



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2023 – 07:53 AM EDT

PDB ID : 3H17
Title : Crystal structure of EstE5-PMSF (I)
Authors : Hwang, K.Y.; Nam, K.H.
Deposited on : 2009-04-11
Resolution : 2.50 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

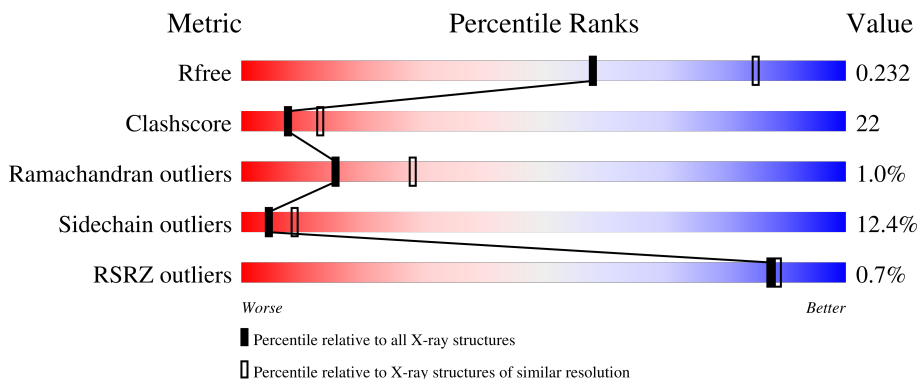
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	322	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2226 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.

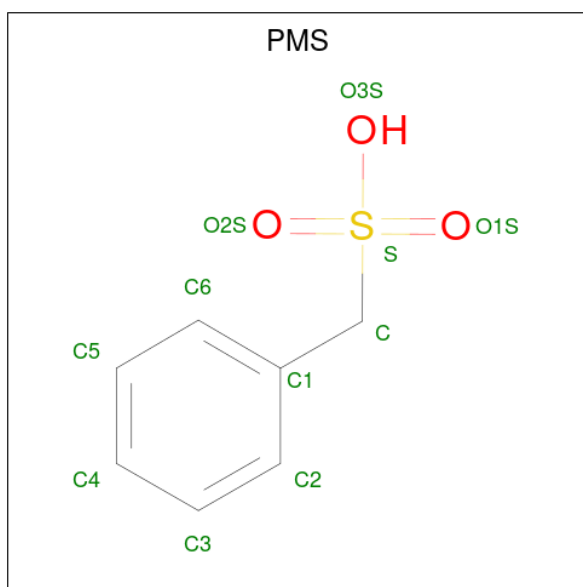
- Molecule 1 is a protein called Esterase/lipase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	292	2206	1403	388	402	13	0	0	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	expression tag	UNP Q0GMU2
A	-11	ALA	-	expression tag	UNP Q0GMU2
A	-10	SER	-	expression tag	UNP Q0GMU2
A	-9	MET	-	expression tag	UNP Q0GMU2
A	-8	THR	-	expression tag	UNP Q0GMU2
A	-7	GLY	-	expression tag	UNP Q0GMU2
A	-6	GLY	-	expression tag	UNP Q0GMU2
A	-5	GLN	-	expression tag	UNP Q0GMU2
A	-4	GLN	-	expression tag	UNP Q0GMU2
A	-3	MET	-	expression tag	UNP Q0GMU2
A	-2	GLY	-	expression tag	UNP Q0GMU2
A	-1	ARG	-	expression tag	UNP Q0GMU2
A	0	GLY	-	expression tag	UNP Q0GMU2
A	298	LEU	-	expression tag	UNP Q0GMU2
A	299	ALA	-	expression tag	UNP Q0GMU2
A	300	ALA	-	expression tag	UNP Q0GMU2
A	301	ALA	-	expression tag	UNP Q0GMU2
A	302	LEU	-	expression tag	UNP Q0GMU2
A	303	GLU	-	expression tag	UNP Q0GMU2
A	304	HIS	-	expression tag	UNP Q0GMU2
A	305	HIS	-	expression tag	UNP Q0GMU2
A	306	HIS	-	expression tag	UNP Q0GMU2
A	307	HIS	-	expression tag	UNP Q0GMU2
A	308	HIS	-	expression tag	UNP Q0GMU2
A	309	HIS	-	expression tag	UNP Q0GMU2

- Molecule 2 is phenylmethanesulfonic acid (three-letter code: PMS) (formula: C₇H₈O₃S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			10	7	2	1		

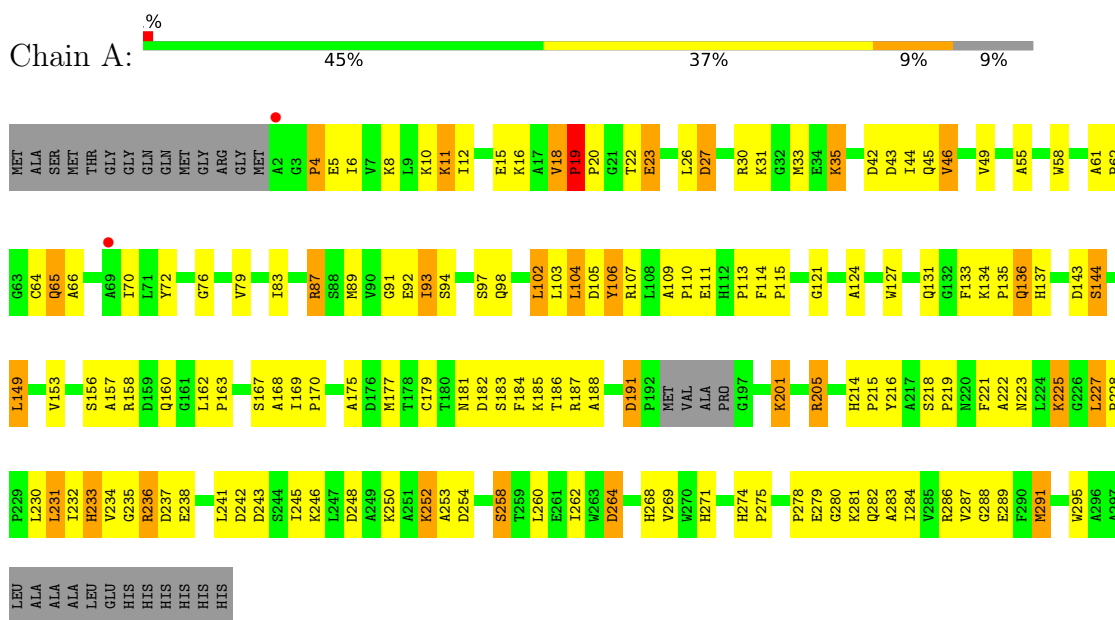
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		

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: Esterase/lipase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	61.14Å 61.14Å 148.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.25 – 2.50 47.25 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.2 (47.25-2.50) 92.0 (47.25-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.51Å)	Xtrriage
Refinement program	CNS, REFMAC 5.2.0019	Depositor
R, R_{free}	0.187 , 0.235 0.206 , 0.232	Depositor DCC
R_{free} test set	452 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtrriage
Anisotropy	0.174	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2226	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.25% 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: PMS

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	1.45	9/2258 (0.4%)	1.43	24/3064 (0.8%)

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	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	CYS	CB-SG	-6.31	1.71	1.82
1	A	106	TYR	CD2-CE2	6.18	1.48	1.39
1	A	295	TRP	CB-CG	-5.99	1.39	1.50
1	A	106	TYR	CE1-CZ	5.57	1.45	1.38
1	A	133	PHE	CD1-CE1	5.45	1.50	1.39
1	A	221	PHE	CE2-CZ	5.42	1.47	1.37
1	A	111	GLU	CG-CD	5.17	1.59	1.51
1	A	35	LYS	CD-CE	5.15	1.64	1.51
1	A	23	GLU	CG-CD	5.04	1.59	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	ARG	NE-CZ-NH2	-10.37	115.11	120.30
1	A	18	VAL	CB-CA-C	8.43	127.41	111.40
1	A	191	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	A	102	LEU	CB-CG-CD2	7.44	123.64	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	PRO	CB-CA-C	7.39	130.47	112.00
1	A	27	ASP	CB-CG-OD1	-7.28	111.75	118.30
1	A	252	LYS	CD-CE-NZ	-7.05	95.48	111.70
1	A	191	ASP	C-N-CD	-6.82	105.61	120.60
1	A	191	ASP	CB-CG-OD1	6.82	124.43	118.30
1	A	241	LEU	CA-CB-CG	6.62	130.53	115.30
1	A	87	ARG	NE-CZ-NH1	-6.46	117.07	120.30
1	A	149	LEU	CA-CB-CG	6.21	129.57	115.30
1	A	107	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	A	236	ARG	NE-CZ-NH1	-6.12	117.24	120.30
1	A	227	LEU	CA-CB-CG	6.03	129.17	115.30
1	A	43	ASP	CB-CG-OD1	-5.96	112.93	118.30
1	A	30	ARG	NE-CZ-NH2	5.81	123.21	120.30
1	A	76	GLY	C-N-CA	-5.59	110.56	122.30
1	A	264	ASP	CB-CG-OD1	5.45	123.20	118.30
1	A	72	TYR	CA-CB-CG	-5.27	103.39	113.40
1	A	264	ASP	CB-CG-OD2	-5.16	113.65	118.30
1	A	158	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	30	ARG	NE-CZ-NH1	-5.02	117.79	120.30
1	A	58	TRP	N-CA-C	-5.00	97.50	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	PRO	Peptide
1	A	191	ASP	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	2206	0	2210	95	0
2	A	10	0	7	3	0
3	A	10	0	0	1	0
All	All	2226	0	2217	97	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 22.

All (97) 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:93:ILE:C	1:A:93:ILE:HD12	1.72	1.06
1:A:169:ILE:HG21	1:A:287:VAL:HG13	1.51	0.89
1:A:136:GLN:H	1:A:136:GLN:HE21	1.14	0.87
1:A:136:GLN:H	1:A:136:GLN:NE2	1.73	0.86
1:A:109:ALA:HB1	1:A:110:PRO:HA	1.61	0.83
1:A:168:ALA:C	1:A:169:ILE:HD12	2.00	0.82
1:A:260:LEU:HD22	1:A:262:ILE:HG13	1.67	0.77
1:A:44:ILE:HD13	1:A:91:GLY:HA3	1.70	0.74
1:A:187:ARG:HD3	1:A:236:ARG:O	1.87	0.74
1:A:278:PRO:O	1:A:282:GLN:HG3	1.89	0.73
1:A:136:GLN:HE21	1:A:136:GLN:N	1.85	0.73
1:A:169:ILE:HD12	1:A:169:ILE:N	2.06	0.70
1:A:175:ALA:HB1	1:A:219:PRO:HD2	1.75	0.68
1:A:187:ARG:CD	1:A:236:ARG:O	2.41	0.68
1:A:65:GLN:HE21	1:A:66:ALA:N	1.91	0.68
1:A:134:LYS:O	1:A:137:HIS:N	2.24	0.68
1:A:8:LYS:O	1:A:12:ILE:HG12	1.94	0.67
1:A:27:ASP:HB2	1:A:31:LYS:NZ	2.09	0.67
1:A:64:CYS:HB2	3:A:407:HOH:O	1.94	0.67
1:A:11:LYS:O	1:A:15:GLU:HG2	1.95	0.66
1:A:44:ILE:CD1	1:A:91:GLY:HA3	2.26	0.65
1:A:127:TRP:O	1:A:131:GLN:HG2	1.97	0.65
1:A:181:ASN:HB3	1:A:242:ASP:CB	2.27	0.65
1:A:181:ASN:HB3	1:A:242:ASP:HB2	1.77	0.65
1:A:250:LYS:O	1:A:253:ALA:HB3	1.97	0.65
1:A:93:ILE:HD13	1:A:291:MET:CE	2.27	0.64
1:A:271:HIS:H	1:A:271:HIS:HD1	1.45	0.63
1:A:70:ILE:CD1	1:A:93:ILE:HD11	2.29	0.62
1:A:283:ALA:O	1:A:287:VAL:HG23	1.99	0.62
1:A:201:LYS:HE3	1:A:205:ARG:CZ	2.30	0.62
1:A:222:ALA:O	1:A:250:LYS:NZ	2.32	0.62
1:A:104:LEU:HD13	1:A:106:TYR:HB3	1.81	0.62
1:A:268:HIS:NE2	2:A:310:PMS:H2A	2.16	0.61
1:A:93:ILE:HD12	1:A:94:SER:N	2.15	0.60
1:A:214:HIS:CE1	1:A:216:TYR:HB2	2.36	0.60
1:A:230:LEU:HD23	1:A:232:ILE:HD11	1.86	0.58
2:A:310:PMS:C2	2:A:310:PMS:O2S	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ILE:C	1:A:93:ILE:CD1	2.58	0.57
1:A:248:ASP:O	1:A:252:LYS:HG2	2.04	0.56
1:A:92:GLU:HG3	1:A:274:HIS:CE1	2.41	0.56
1:A:79:VAL:HA	1:A:109:ALA:O	2.04	0.56
1:A:233:HIS:HD2	1:A:271:HIS:NE2	2.03	0.56
1:A:83:ILE:HG23	1:A:103:LEU:HD23	1.87	0.55
1:A:93:ILE:HD13	1:A:291:MET:HE3	1.88	0.54
1:A:223:ASN:HD21	1:A:225:LYS:HB2	1.72	0.54
1:A:156:SER:O	1:A:160:GLN:HG3	2.07	0.54
1:A:181:ASN:O	1:A:184:PHE:HD1	1.91	0.53
1:A:143:ASP:O	1:A:144:SER:CB	2.55	0.53
1:A:93:ILE:HD12	1:A:93:ILE:O	2.06	0.53
1:A:27:ASP:HB2	1:A:31:LYS:HZ3	1.73	0.53
1:A:169:ILE:HG21	1:A:287:VAL:CG1	2.32	0.53
1:A:230:LEU:O	1:A:258:SER:HA	2.09	0.53
1:A:10:LYS:NZ	1:A:237:ASP:OD2	2.41	0.53
1:A:114:PHE:CD1	1:A:115:PRO:HA	2.44	0.52
1:A:42:ASP:O	1:A:42:ASP:OD2	2.27	0.52
1:A:46:VAL:HG21	1:A:87:ARG:HD3	1.91	0.52
1:A:235:GLY:O	1:A:238:GLU:HG2	2.10	0.51
1:A:177:MET:HG2	1:A:218:SER:OG	2.11	0.51
1:A:201:LYS:HE3	1:A:205:ARG:NE	2.27	0.50
1:A:18:VAL:HG23	1:A:22:THR:OG1	2.12	0.49
1:A:280:GLY:O	1:A:284:ILE:HG13	2.11	0.49
1:A:274:HIS:CD2	1:A:275:PRO:HD3	2.48	0.49
1:A:70:ILE:HD13	1:A:93:ILE:HD11	1.95	0.48
1:A:61:ALA:HB1	1:A:62:PRO:HD2	1.94	0.48
1:A:250:LYS:O	1:A:254:ASP:N	2.46	0.48
1:A:245:ILE:HA	1:A:260:LEU:HD11	1.96	0.47
1:A:260:LEU:CD2	1:A:262:ILE:HG13	2.43	0.47
1:A:169:ILE:N	1:A:169:ILE:CD1	2.76	0.47
1:A:4:PRO:HD2	1:A:5:GLU:OE1	2.15	0.47
1:A:89:MET:O	1:A:93:ILE:HG23	2.15	0.46
1:A:113:PRO:O	1:A:114:PHE:C	2.50	0.46
1:A:170:PRO:HD2	1:A:231:LEU:O	2.16	0.46
1:A:184:PHE:O	1:A:188:ALA:HB2	2.16	0.46
1:A:183:SER:O	1:A:187:ARG:HB2	2.15	0.46
1:A:143:ASP:O	1:A:144:SER:HB3	2.16	0.46
1:A:223:ASN:ND2	1:A:225:LYS:H	2.13	0.45
1:A:279:GLU:OE1	1:A:279:GLU:N	2.42	0.45
1:A:286:ARG:HA	1:A:289:GLU:OE2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:HIS:HA	1:A:215:PRO:HD3	1.82	0.45
1:A:162:LEU:HA	1:A:163:PRO:HD2	1.62	0.45
1:A:227:LEU:HB3	1:A:228:PRO:CD	2.46	0.45
1:A:27:ASP:HB2	1:A:31:LYS:HZ2	1.82	0.45
1:A:121:GLY:HA3	1:A:153:VAL:HG21	1.99	0.44
1:A:182:ASP:O	1:A:185:LYS:N	2.48	0.44
1:A:187:ARG:HD2	1:A:236:ARG:O	2.16	0.44
1:A:55:ALA:O	1:A:105:ASP:HB3	2.17	0.44
1:A:157:ALA:HB1	1:A:162:LEU:HB2	1.99	0.43
2:A:310:PMS:C6	2:A:310:PMS:O1S	2.65	0.43
1:A:134:LYS:O	1:A:136:GLN:N	2.52	0.42
1:A:268:HIS:CD2	1:A:269:VAL:HG23	2.55	0.42
1:A:97:SER:HB3	1:A:288:GLY:HA2	2.01	0.41
1:A:124:ALA:O	1:A:127:TRP:HB3	2.21	0.41
1:A:134:LYS:O	1:A:135:PRO:C	2.59	0.41
1:A:242:ASP:O	1:A:246:LYS:HG3	2.21	0.41
1:A:162:LEU:HA	1:A:162:LEU:HD23	1.83	0.41
1:A:181:ASN:HD22	1:A:246:LYS:NZ	2.19	0.40
1:A:19:PRO:HA	1:A:20:PRO:HD2	1.78	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	288/322 (89%)	261 (91%)	24 (8%)	3 (1%)	15 28

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	SER
1	A	4	PRO

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Mol	Chain	Res	Type
1	A	234	VAL

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	225/246 (92%)	197 (88%)	28 (12%)	4 9

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	11	LYS
1	A	16	LYS
1	A	23	GLU
1	A	26	LEU
1	A	33	MET
1	A	35	LYS
1	A	45	GLN
1	A	46	VAL
1	A	49	VAL
1	A	65	GLN
1	A	93	ILE
1	A	98	GLN
1	A	102	LEU
1	A	104	LEU
1	A	136	GLN
1	A	149	LEU
1	A	167	SER
1	A	186	THR
1	A	201	LYS
1	A	225	LYS
1	A	231	LEU
1	A	233	HIS
1	A	243	ASP
1	A	258	SER

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Mol	Chain	Res	Type
1	A	264	ASP
1	A	281	LYS
1	A	291	MET

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	65	GLN
1	A	136	GLN
1	A	181	ASN
1	A	200	ASN
1	A	223	ASN
1	A	233	HIS
1	A	274	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	PMS	A	310	1	7,10,11	2.15	4 (57%)	11,12,15	4.22	4 (36%)

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	PMS	A	310	1	-	0/4/4/5	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	310	PMS	C4-C3	2.83	1.45	1.38
2	A	310	PMS	C5-C4	2.78	1.45	1.38
2	A	310	PMS	C6-C1	2.49	1.44	1.38
2	A	310	PMS	C3-C2	2.09	1.43	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	310	PMS	O2S-S-C	-9.77	89.73	105.56
2	A	310	PMS	O1S-S-C	-8.62	91.59	105.56
2	A	310	PMS	C6-C1-C2	3.04	122.94	118.17
2	A	310	PMS	C3-C2-C1	-2.33	117.05	120.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	310	PMS	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	292/322 (90%)	-0.16	2 (0%) 87 89	36, 48, 67, 73	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	2.3
1	A	69	ALA	2.2

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 monosaccharides 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
2	PMS	A	310	10/11	0.97	0.23	41,49,58,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.