



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 23, 2026 – 12:44 AM UTC

PDB ID : 8B4M / pdb_00008b4m
Title : Crystal structure of a hydropyrene synthase (M75L variant) in its closed con-
formation
Authors : Helmer, C.P.O.; Driller, R.; Loll, B.
Deposited on : 2022-09-20
Resolution : 3.04 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 ⓘ 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

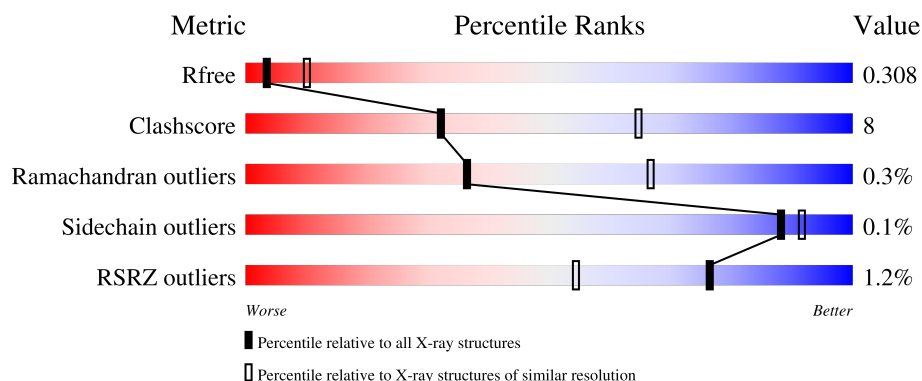
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.04 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	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

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 $\leq 5\%$. 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	78% 18% .
1	B	322	80% 15% 5%
1	C	322	76% 17% 6%
1	D	322	76% 19% 5%
1	E	322	73% 23% .

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Mol	Chain	Length	Quality of chain
1	F	322	% 78% 18% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14633 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 Terpene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2425	1521	441	451	12			
1	B	307	Total	C	N	O	S	0	0	0
			2433	1528	446	448	11			
1	C	302	Total	C	N	O	S	0	0	0
			2388	1499	435	442	12			
1	D	305	Total	C	N	O	S	0	0	0
			2418	1519	444	444	11			
1	E	308	Total	C	N	O	S	0	1	0
			2443	1532	445	454	12			
1	F	311	Total	C	N	O	S	0	0	0
			2458	1540	450	456	12			

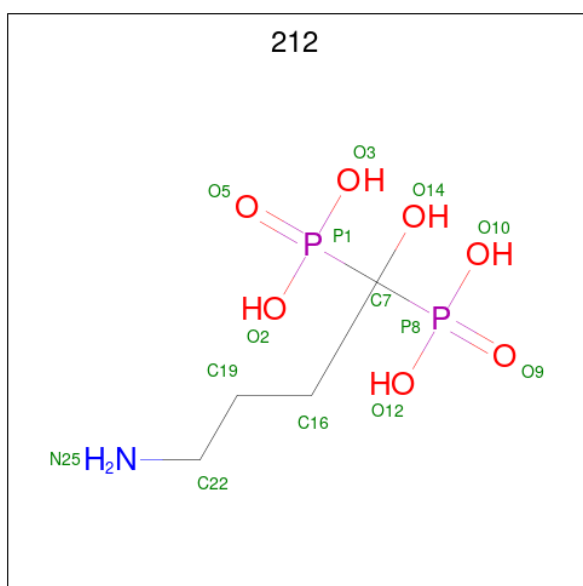
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ASP	-	expression tag	UNP D5SK09
A	75	LEU	MET	engineered mutation	UNP D5SK09
B	0	ASP	-	expression tag	UNP D5SK09
B	75	LEU	MET	engineered mutation	UNP D5SK09
C	0	ASP	-	expression tag	UNP D5SK09
C	75	LEU	MET	engineered mutation	UNP D5SK09
D	0	ASP	-	expression tag	UNP D5SK09
D	75	LEU	MET	engineered mutation	UNP D5SK09
E	0	ASP	-	expression tag	UNP D5SK09
E	75	LEU	MET	engineered mutation	UNP D5SK09
F	0	ASP	-	expression tag	UNP D5SK09
F	75	LEU	MET	engineered mutation	UNP D5SK09

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total 3 Mg 3	0	0
2	D	3	Total 3 Mg 3	0	0
2	E	3	Total 3 Mg 3	0	0
2	F	3	Total 3 Mg 3	0	0

- Molecule 3 is ALENDRONATE (CCD ID: 212) (formula: $C_4H_{13}NO_7P_2$).

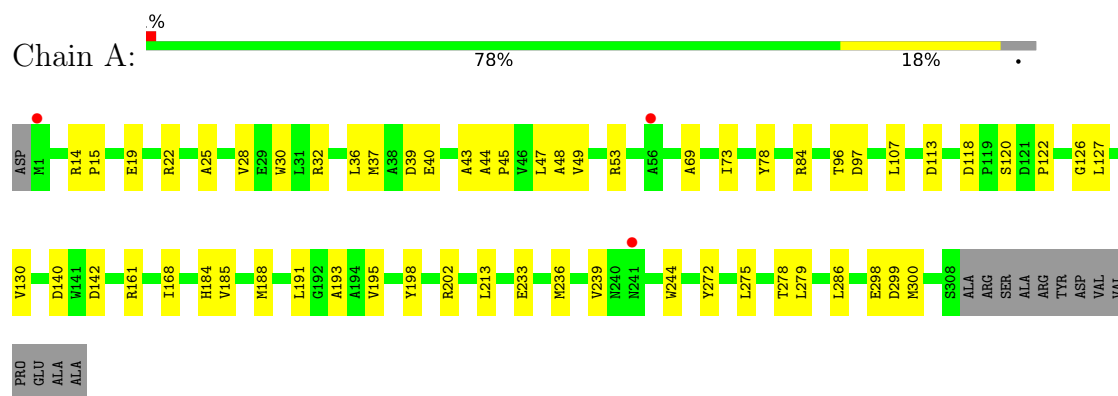


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total 14 C 4 N 1 O 7 P 2	0	0
3	D	1	Total 14 C 4 N 1 O 7 P 2	0	0
3	E	1	Total 14 C 4 N 1 O 7 P 2	0	0
3	F	1	Total 14 C 4 N 1 O 7 P 2	0	0

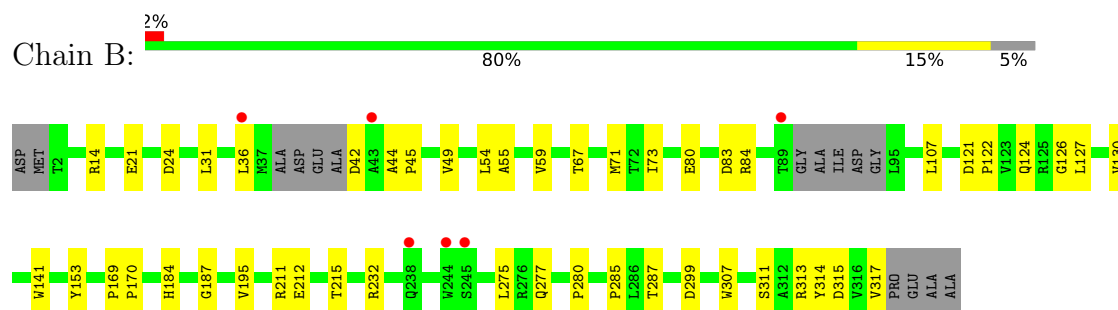
3 Residue-property plots [i](#)

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.

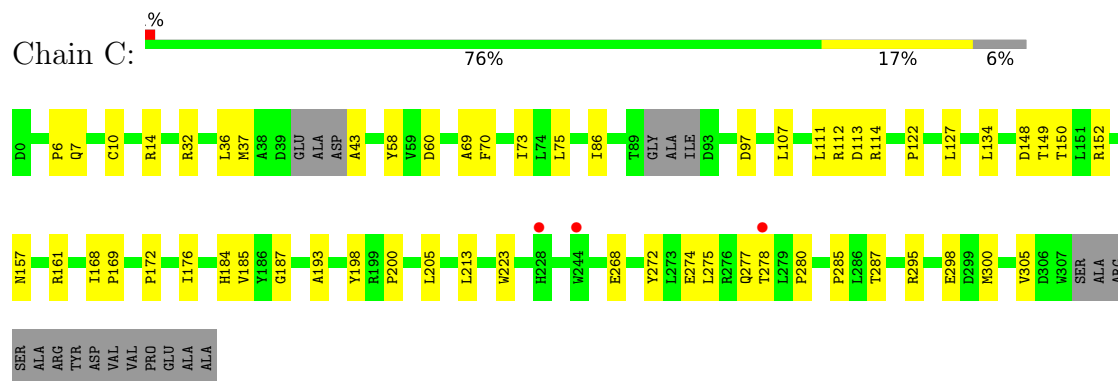
• Molecule 1: Terpene synthase



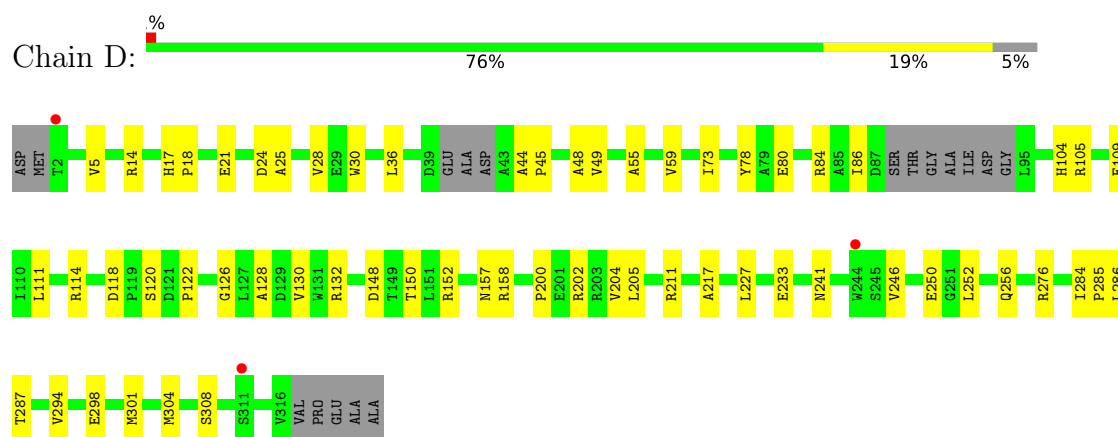
• Molecule 1: Terpene synthase



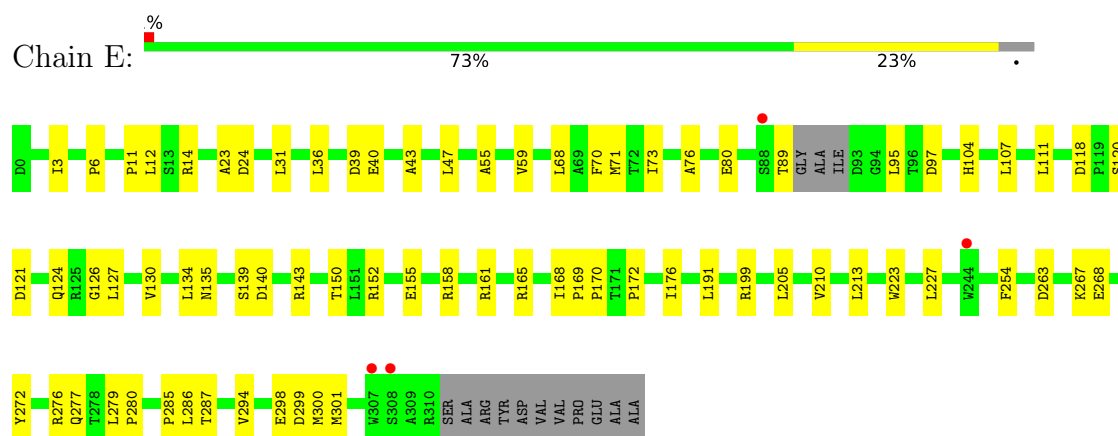
• Molecule 1: Terpene synthase



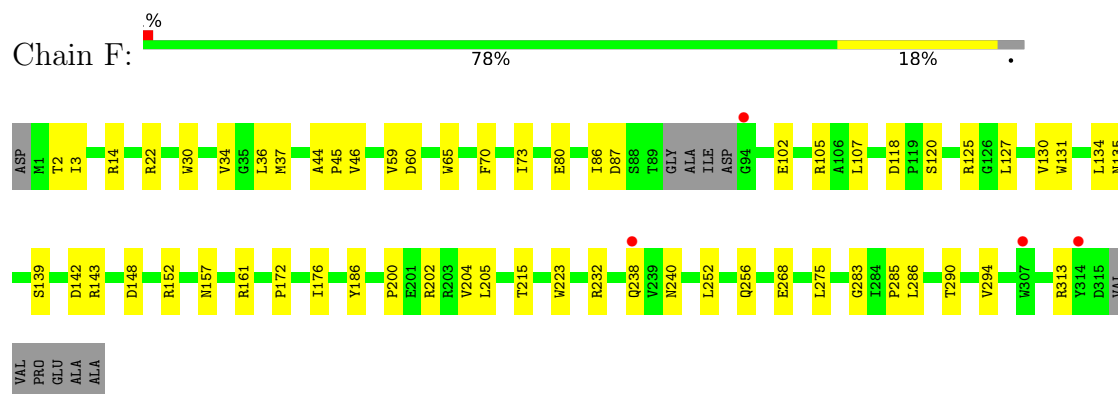
• Molecule 1: Terpene synthase



- Molecule 1: Terpene synthase



- Molecule 1: Terpene synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.72Å 82.32Å 148.29Å 90.00° 92.31° 90.00°	Depositor
Resolution (Å)	49.54 – 3.04 49.54 – 3.04	Depositor EDS
% Data completeness (in resolution range)	96.8 (49.54-3.04) 96.9 (49.54-3.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.252 , 0.307 0.254 , 0.308	Depositor DCC
R_{free} test set	2101 reflections (4.21%)	wwPDB-VP
Wilson B-factor (Å ²)	64.7	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	14633	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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: 212, MG

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	0/2486	0.43	0/3390
1	B	0.18	0/2493	0.41	0/3397
1	C	0.19	0/2447	0.41	0/3334
1	D	0.18	0/2478	0.41	0/3376
1	E	0.18	0/2504	0.43	0/3412
1	F	0.19	0/2519	0.43	0/3432
All	All	0.18	0/14927	0.42	0/20341

There are no bond length outliers.

There are no bond angle outliers.

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	2425	0	2331	36	0
1	B	2433	0	2342	31	0
1	C	2388	0	2294	37	0
1	D	2418	0	2326	41	0
1	E	2443	0	2340	51	0
1	F	2458	0	2360	37	0
2	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
3	B	14	0	9	0	0
3	D	14	0	9	1	0
3	E	14	0	9	0	0
3	F	14	0	9	0	0
All	All	14633	0	14029	229	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 8.

The worst 5 of 229 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:B:14:ARG:NH2	1:B:59:VAL:O	2.07	0.86
1:E:140:ASP:O	1:E:199:ARG:NH1	2.21	0.73
1:E:14:ARG:NH2	1:E:59:VAL:O	2.23	0.68
1:C:223:TRP:CZ3	1:C:268:GLU:HG3	2.29	0.67
1:D:36:LEU:HD13	1:D:80:GLU:HG2	1.76	0.67

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	306/322 (95%)	292 (95%)	11 (4%)	3 (1%)	12	41
1	B	301/322 (94%)	288 (96%)	13 (4%)	0	100	100
1	C	296/322 (92%)	287 (97%)	8 (3%)	1 (0%)	36	67
1	D	299/322 (93%)	291 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	305/322 (95%)	294 (96%)	11 (4%)	0	100	100
1	F	307/322 (95%)	295 (96%)	11 (4%)	1 (0%)	36	67
All	All	1814/1932 (94%)	1747 (96%)	62 (3%)	5 (0%)	36	67

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	ASP
1	A	140	ASP
1	F	139	SER
1	C	113	ASP
1	A	113	ASP

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	246/256 (96%)	246 (100%)	0	100	100
1	B	248/256 (97%)	247 (100%)	1 (0%)	84	87
1	C	243/256 (95%)	243 (100%)	0	100	100
1	D	245/256 (96%)	245 (100%)	0	100	100
1	E	248/256 (97%)	248 (100%)	0	100	100
1	F	249/256 (97%)	249 (100%)	0	100	100
All	All	1479/1536 (96%)	1478 (100%)	1 (0%)	88	91

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	275	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	181	HIS
1	D	234	HIS
1	F	228	HIS
1	F	175	HIS
1	F	181	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 12 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	$\# Z > 2$
3	212	F	404	2	13,13,13	1.71	3 (23%)	19,21,21	1.38	1 (5%)
3	212	E	404	2	13,13,13	1.82	3 (23%)	19,21,21	1.44	3 (15%)
3	212	B	404	2	13,13,13	1.52	3 (23%)	19,21,21	1.49	2 (10%)
3	212	D	404	2	13,13,13	1.41	2 (15%)	19,21,21	1.49	2 (10%)

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
3	212	F	404	2	-	3/23/23/23	-
3	212	E	404	2	-	3/23/23/23	-
3	212	B	404	2	-	3/23/23/23	-
3	212	D	404	2	-	3/23/23/23	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	404	212	P1-C7	3.79	1.87	1.85
3	E	404	212	P8-C7	3.32	1.87	1.85
3	B	404	212	O14-C7	-3.30	1.40	1.44
3	F	404	212	P1-C7	3.27	1.87	1.85
3	D	404	212	O14-C7	-3.26	1.40	1.44

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	404	212	C19-C16-C7	-4.20	108.72	116.02
3	B	404	212	C19-C16-C7	-4.05	108.98	116.02
3	E	404	212	C19-C16-C7	-3.61	109.74	116.02
3	F	404	212	C19-C16-C7	-2.85	111.06	116.02
3	D	404	212	P8-C7-P1	-2.27	108.66	112.72

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	404	212	C19-C16-C7-P1
3	B	404	212	C19-C16-C7-P8
3	B	404	212	C19-C16-C7-O14
3	D	404	212	C19-C16-C7-P1
3	D	404	212	C19-C16-C7-P8

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	404	212	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 [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	308/322 (95%)	0.36	3 (0%) 79 58	39, 61, 90, 118	0
1	B	307/322 (95%)	0.35	6 (1%) 65 41	33, 60, 92, 127	0
1	C	302/322 (93%)	0.15	3 (0%) 79 58	33, 50, 75, 100	0
1	D	305/322 (94%)	0.30	3 (0%) 79 58	29, 57, 84, 104	0
1	E	308/322 (95%)	0.27	4 (1%) 75 52	25, 52, 84, 115	1 (0%)
1	F	311/322 (96%)	0.31	4 (1%) 75 52	29, 53, 90, 120	0
All	All	1841/1932 (95%)	0.29	23 (1%) 76 54	25, 55, 87, 127	1 (0%)

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	244	TRP	3.3
1	B	244	TRP	3.2
1	E	307	TRP	2.9
1	A	56	ALA	2.6
1	B	89	THR	2.6

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

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	MG	D	401	1/1	0.47	0.13	79,79,79,79	0
2	MG	F	403	1/1	0.68	0.14	81,81,81,81	0
2	MG	B	403	1/1	0.73	0.17	66,66,66,66	0
2	MG	E	401	1/1	0.76	0.17	86,86,86,86	0
2	MG	B	401	1/1	0.76	0.12	74,74,74,74	0
3	212	E	404	14/14	0.79	0.12	72,85,98,100	0
3	212	F	404	14/14	0.79	0.15	58,79,92,107	0
2	MG	E	403	1/1	0.84	0.07	65,65,65,65	0
2	MG	D	403	1/1	0.86	0.14	68,68,68,68	0
3	212	B	404	14/14	0.88	0.10	55,72,92,96	0
3	212	D	404	14/14	0.89	0.09	65,78,85,85	0
2	MG	F	402	1/1	0.90	0.11	71,71,71,71	0
2	MG	E	402	1/1	0.92	0.17	64,64,64,64	0
2	MG	F	401	1/1	0.94	0.06	66,66,66,66	0
2	MG	B	402	1/1	0.95	0.06	73,73,73,73	0
2	MG	D	402	1/1	0.97	0.05	54,54,54,54	0

6.5 Other polymers

There are no such residues in this entry.