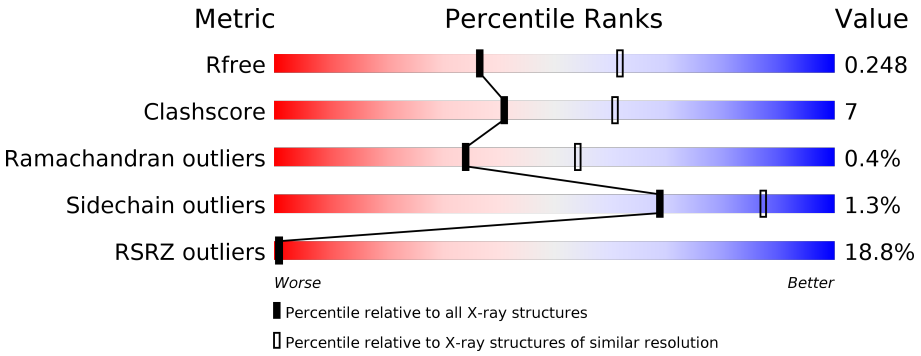
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.49 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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	402	% 75% 12% 12%
1	B	402	2% 74% 12% 13%
1	C	402	26% 73% 10% • 16%
1	D	402	35% 72% 10% 18%
2	E	25	8% 28% 16% 56%
2	F	25	4% 24% 16% 60%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	D	606	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10400 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 F-box-like/WD repeat-containing protein TBL1XR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2654	1669	457	513	15			
1	B	348	Total	C	N	O	S	0	0	0
			2616	1651	452	498	15			
1	C	339	Total	C	N	O	S	0	0	0
			2235	1395	399	430	11			
1	D	331	Total	C	N	O	S	0	0	0
			2114	1309	384	410	11			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	MET	-	initiating methionine	UNP Q8BHJ5
A	114	GLY	-	expression tag	UNP Q8BHJ5
A	115	SER	-	expression tag	UNP Q8BHJ5
A	116	SER	-	expression tag	UNP Q8BHJ5
A	117	HIS	-	expression tag	UNP Q8BHJ5
A	118	HIS	-	expression tag	UNP Q8BHJ5
A	119	HIS	-	expression tag	UNP Q8BHJ5
A	120	HIS	-	expression tag	UNP Q8BHJ5
A	121	HIS	-	expression tag	UNP Q8BHJ5
A	122	HIS	-	expression tag	UNP Q8BHJ5
A	123	SER	-	expression tag	UNP Q8BHJ5
A	124	SER	-	expression tag	UNP Q8BHJ5
A	125	GLY	-	expression tag	UNP Q8BHJ5
A	126	LEU	-	expression tag	UNP Q8BHJ5
A	127	GLU	-	expression tag	UNP Q8BHJ5
A	128	VAL	-	expression tag	UNP Q8BHJ5
A	129	LEU	-	expression tag	UNP Q8BHJ5
A	130	PHE	-	expression tag	UNP Q8BHJ5
A	131	GLN	-	expression tag	UNP Q8BHJ5
A	132	GLY	-	expression tag	UNP Q8BHJ5
A	133	PRO	-	expression tag	UNP Q8BHJ5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	113	MET	-	initiating methionine	UNP Q8BHJ5
B	114	GLY	-	expression tag	UNP Q8BHJ5
B	115	SER	-	expression tag	UNP Q8BHJ5
B	116	SER	-	expression tag	UNP Q8BHJ5
B	117	HIS	-	expression tag	UNP Q8BHJ5
B	118	HIS	-	expression tag	UNP Q8BHJ5
B	119	HIS	-	expression tag	UNP Q8BHJ5
B	120	HIS	-	expression tag	UNP Q8BHJ5
B	121	HIS	-	expression tag	UNP Q8BHJ5
B	122	HIS	-	expression tag	UNP Q8BHJ5
B	123	SER	-	expression tag	UNP Q8BHJ5
B	124	SER	-	expression tag	UNP Q8BHJ5
B	125	GLY	-	expression tag	UNP Q8BHJ5
B	126	LEU	-	expression tag	UNP Q8BHJ5
B	127	GLU	-	expression tag	UNP Q8BHJ5
B	128	VAL	-	expression tag	UNP Q8BHJ5
B	129	LEU	-	expression tag	UNP Q8BHJ5
B	130	PHE	-	expression tag	UNP Q8BHJ5
B	131	GLN	-	expression tag	UNP Q8BHJ5
B	132	GLY	-	expression tag	UNP Q8BHJ5
B	133	PRO	-	expression tag	UNP Q8BHJ5
C	113	MET	-	initiating methionine	UNP Q8BHJ5
C	114	GLY	-	expression tag	UNP Q8BHJ5
C	115	SER	-	expression tag	UNP Q8BHJ5
C	116	SER	-	expression tag	UNP Q8BHJ5
C	117	HIS	-	expression tag	UNP Q8BHJ5
C	118	HIS	-	expression tag	UNP Q8BHJ5
C	119	HIS	-	expression tag	UNP Q8BHJ5
C	120	HIS	-	expression tag	UNP Q8BHJ5
C	121	HIS	-	expression tag	UNP Q8BHJ5
C	122	HIS	-	expression tag	UNP Q8BHJ5
C	123	SER	-	expression tag	UNP Q8BHJ5
C	124	SER	-	expression tag	UNP Q8BHJ5
C	125	GLY	-	expression tag	UNP Q8BHJ5
C	126	LEU	-	expression tag	UNP Q8BHJ5
C	127	GLU	-	expression tag	UNP Q8BHJ5
C	128	VAL	-	expression tag	UNP Q8BHJ5
C	129	LEU	-	expression tag	UNP Q8BHJ5
C	130	PHE	-	expression tag	UNP Q8BHJ5
C	131	GLN	-	expression tag	UNP Q8BHJ5
C	132	GLY	-	expression tag	UNP Q8BHJ5
C	133	PRO	-	expression tag	UNP Q8BHJ5

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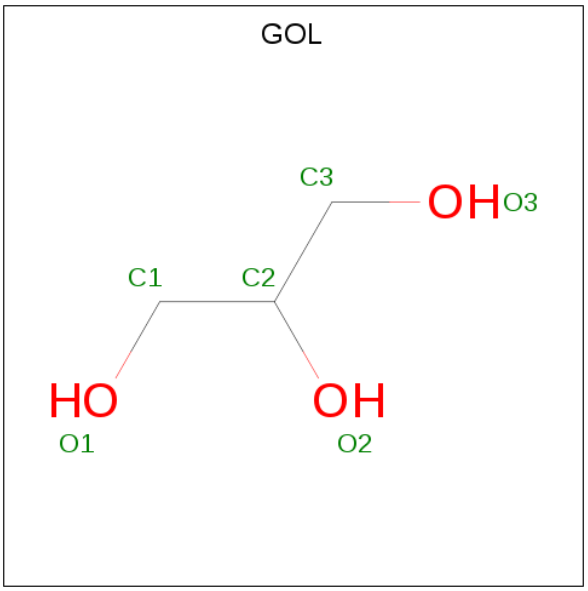
Chain	Residue	Modelled	Actual	Comment	Reference
D	113	MET	-	initiating methionine	UNP Q8BHJ5
D	114	GLY	-	expression tag	UNP Q8BHJ5
D	115	SER	-	expression tag	UNP Q8BHJ5
D	116	SER	-	expression tag	UNP Q8BHJ5
D	117	HIS	-	expression tag	UNP Q8BHJ5
D	118	HIS	-	expression tag	UNP Q8BHJ5
D	119	HIS	-	expression tag	UNP Q8BHJ5
D	120	HIS	-	expression tag	UNP Q8BHJ5
D	121	HIS	-	expression tag	UNP Q8BHJ5
D	122	HIS	-	expression tag	UNP Q8BHJ5
D	123	SER	-	expression tag	UNP Q8BHJ5
D	124	SER	-	expression tag	UNP Q8BHJ5
D	125	GLY	-	expression tag	UNP Q8BHJ5
D	126	LEU	-	expression tag	UNP Q8BHJ5
D	127	GLU	-	expression tag	UNP Q8BHJ5
D	128	VAL	-	expression tag	UNP Q8BHJ5
D	129	LEU	-	expression tag	UNP Q8BHJ5
D	130	PHE	-	expression tag	UNP Q8BHJ5
D	131	GLN	-	expression tag	UNP Q8BHJ5
D	132	GLY	-	expression tag	UNP Q8BHJ5
D	133	PRO	-	expression tag	UNP Q8BHJ5

- Molecule 2 is a protein called Methyl-CpG-binding protein 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	11	Total	C	N	O	0	0	0
			81	52	18	11			
2	F	10	Total	C	N	O	0	0	0
			72	47	14	11			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

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

- Molecule 4 is water.

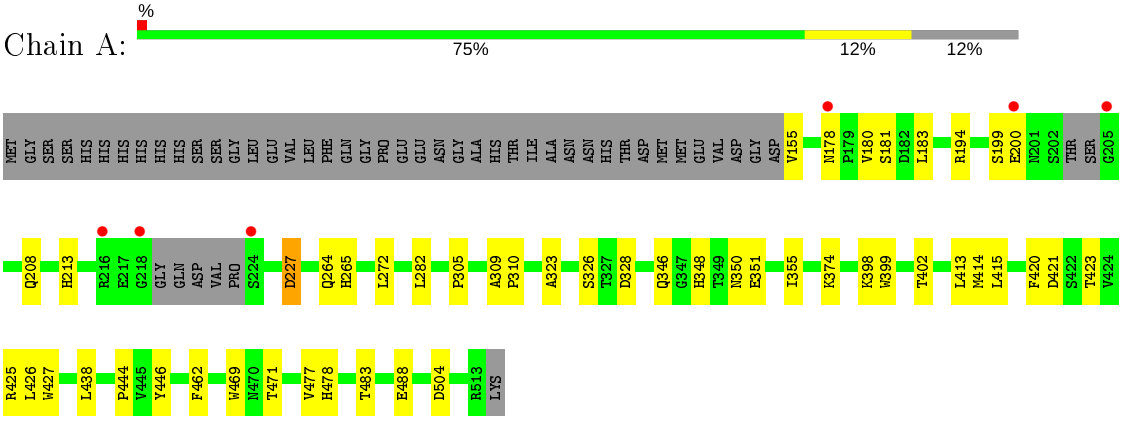
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	202	Total O 202 202	0	0
4	B	187	Total O 187 187	0	0
4	C	74	Total O 74 74	0	0
4	D	40	Total O 40 40	0	0
4	E	5	Total O 5 5	0	0
4	F	6	Total O 6 6	0	0

3 Residue-property plots (i)

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

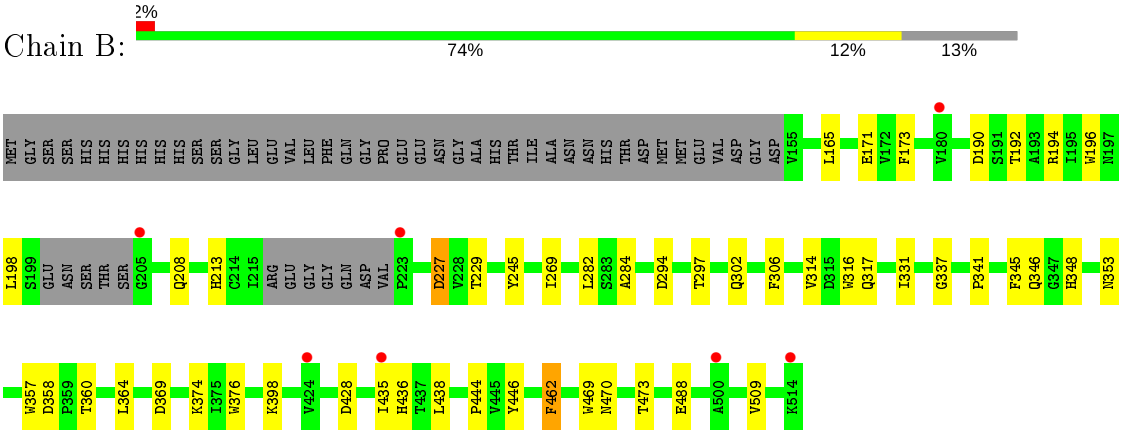
• Molecule 1: F-box-like/WD repeat-containing protein TBL1XR1

Chain A:



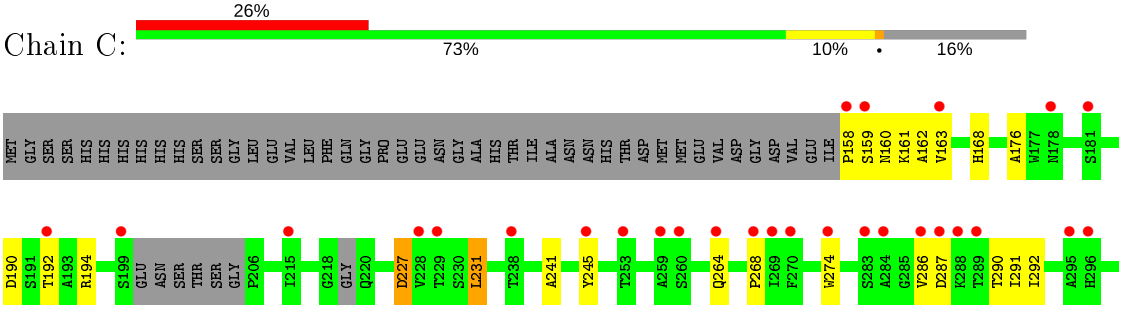
• Molecule 1: F-box-like/WD repeat-containing protein TBL1XR1

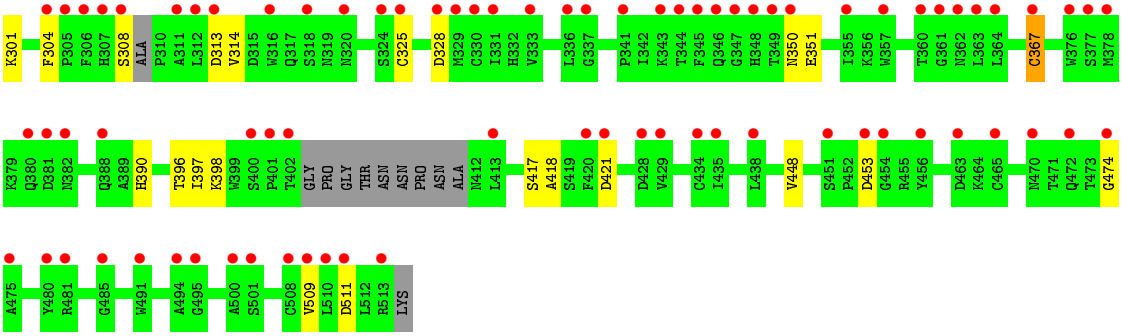
Chain B:



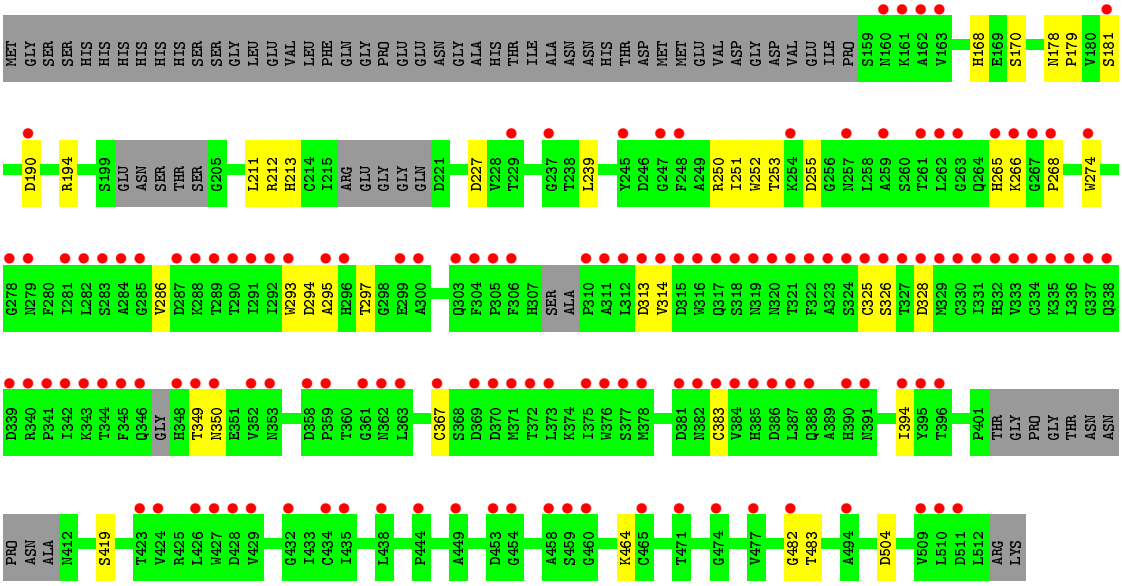
• Molecule 1: F-box-like/WD repeat-containing protein TBL1XR1

Chain C:

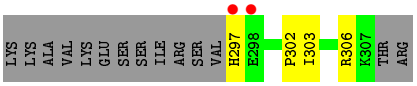




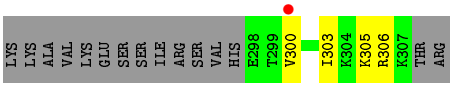
• Molecule 1: F-box-like/WD repeat-containing protein TBL1XR1



• Molecule 2: Methyl-CpG-binding protein 2



• Molecule 2: Methyl-CpG-binding protein 2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	42.63Å 58.64Å 155.10Å 97.63° 91.17° 90.24°	Depositor
Resolution (Å)	49.64 – 2.49 49.64 – 2.49	Depositor EDS
% Data completeness (in resolution range)	97.5 (49.64-2.49) 97.5 (49.64-2.49)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.48Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.203 , 0.248 0.203 , 0.248	Depositor DCC
R_{free} test set	2513 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	33.9	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 66.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10400	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.55% 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

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	0.28	0/2720	0.53	0/3710
1	B	0.29	0/2682	0.52	0/3658
1	C	0.30	0/2286	0.57	2/3138 (0.1%)
1	D	0.34	0/2157	0.54	0/2966
2	E	0.26	0/82	0.50	0/109
2	F	0.28	0/72	0.55	0/95
All	All	0.30	0/9999	0.54	2/13676 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	231	LEU	CB-CG-CD2	-11.20	91.97	111.00
1	C	231	LEU	CB-CG-CD1	5.91	121.05	111.00

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	2654	0	2472	35	0
1	B	2616	0	2456	32	1
1	C	2235	0	1708	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2114	0	1569	27	0
2	E	81	0	77	3	0
2	F	72	0	80	4	0
3	A	42	0	56	0	1
3	B	30	0	40	0	0
3	C	6	0	8	0	0
3	D	36	0	47	0	0
4	A	202	0	0	5	1
4	B	187	0	0	3	1
4	C	74	0	0	7	0
4	D	40	0	0	3	0
4	E	5	0	0	1	0
4	F	6	0	0	0	0
All	All	10400	0	8513	130	2

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 7.

All (130) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:HIS:HE2	1:D:293:TRP:HZ2	1.11	0.92
1:A:194:ARG:HH11	1:A:208:GLN:NE2	1.68	0.91
1:B:302:GLN:HE22	1:B:337:GLY:H	1.23	0.87
1:A:194:ARG:HH11	1:A:208:GLN:HE21	1.18	0.84
1:D:483:THR:OG1	1:D:504:ASP:OD2	1.95	0.83
1:D:250:ARG:NH1	4:D:701:HOH:O	2.10	0.83
1:B:194:ARG:NH1	1:B:208:GLN:OE1	2.11	0.82
1:D:265:HIS:NE2	1:D:293:TRP:HZ2	1.77	0.82
1:B:470:ASN:HD22	1:B:473:THR:H	1.28	0.81
1:D:253:THR:HG22	1:D:255:ASP:H	1.45	0.81
1:D:383:CYS:SG	4:D:708:HOH:O	2.47	0.73
1:C:398:LYS:NZ	4:C:704:HOH:O	2.21	0.73
1:D:313:ASP:OD1	1:D:314:VAL:N	2.23	0.72
1:C:367:CYS:HB3	1:C:397:ILE:HG12	1.72	0.71
1:C:190:ASP:OD1	1:C:192:THR:HG22	1.91	0.69
1:A:425:ARG:NH2	4:A:706:HOH:O	2.25	0.69
1:B:488:GLU:OE2	4:B:701:HOH:O	2.10	0.69
1:C:313:ASP:OD2	1:C:314:VAL:N	2.26	0.69
1:D:212:ARG:NH1	4:D:702:HOH:O	2.24	0.69
1:D:168:HIS:CE1	1:D:194:ARG:HD2	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ARG:NH1	1:A:208:GLN:NE2	2.40	0.68
1:A:488:GLU:OE2	4:A:701:HOH:O	2.12	0.68
1:B:470:ASN:ND2	1:B:473:THR:H	1.91	0.67
1:B:428:ASP:OD1	4:B:702:HOH:O	2.13	0.67
1:D:294:ASP:OD2	1:D:297:THR:N	2.29	0.65
1:A:348:HIS:CE1	1:A:374:LYS:HD2	2.33	0.64
1:D:239:LEU:HD12	1:D:251:ILE:HG22	1.80	0.62
1:A:178:ASN:HD22	1:A:181:SER:H	1.48	0.61
1:A:178:ASN:ND2	1:A:180:VAL:H	1.99	0.60
1:A:178:ASN:HD21	1:A:180:VAL:HG22	1.66	0.60
1:B:173:PHE:O	4:B:703:HOH:O	2.17	0.59
1:D:349:THR:O	1:D:350:ASN:ND2	2.35	0.59
2:F:303:ILE:HA	2:F:306:ARG:HD2	1.85	0.58
1:A:178:ASN:HD22	1:A:180:VAL:H	1.51	0.58
1:B:294:ASP:OD2	1:B:297:THR:N	2.35	0.58
1:B:428:ASP:HB2	1:B:435:ILE:HD11	1.87	0.57
1:A:178:ASN:HB2	1:A:183:LEU:HB2	1.87	0.56
1:B:462:PHE:CE2	2:F:300:VAL:HB	2.40	0.56
1:C:245:TYR:CG	1:C:268:PRO:HB3	2.41	0.56
1:D:178:ASN:ND2	1:D:179:PRO:HD2	2.21	0.55
1:B:317:GLN:HB2	1:B:357:TRP:CE2	2.41	0.55
1:C:241:ALA:HB2	1:C:274:TRP:CZ2	2.41	0.54
1:B:369:ASP:OD2	2:F:305:LYS:NZ	2.40	0.54
1:A:155:VAL:N	4:A:715:HOH:O	2.41	0.54
1:A:438:LEU:HD13	1:A:469:TRP:CG	2.42	0.54
1:B:353:ASN:HD21	2:F:305:LYS:NZ	2.06	0.54
1:B:198:LEU:HD22	1:B:509:VAL:HG11	1.89	0.53
1:B:438:LEU:HD13	1:B:469:TRP:CD2	2.44	0.53
1:C:163:VAL:HG12	1:C:509:VAL:HB	1.91	0.53
1:C:287:ASP:N	1:C:287:ASP:OD2	2.42	0.52
1:D:253:THR:HG22	1:D:255:ASP:N	2.22	0.51
1:A:323:ALA:HB3	1:A:355:ILE:HD13	1.93	0.51
1:B:358:ASP:OD1	1:B:360:THR:OG1	2.22	0.51
1:C:474:GLY:O	4:C:701:HOH:O	2.19	0.51
1:C:453:ASP:OD2	4:C:702:HOH:O	2.19	0.51
1:C:241:ALA:HB2	1:C:274:TRP:CE2	2.47	0.50
1:C:245:TYR:CD1	1:C:268:PRO:HB3	2.46	0.50
1:B:435:ILE:HG22	1:B:436:HIS:CD2	2.47	0.49
1:D:178:ASN:HB3	1:D:181:SER:O	2.12	0.49
1:C:163:VAL:CG1	1:C:509:VAL:HB	2.43	0.49
1:B:444:PRO:HB2	1:B:446:TYR:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:LEU:HB3	1:B:376:TRP:HB2	1.94	0.48
1:C:398:LYS:HG3	1:C:448:VAL:HG23	1.95	0.48
1:C:162:ALA:O	4:C:703:HOH:O	2.20	0.48
1:C:390:HIS:ND1	1:C:421:ASP:OD2	2.45	0.48
1:B:284:ALA:HB2	1:B:314:VAL:HG13	1.95	0.48
1:A:414:MET:HE3	1:A:426:LEU:HD22	1.96	0.48
1:A:438:LEU:HD13	1:A:469:TRP:CD2	2.49	0.48
1:A:402:THR:OG1	1:A:413:LEU:HA	2.14	0.47
1:B:227:ASP:OD2	1:B:227:ASP:N	2.47	0.47
1:D:394:ILE:HA	1:D:419:SER:HA	1.96	0.47
1:B:331:ILE:HB	1:B:345:PHE:HB2	1.94	0.47
1:C:291:ILE:HB	4:C:705:HOH:O	2.14	0.47
1:D:250:ARG:HG3	1:D:250:ARG:HH11	1.79	0.47
1:D:250:ARG:NH1	1:D:250:ARG:HG3	2.30	0.47
1:C:396:THR:HG22	1:C:418:ALA:HB3	1.96	0.46
1:A:477:VAL:HG12	1:A:478:HIS:CD2	2.51	0.46
1:D:170:SER:OG	1:D:190:ASP:N	2.49	0.46
1:A:326:SER:HB3	1:A:328:ASP:OD1	2.16	0.46
1:D:265:HIS:NE2	1:D:293:TRP:CZ2	2.68	0.46
1:C:268:PRO:O	1:C:286:VAL:HG23	2.16	0.45
1:B:438:LEU:HD13	1:B:469:TRP:CG	2.52	0.45
1:B:302:GLN:NE2	1:B:337:GLY:H	2.03	0.45
1:A:309:ALA:HB1	1:A:310:PRO:HD2	1.98	0.45
1:D:464:LYS:O	1:D:482:GLY:N	2.44	0.45
1:B:306:PHE:CE1	1:B:341:PRO:HD3	2.52	0.45
1:A:350:ASN:OD1	1:A:351:GLU:N	2.34	0.44
1:C:227:ASP:N	1:C:227:ASP:OD2	2.50	0.44
1:A:398:LYS:HD3	1:A:398:LYS:HA	1.83	0.44
1:A:483:THR:OG1	1:A:504:ASP:OD2	2.27	0.44
1:B:348:HIS:CE1	1:B:374:LYS:HD2	2.52	0.44
1:C:161:LYS:HB3	1:C:511:ASP:HB3	2.00	0.44
1:D:326:SER:HB2	1:D:328:ASP:OD1	2.18	0.44
1:D:274:TRP:HZ3	1:D:295:ALA:HB2	1.82	0.43
1:C:290:THR:HG22	1:C:304:PHE:HB2	2.00	0.43
1:C:161:LYS:N	4:C:710:HOH:O	2.51	0.43
1:C:290:THR:HG23	1:C:304:PHE:CD2	2.53	0.43
1:D:227:ASP:OD2	1:D:227:ASP:N	2.52	0.43
2:E:297:HIS:N	4:E:402:HOH:O	2.51	0.43
1:C:168:HIS:CE1	1:C:194:ARG:HD2	2.54	0.43
1:A:227:ASP:OD1	1:A:227:ASP:N	2.51	0.43
1:C:192:THR:HG21	1:C:194:ARG:HE	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:ASN:OD1	1:C:351:GLU:N	2.45	0.42
1:B:282:LEU:HB2	1:B:316:TRP:CZ2	2.54	0.42
1:C:159:SER:N	4:C:710:HOH:O	2.52	0.42
1:C:308:SER:N	1:C:328:ASP:OD2	2.53	0.42
1:A:420:PHE:HA	1:A:444:PRO:HB3	2.00	0.42
1:C:397:ILE:HG22	1:C:417:SER:HA	2.01	0.42
1:B:229:THR:OG1	1:B:269:ILE:O	2.24	0.42
1:D:265:HIS:CE1	1:D:293:TRP:HZ2	2.36	0.42
1:A:264:GLN:HG2	1:A:265:HIS:O	2.20	0.41
1:B:398:LYS:HD3	1:B:398:LYS:HA	1.83	0.41
1:A:305:PRO:O	4:A:702:HOH:O	2.22	0.41
1:A:346:GLN:HE21	1:A:346:GLN:HB3	1.73	0.41
1:B:165:LEU:HB3	1:B:196:TRP:CZ3	2.56	0.41
1:A:446:TYR:CZ	2:E:302:PRO:HD3	2.55	0.41
1:C:158:PRO:C	1:C:160:ASN:H	2.22	0.41
1:C:176:ALA:HB3	1:C:231:LEU:HD11	2.02	0.41
1:A:421:ASP:OD1	1:A:423:THR:OG1	2.30	0.41
1:A:414:MET:HE1	1:A:471:THR:HB	2.03	0.41
1:A:213:HIS:ND1	4:A:710:HOH:O	2.37	0.41
1:A:425:ARG:HD3	1:A:427:TRP:CZ2	2.55	0.41
1:D:268:PRO:HD2	1:D:286:VAL:HG11	2.03	0.41
1:B:190:ASP:OD1	1:B:192:THR:OG1	2.31	0.41
1:B:227:ASP:O	1:B:245:TYR:N	2.54	0.41
2:E:303:ILE:HA	2:E:306:ARG:HD2	2.03	0.41
1:D:211:LEU:HD23	1:D:252:TRP:CG	2.56	0.40
1:A:272:LEU:HD12	1:A:282:LEU:O	2.21	0.40
1:A:399:TRP:CE2	1:A:415:LEU:HD13	2.57	0.40
1:C:292:ILE:O	1:C:301:LYS:N	2.52	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:GLN:NE2	3:A:605:GOL:O3[1_565]	2.16	0.04
4:A:844:HOH:O	4:B:859:HOH:O[1_545]	2.19	0.01

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	346/402 (86%)	329 (95%)	15 (4%)	2 (1%)	25	43
1	B	342/402 (85%)	328 (96%)	13 (4%)	1 (0%)	41	61
1	C	329/402 (82%)	312 (95%)	16 (5%)	1 (0%)	41	61
1	D	319/402 (79%)	304 (95%)	14 (4%)	1 (0%)	41	61
2	E	9/25 (36%)	9 (100%)	0	0	100	100
2	F	8/25 (32%)	8 (100%)	0	0	100	100
All	All	1353/1658 (82%)	1290 (95%)	58 (4%)	5 (0%)	34	54

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	266	LYS
1	C	264	GLN
1	A	199	SER
1	A	200	GLU
1	B	213	HIS

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	276/338 (82%)	274 (99%)	2 (1%)	84	94
1	B	273/338 (81%)	270 (99%)	3 (1%)	73	89
1	C	159/338 (47%)	156 (98%)	3 (2%)	57	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	141/338 (42%)	138 (98%)	3 (2%)	53 78
2	E	6/24 (25%)	6 (100%)	0	100 100
2	F	7/24 (29%)	7 (100%)	0	100 100
All	All	862/1400 (62%)	851 (99%)	11 (1%)	69 87

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	227	ASP
1	A	462	PHE
1	B	171	GLU
1	B	227	ASP
1	B	462	PHE
1	C	227	ASP
1	C	325	CYS
1	C	367	CYS
1	D	213	HIS
1	D	325	CYS
1	D	367	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	ASN
1	A	208	GLN
1	B	302	GLN
1	B	353	ASN
1	B	470	ASN
1	C	213	HIS
1	D	160	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

19 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	$\#\|Z\|>2$
3	GOL	B	601	-	5,5,5	0.38	0	5,5,5	0.28	0
3	GOL	A	601	-	5,5,5	0.35	0	5,5,5	0.26	0
3	GOL	D	601	-	5,5,5	0.37	0	5,5,5	0.27	0
3	GOL	C	601	-	5,5,5	0.37	0	5,5,5	0.26	0
3	GOL	B	605	-	5,5,5	0.36	0	5,5,5	0.25	0
3	GOL	A	605	-	5,5,5	0.36	0	5,5,5	0.38	0
3	GOL	A	602	-	5,5,5	0.37	0	5,5,5	0.30	0
3	GOL	D	604	-	5,5,5	0.38	0	5,5,5	0.30	0
3	GOL	A	606	-	5,5,5	0.37	0	5,5,5	0.16	0
3	GOL	B	603	-	5,5,5	0.36	0	5,5,5	0.31	0
3	GOL	B	604	-	5,5,5	0.40	0	5,5,5	0.24	0
3	GOL	A	603	-	5,5,5	0.37	0	5,5,5	0.26	0
3	GOL	D	603	-	5,5,5	0.37	0	5,5,5	0.30	0
3	GOL	A	607	-	5,5,5	0.36	0	5,5,5	0.19	0
3	GOL	B	602	-	5,5,5	0.38	0	5,5,5	0.21	0
3	GOL	A	604	-	5,5,5	0.37	0	5,5,5	0.36	0
3	GOL	D	606	-	5,5,5	0.77	0	5,5,5	0.60	0
3	GOL	D	605	-	5,5,5	0.37	0	5,5,5	0.26	0
3	GOL	D	602	-	5,5,5	0.37	0	5,5,5	0.28	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
3	GOL	B	601	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	601	-	-	2/4/4/4	-
3	GOL	D	601	-	-	2/4/4/4	-
3	GOL	C	601	-	-	2/4/4/4	-
3	GOL	B	605	-	-	4/4/4/4	-
3	GOL	A	605	-	-	0/4/4/4	-
3	GOL	A	602	-	-	2/4/4/4	-
3	GOL	D	604	-	-	2/4/4/4	-
3	GOL	A	606	-	-	2/4/4/4	-
3	GOL	B	603	-	-	2/4/4/4	-
3	GOL	B	604	-	-	2/4/4/4	-
3	GOL	A	603	-	-	2/4/4/4	-
3	GOL	D	603	-	-	2/4/4/4	-
3	GOL	A	607	-	-	2/4/4/4	-
3	GOL	B	602	-	-	0/4/4/4	-
3	GOL	A	604	-	-	4/4/4/4	-
3	GOL	D	606	-	-	0/4/4/4	-
3	GOL	D	605	-	-	2/4/4/4	-
3	GOL	D	602	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	601	GOL	O1-C1-C2-C3
3	C	601	GOL	O1-C1-C2-C3
3	B	605	GOL	O1-C1-C2-C3
3	A	602	GOL	O1-C1-C2-C3
3	D	604	GOL	O1-C1-C2-C3
3	B	603	GOL	O1-C1-C2-C3
3	A	603	GOL	O1-C1-C2-C3
3	D	603	GOL	O1-C1-C2-C3
3	A	607	GOL	O1-C1-C2-C3
3	A	604	GOL	O1-C1-C2-C3
3	D	605	GOL	O1-C1-C2-O2
3	D	605	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	B	601	GOL	O1-C1-C2-C3
3	B	605	GOL	C1-C2-C3-O3
3	A	606	GOL	C1-C2-C3-O3
3	B	604	GOL	O1-C1-C2-C3
3	D	601	GOL	O1-C1-C2-O2
3	C	601	GOL	O1-C1-C2-O2
3	A	602	GOL	O1-C1-C2-O2
3	B	603	GOL	O1-C1-C2-O2
3	A	603	GOL	O1-C1-C2-O2
3	D	603	GOL	O1-C1-C2-O2
3	B	601	GOL	O1-C1-C2-O2
3	B	605	GOL	O1-C1-C2-O2
3	B	605	GOL	O2-C2-C3-O3
3	B	604	GOL	O1-C1-C2-O2
3	A	607	GOL	O1-C1-C2-O2
3	A	601	GOL	O1-C1-C2-O2
3	A	606	GOL	O2-C2-C3-O3
3	A	604	GOL	O1-C1-C2-O2
3	D	604	GOL	O1-C1-C2-O2
3	D	602	GOL	O1-C1-C2-O2
3	D	602	GOL	O1-C1-C2-C3
3	A	601	GOL	O1-C1-C2-C3
3	A	604	GOL	C1-C2-C3-O3
3	A	604	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	605	GOL	0	1

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	352/402 (87%)	0.55	6 (1%) 70 72	17, 28, 50, 127	0
1	B	348/402 (86%)	0.60	7 (2%) 65 68	18, 29, 48, 97	0
1	C	339/402 (84%)	1.63	106 (31%) 0 0	29, 70, 109, 135	0
1	D	331/402 (82%)	2.16	140 (42%) 0 0	32, 75, 125, 155	0
2	E	11/25 (44%)	1.28	2 (18%) 1 1	30, 35, 86, 89	0
2	F	10/25 (40%)	0.85	1 (10%) 7 6	28, 40, 61, 77	0
All	All	1391/1658 (83%)	1.22	262 (18%) 1 1	17, 44, 109, 155	0

All (262) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	306	PHE	10.4
1	D	329	MET	9.4
1	D	330	CYS	8.3
1	D	340	ARG	7.6
1	D	361	GLY	7.4
1	D	344	THR	7.3
1	D	343	LYS	7.1
1	D	377	SER	7.0
1	D	378	MET	6.9
1	D	315	ASP	6.8
1	D	384	VAL	6.7
1	D	376	TRP	6.4
1	C	158	PRO	6.2
1	D	339	ASP	6.1
1	D	295	ALA	6.1
1	C	361	GLY	5.8
1	D	326	SER	5.7
1	D	305	PRO	5.7
1	D	385	HIS	5.7

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Mol	Chain	Res	Type	RSRZ
1	C	378	MET	5.7
1	D	423	THR	5.6
1	D	323	ALA	5.6
1	D	349	THR	5.6
1	D	328	ASP	5.5
1	C	345	PHE	5.5
1	D	434	CYS	5.5
1	D	345	PHE	5.5
1	D	341	PRO	5.4
1	D	278	GLY	5.3
1	D	320	ASN	5.2
1	D	424	VAL	5.2
1	D	348	HIS	5.2
1	C	295	ALA	5.1
1	D	334	CYS	5.0
1	D	342	ILE	5.0
1	D	325	CYS	5.0
1	D	350	ASN	4.9
1	D	318	SER	4.9
1	C	296	HIS	4.8
1	D	367	CYS	4.8
1	D	324	SER	4.8
1	D	259	ALA	4.7
1	D	287	ASP	4.7
1	D	429	VAL	4.7
1	C	274	TRP	4.6
1	D	335	LYS	4.6
1	D	332	HIS	4.6
1	C	510	LEU	4.6
1	D	304	PHE	4.6
1	D	290	THR	4.5
1	C	287	ASP	4.5
1	C	305	PRO	4.5
1	D	381	ASP	4.5
1	C	377	SER	4.5
1	C	382	ASN	4.5
1	C	429	VAL	4.5
1	D	336	LEU	4.5
1	C	474	GLY	4.5
1	C	347	GLY	4.4
1	D	321	THR	4.4
1	D	288	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	331	ILE	4.4
1	D	317	GLN	4.4
1	C	367	CYS	4.4
1	C	362	ASN	4.3
1	C	199	SER	4.3
1	C	336	LEU	4.3
1	D	362	ASN	4.3
1	C	306	PHE	4.2
1	C	434	CYS	4.2
1	D	322	PHE	4.2
1	C	307	HIS	4.2
1	C	480	TYR	4.2
1	D	310	PRO	4.0
1	D	289	THR	4.0
1	D	388	GLN	4.0
1	D	395	TYR	4.0
1	C	333	VAL	4.0
1	C	491	TRP	3.9
1	D	311	ALA	3.9
1	D	263	GLY	3.9
1	C	343	LYS	3.9
2	E	298	GLU	3.9
1	D	292	ILE	3.9
1	C	381	ASP	3.8
1	D	391	ASN	3.8
1	D	372	THR	3.8
1	C	494	ALA	3.8
1	C	324	SER	3.8
1	C	348	HIS	3.8
1	D	284	ALA	3.8
1	D	181	SER	3.8
1	D	314	VAL	3.7
1	D	383	CYS	3.7
1	D	346	GLN	3.7
1	D	245	TYR	3.7
1	D	262	LEU	3.7
1	C	509	VAL	3.7
1	D	282	LEU	3.6
1	C	330	CYS	3.6
1	D	369	ASP	3.6
1	D	373	LEU	3.6
2	E	297	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	485	GLY	3.6
1	C	363	LEU	3.6
1	C	270	PHE	3.5
1	D	299	GLU	3.5
1	D	281	ILE	3.5
1	D	333	VAL	3.5
1	D	319	ASN	3.5
1	C	344	THR	3.4
1	C	229	THR	3.4
1	C	289	THR	3.4
1	D	291	ILE	3.3
1	D	268	PRO	3.3
1	D	375	ILE	3.3
1	D	432	GLY	3.3
1	C	420	PHE	3.3
1	C	350	ASN	3.3
1	C	475	ALA	3.3
1	A	205	GLY	3.2
1	C	388	GLN	3.2
1	D	353	ASN	3.2
1	D	352	VAL	3.2
1	C	318	SER	3.1
1	C	360	THR	3.1
1	C	329	MET	3.1
1	C	421	ASP	3.1
1	D	229	THR	3.1
1	D	370	ASP	3.1
1	D	482	GLY	3.1
1	C	268	PRO	3.1
1	A	216	ARG	3.1
1	B	223	PRO	3.0
1	D	316	TRP	3.0
1	D	427	TRP	3.0
1	A	200	GLU	3.0
1	C	328	ASP	3.0
1	D	359	PRO	3.0
1	C	316	TRP	3.0
1	C	465	CYS	3.0
1	D	382	ASN	2.9
1	C	331	ILE	2.9
1	D	248	PHE	2.9
1	D	303	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	438	LEU	2.9
1	C	159	SER	2.9
1	D	453	ASP	2.9
1	C	438	LEU	2.9
1	B	514	LYS	2.8
1	D	279	ASN	2.8
1	C	380	GLN	2.8
1	C	508	CYS	2.8
1	B	205	GLY	2.8
1	C	181	SER	2.8
1	C	163	VAL	2.8
1	C	495	GLY	2.8
1	C	178	ASN	2.8
1	D	337	GLY	2.8
1	D	283	SER	2.8
1	C	311	ALA	2.7
1	D	296	HIS	2.7
1	A	218	GLY	2.7
1	C	245	TYR	2.7
1	C	325	CYS	2.7
1	D	327	THR	2.7
1	D	510	LEU	2.7
1	D	265	HIS	2.7
1	C	320	ASN	2.7
1	C	238	THR	2.7
1	C	337	GLY	2.7
1	D	285	GLY	2.7
1	D	386	ASP	2.7
1	C	284	ALA	2.7
1	D	267	GLY	2.7
1	D	312	LEU	2.6
1	D	257	ASN	2.6
1	D	471	THR	2.6
1	D	444	PRO	2.6
1	A	224	SER	2.6
1	D	494	ALA	2.6
1	C	288	LYS	2.6
1	C	413	LEU	2.6
1	C	264	GLN	2.6
1	D	396	THR	2.6
1	C	470	ASN	2.6
1	C	341	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	304	PHE	2.6
1	C	260	SER	2.6
1	C	463	ASP	2.6
1	D	358	ASP	2.6
1	D	313	ASP	2.5
1	D	511	ASP	2.5
1	D	426	LEU	2.5
1	C	355	ILE	2.5
1	C	472	GLN	2.5
1	C	313	ASP	2.5
1	D	449	ALA	2.5
1	D	163	VAL	2.5
1	D	190	ASP	2.5
1	D	458	ALA	2.4
1	D	161	LYS	2.4
1	D	460	GLY	2.4
1	B	424	VAL	2.4
1	C	454	GLY	2.4
1	D	237	GLY	2.4
1	D	162	ALA	2.4
1	C	253	THR	2.4
1	C	402	THR	2.4
1	C	451	SER	2.4
1	C	501	SER	2.3
1	C	312	LEU	2.3
1	D	160	ASN	2.3
1	C	286	VAL	2.3
1	D	266	LYS	2.3
2	F	300	VAL	2.3
1	A	178	ASN	2.3
1	D	363	LEU	2.3
1	D	465	CYS	2.3
1	C	269	ILE	2.3
1	D	338	GLN	2.3
1	C	500	ALA	2.2
1	C	349	THR	2.2
1	D	387	LEU	2.2
1	C	401	PRO	2.2
1	C	259	ALA	2.2
1	C	376	TRP	2.2
1	C	481	ARG	2.2
1	C	192	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	428	ASP	2.2
1	C	308	SER	2.2
1	D	300	ALA	2.2
1	C	513	ARG	2.2
1	D	274	TRP	2.2
1	C	428	ASP	2.2
1	D	394	ILE	2.2
1	D	435	ILE	2.2
1	D	293	TRP	2.1
1	C	435	ILE	2.1
1	D	261	THR	2.1
1	C	456	TYR	2.1
1	D	371	MET	2.1
1	D	477	VAL	2.1
1	D	247	GLY	2.1
1	B	435	ILE	2.1
1	C	364	LEU	2.1
1	C	283	SER	2.1
1	C	400	SER	2.1
1	B	180	VAL	2.1
1	C	346	GLN	2.1
1	C	453	ASP	2.1
1	C	511	ASP	2.1
1	D	474	GLY	2.1
1	C	228	VAL	2.1
1	D	459	SER	2.1
1	D	509	VAL	2.0
1	D	390	HIS	2.0
1	C	357	TRP	2.0
1	C	215	ILE	2.0
1	B	500	ALA	2.0
1	D	454	GLY	2.0
1	D	254	LYS	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 carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
3	GOL	D	606	6/6	0.24	0.52	67,70,71,74	0
3	GOL	A	601	6/6	0.43	0.31	64,68,69,69	0
3	GOL	A	606	6/6	0.64	0.33	62,67,69,72	0
3	GOL	A	602	6/6	0.65	0.26	63,65,66,66	0
3	GOL	B	604	6/6	0.69	0.30	40,57,61,62	0
3	GOL	D	605	6/6	0.71	0.21	68,71,73,73	0
3	GOL	D	601	6/6	0.72	0.18	68,74,76,77	0
3	GOL	D	603	6/6	0.72	0.20	58,61,64,65	0
3	GOL	D	602	6/6	0.73	0.21	52,53,54,55	0
3	GOL	B	602	6/6	0.74	0.29	45,49,52,53	0
3	GOL	D	604	6/6	0.76	0.20	68,71,75,78	0
3	GOL	C	601	6/6	0.77	0.21	63,66,67,67	0
3	GOL	B	605	6/6	0.78	0.22	47,50,54,57	0
3	GOL	B	601	6/6	0.79	0.19	60,61,62,64	0
3	GOL	B	603	6/6	0.81	0.35	61,70,75,75	0
3	GOL	A	603	6/6	0.83	0.36	57,60,63,67	0
3	GOL	A	607	6/6	0.83	0.19	53,56,59,59	0
3	GOL	A	604	6/6	0.84	0.35	39,45,46,47	0
3	GOL	A	605	6/6	0.84	0.23	59,60,62,63	0

6.5 Other polymers

There are no such residues in this entry.