wwPDB X-ray Structure Validation Summary Report (i)

Oct 30, 2023 – 06:41 PM JST

PDB ID	:	4XVC
Title	:	Crystal structure of an esterase from the bacterial hormone-sensitive lipase (HSL) family
Authors	:	Zhang, Y.; Li, P.
Deposited on	:	2015-01-27
Resolution	:	2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

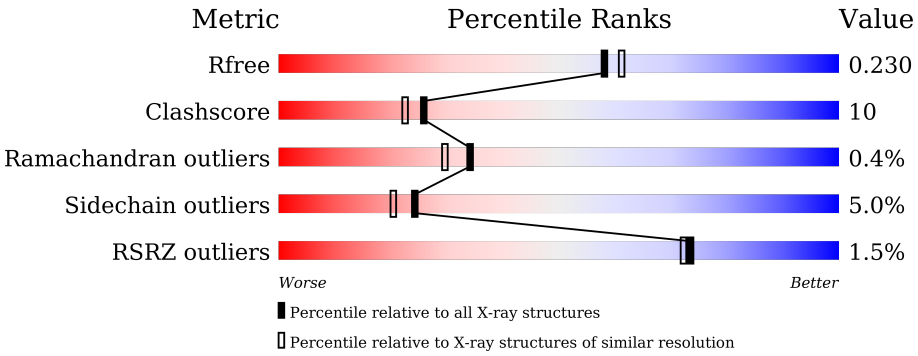
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	317	2% 76% 15% • 6%
1	B	317	2% 79% 11% • 6%
1	C	317	% 79% 12% • 6%
1	D	317	% 77% 14% • 6%
1	E	317	2% 80% 10% • 6%
1	F	317	2% 77% 13% • 6%

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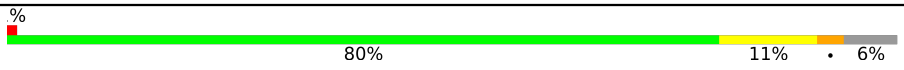
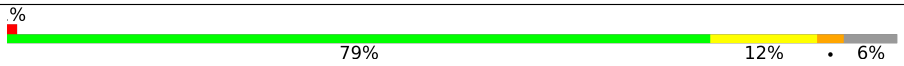
Mol	Chain	Length	Quality of chain
1	G	317	
1	H	317	

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	PMS	C	301	-	-	X	-
2	PMS	D	301	-	-	X	-
2	PMS	E	301	-	-	X	-

2 Entry composition (i)

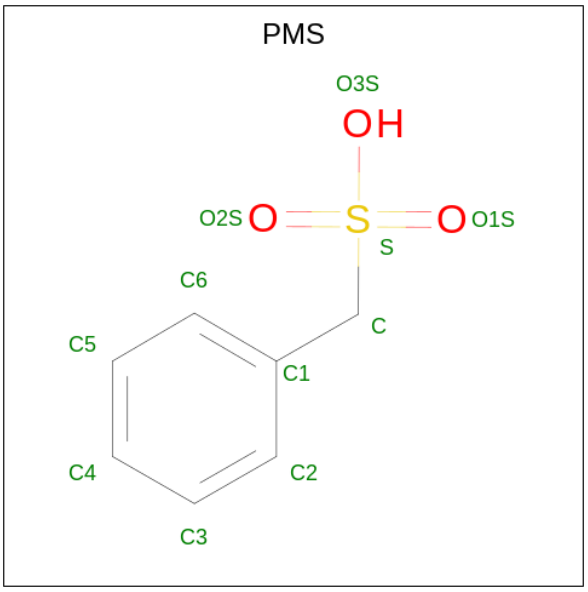
There are 3 unique types of molecules in this entry. The entry contains 20210 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 E40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	3	0
			2277	1442	399	424	12			
1	B	297	Total	C	N	O	S	0	4	0
			2283	1445	400	426	12			
1	C	297	Total	C	N	O	S	0	1	0
			2262	1432	397	421	12			
1	D	297	Total	C	N	O	S	0	2	0
			2269	1436	398	423	12			
1	E	297	Total	C	N	O	S	0	1	0
			2263	1433	397	421	12			
1	F	297	Total	C	N	O	S	0	2	0
			2271	1439	398	422	12			
1	G	297	Total	C	N	O	S	0	0	0
			2256	1429	396	419	12			
1	H	297	Total	C	N	O	S	0	0	0
			2256	1429	396	419	12			

- Molecule 2 is phenylmethanesulfonic acid (three-letter code: PMS) (formula: $C_7H_8O_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O S 10 7 2 1	0	0
2	B	1	Total C O S 10 7 2 1	0	0
2	C	1	Total C O S 10 7 2 1	0	0
2	D	1	Total C O S 10 7 2 1	0	0
2	E	1	Total C O S 10 7 2 1	0	0
2	F	1	Total C O S 10 7 2 1	0	0
2	G	1	Total C O S 10 7 2 1	0	0
2	H	1	Total C O S 10 7 2 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	257	Total O 257 257	0	0
3	B	250	Total O 250 250	0	0
3	C	241	Total O 241 241	0	0
3	D	245	Total O 245 245	0	0

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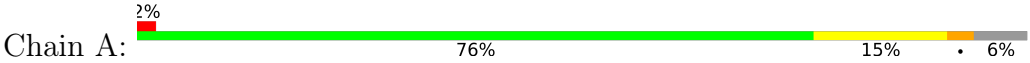
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	244	Total O 244 244	0	0
3	F	253	Total O 253 253	0	0
3	G	260	Total O 260 260	0	0
3	H	243	Total O 243 243	0	0

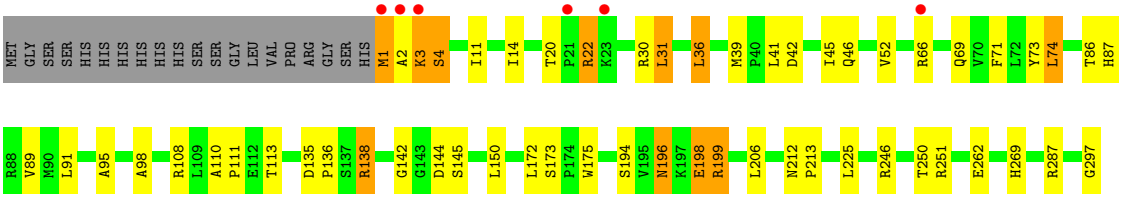
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Esterase E40

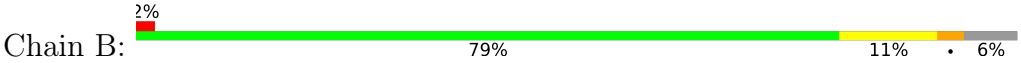
Chain A:

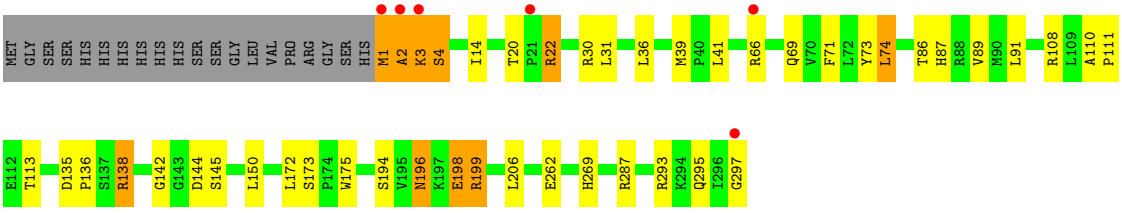




• Molecule 1: Esterase E40

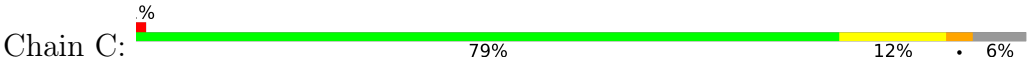
Chain B:

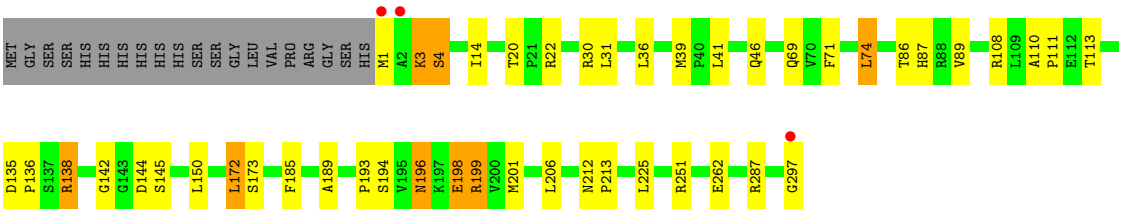




• Molecule 1: Esterase E40

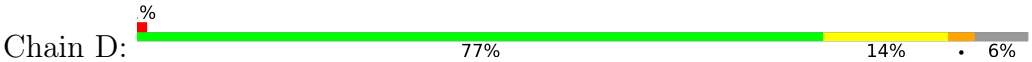
Chain C:

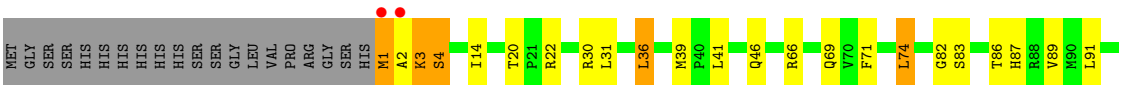


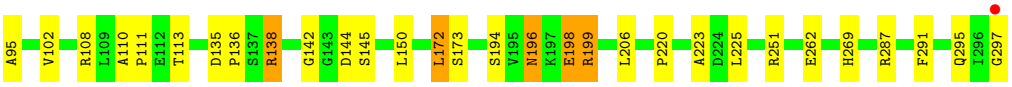


• Molecule 1: Esterase E40

Chain D:

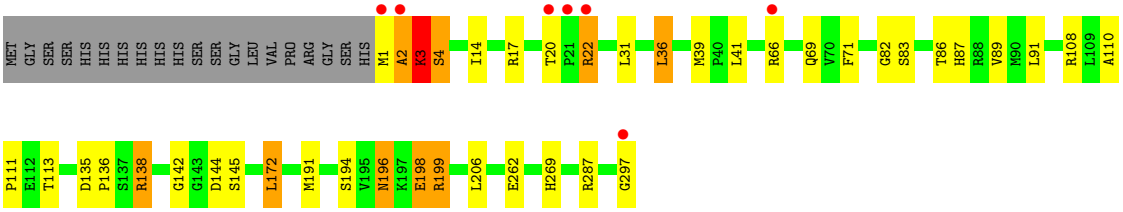






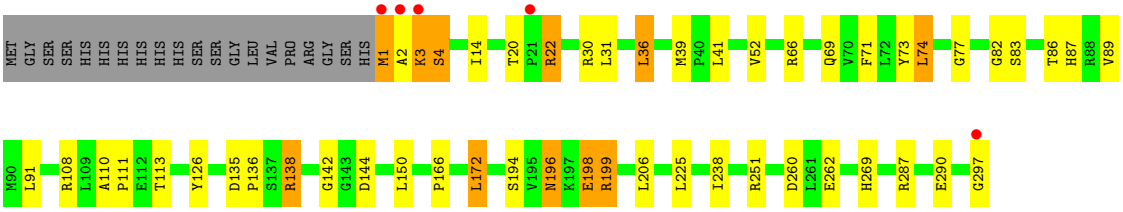
• Molecule 1: Esterase E40

Chain E:



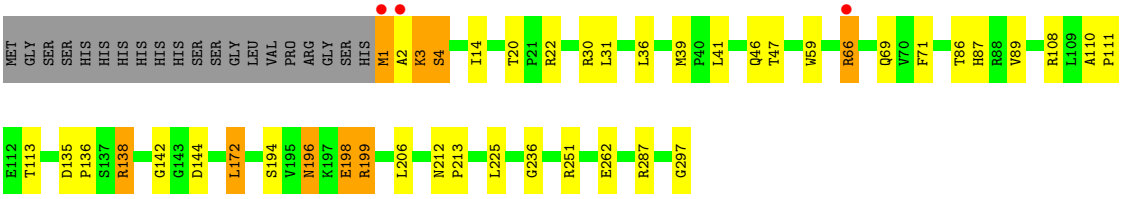
• Molecule 1: Esterase E40

Chain F:



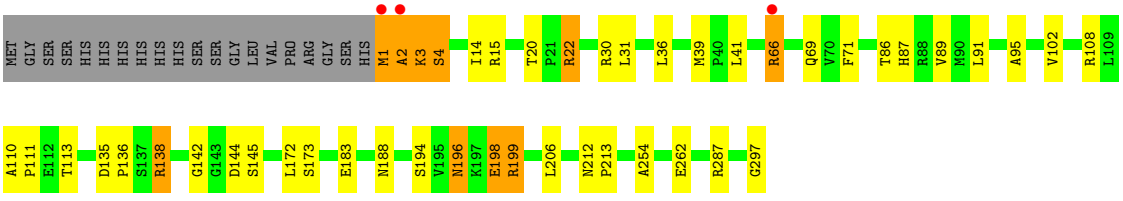
• Molecule 1: Esterase E40

Chain G:



• Molecule 1: Esterase E40

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	74.63Å 76.17Å 130.19Å 74.04° 75.15° 72.60°	Depositor
Resolution (Å)	39.33 – 2.00 39.33 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.7 (39.33-2.00) 96.9 (39.33-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.79 (at 2.00Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6.4_486)	Depositor
R, R_{free}	0.196 , 0.232 0.197 , 0.230	Depositor DCC
R_{free} test set	8460 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	12.5	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.259 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	20210	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 88.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0835e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.39	0/2329	0.55	0/3174
1	B	0.38	0/2335	0.53	0/3182
1	C	0.39	0/2314	0.55	0/3153
1	D	0.39	0/2321	0.54	0/3163
1	E	0.39	0/2315	0.56	1/3155 (0.0%)
1	F	0.38	0/2323	0.54	0/3166
1	G	0.40	0/2308	0.55	1/3145 (0.0%)
1	H	0.39	0/2308	0.55	1/3145 (0.0%)
All	All	0.39	0/18553	0.55	3/25283 (0.0%)

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	E	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	66	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	E	3	LYS	N-CA-C	-6.03	94.72	111.00
1	H	66	ARG	NE-CZ-NH1	-5.07	117.77	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	2	ALA	Peptide

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	2277	0	2273	52	0
1	B	2283	0	2277	53	0
1	C	2262	0	2257	47	0
1	D	2269	0	2263	78	0
1	E	2263	0	2259	48	0
1	F	2271	0	2268	48	0
1	G	2256	0	2252	52	0
1	H	2256	0	2253	33	0
2	A	10	0	7	1	0
2	B	10	0	7	1	0
2	C	10	0	7	6	0
2	D	10	0	7	4	0
2	E	10	0	7	19	0
2	F	10	0	7	3	0
2	G	10	0	7	0	0
2	H	10	0	7	0	0
3	A	257	0	0	11	0
3	B	250	0	0	6	0
3	C	241	0	0	3	0
3	D	245	0	0	13	0
3	E	244	0	0	7	0
3	F	253	0	0	5	0
3	G	260	0	0	5	0
3	H	243	0	0	4	0
All	All	20210	0	18158	382	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 10.

The worst 5 of 382 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:D:145:SER:HB2	2:D:301:PMS:S	1.37	1.58
1:E:145:SER:CB	2:E:301:PMS:S	2.09	1.41
1:C:145:SER:CB	2:C:301:PMS:S	2.11	1.36
1:D:145:SER:CB	2:D:301:PMS:S	2.17	1.31
1:D:66:ARG:CG	1:G:66:ARG:HH12	1.58	1.16

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	298/317 (94%)	288 (97%)	9 (3%)	1 (0%)	41	37
1	B	299/317 (94%)	287 (96%)	10 (3%)	2 (1%)	22	16
1	C	296/317 (93%)	286 (97%)	9 (3%)	1 (0%)	41	37
1	D	297/317 (94%)	288 (97%)	8 (3%)	1 (0%)	41	37
1	E	296/317 (93%)	285 (96%)	10 (3%)	1 (0%)	41	37
1	F	297/317 (94%)	289 (97%)	7 (2%)	1 (0%)	41	37
1	G	295/317 (93%)	285 (97%)	9 (3%)	1 (0%)	41	37
1	H	295/317 (93%)	286 (97%)	7 (2%)	2 (1%)	22	16
All	All	2373/2536 (94%)	2294 (97%)	69 (3%)	10 (0%)	34	30

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	B	2	ALA
1	B	4	SER
1	C	4	SER
1	D	4	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	234/248 (94%)	220 (94%)	14 (6%)	19	14
1	B	235/248 (95%)	222 (94%)	13 (6%)	21	17
1	C	232/248 (94%)	221 (95%)	11 (5%)	26	22
1	D	233/248 (94%)	221 (95%)	12 (5%)	23	19
1	E	232/248 (94%)	222 (96%)	10 (4%)	29	26
1	F	233/248 (94%)	220 (94%)	13 (6%)	21	17
1	G	231/248 (93%)	220 (95%)	11 (5%)	25	22
1	H	231/248 (93%)	220 (95%)	11 (5%)	25	22
All	All	1861/1984 (94%)	1766 (95%)	95 (5%)	24	19

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	198	GLU
1	F	199	ARG
1	E	206	LEU
1	F	74[A]	LEU
1	G	22	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	196	ASN
1	G	295	GLN
1	F	295	GLN
1	G	132	HIS
1	H	132	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)

8 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	$\#\|Z\| > 2$
2	PMS	E	301	-	7,10,11	1.31	1 (14%)	11,12,15	1.72	2 (18%)
2	PMS	G	301	-	7,10,11	1.35	2 (28%)	11,12,15	1.13	2 (18%)
2	PMS	D	301	-	7,10,11	1.26	2 (28%)	11,12,15	1.05	1 (9%)
2	PMS	H	301	-	7,10,11	1.37	2 (28%)	11,12,15	1.14	2 (18%)
2	PMS	C	301	-	7,10,11	1.32	2 (28%)	11,12,15	0.83	0
2	PMS	F	301	-	7,10,11	1.22	1 (14%)	11,12,15	1.27	2 (18%)
2	PMS	B	301	1	7,10,11	1.31	1 (14%)	11,12,15	1.32	2 (18%)
2	PMS	A	301	1	7,10,11	1.31	2 (28%)	11,12,15	1.22	2 (18%)

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	E	301	-	-	3/4/4/5	0/1/1/1
2	PMS	G	301	-	-	0/4/4/5	0/1/1/1
2	PMS	D	301	-	-	0/4/4/5	0/1/1/1
2	PMS	H	301	-	-	0/4/4/5	0/1/1/1
2	PMS	C	301	-	-	2/4/4/5	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PMS	F	301	-	-	2/4/4/5	0/1/1/1
2	PMS	B	301	1	-	0/4/4/5	0/1/1/1
2	PMS	A	301	1	-	0/4/4/5	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	301	PMS	C2-C1	2.75	1.44	1.38
2	G	301	PMS	C2-C1	2.73	1.44	1.38
2	C	301	PMS	C2-C1	2.64	1.44	1.38
2	B	301	PMS	C2-C1	2.62	1.44	1.38
2	E	301	PMS	C2-C1	2.60	1.44	1.38

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	301	PMS	C1-C-S	4.16	121.44	110.60
2	E	301	PMS	O1S-S-C	2.88	110.22	105.56
2	F	301	PMS	O2S-S-C	2.71	109.96	105.56
2	B	301	PMS	O2S-S-C	2.51	109.63	105.56
2	D	301	PMS	C1-C-S	2.44	116.97	110.60

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	301	PMS	S-C-C1-C2
2	E	301	PMS	S-C-C1-C6
2	F	301	PMS	S-C-C1-C2
2	F	301	PMS	S-C-C1-C6
2	E	301	PMS	C1-C-S-O1S

There are no ring outliers.

6 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	PMS	19	0
2	D	301	PMS	4	0
2	C	301	PMS	6	0
2	F	301	PMS	3	0
2	B	301	PMS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	PMS	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, 95^{th} 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	297/317 (93%)	-0.25	6 (2%)	65	63	6, 12, 32, 61	0
1	B	297/317 (93%)	-0.19	6 (2%)	65	63	5, 12, 32, 62	0
1	C	297/317 (93%)	-0.30	3 (1%)	82	81	6, 12, 31, 63	0
1	D	297/317 (93%)	-0.30	3 (1%)	82	81	5, 12, 32, 72	0
1	E	297/317 (93%)	-0.25	7 (2%)	59	57	6, 12, 31, 64	0
1	F	297/317 (93%)	-0.27	5 (1%)	70	68	6, 13, 31, 62	0
1	G	297/317 (93%)	-0.30	3 (1%)	82	81	5, 12, 30, 62	0
1	H	297/317 (93%)	-0.32	3 (1%)	82	81	5, 12, 30, 63	0
All	All	2376/2536 (93%)	-0.27	36 (1%)	73	72	5, 12, 32, 72	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	11.7
1	H	2	ALA	10.8
1	G	2	ALA	10.4
1	D	1	MET	10.2
1	F	2	ALA	9.7

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

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, 95^{th} 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	F	301	10/11	0.65	0.38	33,40,44,44	0
2	PMS	C	301	10/11	0.74	0.28	33,40,44,44	0
2	PMS	H	301	10/11	0.78	0.25	33,40,44,44	0
2	PMS	A	301	10/11	0.81	0.23	33,40,44,44	0
2	PMS	E	301	10/11	0.81	0.25	33,40,44,44	0
2	PMS	G	301	10/11	0.83	0.23	33,40,44,44	0
2	PMS	D	301	10/11	0.83	0.21	33,40,44,44	0
2	PMS	B	301	10/11	0.85	0.22	33,40,44,44	0

6.5 Other polymers (i)

There are no such residues in this entry.