



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 01:44 am BST

PDB ID : 6F2P
Title : Structure of Paenibacillus xanthan lyase to 2.6 Å resolution
Authors : Lo Leggio, L.; Kadziola, A.
Deposited on : 2017-11-27
Resolution : 2.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

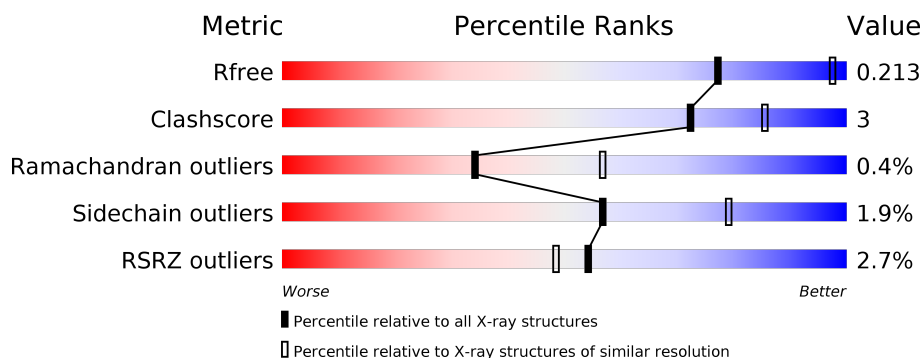
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1040	<div> <div>3%</div> <div>92%</div> <div>8%</div> </div>

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
5	MRD	A	1140	-	-	-	X
6	MPD	A	1129	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8747 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Paenibacillus xanthan lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1040	Total	C	N	O	S	0	3	0
			7989	5019	1350	1591	29			

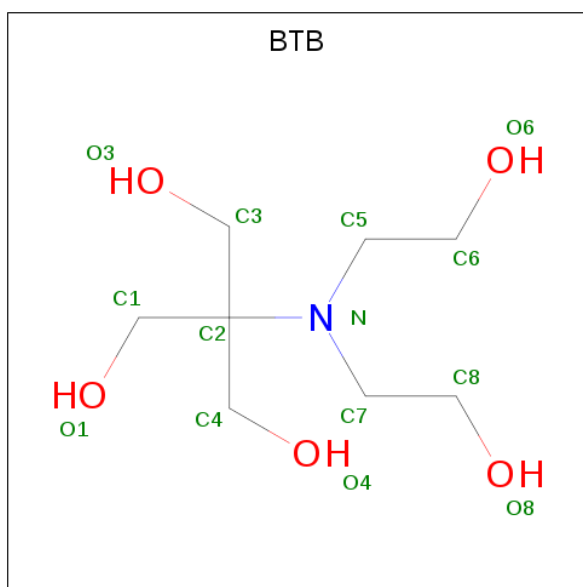
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total	Ca	0	0
			9	9		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

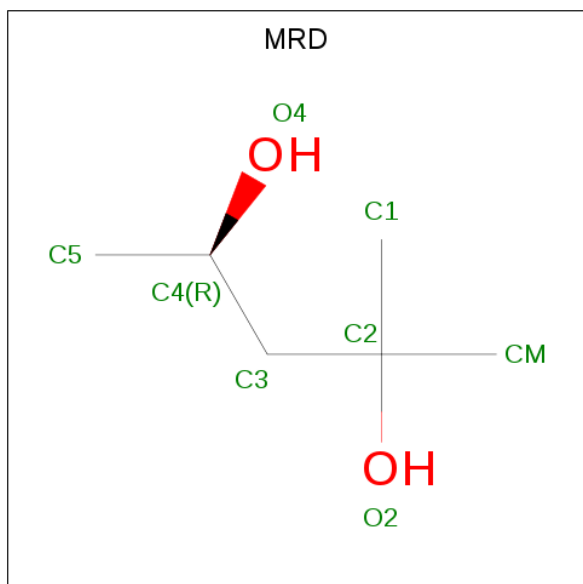
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Cl	0	0
			4	4		

- Molecule 4 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C₈H₁₉NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		
6	A	1	Total	C	O	0	0
			8	6	2		
6	A	1	Total	C	O	0	0
			8	6	2		
6	A	1	Total	C	O	0	0
			8	6	2		
6	A	1	Total	C	O	0	0
			8	6	2		
6	A	1	Total	C	O	0	0
			8	6	2		
6	A	1	Total	C	O	0	0
			8	6	2		
6	A	1	Total	C	O	0	0
			8	6	2		

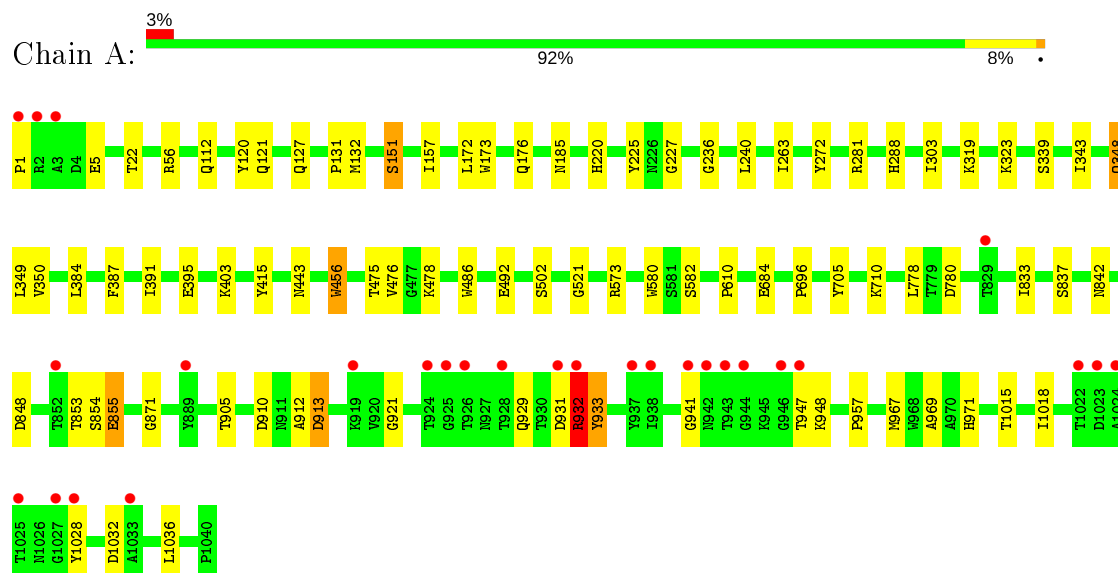
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	515	Total	O	0	0
			515	515		

3 Residue-property plots [i](#)

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

- Molecule 1: Paenibacillus xanthan lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.61Å 100.61Å 324.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.05 – 2.60 48.05 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.05-2.60) 98.7 (48.05-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.165 , 0.213 0.166 , 0.213	Depositor DCC
R_{free} test set	2000 reflections (3.86%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.770	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8747	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 2.57% 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: MRD, MPD, BTB, CA, CL

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	0.32	0/8167	0.52	0/11118

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7989	0	7709	47	0
2	A	9	0	0	0	0
3	A	4	0	0	0	0
4	A	14	0	19	0	0
5	A	136	0	238	10	0
6	A	80	0	140	5	0
7	A	515	0	0	3	0
All	All	8747	0	8106	56	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 3.

All (56) 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:A:185:ASN:HD21	5:A:1119:MRD:H3C2	1.43	0.83
1:A:151:SER:OG	5:A:1119:MRD:H1C2	1.95	0.66
1:A:151:SER:HB2	5:A:1119:MRD:HMC2	1.80	0.61
1:A:172:LEU:HD21	1:A:236:GLY:HA3	1.83	0.61
1:A:931:ASP:HB3	1:A:969:ALA:HA	1.84	0.59
1:A:912:ALA:HA	1:A:913:ASP:O	2.05	0.57
1:A:853:THR:OG1	1:A:855:GLU:OE2	2.18	0.56
6:A:1122:MPD:O4	6:A:1122:MPD:O2	2.19	0.56
1:A:1:PRO:H3	1:A:5:GLU:H	1.54	0.55
1:A:227:GLY:HA3	1:A:281:ARG:HG2	1.89	0.54
1:A:288:HIS:HB3	1:A:580:TRP:CG	2.43	0.54
1:A:837:SER:HB3	1:A:842:ASN:HD22	1.71	0.53
1:A:220:HIS:ND1	1:A:395:GLU:OE1	2.31	0.52
1:A:323:LYS:HE3	1:A:350:VAL:HA	1.91	0.51
1:A:705:TYR:CE1	1:A:871:GLY:HA2	2.45	0.51
1:A:931:ASP:CB	1:A:969:ALA:HA	2.41	0.51
1:A:443:ASN:O	7:A:1201:HOH:O	2.20	0.49
1:A:967:MET:O	1:A:1032:ASP:HB3	2.13	0.49
1:A:403:LYS:HD2	1:A:582:SER:HB3	1.95	0.47
1:A:112:GLN:NE2	1:A:120:TYR:OH	2.47	0.47
1:A:475:THR:HB	1:A:478:LYS:HB2	1.97	0.47
1:A:272:TYR:CD2	1:A:415:TYR:HB3	2.50	0.47
1:A:131:PRO:HB3	1:A:157:ILE:HG23	1.97	0.47
5:A:1120:MRD:H1C1	5:A:1120:MRD:H4	1.66	0.47
1:A:502:SER:HB3	1:A:610:PRO:HD2	1.97	0.47
1:A:932[A]:ARG:HB3	1:A:967:MET:SD	2.55	0.47
1:A:349:LEU:HB2	6:A:1127:MPD:HM3	1.98	0.45
1:A:127:GLN:NE2	7:A:1224:HOH:O	2.50	0.45
5:A:1116:MRD:H4	5:A:1116:MRD:HMC1	1.77	0.44
1:A:833:ILE:HG12	1:A:848:ASP:HA	2.00	0.44
1:A:921:GLY:HA3	1:A:948:LYS:HD3	1.99	0.44
1:A:778:LEU:HD12	1:A:780:ASP:O	2.18	0.44
1:A:173:TRP:HD1	1:A:176:GLN:NE2	2.16	0.44
1:A:339:SER:O	1:A:343:ILE:HG13	2.17	0.43
1:A:910:ASP:O	1:A:913:ASP:HB2	2.19	0.43
1:A:521:GLY:O	1:A:573:ARG:HD3	2.18	0.43
1:A:56:ARG:HB3	7:A:1419:HOH:O	2.18	0.43
5:A:1121:MRD:H1C1	5:A:1121:MRD:H4	1.88	0.43
1:A:240:LEU:HA	1:A:240:LEU:HD23	1.76	0.43
1:A:905:THR:HA	1:A:957:PRO:HG2	2.01	0.43
5:A:1141:MRD:O2	5:A:1141:MRD:O4	2.18	0.43
1:A:387:PHE:HB2	1:A:391:ILE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:GLN:NE2	6:A:1127:MPD:H11	2.34	0.42
1:A:384:LEU:HD11	1:A:486:TRP:CE2	2.53	0.42
5:A:1132:MRD:HMC3	5:A:1132:MRD:H4	1.77	0.42
1:A:1018:ILE:HD11	1:A:1036:LEU:HD11	2.02	0.42
5:A:1115:MRD:HMC3	5:A:1115:MRD:H4	1.83	0.41
1:A:288:HIS:HB3	1:A:580:TRP:CD2	2.56	0.41
5:A:1119:MRD:H1C3	5:A:1119:MRD:H4	1.81	0.41
1:A:456:TRP:CH2	1:A:696:PRO:HG2	2.56	0.41
1:A:684:GLU:OE2	1:A:710:LYS:HE2	2.21	0.41
1:A:319:LYS:HB3	1:A:349:LEU:HD11	2.02	0.41
1:A:941:GLY:HA2	1:A:1028:TYR:HE1	1.85	0.40
1:A:263:ILE:HD12	1:A:303:ILE:HG12	2.02	0.40
6:A:1136:MPD:HM3	6:A:1136:MPD:H4	1.88	0.40
1:A:348:GLN:HE22	6:A:1127:MPD:H11	1.85	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	
1	A	1041/1040 (100%)	992 (95%)	44 (4%)	5 (0%)	29	52

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	933	TYR
1	A	932[A]	ARG
1	A	932[B]	ARG
1	A	913	ASP
1	A	971	HIS

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	864/861 (100%)	847 (98%)	17 (2%)	55 78

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	121	GLN
1	A	132	MET
1	A	151	SER
1	A	225	TYR
1	A	348	GLN
1	A	456	TRP
1	A	476	VAL
1	A	492	GLU
1	A	854	SER
1	A	855	GLU
1	A	929	GLN
1	A	932[A]	ARG
1	A	932[B]	ARG
1	A	933	TYR
1	A	947	THR
1	A	1015	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	112	GLN
1	A	127	GLN
1	A	176	GLN
1	A	348	GLN
1	A	612	ASN
1	A	842	ASN
1	A	929	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 41 ligands modelled in this entry, 13 are monoatomic - leaving 28 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	$\# Z > 2$
5	MRD	A	1115	-	7,7,7	0.59	0	9,10,10	0.24	0
5	MRD	A	1140	-	7,7,7	0.49	0	9,10,10	0.29	0
5	MRD	A	1121	-	7,7,7	0.54	0	9,10,10	0.32	0
6	MPD	A	1137	-	7,7,7	0.52	0	9,10,10	0.48	0
6	MPD	A	1129	-	7,7,7	0.52	0	9,10,10	0.43	0
5	MRD	A	1128	-	7,7,7	0.65	0	9,10,10	0.41	0
5	MRD	A	1126	-	7,7,7	0.52	0	9,10,10	0.43	0
5	MRD	A	1141	-	7,7,7	0.53	0	9,10,10	0.55	0
5	MRD	A	1120	-	7,7,7	0.52	0	9,10,10	0.24	0
5	MRD	A	1130	-	7,7,7	0.60	0	9,10,10	0.34	0
5	MRD	A	1118	-	7,7,7	0.49	0	9,10,10	0.32	0
6	MPD	A	1125	-	7,7,7	0.49	0	9,10,10	0.39	0
5	MRD	A	1132	-	7,7,7	0.63	0	9,10,10	0.42	0
6	MPD	A	1127	-	7,7,7	0.56	0	9,10,10	0.35	0
5	MRD	A	1116	-	7,7,7	0.58	0	9,10,10	0.35	0
6	MPD	A	1124	-	7,7,7	0.59	0	9,10,10	0.36	0
4	BTB	A	1114	-	13,13,13	0.62	0	7,16,16	0.69	0
5	MRD	A	1119	-	7,7,7	0.54	0	9,10,10	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MPD	A	1122	-	7,7,7	0.55	0	9,10,10	0.37	0
6	MPD	A	1139	-	7,7,7	0.52	0	9,10,10	0.25	0
5	MRD	A	1131	-	7,7,7	0.52	0	9,10,10	0.32	0
5	MRD	A	1133	-	7,7,7	0.48	0	9,10,10	0.49	0
5	MRD	A	1134	-	7,7,7	0.43	0	9,10,10	0.65	0
5	MRD	A	1117	-	7,7,7	0.55	0	9,10,10	0.46	0
5	MRD	A	1123	-	7,7,7	0.57	0	9,10,10	0.33	0
6	MPD	A	1138	-	7,7,7	0.48	0	9,10,10	0.41	0
6	MPD	A	1136	-	7,7,7	0.56	0	9,10,10	0.29	0
6	MPD	A	1135	-	7,7,7	0.51	0	9,10,10	0.35	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
5	MRD	A	1115	-	-	0/5/5/5	-
5	MRD	A	1140	-	-	1/5/5/5	-
5	MRD	A	1121	-	-	2/5/5/5	-
6	MPD	A	1137	-	-	4/5/5/5	-
6	MPD	A	1129	-	-	1/5/5/5	-
5	MRD	A	1128	-	-	1/5/5/5	-
5	MRD	A	1126	-	-	5/5/5/5	-
5	MRD	A	1141	-	-	3/5/5/5	-
5	MRD	A	1120	-	-	4/5/5/5	-
5	MRD	A	1130	-	-	1/5/5/5	-
5	MRD	A	1118	-	-	0/5/5/5	-
6	MPD	A	1125	-	-	0/5/5/5	-
5	MRD	A	1132	-	-	1/5/5/5	-
6	MPD	A	1127	-	-	2/5/5/5	-
5	MRD	A	1116	-	-	1/5/5/5	-
6	MPD	A	1124	-	-	1/5/5/5	-
4	BTB	A	1114	-	-	8/21/21/21	-
5	MRD	A	1119	-	-	4/5/5/5	-
6	MPD	A	1122	-	-	3/5/5/5	-
6	MPD	A	1139	-	-	4/5/5/5	-
5	MRD	A	1131	-	-	2/5/5/5	-
5	MRD	A	1133	-	-	5/5/5/5	-
5	MRD	A	1134	-	-	2/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MRD	A	1117	-	-	3/5/5/5	-
5	MRD	A	1123	-	-	0/5/5/5	-
6	MPD	A	1138	-	-	4/5/5/5	-
6	MPD	A	1136	-	-	2/5/5/5	-
6	MPD	A	1135	-	-	2/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1137	MPD	CM-C2-C3-C4
6	A	1137	MPD	C2-C3-C4-O4
5	A	1141	MRD	C2-C3-C4-O4
5	A	1120	MRD	C2-C3-C4-O4
5	A	1116	MRD	C2-C3-C4-O4
4	A	1114	BTB	C1-C2-C3-O3
4	A	1114	BTB	C4-C2-C3-O3
4	A	1114	BTB	N-C2-C3-O3
4	A	1114	BTB	C1-C2-C4-O4
4	A	1114	BTB	C3-C2-C4-O4
4	A	1114	BTB	N-C2-C4-O4
5	A	1119	MRD	C2-C3-C4-O4
6	A	1139	MPD	C2-C3-C4-O4
5	A	1133	MRD	O2-C2-C3-C4
5	A	1133	MRD	C2-C3-C4-O4
5	A	1134	MRD	C2-C3-C4-C5
5	A	1117	MRD	C2-C3-C4-O4
4	A	1114	BTB	N-C5-C6-O6
4	A	1114	BTB	N-C7-C8-O8
5	A	1126	MRD	O2-C2-C3-C4
6	A	1127	MPD	O2-C2-C3-C4
6	A	1139	MPD	O2-C2-C3-C4
5	A	1121	MRD	C2-C3-C4-C5
6	A	1129	MPD	C2-C3-C4-C5
5	A	1128	MRD	C2-C3-C4-C5
5	A	1141	MRD	C2-C3-C4-C5
5	A	1120	MRD	C2-C3-C4-C5
5	A	1130	MRD	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
5	A	1119	MRD	C2-C3-C4-C5
6	A	1139	MPD	C2-C3-C4-C5
5	A	1117	MRD	C2-C3-C4-C5
6	A	1136	MPD	C2-C3-C4-C5
5	A	1126	MRD	C1-C2-C3-C4
5	A	1126	MRD	CM-C2-C3-C4
5	A	1141	MRD	C1-C2-C3-C4
5	A	1120	MRD	C1-C2-C3-C4
6	A	1127	MPD	C1-C2-C3-C4
5	A	1119	MRD	C1-C2-C3-C4
5	A	1119	MRD	CM-C2-C3-C4
6	A	1122	MPD	CM-C2-C3-C4
6	A	1139	MPD	C1-C2-C3-C4
5	A	1133	MRD	C1-C2-C3-C4
5	A	1133	MRD	CM-C2-C3-C4
5	A	1117	MRD	C1-C2-C3-C4
6	A	1138	MPD	C1-C2-C3-C4
6	A	1135	MPD	CM-C2-C3-C4
6	A	1137	MPD	O2-C2-C3-C4
5	A	1120	MRD	O2-C2-C3-C4
6	A	1122	MPD	O2-C2-C3-C4
6	A	1138	MPD	O2-C2-C3-C4
6	A	1135	MPD	O2-C2-C3-C4
6	A	1137	MPD	C2-C3-C4-C5
5	A	1140	MRD	C2-C3-C4-C5
5	A	1126	MRD	C2-C3-C4-C5
5	A	1132	MRD	C2-C3-C4-C5
6	A	1124	MPD	C2-C3-C4-C5
5	A	1131	MRD	C2-C3-C4-C5
5	A	1133	MRD	C2-C3-C4-C5
6	A	1138	MPD	C2-C3-C4-C5
5	A	1121	MRD	C2-C3-C4-O4
5	A	1126	MRD	C2-C3-C4-O4
6	A	1122	MPD	C2-C3-C4-O4
5	A	1131	MRD	C2-C3-C4-O4
5	A	1134	MRD	C2-C3-C4-O4
6	A	1138	MPD	C2-C3-C4-O4
6	A	1136	MPD	C2-C3-C4-O4

There are no ring outliers.

10 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1115	MRD	1	0
5	A	1121	MRD	1	0
5	A	1141	MRD	1	0
5	A	1120	MRD	1	0
5	A	1132	MRD	1	0
6	A	1127	MPD	3	0
5	A	1116	MRD	1	0
5	A	1119	MRD	4	0
6	A	1122	MPD	1	0
6	A	1136	MPD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1040/1040 (100%)	-0.33	28 (2%) 54 48	12, 22, 53, 81	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ARG	9.4
1	A	937	TYR	4.7
1	A	1	PRO	4.1
1	A	944	GLY	4.1
1	A	1022	THR	3.8
1	A	942	ASN	3.6
1	A	925	GLY	3.1
1	A	852	THR	3.0
1	A	1025	THR	3.0
1	A	1023	ASP	3.0
1	A	931	ASP	2.9
1	A	947	THR	2.8
1	A	3	ALA	2.8
1	A	1033	ALA	2.8
1	A	946	GLY	2.5
1	A	1024	ALA	2.4
1	A	924	THR	2.4
1	A	938	ILE	2.3
1	A	926	THR	2.3
1	A	928	THR	2.3
1	A	943	THR	2.3
1	A	1027	GLY	2.3
1	A	829	THR	2.2
1	A	919	LYS	2.2
1	A	889	TYR	2.2
1	A	932[A]	ARG	2.1
1	A	941	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1028	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [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(\AA^2)	Q<0.9
5	MRD	A	1140	8/8	0.73	0.49	37,63,75,80	0
6	MPD	A	1125	8/8	0.76	0.27	36,53,62,65	0
6	MPD	A	1129	8/8	0.79	0.48	39,54,65,66	0
6	MPD	A	1139	8/8	0.79	0.28	30,48,64,68	0
3	CL	A	1113	1/1	0.82	0.14	67,67,67,67	0
5	MRD	A	1131	8/8	0.82	0.26	39,44,64,65	0
4	BTB	A	1114	14/14	0.83	0.25	32,53,59,59	0
5	MRD	A	1121	8/8	0.85	0.22	35,47,56,59	0
5	MRD	A	1119	8/8	0.85	0.29	32,45,52,58	0
5	MRD	A	1133	8/8	0.85	0.29	46,59,69,70	0
6	MPD	A	1136	8/8	0.85	0.23	50,62,72,73	0
5	MRD	A	1128	8/8	0.87	0.47	36,61,70,72	0
5	MRD	A	1132	8/8	0.87	0.20	64,68,74,76	0
5	MRD	A	1134	8/8	0.87	0.69	39,48,56,58	0
5	MRD	A	1120	8/8	0.87	0.27	32,49,54,56	0
5	MRD	A	1130	8/8	0.89	0.18	54,60,65,67	0
6	MPD	A	1135	8/8	0.89	0.34	46,56,61,66	0
6	MPD	A	1127	8/8	0.90	0.68	45,55,62,69	0
5	MRD	A	1123	8/8	0.90	0.34	38,54,68,78	0
6	MPD	A	1124	8/8	0.90	0.35	41,57,69,69	0
6	MPD	A	1122	8/8	0.90	0.17	45,50,68,71	0
5	MRD	A	1126	8/8	0.91	0.19	53,62,68,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MRD	A	1117	8/8	0.92	0.18	26,44,50,51	0
6	MPD	A	1137	8/8	0.92	0.21	38,55,57,64	0
5	MRD	A	1116	8/8	0.93	0.21	27,37,44,53	0
2	CA	A	1103	1/1	0.94	0.05	41,41,41,41	0
5	MRD	A	1141	8/8	0.94	0.20	33,41,52,66	0
2	CA	A	1108	1/1	0.94	0.14	39,39,39,39	0
2	CA	A	1107	1/1	0.95	0.17	67,67,67,67	0
5	MRD	A	1115	8/8	0.95	0.25	21,28,36,42	0
2	CA	A	1106	1/1	0.96	0.05	58,58,58,58	0
2	CA	A	1101	1/1	0.96	0.14	20,20,20,20	0
5	MRD	A	1118	8/8	0.96	0.14	17,31,33,42	0
3	CL	A	1111	1/1	0.97	0.09	39,39,39,39	0
2	CA	A	1109	1/1	0.97	0.09	45,45,45,45	0
6	MPD	A	1138	8/8	0.97	0.16	29,46,50,52	0
2	CA	A	1104	1/1	0.98	0.06	28,28,28,28	0
3	CL	A	1112	1/1	0.99	0.08	27,27,27,27	0
3	CL	A	1110	1/1	0.99	0.08	24,24,24,24	0
2	CA	A	1105	1/1	0.99	0.08	16,16,16,16	0
2	CA	A	1102	1/1	0.99	0.08	24,24,24,24	0

6.5 Other polymers

There are no such residues in this entry.