



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 06:20 AM UTC

PDB ID : 5BN1 / pdb_00005bn1
Title : Structure of Axe2-W215I, an acetyl xylan esterase from *Geobacillus stearothermophilus*
Authors : Lansky, S.; Alalouf, O.; Shoham, Y.; Shoham, G.
Deposited on : 2015-05-25
Resolution : 1.60 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

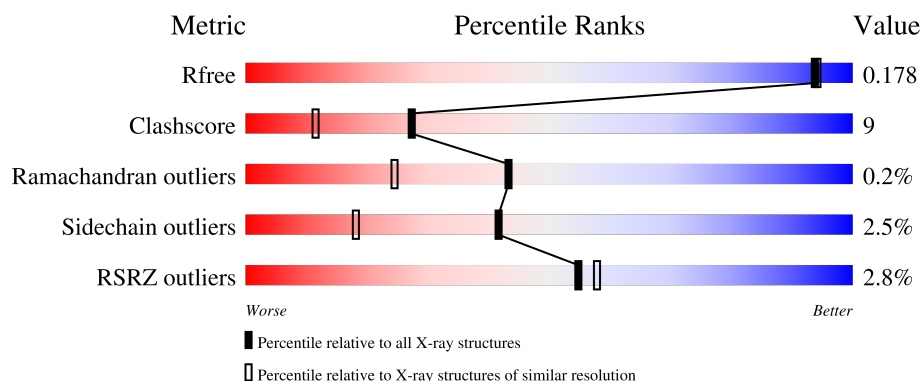
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	219	3% 67% 27% • •
1	B	219	3% 76% 21% •

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
2	GOL	B	305	-	X	-	-
4	IMD	A	304	-	X	-	-
5	TRS	B	304	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4113 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.

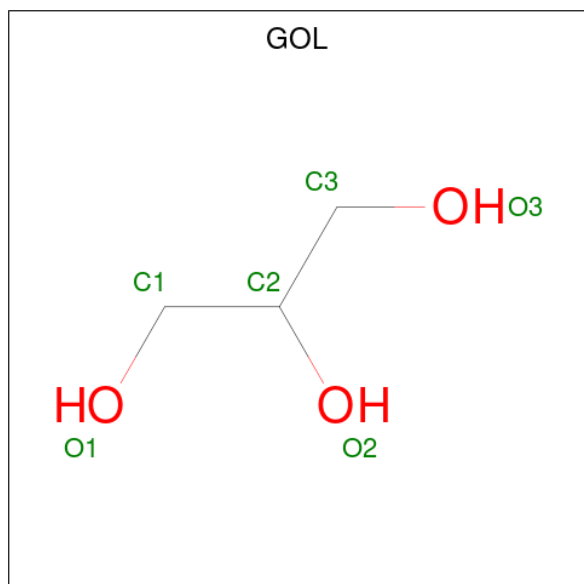
- Molecule 1 is a protein called Acetyl xylan esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	6	0
			1758	1130	298	322	8			
1	B	218	Total	C	N	O	S	0	6	0
			1758	1132	296	322	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	215	ILE	TRP	engineered mutation	UNP Q09LX1
B	215	ILE	TRP	engineered mutation	UNP Q09LX1

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

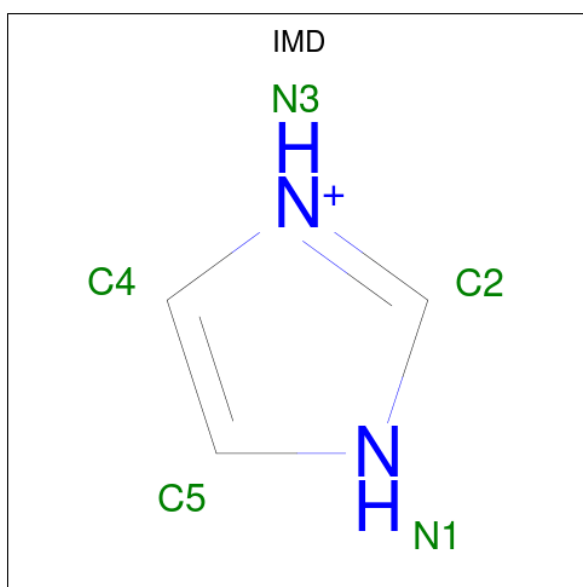
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		

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

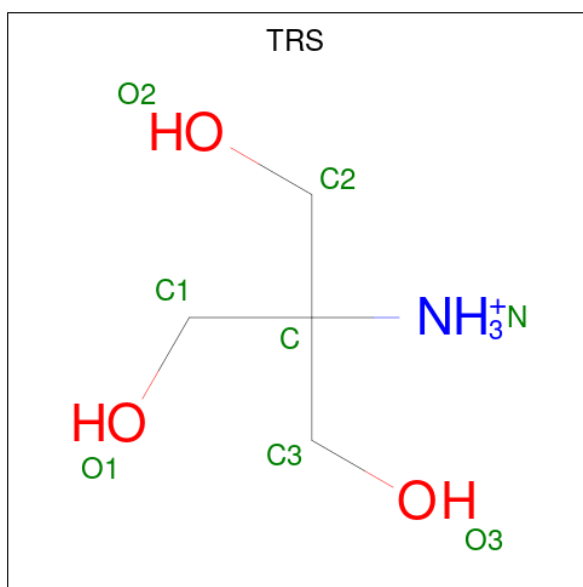
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is IMIDAZOLE (CCD ID: IMD) (formula: C₃H₅N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			5	3	2		
4	A	1	Total	C	N	0	0
			5	3	2		
4	B	1	Total	C	N	0	0
			5	3	2		
4	B	1	Total	C	N	0	0
			5	3	2		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



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

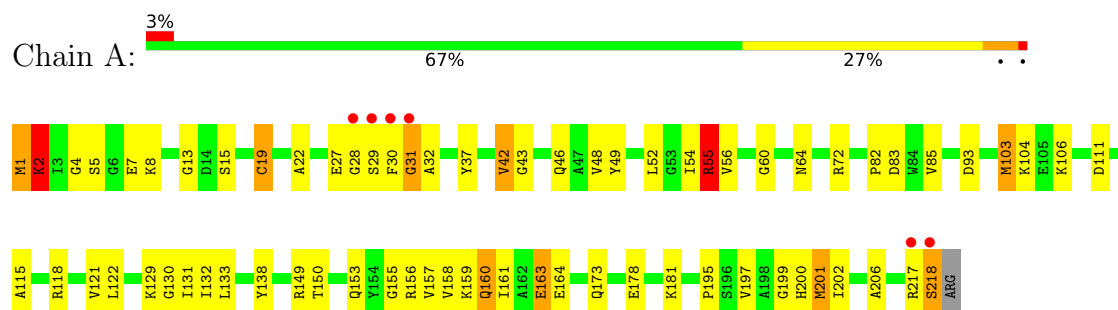
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	269	Total	O	0	0
			269	269		
6	B	286	Total	O	0	0
			286	286		

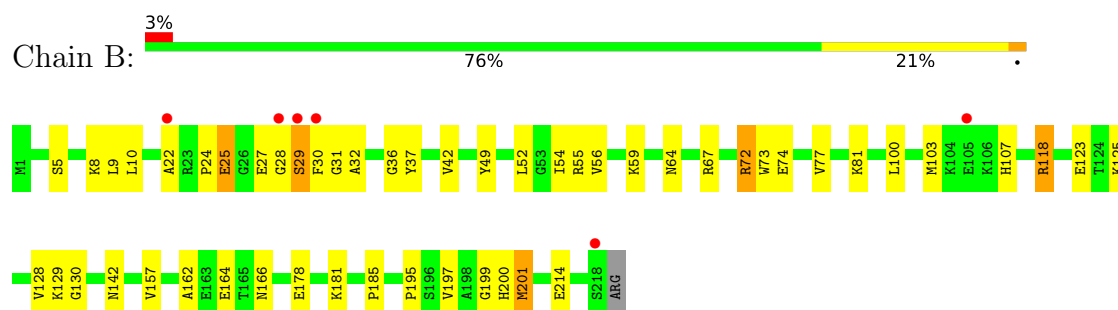
3 Residue-property plots

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: Acetyl xylan esterase



• Molecule 1: Acetyl xylan esterase



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	108.88Å 108.88Å 216.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.60 30.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-1.60) 99.9 (30.00-1.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.144 , 0.166 0.159 , 0.178	Depositor DCC
R_{free} test set	4273 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.637	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.1	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	0.97	EDS
Total number of atoms	4113	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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: IMD, CL, GOL, TRS

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	1.88	35/1812 (1.9%)	1.70	23/2452 (0.9%)
1	B	1.69	14/1812 (0.8%)	1.55	15/2453 (0.6%)
All	All	1.79	49/3624 (1.4%)	1.63	38/4905 (0.8%)

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	118	ARG	NE-CZ	9.20	1.43	1.33
1	B	22	ALA	N-CA	7.55	1.55	1.46
1	A	130	GLY	CA-C	7.33	1.59	1.51
1	A	55[A]	ARG	C-O	-7.08	1.15	1.24
1	A	55[B]	ARG	C-O	-7.08	1.15	1.24
1	A	48	VAL	CA-C	6.97	1.59	1.52
1	A	163	GLU	N-CA	6.71	1.54	1.46
1	B	128	VAL	CA-C	-6.66	1.44	1.52
1	B	118	ARG	CZ-NH1	6.60	1.42	1.32
1	A	4	GLY	CA-C	-6.59	1.45	1.52
1	A	121	VAL	CA-CB	-6.50	1.46	1.54
1	A	60	GLY	C-O	6.46	1.30	1.23
1	B	73	TRP	N-CA	-6.31	1.38	1.46
1	A	31	GLY	N-CA	-6.25	1.36	1.45
1	A	49	TYR	C-N	6.22	1.41	1.34
1	A	206	ALA	C-O	6.20	1.31	1.24
1	A	43	GLY	CA-C	-6.19	1.45	1.52
1	A	22	ALA	N-CA	6.16	1.53	1.46
1	A	160	GLN	CG-CD	6.14	1.67	1.52
1	A	7	GLU	CA-CB	-6.09	1.44	1.53
1	B	130	GLY	CA-C	6.05	1.58	1.51
1	A	115	ALA	CA-C	-5.95	1.45	1.52
1	A	130	GLY	N-CA	-5.91	1.38	1.45
1	A	159	LYS	CA-CB	-5.89	1.44	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	CYS	CA-CB	-5.72	1.44	1.53
1	A	122	LEU	CA-C	-5.68	1.45	1.52
1	A	42	VAL	CA-CB	-5.59	1.47	1.54
1	B	10	LEU	N-CA	-5.57	1.39	1.46
1	A	122	LEU	C-O	5.53	1.31	1.24
1	A	149	ARG	NE-CZ	5.51	1.39	1.33
1	A	82	PRO	N-CA	-5.50	1.40	1.47
1	B	107	HIS	CA-CB	-5.49	1.45	1.53
1	A	202	ILE	N-CA	5.47	1.52	1.46
1	A	103	MET	CA-CB	-5.45	1.44	1.53
1	A	13	GLY	N-CA	-5.40	1.40	1.45
1	B	142	ASN	CA-C	-5.40	1.46	1.52
1	A	157	VAL	CA-C	-5.39	1.46	1.52
1	B	77	VAL	N-CA	-5.37	1.39	1.46
1	A	7	GLU	N-CA	5.33	1.52	1.45
1	B	8	LYS	CA-C	5.32	1.59	1.52
1	A	46	GLN	CA-CB	-5.29	1.44	1.53
1	B	201	MET	N-CA	-5.27	1.39	1.46
1	A	160	GLN	C-O	5.22	1.30	1.24
1	A	156	ARG	N-CA	5.21	1.52	1.46
1	B	67	ARG	CD-NE	-5.21	1.39	1.46
1	A	131	ILE	C-N	5.20	1.39	1.33
1	B	178	GLU	N-CA	5.10	1.52	1.46
1	A	82	PRO	CA-C	-5.05	1.46	1.52
1	A	132	ILE	N-CA	-5.03	1.39	1.46

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	GLN	CB-CG-CD	9.66	129.02	112.60
1	A	150	THR	CA-C-O	7.43	128.63	120.82
1	A	129	LYS	N-CA-C	7.07	119.07	111.36
1	B	81	LYS	CA-C-O	7.03	125.32	120.47
1	A	48	VAL	N-CA-C	-6.78	106.41	111.90
1	A	93	ASP	CA-C-N	6.72	129.08	120.88
1	A	93	ASP	C-N-CA	6.72	129.08	120.88
1	B	36	GLY	O-C-N	-6.72	116.52	123.31
1	A	7	GLU	CG-CD-OE2	6.66	133.71	118.40
1	A	153	GLN	O-C-N	-6.65	115.07	122.12
1	A	118	ARG	NE-CZ-NH1	6.51	128.01	121.50
1	A	49	TYR	O-C-N	-6.44	115.18	121.17
1	B	129	LYS	N-CA-C	6.40	118.33	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	GLY	O-C-N	6.39	128.32	122.19
1	B	103	MET	N-CA-CB	6.27	117.38	110.35
1	A	133	LEU	CA-C-O	6.20	127.00	120.36
1	A	164	GLU	CA-CB-CG	6.11	126.33	114.10
1	B	49	TYR	O-C-N	-5.84	115.74	121.17
1	A	161	ILE	N-CA-CB	5.77	117.30	110.55
1	A	82	PRO	N-CA-C	5.69	119.95	111.41
1	B	197	VAL	CA-C-O	5.68	126.95	121.05
1	B	162	ALA	O-C-N	5.65	128.11	122.12
1	A	197	VAL	O-C-N	-5.60	116.41	121.89
1	B	100	LEU	CA-C-N	5.59	125.26	119.56
1	B	100	LEU	C-N-CA	5.59	125.26	119.56
1	A	2	LYS	CB-CG-CD	5.56	124.09	111.30
1	B	72	ARG	CA-C-N	5.55	127.71	120.28
1	B	72	ARG	C-N-CA	5.55	127.71	120.28
1	B	125	LYS	CA-C-N	-5.44	114.06	119.56
1	B	125	LYS	C-N-CA	-5.44	114.06	119.56
1	A	83	ASP	CA-C-O	5.40	125.92	119.60
1	A	158	VAL	O-C-N	5.21	127.15	121.94
1	A	201	MET	CG-SD-CE	-5.20	89.46	100.90
1	A	85	VAL	CA-C-O	5.19	125.79	120.39
1	A	111	ASP	N-CA-C	5.10	116.83	111.28
1	B	164	GLU	CA-CB-CG	-5.08	103.93	114.10
1	A	150	THR	N-CA-C	5.07	116.50	111.07
1	B	36	GLY	CA-C-O	5.04	126.56	121.72

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	1758	0	1788	36	0
1	B	1758	0	1789	27	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	1	0
3	B	1	0	0	0	0
4	A	10	0	10	2	0
4	B	10	0	10	5	0
5	B	8	0	12	1	0
6	A	269	0	0	9	0
6	B	286	0	0	5	0
All	All	4113	0	3625	65	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 9.

All (65) 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:55[B]:ARG:HH11	1:A:55[B]:ARG:HG3	1.14	1.09
1:A:138:TYR:H	1:A:173:GLN:HE22	1.27	0.83
1:A:55[B]:ARG:HH11	1:A:55[B]:ARG:CG	1.96	0.76
1:B:64:ASN:HD21	1:B:72:ARG:HE	1.34	0.75
1:A:1:MET:HA	1:A:1:MET:HE2	1.69	0.74
1:A:64:ASN:HD21	1:A:72:ARG:HE	1.37	0.72
1:A:30:PHE:O	1:A:31:GLY:C	2.34	0.70
5:B:304:TRS:H11	6:B:441:HOH:O	1.89	0.70
1:A:178:GLU:HG2	6:A:614:HOH:O	1.92	0.70
1:A:104:LYS:HD3	6:A:468:HOH:O	1.91	0.69
1:B:74:GLU:OE2	4:B:302:IMD:H2	1.96	0.65
4:A:304:IMD:H4	6:A:605:HOH:O	1.96	0.64
1:A:29:SER:HB2	6:A:576:HOH:O	1.99	0.63
1:B:123:GLU:CG	4:B:302:IMD:HN3	2.15	0.59
1:A:30:PHE:HD2	6:A:401:HOH:O	1.87	0.56
1:B:30:PHE:O	1:B:31:GLY:C	2.50	0.55
1:A:201:MET:HE1	1:B:201:MET:HE1	1.87	0.55
4:A:304:IMD:C4	6:A:605:HOH:O	2.51	0.54
1:B:64:ASN:ND2	1:B:72:ARG:HE	2.03	0.53
1:A:27[A]:GLU:OE2	1:A:55[A]:ARG:NH2	2.24	0.53
1:B:55:ARG:HH11	1:B:55:ARG:HG3	1.74	0.53
1:A:103:MET:HE2	1:A:106:LYS:HD2	1.90	0.52
1:A:200:HIS:HE1	6:A:617:HOH:O	1.93	0.51
1:A:27[A]:GLU:CD	1:A:55[A]:ARG:HH21	2.17	0.50
1:B:42:VAL:HG22	1:B:56:VAL:HG21	1.92	0.50
1:A:217:ARG:O	1:A:218:SER:HB2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:PRO:HB2	1:A:199:GLY:HA3	1.93	0.50
1:A:27[A]:GLU:HG3	1:A:56:VAL:O	2.13	0.49
1:B:37:TYR:H	1:B:200:HIS:CD2	2.31	0.49
1:A:30:PHE:C	1:A:32:ALA:N	2.66	0.49
1:A:1:MET:HE2	1:A:1:MET:CA	2.41	0.48
1:B:25:GLU:H	1:B:25:GLU:CD	2.21	0.48
1:B:9:LEU:HB3	1:B:54[B]:ILE:HD11	1.96	0.48
1:A:55[B]:ARG:HG3	1:A:55[B]:ARG:NH1	1.98	0.48
1:A:138:TYR:H	1:A:173:GLN:NE2	2.05	0.48
1:A:42:VAL:HG22	1:A:56:VAL:HG21	1.96	0.48
1:B:118:ARG:NH1	6:B:405:HOH:O	2.43	0.47
1:B:24:PRO:O	1:B:59:LYS:NZ	2.45	0.46
1:A:37:TYR:H	1:A:200:HIS:CD2	2.34	0.46
1:B:200:HIS:HE1	6:B:634:HOH:O	1.99	0.46
1:B:28:GLY:O	1:B:29:SER:HB3	2.15	0.46
1:A:28:GLY:O	1:A:29:SER:HB3	2.17	0.45
1:A:52:LEU:HG	1:A:54:ILE:HG23	1.97	0.45
1:B:37:TYR:H	1:B:200:HIS:HD2	1.66	0.44
1:B:123:GLU:HG3	4:B:302:IMD:HN3	1.83	0.44
1:A:29:SER:O	1:A:32:ALA:HB3	2.17	0.44
1:B:55:ARG:HG3	1:B:55:ARG:NH1	2.32	0.44
1:B:52:LEU:HG	1:B:54[A]:ILE:HG23	2.00	0.43
1:A:15:SER:OG	3:A:302:CL:CL	2.70	0.43
1:B:214:GLU:HG3	4:B:303:IMD:H2	2.00	0.43
1:A:160:GLN:OE1	1:A:163:GLU:OE2	2.37	0.43
1:B:166[A]:ASN:ND2	6:B:403:HOH:O	2.41	0.43
1:A:64:ASN:ND2	1:A:72:ARG:HE	2.09	0.43
1:A:2:LYS:HB3	1:A:2:LYS:NZ	2.35	0.42
1:B:64:ASN:HD21	1:B:72:ARG:NE	2.09	0.42
1:B:195:PRO:HB2	1:B:199:GLY:HA3	2.01	0.42
1:A:2:LYS:NZ	1:A:2:LYS:CB	2.81	0.41
1:B:29:SER:O	1:B:32:ALA:HB3	2.20	0.41
1:A:19:CYS:HB3	6:A:571:HOH:O	2.21	0.41
1:B:214:GLU:HG3	4:B:303:IMD:C2	2.51	0.41
1:A:8:LYS:HA	1:A:55[B]:ARG:HB2	2.02	0.41
1:B:181:LYS:HE3	6:B:589:HOH:O	2.21	0.40
1:A:181:LYS:HE3	6:A:577:HOH:O	2.21	0.40
1:A:1:MET:CA	1:A:1:MET:CE	2.98	0.40
1:B:27[A]:GLU:HG3	1:B:56:VAL:O	2.22	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	222/219 (101%)	212 (96%)	10 (4%)	0	100	100
1	B	222/219 (101%)	213 (96%)	8 (4%)	1 (0%)	24	10
All	All	444/438 (101%)	425 (96%)	18 (4%)	1 (0%)	43	24

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	29	SER

5.3.2 Protein sidechains [i](#)

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	189/184 (103%)	183 (97%)	6 (3%)	34	12
1	B	189/184 (103%)	185 (98%)	4 (2%)	47	23
All	All	378/368 (103%)	368 (97%)	10 (3%)	42	17

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	LYS
1	A	5	SER
1	A	55[A]	ARG
1	A	55[B]	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	218	SER
1	B	5	SER
1	B	25	GLU
1	B	157	VAL
1	B	185	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	80	GLN
1	A	173	GLN
1	A	200	HIS
1	B	64	ASN
1	B	144	GLN
1	B	200	HIS

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 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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
4	IMD	B	302	-	5,5,5	0.65	0	5,5,5	0.87	0
4	IMD	B	303	-	5,5,5	1.24	1 (20%)	5,5,5	1.05	0
2	GOL	A	301	-	5,5,5	0.56	0	5,5,5	1.39	1 (20%)
5	TRS	B	304	-	7,7,7	1.02	0	9,9,9	2.54	3 (33%)
4	IMD	A	304	-	5,5,5	1.72	1 (20%)	5,5,5	2.16	4 (80%)
4	IMD	A	303	-	5,5,5	1.14	0	5,5,5	0.89	0
2	GOL	B	305	-	5,5,5	1.32	2 (40%)	5,5,5	2.66	2 (40%)

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	IMD	B	302	-	-	-	0/1/1/1
4	IMD	B	303	-	-	-	0/1/1/1
2	GOL	A	301	-	-	4/4/4/4	-
5	TRS	B	304	-	-	9/9/9/9	-
4	IMD	A	304	-	-	-	0/1/1/1
4	IMD	A	303	-	-	-	0/1/1/1
2	GOL	B	305	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	304	IMD	C2-N1	2.95	1.45	1.34
2	B	305	GOL	O2-C2	2.06	1.49	1.43
2	B	305	GOL	C1-C2	2.02	1.59	1.51
4	B	303	IMD	C2-N3	2.01	1.41	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	304	TRS	O1-C1-C	5.77	126.97	110.88
2	B	305	GOL	O3-C3-C2	5.35	134.48	110.38
4	A	304	IMD	C5-N1-C2	2.85	113.33	107.19
5	B	304	TRS	C3-C-C2	2.81	118.15	110.66
5	B	304	TRS	O3-C3-C	2.60	118.12	110.88
4	A	304	IMD	C4-C5-N1	-2.30	100.90	106.79
4	A	304	IMD	N1-C2-N3	-2.27	100.98	110.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	305	GOL	O2-C2-C3	-2.25	99.87	109.18
4	A	304	IMD	C4-N3-C2	2.12	114.59	106.40
2	A	301	GOL	O2-C2-C1	-2.02	100.81	109.18

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	305	GOL	C1-C2-C3-O3
5	B	304	TRS	C2-C-C1-O1
5	B	304	TRS	C3-C-C1-O1
5	B	304	TRS	N-C-C1-O1
5	B	304	TRS	N-C-C2-O2
5	B	304	TRS	C1-C-C3-O3
2	A	301	GOL	O1-C1-C2-O2
2	A	301	GOL	O1-C1-C2-C3
2	A	301	GOL	C1-C2-C3-O3
2	A	301	GOL	O2-C2-C3-O3
2	B	305	GOL	O2-C2-C3-O3
5	B	304	TRS	C3-C-C2-O2
5	B	304	TRS	C2-C-C3-O3
5	B	304	TRS	C1-C-C2-O2
5	B	304	TRS	N-C-C3-O3

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	302	IMD	3	0
4	B	303	IMD	2	0
5	B	304	TRS	1	0
4	A	304	IMD	2	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 [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	218/219 (99%)	-0.18	6 (2%) 55 58	9, 17, 35, 57	6 (2%)
1	B	218/219 (99%)	-0.21	6 (2%) 55 58	9, 17, 34, 46	6 (2%)
All	All	436/438 (99%)	-0.20	12 (2%) 55 58	9, 17, 35, 57	12 (2%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	30	PHE	7.7
1	B	30	PHE	6.1
1	A	29	SER	3.2
1	B	28	GLY	3.1
1	B	218	SER	2.9
1	B	22	ALA	2.6
1	A	28	GLY	2.5
1	A	217	ARG	2.3
1	B	29	SER	2.3
1	B	105	GLU	2.1
1	A	31	GLY	2.1
1	A	218	SER	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(Å ²)	Q<0.9
4	IMD	B	303	5/5	0.62	0.20	42,47,51,52	0
4	IMD	A	303	5/5	0.66	0.20	46,50,56,56	0
4	IMD	A	304	5/5	0.82	0.15	23,25,34,35	0
2	GOL	B	305	6/6	0.87	0.14	22,32,35,47	0
5	TRS	B	304	8/8	0.87	0.14	24,40,56,58	0
4	IMD	B	302	5/5	0.89	0.10	25,30,34,38	0
2	GOL	A	301	6/6	0.92	0.12	26,42,46,48	0
3	CL	A	302	1/1	0.99	0.09	21,21,21,21	1
3	CL	B	301	1/1	1.00	0.14	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.