



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:08 AM UTC

PDB ID : 1TZ7 / pdb_00001tz7
Title : Aquifex aeolicus amylomaltase
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Deposited on : 2004-07-09
Resolution : 2.15 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

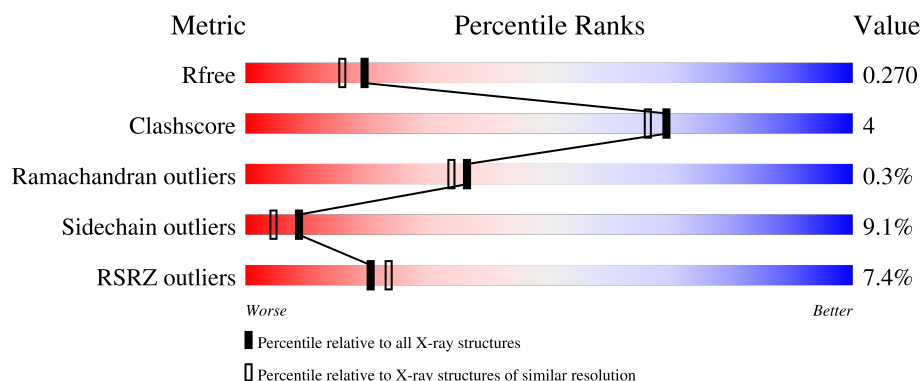
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	505	7% 83% 11% • •
1	B	505	8% 82% 12% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8508 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 4-alpha-glucanotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	0	0
			4147	2714	695	732	6			
1	B	487	Total	C	N	O	S	0	0	0
			4143	2712	694	731	6			

There are 42 discrepancies between the modelled and reference sequences:

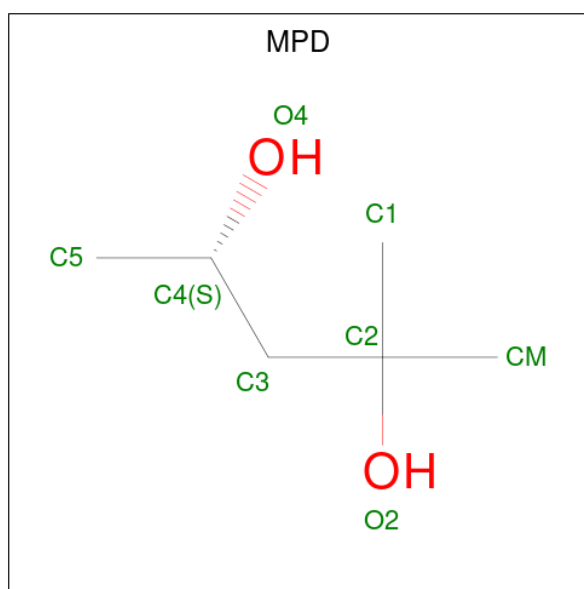
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP O66937
A	-18	GLY	-	expression tag	UNP O66937
A	-17	SER	-	expression tag	UNP O66937
A	-16	SER	-	expression tag	UNP O66937
A	-15	HIS	-	expression tag	UNP O66937
A	-14	HIS	-	expression tag	UNP O66937
A	-13	HIS	-	expression tag	UNP O66937
A	-12	HIS	-	expression tag	UNP O66937
A	-11	HIS	-	expression tag	UNP O66937
A	-10	HIS	-	expression tag	UNP O66937
A	-9	SER	-	expression tag	UNP O66937
A	-8	SER	-	expression tag	UNP O66937
A	-7	GLY	-	expression tag	UNP O66937
A	-6	LEU	-	expression tag	UNP O66937
A	-5	VAL	-	expression tag	UNP O66937
A	-4	PRO	-	expression tag	UNP O66937
A	-3	ARG	-	expression tag	UNP O66937
A	-2	GLY	-	expression tag	UNP O66937
A	-1	SER	-	expression tag	UNP O66937
A	0	HIS	-	expression tag	UNP O66937
A	274	LEU	HIS	conflict	UNP O66937
B	-19	MET	-	expression tag	UNP O66937
B	-18	GLY	-	expression tag	UNP O66937
B	-17	SER	-	expression tag	UNP O66937
B	-16	SER	-	expression tag	UNP O66937

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP O66937
B	-14	HIS	-	expression tag	UNP O66937
B	-13	HIS	-	expression tag	UNP O66937
B	-12	HIS	-	expression tag	UNP O66937
B	-11	HIS	-	expression tag	UNP O66937
B	-10	HIS	-	expression tag	UNP O66937
B	-9	SER	-	expression tag	UNP O66937
B	-8	SER	-	expression tag	UNP O66937
B	-7	GLY	-	expression tag	UNP O66937
B	-6	LEU	-	expression tag	UNP O66937
B	-5	VAL	-	expression tag	UNP O66937
B	-4	PRO	-	expression tag	UNP O66937
B	-3	ARG	-	expression tag	UNP O66937
B	-2	GLY	-	expression tag	UNP O66937
B	-1	SER	-	expression tag	UNP O66937
B	0	HIS	-	expression tag	UNP O66937
B	274	LEU	HIS	conflict	UNP O66937

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



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

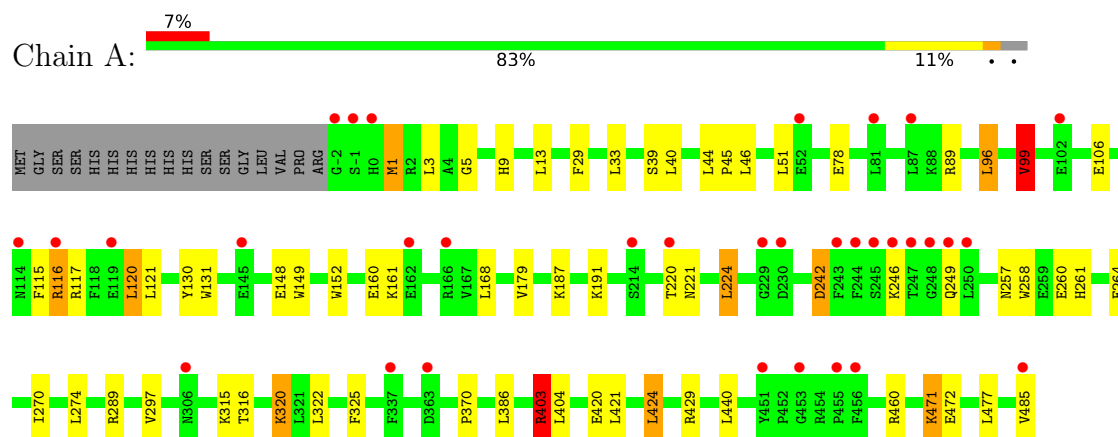
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	98	Total 98	O 98	0	0
3	B	112	Total 112	O 112	0	0

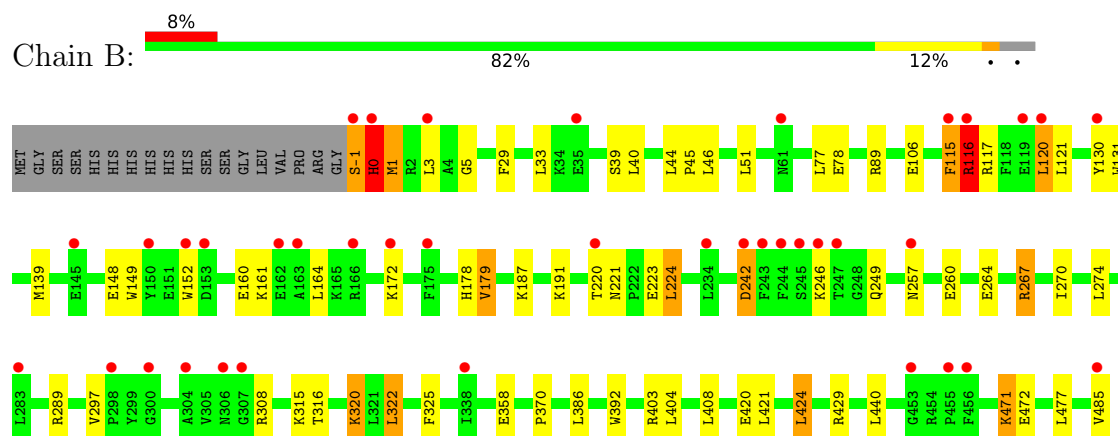
3 Residue-property plots [i](#)

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: 4-alpha-glucanotransferase



• Molecule 1: 4-alpha-glucanotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	156.75Å 156.75Å 169.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.15 15.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.8 (15.00-2.15) 99.4 (15.00-2.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.99 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.215 , 0.243 0.258 , 0.270	Depositor DCC
R_{free} test set	3380 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8508	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.94% 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: MPD

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	0.61	1/4273 (0.0%)	0.67	6/5768 (0.1%)
1	B	0.61	1/4269 (0.0%)	0.70	9/5763 (0.2%)
All	All	0.61	2/8542 (0.0%)	0.68	15/11531 (0.1%)

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
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	179	VAL	CA-CB	5.19	1.61	1.54
1	A	99	VAL	CA-CB	5.08	1.61	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	403	ARG	NE-CZ-NH2	7.29	125.76	119.20
1	B	403	ARG	NE-CZ-NH1	-7.24	114.26	121.50
1	B	429	ARG	NE-CZ-NH2	6.80	125.32	119.20
1	A	460	ARG	NE-CZ-NH2	6.32	124.88	119.20
1	B	267	ARG	NE-CZ-NH2	6.28	124.85	119.20
1	B	429	ARG	NE-CZ-NH1	-6.23	115.27	121.50
1	B	308	ARG	NE-CZ-NH2	6.09	124.68	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172	LYS	CB-CA-C	5.98	121.01	110.85
1	A	403	ARG	CD-NE-CZ	5.79	132.51	124.40
1	B	267	ARG	NE-CZ-NH1	-5.76	115.74	121.50
1	A	460	ARG	NE-CZ-NH1	-5.75	115.75	121.50
1	B	308	ARG	NE-CZ-NH1	-5.69	115.81	121.50
1	A	403	ARG	NE-CZ-NH2	-5.51	114.24	119.20
1	A	403	ARG	CG-CD-NE	5.29	123.64	112.00
1	A	403	ARG	NE-CZ-NH1	5.19	126.69	121.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	PHE	Peptide
1	B	115	PHE	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	4147	0	4071	27	0
1	B	4143	0	4068	31	0
2	A	8	0	14	0	0
3	A	98	0	0	1	0
3	B	112	0	0	1	0
All	All	8508	0	8153	58	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 (58) 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:B:-1:SER:HA	1:B:0:HIS:CB	1.90	1.01
1:B:-1:SER:HA	1:B:0:HIS:HB2	1.41	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LEU:HG	1:A:261:HIS:CE1	2.04	0.92
1:B:1:SER:HA	1:B:0:HIS:CG	2.07	0.88
1:B:1:SER:CA	1:B:0:HIS:HB2	2.10	0.82
1:B:257:ASN:HD22	1:B:260:GLU:HB2	1.50	0.77
1:A:257:ASN:HD22	1:A:260:GLU:HB2	1.51	0.75
1:B:29:PHE:CZ	1:B:33:LEU:HD21	2.28	0.68
1:A:29:PHE:CZ	1:A:33:LEU:HD21	2.31	0.65
1:A:3:LEU:HD23	1:A:39:SER:CB	2.26	0.65
1:B:3:LEU:HD23	1:B:39:SER:CB	2.27	0.64
1:A:29:PHE:O	1:A:33:LEU:HD23	1.99	0.63
1:A:3:LEU:HD23	1:A:39:SER:HB2	1.83	0.61
1:A:242:ASP:OD1	1:A:242:ASP:N	2.35	0.59
1:B:242:ASP:N	1:B:242:ASP:OD1	2.35	0.58
1:B:3:LEU:HD23	1:B:39:SER:HB2	1.85	0.58
1:B:29:PHE:O	1:B:33:LEU:HD23	2.04	0.58
1:A:258:TRP:HA	1:A:261:HIS:HD2	1.68	0.58
1:A:270:ILE:HD11	1:A:320:LYS:HD3	1.91	0.53
1:B:270:ILE:HD11	1:B:320:LYS:HD3	1.90	0.52
1:A:96:LEU:HB3	1:A:99:VAL:HG13	1.92	0.51
1:A:370:PRO:HG2	1:A:424:LEU:HG	1.92	0.51
1:A:485:VAL:HG11	3:A:3288:HOH:O	2.10	0.51
1:A:221:ASN:HB3	1:A:224:LEU:HD22	1.93	0.50
1:B:370:PRO:HG2	1:B:424:LEU:HG	1.93	0.49
1:B:139:MET:HB3	1:B:178:HIS:CE1	2.47	0.49
1:B:149:TRP:HA	1:B:152:TRP:CD2	2.47	0.49
1:A:5:GLY:HA3	1:A:40:LEU:HB2	1.94	0.49
1:B:5:GLY:HA3	1:B:40:LEU:HB2	1.94	0.49
1:B:115:PHE:HA	1:B:116:ARG:HB2	1.95	0.48
1:B:221:ASN:HB3	1:B:224:LEU:HD22	1.94	0.47
1:A:274:LEU:HD12	1:A:325:PHE:HE2	1.80	0.47
1:A:149:TRP:HA	1:A:152:TRP:CD2	2.49	0.47
1:A:471:LYS:HG3	1:A:472:GLU:N	2.30	0.46
1:B:130:TYR:CE1	1:B:131:TRP:HD1	2.33	0.46
1:A:130:TYR:CE1	1:A:131:TRP:HD1	2.34	0.46
1:B:485:VAL:HG11	3:B:498:HOH:O	2.15	0.46
1:A:404:LEU:HD11	1:A:421:LEU:HD21	1.97	0.45
1:B:44:LEU:HB3	1:B:45:PRO:HD2	1.98	0.45
1:A:44:LEU:HB3	1:A:45:PRO:HD2	1.99	0.45
1:B:404:LEU:HD11	1:B:421:LEU:HD21	1.97	0.45
1:A:224:LEU:HG	1:A:261:HIS:ND1	2.32	0.45
1:B:44:LEU:HB3	1:B:45:PRO:CD	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:HIS:CE1	1:A:44:LEU:HB2	2.52	0.44
1:B:1:MET:O	1:B:1:MET:HG3	2.16	0.44
1:B:471:LYS:HG3	1:B:472:GLU:N	2.32	0.44
1:A:44:LEU:HB3	1:A:45:PRO:CD	2.48	0.43
1:B:29:PHE:CE2	1:B:33:LEU:HD21	2.53	0.43
1:A:403:ARG:HG3	1:A:403:ARG:HH11	1.83	0.43
1:B:274:LEU:HD12	1:B:325:PHE:HE2	1.84	0.43
1:B:117:ARG:HG2	1:B:120:LEU:HD23	2.01	0.42
1:A:1:MET:O	1:A:1:MET:HG3	2.16	0.42
1:B:322:LEU:HD13	1:B:322:LEU:HA	1.94	0.42
1:A:258:TRP:HA	1:A:261:HIS:CD2	2.50	0.41
1:A:117:ARG:HG2	1:A:120:LEU:HD12	2.01	0.41
1:B:-1:SER:CB	1:B:0:HIS:HB2	2.51	0.40
1:B:257:ASN:ND2	1:B:260:GLU:HB2	2.25	0.40
1:B:358:GLU:HG3	1:B:392:TRP:CD2	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	
1	A	486/505 (96%)	475 (98%)	10 (2%)	1 (0%)	43	44
1	B	485/505 (96%)	474 (98%)	9 (2%)	2 (0%)	30	26
All	All	971/1010 (96%)	949 (98%)	19 (2%)	3 (0%)	36	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	0	HIS
1	B	116	ARG
1	A	116	ARG

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	436/451 (97%)	397 (91%)	39 (9%)	9	5
1	B	436/451 (97%)	396 (91%)	40 (9%)	8	4
All	All	872/902 (97%)	793 (91%)	79 (9%)	9	4

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	13	LEU
1	A	46	LEU
1	A	51	LEU
1	A	78	GLU
1	A	89	ARG
1	A	96	LEU
1	A	99	VAL
1	A	106	GLU
1	A	116	ARG
1	A	120	LEU
1	A	121	LEU
1	A	148	GLU
1	A	160	GLU
1	A	161	LYS
1	A	168	LEU
1	A	179	VAL
1	A	187	LYS
1	A	191	LYS
1	A	220	THR
1	A	224	LEU
1	A	242	ASP
1	A	246	LYS
1	A	249	GLN
1	A	264	GLU
1	A	289	ARG
1	A	297	VAL

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Mol	Chain	Res	Type
1	A	315	LYS
1	A	316	THR
1	A	320	LYS
1	A	322	LEU
1	A	386	LEU
1	A	403	ARG
1	A	420	GLU
1	A	424	LEU
1	A	429	ARG
1	A	440	LEU
1	A	471	LYS
1	A	477	LEU
1	B	-1	SER
1	B	0	HIS
1	B	1	MET
1	B	46	LEU
1	B	51	LEU
1	B	77	LEU
1	B	78	GLU
1	B	89	ARG
1	B	106	GLU
1	B	116	ARG
1	B	120	LEU
1	B	121	LEU
1	B	148	GLU
1	B	160	GLU
1	B	161	LYS
1	B	164	LEU
1	B	179	VAL
1	B	187	LYS
1	B	191	LYS
1	B	220	THR
1	B	223	GLU
1	B	224	LEU
1	B	242	ASP
1	B	246	LYS
1	B	249	GLN
1	B	264	GLU
1	B	267	ARG
1	B	289	ARG
1	B	297	VAL
1	B	315	LYS

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Mol	Chain	Res	Type
1	B	316	THR
1	B	320	LYS
1	B	322	LEU
1	B	386	LEU
1	B	408	LEU
1	B	420	GLU
1	B	424	LEU
1	B	440	LEU
1	B	471	LYS
1	B	477	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	114	ASN
1	A	249	GLN
1	A	257	ASN
1	A	436	GLN
1	A	445	ASN
1	B	42	GLN
1	B	114	ASN
1	B	178	HIS
1	B	249	GLN
1	B	257	ASN
1	B	384	HIS
1	B	436	GLN
1	B	445	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MPD	A	3282	-	7,7,7	0.36	0	9,10,10	0.20	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
2	MPD	A	3282	-	-	0/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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	488/505 (96%)	0.58	33 (6%)	23 26	21, 32, 56, 107	0
1	B	487/505 (96%)	0.67	39 (8%)	18 20	16, 32, 56, 98	0
All	All	975/1010 (96%)	0.63	72 (7%)	20 23	16, 32, 56, 107	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	455	PRO	5.2
1	B	243	PHE	4.8
1	B	153	ASP	4.4
1	B	453	GLY	4.3
1	B	172	LYS	4.2
1	B	-1	SER	4.1
1	A	-2	GLY	4.1
1	B	247	THR	3.9
1	A	243	PHE	3.8
1	A	453	GLY	3.7
1	B	244	PHE	3.5
1	B	0	HIS	3.4
1	A	214	SER	3.3
1	B	300	GLY	3.2
1	B	150	TYR	3.1
1	A	116	ARG	2.9
1	A	0	HIS	2.9
1	B	35	GLU	2.9
1	B	175	PHE	2.8
1	B	456	PHE	2.8
1	B	163	ALA	2.8
1	A	244	PHE	2.8
1	B	145	GLU	2.8
1	A	250	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	119	GLU	2.6
1	B	115	PHE	2.6
1	A	-1	SER	2.6
1	B	130	TYR	2.6
1	A	485	VAL	2.6
1	B	3	LEU	2.4
1	A	248	GLY	2.4
1	A	456	PHE	2.4
1	B	119	GLU	2.4
1	A	363	ASP	2.4
1	A	246	LYS	2.4
1	B	120	LEU	2.4
1	B	257	ASN	2.4
1	B	162	GLU	2.4
1	B	242	ASP	2.4
1	A	245	SER	2.4
1	B	246	LYS	2.4
1	A	230	ASP	2.3
1	B	283	LEU	2.3
1	B	485	VAL	2.3
1	B	152	TRP	2.3
1	A	166	ARG	2.3
1	B	166	ARG	2.3
1	B	234	LEU	2.3
1	A	451	TYR	2.3
1	B	245	SER	2.2
1	B	116	ARG	2.2
1	B	304	ALA	2.2
1	B	306	ASN	2.2
1	A	247	THR	2.2
1	B	338	ILE	2.2
1	A	145	GLU	2.1
1	A	162	GLU	2.1
1	B	307	GLY	2.1
1	B	61	ASN	2.1
1	A	52	GLU	2.1
1	A	220	THR	2.1
1	A	229	GLY	2.1
1	A	87	LEU	2.1
1	A	102	GLU	2.1
1	A	249	GLN	2.1
1	A	114	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	306	ASN	2.1
1	A	455	PRO	2.1
1	B	220	THR	2.1
1	B	298	PRO	2.1
1	A	81	LEU	2.0
1	A	337	PHE	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
2	MPD	A	3282	8/8	0.87	0.17	57,65,66,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.