



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:02 PM UTC

PDB ID : 9L9S / pdb_00009l9s
Title : The crystal structure of UG15
Authors : Chen, Q.; Yu, Y.; Jia, T.
Deposited on : 2024-12-31
Resolution : 3.31 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

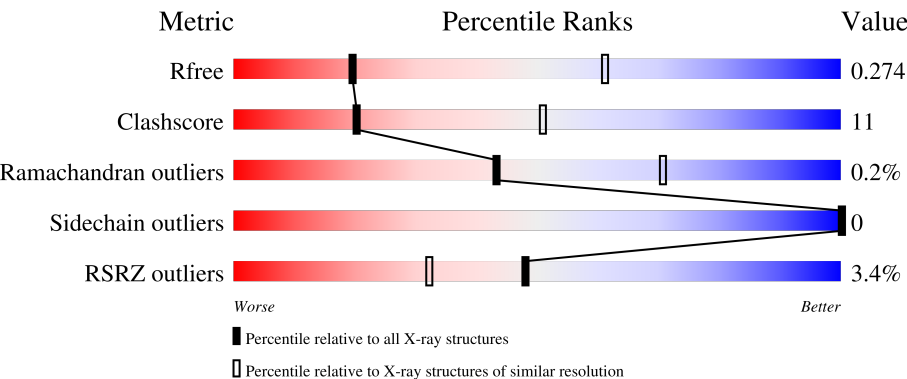
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.31 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	540	3% 77% 23%
1	B	540	2% 80% 20%
1	C	540	4% 75% 24%
2	D	6	17% 67% 17% 17%
2	E	6	17% 33% 50% 17%

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Mol	Chain	Length	Quality of chain
2	F	6	33% 33% 67%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26567 atoms, of which 12957 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 UG15.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	538	Total	C	H	N	O	S	0	0	0
			8659	2810	4257	727	840	25			
1	B	539	Total	C	H	N	O	S	0	0	0
			8684	2822	4268	728	841	25			
1	C	539	Total	C	H	N	O	S	0	1	0
			8689	2822	4273	728	841	25			

- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	5	Total	C	H	N	O	P	0	0	0
			145	50	40	25	25	5			
2	E	5	Total	C	H	N	O	P	0	0	0
			145	50	40	25	25	5			
2	F	6	Total	C	H	N	O	P	0	0	0
			166	60	40	30	30	6			

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
3	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
3	C	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

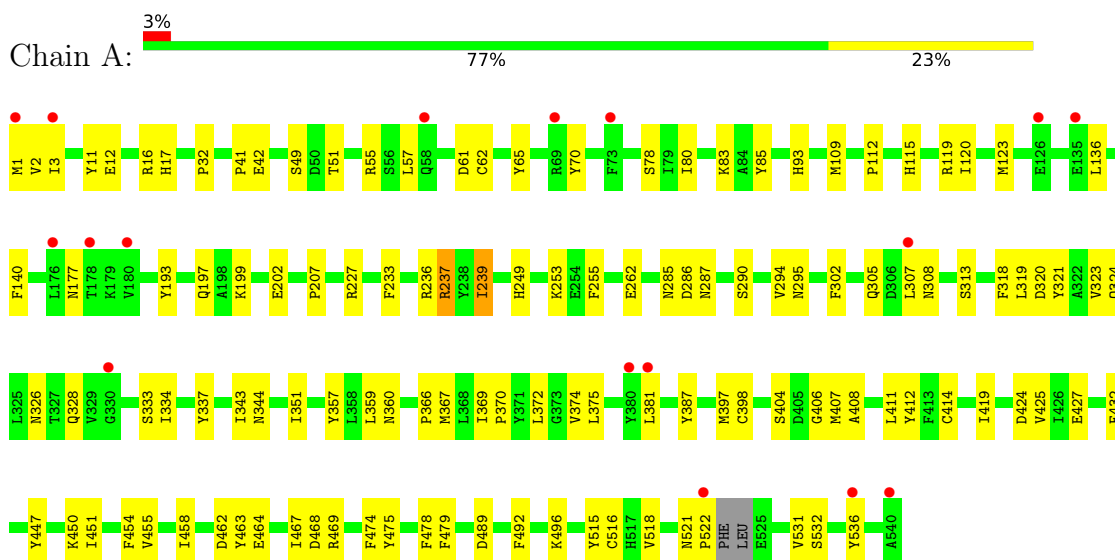
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	B	1	Total	O	0	0
			1	1		

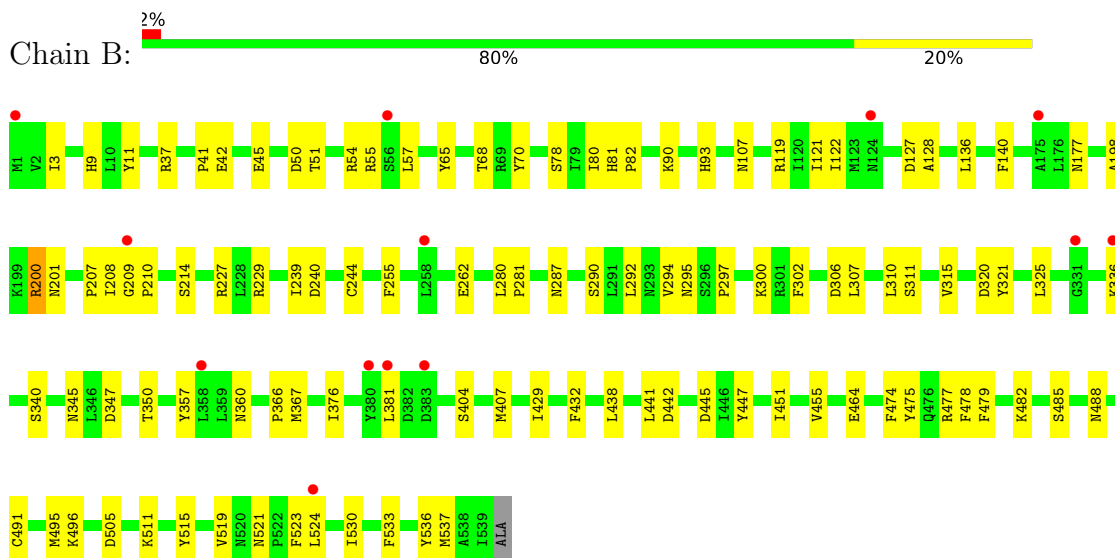
3 Residue-property plots [i](#)

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

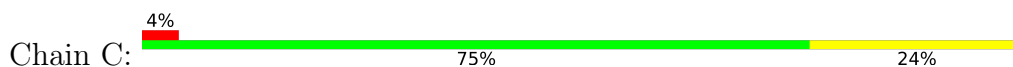
• Molecule 1: UG15

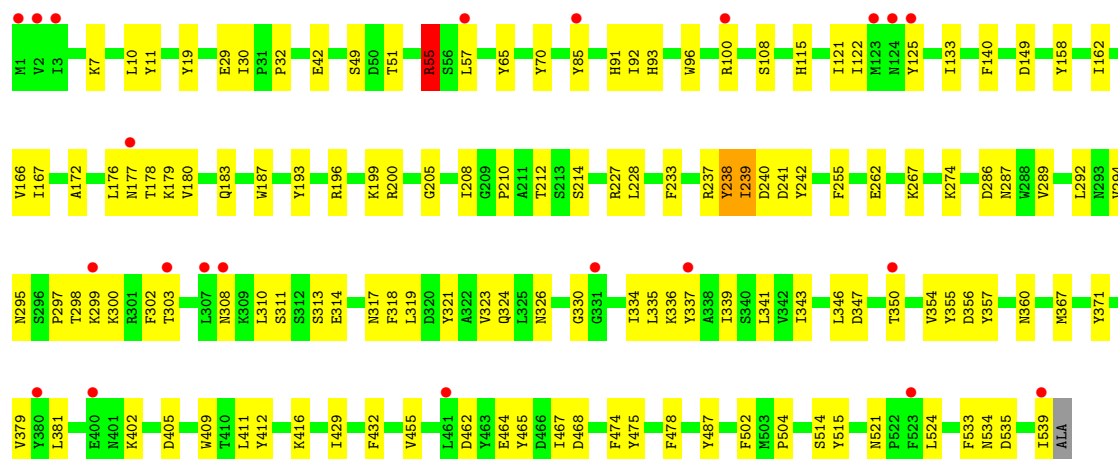


• Molecule 1: UG15

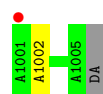


• Molecule 1: UG15

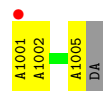




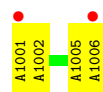
- Molecule 2: DNA (5'-D(P*AP*AP*AP*AP*AP*A)-3')



- Molecule 2: DNA (5'-D(P*AP*AP*AP*AP*AP*A)-3')



- Molecule 2: DNA (5'-D(P*AP*AP*AP*AP*AP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	198.59Å 198.59Å 349.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.10 – 3.31 35.10 – 3.31	Depositor EDS
% Data completeness (in resolution range)	99.7 (35.10-3.31) 99.6 (35.10-3.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 3.32Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, R_{free}	0.260 , 0.284 0.260 , 0.274	Depositor DCC
R_{free} test set	1052 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	90.0	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 24.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	26567	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: MES

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	0.34	0/4506	0.56	2/6100 (0.0%)
1	B	0.32	0/4522	0.55	2/6123 (0.0%)
1	C	0.33	0/4530	0.61	3/6134 (0.0%)
2	D	0.46	0/119	0.45	0/181
2	E	0.52	0/119	0.62	0/181
2	F	0.58	0/143	0.51	0/218
All	All	0.34	0/13939	0.57	7/18937 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	55	ARG	CD-NE-CZ	14.52	144.72	124.40
1	A	237	ARG	CD-NE-CZ	11.43	140.40	124.40
1	B	200	ARG	CD-NE-CZ	8.40	136.16	124.40
1	A	237	ARG	NE-CZ-NH1	-7.61	113.89	121.50
1	C	238	TYR	N-CA-C	-7.21	95.18	108.02
1	C	55	ARG	NE-CZ-NH1	-5.53	115.97	121.50
1	B	200	ARG	NE-CZ-NH1	-5.14	116.36	121.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	237	ARG	Sidechain
1	B	200	ARG	Sidechain
1	C	55	ARG	Sidechain

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	4402	4257	4271	95	1
1	B	4416	4268	4287	93	1
1	C	4416	4273	4276	127	1
2	D	105	40	56	1	0
2	E	105	40	56	6	0
2	F	126	40	67	8	0
3	A	12	13	13	0	0
3	B	12	13	13	0	0
3	C	12	13	13	0	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
All	All	13610	12957	13052	300	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 11.

All (300) 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:C:19:TYR:CD1	1:C:85:TYR:CE2	2.59	0.91
1:C:521:ASN:HB3	1:C:524:LEU:HD23	1.61	0.82
1:B:521:ASN:HB3	1:B:524:LEU:HD12	1.62	0.81
1:A:123:MET:HE2	1:A:239:ILE:HD11	1.62	0.81
2:E:1001:DA:H2''	2:E:1002:DA:O5'	1.81	0.81
1:C:19:TYR:HD1	1:C:85:TYR:CE2	2.05	0.74
1:A:2:VAL:HG12	1:A:3:ILE:H	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:GLU:OE2	1:A:450:LYS:NZ	2.16	0.72
2:F:1005:DA:H3'	2:F:1006:DA:H5'	1.73	0.71
1:C:521:ASN:CB	1:C:524:LEU:HD23	2.21	0.70
1:A:407:MET:HE1	1:A:432:PHE:CD1	2.28	0.69
1:C:19:TYR:HD1	1:C:85:TYR:HE2	1.39	0.68
1:C:356:ASP:O	1:C:360:ASN:ND2	2.28	0.66
1:B:300:LYS:HB3	1:B:302:PHE:HD2	1.62	0.65
1:B:57:LEU:O	1:B:57:LEU:HD12	1.97	0.64
1:C:70:TYR:HA	1:C:367:MET:SD	2.38	0.64
1:B:127:ASP:OD1	1:B:128:ALA:N	2.30	0.64
1:C:85:TYR:O	1:C:85:TYR:HD1	1.81	0.63
1:C:85:TYR:O	1:C:85:TYR:CD1	2.51	0.63
1:B:54:ARG:O	1:B:488:ASN:ND2	2.31	0.63
1:A:313:SER:OG	1:C:299:LYS:NZ	2.32	0.62
1:C:42:GLU:HB3	1:C:533:PHE:CE1	2.34	0.62
1:C:149:ASP:OD2	1:C:274:LYS:HD3	2.00	0.62
1:C:199:LYS:NZ	1:C:205:GLY:O	2.33	0.62
1:B:310:LEU:HD12	1:B:315:VAL:CG2	2.29	0.62
1:C:478:PHE:CG	1:C:478:PHE:O	2.53	0.62
1:C:19:TYR:CE1	1:C:85:TYR:CD2	2.89	0.61
1:B:244:CYS:HB2	1:B:255:PHE:CE1	2.36	0.61
1:B:515:TYR:HB2	1:B:536:TYR:CD1	2.35	0.60
1:B:42:GLU:HB3	1:B:533:PHE:CD1	2.36	0.60
1:A:3:ILE:HG21	1:A:115:HIS:O	2.02	0.60
1:C:475:TYR:CG	1:C:475:TYR:O	2.55	0.59
1:A:360:ASN:OD1	1:C:140:PHE:HB2	2.02	0.59
1:C:178:THR:HG22	1:C:180:VAL:HG22	1.84	0.59
1:C:108:SER:HB2	1:C:237:ARG:HH21	1.67	0.58
1:B:70:TYR:HA	1:B:367:MET:SD	2.43	0.58
1:B:57:LEU:HD11	1:B:464:GLU:HB2	1.86	0.58
1:C:108:SER:HB2	1:C:237:ARG:NH2	2.20	0.57
1:A:359:LEU:HD12	1:A:372:LEU:HD21	1.86	0.57
1:B:42:GLU:OE1	1:B:42:GLU:N	2.36	0.57
1:A:424:ASP:OD1	1:A:425:VAL:N	2.37	0.57
1:C:228:LEU:HD13	1:C:255:PHE:HE2	1.70	0.56
1:A:123:MET:HE2	1:A:239:ILE:CD1	2.33	0.56
1:B:442:ASP:OD1	1:B:477:ARG:NH1	2.38	0.56
1:C:298:THR:HG22	1:C:310:LEU:HD21	1.88	0.56
1:C:162:ILE:O	1:C:166:VAL:HG23	2.06	0.56
1:A:1:MET:HE1	1:A:16:ARG:HH12	1.71	0.56
1:A:407:MET:HE1	1:A:432:PHE:HD1	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:478:PHE:O	1:C:478:PHE:CD1	2.59	0.56
1:C:402:LYS:HA	1:C:432:PHE:CE1	2.41	0.55
1:C:515:TYR:CE1	1:C:533:PHE:HA	2.41	0.55
2:F:1005:DA:H4'	2:F:1006:DA:OP2	2.06	0.55
1:B:310:LEU:HD12	1:B:315:VAL:HG22	1.88	0.55
1:A:455:VAL:HG13	1:A:474:PHE:CE1	2.41	0.55
1:B:310:LEU:HD13	1:B:311:SER:N	2.22	0.55
1:B:515:TYR:HB2	1:B:536:TYR:CE1	2.42	0.55
1:C:29:GLU:HG2	2:F:1006:DA:H61	1.72	0.54
1:B:70:TYR:CA	1:B:367:MET:HE1	2.37	0.54
1:C:313:SER:HB2	2:E:1001:DA:OP1	2.08	0.54
1:C:515:TYR:HE1	1:C:533:PHE:HA	1.73	0.54
1:A:1:MET:HE3	1:A:12:GLU:OE2	2.08	0.53
1:A:521:ASN:OD1	1:A:522:PRO:HD2	2.07	0.53
1:C:42:GLU:HB3	1:C:533:PHE:CD1	2.43	0.53
1:C:55:ARG:HG2	1:C:464:GLU:OE1	2.08	0.53
1:A:57:LEU:HD11	1:A:463:TYR:CE2	2.44	0.53
1:A:305:GLN:HA	1:A:308:ASN:HB3	1.91	0.53
1:B:240:ASP:CG	2:E:1005:DA:HO3'	2.17	0.52
1:C:115:HIS:CE1	1:C:122:ILE:HD11	2.44	0.52
1:A:324:GLN:O	1:A:328:GLN:HG3	2.08	0.52
1:C:57:LEU:HD13	1:C:465:TYR:CE1	2.43	0.52
1:B:3:ILE:HD13	1:B:9:HIS:HA	1.92	0.52
1:C:535:ASP:O	1:C:539:ILE:HD12	2.10	0.52
1:C:158:TYR:HD1	1:C:267:LYS:HG3	1.74	0.52
1:A:227:ARG:HG2	1:A:262:GLU:OE2	2.10	0.52
1:B:70:TYR:HA	1:B:367:MET:HE1	1.92	0.52
1:C:42:GLU:CB	1:C:533:PHE:CE1	2.93	0.52
1:C:475:TYR:O	1:C:475:TYR:CD1	2.63	0.51
1:C:347:ASP:OD2	1:C:350:THR:HG22	2.10	0.51
1:B:336:LYS:HD2	1:B:367:MET:HE2	1.91	0.51
1:A:536:TYR:HD1	1:A:536:TYR:O	1.92	0.51
1:C:297:PRO:HB2	1:C:310:LEU:HD11	1.91	0.51
1:C:318:PHE:O	1:C:321:TYR:HB3	2.11	0.51
1:C:429:ILE:O	1:C:432:PHE:HB3	2.11	0.51
1:A:432:PHE:C	1:A:432:PHE:CD2	2.88	0.51
1:B:37:ARG:NH2	1:B:505:ASP:O	2.42	0.51
1:B:140:PHE:CD2	1:C:360:ASN:HA	2.46	0.51
1:C:233:PHE:CE1	1:C:255:PHE:HB2	2.45	0.51
1:A:193:TYR:O	1:A:197:GLN:HG2	2.10	0.50
1:B:294:VAL:CG1	1:C:295:ASN:HB3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1001:DA:H2''	2:E:1002:DA:C5'	2.40	0.50
1:A:70:TYR:HA	1:A:367:MET:SD	2.52	0.50
1:A:479:PHE:O	1:A:479:PHE:CD1	2.64	0.50
1:B:140:PHE:HD2	1:C:360:ASN:HA	1.76	0.50
1:C:149:ASP:OD2	1:C:274:LYS:CD	2.60	0.50
1:B:479:PHE:O	1:B:479:PHE:CG	2.64	0.50
1:C:30:ILE:HG22	1:C:65:TYR:CE1	2.46	0.50
2:F:1001:DA:H2''	2:F:1002:DA:O5'	2.11	0.50
1:A:357:TYR:HD1	1:A:357:TYR:O	1.95	0.49
1:C:346:LEU:HD21	1:C:354:VAL:HG11	1.94	0.49
1:C:326:ASN:OD1	1:C:335:LEU:HG	2.12	0.49
1:C:343:ILE:HA	1:C:346:LEU:HD11	1.95	0.49
1:C:65:TYR:HE2	1:C:405:ASP:N	2.11	0.49
1:C:122:ILE:HD12	1:C:125:TYR:HB2	1.95	0.49
1:C:300:LYS:HB3	1:C:302:PHE:CZ	2.48	0.49
1:A:343:ILE:HG23	1:A:344:ASN:N	2.28	0.48
1:C:11:TYR:CD1	1:C:93:HIS:CG	3.01	0.48
1:A:302:PHE:CD2	1:B:307:LEU:HD21	2.48	0.48
1:B:70:TYR:HB3	1:B:367:MET:HE1	1.95	0.48
1:A:1:MET:HE1	1:A:16:ARG:NH1	2.28	0.48
1:A:62:CYS:O	1:A:469:ARG:HA	2.13	0.48
1:B:140:PHE:HB2	1:C:360:ASN:OD1	2.13	0.48
1:A:42:GLU:OE1	1:A:42:GLU:N	2.44	0.48
1:B:306:ASP:OD1	1:B:306:ASP:C	2.57	0.48
1:C:326:ASN:O	1:C:330:GLY:HA2	2.13	0.48
1:C:237:ARG:HD3	1:C:242:TYR:CZ	2.48	0.48
1:C:455:VAL:HG13	1:C:474:PHE:CE1	2.49	0.48
1:A:32:PRO:HD2	1:A:412:TYR:CE1	2.48	0.48
1:C:240:ASP:CG	2:F:1006:DA:H5''	2.38	0.48
1:C:240:ASP:OD2	2:F:1006:DA:H5''	2.14	0.48
1:C:468:ASP:OD1	1:C:487:TYR:OH	2.30	0.48
1:A:55:ARG:HG2	1:A:464:GLU:OE1	2.14	0.48
1:B:65:TYR:CD2	1:B:404:SER:HB3	2.49	0.47
1:C:85:TYR:CE1	1:C:212:THR:HG21	2.49	0.47
1:C:411:LEU:O	1:C:412:TYR:C	2.56	0.47
1:B:127:ASP:OD1	1:B:127:ASP:C	2.57	0.47
1:A:307:LEU:HD11	1:C:303:THR:CG2	2.44	0.47
1:B:297:PRO:CG	1:B:310:LEU:HD21	2.44	0.47
1:B:455:VAL:HG13	1:B:474:PHE:CE1	2.50	0.47
1:A:11:TYR:CD1	1:A:93:HIS:CG	3.02	0.47
1:C:30:ILE:HG22	1:C:65:TYR:HE1	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:PHE:HB2	1:B:360:ASN:OD1	2.15	0.47
1:B:45:GLU:OE2	1:B:90:LYS:HE2	2.15	0.47
1:C:292:LEU:HD11	1:C:334:ILE:HG23	1.95	0.47
1:C:355:TYR:CG	1:C:379:VAL:HG21	2.50	0.47
1:B:121:ILE:HD13	1:B:214:SER:CB	2.44	0.47
1:B:340:SER:OG	2:E:1002:DA:H2''	2.14	0.47
1:C:65:TYR:OH	1:C:405:ASP:HA	2.15	0.47
1:C:412:TYR:C	1:C:412:TYR:CD2	2.93	0.47
1:B:11:TYR:CD1	1:B:93:HIS:CG	3.03	0.47
1:B:292:LEU:CD2	1:B:325:LEU:HD23	2.45	0.47
1:A:318:PHE:O	1:A:321:TYR:HB3	2.15	0.46
1:C:199:LYS:NZ	1:C:205:GLY:C	2.72	0.46
1:A:454:PHE:HE2	1:A:458:ILE:HD11	1.81	0.46
1:C:199:LYS:HG3	1:C:200:ARG:NH1	2.30	0.46
1:C:319:LEU:O	1:C:323:VAL:HG23	2.16	0.46
1:C:289:VAL:HG13	1:C:337:TYR:HE2	1.80	0.46
1:A:307:LEU:CD1	1:C:303:THR:OG1	2.63	0.46
1:C:233:PHE:CZ	1:C:255:PHE:HB2	2.51	0.46
1:A:12:GLU:OE2	1:A:516:CYS:HB3	2.16	0.46
1:C:7:LYS:HG3	1:C:100:ARG:NH2	2.31	0.46
1:B:55:ARG:HG3	1:B:464:GLU:OE1	2.16	0.46
1:B:347:ASP:HB3	1:B:350:THR:HG22	1.97	0.45
1:B:438:LEU:HD23	1:B:441:LEU:HD12	1.98	0.45
1:C:238:TYR:O	1:C:239:ILE:C	2.59	0.45
1:C:199:LYS:HZ1	1:C:205:GLY:C	2.24	0.45
1:A:294:VAL:CG1	1:B:295:ASN:HB3	2.47	0.45
1:B:310:LEU:HD13	1:B:310:LEU:C	2.42	0.45
1:C:29:GLU:CG	2:F:1006:DA:H61	2.30	0.45
1:C:178:THR:CG2	1:C:180:VAL:HG22	2.45	0.45
2:F:1001:DA:OP2	2:F:1001:DA:C8	2.69	0.45
1:B:310:LEU:HD12	1:B:315:VAL:HG23	1.97	0.45
2:E:1001:DA:H4'	2:E:1002:DA:OP1	2.17	0.45
1:C:121:ILE:HD13	1:C:214:SER:CB	2.47	0.45
1:C:313:SER:O	1:C:317:ASN:ND2	2.50	0.45
1:A:295:ASN:HB3	1:C:294:VAL:CG1	2.47	0.45
1:A:369:ILE:N	1:A:370:PRO:CD	2.80	0.45
1:C:92:ILE:O	1:C:96:TRP:HB2	2.17	0.45
1:A:112:PRO:HA	1:A:120:ILE:O	2.17	0.45
1:B:201:ASN:O	1:B:201:ASN:ND2	2.44	0.45
1:C:337:TYR:O	1:C:337:TYR:CD1	2.69	0.45
1:B:80:ILE:CG2	1:B:198:ALA:HB1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ILE:HG13	1:A:3:ILE:O	2.17	0.44
1:C:10:LEU:HD22	1:C:96:TRP:CD2	2.52	0.44
1:C:91:HIS:NE2	1:C:187:TRP:O	2.41	0.44
1:C:409:TRP:O	1:C:412:TYR:HB3	2.17	0.44
1:C:467:ILE:HG23	1:C:474:PHE:CD2	2.52	0.44
1:B:290:SER:O	1:B:294:VAL:HG23	2.17	0.44
1:A:115:HIS:HB2	1:A:119:ARG:O	2.18	0.44
1:A:249:HIS:NE2	1:A:253:LYS:HE3	2.33	0.44
1:B:107:ASN:OD1	1:B:229:ARG:HD3	2.17	0.44
1:C:96:TRP:CD1	1:C:100:ARG:HE	2.35	0.44
1:A:12:GLU:HG2	1:A:16:ARG:HD3	1.99	0.44
1:A:326:ASN:HA	1:A:334:ILE:HD12	1.98	0.44
1:A:343:ILE:HG13	1:A:374:VAL:HG11	2.00	0.44
1:C:49:SER:O	1:C:51:THR:HG23	2.17	0.44
1:A:290:SER:OG	1:B:320:ASP:HB3	2.18	0.44
1:A:414:CYS:HA	1:A:419:ILE:HB	1.98	0.44
1:A:467:ILE:HG23	1:A:474:PHE:CE2	2.52	0.44
1:B:479:PHE:HA	1:B:496:LYS:HE3	2.00	0.44
1:B:310:LEU:CD1	1:B:315:VAL:CG2	2.94	0.44
1:B:209:GLY:N	1:B:210:PRO:HD2	2.33	0.44
1:A:17:HIS:HB3	1:A:119:ARG:HG2	2.00	0.44
1:A:302:PHE:HD2	1:B:307:LEU:HD21	1.82	0.44
1:A:320:ASP:O	1:A:324:GLN:HG2	2.18	0.44
1:B:310:LEU:CD1	1:B:315:VAL:HG22	2.48	0.44
1:B:50:ASP:OD1	1:B:51:THR:N	2.51	0.43
1:B:78:SER:HB2	1:B:207:PRO:HB3	2.00	0.43
1:A:49:SER:O	1:A:51:THR:HG23	2.18	0.43
1:C:149:ASP:OD1	1:C:241:ASP:HA	2.17	0.43
1:C:193:TYR:HB2	1:C:196:ARG:HH21	1.82	0.43
1:A:136:LEU:HD21	1:B:357:TYR:HD2	1.83	0.43
1:C:238:TYR:O	1:C:240:ASP:N	2.52	0.43
1:B:475:TYR:CD1	1:B:475:TYR:C	2.96	0.43
1:B:294:VAL:HG11	1:C:295:ASN:HB3	2.00	0.43
1:C:179:LYS:HA	1:C:183:GLN:HB3	1.99	0.43
1:A:515:TYR:HD2	1:A:536:TYR:CD2	2.36	0.43
1:C:357:TYR:HA	1:C:360:ASN:HD22	1.83	0.43
1:A:70:TYR:HB3	1:A:333:SER:HB3	2.01	0.43
1:A:109:MET:HE3	1:A:236:ARG:HD2	2.01	0.43
1:B:11:TYR:CD2	1:B:41:PRO:HB3	2.54	0.43
1:B:136:LEU:HD22	1:C:360:ASN:HD22	1.83	0.43
1:C:133:ILE:HG22	1:C:133:ILE:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:VAL:HG21	1:A:536:TYR:HE2	1.83	0.43
1:B:70:TYR:CB	1:B:367:MET:HE1	2.49	0.43
1:B:140:PHE:CD2	1:C:360:ASN:OD1	2.72	0.43
1:B:511:LYS:NZ	1:B:536:TYR:O	2.51	0.43
1:C:19:TYR:CD1	1:C:85:TYR:CD2	3.03	0.43
1:C:379:VAL:O	1:C:381:LEU:HD22	2.18	0.43
1:A:381:LEU:HA	1:A:387:TYR:HD2	1.84	0.43
1:B:287:ASN:HB2	1:C:324:GLN:OE1	2.19	0.43
1:A:61:ASP:HB3	1:A:468:ASP:HB2	2.00	0.42
1:B:345:ASN:N	1:B:345:ASN:OD1	2.49	0.42
1:B:119:ARG:CZ	1:B:122:ILE:HD12	2.50	0.42
1:B:321:TYR:O	1:B:321:TYR:CG	2.72	0.42
1:A:337:TYR:CE1	2:D:1002:DA:H2'	2.53	0.42
1:A:398:CYS:SG	1:A:406:GLY:HA3	2.60	0.42
1:B:208:ILE:C	1:B:210:PRO:HD2	2.44	0.42
1:C:32:PRO:HD2	1:C:412:TYR:CE1	2.53	0.42
1:C:502:PHE:C	1:C:504:PRO:HD3	2.44	0.42
1:B:523:PHE:O	1:B:524:LEU:C	2.61	0.42
1:C:297:PRO:HD3	1:C:318:PHE:CD1	2.54	0.42
1:C:514:SER:O	1:C:515:TYR:C	2.63	0.42
1:A:233:PHE:CE1	1:A:255:PHE:HB2	2.54	0.42
1:B:407:MET:SD	1:B:429:ILE:HG12	2.60	0.42
1:A:65:TYR:CD2	1:A:404:SER:HB3	2.54	0.42
1:A:80:ILE:HD12	1:A:85:TYR:HD2	1.85	0.42
1:A:294:VAL:HG13	1:B:295:ASN:HB3	2.01	0.42
1:B:447:TYR:O	1:B:451:ILE:HG12	2.20	0.42
1:C:108:SER:CB	1:C:237:ARG:NH2	2.82	0.42
1:C:321:TYR:C	1:C:321:TYR:CD2	2.98	0.42
1:C:339:ILE:C	1:C:341:LEU:N	2.78	0.42
1:A:374:VAL:HG12	1:A:375:LEU:HD23	2.01	0.41
1:C:286:ASP:O	1:C:287:ASN:C	2.62	0.41
1:B:70:TYR:HA	1:B:367:MET:CE	2.50	0.41
1:B:300:LYS:HB3	1:B:302:PHE:CD2	2.47	0.41
1:C:347:ASP:OD1	1:C:347:ASP:O	2.38	0.41
1:B:491:CYS:SG	1:B:495:MET:HE2	2.60	0.41
1:C:533:PHE:O	1:C:534:ASN:C	2.63	0.41
1:A:2:VAL:HG12	1:A:3:ILE:N	2.27	0.41
1:A:285:ASN:O	1:A:286:ASP:C	2.63	0.41
1:A:286:ASP:O	1:A:287:ASN:C	2.62	0.41
1:A:475:TYR:CD1	1:A:475:TYR:C	2.99	0.41
1:A:479:PHE:CD2	1:A:496:LYS:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:HIS:CG	1:B:82:PRO:HD2	2.55	0.41
1:B:376:ILE:HG13	1:B:381:LEU:HD21	2.01	0.41
1:B:478:PHE:CD1	1:B:485:SER:HB2	2.55	0.41
1:B:515:TYR:HB2	1:B:536:TYR:HD1	1.81	0.41
1:C:176:LEU:O	1:C:177:ASN:HB2	2.21	0.41
1:A:199:LYS:O	1:A:202:GLU:HB2	2.21	0.41
1:A:319:LEU:O	1:A:323:VAL:HG23	2.21	0.41
1:A:411:LEU:O	1:A:412:TYR:C	2.63	0.41
1:A:478:PHE:CD1	1:A:492:PHE:HB3	2.56	0.41
1:B:227:ARG:HG2	1:B:262:GLU:CD	2.44	0.41
1:B:478:PHE:CE1	1:B:485:SER:HB2	2.55	0.41
1:C:432:PHE:CD2	1:C:432:PHE:C	2.99	0.41
1:A:78:SER:HB2	1:A:207:PRO:HB3	2.02	0.41
1:C:167:ILE:HD11	1:C:172:ALA:HA	2.02	0.41
1:A:295:ASN:HB3	1:C:294:VAL:HG13	2.02	0.41
1:B:479:PHE:HD2	1:B:496:LYS:HG3	1.86	0.41
1:A:11:TYR:CD2	1:A:41:PRO:HB3	2.56	0.41
1:A:366:PRO:HG3	1:A:397:MET:HE1	2.02	0.41
1:B:68:THR:HG21	1:B:366:PRO:HD2	2.02	0.41
1:A:255:PHE:O	1:A:255:PHE:CG	2.74	0.41
1:A:531:VAL:HG22	1:A:532:SER:N	2.36	0.41
1:C:96:TRP:NE1	1:C:100:ARG:HE	2.19	0.41
1:C:227:ARG:HG2	1:C:262:GLU:CD	2.45	0.41
1:B:432:PHE:C	1:B:432:PHE:CD2	2.98	0.41
1:C:402:LYS:HA	1:C:432:PHE:CZ	2.56	0.41
1:A:83:LYS:HD2	1:A:489:ASP:OD2	2.21	0.40
1:A:447:TYR:O	1:A:451:ILE:HG12	2.21	0.40
1:A:515:TYR:O	1:A:515:TYR:CD1	2.73	0.40
1:A:366:PRO:O	1:A:369:ILE:HG13	2.21	0.40
1:A:407:MET:O	1:A:408:ALA:C	2.64	0.40
1:B:519:VAL:O	1:B:519:VAL:HG22	2.20	0.40
1:B:530:ILE:HD12	1:B:530:ILE:C	2.47	0.40
1:C:299:LYS:HA	1:C:299:LYS:HD3	1.91	0.40
1:C:311:SER:HB3	1:C:314:GLU:HG3	2.03	0.40
1:C:336:LYS:HD2	1:C:371:TYR:HE2	1.85	0.40
1:A:432:PHE:C	1:A:432:PHE:HD2	2.28	0.40
1:A:479:PHE:HD2	1:A:496:LYS:HA	1.87	0.40
1:B:280:LEU:HA	1:B:281:PRO:C	2.47	0.40
1:A:136:LEU:HD21	1:B:357:TYR:CD2	2.56	0.40
1:B:445:ASP:OD1	1:B:482:LYS:NZ	2.45	0.40
1:C:297:PRO:CD	1:C:318:PHE:CD1	3.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ILE:HD12	1:A:85:TYR:CD2	2.56	0.40
1:A:351:ILE:CD1	1:A:375:LEU:HD22	2.52	0.40
1:B:533:PHE:CE2	1:B:537:MET:CG	3.04	0.40
1:C:208:ILE:C	1:C:210:PRO:HD2	2.46	0.40
1:C:302:PHE:N	1:C:308:ASN:OD1	2.51	0.40
1:C:416:LYS:HG2	1:C:416:LYS:O	2.21	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:A:177:ASN:ND2	1:A:462:ASP:O[10_655]	2.01	0.19
1:B:177:ASN:HD21	1:C:462:ASP:O[10_655]	1.54	0.06

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	534/540 (99%)	486 (91%)	47 (9%)	1 (0%)	43	71
1	B	537/540 (99%)	484 (90%)	52 (10%)	1 (0%)	43	71
1	C	538/540 (100%)	490 (91%)	47 (9%)	1 (0%)	43	71
All	All	1609/1620 (99%)	1460 (91%)	146 (9%)	3 (0%)	43	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	239	ILE
1	A	239	ILE
1	B	239	ILE

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	492/494 (100%)	492 (100%)	0	100	100
1	B	494/494 (100%)	494 (100%)	0	100	100
1	C	495/494 (100%)	495 (100%)	0	100	100
All	All	1481/1482 (100%)	1481 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	HIS
1	A	257	HIS
1	A	285	ASN
1	A	293	ASN
1	A	520	ASN
1	B	93	HIS
1	B	147	ASN
1	B	204	HIS
1	B	293	ASN
1	B	317	ASN
1	B	364	HIS
1	B	401	ASN
1	C	204	HIS
1	C	295	ASN
1	C	345	ASN
1	C	360	ASN
1	C	392	ASN
1	C	517	HIS

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	MES	A	1101	-	12,12,12	1.81	1 (8%)	15,16,16	1.47	3 (20%)
3	MES	C	1101	-	12,12,12	1.65	3 (25%)	15,16,16	1.69	2 (13%)
3	MES	B	1101	-	12,12,12	1.94	1 (8%)	15,16,16	1.30	3 (20%)

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	MES	A	1101	-	-	3/6/14/14	0/1/1/1
3	MES	C	1101	-	-	5/6/14/14	0/1/1/1
3	MES	B	1101	-	-	4/6/14/14	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1101	MES	C8-S	-6.04	1.69	1.77
3	A	1101	MES	C8-S	-5.56	1.69	1.77
3	C	1101	MES	C8-S	-4.65	1.71	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1101	MES	O2S-S	2.09	1.51	1.45
3	C	1101	MES	O1S-S	2.07	1.51	1.45

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1101	MES	O2S-S-C8	4.71	113.85	106.73
3	A	1101	MES	C5-N4-C3	3.20	115.74	108.84
3	A	1101	MES	O2S-S-C8	2.64	110.72	106.73
3	C	1101	MES	C5-N4-C3	2.47	114.17	108.84
3	A	1101	MES	O1S-S-C8	2.33	110.25	106.73
3	B	1101	MES	C5-N4-C3	2.20	113.59	108.84
3	B	1101	MES	C7-N4-C5	2.18	117.04	111.24
3	B	1101	MES	O3S-S-C8	2.00	109.92	106.00

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	MES	C7-C8-S-O1S
3	A	1101	MES	C7-C8-S-O2S
3	A	1101	MES	C7-C8-S-O3S
3	B	1101	MES	C8-C7-N4-C5
3	B	1101	MES	C7-C8-S-O1S
3	C	1101	MES	C7-C8-S-O1S
3	C	1101	MES	C7-C8-S-O3S
3	B	1101	MES	C7-C8-S-O3S
3	C	1101	MES	C8-C7-N4-C5
3	B	1101	MES	C7-C8-S-O2S
3	C	1101	MES	C7-C8-S-O2S
3	C	1101	MES	C8-C7-N4-C3

There are no ring outliers.

No monomer is involved in short contacts.

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	538/540 (99%)	0.33	17 (3%)	50 34	76, 84, 118, 138	0
1	B	539/540 (99%)	0.42	13 (2%)	59 40	83, 93, 126, 143	0
1	C	539/540 (99%)	0.50	22 (4%)	41 27	80, 96, 126, 150	0
2	D	5/6 (83%)	1.37	1 (20%)	3 2	92, 94, 97, 98	0
2	E	5/6 (83%)	1.24	1 (20%)	3 2	98, 99, 104, 104	0
2	F	6/6 (100%)	1.61	2 (33%)	1 1	90, 97, 102, 104	0
All	All	1632/1638 (99%)	0.42	56 (3%)	48 32	76, 93, 123, 150	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	522	PRO	4.2
1	A	3	ILE	4.0
1	B	381	LEU	3.9
2	F	1006	DA	3.5
1	A	73	PHE	3.3
1	C	125	TYR	3.2
1	C	3	ILE	3.2
1	A	536	TYR	3.0
2	D	1001	DA	3.0
1	A	135	GLU	3.0
1	B	1	MET	3.0
1	C	539	ILE	2.9
1	C	307	LEU	2.9
1	C	350	THR	2.9
1	C	85	TYR	2.9
1	C	123	MET	2.8
1	A	1	MET	2.7
1	C	1	MET	2.7
2	E	1001	DA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	307	LEU	2.7
1	A	58	GLN	2.6
1	C	523	PHE	2.6
1	C	2	VAL	2.6
1	B	524	LEU	2.5
1	A	540	ALA	2.5
1	B	331	GLY	2.5
1	B	358	LEU	2.5
1	A	381	LEU	2.5
1	C	124	ASN	2.4
1	C	303	THR	2.4
1	A	330	GLY	2.4
1	B	258	LEU	2.4
1	A	126	GLU	2.3
1	A	380	TYR	2.3
1	B	124	ASN	2.3
1	A	180	VAL	2.3
1	C	337	TYR	2.3
1	C	100	ARG	2.3
2	F	1001	DA	2.2
1	A	178	THR	2.2
1	C	57	LEU	2.2
1	B	56	SER	2.2
1	C	177	ASN	2.2
1	B	209	GLY	2.2
1	B	383	ASP	2.2
1	C	299	LYS	2.2
1	C	308	ASN	2.2
1	C	400	GLU	2.2
1	A	176	LEU	2.1
1	B	380	TYR	2.1
1	A	69	ARG	2.1
1	B	175	ALA	2.1
1	C	380	TYR	2.1
1	B	336	LYS	2.0
1	C	331	GLY	2.0
1	C	461	LEU	2.0

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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MES	B	1101	12/12	0.76	0.20	87,92,105,106	0
3	MES	C	1101	12/12	0.80	0.19	78,83,95,96	0
3	MES	A	1101	12/12	0.85	0.18	76,78,92,92	0

6.5 Other polymers [i](#)

There are no such residues in this entry.