



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:36 AM UTC

PDB ID : 5D8H / pdb_00005d8h
Title : CRYSTAL STRUCTURE OF THE BASE OF THE RIBOSOMAL P
STALK FROM METHANOCOCCUS JANNASCHII WITH ANTIBIOTIC
THIOSTREPTON
Authors : Gabdulkhakov, A.G.; Mitroshin, I.V.; Garber, M.B.
Deposited on : 2015-08-17
Resolution : 2.80 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

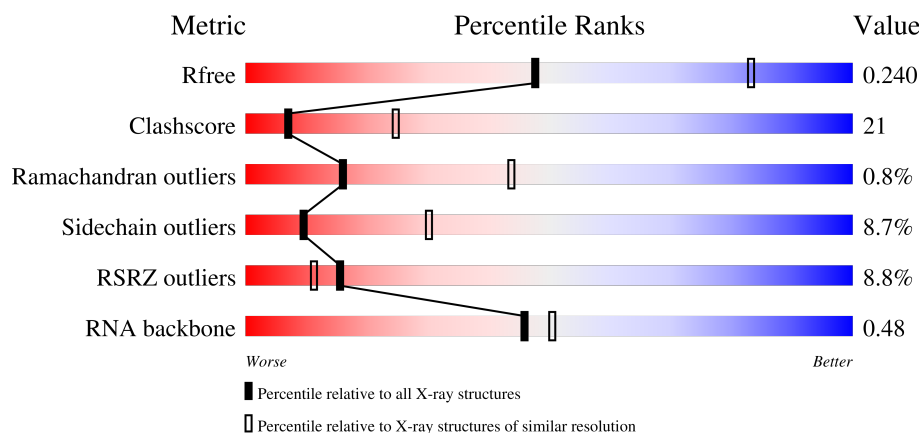
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

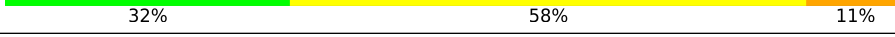
The reported resolution of this entry is 2.80 Å.

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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

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	74	 10% (upper bar), 65% (green), 31% (yellow), . (orange/red)
2	B	213	 10% (upper bar), 59% (green), 28% (yellow), 9% (orange), .. (red/grey)
3	C	161	 11% (upper bar), 50% (green), 37% (yellow), 9% (orange), .. (red/grey)
4	D	19	 32% (green), 58% (yellow), 11% (orange)

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DBU	D	8	-	X	-	-
6	NA	A	1312	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4592 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	74	Total	C	N	O	P	0	0	0
			1588	708	293	513	74			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1224	C	-	expression tag	REF 470491724

- Molecule 2 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	207	Total	C	N	O	S	Se	0	0	0
			1589	1024	268	290	1	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	9	MSE	VAL	engineered mutation	UNP P54049

- Molecule 3 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	158	Total	C	N	O	S	Se	0	0	0
			1197	762	197	232	1	5			

- Molecule 4 is a protein called THIOSTREPTON.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	19	Total	C	N	O	S	1	0	1
			114	72	19	18	5			

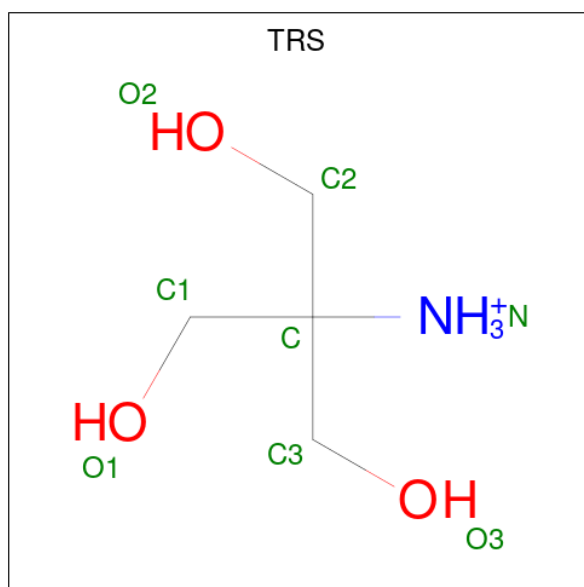
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total	Mg	0	0
			10	10		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	Na	0	0
			3	3		
6	B	1	Total	Na	0	0
			1	1		

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			8	4	1	3		
7	A	1	Total	C	N	O	0	0
			8	4	1	3		
7	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	58	Total 58	O 58	0	0
8	B	4	Total 4	O 4	0	0
8	C	3	Total 3	O 3	0	0

3 Residue-property plots [i](#)

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

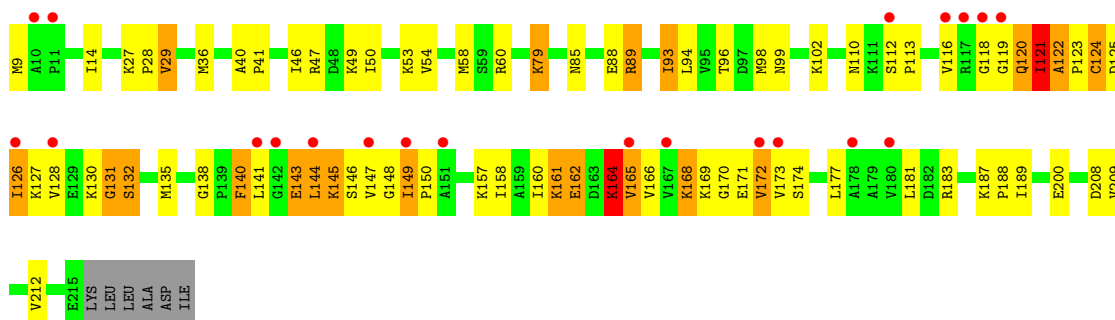
- Molecule 1: 23S ribosomal RNA

Chain A: 



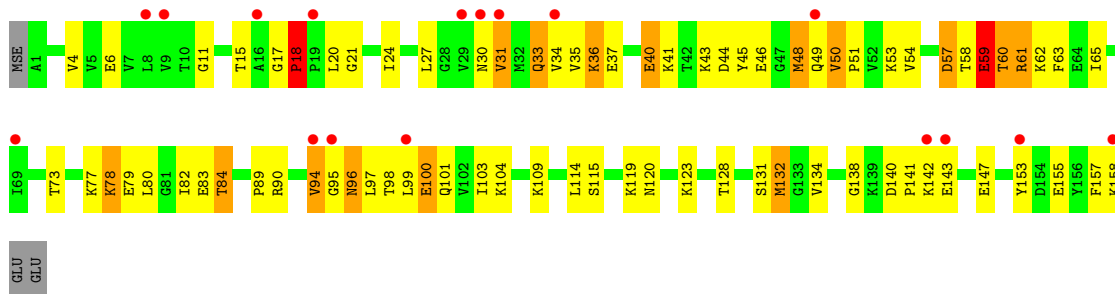
- Molecule 2: 50S ribosomal protein L10

Chain B: 

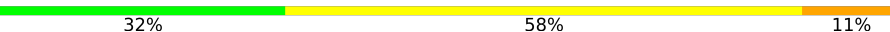


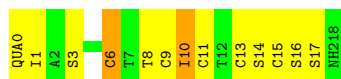
- Molecule 3: 50S ribosomal protein L11

Chain C: 



- Molecule 4: THIOSTREPTON

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	125.07Å 127.16Å 132.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.55 – 2.80 45.55 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (45.55-2.80) 99.9 (45.55-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.208 , 0.245 (Not available) , 0.240	Depositor DCC
R_{free} test set	1322 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	75.0	Xtriage
Anisotropy	0.799	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 62.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4592	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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: TRS, MG, NA, TS9, DBU, DCY, QUA, NH2, MH6, BB9, DHA

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	0.46	0/1777	0.72	0/2768
2	B	0.84	2/1607 (0.1%)	1.35	24/2161 (1.1%)
3	C	1.25	6/1208 (0.5%)	1.58	26/1624 (1.6%)
4	D	0.80	0/31	0.78	0/38
All	All	0.86	8/4623 (0.2%)	1.20	50/6591 (0.8%)

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
2	B	0	3
3	C	0	2
All	All	0	5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	44	ASP	C-N	-31.13	0.92	1.33
3	C	41	LYS	C-N	13.09	1.52	1.33
2	B	140	PHE	C-O	-7.21	1.15	1.24
2	B	165	VAL	CA-CB	6.31	1.62	1.54
3	C	59	GLU	CA-C	6.18	1.61	1.52
3	C	31	VAL	CA-C	5.37	1.59	1.52
3	C	57	ASP	CA-C	5.20	1.59	1.52
3	C	61	ARG	N-CA	5.07	1.52	1.46

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	44	ASP	CA-C-N	20.57	155.57	122.65
3	C	44	ASP	C-N-CA	20.57	155.57	122.65
3	C	59	GLU	CA-C-N	11.64	140.66	122.86
3	C	59	GLU	C-N-CA	11.64	140.66	122.86
3	C	44	ASP	O-C-N	-10.02	109.37	122.39
2	B	122	ALA	CA-C-N	9.99	129.78	119.19
2	B	122	ALA	C-N-CA	9.99	129.78	119.19
2	B	144	LEU	N-CA-C	-9.93	100.00	113.30
3	C	41	LYS	CA-C-N	-9.86	107.02	122.49
3	C	41	LYS	C-N-CA	-9.86	107.02	122.49
3	C	31	VAL	N-CA-C	9.16	119.71	110.82
2	B	172	VAL	N-CA-C	7.99	119.43	108.89
3	C	30	ASN	CB-CA-C	7.74	123.48	109.62
3	C	59	GLU	N-CA-CB	-7.71	97.47	110.49
2	B	131	GLY	N-CA-C	-6.87	101.93	111.76
3	C	132	MSE	N-CA-C	6.77	121.70	113.17
3	C	60	THR	N-CA-C	6.55	120.91	112.26
3	C	61	ARG	N-CA-C	6.28	124.17	110.80
3	C	61	ARG	CB-CA-C	-6.22	98.04	110.42
2	B	89	ARG	CB-CA-C	-6.19	109.45	116.63
2	B	119	GLY	CA-C-N	-6.15	111.71	121.86
2	B	119	GLY	C-N-CA	-6.15	111.71	121.86
2	B	121	ILE	N-CA-C	6.12	122.07	109.34
3	C	17	GLY	C-N-CD	6.01	133.82	120.60
2	B	187	LYS	CA-C-N	5.89	125.44	119.19
2	B	187	LYS	C-N-CA	5.89	125.44	119.19
2	B	148	GLY	CA-C-N	-5.74	118.70	122.60
2	B	148	GLY	C-N-CA	-5.74	118.70	122.60
2	B	79	LYS	CA-C-N	-5.73	113.08	122.54
2	B	79	LYS	C-N-CA	-5.73	113.08	122.54
3	C	59	GLU	N-CA-C	5.69	122.93	110.80
3	C	58	THR	CA-C-N	5.55	132.13	121.54
3	C	58	THR	C-N-CA	5.55	132.13	121.54
2	B	140	PHE	O-C-N	-5.46	116.45	122.07
2	B	118	GLY	N-CA-C	5.45	126.09	113.18
2	B	170	GLY	N-CA-C	5.43	122.24	114.64
2	B	162	GLU	CA-CB-CG	5.43	124.96	114.10
2	B	140	PHE	N-CA-C	-5.34	105.36	111.07
3	C	96	ASN	N-CA-C	5.33	118.08	109.40
3	C	30	ASN	CA-CB-CG	5.31	117.91	112.60
3	C	79	GLU	N-CA-C	-5.27	106.70	113.23
3	C	157	PHE	N-CA-C	5.23	117.81	109.65
3	C	61	ARG	CA-CB-CG	5.20	124.50	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	162	GLU	N-CA-C	5.20	116.97	109.07
2	B	149	ILE	CA-C-O	5.15	122.00	119.12
3	C	17	GLY	CA-C-N	-5.13	114.69	127.00
3	C	17	GLY	C-N-CA	-5.13	114.69	127.00
3	C	30	ASN	N-CA-CB	-5.04	102.63	110.04
2	B	138	GLY	CA-C-N	5.04	124.65	119.56
2	B	138	GLY	C-N-CA	5.04	124.65	119.56

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	121	ILE	Peptide
2	B	126	ILE	Peptide
2	B	164	LYS	Peptide
3	C	18	PRO	Peptide
3	C	94	VAL	Peptide

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	1588	0	802	20	0
2	B	1589	0	1720	92	0
3	C	1197	0	1255	66	0
4	D	114	0	80	9	0
5	A	10	0	0	0	0
5	C	1	0	0	0	0
6	A	3	0	0	0	0
6	B	1	0	0	0	0
7	A	16	0	24	0	0
7	B	8	0	12	2	0
8	A	58	0	0	3	0
8	B	4	0	0	0	0
8	C	3	0	0	0	0
All	All	4592	0	3893	173	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (173) 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)
4:D:0:QUA:C7	4:D:1:ILE:N	1.68	1.51
2:B:120:GLN:O	2:B:121:ILE:HG13	1.33	1.26
3:C:59:GLU:CD	3:C:60:THR:H	1.65	1.03
3:C:98:THR:HG22	3:C:101:GLN:HG3	1.43	0.98
2:B:120:GLN:C	2:B:121:ILE:HG13	1.82	0.98
2:B:127:LYS:HD2	2:B:165:VAL:HA	1.43	0.98
4:D:0:QUA:C7	4:D:1:ILE:H3	1.52	0.95
2:B:126:ILE:HD12	2:B:127:LYS:HA	1.47	0.95
1:A:1183:A:OP1	8:A:1401:HOH:O	1.89	0.89
4:D:0:QUA:C8	4:D:1:ILE:N	2.38	0.87
2:B:121:ILE:HG12	2:B:172:VAL:HA	1.57	0.84
2:B:120:GLN:O	2:B:121:ILE:CG1	2.24	0.83
2:B:145:LYS:HG3	2:B:146:SER:H	1.44	0.82
2:B:127:LYS:HE3	2:B:166:VAL:H	1.46	0.81
3:C:18:PRO:O	3:C:21:GLY:N	2.13	0.80
3:C:59:GLU:HG2	3:C:60:THR:HG23	1.64	0.79
2:B:161:LYS:O	2:B:161:LYS:HD2	1.82	0.78
3:C:34:VAL:HG13	3:C:65:ILE:HD11	1.66	0.78
2:B:121:ILE:HG22	2:B:122:ALA:H	1.48	0.77
2:B:147:VAL:HG23	2:B:149:ILE:H	1.52	0.74
3:C:98:THR:HG23	3:C:100:GLU:HG2	1.70	0.73
2:B:162:GLU:HG3	2:B:164:LYS:HB2	1.71	0.73
2:B:121:ILE:HG21	2:B:171:GLU:O	1.88	0.73
3:C:59:GLU:CG	3:C:60:THR:H	2.01	0.73
3:C:60:THR:O	3:C:61:ARG:NH2	2.23	0.71
3:C:94:VAL:H	3:C:95:GLY:HA3	1.55	0.70
1:A:1163:G:H21	2:B:36:MSE:CE	2.05	0.70
2:B:130:LYS:HG3	2:B:131:GLY:H	1.57	0.69
3:C:59:GLU:CD	3:C:60:THR:N	2.46	0.69
2:B:125:ASP:OD1	2:B:168:LYS:HG3	1.93	0.68
2:B:147:VAL:HG21	2:B:149:ILE:HD12	1.76	0.67
2:B:141:LEU:C	2:B:143:GLU:H	2.01	0.66
2:B:99:ASN:HD21	2:B:102:LYS:HG2	1.60	0.65
1:A:1196:A:O2'	1:A:1213:A:N1	2.27	0.65
2:B:123:PRO:O	2:B:169:LYS:NZ	2.30	0.64
2:B:145:LYS:HG3	2:B:146:SER:N	2.12	0.62
3:C:33:GLN:NE2	3:C:36:LYS:HE2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:MSE:HB3	2:B:14:ILE:HD11	1.82	0.62
2:B:161:LYS:HE3	2:B:162:GLU:HB2	1.82	0.62
3:C:34:VAL:HG12	3:C:34:VAL:O	2.00	0.62
3:C:140:ASP:OD1	3:C:141:PRO:HD2	2.00	0.61
2:B:85:ASN:ND2	7:B:302:TRS:O2	2.32	0.61
2:B:122:ALA:HB1	2:B:124:CYS:O	1.99	0.61
1:A:1223:G:O6	8:A:1402:HOH:O	2.12	0.60
2:B:121:ILE:HG22	2:B:122:ALA:N	2.14	0.60
3:C:95:GLY:HA2	3:C:134:VAL:HG22	1.84	0.59
3:C:48:MSE:SE	3:C:78:LYS:HE2	2.53	0.59
2:B:116:VAL:HG23	2:B:188:PRO:HG2	1.85	0.58
2:B:127:LYS:CD	2:B:165:VAL:HA	2.27	0.58
3:C:6:GLU:HB2	3:C:53:LYS:HG3	1.85	0.58
2:B:147:VAL:HG23	2:B:149:ILE:N	2.19	0.57
2:B:140:PHE:CZ	2:B:183:ARG:HG2	2.39	0.57
2:B:120:GLN:C	2:B:121:ILE:CG1	2.69	0.57
1:A:1168:G:H1'	3:C:114:LEU:HG	1.87	0.57
2:B:143:GLU:O	2:B:143:GLU:HG3	2.05	0.57
2:B:125:ASP:OD1	2:B:168:LYS:HA	2.05	0.56
2:B:130:LYS:HD3	2:B:161:LYS:C	2.30	0.56
3:C:59:GLU:OE1	3:C:60:THR:N	2.38	0.56
2:B:140:PHE:CE1	2:B:183:ARG:HG2	2.39	0.56
1:A:1182:C:N3	1:A:1202:C:N4	2.52	0.56
2:B:145:LYS:HE2	2:B:146:SER:OG	2.05	0.56
3:C:31:VAL:O	3:C:35:VAL:HG23	2.05	0.56
3:C:59:GLU:OE1	3:C:59:GLU:N	2.39	0.55
2:B:130:LYS:HB2	2:B:160:ILE:HG13	1.87	0.55
3:C:34:VAL:CG1	3:C:65:ILE:HD11	2.36	0.55
2:B:29:VAL:HG12	2:B:200:GLU:HG3	1.89	0.54
3:C:57:ASP:HB2	3:C:59:GLU:CD	2.33	0.54
3:C:73:THR:O	3:C:77:LYS:HG3	2.07	0.54
1:A:1173:G:H4'	3:C:132:MSE:HG2	1.89	0.54
2:B:140:PHE:O	2:B:143:GLU:HB3	2.07	0.54
1:A:1216:C:H4'	2:B:58:MSE:HE3	1.89	0.54
3:C:34:VAL:HG11	3:C:54:VAL:HG11	1.90	0.54
3:C:140:ASP:OD1	3:C:141:PRO:CD	2.56	0.54
1:A:1163:G:H21	2:B:36:MSE:HE3	1.71	0.54
2:B:130:LYS:CG	2:B:131:GLY:N	2.71	0.54
2:B:132:SER:HB3	2:B:157:LYS:CE	2.38	0.53
1:A:1156:A:C5	2:B:9:MSE:SE	3.11	0.53
2:B:121:ILE:HG23	2:B:173:VAL:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:LYS:HG3	2:B:131:GLY:N	2.22	0.53
4:D:0:QUA:HC8	4:D:1:ILE:N	2.23	0.53
1:A:1164:G:O6	8:A:1403:HOH:O	2.19	0.53
3:C:57:ASP:OD1	3:C:62:LYS:N	2.42	0.53
3:C:60:THR:C	3:C:61:ARG:HG3	2.34	0.52
3:C:4:VAL:HG11	3:C:53:LYS:HE3	1.91	0.52
3:C:96:ASN:HD21	3:C:138:GLY:HA2	1.73	0.52
1:A:1170:U:OP2	3:C:109:LYS:NZ	2.43	0.52
3:C:80:LEU:HD21	3:C:97:LEU:HG	1.91	0.51
4:D:0:QUA:O16	4:D:10:TS9:HD13	2.11	0.51
3:C:94:VAL:N	3:C:95:GLY:HA3	2.20	0.51
1:A:1194:A:OP1	2:B:47:ARG:NH2	2.43	0.51
2:B:53:LYS:O	2:B:96:THR:OG1	2.28	0.50
3:C:57:ASP:OD2	3:C:62:LYS:HB2	2.11	0.50
2:B:135:MSE:HE3	2:B:140:PHE:CE2	2.45	0.50
3:C:99:LEU:HD22	3:C:153:TYR:CD2	2.46	0.50
3:C:128:THR:O	3:C:131:SER:OG	2.28	0.50
3:C:153:TYR:O	3:C:155:GLU:N	2.40	0.50
1:A:1157:G:OP1	2:B:60:ARG:NH1	2.44	0.49
3:C:119:LYS:O	3:C:123:LYS:HG3	2.13	0.49
2:B:177:LEU:O	2:B:181:LEU:HG	2.12	0.49
3:C:24:ILE:O	3:C:27:LEU:N	2.25	0.48
4:D:0:QUA:HC8	4:D:1:ILE:CA	2.42	0.48
2:B:147:VAL:CG2	2:B:149:ILE:H	2.23	0.48
4:D:0:QUA:C7	4:D:1:ILE:CA	2.81	0.48
1:A:1166:G:H5''	1:A:1167:A:H5'	1.95	0.47
2:B:49:LYS:NZ	2:B:110:ASN:OD1	2.28	0.47
3:C:147:GLU:OE1	3:C:153:TYR:HE1	1.96	0.47
2:B:127:LYS:HZ1	2:B:128:VAL:HG22	1.80	0.47
2:B:150:PRO:HB2	2:B:161:LYS:HB3	1.96	0.47
3:C:141:PRO:C	3:C:143:GLU:N	2.72	0.47
3:C:33:GLN:HE22	3:C:36:LYS:HE2	1.78	0.47
1:A:1164:G:H1'	2:B:36:MSE:HE2	1.96	0.46
1:A:1156:A:C4	2:B:9:MSE:SE	3.19	0.46
2:B:49:LYS:HE3	2:B:49:LYS:HB3	1.53	0.46
2:B:144:LEU:HD13	2:B:160:ILE:HG22	1.97	0.46
2:B:162:GLU:CG	2:B:164:LYS:HB2	2.44	0.46
2:B:93:ILE:HA	2:B:93:ILE:HD13	1.77	0.46
2:B:121:ILE:CG2	2:B:122:ALA:H	2.17	0.45
2:B:140:PHE:HB3	2:B:158:ILE:CD1	2.46	0.45
3:C:11:GLY:O	3:C:46:GLU:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:98:THR:O	3:C:101:GLN:HB2	2.16	0.45
3:C:99:LEU:O	3:C:103:ILE:HG13	2.17	0.45
1:A:1180:A:C8	1:A:1207:C:O5'	2.70	0.45
2:B:125:ASP:CG	2:B:168:LYS:HZ2	2.23	0.44
2:B:140:PHE:O	2:B:141:LEU:C	2.59	0.44
4:D:0:QUA:O15	4:D:6:BB9:HB	2.16	0.44
3:C:49:GLN:N	3:C:49:GLN:OE1	2.50	0.44
3:C:115:SER:HB3	3:C:120:ASN:HB3	2.00	0.44
3:C:57:ASP:CG	3:C:59:GLU:OE2	2.61	0.44
3:C:100:GLU:O	3:C:104:LYS:HG2	2.18	0.44
1:A:1186:C:HI'	3:C:89:PRO:HD2	1.98	0.44
2:B:46:ILE:O	2:B:50:ILE:HG12	2.17	0.44
3:C:37:GLU:OE1	3:C:65:ILE:HG13	2.17	0.44
3:C:45:TYR:CD2	3:C:50:VAL:HG21	2.53	0.44
2:B:96:THR:HG23	2:B:98:MSE:H	1.83	0.43
2:B:144:LEU:HB3	2:B:149:ILE:O	2.18	0.43
3:C:18:PRO:HD2	4:D:9:DCY:HB2	1.99	0.43
2:B:145:LYS:CG	2:B:146:SER:N	2.81	0.43
2:B:161:LYS:HD2	2:B:161:LYS:C	2.43	0.43
2:B:174:SER:HB3	2:B:177:LEU:HB3	2.01	0.43
3:C:90:ARG:NH2	3:C:142:LYS:HG3	2.34	0.43
2:B:132:SER:HB3	2:B:157:LYS:HE2	2.01	0.43
3:C:45:TYR:HA	3:C:48:MSE:HE2	1.99	0.43
2:B:85:ASN:HD21	7:B:302:TRS:C2	2.31	0.43
3:C:37:GLU:HA	3:C:40:GLU:HB3	2.00	0.43
2:B:98:MSE:HE2	2:B:102:LYS:HB3	2.02	0.42
1:A:1174:C:H5''	3:C:84:THR:HG23	2.01	0.42
2:B:88:GLU:HG2	2:B:89:ARG:N	2.34	0.42
3:C:98:THR:CG2	3:C:100:GLU:HG2	2.47	0.42
3:C:20:LEU:O	3:C:24:ILE:HG12	2.20	0.42
2:B:127:LYS:HA	2:B:127:LYS:HE2	2.02	0.41
2:B:141:LEU:C	2:B:143:GLU:N	2.72	0.41
2:B:162:GLU:HG3	2:B:164:LYS:CB	2.47	0.41
3:C:50:VAL:HA	3:C:51:PRO:HD3	1.91	0.41
3:C:82:ILE:HG22	3:C:83:GLU:H	1.85	0.41
2:B:143:GLU:HA	2:B:145:LYS:NZ	2.35	0.41
3:C:82:ILE:HG22	3:C:83:GLU:N	2.35	0.41
2:B:127:LYS:NZ	2:B:166:VAL:HG23	2.35	0.41
2:B:27:LYS:HB3	2:B:28:PRO:HD2	2.02	0.41
2:B:122:ALA:HA	2:B:123:PRO:HD2	1.65	0.41
2:B:144:LEU:HB3	2:B:149:ILE:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:PRO:HG2	2:B:161:LYS:HG3	2.02	0.41
2:B:40:ALA:HB3	2:B:41:PRO:HD3	2.03	0.41
2:B:113:PRO:HA	2:B:189:ILE:O	2.21	0.41
2:B:121:ILE:CG1	2:B:172:VAL:HA	2.39	0.41
3:C:97:LEU:HD12	3:C:134:VAL:HG11	2.01	0.41
2:B:9:MSE:N	2:B:9:MSE:HE2	2.36	0.41
3:C:59:GLU:CG	3:C:60:THR:N	2.79	0.40
3:C:153:TYR:C	3:C:155:GLU:H	2.26	0.40
2:B:94:LEU:C	2:B:94:LEU:HD23	2.45	0.40
2:B:29:VAL:HG22	2:B:96:THR:O	2.21	0.40
2:B:140:PHE:HB3	2:B:158:ILE:HD13	2.04	0.40
2:B:209:VAL:O	2:B:212:VAL:HG22	2.22	0.40
3:C:34:VAL:HG22	3:C:63:PHE:CG	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	205/213 (96%)	193 (94%)	11 (5%)	1 (0%)	24	55
3	C	156/161 (97%)	146 (94%)	8 (5%)	2 (1%)	9	31
4	D	5/19 (26%)	4 (80%)	1 (20%)	0	100	100
All	All	366/393 (93%)	343 (94%)	20 (6%)	3 (1%)	16	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	121	ILE
3	C	59	GLU
3	C	18	PRO

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	
2	B	175/174 (101%)	160 (91%)	15 (9%)	10	31
3	C	132/129 (102%)	120 (91%)	12 (9%)	9	28
4	D	3/4 (75%)	3 (100%)	0	100	100
All	All	310/307 (101%)	283 (91%)	27 (9%)	9	30

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	29	VAL
2	B	54	VAL
2	B	79	LYS
2	B	93	ILE
2	B	112	SER
2	B	120	GLN
2	B	121	ILE
2	B	124	CYS
2	B	132	SER
2	B	143	GLU
2	B	145	LYS
2	B	161	LYS
2	B	164	LYS
2	B	168	LYS
2	B	208	ASP
3	C	15	THR
3	C	33	GLN
3	C	36	LYS
3	C	40	GLU
3	C	43	LYS
3	C	48	MSE
3	C	50	VAL
3	C	59	GLU
3	C	78	LYS
3	C	84	THR
3	C	100	GLU

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Mol	Chain	Res	Type
3	C	158	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	85	ASN
2	B	99	ASN
2	B	120	GLN
3	C	30	ASN
3	C	33	GLN
3	C	96	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	73/74 (98%)	8 (10%)	1 (1%)

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	1170	U
1	A	1179	A
1	A	1180	A
1	A	1193	U
1	A	1198	A
1	A	1207	C
1	A	1221	A
1	A	1222	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1180	A

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

11 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
4	DHA	D	3	4	3,4,5	1.11	0	2,4,6	2.78	1 (50%)
4	DBU	D	8	4	3,4,6	1.23	1 (33%)	3,4,7	2.92	3 (100%)
4	TS9	D	10	4	7,8,10	0.45	0	6,12,15	1.77	2 (33%)
4	DHA	D	17	4	3,4,5	1.07	0	2,4,6	3.10	2 (100%)
4	MH6	D	14	4	3,3,6	1.95	1 (33%)	1,3,7	1.80	0
4	BB9	D	6	4	2,5,6	1.82	1 (50%)	1,5,7	4.75	1 (100%)
4	BB9	D	13	4	2,4,6	1.02	0	3,4,7	4.84	2 (66%)
4	BB9	D	11	4	2,5,6	1.18	0	1,5,7	3.88	1 (100%)
4	BB9	D	15	4	2,5,6	1.66	0	1,5,7	4.41	1 (100%)
4	DHA	D	16	4	3,4,5	1.60	1 (33%)	2,4,6	2.48	2 (100%)

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
4	DHA	D	3	4	-	0/0/2/4	-
4	DBU	D	8	4	-	0/1/2/6	-
4	TS9	D	10	4	-	0/9/12/16	-
4	DHA	D	17	4	-	0/0/2/4	-
4	BB9	D	6	4	-	0/0/4/6	-
4	BB9	D	13	4	-	0/0/2/6	-
4	BB9	D	11	4	-	0/0/4/6	-
4	BB9	D	15	4	-	0/0/4/6	-
4	DHA	D	16	4	-	0/0/2/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	14	MH6	C-CA	-3.23	1.45	1.49
4	D	16	DHA	O-C	2.10	1.26	1.22
4	D	6	BB9	O-C	2.09	1.26	1.22
4	D	8	DBU	C-CA	-2.01	1.44	1.49

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	13	BB9	C-CA-N	7.43	124.56	116.44
4	D	6	BB9	O-C-CA	-4.75	119.43	125.39
4	D	15	BB9	O-C-CA	-4.41	119.87	125.39
4	D	3	DHA	O-C-CA	-3.93	118.16	125.53
4	D	11	BB9	O-C-CA	-3.88	120.53	125.39
4	D	13	BB9	CB-CA-N	-3.63	111.36	122.53
4	D	17	DHA	O-C-CA	-3.54	118.89	125.53
4	D	8	DBU	C-CA-N	3.01	119.73	116.44
4	D	10	TS9	C-CA-N	2.98	115.35	109.33
4	D	8	DBU	C-CA-CB	-2.89	115.61	121.25
4	D	8	DBU	CB-CA-N	2.85	124.55	122.88
4	D	16	DHA	O-C-CA	-2.81	120.26	125.53
4	D	17	DHA	CB-CA-N	-2.58	119.54	125.76
4	D	10	TS9	OD2-CG1-CD1	2.11	113.76	108.92
4	D	16	DHA	CB-CA-N	-2.10	120.71	125.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	10	TS9	1	0
4	D	6	BB9	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 15 are monoatomic - leaving 3 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
7	TRS	A	1314	-	7,7,7	0.34	0	9,9,9	0.34	0
7	TRS	A	1315	-	7,7,7	0.53	0	9,9,9	1.14	0
7	TRS	B	302	-	7,7,7	0.32	0	9,9,9	0.76	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	TRS	A	1314	-	-	6/9/9/9	-
7	TRS	A	1315	-	-	4/9/9/9	-
7	TRS	B	302	-	-	2/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1314	TRS	C2-C-C1-O1
7	A	1315	TRS	N-C-C2-O2
7	A	1314	TRS	C3-C-C1-O1
7	A	1314	TRS	N-C-C1-O1
7	A	1315	TRS	C1-C-C2-O2
7	A	1314	TRS	C1-C-C3-O3
7	A	1314	TRS	C2-C-C3-O3
7	A	1314	TRS	N-C-C3-O3
7	A	1315	TRS	C3-C-C2-O2
7	B	302	TRS	C1-C-C3-O3
7	A	1315	TRS	N-C-C3-O3
7	B	302	TRS	N-C-C3-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	302	TRS	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	D	2
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	0:QUA	C7	1:ILE	N	1.68
1	D	11:BB9	C	12:THR	N	1.17
1	C	44:ASP	C	45:TYR	N	0.91

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	74/74 (100%)	-0.34	0 100 100	62, 72, 84, 93	0
2	B	201/213 (94%)	0.57	21 (10%) 11 8	63, 95, 170, 178	0
3	C	153/161 (95%)	0.92	17 (11%) 10 7	24, 112, 164, 177	0
4	D	6/19 (31%)	0.15	0 100 100	76, 77, 84, 87	0
All	All	434/467 (92%)	0.53	38 (8%) 15 11	24, 98, 168, 178	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	143	GLU	6.9
2	B	178	ALA	4.8
3	C	34	VAL	4.4
2	B	10	ALA	4.1
2	B	117	ARG	3.7
2	B	180	VAL	3.4
3	C	19	PRO	3.3
3	C	49	GLN	3.2
3	C	95	GLY	3.1
2	B	167	VAL	2.9
2	B	149	ILE	2.9
3	C	31	VAL	2.9
2	B	118	GLY	2.8
2	B	126	ILE	2.8
2	B	151	ALA	2.8
3	C	99	LEU	2.8
3	C	30	ASN	2.7
3	C	16	ALA	2.7
2	B	116	VAL	2.6
2	B	165	VAL	2.6
2	B	112	SER	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	8	LEU	2.4
3	C	153	TYR	2.4
2	B	119	GLY	2.4
2	B	147	VAL	2.4
3	C	69	ILE	2.3
3	C	158	LYS	2.3
2	B	128	VAL	2.2
2	B	172	VAL	2.2
3	C	94	VAL	2.1
2	B	144	LEU	2.1
2	B	11	PRO	2.0
3	C	142	LYS	2.0
2	B	173	VAL	2.0
3	C	29	VAL	2.0
2	B	141	LEU	2.0
2	B	142	GLY	2.0
3	C	9	VAL	2.0

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

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(Å ²)	Q<0.9
4	DHA	D	16	5/6	0.28	0.18	121,122,130,130	0
4	DHA	D	17	5/6	0.40	0.18	122,127,128,129	1
4	MH6	D	14	4/7	0.84	0.09	80,80,80,87	0
4	BB9	D	15	6/7	0.84	0.09	97,107,112,114	0
4	TS9	D	10	9/11	0.90	0.12	74,85,90,92	0
4	DCY	D	9	6/7	0.91	0.11	85,88,95,101	0
4	DHA	D	3	5/6	0.91	0.12	77,79,81,83	0
4	BB9	D	6	6/7	0.91	0.12	63,68,71,77	0
4	BB9	D	11	6/7	0.95	0.10	85,86,89,97	0
4	BB9	D	13	5/7	0.95	0.10	76,76,83,83	0
4	DBU	D	8	5/7	0.97	0.14	79,81,83,83	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
6	NA	A	1312	1/1	0.58	0.56	114,114,114,114	0
6	NA	A	1313	1/1	0.74	0.31	84,84,84,84	0
6	NA	A	1311	1/1	0.79	0.37	87,87,87,87	0
7	TRS	B	302	8/8	0.79	0.11	83,86,93,100	0
7	TRS	A	1315	8/8	0.85	0.32	75,82,90,91	0
5	MG	A	1308	1/1	0.88	0.10	109,109,109,109	0
7	TRS	A	1314	8/8	0.88	0.21	87,91,95,95	0
6	NA	B	301	1/1	0.89	0.34	86,86,86,86	0
5	MG	A	1310	1/1	0.90	0.39	125,125,125,125	0
5	MG	A	1309	1/1	0.90	0.09	82,82,82,82	0
5	MG	A	1303	1/1	0.91	0.22	68,68,68,68	0
5	MG	A	1307	1/1	0.95	0.14	77,77,77,77	0
5	MG	C	201	1/1	0.96	0.06	92,92,92,92	0
5	MG	A	1302	1/1	0.96	0.06	71,71,71,71	0
5	MG	A	1305	1/1	0.98	0.07	64,64,64,64	0
5	MG	A	1306	1/1	0.98	0.07	95,95,95,95	0
5	MG	A	1301	1/1	0.99	0.03	60,60,60,60	0
5	MG	A	1304	1/1	0.99	0.04	65,65,65,65	0

6.5 Other polymers

There are no such residues in this entry.