



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:50 PM UTC

PDB ID : 6F2P / pdb_00006f2p
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 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

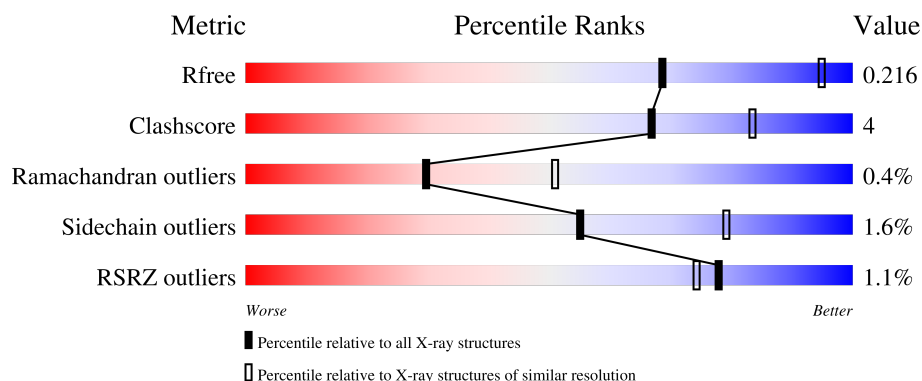
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 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	1040	

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 (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

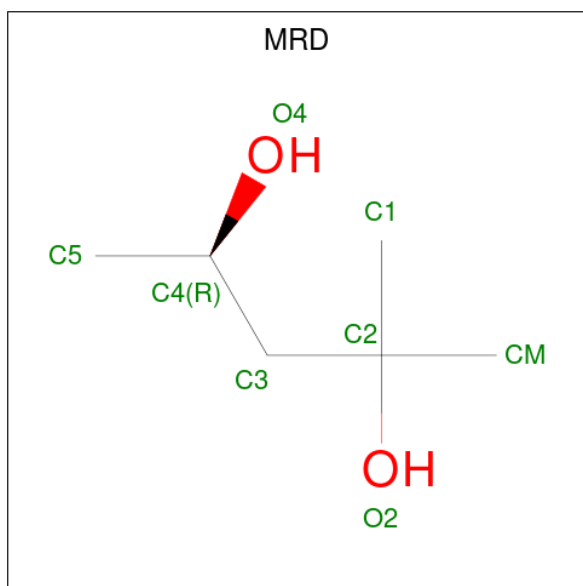
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Cl	0	0
			4	4		

- Molecule 4 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: 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 (CCD ID: 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		
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		

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



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

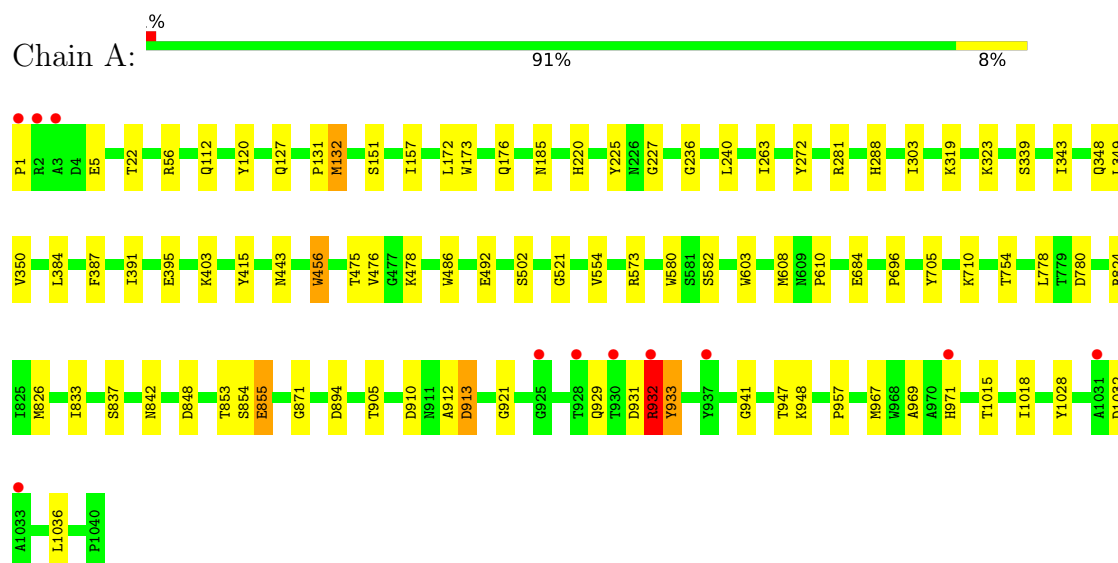
- Molecule 7 is water.

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

3 Residue-property plots

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: *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 0.169 , 0.216	Depositor DCC
R_{free} test set	2000 reflections (3.81%)	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)	0.35 , 49.0	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MRD, MPD, CL, BTB

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	0.40	0/8167	0.77	2/11118 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	603	TRP	N-CA-C	5.36	116.43	108.60
1	A	933	TYR	N-CA-C	5.34	122.17	110.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	52	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	11	0
6	A	80	0	140	5	0
7	A	515	0	0	3	0
All	All	8747	0	8106	61	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 4.

All (61) 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:132:MET:HE2	5:A:1133:MRD:H5C3	1.81	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:824:ARG:NH1	1:A:826:MET:HE1	2.25	0.52
5:A:1141:MRD:O4	5:A:1141:MRD:O2	2.18	0.51
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:826:MET:HE3	1:A:894:ASP:HB2	1.93	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:132:MET:HE1	1:A:176:GLN:NE2	2.29	0.48
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
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
5:A:1120:MRD:H1C1	5:A:1120:MRD:H4	1.66	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:HMC1	5:A:1116:MRD:H4	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:240:LEU:HD23	1:A:240:LEU:HA	1.76	0.43
1:A:905:THR:HA	1:A:957:PRO:HG2	2.01	0.43
5:A:1121:MRD:H1C1	5:A:1121:MRD:H4	1.88	0.43
1:A:387:PHE:HB2	1:A:391:ILE:O	2.18	0.43
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:H4	5:A:1132:MRD:HMC3	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:H4	5:A:1119:MRD:H1C3	1.81	0.41
1:A:456:TRP:CH2	1:A:696:PRO:HG2	2.56	0.41
1:A:608:MET:HE2	1:A:608:MET:HB3	1.84	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:263:ILE:HD12	1:A:303:ILE:HG12	2.02	0.40
1:A:941:GLY:HA2	1:A:1028:TYR:HE1	1.85	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%)	24 46

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%)	849 (98%)	15 (2%)	53 78

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	132	MET
1	A	225	TYR
1	A	456	TRP
1	A	476	VAL
1	A	492	GLU
1	A	554	VAL
1	A	754	THR
1	A	854	SER
1	A	855	GLU
1	A	929	GLN
1	A	932[A]	ARG
1	A	932[B]	ARG
1	A	947	THR
1	A	1015	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	112	GLN
1	A	127	GLN
1	A	176	GLN
1	A	348	GLN
1	A	443	ASN
1	A	738	ASN
1	A	842	ASN
1	A	929	GLN
1	A	942	ASN
1	A	973	ASN
1	A	996	GLN
1	A	998	ASN

5.3.3 RNA [i](#)

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](#)

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	0.64	0	9,10,10	0.25	0
6	MPD	A	1127	-	7,7,7	0.60	0	9,10,10	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MRD	A	1132	-	7,7,7	0.67	0	9,10,10	0.41	0
5	MRD	A	1118	-	7,7,7	0.53	0	9,10,10	0.34	0
5	MRD	A	1123	-	7,7,7	0.61	0	9,10,10	0.37	0
6	MPD	A	1122	-	7,7,7	0.59	0	9,10,10	0.39	0
5	MRD	A	1117	-	7,7,7	0.60	0	9,10,10	0.50	0
6	MPD	A	1137	-	7,7,7	0.56	0	9,10,10	0.46	0
4	BTB	A	1114	-	13,13,13	0.67	0	7,16,16	0.77	0
5	MRD	A	1120	-	7,7,7	0.56	0	9,10,10	0.27	0
6	MPD	A	1125	-	7,7,7	0.53	0	9,10,10	0.37	0
5	MRD	A	1141	-	7,7,7	0.57	0	9,10,10	0.60	0
6	MPD	A	1124	-	7,7,7	0.63	0	9,10,10	0.36	0
5	MRD	A	1128	-	7,7,7	0.70	0	9,10,10	0.42	0
5	MRD	A	1130	-	7,7,7	0.64	0	9,10,10	0.33	0
6	MPD	A	1138	-	7,7,7	0.52	0	9,10,10	0.44	0
6	MPD	A	1136	-	7,7,7	0.61	0	9,10,10	0.30	0
5	MRD	A	1126	-	7,7,7	0.56	0	9,10,10	0.45	0
5	MRD	A	1121	-	7,7,7	0.58	0	9,10,10	0.31	0
5	MRD	A	1140	-	7,7,7	0.53	0	9,10,10	0.29	0
5	MRD	A	1134	-	7,7,7	0.46	0	9,10,10	0.67	0
6	MPD	A	1135	-	7,7,7	0.56	0	9,10,10	0.35	0
5	MRD	A	1119	-	7,7,7	0.58	0	9,10,10	0.55	0
5	MRD	A	1116	-	7,7,7	0.62	0	9,10,10	0.36	0
6	MPD	A	1139	-	7,7,7	0.56	0	9,10,10	0.29	0
5	MRD	A	1131	-	7,7,7	0.56	0	9,10,10	0.34	0
5	MRD	A	1133	-	7,7,7	0.52	0	9,10,10	0.55	0
6	MPD	A	1129	-	7,7,7	0.56	0	9,10,10	0.45	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	-
6	MPD	A	1127	-	-	3/5/5/5	-
5	MRD	A	1132	-	-	1/5/5/5	-
5	MRD	A	1118	-	-	0/5/5/5	-
5	MRD	A	1123	-	-	0/5/5/5	-
6	MPD	A	1122	-	-	3/5/5/5	-
5	MRD	A	1117	-	-	4/5/5/5	-
6	MPD	A	1137	-	-	4/5/5/5	-
4	BTB	A	1114	-	-	8/21/21/21	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MRD	A	1120	-	-	4/5/5/5	-
6	MPD	A	1125	-	-	1/5/5/5	-
5	MRD	A	1141	-	-	4/5/5/5	-
6	MPD	A	1124	-	-	0/5/5/5	-
5	MRD	A	1128	-	-	1/5/5/5	-
5	MRD	A	1130	-	-	2/5/5/5	-
6	MPD	A	1138	-	-	4/5/5/5	-
6	MPD	A	1136	-	-	3/5/5/5	-
5	MRD	A	1126	-	-	4/5/5/5	-
5	MRD	A	1121	-	-	3/5/5/5	-
5	MRD	A	1140	-	-	1/5/5/5	-
5	MRD	A	1134	-	-	3/5/5/5	-
6	MPD	A	1135	-	-	2/5/5/5	-
5	MRD	A	1119	-	-	4/5/5/5	-
5	MRD	A	1116	-	-	2/5/5/5	-
6	MPD	A	1139	-	-	5/5/5/5	-
5	MRD	A	1131	-	-	2/5/5/5	-
5	MRD	A	1133	-	-	5/5/5/5	-
6	MPD	A	1129	-	-	2/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	1116	MRD	C2-C3-C4-O4
5	A	1116	MRD	C2-C3-C4-C5
5	A	1117	MRD	C2-C3-C4-O4
5	A	1119	MRD	C2-C3-C4-O4
5	A	1120	MRD	C2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
5	A	1120	MRD	C2-C3-C4-C5
5	A	1133	MRD	C2-C3-C4-O4
5	A	1133	MRD	C2-C3-C4-C5
5	A	1134	MRD	C2-C3-C4-C5
5	A	1141	MRD	C2-C3-C4-O4
6	A	1137	MPD	CM-C2-C3-C4
6	A	1137	MPD	C2-C3-C4-O4
6	A	1137	MPD	C2-C3-C4-C5
6	A	1139	MPD	C2-C3-C4-O4
6	A	1139	MPD	C2-C3-C4-C5
4	A	1114	BTB	N-C5-C6-O6
4	A	1114	BTB	N-C7-C8-O8
5	A	1130	MRD	O2-C2-C3-C4
5	A	1133	MRD	O2-C2-C3-C4
6	A	1129	MPD	O2-C2-C3-C4
5	A	1117	MRD	C1-C2-C3-C4
5	A	1119	MRD	C1-C2-C3-C4
5	A	1119	MRD	CM-C2-C3-C4
5	A	1120	MRD	C1-C2-C3-C4
5	A	1126	MRD	C1-C2-C3-C4
5	A	1126	MRD	CM-C2-C3-C4
5	A	1133	MRD	C1-C2-C3-C4
5	A	1133	MRD	CM-C2-C3-C4
5	A	1141	MRD	C1-C2-C3-C4
6	A	1122	MPD	CM-C2-C3-C4
6	A	1127	MPD	C1-C2-C3-C4
6	A	1135	MPD	CM-C2-C3-C4
6	A	1138	MPD	C1-C2-C3-C4
6	A	1139	MPD	C1-C2-C3-C4
5	A	1117	MRD	C2-C3-C4-C5
5	A	1119	MRD	C2-C3-C4-C5
5	A	1121	MRD	C2-C3-C4-C5
5	A	1128	MRD	C2-C3-C4-C5
5	A	1130	MRD	C2-C3-C4-C5
5	A	1141	MRD	C2-C3-C4-C5
6	A	1129	MPD	C2-C3-C4-C5
6	A	1136	MPD	C2-C3-C4-C5
5	A	1121	MRD	O2-C2-C3-C4
5	A	1126	MRD	O2-C2-C3-C4
5	A	1131	MRD	O2-C2-C3-C4
5	A	1132	MRD	O2-C2-C3-C4
5	A	1140	MRD	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
6	A	1127	MPD	O2-C2-C3-C4
6	A	1136	MPD	O2-C2-C3-C4
6	A	1138	MPD	O2-C2-C3-C4
6	A	1139	MPD	O2-C2-C3-C4
5	A	1121	MRD	C2-C3-C4-O4
5	A	1126	MRD	C2-C3-C4-O4
5	A	1131	MRD	C2-C3-C4-O4
5	A	1134	MRD	C2-C3-C4-O4
6	A	1122	MPD	C2-C3-C4-O4
6	A	1136	MPD	C2-C3-C4-O4
6	A	1138	MPD	C2-C3-C4-O4
5	A	1117	MRD	CM-C2-C3-C4
5	A	1120	MRD	CM-C2-C3-C4
5	A	1134	MRD	CM-C2-C3-C4
5	A	1141	MRD	CM-C2-C3-C4
6	A	1122	MPD	C1-C2-C3-C4
6	A	1125	MPD	CM-C2-C3-C4
6	A	1127	MPD	CM-C2-C3-C4
6	A	1135	MPD	C1-C2-C3-C4
6	A	1137	MPD	C1-C2-C3-C4
6	A	1138	MPD	CM-C2-C3-C4
6	A	1139	MPD	CM-C2-C3-C4

There are no ring outliers.

11 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1115	MRD	1	0
6	A	1127	MPD	3	0
5	A	1132	MRD	1	0
6	A	1122	MPD	1	0
5	A	1120	MRD	1	0
5	A	1141	MRD	1	0
6	A	1136	MPD	1	0
5	A	1121	MRD	1	0
5	A	1119	MRD	4	0
5	A	1116	MRD	1	0
5	A	1133	MRD	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.60	11 (1%) 78 74	9, 22, 53, 81	3 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ARG	5.8
1	A	1	PRO	5.5
1	A	932[A]	ARG	5.2
1	A	3	ALA	3.6
1	A	1033	ALA	3.0
1	A	925	GLY	2.9
1	A	937	TYR	2.4
1	A	971	HIS	2.1
1	A	928	THR	2.1
1	A	1031	ALA	2.1
1	A	930	THR	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 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
5	MRD	A	1130	8/8	0.57	0.30	54,60,65,67	0
5	MRD	A	1131	8/8	0.71	0.22	39,44,64,65	0
6	MPD	A	1125	8/8	0.72	0.20	36,53,62,65	0
6	MPD	A	1137	8/8	0.73	0.23	38,55,57,64	0
5	MRD	A	1119	8/8	0.75	0.15	32,45,52,58	0
5	MRD	A	1133	8/8	0.77	0.23	46,59,69,70	0
5	MRD	A	1140	8/8	0.77	0.23	37,63,75,80	0
6	MPD	A	1129	8/8	0.78	0.30	39,54,65,66	0
5	MRD	A	1128	8/8	0.79	0.23	36,61,70,72	0
5	MRD	A	1121	8/8	0.79	0.19	35,47,56,59	0
4	BTB	A	1114	14/14	0.80	0.18	32,53,59,59	0
5	MRD	A	1134	8/8	0.80	0.27	39,48,56,58	0
5	MRD	A	1132	8/8	0.80	0.23	64,68,74,76	0
6	MPD	A	1139	8/8	0.80	0.17	30,48,64,68	0
6	MPD	A	1135	8/8	0.82	0.23	46,56,61,66	0
6	MPD	A	1136	8/8	0.82	0.19	50,62,72,73	0
6	MPD	A	1124	8/8	0.83	0.17	41,57,69,69	0
5	MRD	A	1126	8/8	0.83	0.20	53,62,68,70	0
6	MPD	A	1127	8/8	0.83	0.23	45,55,62,69	0
5	MRD	A	1123	8/8	0.83	0.14	38,54,68,78	0
5	MRD	A	1120	8/8	0.84	0.16	32,49,54,56	0
6	MPD	A	1122	8/8	0.85	0.18	45,50,68,71	0
5	MRD	A	1117	8/8	0.88	0.15	26,44,50,51	0
3	CL	A	1113	1/1	0.88	0.12	67,67,67,67	0
5	MRD	A	1115	8/8	0.89	0.12	21,28,36,42	0
6	MPD	A	1138	8/8	0.91	0.13	29,46,50,52	0
2	CA	A	1107	1/1	0.92	0.06	67,67,67,67	0
5	MRD	A	1141	8/8	0.92	0.12	33,41,52,66	0
5	MRD	A	1116	8/8	0.92	0.11	27,37,44,53	0
2	CA	A	1103	1/1	0.93	0.08	41,41,41,41	0
5	MRD	A	1118	8/8	0.94	0.09	17,31,33,42	0
2	CA	A	1109	1/1	0.95	0.06	45,45,45,45	0
2	CA	A	1108	1/1	0.97	0.04	39,39,39,39	0
2	CA	A	1101	1/1	0.98	0.03	20,20,20,20	0
2	CA	A	1106	1/1	0.98	0.04	58,58,58,58	0
3	CL	A	1112	1/1	0.99	0.08	27,27,27,27	0
2	CA	A	1104	1/1	0.99	0.02	28,28,28,28	0
2	CA	A	1105	1/1	0.99	0.02	16,16,16,16	0
2	CA	A	1102	1/1	0.99	0.02	24,24,24,24	0
3	CL	A	1111	1/1	0.99	0.06	39,39,39,39	0
3	CL	A	1110	1/1	1.00	0.05	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.