



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:51 PM GMT

PDB ID : 3KEE
Title : HCV NS3/NS4A complexed with Non-covalent macrocyclic compound
TMC435
Authors : Lindberg, J.D.; Nystrom, S.; Cummings, M.D.
Deposited on : 2009-10-26
Resolution : 2.40 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

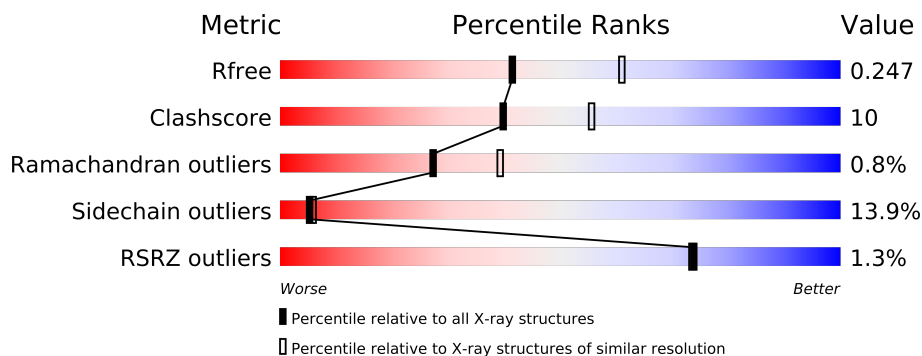
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.40 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}	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	190	
1	B	190	
1	C	190	
1	D	190	
2	E	23	
2	F	23	
2	G	23	
2	H	23	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	GOL	C	3968[A]	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
5	GOL	C	3968[B]	-	X
5	GOL	D	3968[A]	-	X
5	GOL	D	3968[B]	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5877 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1312	815	238	249	10			
1	B	178	Total	C	N	O	S	0	0	0
			1312	815	238	249	10			
1	C	178	Total	C	N	O	S	0	0	0
			1312	815	238	249	10			
1	D	178	Total	C	N	O	S	0	0	0
			1312	815	238	249	10			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP P90191
A	181	SER	-	EXPRESSION TAG	UNP P90191
A	182	GLY	-	EXPRESSION TAG	UNP P90191
A	183	SER	-	EXPRESSION TAG	UNP P90191
A	184	HIS	-	EXPRESSION TAG	UNP P90191
A	185	HIS	-	EXPRESSION TAG	UNP P90191
A	186	HIS	-	EXPRESSION TAG	UNP P90191
A	187	HIS	-	EXPRESSION TAG	UNP P90191
A	188	HIS	-	EXPRESSION TAG	UNP P90191
A	189	HIS	-	EXPRESSION TAG	UNP P90191
B	0	MET	-	EXPRESSION TAG	UNP P90191
B	181	SER	-	EXPRESSION TAG	UNP P90191
B	182	GLY	-	EXPRESSION TAG	UNP P90191
B	183	SER	-	EXPRESSION TAG	UNP P90191
B	184	HIS	-	EXPRESSION TAG	UNP P90191
B	185	HIS	-	EXPRESSION TAG	UNP P90191
B	186	HIS	-	EXPRESSION TAG	UNP P90191
B	187	HIS	-	EXPRESSION TAG	UNP P90191
B	188	HIS	-	EXPRESSION TAG	UNP P90191
B	189	HIS	-	EXPRESSION TAG	UNP P90191
C	0	MET	-	EXPRESSION TAG	UNP P90191

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Chain	Residue	Modelled	Actual	Comment	Reference
C	181	SER	-	EXPRESSION TAG	UNP P90191
C	182	GLY	-	EXPRESSION TAG	UNP P90191
C	183	SER	-	EXPRESSION TAG	UNP P90191
C	184	HIS	-	EXPRESSION TAG	UNP P90191
C	185	HIS	-	EXPRESSION TAG	UNP P90191
C	186	HIS	-	EXPRESSION TAG	UNP P90191
C	187	HIS	-	EXPRESSION TAG	UNP P90191
C	188	HIS	-	EXPRESSION TAG	UNP P90191
C	189	HIS	-	EXPRESSION TAG	UNP P90191
D	0	MET	-	EXPRESSION TAG	UNP P90191
D	181	SER	-	EXPRESSION TAG	UNP P90191
D	182	GLY	-	EXPRESSION TAG	UNP P90191
D	183	SER	-	EXPRESSION TAG	UNP P90191
D	184	HIS	-	EXPRESSION TAG	UNP P90191
D	185	HIS	-	EXPRESSION TAG	UNP P90191
D	186	HIS	-	EXPRESSION TAG	UNP P90191
D	187	HIS	-	EXPRESSION TAG	UNP P90191
D	188	HIS	-	EXPRESSION TAG	UNP P90191
D	189	HIS	-	EXPRESSION TAG	UNP P90191

- Molecule 2 is a protein called 19-mer peptide from Genome polyprotein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	12	Total	C	N	O	0	0	0
			86	57	16	13			
2	F	12	Total	C	N	O	0	0	0
			86	57	16	13			
2	G	12	Total	C	N	O	0	0	0
			86	57	16	13			
2	H	12	Total	C	N	O	0	0	0
			86	57	16	13			

There are 16 discrepancies between the modelled and reference sequences:

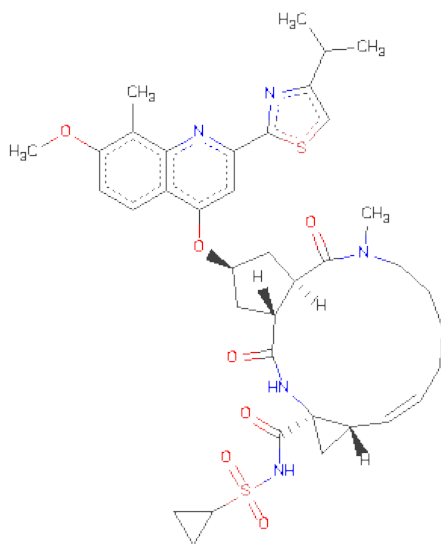
Chain	Residue	Modelled	Actual	Comment	Reference
E	19	LYS	-	EXPRESSION TAG	UNP Q6GYR8
E	20	LYS	-	EXPRESSION TAG	UNP Q6GYR8
E	40	LYS	-	EXPRESSION TAG	UNP Q6GYR8
E	41	LYS	-	EXPRESSION TAG	UNP Q6GYR8
F	19	LYS	-	EXPRESSION TAG	UNP Q6GYR8
F	20	LYS	-	EXPRESSION TAG	UNP Q6GYR8
F	40	LYS	-	EXPRESSION TAG	UNP Q6GYR8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	41	LYS	-	EXPRESSION TAG	UNP Q6GYR8
G	19	LYS	-	EXPRESSION TAG	UNP Q6GYR8
G	20	LYS	-	EXPRESSION TAG	UNP Q6GYR8
G	40	LYS	-	EXPRESSION TAG	UNP Q6GYR8
G	41	LYS	-	EXPRESSION TAG	UNP Q6GYR8
H	19	LYS	-	EXPRESSION TAG	UNP Q6GYR8
H	20	LYS	-	EXPRESSION TAG	UNP Q6GYR8
H	40	LYS	-	EXPRESSION TAG	UNP Q6GYR8
H	41	LYS	-	EXPRESSION TAG	UNP Q6GYR8

- Molecule 3 is (2R,3AR,10Z,11AS,12AR,14AR)-N-(CYCLOPROPYLSULFONYL)-2-({7-METHOXY-8-METHYL-2-[4-(1-METHYLETHYL)-1,3-THIAZOL-2-YL]QUINOLIN-4-YL} OXY)-5-METHYL-4,14-DIOXO-2,3,3A,4,5,6,7,8,9,11A,12,13,14,14A-TETRADECAHYDROCYCLOPENTA[C]CYCLOPROPA[G][1,6]DIAZACYCLOTETRADECINE-12A(1H)-CARBOXAMIDE (three-letter code: 30B) (formula: C₃₈H₄₇N₅O₇S₂).

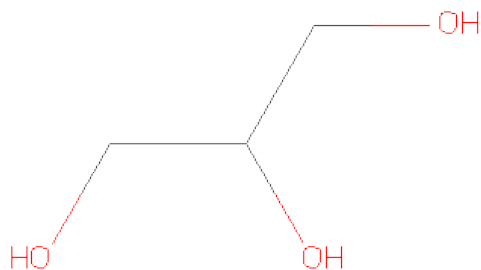


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			52	38	5	7	2		
3	B	1	Total	C	N	O	S	0	0
			52	38	5	7	2		
3	C	1	Total	C	N	O	S	0	0
			52	38	5	7	2		
3	D	1	Total	C	N	O	S	0	0
			52	38	5	7	2		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Zn 1 1	0	0
4	A	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0
4	C	1	Total Zn 1 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 12 6 6	0	1
5	D	1	Total C O 12 6 6	0	1

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	11	Total O 11 11	0	0
6	E	1	Total O 1 1	0	0
6	B	11	Total O 11 11	0	0
6	F	1	Total O 1 1	0	0

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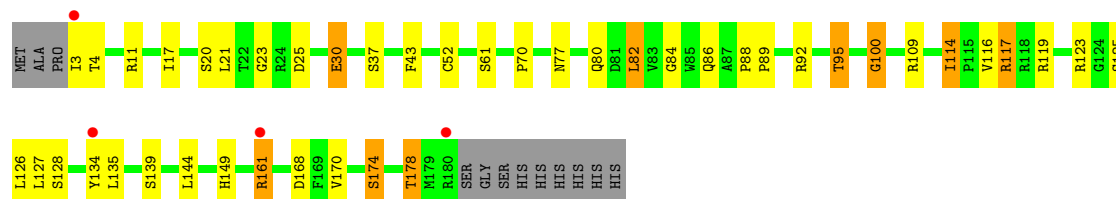
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	10	Total 10	O 10	0	0
6	D	13	Total 13	O 13	0	0
6	H	2	Total 2	O 2	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

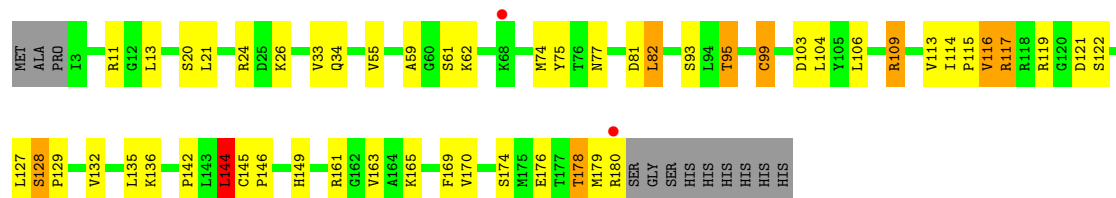
• Molecule 1: Genome polyprotein

Chain A: 



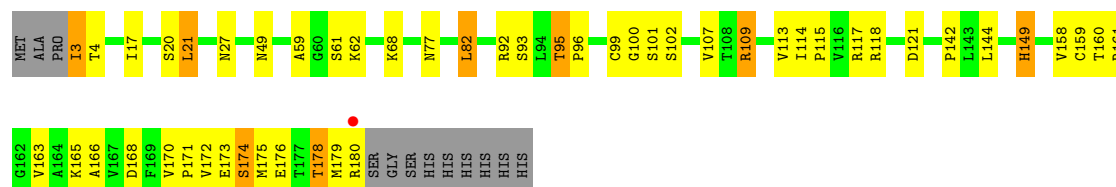
• Molecule 1: Genome polyprotein

Chain B: 



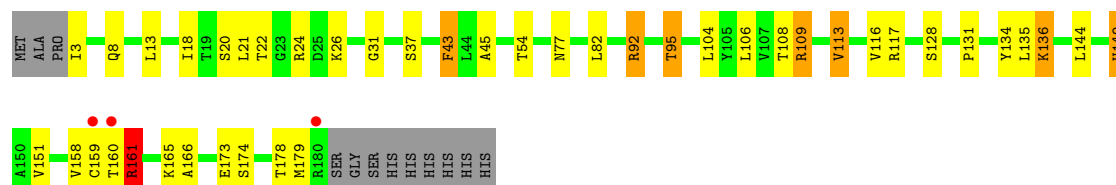
• Molecule 1: Genome polyprotein

Chain C: 



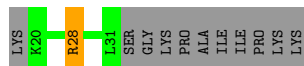
• Molecule 1: Genome polyprotein

Chain D: 



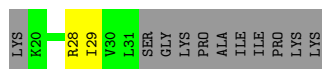
- Molecule 2: 19-mer peptide from Genome polyprotein

Chain E: 



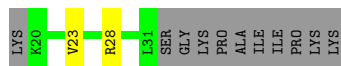
- Molecule 2: 19-mer peptide from Genome polyprotein

Chain F: 



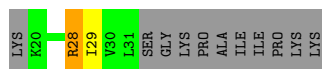
- Molecule 2: 19-mer peptide from Genome polyprotein

Chain G: 



- Molecule 2: 19-mer peptide from Genome polyprotein

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	48.03Å 54.45Å 85.50Å 92.44° 93.16° 116.04°	Depositor
Resolution (Å)	48.80 – 2.40 48.79 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.9 (48.80-2.40) 95.9 (48.79-2.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.196 , 0.246 0.197 , 0.247	Depositor DCC
R_{free} test set	1461 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 17.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 29045 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5877	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, 30B

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	0.73	0/1337	0.82	1/1820 (0.1%)
1	B	0.68	0/1337	0.88	2/1820 (0.1%)
1	C	0.71	0/1337	0.83	0/1820
1	D	0.70	1/1337 (0.1%)	0.84	2/1820 (0.1%)
2	E	0.83	0/85	0.77	0/113
2	F	0.82	0/85	0.76	0/113
2	G	0.72	0/85	0.79	0/113
2	H	0.73	0/85	0.78	0/113
All	All	0.71	1/5688 (0.0%)	0.84	5/7732 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	159	CYS	CB-SG	5.22	1.91	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	109	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	B	99	CYS	CA-C-N	6.50	129.21	116.20
1	D	109	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	A	92	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	B	144	LEU	CA-CB-CG	5.54	128.04	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1312	0	1318	34	0
1	B	1312	0	1318	32	0
1	C	1312	0	1318	37	0
1	D	1312	0	1318	26	0
2	E	86	0	105	1	0
2	F	86	0	105	1	0
2	G	86	0	105	1	0
2	H	86	0	105	3	0
3	A	52	0	47	2	0
3	B	52	0	47	0	0
3	C	52	0	47	1	0
3	D	52	0	47	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	C	12	0	16	1	0
5	D	12	0	16	2	0
6	A	11	0	0	3	0
6	B	11	0	0	1	0
6	C	10	0	0	0	0
6	D	13	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	H	2	0	0	0	0
All	All	5877	0	5912	112	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (112) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:95:THR:CG2	1:C:95:THR:HG22	1.61	1.31
1:A:114:ILE:HG21	6:A:196:HOH:O	1.46	1.12

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:95:THR:HG23	1:C:95:THR:HG22	1.28	1.10
1:A:114:ILE:HD11	1:A:126:LEU:HD22	1.21	1.08
1:B:95:THR:HG22	1:D:95:THR:CG2	1.86	1.05
1:B:95:THR:HG22	1:D:95:THR:HG23	1.33	1.04
1:D:160:THR:O	1:D:161:ARG:HB2	1.56	1.02
1:C:179:MET:O	1:C:180:ARG:HB2	1.57	1.02
1:A:174:SER:O	1:A:178:THR:HG23	1.67	0.93
1:A:95:THR:HG23	1:C:95:THR:CG2	2.02	0.89
1:A:95:THR:HG21	1:C:95:THR:HG22	1.56	0.87
1:D:174:SER:O	1:D:178:THR:HG23	1.75	0.86
1:A:95:THR:CG2	1:C:95:THR:CG2	2.52	0.86
1:C:142:PRO:HB2	1:C:144:LEU:HD13	1.65	0.76
1:A:95:THR:HB	1:C:93:SER:O	1.87	0.75
1:C:179:MET:O	1:C:180:ARG:CB	2.35	0.74
1:A:161:ARG:HB3	1:A:161:ARG:HH11	1.50	0.74
1:B:82:LEU:HG	1:B:170:VAL:HG11	1.69	0.73
1:D:158:VAL:HB	1:D:166:ALA:HB3	1.70	0.72
1:B:99:CYS:SG	1:B:99:CYS:O	2.47	0.71
1:A:161:ARG:HB3	1:A:161:ARG:NH1	2.06	0.70
1:B:149:HIS:CE1	1:D:149:HIS:HE1	2.11	0.68
1:B:109:ARG:NH1	5:D:3968[A]:GOL:H11	2.09	0.67
1:C:174:SER:O	1:C:178:THR:HG22	1.95	0.67
1:B:95:THR:HG22	1:D:95:THR:HG21	1.74	0.66
1:C:62:LYS:HB2	2:G:23:VAL:HG23	1.77	0.66
1:B:142:PRO:HB2	1:B:144:LEU:HD13	1.79	0.65
1:C:107:VAL:HB	1:C:142:PRO:HG2	1.78	0.65
1:C:142:PRO:HB2	1:C:144:LEU:CD1	2.26	0.64
1:A:86:GLN:OE1	1:C:68:LYS:HE3	1.97	0.64
1:A:114:ILE:HD11	1:A:126:LEU:CD2	2.14	0.62
1:C:59:ALA:O	1:C:62:LYS:HG2	2.00	0.60
1:A:123:ARG:NH1	1:A:168:ASP:OD1	2.35	0.60
1:B:24:ARG:HE	1:B:26:LYS:HE3	1.67	0.59
1:D:160:THR:O	1:D:161:ARG:CB	2.41	0.58
1:C:158:VAL:HB	1:C:166:ALA:HB3	1.86	0.58
1:B:74:MET:HB2	1:B:75:TYR:CD2	2.39	0.57
1:C:49:ASN:HD21	1:C:96:PRO:CG	2.17	0.57
1:B:149:HIS:CE1	1:D:149:HIS:CE1	2.93	0.57
1:B:122:SER:HB2	1:B:169:PHE:O	2.06	0.56
1:D:108:THR:O	2:H:29:ILE:CD1	2.54	0.55
1:C:102:SER:HA	1:C:118:ARG:HB3	1.88	0.55
1:A:86:GLN:OE1	1:C:68:LYS:CE	2.55	0.55
1:B:33:VAL:HB	2:F:29:ILE:HB	1.89	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:115:PRO:HB2	1:B:127:LEU:HG	1.90	0.52
1:A:30:GLU:HG3	2:E:28:ARG:CZ	2.40	0.52
1:A:95:THR:HG21	1:C:95:THR:CG2	2.31	0.51
1:A:17:ILE:O	1:A:20:SER:HB3	2.11	0.51
1:B:93:SER:O	1:D:95:THR:CG2	2.60	0.50
1:C:82:LEU:HG	1:C:170:VAL:HG11	1.93	0.50
1:D:18:ILE:O	1:D:22:THR:HG23	2.12	0.50
1:A:3:ILE:N	1:A:3:ILE:HD12	2.27	0.50
1:C:160:THR:O	1:C:163:VAL:HG22	2.11	0.49
1:B:59:ALA:O	1:B:62:LYS:HG3	2.13	0.49
1:D:43:PHE:CD1	1:D:43:PHE:N	2.79	0.49
1:C:99:CYS:O	1:C:101:SER:N	2.46	0.49
1:A:11:ARG:HH12	1:A:25:ASP:CG	2.16	0.48
1:A:134:TYR:HE2	6:A:196:HOH:O	1.97	0.48
1:C:109:ARG:HD3	5:C:3968[B]:GOL:O2	2.12	0.48
1:D:31:GLY:H	1:D:92:ARG:HD3	1.78	0.48
1:B:178:THR:C	1:B:180:ARG:H	2.17	0.47
1:B:34:GLN:NE2	6:B:194:HOH:O	2.46	0.47
1:A:119:ARG:HD3	1:A:125:SER:HB3	1.96	0.47
1:D:160:THR:O	1:D:160:THR:HG22	2.15	0.47
1:C:171:PRO:HB2	1:C:173:GLU:HG2	1.96	0.47
1:C:17:ILE:O	1:C:21:LEU:HD22	2.15	0.47
1:C:174:SER:O	1:C:178:THR:CG2	2.62	0.47
1:A:117:ARG:HH22	1:B:119:ARG:HB3	1.80	0.47
1:B:104:LEU:HB2	1:B:116:VAL:HG22	1.96	0.46
1:B:109:ARG:HH11	5:D:3968[A]:GOL:H11	1.80	0.46
1:D:131:PRO:O	1:D:134:TYR:HB3	2.16	0.46
1:C:107:VAL:HB	1:C:142:PRO:CG	2.46	0.46
1:B:149:HIS:HE1	1:D:149:HIS:CE1	2.33	0.46
1:C:176:GLU:HA	1:C:179:MET:CE	2.46	0.46
1:A:149:HIS:HE1	1:C:149:HIS:CE1	2.34	0.46
1:B:115:PRO:O	1:B:116:VAL:HG12	2.16	0.45
1:A:77:ASN:OD1	1:A:80:GLN:HB2	2.17	0.45
1:D:173:GLU:H	1:D:173:GLU:CD	2.20	0.45
1:D:8:GLN:OE1	2:H:28:ARG:HD3	2.16	0.45
1:D:24:ARG:HE	1:D:26:LYS:HE2	1.83	0.44
1:A:139:SER:HB3	3:A:500:30B:C12	2.48	0.44
1:C:159:CYS:HA	1:C:163:VAL:O	2.18	0.44
1:A:82:LEU:HG	1:A:170:VAL:HG11	1.99	0.44
1:B:104:LEU:HA	1:B:144:LEU:O	2.18	0.43
1:C:114:ILE:HA	1:C:115:PRO:HD3	1.79	0.43
1:D:108:THR:O	2:H:29:ILE:HD11	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:55:VAL:HA	1:B:81:ASP:O	2.17	0.43
1:C:3:ILE:HG21	1:C:144:LEU:HD23	1.99	0.43
3:D:500:30B:H11	3:D:500:30B:H21	1.78	0.43
1:A:100:GLY:O	1:B:117:ARG:NH1	2.42	0.43
1:A:114:ILE:HD13	6:A:196:HOH:O	2.19	0.43
1:A:43:PHE:CD1	1:A:43:PHE:N	2.87	0.42
1:A:23:GLY:HA3	1:A:70:PRO:HG3	2.01	0.42
1:C:49:ASN:HD21	1:C:96:PRO:HG3	1.83	0.42
3:A:500:30B:H2	3:A:500:30B:H15B	1.98	0.42
1:B:106:LEU:HD23	1:B:114:ILE:HD11	2.02	0.42
1:C:59:ALA:O	1:C:62:LYS:CG	2.65	0.42
3:C:500:30B:H21	3:C:500:30B:H11	1.99	0.42
1:B:145:CYS:HB2	1:B:146:PRO:CD	2.50	0.42
1:D:104:LEU:HD22	1:D:151:VAL:HG21	2.02	0.42
1:B:128:SER:HA	1:B:129:PRO:HD2	1.75	0.41
1:C:17:ILE:O	1:C:20:SER:HB3	2.20	0.41
1:C:175:MET:O	1:C:179:MET:HG3	2.21	0.41
1:D:136:LYS:HD2	3:D:500:30B:O49	2.19	0.41
1:A:117:ARG:HH12	1:B:119:ARG:HD2	1.85	0.41
1:D:92:ARG:HG2	1:D:92:ARG:NH1	2.35	0.41
1:B:24:ARG:HH21	1:B:26:LYS:NZ	2.19	0.41
1:D:45:ALA:HB2	1:D:54:THR:HB	2.03	0.41
1:D:106:LEU:O	1:D:113:VAL:HA	2.21	0.41
1:A:88:PRO:HA	1:A:89:PRO:HD3	1.98	0.40
1:B:174:SER:O	1:B:178:THR:CG2	2.69	0.40
1:A:52:CYS:O	1:A:84:GLY:HA2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	176/190 (93%)	170 (97%)	5 (3%)	1 (1%)	33	47
1	B	176/190 (93%)	170 (97%)	5 (3%)	1 (1%)	33	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	176/190 (93%)	168 (96%)	6 (3%)	2 (1%)	21	29
1	D	176/190 (93%)	170 (97%)	4 (2%)	2 (1%)	21	29
2	E	10/23 (44%)	10 (100%)	0	0	100	100
2	F	10/23 (44%)	10 (100%)	0	0	100	100
2	G	10/23 (44%)	10 (100%)	0	0	100	100
2	H	10/23 (44%)	10 (100%)	0	0	100	100
All	All	744/852 (87%)	718 (96%)	20 (3%)	6 (1%)	27	39

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	100	GLY
1	D	161	ARG
1	A	100	GLY
1	C	27	ASN
1	B	179	MET
1	D	179	MET

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	145/155 (94%)	127 (88%)	18 (12%)	7	8
1	B	145/155 (94%)	121 (83%)	24 (17%)	3	3
1	C	145/155 (94%)	126 (87%)	19 (13%)	6	7
1	D	145/155 (94%)	124 (86%)	21 (14%)	5	5
2	E	10/19 (53%)	9 (90%)	1 (10%)	11	16
2	F	10/19 (53%)	9 (90%)	1 (10%)	11	16
2	G	10/19 (53%)	9 (90%)	1 (10%)	11	16
2	H	10/19 (53%)	9 (90%)	1 (10%)	11	16
All	All	620/696 (89%)	534 (86%)	86 (14%)	5	6

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	21	LEU
1	A	30	GLU
1	A	37	SER
1	A	61	SER
1	A	82	LEU
1	A	95	THR
1	A	109	ARG
1	A	114	ILE
1	A	116	VAL
1	A	117	ARG
1	A	127	LEU
1	A	128	SER
1	A	135	LEU
1	A	144	LEU
1	A	161	ARG
1	A	174	SER
1	A	178	THR
2	E	28	ARG
1	B	11	ARG
1	B	13	LEU
1	B	20	SER
1	B	21	LEU
1	B	61	SER
1	B	77	ASN
1	B	82	LEU
1	B	95	THR
1	B	103	ASP
1	B	109	ARG
1	B	113	VAL
1	B	116	VAL
1	B	117	ARG
1	B	121	ASP
1	B	128	SER
1	B	132	VAL
1	B	135	LEU
1	B	136	LYS
1	B	144	LEU
1	B	161	ARG
1	B	163	VAL
1	B	165	LYS
1	B	176	GLU

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Mol	Chain	Res	Type
1	B	178	THR
2	F	28	ARG
1	C	3	ILE
1	C	4	THR
1	C	21	LEU
1	C	61	SER
1	C	77	ASN
1	C	82	LEU
1	C	92	ARG
1	C	95	THR
1	C	109	ARG
1	C	113	VAL
1	C	117	ARG
1	C	121	ASP
1	C	149	HIS
1	C	161	ARG
1	C	165	LYS
1	C	168	ASP
1	C	172	VAL
1	C	174	SER
1	C	178	THR
2	G	28	ARG
1	D	3	ILE
1	D	13	LEU
1	D	20	SER
1	D	21	LEU
1	D	37	SER
1	D	43	PHE
1	D	77	ASN
1	D	82	LEU
1	D	92	ARG
1	D	95	THR
1	D	109	ARG
1	D	113	VAL
1	D	116	VAL
1	D	117	ARG
1	D	128	SER
1	D	135	LEU
1	D	136	LYS
1	D	144	LEU
1	D	149	HIS
1	D	161	ARG

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Mol	Chain	Res	Type
1	D	165	LYS
2	H	28	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	34	GLN
1	A	149	HIS
1	B	27	ASN
1	B	34	GLN
1	B	77	ASN
1	B	149	HIS
1	C	9	GLN
1	C	27	ASN
1	C	49	ASN
1	C	77	ASN
1	D	9	GLN
1	D	27	ASN
1	D	49	ASN
1	D	149	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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	30B	A	500	-	58,58,58	1.59	10 (17%)	85,88,88	2.83	26 (30%)
3	30B	B	500	-	58,58,58	1.63	9 (15%)	85,88,88	2.83	28 (32%)
5	GOL	C	3968[A]	-	5,5,5	0.22	0	5,5,5	0.41	0
5	GOL	C	3968[B]	-	5,5,5	0.29	0	5,5,5	0.31	0
3	30B	C	500	-	58,58,58	1.62	8 (13%)	85,88,88	2.72	22 (25%)
5	GOL	D	3968[A]	-	5,5,5	0.35	0	5,5,5	0.33	0
5	GOL	D	3968[B]	-	5,5,5	0.35	0	5,5,5	0.32	0
3	30B	D	500	-	58,58,58	1.64	10 (17%)	85,88,88	2.54	27 (31%)

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	30B	A	500	-	-	0/55/79/79	0/1/7/7
3	30B	B	500	-	-	0/55/79/79	0/1/7/7
5	GOL	C	3968[A]	-	-	0/4/4/4	0/0/0/0
5	GOL	C	3968[B]	-	-	0/4/4/4	0/0/0/0
3	30B	C	500	-	-	0/55/79/79	0/1/7/7
5	GOL	D	3968[A]	-	-	0/4/4/4	0/0/0/0
5	GOL	D	3968[B]	-	-	0/4/4/4	0/0/0/0
3	30B	D	500	-	-	0/55/79/79	0/1/7/7

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	500	30B	C36-S35	6.33	1.80	1.70
3	B	500	30B	C36-S35	5.44	1.79	1.70
3	A	500	30B	C12-N45	-5.26	1.32	1.38
3	C	500	30B	C36-S35	5.11	1.78	1.70
3	B	500	30B	C29-C28	-4.94	1.37	1.43
3	C	500	30B	C48-S47	-4.66	1.67	1.78
3	B	500	30B	C48-S47	-4.16	1.68	1.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	500	30B	O42-C24	3.84	1.43	1.37
3	A	500	30B	C36-S35	3.84	1.76	1.70
3	A	500	30B	C48-S47	-3.84	1.69	1.78
3	C	500	30B	C29-C28	-3.61	1.39	1.43
3	D	500	30B	C48-S47	-3.54	1.70	1.78
3	D	500	30B	O42-C24	3.50	1.42	1.37
3	C	500	30B	C11-C18	3.49	1.54	1.49
3	B	500	30B	O42-C24	3.48	1.42	1.37
3	A	500	30B	C11-C18	3.42	1.54	1.49
3	B	500	30B	C11-C18	3.39	1.53	1.49
3	C	500	30B	S47-N45	-3.36	1.53	1.61
3	C	500	30B	C12-N45	-3.35	1.34	1.38
3	D	500	30B	C29-C28	-3.34	1.39	1.43
3	A	500	30B	S47-N45	-3.21	1.53	1.61
3	D	500	30B	C11-C18	3.13	1.53	1.49
3	B	500	30B	S47-N45	-3.07	1.54	1.61
3	D	500	30B	C52-C48	2.96	1.54	1.50
3	C	500	30B	O49-S47	-2.83	1.41	1.44
3	A	500	30B	C34-S35	2.76	1.77	1.73
3	D	500	30B	C12-N45	-2.56	1.35	1.38
3	D	500	30B	C34-S35	2.53	1.77	1.73
3	B	500	30B	C12-N45	-2.50	1.35	1.38
3	D	500	30B	S47-N45	-2.23	1.56	1.61
3	A	500	30B	C17-C16	2.21	1.53	1.51
3	B	500	30B	C28-N33	-2.20	1.32	1.37
3	A	500	30B	C3-C6	2.19	1.55	1.51
3	A	500	30B	C52-C48	2.19	1.53	1.50
3	D	500	30B	C17-C16	2.13	1.53	1.51
3	B	500	30B	O49-S47	-2.10	1.42	1.44
3	A	500	30B	C26-C25	2.06	1.40	1.36

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	30B	C36-C37-C39	-13.43	108.64	129.30
3	C	500	30B	C36-C37-C39	-10.03	113.86	129.30
3	B	500	30B	C11-C16-N8	-9.73	98.55	117.79
3	B	500	30B	C12-C16-N8	9.31	125.46	117.23
3	B	500	30B	C36-C37-C39	-9.27	115.03	129.30
3	C	500	30B	C12-C16-N8	8.85	125.06	117.23
3	A	500	30B	C12-C16-N8	8.77	124.98	117.23
3	B	500	30B	O42-C24-C29	8.53	122.31	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	500	30B	C11-C16-N8	-8.24	101.50	117.79
3	C	500	30B	C11-C16-N8	-8.17	101.63	117.79
3	A	500	30B	C11-C16-N8	-8.13	101.71	117.79
3	D	500	30B	O50-S47-O49	-7.35	106.16	120.33
3	C	500	30B	O50-S47-O49	-7.31	106.24	120.33
3	D	500	30B	C12-C16-N8	7.14	123.55	117.23
3	D	500	30B	C36-C37-C39	-7.08	118.41	129.30
3	A	500	30B	C39-C37-N38	6.99	131.75	120.27
3	D	500	30B	O42-C24-C29	6.92	120.95	115.13
3	A	500	30B	C4-C3-C6	6.22	127.30	114.11
3	B	500	30B	C32-C34-N38	6.19	135.69	123.93
3	C	500	30B	C51-C48-S47	-5.95	108.12	119.60
3	A	500	30B	C36-C37-N38	5.35	119.51	109.56
3	C	500	30B	O42-C24-C29	5.14	119.45	115.13
3	C	500	30B	C52-C48-S47	-5.12	109.71	119.60
3	B	500	30B	O50-S47-O49	-5.06	110.58	120.33
3	C	500	30B	C32-C34-N38	5.02	133.47	123.93
3	C	500	30B	C39-C37-N38	4.94	128.38	120.27
3	B	500	30B	C51-C48-S47	-4.72	110.48	119.60
3	B	500	30B	C36-C37-N38	4.67	118.23	109.56
3	B	500	30B	O42-C24-C25	-4.53	116.89	124.37
3	C	500	30B	O50-S47-C48	4.43	113.70	107.73
3	C	500	30B	C36-C37-N38	4.35	117.64	109.56
3	D	500	30B	O42-C24-C25	-4.33	117.21	124.37
3	B	500	30B	C12-N45-S47	-4.28	120.07	124.21
3	A	500	30B	O50-S47-O49	-4.24	112.15	120.33
3	A	500	30B	C52-C48-S47	-4.19	111.51	119.60
3	A	500	30B	C32-C34-N38	4.19	131.88	123.93
3	A	500	30B	C17-C11-C18	-4.15	113.57	119.66
3	D	500	30B	C34-C32-N33	4.03	121.97	115.73
3	D	500	30B	C4-C3-C6	3.95	122.47	114.11
3	B	500	30B	O50-S47-C48	3.94	113.03	107.73
3	B	500	30B	C39-C37-N38	3.93	126.72	120.27
3	C	500	30B	C17-C16-C12	-3.83	110.71	116.62
3	D	500	30B	C16-C12-N45	3.64	121.42	116.15
3	D	500	30B	C32-C34-N38	3.54	130.65	123.93
3	B	500	30B	O23-C30-C27	3.52	119.97	114.52
3	A	500	30B	O42-C24-C29	3.51	118.08	115.13
3	D	500	30B	C36-C37-N38	3.46	115.99	109.56
3	D	500	30B	C51-C48-S47	-3.37	113.10	119.60
3	D	500	30B	O50-S47-C48	3.35	112.25	107.73
3	A	500	30B	O23-C30-C27	3.30	119.63	114.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	30B	C51-C48-S47	-3.30	113.23	119.60
3	B	500	30B	C4-C3-C6	3.29	121.08	114.11
3	A	500	30B	O42-C24-C25	-3.27	118.97	124.37
3	D	500	30B	C39-C37-N38	3.25	125.61	120.27
3	A	500	30B	C11-C18-C22	-3.23	118.86	125.10
3	D	500	30B	O23-C30-C27	3.22	119.51	114.52
3	C	500	30B	C16-N8-C6	3.16	131.02	122.22
3	C	500	30B	O42-C24-C25	-3.14	119.19	124.37
3	A	500	30B	C12-N45-S47	-2.93	121.38	124.21
3	C	500	30B	C4-C5-C1	2.89	109.06	104.60
3	A	500	30B	C41-C39-C37	-2.87	105.36	111.92
3	D	500	30B	C29-C28-N33	2.86	120.69	117.73
3	B	500	30B	C52-C48-S47	-2.85	114.10	119.60
3	D	500	30B	C16-N8-C6	2.84	130.13	122.22
3	D	500	30B	C31-C32-C34	-2.84	115.82	121.14
3	A	500	30B	C29-C28-N33	2.83	120.66	117.73
3	B	500	30B	C17-C16-C12	-2.81	112.28	116.62
3	B	500	30B	C25-C26-C27	-2.76	117.04	121.15
3	D	500	30B	C52-C48-S47	-2.76	114.27	119.60
3	D	500	30B	C12-N45-S47	-2.72	121.58	124.21
3	C	500	30B	C34-C32-N33	2.71	119.93	115.73
3	C	500	30B	O23-C30-C27	2.68	118.68	114.52
3	A	500	30B	C37-C36-S35	-2.66	103.86	110.63
3	B	500	30B	C17-C11-C18	-2.66	115.76	119.66
3	C	500	30B	C4-C3-C6	2.65	119.72	114.11
3	C	500	30B	C17-C16-N8	2.65	120.91	117.67
3	B	500	30B	C37-C36-S35	-2.63	103.95	110.63
3	D	500	30B	C3-C6-N8	-2.60	112.66	116.28
3	C	500	30B	C3-C6-N8	-2.59	112.67	116.28
3	D	500	30B	C43-O42-C24	2.55	121.35	117.59
3	B	500	30B	C19-C14-N13	-2.50	103.17	112.53
3	B	500	30B	C4-C5-C1	2.49	108.44	104.60
3	C	500	30B	C37-C36-S35	-2.47	104.35	110.63
3	B	500	30B	C32-N33-C28	2.47	120.33	118.42
3	B	500	30B	C40-C39-C37	-2.46	106.31	111.92
3	B	500	30B	C44-C29-C24	2.43	124.17	120.60
3	C	500	30B	C16-C11-C18	-2.39	117.35	121.51
3	D	500	30B	C40-C39-C37	-2.37	106.51	111.92
3	B	500	30B	C11-C16-C12	2.36	120.95	116.94
3	D	500	30B	C48-S47-N45	2.35	112.46	106.51
3	B	500	30B	O7-C6-C3	2.34	124.22	121.51
3	B	500	30B	C3-C6-N8	-2.33	113.03	116.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	30B	O50-S47-C48	2.32	110.86	107.73
3	A	500	30B	C34-C32-N33	2.31	119.31	115.73
3	A	500	30B	C16-N8-C6	2.30	128.62	122.22
3	A	500	30B	O46-C12-N45	-2.21	118.55	120.95
3	A	500	30B	O23-C5-C4	2.17	114.48	108.75
3	D	500	30B	C44-C29-C28	-2.10	117.07	119.24
3	D	500	30B	O23-C30-C31	-2.09	120.87	125.24
3	D	500	30B	O7-C6-C3	2.08	123.92	121.51
3	A	500	30B	C26-C25-C24	-2.06	116.35	119.75
3	A	500	30B	O46-C12-C16	2.01	123.05	120.72
3	B	500	30B	C1-C2-C9	2.01	117.75	113.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	178/190 (93%)	-0.19	4 (2%) 59 57	11, 22, 36, 51	1 (0%)
1	B	178/190 (93%)	-0.24	2 (1%) 77 77	13, 24, 38, 46	1 (0%)
1	C	178/190 (93%)	-0.29	1 (0%) 86 86	11, 24, 39, 48	1 (0%)
1	D	178/190 (93%)	-0.22	3 (1%) 67 65	12, 24, 39, 49	1 (0%)
2	E	12/23 (52%)	-0.31	0 100 100	19, 24, 31, 35	0
2	F	12/23 (52%)	-0.42	0 100 100	19, 23, 28, 37	0
2	G	12/23 (52%)	-0.31	0 100 100	19, 22, 29, 39	0
2	H	12/23 (52%)	-0.48	0 100 100	19, 24, 32, 37	0
All	All	760/852 (89%)	-0.24	10 (1%) 74 73	11, 24, 38, 51	4 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	180	ARG	5.0
1	A	161	ARG	4.1
1	B	180	ARG	4.0
1	C	180	ARG	3.5
1	D	180	ARG	3.3
1	A	134	TYR	2.6
1	D	160	THR	2.3
1	A	3	ILE	2.2
1	D	159	CYS	2.1
1	B	68	LYS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	GOL	C	3968[B]	6/6	0.20	7.58	28,29,30,31	6
5	GOL	C	3968[A]	6/6	0.20	7.58	34,35,35,35	6
5	GOL	D	3968[A]	6/6	0.19	5.98	33,34,34,34	6
5	GOL	D	3968[B]	6/6	0.19	5.98	25,27,27,28	6
4	ZN	C	2000	1/1	0.11	-0.12	31,31,31,31	0
4	ZN	D	2000	1/1	0.10	-0.38	27,27,27,27	0
3	30B	C	500	52/52	0.12	-0.51	9,14,17,18	0
3	30B	B	500	52/52	0.11	-0.56	5,13,17,19	0
3	30B	A	500	52/52	0.11	-0.67	4,10,17,17	0
3	30B	D	500	52/52	0.11	-0.76	6,15,19,23	0
4	ZN	B	2000	1/1	0.12	-0.79	32,32,32,32	0
4	ZN	A	2000	1/1	0.09	-1.18	24,24,24,24	0

6.5 Other polymers ⓘ

There are no such residues in this entry.