



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:35 PM UTC

PDB ID : 8B4L / pdb_00008b4l
Title : Crystal structure of a selenomethionine-labeled hydropyrene synthase (M75L variant) in its closed conformation
Authors : Helmer, C.P.O.; Driller, R.; Loll, B.
Deposited on : 2022-09-20
Resolution : 3.39 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

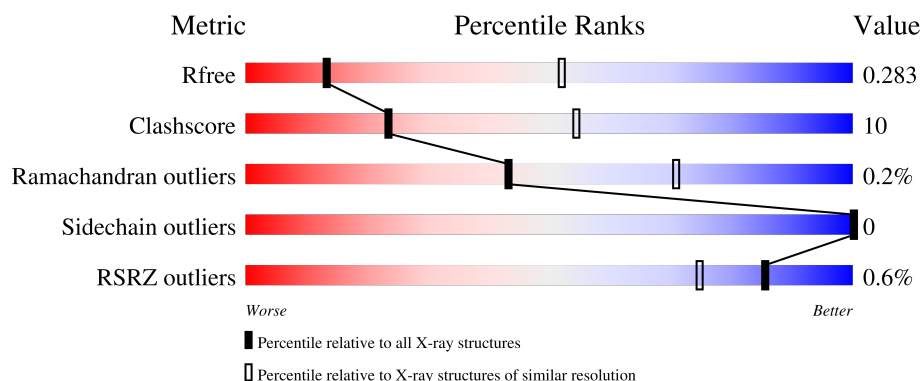
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.39 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	323	% 72% 23% 5%
1	B	323	72% 23% 5%
1	C	323	73% 23% .
1	D	323	% 70% 24% 6%
1	E	323	% 67% 27% 6%

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Mol	Chain	Length	Quality of chain
1	F	323	 A horizontal bar chart showing the quality of the chain. The bar is divided into three segments: a green segment representing 72%, a yellow segment representing 23%, and a small grey segment at the end. A small black dot is located at the far right end of the bar.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14704 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	E	304	Total	C	N	O	S	Se	0	1	0
			2411	1515	438	446	3	9			
1	A	306	Total	C	N	O	S	Se	0	1	0
			2427	1523	440	452	3	9			
1	B	308	Total	C	N	O	S	Se	0	1	0
			2442	1531	448	452	3	8			
1	C	311	Total	C	N	O	S	Se	0	1	0
			2459	1541	448	458	3	9			
1	D	305	Total	C	N	O	S	Se	0	1	0
			2416	1518	439	447	3	9			
1	F	309	Total	C	N	O	S	Se	0	1	0
			2449	1535	446	456	3	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ALA	-	expression tag	UNP D5SK09
E	0	ASP	-	expression tag	UNP D5SK09
E	75	LEU	MET	engineered mutation	UNP D5SK09
A	-1	ALA	-	expression tag	UNP D5SK09
A	0	ASP	-	expression tag	UNP D5SK09
A	75	LEU	MET	engineered mutation	UNP D5SK09
B	-1	ALA	-	expression tag	UNP D5SK09
B	0	ASP	-	expression tag	UNP D5SK09
B	75	LEU	MET	engineered mutation	UNP D5SK09
C	-1	ALA	-	expression tag	UNP D5SK09
C	0	ASP	-	expression tag	UNP D5SK09
C	75	LEU	MET	engineered mutation	UNP D5SK09
D	-1	ALA	-	expression tag	UNP D5SK09
D	0	ASP	-	expression tag	UNP D5SK09
D	75	LEU	MET	engineered mutation	UNP D5SK09
F	-1	ALA	-	expression tag	UNP D5SK09
F	0	ASP	-	expression tag	UNP D5SK09

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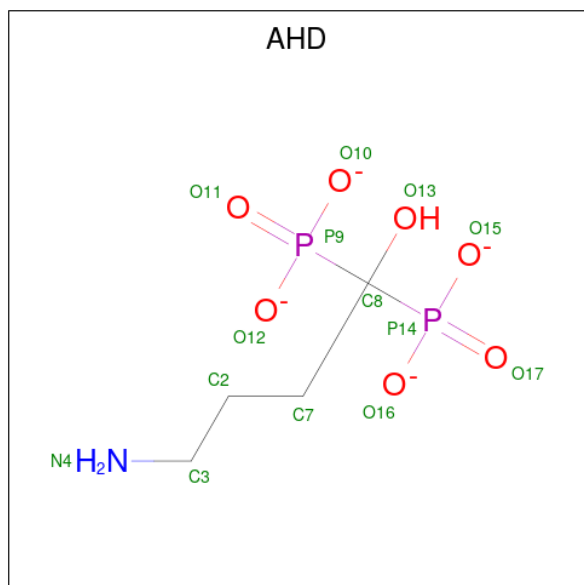
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Chain	Residue	Modelled	Actual	Comment	Reference
F	75	LEU	MET	engineered mutation	UNP D5SK09

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	3	Total	Mg	0	0
			3	3		
2	A	3	Total	Mg	0	0
			3	3		
2	B	3	Total	Mg	0	0
			3	3		
2	C	3	Total	Mg	0	0
			3	3		
2	D	3	Total	Mg	0	0
			3	3		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 4-AMINO-1-HYDROXYBUTANE-1,1-DIYLDIPHOSPHONATE (CCD ID: AHD) (formula: C₄H₉NO₇P₂).



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

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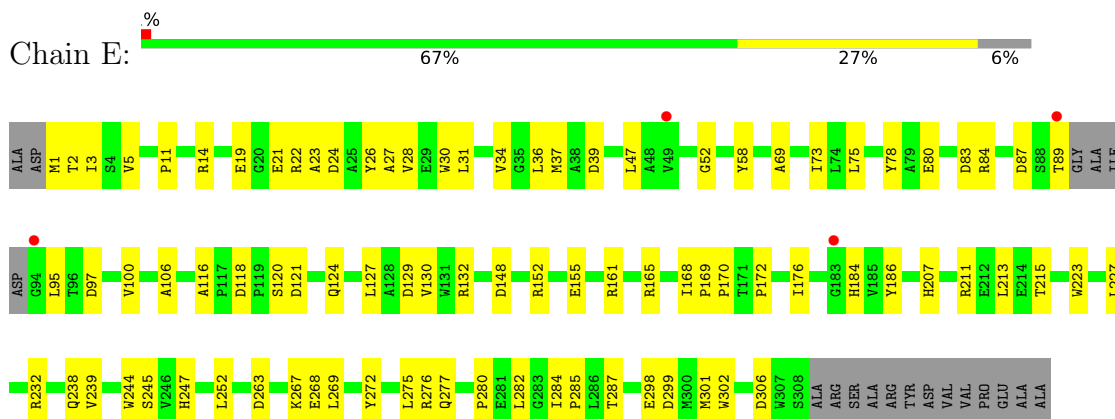
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	C	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	D	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	F	1	Total	C	N	O	P	0	0
			14	4	1	7	2		

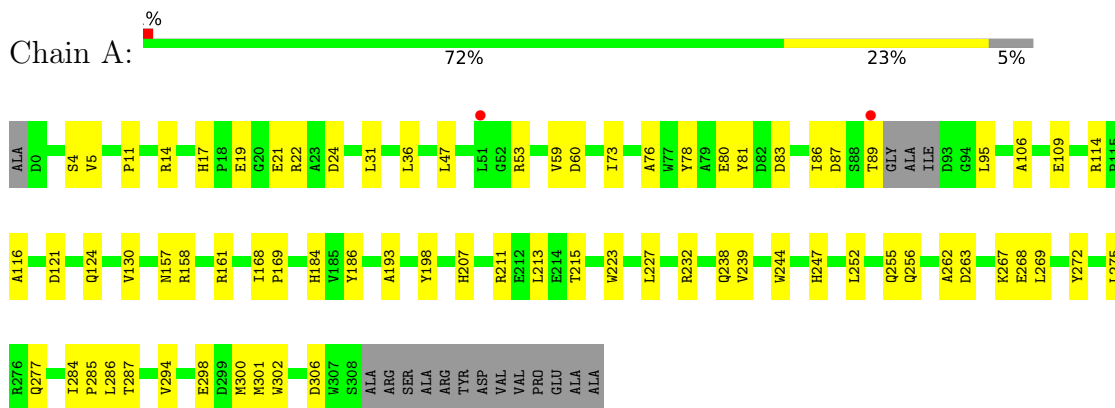
3 Residue-property plots [i](#)

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.

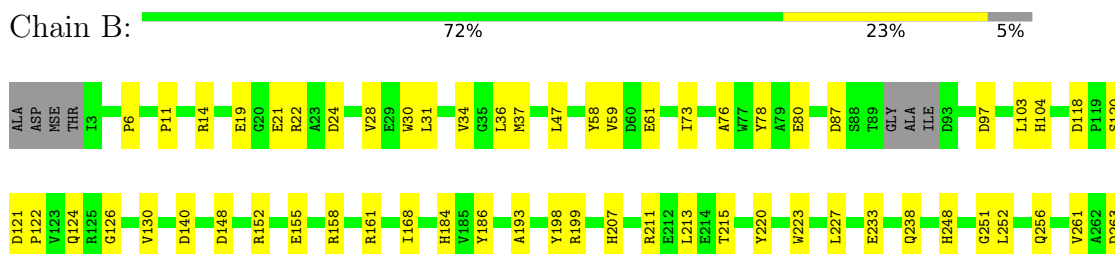
• Molecule 1: Terpene synthase

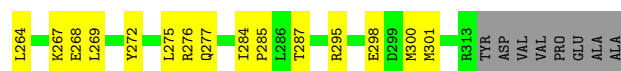


• Molecule 1: Terpene synthase



• Molecule 1: Terpene synthase

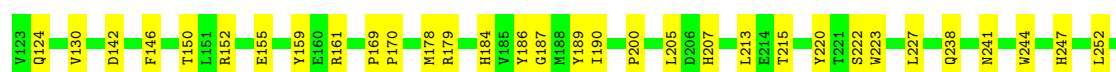
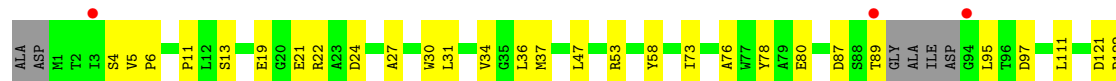




• Molecule 1: Terpene synthase



• Molecule 1: Terpene synthase



• Molecule 1: Terpene synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.70Å 176.69Å 185.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.11 – 3.39 49.11 – 3.39	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.11-3.39) 99.6 (49.11-3.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.237 , 0.275 0.241 , 0.283	Depositor DCC
R_{free} test set	1113 reflections (2.97%)	wwPDB-VP
Wilson B-factor (Å ²)	104.5	Xtriage
Anisotropy	0.656	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14704	wwPDB-VP
Average B, all atoms (Å ²)	107.0	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 40.32 % 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 2.7831e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: MG, AHD

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	0.15	0/2479	0.36	0/3364
1	B	0.15	0/2495	0.36	0/3386
1	C	0.16	0/2511	0.37	0/3407
1	D	0.15	0/2469	0.36	0/3352
1	E	0.15	0/2464	0.37	0/3345
1	F	0.15	0/2501	0.37	0/3393
All	All	0.15	0/14919	0.36	0/20247

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 [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	2427	0	2322	47	0
1	B	2442	0	2340	52	0
1	C	2459	0	2355	48	0
1	D	2416	0	2319	48	0
1	E	2411	0	2314	58	0
1	F	2449	0	2345	49	0
2	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	1	0	0	0	0
3	A	14	0	9	0	0
3	B	14	0	9	0	0
3	C	14	0	9	0	0
3	D	14	0	9	0	0
3	E	14	0	9	0	0
3	F	14	0	9	0	0
All	All	14704	0	14049	292	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 292 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:121:ASP:HB3	1:A:124:GLN:HG3	1.68	0.75
1:E:121:ASP:HB3	1:E:124:GLN:HG3	1.69	0.75
1:E:247:HIS:NE2	1:B:61:GLU:OE2	2.20	0.74
1:D:121:ASP:HB3	1:D:124:GLN:HG3	1.69	0.74
1:A:89:THR:HG22	1:A:95:LEU:H	1.56	0.71

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	303/323 (94%)	292 (96%)	11 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	305/323 (94%)	294 (96%)	11 (4%)	0	100	100
1	C	308/323 (95%)	296 (96%)	11 (4%)	1 (0%)	36	65
1	D	302/323 (94%)	291 (96%)	10 (3%)	1 (0%)	36	65
1	E	301/323 (93%)	291 (97%)	9 (3%)	1 (0%)	36	65
1	F	306/323 (95%)	294 (96%)	11 (4%)	1 (0%)	36	65
All	All	1825/1938 (94%)	1758 (96%)	63 (4%)	4 (0%)	43	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	39	ASP
1	C	311	SER
1	D	4	SER
1	F	3	ILE

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	247/247 (100%)	247 (100%)	0	100	100
1	B	247/247 (100%)	247 (100%)	0	100	100
1	C	249/247 (101%)	249 (100%)	0	100	100
1	D	245/247 (99%)	245 (100%)	0	100	100
1	E	245/247 (99%)	245 (100%)	0	100	100
1	F	249/247 (101%)	249 (100%)	0	100	100
All	All	1482/1482 (100%)	1482 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	157	ASN
1	C	163	ASN
1	F	157	ASN
1	C	181	HIS
1	B	104	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 22 ligands modelled in this entry, 16 are monoatomic - leaving 6 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	AHD	E	404	2	13,13,13	1.65	3 (23%)	19,21,21	1.40	2 (10%)
3	AHD	A	404	2	13,13,13	1.54	3 (23%)	19,21,21	1.36	1 (5%)
3	AHD	F	402	2	13,13,13	1.52	3 (23%)	19,21,21	1.50	2 (10%)
3	AHD	D	404	2	13,13,13	1.60	3 (23%)	19,21,21	1.40	2 (10%)
3	AHD	C	404	2	13,13,13	1.50	3 (23%)	19,21,21	1.46	2 (10%)
3	AHD	B	404	2	13,13,13	1.49	2 (15%)	19,21,21	1.46	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	AHD	E	404	2	-	3/23/23/23	-
3	AHD	A	404	2	-	4/23/23/23	-
3	AHD	F	402	2	-	3/23/23/23	-
3	AHD	D	404	2	-	4/23/23/23	-
3	AHD	C	404	2	-	4/23/23/23	-
3	AHD	B	404	2	-	3/23/23/23	-

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	404	AHD	P14-C8	3.37	1.87	1.85
3	B	404	AHD	O13-C8	-3.28	1.40	1.44
3	C	404	AHD	O13-C8	-3.26	1.40	1.44
3	A	404	AHD	O13-C8	-3.25	1.40	1.44
3	D	404	AHD	O13-C8	-3.18	1.40	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	404	AHD	C2-C7-C8	-3.91	109.22	116.02
3	F	402	AHD	C2-C7-C8	-3.84	109.34	116.02
3	B	404	AHD	C2-C7-C8	-3.64	109.70	116.02
3	E	404	AHD	C2-C7-C8	-3.37	110.17	116.02
3	D	404	AHD	C2-C7-C8	-3.35	110.19	116.02

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	404	AHD	C2-C7-C8-P9
3	E	404	AHD	C2-C7-C8-P14
3	E	404	AHD	C2-C7-C8-O13
3	A	404	AHD	C2-C7-C8-P9
3	A	404	AHD	C2-C7-C8-P14

There are no ring outliers.

No monomer is involved in short contacts.

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	297/323 (91%)	-0.31	2 (0%) 84 73	44, 95, 128, 163	1 (0%)
1	B	300/323 (92%)	-0.18	0 100 100	55, 105, 156, 196	1 (0%)
1	C	302/323 (93%)	-0.18	1 (0%) 90 84	52, 103, 147, 185	1 (0%)
1	D	296/323 (91%)	-0.23	3 (1%) 79 66	46, 104, 139, 184	1 (0%)
1	E	295/323 (91%)	-0.23	4 (1%) 73 59	45, 100, 133, 151	1 (0%)
1	F	300/323 (92%)	-0.14	1 (0%) 90 84	48, 110, 152, 185	1 (0%)
All	All	1790/1938 (92%)	-0.21	11 (0%) 85 75	44, 103, 145, 196	6 (0%)

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	89	THR	3.5
1	C	312	ALA	3.4
1	A	89	THR	3.2
1	E	89	THR	2.5
1	E	183	GLY	2.3

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
2	MG	C	401	1/1	0.56	0.16	138,138,138,138	0
2	MG	D	401	1/1	0.64	0.12	143,143,143,143	0
2	MG	B	401	1/1	0.69	0.10	127,127,127,127	0
2	MG	E	403	1/1	0.77	0.08	117,117,117,117	0
3	AHD	E	404	14/14	0.82	0.14	112,132,144,145	0
3	AHD	A	404	14/14	0.85	0.10	112,122,138,142	0
2	MG	D	403	1/1	0.87	0.05	128,128,128,128	0
2	MG	E	401	1/1	0.87	0.08	96,96,96,96	0
2	MG	B	403	1/1	0.87	0.06	139,139,139,139	0
2	MG	A	401	1/1	0.89	0.06	119,119,119,119	0
3	AHD	F	402	14/14	0.90	0.09	123,154,165,180	0
3	AHD	D	404	14/14	0.91	0.09	113,144,158,161	0
3	AHD	C	404	14/14	0.92	0.08	113,134,142,150	0
2	MG	A	403	1/1	0.93	0.07	119,119,119,119	0
2	MG	B	402	1/1	0.94	0.05	113,113,113,113	0
2	MG	C	403	1/1	0.94	0.05	132,132,132,132	0
3	AHD	B	404	14/14	0.94	0.07	126,143,154,154	0
2	MG	F	401	1/1	0.95	0.07	131,131,131,131	0
2	MG	A	402	1/1	0.97	0.04	111,111,111,111	0
2	MG	D	402	1/1	0.98	0.06	128,128,128,128	0
2	MG	E	402	1/1	0.98	0.03	107,107,107,107	0
2	MG	C	402	1/1	0.98	0.05	120,120,120,120	0

6.5 Other polymers [i](#)

There are no such residues in this entry.