



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:45 PM UTC

PDB ID : 4KRT / pdb_00004krt
Title : X-ray structure of endolysin from clostridium perfringens phage phiSM101
Authors : Kamitori, S.; Yoshida, H.
Deposited on : 2013-05-17
Resolution : 1.92 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

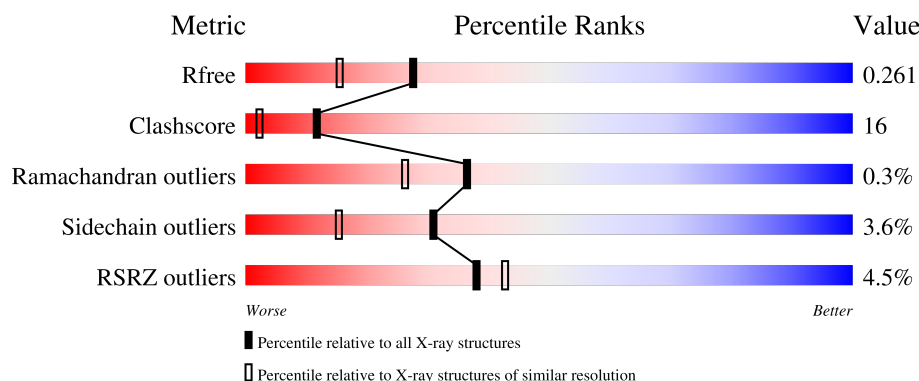
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	353	2% 74% 23% ..
1	B	353	7% 64% 30% ..

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
3	ACT	B	502	-	-	X	-
3	ACT	B	503	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5945 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 Autolytic lysozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2779	1765	468	539	7			
1	B	342	Total	C	N	O	S	0	0	0
			2729	1735	453	534	7			

There are 22 discrepancies between the modelled and reference sequences:

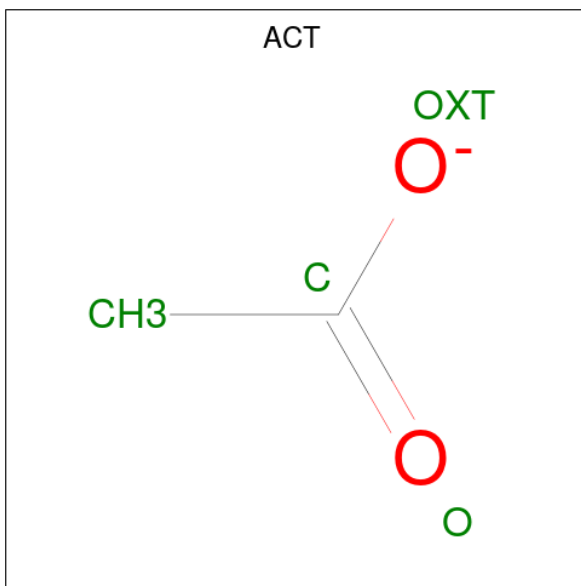
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q0SPG7
A	-10	ASN	-	expression tag	UNP Q0SPG7
A	-9	HIS	-	expression tag	UNP Q0SPG7
A	-8	LYS	-	expression tag	UNP Q0SPG7
A	-7	VAL	-	expression tag	UNP Q0SPG7
A	-6	HIS	-	expression tag	UNP Q0SPG7
A	-5	HIS	-	expression tag	UNP Q0SPG7
A	-4	HIS	-	expression tag	UNP Q0SPG7
A	-3	HIS	-	expression tag	UNP Q0SPG7
A	-2	HIS	-	expression tag	UNP Q0SPG7
A	-1	HIS	-	expression tag	UNP Q0SPG7
B	-10	MET	-	expression tag	UNP Q0SPG7
B	-9	ASN	-	expression tag	UNP Q0SPG7
B	-8	HIS	-	expression tag	UNP Q0SPG7
B	-7	LYS	-	expression tag	UNP Q0SPG7
B	-6	VAL	-	expression tag	UNP Q0SPG7
B	-5	HIS	-	expression tag	UNP Q0SPG7
B	-4	HIS	-	expression tag	UNP Q0SPG7
B	-3	HIS	-	expression tag	UNP Q0SPG7
B	-2	HIS	-	expression tag	UNP Q0SPG7
B	-1	HIS	-	expression tag	UNP Q0SPG7
B	0	HIS	-	expression tag	UNP Q0SPG7

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2^-$).



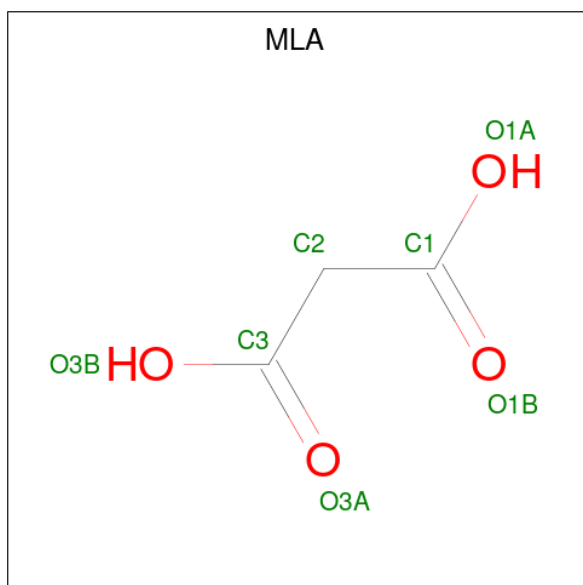
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

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

- Molecule 4 is MALONIC ACID (CCD ID: MLA) (formula: $C_3H_4O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 7	C 3	O 4	0	0
4	B	1	Total 7	C 3	O 4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	204	Total 204	O 204	0	0
5	B	148	Total 148	O 148	0	0

- Molecule 1: Autolytic lysozyme



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.60Å 112.90Å 64.95Å 90.00° 91.35° 90.00°	Depositor
Resolution (Å)	22.36 – 1.92 22.36 – 1.92	Depositor EDS
% Data completeness (in resolution range)	91.1 (22.36-1.92) 91.2 (22.36-1.92)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 1.92Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.226 , 0.261 0.226 , 0.261	Depositor DCC
R_{free} test set	2815 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5945	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% 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: MLA, EPE, ACT

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	0.39	0/2843	0.89	8/3849 (0.2%)
1	B	0.37	0/2788	0.87	6/3774 (0.2%)
All	All	0.38	0/5631	0.88	14/7623 (0.2%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	202	ILE	N-CA-C	7.90	117.96	110.53
1	A	230	ASN	N-CA-C	-6.41	105.46	113.28
1	A	174	VAL	N-CA-C	-6.32	106.02	113.42
1	A	323	ARG	N-CA-C	-5.68	100.03	109.46
1	B	24	GLU	N-CA-C	-5.67	104.71	111.69
1	A	129	GLY	N-CA-C	-5.61	107.22	115.30
1	A	324	ILE	N-CA-C	5.53	115.57	108.82
1	B	129	GLY	N-CA-C	-5.39	107.54	115.30
1	B	323	ARG	N-CA-C	-5.36	100.56	109.46
1	B	257	TYR	N-CA-C	-5.23	100.65	108.96
1	A	99	ALA	N-CA-C	5.22	117.74	109.24
1	A	63	VAL	N-CA-C	5.19	116.84	108.85
1	B	63	VAL	N-CA-C	5.05	116.63	108.85
1	A	24	GLU	N-CA-C	-5.02	105.81	111.28

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	2779	0	2648	60	0
1	B	2729	0	2613	109	0
2	A	15	0	17	4	0
3	A	28	0	21	2	0
3	B	28	0	21	7	0
4	A	7	0	2	0	0
4	B	7	0	2	0	0
5	A	204	0	0	6	0
5	B	148	0	0	10	0
All	All	5945	0	5324	174	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 16.

All (174) 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:232:LYS:HD2	1:A:232:LYS:H	1.14	1.08
1:B:232:LYS:H	1:B:232:LYS:HD2	1.17	1.04
1:A:285:THR:HG23	1:A:286:PHE:H	1.26	1.00
1:B:228:THR:HG22	1:B:230:ASN:H	1.27	0.99
1:A:123:GLU:O	1:A:127:LEU:HD23	1.64	0.96
1:B:222:ASN:H	3:B:503:ACT:H3	1.27	0.96
1:A:55:GLY:O	1:A:58:GLU:HG2	1.68	0.94
1:B:104:THR:HG22	5:B:653:HOH:O	1.70	0.90
1:B:206:ASN:HD21	1:B:308:ILE:H	1.17	0.89
1:B:232:LYS:H	1:B:232:LYS:CD	1.84	0.89
1:A:232:LYS:H	1:A:232:LYS:CD	1.91	0.82
1:A:238:PRO:HG2	1:A:241:GLU:HG3	1.63	0.81
1:B:232:LYS:HD2	1:B:232:LYS:N	1.95	0.81
1:B:285:THR:HG23	1:B:286:PHE:H	1.49	0.78
1:B:1:MET:HA	3:B:502:ACT:H3	1.65	0.77
1:B:108:VAL:HG11	1:B:116:MET:HE2	1.67	0.75
1:B:238:PRO:HG2	1:B:241:GLU:HG3	1.69	0.73
1:B:108:VAL:HG11	1:B:116:MET:CE	2.18	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:LEU:HA	1:B:116:MET:HE2	1.71	0.73
1:A:322:TYR:CE2	1:A:339:VAL:HG21	2.25	0.71
1:B:113:LEU:HA	1:B:116:MET:CE	2.20	0.71
1:B:114:THR:O	1:B:118:ILE:HG12	1.92	0.70
1:B:298:ARG:HH11	1:B:298:ARG:HB3	1.56	0.70
1:B:222:ASN:N	3:B:503:ACT:H3	2.05	0.70
1:B:2:GLN:HG3	5:B:732:HOH:O	1.92	0.69
1:A:228:THR:HG22	1:A:230:ASN:H	1.58	0.68
1:A:250:GLU:HG2	5:A:645:HOH:O	1.94	0.68
1:A:285:THR:HG23	1:A:286:PHE:N	2.06	0.67
1:A:223:ILE:HD13	1:A:267:VAL:CG1	2.25	0.67
1:A:232:LYS:HD2	1:A:232:LYS:N	1.98	0.66
1:B:172:SER:HA	5:B:732:HOH:O	1.96	0.65
1:B:310:ARG:HD2	1:B:312:ASP:OD1	1.96	0.65
1:A:37:LYS:HB2	1:A:66:TYR:CZ	2.32	0.64
1:B:285:THR:HG23	1:B:286:PHE:N	2.12	0.64
2:A:401:EPE:H92	5:A:632:HOH:O	1.98	0.64
1:A:238:PRO:HG2	1:A:241:GLU:CG	2.28	0.64
1:B:322:TYR:CE2	1:B:339:VAL:HG21	2.33	0.64
1:B:174:VAL:HG12	1:B:199:GLU:HB3	1.80	0.63
1:A:223:ILE:HD11	1:A:237:ILE:HD11	1.81	0.63
1:B:22:ASN:O	1:B:26:VAL:HG23	1.98	0.63
1:B:5:ASN:HB3	1:B:8:ASN:ND2	2.13	0.63
1:B:168:ASN:C	1:B:168:ASN:HD22	2.06	0.63
1:B:238:PRO:HG2	1:B:241:GLU:CG	2.29	0.62
1:B:206:ASN:HD21	1:B:308:ILE:N	1.95	0.62
1:B:155:TRP:HE1	1:B:194:ASN:ND2	1.97	0.62
1:B:182:GLY:HA3	1:B:193:MET:SD	2.39	0.62
1:B:113:LEU:HD12	1:B:116:MET:HE3	1.82	0.61
1:B:40:GLU:HG3	1:B:68:PHE:HB3	1.83	0.60
1:B:206:ASN:HD22	1:B:206:ASN:H	1.48	0.60
1:B:2:GLN:HB2	1:B:173:TRP:NE1	2.17	0.60
1:B:320:GLY:HA2	3:B:506:ACT:H2	1.82	0.59
1:B:8:ASN:HB3	1:B:195:GLU:HG2	1.83	0.59
1:B:8:ASN:CB	1:B:195:GLU:HG2	2.33	0.58
1:A:322:TYR:HE2	1:A:339:VAL:HG21	1.67	0.58
1:B:2:GLN:O	1:B:163:THR:HG23	2.03	0.58
1:B:285:THR:HG22	5:B:711:HOH:O	2.04	0.57
1:B:35:TYR:HA	1:B:64:GLY:O	2.05	0.57
1:B:145:LEU:O	1:B:169:ILE:HD11	2.04	0.57
1:B:207:PHE:CD2	1:B:277:MET:HE1	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:401:EPE:H52	5:A:553:HOH:O	2.05	0.56
1:A:302:LYS:HB3	5:A:512:HOH:O	2.06	0.55
1:B:206:ASN:HD22	1:B:206:ASN:N	2.03	0.55
1:B:114:THR:HG23	1:B:149:LEU:HG	1.90	0.54
1:B:206:ASN:H	1:B:206:ASN:ND2	2.05	0.54
1:B:202:ILE:HG23	5:B:722:HOH:O	2.07	0.54
1:B:18:LYS:HE3	1:B:188:ASN:O	2.08	0.53
1:A:330:LYS:N	1:A:330:LYS:HD2	2.24	0.53
1:B:295:LEU:HD21	5:B:709:HOH:O	2.08	0.53
1:B:5:ASN:OD1	1:B:7:ASN:N	2.39	0.52
1:B:97:LYS:HE3	1:B:201:PHE:O	2.10	0.52
1:A:4:ARG:HB2	1:A:162:ASN:HD21	1.74	0.52
1:B:230:ASN:ND2	5:B:678:HOH:O	2.43	0.52
1:B:68:PHE:HA	1:B:101:ASP:HB3	1.92	0.52
1:B:37:LYS:HB2	1:B:66:TYR:CZ	2.45	0.51
1:A:137:TYR:OH	2:A:401:EPE:H72	2.09	0.51
1:A:220:LYS:N	1:A:220:LYS:HD3	2.25	0.51
1:B:298:ARG:CB	1:B:298:ARG:NH1	2.73	0.51
1:B:20:ASN:HA	5:B:680:HOH:O	2.10	0.51
1:A:53:TYR:CE2	1:A:91:ALA:HA	2.46	0.50
1:B:298:ARG:HH11	1:B:298:ARG:CB	2.24	0.50
1:A:74:GLY:O	1:A:78:GLN:HG3	2.12	0.50
1:B:228:THR:HG22	1:B:230:ASN:N	2.10	0.50
1:B:295:LEU:C	1:B:296:ASN:HD22	2.19	0.50
1:B:21:ILE:HG23	1:B:186:GLY:O	2.12	0.50
1:B:27:LYS:HG3	1:B:28:ASN:N	2.25	0.50
1:B:13:ASP:OD2	1:B:177:GLN:NE2	2.44	0.49
1:B:164:PRO:HG2	3:B:502:ACT:H2	1.94	0.49
1:A:285:THR:CG2	1:A:286:PHE:H	2.09	0.49
1:B:291:GLU:CD	1:B:298:ARG:NH1	2.70	0.49
1:B:5:ASN:HB3	1:B:8:ASN:HD21	1.76	0.49
1:A:1:MET:HE2	1:A:172:SER:C	2.37	0.49
1:B:298:ARG:HB3	1:B:298:ARG:NH1	2.25	0.49
3:B:504:ACT:H1	5:B:658:HOH:O	2.12	0.49
1:A:1:MET:HE2	1:A:172:SER:N	2.27	0.48
1:B:33:VAL:HG22	1:B:62:SER:HB2	1.95	0.48
1:A:4:ARG:HB2	1:A:162:ASN:ND2	2.28	0.48
1:A:220:LYS:HD3	1:A:220:LYS:H	1.77	0.48
1:A:290:ARG:HD3	1:A:294:SER:O	2.12	0.48
1:A:226:LYS:N	1:A:231:SER:OG	2.46	0.48
1:B:324:ILE:C	1:B:324:ILE:HD12	2.38	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:GLU:HB2	1:A:318:PHE:CZ	2.49	0.48
1:A:114:THR:HG23	1:A:149:LEU:HG	1.94	0.47
1:B:4:ARG:HH11	1:B:4:ARG:HG3	1.79	0.47
1:B:164:PRO:HG2	3:B:502:ACT:CH3	2.44	0.47
1:A:324:ILE:C	1:A:324:ILE:HD12	2.38	0.47
1:B:110:VAL:HG22	1:B:144:ASN:HA	1.97	0.47
1:A:123:GLU:CD	1:A:127:LEU:HD21	2.40	0.47
1:A:207:PHE:CE1	1:A:209:LEU:HB2	2.49	0.47
1:B:142:ASN:OD1	1:B:167:ASN:HA	2.15	0.47
1:B:177:GLN:HA	1:B:194:ASN:ND2	2.30	0.47
1:B:108:VAL:HG11	1:B:116:MET:HE1	1.96	0.46
1:B:108:VAL:HG21	1:B:116:MET:HE1	1.98	0.46
1:A:304:ASN:O	1:A:305:SER:C	2.59	0.46
1:A:1:MET:HE2	1:A:172:SER:CA	2.46	0.46
1:A:48:TYR:CZ	3:A:409:ACT:H2	2.51	0.46
1:B:9:LEU:HD11	1:B:201:PHE:CE2	2.51	0.46
1:A:298:ARG:CB	1:A:298:ARG:HH11	2.29	0.45
1:B:100:LEU:HG	1:B:120:PHE:CD1	2.51	0.45
1:B:135:TYR:CD1	1:B:135:TYR:C	2.95	0.45
1:A:58:GLU:HG3	1:A:59:GLN:HE21	1.82	0.45
1:B:285:THR:CG2	1:B:286:PHE:H	2.26	0.45
1:B:224:ARG:HB3	1:B:231:SER:OG	2.17	0.45
1:B:168:ASN:HD22	1:B:169:ILE:HG13	1.80	0.45
1:A:2:GLN:HG2	1:A:173:TRP:CE2	2.52	0.45
1:A:277:MET:CE	1:A:310:ARG:HG3	2.47	0.45
1:A:40:GLU:HB3	1:A:44:PHE:HB3	1.98	0.45
1:A:123:GLU:OE2	1:A:127:LEU:HD21	2.16	0.45
1:B:322:TYR:CD2	1:B:339:VAL:HG21	2.51	0.45
1:A:226:LYS:HA	1:A:266:TYR:CD2	2.51	0.45
1:A:304:ASN:HB2	1:A:307:ASP:OD2	2.17	0.45
1:B:54:GLU:O	1:B:58:GLU:HB2	2.17	0.44
1:B:136:THR:O	1:B:156:ILE:HD13	2.18	0.44
1:A:259:GLU:HA	1:A:263:VAL:O	2.17	0.44
1:B:102:ILE:HG23	1:B:102:ILE:O	2.17	0.44
1:B:164:PRO:HD3	1:B:176:PHE:CZ	2.53	0.44
1:A:292:GLU:HA	1:A:333:PHE:CD1	2.53	0.43
1:A:-4:HIS:CD2	1:A:-3:HIS:N	2.87	0.43
1:A:53:TYR:O	1:A:57:LYS:HG2	2.18	0.43
1:A:277:MET:HE1	1:A:310:ARG:HG3	2.00	0.43
1:B:27:LYS:HB3	1:B:61:LEU:HD21	2.00	0.43
1:A:275:LEU:HD13	1:A:310:ARG:HD2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:GLN:OE1	1:B:172:SER:HB2	2.19	0.42
1:B:177:GLN:HG3	1:B:194:ASN:HD21	1.83	0.42
1:B:13:ASP:HA	1:B:35:TYR:O	2.19	0.42
1:B:311:ILE:HA	1:B:324:ILE:HG22	2.02	0.42
1:A:144:ASN:O	1:A:145:LEU:HD13	2.19	0.42
1:B:319:ILE:HD12	1:B:319:ILE:N	2.34	0.42
1:A:287:LEU:HB3	1:A:303:ILE:HB	2.02	0.42
3:A:402:ACT:H2	5:A:539:HOH:O	2.19	0.42
1:B:137:TYR:CE1	1:B:140:PHE:HB2	2.55	0.42
1:B:23:PHE:O	1:B:59:GLN:HG3	2.20	0.42
1:B:53:TYR:OH	1:B:93:ASN:HB2	2.18	0.42
1:B:106:GLU:HG3	5:B:717:HOH:O	2.20	0.42
1:B:168:ASN:ND2	1:B:169:ILE:HG13	2.35	0.42
1:A:223:ILE:HD11	1:A:237:ILE:CD1	2.49	0.42
1:A:228:THR:CG2	1:A:230:ASN:HB2	2.50	0.42
1:B:246:LYS:HE2	1:B:247:TRP:CZ3	2.55	0.42
1:B:113:LEU:HA	1:B:116:MET:HE3	1.98	0.41
1:B:228:THR:HG22	1:B:229:THR:N	2.34	0.41
1:B:112:ASP:O	1:B:116:MET:HG3	2.20	0.41
1:B:168:ASN:C	1:B:168:ASN:ND2	2.72	0.41
1:B:9:LEU:O	1:B:195:GLU:HA	2.21	0.41
2:A:401:EPE:H21	5:A:632:HOH:O	2.20	0.41
1:B:135:TYR:CE2	1:B:157:ALA:HB2	2.56	0.41
1:B:30:GLY:O	1:B:31:VAL:C	2.63	0.41
1:B:23:PHE:C	1:B:59:GLN:HG3	2.45	0.41
1:B:154:VAL:HB	1:B:170:TRP:CE2	2.56	0.41
1:A:141:ALA:HB1	1:A:169:ILE:HD12	2.02	0.41
1:A:165:GLY:O	1:A:166:ALA:C	2.64	0.41
1:B:40:GLU:O	1:B:41:GLY:C	2.64	0.41
1:A:313:TRP:CD1	1:A:313:TRP:C	2.99	0.40
1:A:336:ALA:O	1:A:339:VAL:HG22	2.21	0.40
1:B:230:ASN:HD22	1:B:230:ASN:HA	1.64	0.40
1:B:177:GLN:HG3	1:B:194:ASN:ND2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	345/353 (98%)	330 (96%)	15 (4%)	0	100	100
1	B	340/353 (96%)	322 (95%)	16 (5%)	2 (1%)	21	10
All	All	685/706 (97%)	652 (95%)	31 (4%)	2 (0%)	36	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	169	ILE
1	B	31	VAL

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	298/304 (98%)	286 (96%)	12 (4%)	28	12
1	B	293/304 (96%)	284 (97%)	9 (3%)	35	19
All	All	591/608 (97%)	570 (96%)	21 (4%)	31	15

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	VAL
1	A	93	ASN
1	A	95	ASP
1	A	100	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	119	GLU
1	A	145	LEU
1	A	168	ASN
1	A	181	ASN
1	A	219	THR
1	A	220	LYS
1	A	232	LYS
1	A	250	GLU
1	B	95	ASP
1	B	100	LEU
1	B	106	GLU
1	B	156	ILE
1	B	168	ASN
1	B	206	ASN
1	B	220	LYS
1	B	232	LYS
1	B	287	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	20	ASN
1	A	51	GLN
1	A	59	GLN
1	A	87	ASN
1	A	144	ASN
1	A	151	ASN
1	A	162	ASN
1	A	168	ASN
1	A	181	ASN
1	A	230	ASN
1	A	282	ASN
1	A	288	ASN
1	A	328	ASN
1	B	8	ASN
1	B	20	ASN
1	B	51	GLN
1	B	87	ASN
1	B	143	ASN
1	B	144	ASN
1	B	168	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	181	ASN
1	B	194	ASN
1	B	206	ASN
1	B	208	ASN
1	B	222	ASN
1	B	230	ASN
1	B	282	ASN
1	B	296	ASN
1	B	328	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](#)

17 ligands are 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	$\# Z > 2$
3	ACT	A	404	-	3,3,3	0.93	0	3,3,3	0.71	0
3	ACT	A	402	-	3,3,3	0.90	0	3,3,3	0.75	0
3	ACT	A	405	-	3,3,3	0.91	0	3,3,3	0.74	0
3	ACT	A	408	-	3,3,3	0.94	0	3,3,3	0.69	0
3	ACT	B	502	-	3,3,3	0.87	0	3,3,3	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACT	A	406	-	3,3,3	0.89	0	3,3,3	0.78	0
3	ACT	B	506	-	3,3,3	0.97	0	3,3,3	0.66	0
3	ACT	B	508	-	3,3,3	0.93	0	3,3,3	0.75	0
3	ACT	B	504	-	3,3,3	0.89	0	3,3,3	0.77	0
3	ACT	A	407	-	3,3,3	0.91	0	3,3,3	0.78	0
3	ACT	A	409	-	3,3,3	0.89	0	3,3,3	0.81	0
3	ACT	B	501	-	3,3,3	0.93	0	3,3,3	0.79	0
3	ACT	B	507	-	3,3,3	0.88	0	3,3,3	0.80	0
2	EPE	A	401	-	15,15,15	1.39	1 (6%)	19,20,20	1.20	2 (10%)
3	ACT	B	503	-	3,3,3	0.90	0	3,3,3	0.79	0
4	MLA	B	505	-	6,6,6	1.05	0	7,7,7	1.12	0
4	MLA	A	403	-	6,6,6	1.19	0	7,7,7	1.02	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
4	MLA	B	505	-	-	1/4/4/4	-
4	MLA	A	403	-	-	0/4/4/4	-
2	EPE	A	401	-	-	5/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	EPE	C10-S	4.01	1.83	1.77

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	EPE	C3-C2-N1	2.89	116.48	110.65
2	A	401	EPE	O2S-S-C10	2.06	109.83	106.73

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	EPE	C8-C7-N4-C5
2	A	401	EPE	C9-C10-S-O1S
2	A	401	EPE	C9-C10-S-O3S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	505	MLA	O1A-C1-C2-C3
2	A	401	EPE	C9-C10-S-O2S
2	A	401	EPE	N4-C7-C8-O8

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	ACT	1	0
3	B	502	ACT	3	0
3	B	506	ACT	1	0
3	B	504	ACT	1	0
3	A	409	ACT	1	0
2	A	401	EPE	4	0
3	B	503	ACT	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

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	347/353 (98%)	0.22	6 (1%) 69 75	20, 34, 50, 80	1 (0%)
1	B	342/353 (96%)	0.60	25 (7%) 21 25	21, 40, 58, 75	1 (0%)
All	All	689/706 (97%)	0.41	31 (4%) 38 43	20, 37, 56, 80	2 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	3.6
1	A	-2	HIS	3.5
1	B	3	SER	3.4
1	B	262	GLY	3.4
1	B	159	TYR	3.3
1	B	166	ALA	3.3
1	B	2	GLN	3.2
1	B	161	VAL	3.0
1	A	-1	HIS	2.9
1	B	185	ALA	2.8
1	B	160	GLY	2.7
1	B	31	VAL	2.7
1	A	-3	HIS	2.6
1	B	182	GLY	2.6
1	B	174	VAL	2.6
1	B	9	LEU	2.5
1	B	164	PRO	2.5
1	B	295	LEU	2.4
1	B	30	GLY	2.4
1	B	178	TYR	2.4
1	B	165	GLY	2.3
1	A	219	THR	2.3
1	B	158	HIS	2.3
1	A	262	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	156	ILE	2.2
1	B	171	SER	2.2
1	A	198	GLU	2.2
1	B	202	ILE	2.1
1	B	61	LEU	2.0
1	B	195	GLU	2.0
1	B	7	ASN	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
3	ACT	B	503	4/4	0.61	0.22	56,58,58,58	0
3	ACT	A	408	4/4	0.69	0.24	67,67,67,67	0
3	ACT	B	501	4/4	0.72	0.14	47,47,48,49	0
3	ACT	A	404	4/4	0.79	0.15	46,48,49,50	0
3	ACT	B	506	4/4	0.82	0.13	44,45,45,46	0
3	ACT	B	507	4/4	0.82	0.17	63,63,64,64	0
3	ACT	A	409	4/4	0.85	0.14	63,65,65,65	0
3	ACT	A	406	4/4	0.86	0.12	37,38,39,40	0
2	EPE	A	401	15/15	0.87	0.14	48,49,51,52	0
3	ACT	A	402	4/4	0.87	0.13	61,61,61,62	0
3	ACT	B	508	4/4	0.87	0.11	63,63,64,64	0
3	ACT	A	407	4/4	0.89	0.15	62,62,62,64	0
3	ACT	B	502	4/4	0.89	0.12	56,56,57,58	0
3	ACT	B	504	4/4	0.92	0.13	43,44,45,45	0
3	ACT	A	405	4/4	0.94	0.07	40,41,42,43	0
4	MLA	A	403	7/7	0.94	0.07	38,39,40,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MLA	B	505	7/7	0.96	0.06	27,31,33,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.