



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:29 PM UTC

PDB ID : 9QBP / pdb_00009qbp
Title : Crystal structure of Enhydrobacter aerosaccus apo SPARDA complex
Authors : Manakova, E.N.; Grazulis, S.; Zaremba, M.
Deposited on : 2025-03-03
Resolution : 2.45 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

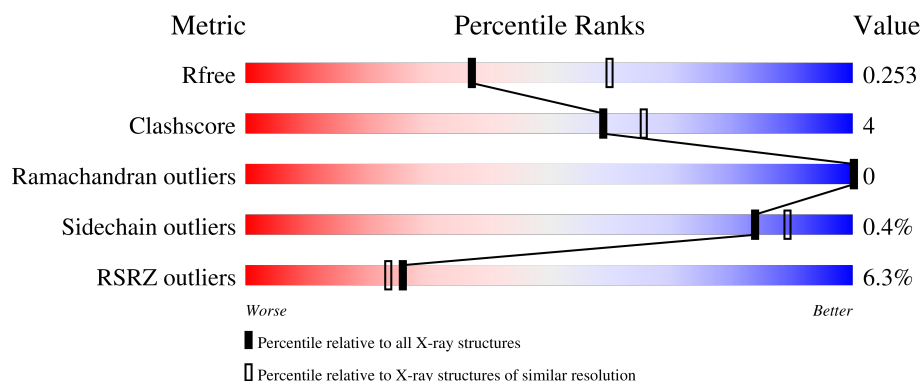
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	467	<div> <div>7%</div> <div>53%</div> <div>7%</div> <div>40%</div> </div>
1	C	467	<div> <div>4%</div> <div>81%</div> <div>7%</div> <div>11%</div> </div>
2	B	484	<div> <div>4%</div> <div>86%</div> <div>10%</div> <div>.</div> </div>
2	D	484	<div> <div>6%</div> <div>85%</div> <div>12%</div> <div>.</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13521 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 DUF4365 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	43	3	0
			2341	1492	424	422	3			
1	C	414	Total	C	N	O	S	37	0	0
			3347	2124	597	621	5			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP A0A1T4TDU6
A	-19	GLY	-	expression tag	UNP A0A1T4TDU6
A	-18	GLY	-	expression tag	UNP A0A1T4TDU6
A	-17	SER	-	expression tag	UNP A0A1T4TDU6
A	-16	HIS	-	expression tag	UNP A0A1T4TDU6
A	-15	HIS	-	expression tag	UNP A0A1T4TDU6
A	-14	HIS	-	expression tag	UNP A0A1T4TDU6
A	-13	HIS	-	expression tag	UNP A0A1T4TDU6
A	-12	HIS	-	expression tag	UNP A0A1T4TDU6
A	-11	HIS	-	expression tag	UNP A0A1T4TDU6
A	-10	GLY	-	expression tag	UNP A0A1T4TDU6
A	-9	MET	-	expression tag	UNP A0A1T4TDU6
A	-8	ALA	-	expression tag	UNP A0A1T4TDU6
A	-7	SER	-	expression tag	UNP A0A1T4TDU6
A	-6	GLU	-	expression tag	UNP A0A1T4TDU6
A	-5	ASN	-	expression tag	UNP A0A1T4TDU6
A	-4	LEU	-	expression tag	UNP A0A1T4TDU6
A	-3	TYR	-	expression tag	UNP A0A1T4TDU6
A	-2	PHE	-	expression tag	UNP A0A1T4TDU6
A	-1	GLN	-	expression tag	UNP A0A1T4TDU6
A	0	GLY	-	expression tag	UNP A0A1T4TDU6
A	1	GLY	-	expression tag	UNP A0A1T4TDU6
C	-20	MET	-	initiating methionine	UNP A0A1T4TDU6
C	-19	GLY	-	expression tag	UNP A0A1T4TDU6
C	-18	GLY	-	expression tag	UNP A0A1T4TDU6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	SER	-	expression tag	UNP A0A1T4TDU6
C	-16	HIS	-	expression tag	UNP A0A1T4TDU6
C	-15	HIS	-	expression tag	UNP A0A1T4TDU6
C	-14	HIS	-	expression tag	UNP A0A1T4TDU6
C	-13	HIS	-	expression tag	UNP A0A1T4TDU6
C	-12	HIS	-	expression tag	UNP A0A1T4TDU6
C	-11	HIS	-	expression tag	UNP A0A1T4TDU6
C	-10	GLY	-	expression tag	UNP A0A1T4TDU6
C	-9	MET	-	expression tag	UNP A0A1T4TDU6
C	-8	ALA	-	expression tag	UNP A0A1T4TDU6
C	-7	SER	-	expression tag	UNP A0A1T4TDU6
C	-6	GLU	-	expression tag	UNP A0A1T4TDU6
C	-5	ASN	-	expression tag	UNP A0A1T4TDU6
C	-4	LEU	-	expression tag	UNP A0A1T4TDU6
C	-3	TYR	-	expression tag	UNP A0A1T4TDU6
C	-2	PHE	-	expression tag	UNP A0A1T4TDU6
C	-1	GLN	-	expression tag	UNP A0A1T4TDU6
C	0	GLY	-	expression tag	UNP A0A1T4TDU6
C	1	GLY	-	expression tag	UNP A0A1T4TDU6

- Molecule 2 is a protein called Protein argonaute.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	465	Total	C	N	O	S	14	1	0
			3676	2338	660	674	4			
2	D	470	Total	C	N	O	S	19	4	0
			3744	2376	675	689	4			

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

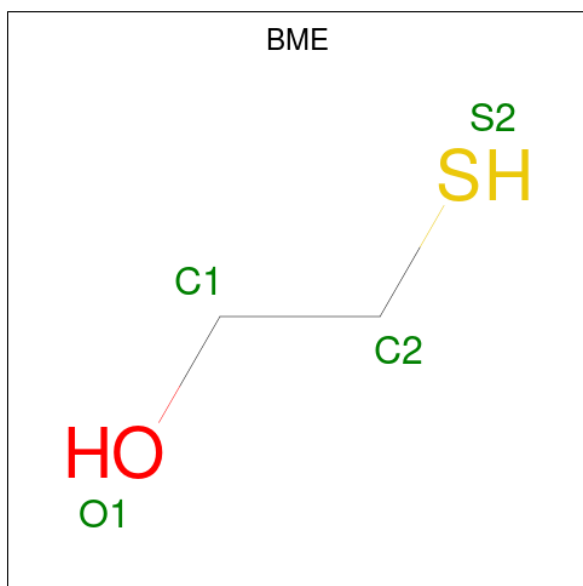
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		
3	B	3	Total	Cl	0	0
			3	3		
3	C	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



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

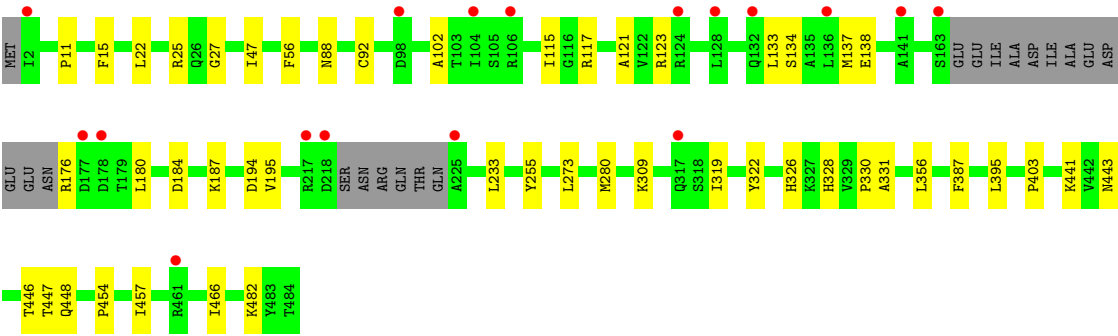
- Molecule 5 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



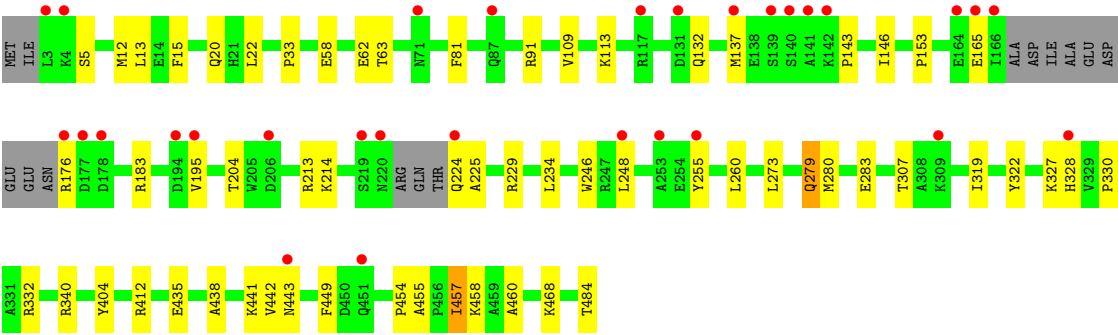
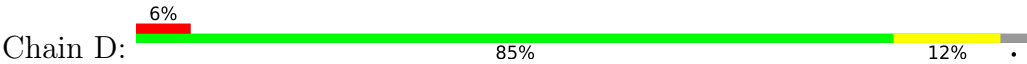
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	32	Total 32	O 32	0	0
6	B	128	Total 128	O 128	0	0
6	C	63	Total 63	O 63	0	0
6	D	163	Total 163	O 163	0	0



● Molecule 2: Protein argonaute



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.18Å 127.24Å 191.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.17 – 2.45 94.17 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.7 (94.17-2.45) 99.9 (94.17-2.45)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.45Å)	Xtriage
Refinement program	PHENIX (1.20_4459: ???)	Depositor
R, R_{free}	0.205 , 0.248 0.211 , 0.253	Depositor DCC
R_{free} test set	9815 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å ²)	53.0	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13521	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: BME, CL, 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	0.17	0/2394	0.34	1/3241 (0.0%)
1	C	0.17	0/3418	0.35	0/4626
2	B	0.20	0/3756	0.36	0/5095
2	D	0.19	0/3827	0.36	0/5188
All	All	0.18	0/13395	0.35	1/18150 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	PHE	CA-CB-CG	5.00	118.80	113.80

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	2341	0	2324	27	0
1	C	3347	0	3323	28	0
2	B	3676	0	3714	31	0
2	D	3744	0	3778	40	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	B	8	0	12	0	0
5	D	12	0	18	1	0
6	A	32	0	0	0	0
6	B	128	0	0	0	0
6	C	63	0	0	0	0
6	D	163	0	0	0	0
All	All	13521	0	13169	114	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 (114) 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)
2:D:260:LEU:HD13	2:D:280:MET:HE3	1.57	0.84
1:A:307:ALA:HA	1:A:320:VAL:HG12	1.60	0.82
1:A:93:LEU:HD13	2:B:22:LEU:HD23	1.61	0.81
2:B:117:ARG:NH1	1:C:212:ARG:HH12	1.80	0.78
2:B:11:PRO:HG2	2:B:441:LYS:HD2	1.70	0.72
2:B:443:ASN:HD21	2:B:446:THR:HG22	1.52	0.72
1:C:98:VAL:H	1:C:116:THR:HG22	1.54	0.71
2:B:117:ARG:HH12	1:C:212:ARG:HH12	1.37	0.71
2:B:454:PRO:HG2	2:B:457:ILE:HD12	1.73	0.71
2:B:117:ARG:NH1	1:C:212:ARG:NH1	2.38	0.70
2:D:441:LYS:O	2:D:443:ASN:ND2	2.28	0.67
1:A:170:LEU:CD2	1:A:339:VAL:HG22	2.24	0.67
1:A:93:LEU:HD13	2:B:22:LEU:CD2	2.27	0.65
1:A:168:ILE:HD13	1:A:170:LEU:HD12	1.79	0.63
2:D:146:ILE:HD12	2:D:195:VAL:HG11	1.81	0.62
1:C:168:ILE:HG12	1:C:170:LEU:HG	1.82	0.62
2:D:280:MET:HE1	2:D:319:ILE:HD13	1.82	0.61
1:A:218:ASP:HB3	1:A:221:GLU:HG3	1.83	0.60
2:D:137:MET:HE2	2:D:195:VAL:HG22	1.84	0.60
2:B:446:THR:HG23	2:B:448:GLN:H	1.69	0.58
2:B:194:ASP:OD1	2:B:482:LYS:HE3	2.03	0.58
2:D:332:ARG:NH2	2:D:435:GLU:OE2	2.37	0.57
1:A:168:ILE:CD1	1:A:170:LEU:HD12	2.34	0.57
1:C:114:ASP:OD1	1:C:116:THR:HG23	2.05	0.56
2:D:255:TYR:HB3	2:D:328:HIS:NE2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:GLY:HA2	2:D:165:GLU:OE1	2.07	0.55
2:D:279:GLN:OE1	2:D:460:ALA:HA	2.08	0.54
2:B:123:ARG:CZ	2:B:180:LEU:HD11	2.37	0.54
1:A:173:ILE:HD11	1:A:338:VAL:HB	1.89	0.54
2:D:248:LEU:HD22	2:D:438:ALA:HB1	1.89	0.54
2:B:137:MET:SD	2:B:195:VAL:HG21	2.48	0.54
1:A:181:ILE:HG22	1:A:214[B]:VAL:HG12	1.90	0.53
2:D:340:ARG:HH11	2:D:340:ARG:HG3	1.74	0.53
2:D:441:LYS:HD2	2:D:449:PHE:HB2	1.91	0.53
2:B:273:LEU:HD21	2:D:273:LEU:HD21	1.90	0.53
1:A:272:LEU:HD21	1:C:352:ARG:HH22	1.74	0.51
1:A:328:ARG:HB3	1:A:339:VAL:HB	1.93	0.51
1:A:168:ILE:HG12	1:A:170:LEU:HG	1.93	0.51
1:C:432:LYS:NZ	1:C:433:GLU:HG2	2.25	0.51
2:D:137:MET:SD	2:D:143:PRO:HD2	2.51	0.51
1:C:60:ALA:HB3	1:C:98:VAL:HG22	1.93	0.50
1:A:88:LEU:HD13	1:A:98:VAL:HG11	1.93	0.50
2:D:183:ARG:NH2	2:D:484:THR:OXT	2.45	0.50
1:A:212[B]:ARG:HG2	1:A:212[B]:ARG:HH11	1.77	0.50
2:D:109:VAL:HG12	2:D:113:LYS:HE2	1.94	0.49
1:A:246:ASP:HB3	1:A:249:ASP:HB2	1.95	0.49
1:C:39:GLY:HA3	1:C:63:VAL:O	2.12	0.49
1:A:291:TYR:CE2	1:A:293:TYR:HB3	2.48	0.48
1:A:288:SER:OG	1:A:307:ALA:N	2.38	0.48
1:A:282:ALA:HB2	1:A:322:HIS:HE1	1.79	0.48
1:C:201:ASN:OD1	1:C:222:TYR:HA	2.13	0.48
2:D:113:LYS:HD3	2:D:153:PRO:HB2	1.94	0.48
2:D:322:TYR:CD1	2:D:330:PRO:HD3	2.49	0.48
1:A:170:LEU:HD23	1:A:339:VAL:HG22	1.94	0.47
1:C:207:VAL:HB	1:C:214:VAL:HG23	1.95	0.47
2:B:115:ILE:HB	2:B:121:ALA:HB2	1.95	0.47
1:C:68:GLU:HA	1:C:106:SER:HB3	1.97	0.47
1:C:258:ARG:HG2	1:C:258:ARG:HH11	1.79	0.47
2:D:307:THR:HB	5:D:504:BME:H21	1.95	0.47
2:B:280:MET:HE1	2:B:319:ILE:HD13	1.96	0.47
2:B:255:TYR:HB2	2:B:331:ALA:HB3	1.96	0.46
1:A:193:VAL:HG21	1:C:356:TYR:CD2	2.50	0.46
2:D:33:PRO:HD2	2:D:91:ARG:HG3	1.96	0.46
2:B:134:SER:O	2:B:138:GLU:HG2	2.16	0.46
2:D:176:ARG:HA	2:D:176:ARG:HD3	1.70	0.46
2:B:319:ILE:HG21	2:B:356:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:TRP:HZ2	2:B:403:PRO:HA	1.81	0.45
2:B:56:PHE:HE1	2:B:233:LEU:HD21	1.81	0.45
1:C:67:LYS:O	1:C:68:GLU:HG2	2.16	0.45
1:A:182:ALA:HB2	1:A:233:VAL:HA	1.97	0.45
1:C:36:LEU:HD23	1:C:36:LEU:HA	1.78	0.45
2:D:454:PRO:HG2	2:D:457:ILE:HD12	1.98	0.45
2:D:327:LYS:HD3	2:D:327:LYS:HA	1.66	0.45
2:D:283:GLU:H	2:D:283:GLU:CD	2.25	0.45
2:D:458:LYS:HE3	2:D:458:LYS:HB2	1.73	0.45
2:D:58:GLU:O	2:D:62:GLU:HG3	2.17	0.45
1:A:214[B]:VAL:HG11	1:A:241:PHE:CZ	2.52	0.44
1:A:207:VAL:HB	1:A:214[B]:VAL:HG23	1.98	0.44
2:D:332:ARG:HH22	2:D:435:GLU:CD	2.25	0.44
1:C:189:GLY:O	1:C:193:VAL:HG23	2.18	0.44
1:C:214:VAL:HG11	1:C:241:PHE:CZ	2.53	0.44
1:C:20:LYS:O	1:C:24:LEU:HG	2.17	0.44
2:D:12:MET:HE3	2:D:20:GLN:HB3	1.99	0.44
1:C:258:ARG:HG2	1:C:258:ARG:NH1	2.33	0.43
1:A:365:LYS:HA	1:A:365:LYS:HD2	1.71	0.43
2:B:194:ASP:O	2:B:194:ASP:CG	2.61	0.43
1:C:209:ARG:HH22	1:C:248:ASP:HA	1.84	0.43
1:C:414:GLU:O	2:D:5:SER:OG	2.36	0.43
2:D:442:VAL:HB	2:D:455:ALA:HB2	2.00	0.42
1:A:208:ILE:HD11	1:A:227:ILE:HD12	2.00	0.42
2:D:225:ALA:O	2:D:229:ARG:HG3	2.19	0.42
2:B:15:PHE:CZ	2:B:27:GLY:HA3	2.54	0.42
2:B:88:ASN:ND2	2:B:92:CYS:H	2.17	0.42
1:C:246:ASP:O	1:C:250:THR:HG23	2.19	0.42
2:D:13:LEU:HB2	2:D:15:PHE:CE1	2.54	0.42
2:B:47:ILE:HG12	2:B:102:ALA:HB3	2.02	0.42
2:B:326:HIS:HB3	2:B:328:HIS:CE1	2.55	0.42
2:D:132:GLN:HA	2:D:132:GLN:OE1	2.20	0.42
2:B:133:LEU:HD12	2:B:133:LEU:HA	1.86	0.42
2:B:322:TYR:CD1	2:B:330:PRO:HD3	2.55	0.42
2:D:81:PHE:CZ	2:D:234:LEU:HD12	2.55	0.42
2:D:22:LEU:HD11	2:D:404:TYR:CG	2.55	0.41
1:A:212[A]:ARG:HA	1:A:212[A]:ARG:HD3	1.89	0.41
2:B:25:ARG:HG3	2:B:447:THR:HB	2.02	0.41
2:D:224:GLN:C	2:D:229:ARG:HH21	2.28	0.41
1:C:205:ASP:OD1	1:C:205:ASP:N	2.42	0.41
2:D:213:ARG:HD2	2:D:214:LYS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:246:TRP:HZ3	2:D:248:LEU:HG	1.85	0.41
2:B:187:LYS:HB2	2:B:466:ILE:HG12	2.03	0.41
2:D:204:THR:O	2:D:229:ARG:HD2	2.21	0.41
2:B:176:ARG:NH2	2:B:184:ASP:OD2	2.54	0.40
2:B:387:PHE:HA	2:B:395:LEU:O	2.22	0.40
1:C:365:LYS:O	2:D:412[A]:ARG:HD3	2.21	0.40
1:C:432:LYS:HZ3	1:C:433:GLU:HG2	1.83	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	277/467 (59%)	264 (95%)	13 (5%)	0	100	100
1	C	408/467 (87%)	396 (97%)	12 (3%)	0	100	100
2	B	460/484 (95%)	446 (97%)	14 (3%)	0	100	100
2	D	468/484 (97%)	458 (98%)	10 (2%)	0	100	100
All	All	1613/1902 (85%)	1564 (97%)	49 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	252/398 (63%)	251 (100%)	1 (0%)	84	89
1	C	358/398 (90%)	358 (100%)	0	100	100
2	B	390/406 (96%)	389 (100%)	1 (0%)	86	91
2	D	398/406 (98%)	394 (99%)	4 (1%)	68	77
All	All	1398/1608 (87%)	1392 (100%)	6 (0%)	84	89

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	PHE
2	B	309	LYS
2	D	63	THR
2	D	279	GLN
2	D	457	ILE
2	D	468	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	322	HIS
2	B	279	GLN
2	B	296	GLN
2	B	469	HIS
1	C	127	GLN
1	C	201	ASN
1	C	376	GLN
2	D	303	HIS
2	D	379	ASN
2	D	469	HIS

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

Of 11 ligands modelled in this entry, 7 are monoatomic - leaving 4 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	BME	D	504	-	3,3,3	0.33	0	2,2,2	0.19	0
5	BME	D	503	-	3,3,3	0.20	0	2,2,2	0.40	0
4	TRS	B	504	-	7,7,7	0.10	0	9,9,9	0.20	0
5	BME	D	502	-	3,3,3	0.20	0	2,2,2	0.29	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	BME	D	504	-	-	0/1/1/1	-
5	BME	D	503	-	-	0/1/1/1	-
4	TRS	B	504	-	-	0/9/9/9	-
5	BME	D	502	-	-	0/1/1/1	-

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	504	BME	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	282/467 (60%)	0.94	35 (12%) 8 7	27, 70, 115, 158	11 (3%)
1	C	414/467 (88%)	0.53	21 (5%) 33 31	42, 67, 96, 149	8 (1%)
2	B	465/484 (96%)	0.31	17 (3%) 45 45	27, 58, 81, 116	5 (1%)
2	D	470/484 (97%)	0.18	30 (6%) 25 23	26, 52, 84, 135	9 (1%)
All	All	1631/1902 (85%)	0.44	103 (6%) 26 23	26, 60, 97, 158	33 (2%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	437	ARG	6.2
1	A	309	THR	5.7
1	A	93	LEU	5.5
1	A	98	VAL	5.5
1	A	318	GLY	5.4
2	D	166	ILE	5.3
1	A	160	LEU	5.1
2	B	2	ILE	4.9
1	C	391	ASN	4.7
2	B	178	ASP	4.6
1	C	7	ASP	4.5
1	A	86	ALA	4.5
2	B	141	ALA	4.3
2	D	141	ALA	4.2
1	A	88	LEU	4.1
2	D	142	LYS	3.9
2	D	443	ASN	3.9
2	D	3	LEU	3.8
1	A	358	GLU	3.6
1	C	124	ARG	3.5
1	A	90	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	148	VAL	3.5
1	A	403	VAL	3.5
1	A	389	SER	3.4
2	D	253	ALA	3.3
2	B	317[A]	GLN	3.2
1	A	258[A]	ARG	3.2
1	C	318	GLY	3.2
1	C	402	ASP	3.2
1	C	297	VAL	3.2
2	D	4	LYS	3.1
2	D	164	GLU	3.1
1	A	294	LEU	3.1
1	C	310	ASN	3.1
1	A	356	TYR	3.0
2	D	117[A]	ARG	3.0
2	D	220	ASN	3.0
2	D	255	TYR	3.0
2	B	177	ASP	3.0
1	C	122	GLU	2.9
2	D	139	SER	2.9
2	D	176	ARG	2.9
2	B	218	ASP	2.8
1	C	356	TYR	2.8
1	A	159	PRO	2.8
2	B	136	LEU	2.7
1	C	9	GLN	2.7
1	A	190	ARG	2.7
1	A	297	VAL	2.6
1	C	309	THR	2.6
1	C	240	ILE	2.6
1	A	349	ASP	2.6
2	D	131	ASP	2.6
2	B	163	SER	2.6
2	D	140	SER	2.6
1	A	308	TYR	2.5
2	B	225	ALA	2.5
1	C	28	PHE	2.5
1	A	170	LEU	2.4
1	A	87	ASP	2.4
2	D	87	GLN	2.4
2	B	124	ARG	2.4
2	D	165	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	355	ARG	2.3
1	A	295	ALA	2.3
2	D	224	GLN	2.3
1	A	319	TYR	2.3
1	A	285	THR	2.3
1	A	96	ILE	2.3
1	C	296	ASN	2.3
1	C	437	ARG	2.3
2	D	248	LEU	2.3
1	A	344	PHE	2.3
2	D	195	VAL	2.3
2	D	194	ASP	2.2
2	D	206	ASP	2.2
1	C	123	GLU	2.2
1	C	150	ARG	2.2
2	B	461	ARG	2.2
2	B	104	ILE	2.2
2	B	217	ARG	2.2
1	C	38	ALA	2.2
2	B	98	ASP	2.2
2	D	178	ASP	2.2
2	D	177	ASP	2.2
1	A	274	LYS	2.2
2	B	106	ARG	2.1
1	A	298	LYS	2.1
2	D	309[A]	LYS	2.1
1	A	91	TRP	2.1
2	D	137	MET	2.1
2	D	451	GLN	2.1
1	A	300	THR	2.1
1	A	212[A]	ARG	2.1
2	B	132	GLN	2.1
1	C	120	ARG	2.1
2	B	128	LEU	2.1
2	D	219	SER	2.1
1	C	85	PRO	2.1
1	A	360	LEU	2.0
2	D	71	ASN	2.0
1	A	323	HIS	2.0
2	D	328	HIS	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(\AA^2)	Q<0.9
5	BME	D	504	4/4	0.70	0.27	53,61,70,91	0
4	TRS	B	504	8/8	0.76	0.20	67,76,81,82	0
3	CL	A	502	1/1	0.81	0.13	108,108,108,108	0
3	CL	B	502	1/1	0.83	0.13	89,89,89,89	0
5	BME	D	502	4/4	0.87	0.18	77,78,80,89	0
3	CL	B	503	1/1	0.87	0.14	99,99,99,99	0
3	CL	C	501	1/1	0.89	0.18	77,77,77,77	0
3	CL	A	501	1/1	0.89	0.14	84,84,84,84	0
5	BME	D	503	4/4	0.90	0.14	60,62,74,84	0
3	CL	B	501	1/1	0.98	0.07	59,59,59,59	0
3	CL	D	501	1/1	0.99	0.04	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.