



Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 05:35 AM GMT

PDB ID : 2OBX
Title : Lumazine synthase RibH2 from Mesorhizobium loti (Gene mll7281, Swiss-Prot entry Q986N2) complexed with inhibitor 5-Nitro-6-(D-Ribitylamino)-2,4(1H, 3H)Pyrimidinedione
Authors : Klinke, S.; Zylberman, V.; Bonomi, H.R.; Haase, I.; Guimaraes, B.G.; Braden, B.C.; Bacher, A.; Fischer, M.; Goldbaum, F.A.
Deposited on : 2006-12-20
Resolution : 2.53 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>

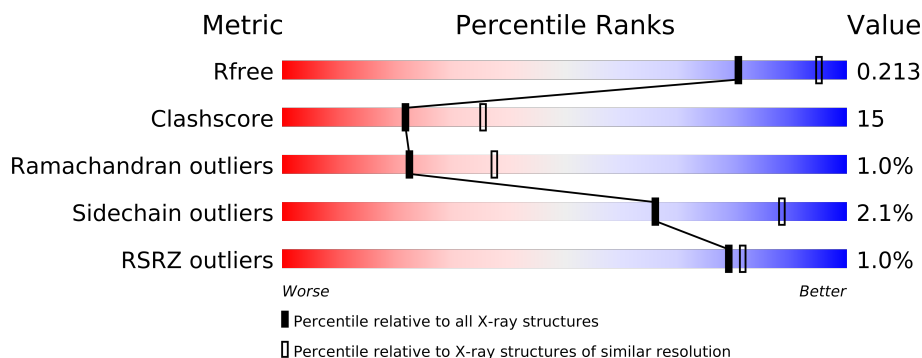
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.53 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	3240 (2.54-2.50)
Clashscore	79885	4080 (2.54-2.50)
Ramachandran outliers	78287	3990 (2.54-2.50)
Sidechain outliers	78261	3992 (2.54-2.50)
RSRZ outliers	66119	3241 (2.54-2.50)

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. 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	157	
1	B	157	
1	C	157	
1	D	157	
1	E	157	
1	F	157	
1	G	157	
1	H	157	
1	I	157	
1	J	157	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	PO4	A	1001	-	X
2	PO4	B	1002	-	X
2	PO4	C	1003	-	X
2	PO4	E	1004	-	X
2	PO4	F	1005	-	X
2	PO4	G	1006	-	X
2	PO4	I	1007	-	X
2	PO4	J	1008	-	X
2	PO4	J	1009	-	X
3	INI	A	201	-	X
3	INI	B	202	-	X
3	INI	C	203	-	X
3	INI	D	204	-	X
3	INI	E	205	-	X
3	INI	F	206	-	X
3	INI	G	207	-	X
3	INI	H	208	-	X
3	INI	I	209	-	X
3	INI	J	210	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11693 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 6,7-dimethyl-8-ribityllumazinesynthase 1.

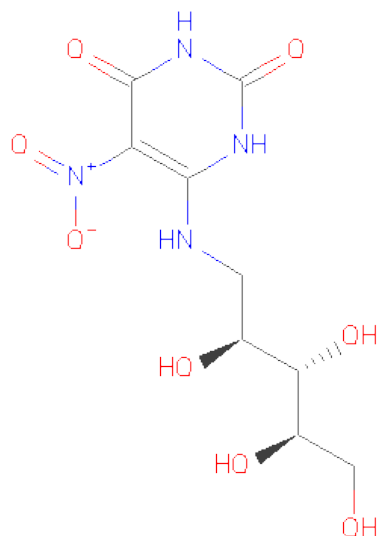
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	0	0
			1145	730	202	208	5			
1	B	147	Total	C	N	O	S	0	0	0
			1124	716	199	204	5			
1	C	147	Total	C	N	O	S	0	0	0
			1116	711	198	202	5			
1	D	146	Total	C	N	O	S	0	0	0
			1118	711	197	205	5			
1	E	146	Total	C	N	O	S	0	0	0
			1111	707	196	203	5			
1	F	148	Total	C	N	O	S	0	0	0
			1130	719	200	206	5			
1	G	148	Total	C	N	O	S	0	0	0
			1126	716	199	206	5			
1	H	147	Total	C	N	O	S	0	0	0
			1125	715	201	204	5			
1	I	146	Total	C	N	O	S	0	0	0
			1112	710	198	199	5			
1	J	146	Total	C	N	O	S	0	0	0
			1112	708	194	205	5			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	I	1	Total	O	P	0	0
			5	4	1		
2	J	1	Total	O	P	0	0
			5	4	1		
2	J	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is 5-NITRO-6-RIBITYL-AMINO-2,4(1H,3H)-PYRIMIDINEDIONE (three-letter code: INI) (formula: C₉H₁₄N₄O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	9	4	8		
3	B	1	Total	C	N	O	0	0
			21	9	4	8		
3	C	1	Total	C	N	O	0	0
			21	9	4	8		
3	D	1	Total	C	N	O	0	0
			21	9	4	8		
3	E	1	Total	C	N	O	0	0
			21	9	4	8		
3	F	1	Total	C	N	O	0	0
			21	9	4	8		
3	G	1	Total	C	N	O	0	0
			21	9	4	8		
3	H	1	Total	C	N	O	0	0
			21	9	4	8		
3	I	1	Total	C	N	O	0	0
			21	9	4	8		
3	J	1	Total	C	N	O	0	0
			21	9	4	8		

- Molecule 4 is water.

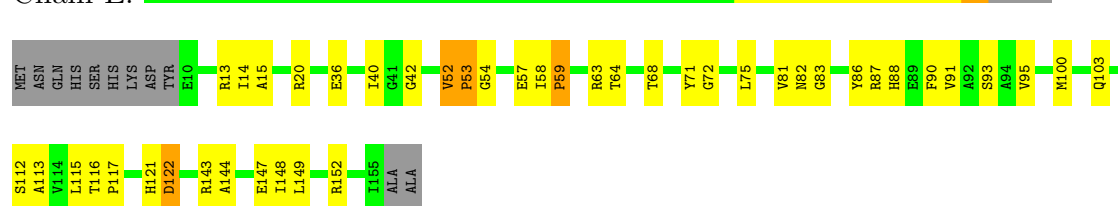
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total	O	0	0
			16	16		
4	B	23	Total	O	0	0
			23	23		

Continued on next page...

Continued from previous page...

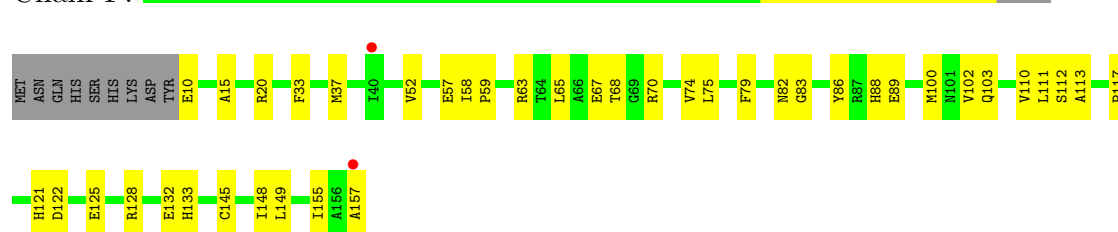
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	22	Total 22	O 22	0	0
4	D	21	Total 21	O 21	0	0
4	E	27	Total 27	O 27	0	0
4	F	20	Total 20	O 20	0	0
4	G	24	Total 24	O 24	0	0
4	H	24	Total 24	O 24	0	0
4	I	16	Total 16	O 16	0	0
4	J	26	Total 26	O 26	0	0

Chain E:



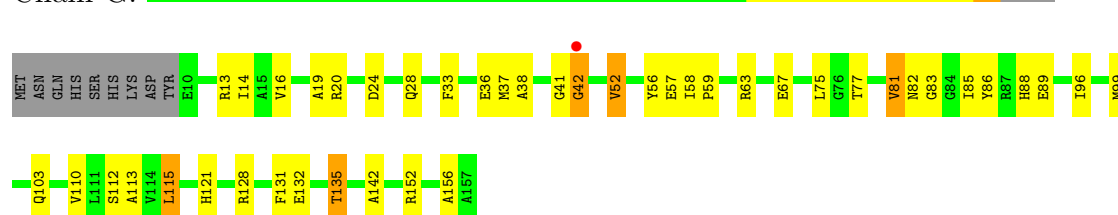
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase 1

Chain F:



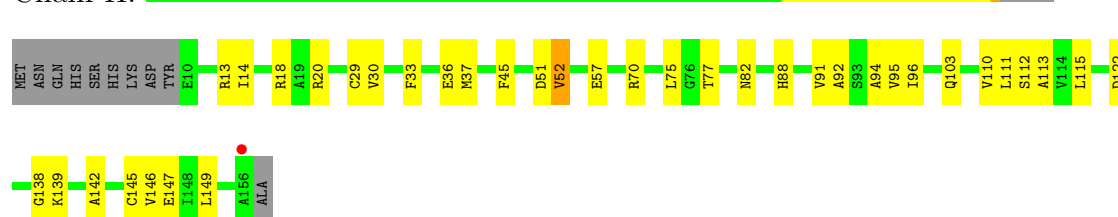
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase 1

Chain G:



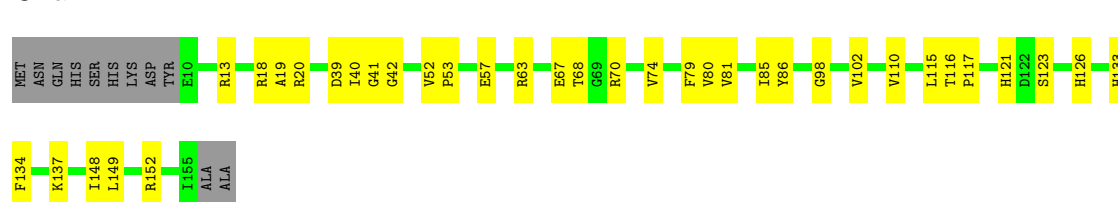
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase 1

Chain H:



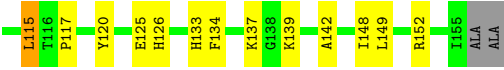
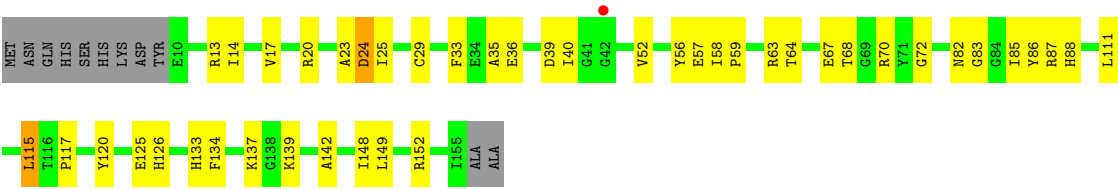
- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase 1

Chain I:



- Molecule 1: 6,7-dimethyl-8-ribityllumazinesynthase 1

Chain J:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	154.38Å 122.22Å 94.93Å 90.00° 125.43° 90.00°	Depositor
Resolution (Å)	50.00 – 2.53 38.98 – 2.53	Depositor EDS
% Data completeness (in resolution range)	96.6 (50.00-2.53) 96.6 (38.98-2.53)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.54Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.213 , 0.281 0.223 , 0.213	Depositor DCC
R_{free} test set	2344 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 10.4	EDS
Estimated twinning fraction	0.003 for k+l,h+l,-l 0.001 for -k+l,-h-l,-l 0.024 for -h-2*l,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 46425 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11693	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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: PO4, INI

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	0.39	0/1172	0.62	0/1594
1	B	0.40	0/1150	0.65	0/1563
1	C	0.37	0/1142	0.60	0/1554
1	D	0.39	0/1144	0.61	0/1556
1	E	0.37	0/1137	0.59	0/1548
1	F	0.37	0/1156	0.59	0/1570
1	G	0.39	0/1152	0.62	0/1566
1	H	0.41	0/1151	0.63	0/1565
1	I	0.38	0/1138	0.61	0/1547
1	J	0.39	0/1138	0.62	0/1549
All	All	0.39	0/11480	0.61	0/15612

There are no bond length outliers.

There are no bond angle outliers.

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	1145	0	1096	28	0
1	B	1124	0	1088	39	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1116	0	1073	37	0
1	D	1118	0	1074	43	0
1	E	1111	0	1061	36	0
1	F	1130	0	1093	34	0
1	G	1126	0	1082	44	0
1	H	1125	0	1086	33	0
1	I	1112	0	1077	29	0
1	J	1112	0	1063	37	0
2	A	5	0	0	3	0
2	B	5	0	0	4	0
2	C	5	0	0	2	0
2	E	5	0	0	3	0
2	F	5	0	0	2	0
2	G	5	0	0	4	0
2	I	5	0	0	2	0
2	J	10	0	0	5	0
3	A	21	0	14	1	0
3	B	21	0	14	2	0
3	C	21	0	14	3	0
3	D	21	0	14	0	0
3	E	21	0	14	1	0
3	F	21	0	14	0	0
3	G	21	0	14	2	0
3	H	21	0	14	3	0
3	I	21	0	14	3	0
3	J	21	0	14	1	0
4	A	16	0	0	0	0
4	B	23	0	0	1	0
4	C	22	0	0	0	0
4	D	21	0	0	1	0
4	E	27	0	0	3	0
4	F	20	0	0	0	0
4	G	24	0	0	1	0
4	H	24	0	0	0	0
4	I	16	0	0	0	0
4	J	26	0	0	0	0
All	All	11693	0	10933	339	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 15.

All (339) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:152:ARG:HH11	1:B:152:ARG:HB3	1.17	1.05
1:B:139:LYS:HE2	1:B:143:ARG:NH2	1.84	0.93
1:B:139:LYS:HE2	1:B:143:ARG:HH22	1.33	0.91
1:C:77:THR:HB	1:C:113:ALA:HB3	1.59	0.85
1:B:152:ARG:NH1	1:B:152:ARG:HB3	1.92	0.85
1:J:52:VAL:HG13	1:J:57:GLU:HB2	1.60	0.83
1:J:52:VAL:CG1	1:J:57:GLU:HB2	2.11	0.80
1:G:128:ARG:O	1:G:132:GLU:HG3	1.84	0.77
1:B:52:VAL:HG13	1:B:57:GLU:HB2	1.68	0.76
1:C:156:ALA:HB3	1:D:70:ARG:NH1	2.02	0.75
1:I:148:ILE:O	1:I:152:ARG:HG3	1.88	0.73
1:B:36:GLU:HG3	1:B:139:LYS:HG3	1.71	0.73
1:B:52:VAL:CG1	1:B:57:GLU:HB2	2.20	0.72
1:I:39:ASP:C	1:I:41:GLY:H	1.93	0.72
1:B:82:ASN:HB2	1:B:88:HIS:CE1	2.25	0.72
1:D:82:ASN:HB3	4:D:356:HOH:O	1.90	0.71
1:B:125:GLU:CD	1:B:125:GLU:H	1.94	0.71
1:H:112:SER:H	3:I:209:INI:H122	1.55	0.71
1:H:37:MET:HE1	1:H:146:VAL:HG23	1.73	0.69
1:C:148:ILE:O	1:C:152:ARG:HG3	1.92	0.69
1:I:116:THR:HG22	1:J:87:ARG:HG3	1.73	0.69
1:J:36:GLU:HG3	1:J:139:LYS:HG2	1.74	0.69
1:I:52:VAL:HG13	1:I:57:GLU:HB2	1.76	0.67
1:D:116:THR:HG22	1:E:87:ARG:HG3	1.75	0.67
1:E:36:GLU:O	1:E:40:ILE:HG12	1.95	0.66
1:C:98:GLY:O	1:C:102:VAL:HG23	1.94	0.66
1:B:150:ALA:O	1:B:153:GLU:HB2	1.95	0.66
1:I:18:ARG:HD2	1:I:20:ARG:NH2	2.09	0.66
1:B:152:ARG:HH11	1:B:152:ARG:CB	2.03	0.66
1:G:19:ALA:HA	1:G:52:VAL:HG12	1.77	0.66
1:C:103:GLN:HB3	1:C:110:VAL:HG23	1.75	0.66
1:D:36:GLU:O	1:D:40:ILE:HG12	1.96	0.66
1:G:13:ARG:C	1:G:14:ILE:HD12	2.15	0.65
1:D:148:ILE:O	1:D:152:ARG:HG3	1.95	0.65
1:G:38:ALA:HA	1:G:42:GLY:HA2	1.78	0.65
1:G:103:GLN:HB3	1:G:110:VAL:HG23	1.77	0.64
1:E:100:MET:HA	1:E:103:GLN:HE21	1.62	0.64
1:H:52:VAL:HG13	1:H:57:GLU:HB2	1.79	0.64
1:F:125:GLU:CD	1:F:125:GLU:H	2.01	0.64
1:D:98:GLY:O	1:D:102:VAL:HG23	1.98	0.64
1:H:91:VAL:O	1:H:95:VAL:HG23	1.98	0.64
1:C:33:PHE:O	1:C:37:MET:HB2	1.97	0.64
1:E:52:VAL:HG13	1:E:57:GLU:HB2	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:77:THR:HB	1:H:113:ALA:HB3	1.79	0.63
1:G:82:ASN:HB2	1:G:88:HIS:CE1	2.34	0.63
1:G:20:ARG:HE	1:G:20:ARG:HA	1.64	0.62
1:H:82:ASN:HB2	1:H:88:HIS:CE1	2.35	0.62
1:C:133:HIS:CE1	1:C:137:LYS:HD3	2.34	0.62
1:F:83:GLY:H	2:F:1005:PO4:P	2.22	0.62
1:D:20:ARG:HA	1:D:20:ARG:NE	2.15	0.62
1:C:82:ASN:HB2	1:C:88:HIS:CE1	2.34	0.62
1:H:37:MET:CE	1:H:146:VAL:HG23	2.28	0.62
1:C:128:ARG:O	1:C:132:GLU:HG3	2.00	0.61
1:J:36:GLU:CG	1:J:139:LYS:HG2	2.31	0.61
4:B:333:HOH:O	1:C:87:ARG:HD2	2.02	0.60
1:A:82:ASN:HB2	1:A:88:HIS:CE1	2.36	0.60
1:J:63:ARG:O	1:J:67:GLU:HG3	2.00	0.60
1:C:156:ALA:HB3	1:D:70:ARG:HH12	1.66	0.60
1:G:20:ARG:HA	1:G:20:ARG:NE	2.16	0.60
1:B:36:GLU:CG	1:B:139:LYS:HG3	2.31	0.60
1:J:86:TYR:CD1	2:J:1008:PO4:O3	2.54	0.60
1:D:41:GLY:O	1:D:42:GLY:O	2.20	0.59
1:G:77:THR:HB	1:G:113:ALA:HB3	1.83	0.59
1:C:20:ARG:HA	1:C:20:ARG:NE	2.17	0.59
1:C:77:THR:CB	1:C:113:ALA:HB3	2.31	0.59
1:E:82:ASN:HB2	1:E:88:HIS:CE1	2.38	0.59
1:F:52:VAL:HG13	1:F:57:GLU:HB2	1.85	0.58
1:G:33:PHE:O	1:G:37:MET:HB2	2.03	0.58
1:F:121:HIS:O	1:F:122:ASP:HB2	2.03	0.58
1:J:82:ASN:HB2	1:J:88:HIS:CE1	2.39	0.58
1:E:113:ALA:O	1:E:115:LEU:HD22	2.04	0.58
1:F:79:PHE:CE2	1:F:117:PRO:HD3	2.39	0.58
1:J:24:ASP:OD1	1:J:25:ILE:HG13	2.04	0.58
1:F:111:LEU:HD12	1:F:111:LEU:N	2.19	0.58
1:E:152:ARG:HD3	4:E:380:HOH:O	2.01	0.58
1:G:24:ASP:OD1	1:G:131:PHE:HD1	1.87	0.58
1:H:14:ILE:CD1	1:H:45:PHE:HD2	2.17	0.57
1:A:148:ILE:O	1:A:152:ARG:HG3	2.04	0.57
1:F:20:ARG:NE	1:F:20:ARG:HA	2.19	0.57
1:C:111:LEU:N	1:C:111:LEU:HD12	2.20	0.57
1:H:112:SER:H	3:I:209:INI:C12	2.18	0.57
1:I:81:VAL:HG12	1:I:117:PRO:HD2	1.87	0.57
1:C:20:ARG:HA	1:C:20:ARG:HE	1.70	0.57
1:H:111:LEU:N	1:H:111:LEU:HD12	2.20	0.56
1:H:20:ARG:NE	1:H:20:ARG:HA	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:115:LEU:N	1:I:115:LEU:HD22	2.20	0.56
1:D:89:GLU:H	1:D:89:GLU:CD	2.09	0.56
1:J:148:ILE:O	1:J:152:ARG:HG3	2.05	0.56
1:C:91:VAL:O	1:C:95:VAL:HG23	2.05	0.56
1:C:133:HIS:HE1	1:C:137:LYS:HD3	1.70	0.56
1:C:13:ARG:HG2	1:C:46:ALA:HB3	1.87	0.56
1:C:52:VAL:HG13	1:C:57:GLU:HB2	1.87	0.56
1:D:36:GLU:HG3	1:D:139:LYS:HG2	1.89	0.55
1:J:85:ILE:HB	2:J:1008:PO4:O3	2.07	0.55
1:G:56:TYR:HB2	3:G:207:INI:H9	1.87	0.55
1:J:68:THR:OG1	1:J:70:ARG:HG3	2.05	0.55
1:D:58:ILE:HB	1:D:59:PRO:HD3	1.88	0.55
1:H:33:PHE:O	1:H:37:MET:HB2	2.06	0.55
1:D:77:THR:HB	1:D:113:ALA:HB3	1.87	0.55
1:C:111:LEU:HD21	1:C:145:CYS:HA	1.88	0.55
1:G:99:MET:O	1:G:103:GLN:HG2	2.07	0.54
1:I:20:ARG:NE	1:I:20:ARG:HA	2.22	0.54
1:D:14:ILE:HG12	1:D:145:CYS:SG	2.48	0.54
1:A:52:VAL:CG1	1:A:57:GLU:HB2	2.37	0.54
1:G:13:ARG:O	1:G:14:ILE:HD12	2.07	0.54
1:A:88:HIS:CE1	1:A:89:GLU:OE2	2.60	0.54
1:F:33:PHE:O	1:F:37:MET:HB2	2.07	0.54
1:D:42:GLY:O	1:D:43:ASP:HB3	2.07	0.54
1:G:81:VAL:HG23	1:G:82:ASN:N	2.23	0.54
1:J:86:TYR:H	2:J:1008:PO4:P	2.30	0.54
1:I:39:ASP:C	1:I:41:GLY:N	2.61	0.54
1:G:132:GLU:O	1:G:135:THR:HG23	2.08	0.54
1:I:68:THR:HB	1:I:70:ARG:NH1	2.23	0.54
1:J:20:ARG:HA	1:J:20:ARG:NE	2.22	0.53
1:E:20:ARG:HA	1:E:20:ARG:NE	2.23	0.53
1:J:20:ARG:O	1:J:23:ALA:HB2	2.08	0.53
1:B:80:VAL:O	1:B:116:THR:HG23	2.08	0.53
1:D:52:VAL:CG1	1:D:57:GLU:HB2	2.37	0.53
1:E:144:ALA:O	1:E:148:ILE:HG22	2.09	0.53
1:I:13:ARG:HB2	1:I:70:ARG:O	2.08	0.53
1:H:77:THR:CB	1:H:113:ALA:HB3	2.38	0.53
1:F:128:ARG:HG2	1:F:132:GLU:OE2	2.09	0.52
1:E:81:VAL:HG12	1:E:117:PRO:CD	2.39	0.52
1:I:63:ARG:O	1:I:67:GLU:HG3	2.08	0.52
1:D:36:GLU:HG3	1:D:139:LYS:CB	2.39	0.52
1:C:85:ILE:HB	2:C:1003:PO4:O3	2.10	0.52
1:B:13:ARG:C	1:B:14:ILE:HD12	2.30	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:20:ARG:NE	1:A:20:ARG:HA	2.25	0.52
1:F:86:TYR:CD2	1:J:115:LEU:HB3	2.45	0.52
1:A:33:PHE:O	1:A:37:MET:HB2	2.08	0.52
1:G:63:ARG:O	1:G:67:GLU:HG3	2.10	0.52
1:B:86:TYR:CD1	2:B:1002:PO4:O1	2.63	0.51
1:F:111:LEU:H	1:F:111:LEU:HD12	1.73	0.51
1:I:52:VAL:HG13	1:I:57:GLU:CB	2.40	0.51
1:I:133:HIS:CE1	1:I:137:LYS:HD3	2.44	0.51
1:A:36:GLU:HG3	1:A:139:LYS:HA	1.93	0.51
1:J:52:VAL:HG13	1:J:57:GLU:CB	2.38	0.51
1:D:133:HIS:CD2	1:J:125:GLU:HG2	2.45	0.51
1:C:148:ILE:HG23	1:C:149:LEU:N	2.26	0.50
1:C:52:VAL:HG13	1:C:53:PRO:HD2	1.92	0.50
1:G:112:SER:O	3:H:208:INI:H122	2.11	0.50
1:B:125:GLU:N	1:B:125:GLU:CD	2.64	0.50
1:A:15:ALA:HB2	1:A:71:TYR:CD2	2.46	0.50
1:D:24:ASP:OD2	1:D:127:HIS:CE1	2.64	0.50
1:E:121:HIS:O	1:E:122:ASP:C	2.48	0.50
1:D:19:ALA:HB1	1:D:54:GLY:HA2	1.94	0.50
1:E:58:ILE:HB	1:E:59:PRO:HD3	1.93	0.50
1:B:36:GLU:O	1:B:40:ILE:HG12	2.12	0.50
1:F:15:ALA:HB1	1:F:65:LEU:HD13	1.94	0.50
1:H:111:LEU:HD21	1:H:145:CYS:HA	1.93	0.50
1:B:77:THR:HB	1:B:113:ALA:HB3	1.94	0.50
1:J:17:VAL:HG12	1:J:58:ILE:HG12	1.94	0.50
1:F:52:VAL:CG1	1:F:57:GLU:HB2	2.42	0.50
1:D:15:ALA:HB2	1:D:71:TYR:CD2	2.46	0.49
1:B:81:VAL:HG12	1:B:117:PRO:HD2	1.93	0.49
1:J:36:GLU:HG3	1:J:139:LYS:HA	1.93	0.49
1:D:21:TRP:O	1:D:22:HIS:HB2	2.12	0.49
1:B:81:VAL:HG12	1:B:117:PRO:CD	2.43	0.49
1:A:98:GLY:O	1:A:102:VAL:HG23	2.13	0.49
1:G:156:ALA:C	1:H:70:ARG:HH22	2.16	0.49
1:I:98:GLY:O	1:I:102:VAL:HG23	2.13	0.49
1:G:86:TYR:HD1	2:G:1006:PO4:O1	1.96	0.49
1:I:80:VAL:HA	3:I:209:INI:O4	2.13	0.49
1:G:103:GLN:HB3	1:G:110:VAL:CG2	2.42	0.49
1:A:140:GLU:HA	1:A:143:ARG:NH1	2.27	0.49
1:H:20:ARG:HD2	1:H:51:ASP:OD2	2.13	0.49
1:B:85:ILE:H	2:B:1002:PO4:P	2.34	0.48
1:B:33:PHE:O	1:B:37:MET:HB2	2.13	0.48
1:E:148:ILE:O	1:E:152:ARG:HG3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:20:ARG:HA	1:B:20:ARG:NE	2.28	0.48
1:G:52:VAL:HG22	1:G:57:GLU:CB	2.43	0.48
1:C:86:TYR:CD1	2:C:1003:PO4:O3	2.66	0.48
1:E:72:GLY:O	1:E:149:LEU:HD21	2.13	0.48
1:G:52:VAL:HG22	1:G:57:GLU:HB2	1.96	0.48
1:G:86:TYR:CD1	2:G:1006:PO4:O1	2.67	0.48
1:I:86:TYR:HD1	2:I:1007:PO4:O4	1.96	0.48
1:G:96:ILE:HG22	1:H:94:ALA:HB2	1.96	0.48
1:E:83:GLY:HA3	2:E:1004:PO4:P	2.54	0.48
1:F:86:TYR:HA	1:J:117:PRO:HA	1.94	0.48
1:B:86:TYR:HD1	2:B:1002:PO4:O1	1.96	0.48
1:G:24:ASP:OD1	1:G:131:PHE:CD1	2.67	0.48
1:A:52:VAL:HG13	1:A:53:PRO:HD2	1.95	0.48
1:J:33:PHE:CE1	1:J:142:ALA:HA	2.48	0.48
1:A:112:SER:H	3:B:202:INI:H122	1.77	0.48
1:G:152:ARG:HD3	4:G:413:HOH:O	2.13	0.48
1:I:133:HIS:HE1	1:I:137:LYS:HD3	1.79	0.48
1:J:72:GLY:O	1:J:149:LEU:HD21	2.14	0.48
1:G:58:ILE:HB	1:G:59:PRO:HD3	1.94	0.48
1:D:36:GLU:CG	1:D:139:LYS:HG2	2.44	0.47
1:I:85:ILE:N	2:I:1007:PO4:O2	2.46	0.47
1:I:74:VAL:O	1:I:110:VAL:HA	2.14	0.47
1:D:128:ARG:O	1:D:132:GLU:HG3	2.14	0.47
1:F:148:ILE:HG23	1:F:149:LEU:N	2.29	0.47
1:B:86:TYR:H	2:B:1002:PO4:P	2.37	0.47
1:H:36:GLU:HG2	1:H:139:LYS:HG2	1.96	0.47
1:C:103:GLN:HB3	1:C:110:VAL:CG2	2.43	0.47
1:D:52:VAL:HG13	1:D:57:GLU:HB2	1.96	0.47
1:D:36:GLU:HG3	1:D:139:LYS:CG	2.45	0.47
1:F:10:GLU:HA	1:F:10:GLU:OE1	2.15	0.47
1:C:121:HIS:HE1	1:G:82:ASN:O	1.97	0.47
1:B:112:SER:H	3:C:203:INI:H122	1.79	0.47
1:G:36:GLU:HB3	1:G:142:ALA:CB	2.45	0.47
1:D:82:ASN:O	1:F:121:HIS:HE1	1.98	0.47
1:I:81:VAL:HG12	1:I:117:PRO:CD	2.44	0.47
1:H:14:ILE:HD11	1:H:45:PHE:HD2	1.78	0.46
1:E:40:ILE:HG13	1:E:40:ILE:O	2.15	0.46
1:A:15:ALA:HB2	1:A:71:TYR:CE2	2.51	0.46
1:A:83:GLY:HA3	2:A:1001:PO4:O3	2.15	0.46
1:A:87:ARG:HG3	1:E:116:THR:HG22	1.96	0.46
1:B:52:VAL:HG13	1:B:53:PRO:HD2	1.96	0.46
1:E:52:VAL:CG1	1:E:57:GLU:HB2	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:156:ALA:O	1:H:70:ARG:NH2	2.49	0.46
1:J:111:LEU:HD12	1:J:111:LEU:N	2.31	0.46
1:D:18:ARG:HD3	1:D:30:VAL:HG21	1.98	0.46
1:J:36:GLU:HG3	1:J:139:LYS:CG	2.45	0.46
1:B:80:VAL:HG11	1:B:92:ALA:HB2	1.97	0.46
1:E:81:VAL:HG12	1:E:117:PRO:CG	2.44	0.46
1:G:112:SER:H	3:H:208:INI:H122	1.80	0.46
1:H:29:CYS:SG	1:H:138:GLY:HA2	2.56	0.46
1:C:18:ARG:HD3	1:C:30:VAL:HG21	1.96	0.46
1:B:139:LYS:CE	1:B:143:ARG:HH22	2.17	0.46
1:J:58:ILE:HB	1:J:59:PRO:HD3	1.98	0.46
1:F:100:MET:HA	1:F:103:GLN:HE21	1.80	0.46
1:A:128:ARG:O	1:A:132:GLU:HG3	2.15	0.46
1:E:81:VAL:HG12	1:E:117:PRO:HD2	1.98	0.45
1:D:18:ARG:NE	1:D:51:ASP:OD1	2.45	0.45
1:E:91:VAL:O	1:E:95:VAL:HG23	2.17	0.45
1:D:20:ARG:HE	1:D:20:ARG:HA	1.80	0.45
1:J:133:HIS:CE1	1:J:137:LYS:HD3	2.52	0.45
1:F:68:THR:OG1	1:F:70:ARG:HG3	2.16	0.45
1:C:148:ILE:CG2	1:C:149:LEU:N	2.80	0.45
1:B:133:HIS:O	1:B:136:VAL:HB	2.17	0.45
1:F:58:ILE:HB	1:F:59:PRO:HD3	1.98	0.45
1:J:83:GLY:C	2:J:1008:PO4:O2	2.56	0.45
1:H:14:ILE:HD13	1:H:45:PHE:HD2	1.82	0.45
1:A:98:GLY:O	1:A:101:ASN:HB3	2.17	0.45
3:A:201:INI:C12	1:E:112:SER:H	2.30	0.45
1:A:24:ASP:OD1	1:A:131:PHE:HD1	1.99	0.45
1:E:63:ARG:HD3	4:E:376:HOH:O	2.16	0.45
1:I:19:ALA:HA	1:I:52:VAL:O	2.16	0.45
1:C:18:ARG:NH1	1:C:27:ASP:OD2	2.49	0.45
1:B:139:LYS:CE	1:B:143:ARG:NH2	2.68	0.44
1:B:56:TYR:HB2	3:B:202:INI:H9	1.98	0.44
1:G:112:SER:H	3:H:208:INI:C12	2.30	0.44
1:H:103:GLN:HB3	1:H:110:VAL:HG23	1.98	0.44
1:E:143:ARG:HB3	1:E:147:GLU:OE2	2.17	0.44
1:B:28:GLN:HB3	1:B:135:THR:HG22	2.00	0.44
1:J:125:GLU:CD	1:J:125:GLU:H	2.20	0.44
1:E:54:GLY:HA3	3:E:205:INI:O9	2.18	0.44
1:B:52:VAL:HG13	1:B:57:GLU:CB	2.42	0.44
1:J:36:GLU:O	1:J:40:ILE:HG12	2.18	0.44
1:I:52:VAL:CG1	1:I:57:GLU:HB2	2.46	0.44
1:H:149:LEU:HD23	1:H:149:LEU:HA	1.90	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:111:LEU:N	1:D:111:LEU:HD12	2.33	0.44
1:G:28:GLN:HB3	1:G:135:THR:HG22	1.98	0.44
1:E:86:TYR:HD1	2:E:1004:PO4:O2	2.00	0.44
1:J:14:ILE:HD12	1:J:14:ILE:N	2.33	0.44
1:H:33:PHE:CE1	1:H:142:ALA:HA	2.53	0.43
1:H:75:LEU:HD11	1:H:113:ALA:HB2	1.99	0.43
1:F:125:GLU:CD	1:F:125:GLU:N	2.68	0.43
1:C:14:ILE:HD11	1:C:45:PHE:HD2	1.83	0.43
1:H:111:LEU:HD12	1:H:111:LEU:H	1.84	0.43
1:B:99:MET:HE2	1:B:114:VAL:HG21	2.00	0.43
1:D:121:HIS:HE1	1:F:82:ASN:O	2.02	0.43
1:A:86:TYR:HD1	2:A:1001:PO4:O2	2.01	0.43
1:J:13:ARG:C	1:J:14:ILE:HD12	2.39	0.43
1:D:99:MET:HB3	1:D:110:VAL:HG11	2.01	0.43
1:I:123:SER:OG	1:I:126:HIS:HB2	2.19	0.43
1:A:8:ASP:HA	1:A:10:GLU:HG3	2.01	0.43
1:E:53:PRO:HD2	1:E:57:GLU:HG2	1.99	0.43
1:H:115:LEU:HD22	1:H:115:LEU:N	2.33	0.43
1:G:38:ALA:HA	1:G:42:GLY:CA	2.46	0.43
1:H:13:ARG:C	1:H:14:ILE:HD12	2.39	0.43
1:H:45:PHE:CD1	1:H:45:PHE:N	2.86	0.43
1:A:82:ASN:O	1:I:121:HIS:HE1	2.02	0.43
1:G:85:ILE:HB	2:G:1006:PO4:O2	2.19	0.43
1:A:121:HIS:O	1:A:122:ASP:C	2.57	0.43
1:G:16:VAL:HG22	1:G:75:LEU:HB3	2.01	0.42
1:E:64:THR:O	1:E:68:THR:HG23	2.19	0.42
1:F:88:HIS:HB3	2:F:1005:PO4:O3	2.19	0.42
1:D:145:CYS:O	1:D:148:ILE:HG22	2.19	0.42
1:C:52:VAL:CG1	1:C:57:GLU:HB2	2.48	0.42
1:H:18:ARG:HD3	1:H:30:VAL:HG21	2.01	0.42
1:C:82:ASN:O	1:G:121:HIS:HE1	2.02	0.42
1:I:152:ARG:NH2	1:J:64:THR:OG1	2.53	0.42
1:E:15:ALA:HB2	1:E:71:TYR:CD2	2.54	0.42
1:C:32:ALA:HB1	1:C:139:LYS:HG3	2.02	0.42
1:I:79:PHE:CE2	1:I:117:PRO:HD3	2.55	0.42
1:C:57:GLU:OE2	3:C:203:INI:H10	2.20	0.42
1:F:63:ARG:O	1:F:67:GLU:HG3	2.20	0.42
1:J:35:ALA:O	1:J:39:ASP:HB2	2.19	0.42
1:D:37:MET:O	1:D:41:GLY:N	2.53	0.42
1:E:75:LEU:HD11	1:E:113:ALA:HB2	2.01	0.42
1:E:83:GLY:HA3	2:E:1004:PO4:O3	2.20	0.42
1:D:12:VAL:HB	1:D:45:PHE:CD2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:147:GLU:HB3	1:I:53:PRO:HG3	2.01	0.42
1:A:149:LEU:HA	1:A:149:LEU:HD23	1.83	0.41
1:C:41:GLY:O	1:C:42:GLY:O	2.38	0.41
1:C:57:GLU:OE2	3:C:203:INI:O12	2.35	0.41
1:E:20:ARG:HE	1:E:20:ARG:HA	1.85	0.41
1:E:90:PHE:HB2	4:E:515:HOH:O	2.20	0.41
1:H:92:ALA:O	1:H:96:ILE:HD13	2.21	0.41
1:A:88:HIS:ND1	1:A:89:GLU:OE2	2.54	0.41
1:B:132:GLU:O	1:B:135:THR:HG23	2.19	0.41
1:F:88:HIS:CE1	1:F:89:GLU:OE2	2.73	0.41
1:B:33:PHE:CE1	1:B:142:ALA:HA	2.55	0.41
1:D:33:PHE:CE1	1:D:142:ALA:HA	2.55	0.41
1:I:148:ILE:HG23	1:I:149:LEU:N	2.35	0.41
1:D:42:GLY:C	1:D:44:ARG:H	2.24	0.41
1:F:112:SER:O	3:G:207:INI:H122	2.20	0.41
1:D:35:ALA:O	1:D:39:ASP:HB2	2.21	0.41
1:J:56:TYR:HB2	3:J:210:INI:H9	2.02	0.41
1:D:82:ASN:O	1:F:121:HIS:CE1	2.73	0.41
1:C:14:ILE:HG12	1:C:145:CYS:SG	2.60	0.41
1:F:63:ARG:HB2	1:F:102:VAL:HG22	2.03	0.41
1:A:24:ASP:OD1	1:A:131:PHE:CD1	2.74	0.41
1:F:75:LEU:HD11	1:F:113:ALA:HB2	2.03	0.41
1:G:82:ASN:HB2	1:G:88:HIS:ND1	2.35	0.41
1:G:20:ARG:CA	1:G:20:ARG:HE	2.33	0.41
1:F:111:LEU:HD21	1:F:145:CYS:HA	2.03	0.41
1:D:17:VAL:HG12	1:D:58:ILE:HG12	2.02	0.41
1:A:83:GLY:HA3	2:A:1001:PO4:P	2.61	0.41
1:F:74:VAL:O	1:F:110:VAL:HA	2.21	0.41
1:D:79:PHE:CE2	1:D:117:PRO:HD3	2.56	0.41
1:D:115:LEU:HB3	1:E:86:TYR:CD2	2.56	0.41
1:F:103:GLN:HB3	1:F:110:VAL:HG23	2.03	0.41
1:G:89:GLU:CD	1:G:89:GLU:H	2.24	0.41
1:G:83:GLY:N	2:G:1006:PO4:O3	2.51	0.40
1:F:155:ILE:O	1:F:157:ALA:N	2.54	0.40
1:A:52:VAL:HG13	1:A:57:GLU:HB2	2.02	0.40
1:J:86:TYR:N	2:J:1008:PO4:O3	2.54	0.40
1:F:133:HIS:CE1	1:G:86:TYR:HE1	2.39	0.40
1:B:148:ILE:HG23	1:B:149:LEU:N	2.36	0.40
1:G:113:ALA:C	1:G:115:LEU:HD13	2.41	0.40
1:E:82:ASN:HB2	1:E:88:HIS:ND1	2.36	0.40
1:E:13:ARG:C	1:E:14:ILE:HD12	2.42	0.40
1:J:120:TYR:CD1	1:J:126:HIS:HB3	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:109:PRO:HG2	1:B:152:ARG:HD2	2.04	0.40
1:A:58:ILE:HB	1:A:59:PRO:HD3	2.03	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	148/157 (94%)	143 (97%)	3 (2%)	2 (1%)	16	27
1	B	145/157 (92%)	140 (97%)	3 (2%)	2 (1%)	16	27
1	C	145/157 (92%)	138 (95%)	6 (4%)	1 (1%)	30	50
1	D	144/157 (92%)	134 (93%)	8 (6%)	2 (1%)	16	27
1	E	144/157 (92%)	135 (94%)	6 (4%)	3 (2%)	11	15
1	F	146/157 (93%)	138 (94%)	8 (6%)	0	100	100
1	G	146/157 (93%)	142 (97%)	2 (1%)	2 (1%)	16	27
1	H	145/157 (92%)	140 (97%)	5 (3%)	0	100	100
1	I	144/157 (92%)	135 (94%)	7 (5%)	2 (1%)	16	27
1	J	144/157 (92%)	136 (94%)	8 (6%)	0	100	100
All	All	1451/1570 (92%)	1381 (95%)	56 (4%)	14 (1%)	22	37

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	42	GLY
1	A	42	GLY
1	B	42	GLY
1	C	42	GLY
1	E	122	ASP
1	G	42	GLY
1	A	122	ASP
1	I	40	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	42	GLY
1	D	56	TYR
1	B	43	ASP
1	E	42	GLY
1	E	53	PRO
1	G	41	GLY

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	113/123 (92%)	111 (98%)	2 (2%)	71	91
1	B	112/123 (91%)	108 (96%)	4 (4%)	47	72
1	C	110/123 (89%)	109 (99%)	1 (1%)	87	97
1	D	112/123 (91%)	110 (98%)	2 (2%)	71	91
1	E	110/123 (89%)	107 (97%)	3 (3%)	57	83
1	F	112/123 (91%)	112 (100%)	0	100	100
1	G	111/123 (90%)	107 (96%)	4 (4%)	47	72
1	H	112/123 (91%)	110 (98%)	2 (2%)	71	91
1	I	110/123 (89%)	109 (99%)	1 (1%)	87	97
1	J	111/123 (90%)	107 (96%)	4 (4%)	47	72
All	All	1113/1230 (90%)	1090 (98%)	23 (2%)	66	88

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
1	A	134	PHE
1	B	37	MET
1	B	134	PHE
1	B	135	THR
1	B	152	ARG
1	C	125	GLU
1	D	122	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	134	PHE
1	E	52	VAL
1	E	59	PRO
1	E	93	SER
1	G	52	VAL
1	G	81	VAL
1	G	115	LEU
1	G	135	THR
1	H	52	VAL
1	H	122	ASP
1	I	134	PHE
1	J	24	ASP
1	J	29	CYS
1	J	115	LEU
1	J	134	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	HIS
1	B	121	HIS
1	C	121	HIS
1	D	121	HIS
1	E	103	GLN
1	F	121	HIS
1	G	121	HIS
1	G	127	HIS
1	I	121	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 ⓘ

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$
2	PO4	A	1001	-	4,4,4	0.87	0	6,6,6	0.31	0
3	INI	A	201	-	21,21,21	3.67	9 (42%)	24,29,29	2.78	12 (50%)
2	PO4	B	1002	-	4,4,4	0.94	0	6,6,6	0.31	0
3	INI	B	202	-	21,21,21	3.53	9 (42%)	24,29,29	2.77	10 (41%)
2	PO4	C	1003	-	4,4,4	0.92	0	6,6,6	0.31	0
3	INI	C	203	-	21,21,21	3.56	9 (42%)	24,29,29	2.84	11 (45%)
3	INI	D	204	-	21,21,21	3.65	9 (42%)	24,29,29	2.81	12 (50%)
2	PO4	E	1004	-	4,4,4	0.90	0	6,6,6	0.31	0
3	INI	E	205	-	21,21,21	3.60	10 (47%)	24,29,29	2.73	12 (50%)
2	PO4	F	1005	-	4,4,4	0.87	0	6,6,6	0.31	0
3	INI	F	206	-	21,21,21	3.73	10 (47%)	24,29,29	2.82	11 (45%)
2	PO4	G	1006	-	4,4,4	0.96	0	6,6,6	0.31	0
3	INI	G	207	-	21,21,21	3.57	9 (42%)	24,29,29	2.73	10 (41%)
3	INI	H	208	-	21,21,21	3.43	10 (47%)	24,29,29	2.81	11 (45%)
2	PO4	I	1007	-	4,4,4	0.95	0	6,6,6	0.31	0
3	INI	I	209	-	21,21,21	3.62	10 (47%)	24,29,29	2.73	11 (45%)
2	PO4	J	1008	-	4,4,4	1.03	0	6,6,6	0.31	0
2	PO4	J	1009	-	4,4,4	0.80	0	6,6,6	0.31	0
3	INI	J	210	-	21,21,21	3.68	10 (47%)	24,29,29	2.85	13 (54%)

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
2	PO4	A	1001	-	-	0/0/0/0	0/0/0/0
3	INI	A	201	-	-	1/17/19/19	0/1/1/1
2	PO4	B	1002	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	INI	B	202	-	-	1/17/19/19	0/1/1/1
2	PO4	C	1003	-	-	0/0/0/0	0/0/0/0
3	INI	C	203	-	-	1/17/19/19	0/1/1/1
3	INI	D	204	-	-	1/17/19/19	0/1/1/1
2	PO4	E	1004	-	-	0/0/0/0	0/0/0/0
3	INI	E	205	-	-	0/17/19/19	0/1/1/1
2	PO4	F	1005	-	-	0/0/0/0	0/0/0/0
3	INI	F	206	-	-	1/17/19/19	0/1/1/1
2	PO4	G	1006	-	-	0/0/0/0	0/0/0/0
3	INI	G	207	-	-	1/17/19/19	0/1/1/1
3	INI	H	208	-	-	1/17/19/19	0/1/1/1
2	PO4	I	1007	-	-	0/0/0/0	0/0/0/0
3	INI	I	209	-	-	1/17/19/19	0/1/1/1
2	PO4	J	1008	-	-	0/0/0/0	0/0/0/0
2	PO4	J	1009	-	-	0/0/0/0	0/0/0/0
3	INI	J	210	-	-	1/17/19/19	0/1/1/1

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	209	INI	C11-C10	8.79	1.71	1.53
3	F	206	INI	C11-C10	8.74	1.71	1.53
3	G	207	INI	C11-C10	8.66	1.71	1.53
3	C	203	INI	C11-C10	8.57	1.71	1.53
3	A	201	INI	C11-C10	8.55	1.71	1.53
3	E	205	INI	C11-C10	8.49	1.71	1.53
3	B	202	INI	C4-C5	8.33	1.58	1.42
3	J	210	INI	C11-C10	8.27	1.70	1.53
3	E	205	INI	C4-C5	8.25	1.58	1.42
3	G	207	INI	C4-C5	8.24	1.58	1.42
3	F	206	INI	C4-C5	8.16	1.58	1.42
3	B	202	INI	C11-C10	8.07	1.70	1.53
3	I	209	INI	C4-C5	8.06	1.57	1.42
3	A	201	INI	C4-C5	8.02	1.57	1.42
3	D	204	INI	C11-C10	8.01	1.70	1.53
3	J	210	INI	C4-C5	8.00	1.57	1.42
3	D	204	INI	C4-C5	7.90	1.57	1.42
3	H	208	INI	C11-C10	7.82	1.69	1.53
3	H	208	INI	C4-C5	7.68	1.57	1.42
3	C	203	INI	C4-C5	7.50	1.56	1.42
3	J	210	INI	C6-N7	7.04	1.44	1.32
3	A	201	INI	C6-N7	6.74	1.43	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	204	INI	C6-N7	6.67	1.43	1.32
3	E	205	INI	C6-N7	6.46	1.43	1.32
3	C	203	INI	C6-N7	6.40	1.43	1.32
3	F	206	INI	C6-N7	6.20	1.42	1.32
3	H	208	INI	C6-N7	6.18	1.42	1.32
3	I	209	INI	C6-N7	6.11	1.42	1.32
3	B	202	INI	C6-N7	6.02	1.42	1.32
3	G	207	INI	C6-N7	5.84	1.42	1.32
3	D	204	INI	C8-C9	5.46	1.60	1.52
3	F	206	INI	C9-C10	5.11	1.64	1.53
3	J	210	INI	C8-C9	5.07	1.59	1.52
3	J	210	INI	C9-C10	5.06	1.64	1.53
3	B	202	INI	C8-C9	5.03	1.59	1.52
3	D	204	INI	C9-C10	4.99	1.63	1.53
3	F	206	INI	C8-C9	4.91	1.59	1.52
3	E	205	INI	C9-C10	4.88	1.63	1.53
3	C	203	INI	C9-C10	4.88	1.63	1.53
3	A	201	INI	C9-C10	4.85	1.63	1.53
3	C	203	INI	C8-C9	4.79	1.59	1.52
3	I	209	INI	C8-C9	4.71	1.59	1.52
3	E	205	INI	C8-C9	4.68	1.59	1.52
3	A	201	INI	C8-C9	4.60	1.59	1.52
3	H	208	INI	C9-C10	4.59	1.63	1.53
3	G	207	INI	C9-C10	4.59	1.63	1.53
3	I	209	INI	C9-C10	4.47	1.62	1.53
3	B	202	INI	C9-C10	4.36	1.62	1.53
3	H	208	INI	C8-C9	4.29	1.58	1.52
3	G	207	INI	C8-C9	4.24	1.58	1.52
3	F	206	INI	C5-C6	3.71	1.50	1.41
3	J	210	INI	C5-C6	3.70	1.50	1.41
3	D	204	INI	C5-C6	3.70	1.50	1.41
3	A	201	INI	O51-N5	-3.64	1.19	1.25
3	I	209	INI	O51-N5	-3.53	1.19	1.25
3	G	207	INI	O51-N5	-3.50	1.19	1.25
3	A	201	INI	C5-C6	3.43	1.49	1.41
3	C	203	INI	C5-C6	3.41	1.49	1.41
3	F	206	INI	O51-N5	-3.32	1.19	1.25
3	G	207	INI	C5-C6	3.30	1.49	1.41
3	D	204	INI	O51-N5	-3.22	1.19	1.25
3	C	203	INI	O51-N5	-3.15	1.19	1.25
3	E	205	INI	O51-N5	-3.14	1.19	1.25
3	H	208	INI	C5-C6	3.12	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	210	INI	O51-N5	-3.11	1.20	1.25
3	B	202	INI	O51-N5	-3.11	1.20	1.25
3	H	208	INI	O51-N5	-3.10	1.20	1.25
3	F	206	INI	C12-C11	3.00	1.61	1.52
3	B	202	INI	C5-C6	2.99	1.48	1.41
3	E	205	INI	C5-C6	2.99	1.48	1.41
3	D	204	INI	C12-C11	2.94	1.60	1.52
3	I	209	INI	C5-C6	2.84	1.48	1.41
3	H	208	INI	C12-C11	2.75	1.60	1.52
3	B	202	INI	C12-C11	2.75	1.60	1.52
3	J	210	INI	C12-C11	2.72	1.60	1.52
3	A	201	INI	C12-C11	2.68	1.60	1.52
3	F	206	INI	C6-N1	2.67	1.41	1.35
3	C	203	INI	C12-C11	2.67	1.60	1.52
3	D	204	INI	C6-N1	2.61	1.41	1.35
3	G	207	INI	C12-C11	2.61	1.59	1.52
3	I	209	INI	C6-N1	2.53	1.41	1.35
3	E	205	INI	C12-C11	2.45	1.59	1.52
3	J	210	INI	C6-N1	2.39	1.41	1.35
3	B	202	INI	C6-N1	2.37	1.41	1.35
3	E	205	INI	C6-N1	2.35	1.41	1.35
3	F	206	INI	C4-N3	2.32	1.41	1.37
3	A	201	INI	C6-N1	2.31	1.41	1.35
3	I	209	INI	C12-C11	2.31	1.59	1.52
3	C	203	INI	C6-N1	2.31	1.41	1.35
3	H	208	INI	C6-N1	2.27	1.41	1.35
3	I	209	INI	C4-N3	2.25	1.41	1.37
3	G	207	INI	C6-N1	2.20	1.40	1.35
3	J	210	INI	C8-N7	2.11	1.49	1.45
3	H	208	INI	C8-N7	2.10	1.49	1.45
3	E	205	INI	C4-N3	2.05	1.40	1.37

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	210	INI	C12-C11-C10	6.97	128.19	112.38
3	C	203	INI	C12-C11-C10	6.92	128.08	112.38
3	H	208	INI	C12-C11-C10	6.86	127.93	112.38
3	G	207	INI	C12-C11-C10	6.84	127.90	112.38
3	B	202	INI	C12-C11-C10	6.80	127.82	112.38
3	F	206	INI	C12-C11-C10	6.79	127.79	112.38
3	A	201	INI	C12-C11-C10	6.75	127.70	112.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	204	INI	C12-C11-C10	6.72	127.62	112.38
3	E	205	INI	C12-C11-C10	6.35	126.78	112.38
3	I	209	INI	C12-C11-C10	6.08	126.17	112.38
3	I	209	INI	O11-C11-C12	-5.48	96.43	109.20
3	C	203	INI	C4-C5-N5	-5.33	117.11	121.94
3	B	202	INI	O11-C11-C12	-5.20	97.08	109.20
3	J	210	INI	C4-C5-N5	-5.20	117.23	121.94
3	D	204	INI	C4-C5-N5	-5.15	117.27	121.94
3	E	205	INI	O11-C11-C12	-5.01	97.53	109.20
3	F	206	INI	C4-C5-N5	-5.00	117.41	121.94
3	C	203	INI	O11-C11-C12	-4.98	97.58	109.20
3	H	208	INI	C4-C5-N5	-4.96	117.44	121.94
3	A	201	INI	C4-C5-N5	-4.95	117.46	121.94
3	J	210	INI	O11-C11-C12	-4.91	97.76	109.20
3	F	206	INI	O11-C11-C12	-4.77	98.09	109.20
3	D	204	INI	O11-C11-C12	-4.75	98.12	109.20
3	G	207	INI	O11-C11-C12	-4.70	98.25	109.20
3	I	209	INI	C4-C5-N5	-4.69	117.69	121.94
3	H	208	INI	O11-C11-C12	-4.67	98.31	109.20
3	B	202	INI	C8-N7-C6	-4.60	112.97	124.59
3	A	201	INI	O11-C11-C12	-4.60	98.49	109.20
3	E	205	INI	C4-C5-N5	-4.42	117.94	121.94
3	G	207	INI	C4-C5-N5	-4.41	117.95	121.94
3	G	207	INI	C8-N7-C6	-4.20	113.97	124.59
3	H	208	INI	C8-N7-C6	-4.19	114.01	124.59
3	B	202	INI	O11-C11-C10	-3.85	99.45	109.05
3	C	203	INI	C8-N7-C6	-3.85	114.86	124.59
3	D	204	INI	C8-C9-C10	3.81	123.86	110.94
3	B	202	INI	C4-C5-N5	-3.81	118.49	121.94
3	D	204	INI	O11-C11-C10	-3.78	99.63	109.05
3	I	209	INI	C8-C9-C10	3.76	123.66	110.94
3	H	208	INI	O11-C11-C10	-3.73	99.75	109.05
3	F	206	INI	C8-N7-C6	-3.72	115.20	124.59
3	J	210	INI	C8-C9-C10	3.69	123.45	110.94
3	C	203	INI	C8-C9-C10	3.65	123.30	110.94
3	F	206	INI	C8-C9-C10	3.64	123.27	110.94
3	D	204	INI	C8-N7-C6	-3.64	115.40	124.59
3	E	205	INI	C8-C9-C10	3.64	123.26	110.94
3	J	210	INI	O11-C11-C10	-3.60	100.08	109.05
3	F	206	INI	C11-C10-C9	3.57	121.32	113.25
3	A	201	INI	C8-C9-C10	3.57	123.03	110.94
3	I	209	INI	C8-N7-C6	-3.50	115.75	124.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	205	INI	O11-C11-C10	-3.44	100.47	109.05
3	C	203	INI	O11-C11-C10	-3.41	100.55	109.05
3	J	210	INI	C8-N7-C6	-3.41	115.98	124.59
3	B	202	INI	C8-C9-C10	3.39	122.44	110.94
3	A	201	INI	C8-N7-C6	-3.39	116.02	124.59
3	E	205	INI	C8-N7-C6	-3.38	116.05	124.59
3	A	201	INI	C11-C10-C9	3.38	120.88	113.25
3	H	208	INI	C8-C9-C10	3.35	122.28	110.94
3	G	207	INI	O11-C11-C10	-3.25	100.96	109.05
3	G	207	INI	C8-C9-C10	3.22	121.86	110.94
3	F	206	INI	O9-C9-C8	-3.22	102.66	109.72
3	I	209	INI	C11-C10-C9	3.19	120.45	113.25
3	A	201	INI	O11-C11-C10	-3.18	101.12	109.05
3	J	210	INI	C11-C10-C9	3.12	120.30	113.25
3	C	203	INI	C11-C10-C9	3.10	120.25	113.25
3	G	207	INI	C11-C10-C9	3.08	120.21	113.25
3	E	205	INI	C11-C10-C9	3.06	120.17	113.25
3	F	206	INI	O11-C11-C10	-3.06	101.43	109.05
3	D	204	INI	N7-C6-N1	-3.06	114.56	120.44
3	I	209	INI	O11-C11-C10	-3.02	101.54	109.05
3	F	206	INI	N7-C6-N1	-2.99	114.68	120.44
3	C	203	INI	N7-C6-N1	-2.99	114.69	120.44
3	I	209	INI	C4-C5-C6	2.97	116.59	114.55
3	G	207	INI	N7-C6-N1	-2.95	114.77	120.44
3	B	202	INI	C11-C10-C9	2.95	119.91	113.25
3	H	208	INI	N7-C6-N1	-2.95	114.77	120.44
3	A	201	INI	N7-C6-N1	-2.92	114.82	120.44
3	H	208	INI	C11-C10-C9	2.92	119.84	113.25
3	A	201	INI	O9-C9-C8	-2.88	103.39	109.72
3	D	204	INI	C11-C10-C9	2.88	119.76	113.25
3	J	210	INI	O9-C9-C8	-2.88	103.39	109.72
3	B	202	INI	N7-C6-N1	-2.85	114.95	120.44
3	I	209	INI	N7-C6-N1	-2.84	114.98	120.44
3	H	208	INI	C4-C5-C6	2.83	116.49	114.55
3	J	210	INI	N7-C6-N1	-2.82	115.01	120.44
3	G	207	INI	O9-C9-C8	-2.78	103.61	109.72
3	E	205	INI	C4-C5-C6	2.78	116.45	114.55
3	E	205	INI	O9-C9-C8	-2.76	103.66	109.72
3	E	205	INI	N7-C6-N1	-2.64	115.37	120.44
3	E	205	INI	O12-C12-C11	-2.60	105.24	111.05
3	A	201	INI	C4-C5-C6	2.53	116.28	114.55
3	H	208	INI	O9-C9-C8	-2.35	104.57	109.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	203	INI	O9-C9-C8	-2.34	104.58	109.72
3	I	209	INI	O9-C9-C10	-2.32	103.28	109.05
3	C	203	INI	C4-C5-C6	2.30	116.13	114.55
3	J	210	INI	C4-C5-C6	2.27	116.10	114.55
3	F	206	INI	O9-C9-C10	-2.23	103.50	109.05
3	J	210	INI	O9-C9-C10	-2.21	103.55	109.05
3	C	203	INI	O9-C9-C10	-2.17	103.64	109.05
3	I	209	INI	O9-C9-C8	-2.16	104.97	109.72
3	B	202	INI	O9-C9-C10	-2.16	103.67	109.05
3	D	204	INI	O9-C9-C10	-2.16	103.68	109.05
3	G	207	INI	O12-C12-C11	-2.15	106.25	111.05
3	E	205	INI	O9-C9-C10	-2.10	103.81	109.05
3	B	202	INI	O9-C9-C8	-2.10	105.11	109.72
3	J	210	INI	C5-C6-N7	2.09	128.96	124.56
3	D	204	INI	C4-C5-C6	2.08	115.98	114.55
3	J	210	INI	O12-C12-C11	-2.08	106.39	111.05
3	A	201	INI	O12-C12-C11	-2.03	106.50	111.05
3	D	204	INI	C5-C6-N7	2.03	128.83	124.56
3	D	204	INI	O9-C9-C8	-2.03	105.26	109.72
3	F	206	INI	C4-C5-C6	2.02	115.93	114.55
3	A	201	INI	O9-C9-C10	-2.02	104.03	109.05
3	H	208	INI	O9-C9-C10	-2.01	104.03	109.05

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	209	INI	N1-C6-N7-C8
3	C	203	INI	N1-C6-N7-C8
3	J	210	INI	N1-C6-N7-C8
3	H	208	INI	N1-C6-N7-C8
3	D	204	INI	N1-C6-N7-C8
3	A	201	INI	N1-C6-N7-C8
3	F	206	INI	N1-C6-N7-C8
3	G	207	INI	N1-C6-N7-C8
3	B	202	INI	N1-C6-N7-C8

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	150/157 (95%)	-0.29	0 100 100	12, 24, 39, 56	2 (1%)
1	B	147/157 (93%)	-0.46	0 100 100	11, 21, 39, 48	3 (2%)
1	C	147/157 (93%)	-0.38	0 100 100	12, 24, 43, 51	0
1	D	146/157 (92%)	-0.33	1 (0%) 84 87	12, 23, 41, 53	2 (1%)
1	E	146/157 (92%)	-0.28	0 100 100	12, 24, 45, 54	2 (1%)
1	F	148/157 (94%)	-0.32	2 (1%) 72 75	14, 25, 43, 60	1 (0%)
1	G	148/157 (94%)	-0.23	1 (0%) 84 87	14, 27, 47, 59	3 (2%)
1	H	147/157 (93%)	-0.40	1 (0%) 84 87	10, 24, 39, 50	0
1	I	146/157 (92%)	-0.36	0 100 100	14, 25, 48, 59	1 (0%)
1	J	146/157 (92%)	-0.28	1 (0%) 84 87	10, 24, 42, 49	2 (1%)
All	All	1471/1570 (93%)	-0.33	6 (0%) 79 92	10, 24, 44, 60	16 (1%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	42	GLY	3.8
1	H	156	ALA	3.7
1	F	40	ILE	3.0
1	D	42	GLY	2.9
1	F	157	ALA	2.5
1	J	42	GLY	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
2	PO4	B	1002	5/5	0.73	25.70	61,61,61,61	5
2	PO4	G	1006	5/5	0.53	18.61	50,50,51,51	5
2	PO4	A	1001	5/5	0.58	17.91	60,61,62,62	5
2	PO4	J	1008	5/5	0.44	17.40	49,49,49,50	5
2	PO4	F	1005	5/5	0.60	17.38	56,57,57,57	5
2	PO4	E	1004	5/5	0.43	11.86	56,57,58,58	5
2	PO4	C	1003	5/5	0.41	11.20	55,56,56,56	5
2	PO4	I	1007	5/5	0.55	9.74	55,56,56,57	5
3	INI	G	207	21/21	0.18	5.51	20,31,40,43	0
3	INI	A	201	21/21	0.20	3.83	24,38,44,47	0
3	INI	C	203	21/21	0.17	3.32	28,34,41,45	0
3	INI	B	202	21/21	0.17	3.30	22,30,40,45	0
3	INI	E	205	21/21	0.17	3.04	27,30,37,39	0
3	INI	I	209	21/21	0.16	2.77	14,28,36,39	0
3	INI	F	206	21/21	0.18	2.73	25,32,42,44	0
3	INI	J	210	21/21	0.16	2.62	30,33,37,40	0
3	INI	D	204	21/21	0.17	2.42	24,35,44,49	0
2	PO4	J	1009	5/5	0.16	2.41	43,44,47,50	5
3	INI	H	208	21/21	0.16	2.34	17,33,42,45	0

6.5 Other polymers ⓘ

There are no such residues in this entry.