Full wwPDB X-ray Structure Validation Report (i)

Mar 22, 2016 – 07:20 PM EDT

PDB ID	:	5F34
Title	:	Crystal structure of membrane associated PatA from Mycobacterium smegmatis in complex with S-hexadecyl Coenzyme A - P21 space group
Authors	:	Albesa-Jove, D.; Svetlikova, Z.; Carreras-Gonzalez, A.; Tersa, M.; Sancho-Vaello, E.; Cifuente, J.O.; Mikusova, K.; Guerin, M.E.
Deposited on	:	2015-12-02
Resolution	:	3.28 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

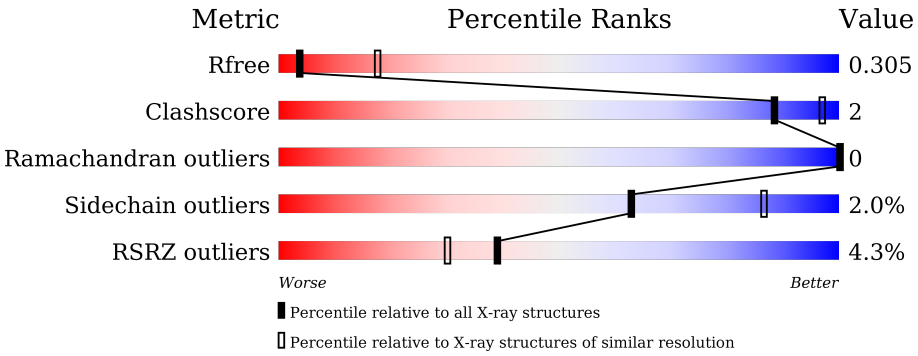
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0122
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

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 3.28 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}	91344	1756 (3.36-3.20)
Clashscore	102246	1941 (3.36-3.20)
Ramachandran outliers	100387	1905 (3.36-3.20)
Sidechain outliers	100360	1903 (3.36-3.20)
RSRZ outliers	91569	1764 (3.36-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	308	2% 73% 8% • 18%
1	B	308	3% 78% • 18%
1	C	308	4% 79% • 18%
1	D	308	5% 78% • 18%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HD6	A	401	-	-	-	X
2	HD6	B	401	-	-	-	X
2	HD6	C	401	-	-	-	X
2	HD6	D	401	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7597 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 Phosphatidylinositol mannoside acyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			1918	1224	338	348	8			
1	B	253	Total	C	N	O	S	0	0	0
			1899	1205	342	344	8			
1	C	252	Total	C	N	O	S	0	0	0
			1812	1165	313	326	8			
1	D	253	Total	C	N	O	S	0	0	0
			1771	1131	301	332	7			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	MET	-	initiating methionine	UNP A0QWG5
A	6	PRO	-	expression tag	UNP A0QWG5
A	7	GLU	-	expression tag	UNP A0QWG5
A	8	VAL	-	expression tag	UNP A0QWG5
A	9	VAL	-	expression tag	UNP A0QWG5
A	10	PHE	-	expression tag	UNP A0QWG5
A	11	GLY	-	expression tag	UNP A0QWG5
A	12	SER	-	expression tag	UNP A0QWG5
A	305	SER	-	expression tag	UNP A0QWG5
A	306	ARG	-	expression tag	UNP A0QWG5
A	307	HIS	-	expression tag	UNP A0QWG5
A	308	HIS	-	expression tag	UNP A0QWG5
A	309	HIS	-	expression tag	UNP A0QWG5
A	310	HIS	-	expression tag	UNP A0QWG5
A	311	HIS	-	expression tag	UNP A0QWG5
A	312	HIS	-	expression tag	UNP A0QWG5
B	5	MET	-	initiating methionine	UNP A0QWG5
B	6	PRO	-	expression tag	UNP A0QWG5
B	7	GLU	-	expression tag	UNP A0QWG5
B	8	VAL	-	expression tag	UNP A0QWG5
B	9	VAL	-	expression tag	UNP A0QWG5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	10	PHE	-	expression tag	UNP A0QWG5
B	11	GLY	-	expression tag	UNP A0QWG5
B	12	SER	-	expression tag	UNP A0QWG5
B	305	SER	-	expression tag	UNP A0QWG5
B	306	ARG	-	expression tag	UNP A0QWG5
B	307	HIS	-	expression tag	UNP A0QWG5
B	308	HIS	-	expression tag	UNP A0QWG5
B	309	HIS	-	expression tag	UNP A0QWG5
B	310	HIS	-	expression tag	UNP A0QWG5
B	311	HIS	-	expression tag	UNP A0QWG5
B	312	HIS	-	expression tag	UNP A0QWG5
C	5	MET	-	initiating methionine	UNP A0QWG5
C	6	PRO	-	expression tag	UNP A0QWG5
C	7	GLU	-	expression tag	UNP A0QWG5
C	8	VAL	-	expression tag	UNP A0QWG5
C	9	VAL	-	expression tag	UNP A0QWG5
C	10	PHE	-	expression tag	UNP A0QWG5
C	11	GLY	-	expression tag	UNP A0QWG5
C	12	SER	-	expression tag	UNP A0QWG5
C	305	SER	-	expression tag	UNP A0QWG5
C	306	ARG	-	expression tag	UNP A0QWG5
C	307	HIS	-	expression tag	UNP A0QWG5
C	308	HIS	-	expression tag	UNP A0QWG5
C	309	HIS	-	expression tag	UNP A0QWG5
C	310	HIS	-	expression tag	UNP A0QWG5
C	311	HIS	-	expression tag	UNP A0QWG5
C	312	HIS	-	expression tag	UNP A0QWG5
D	5	MET	-	initiating methionine	UNP A0QWG5
D	6	PRO	-	expression tag	UNP A0QWG5
D	7	GLU	-	expression tag	UNP A0QWG5
D	8	VAL	-	expression tag	UNP A0QWG5
D	9	VAL	-	expression tag	UNP A0QWG5
D	10	PHE	-	expression tag	UNP A0QWG5
D	11	GLY	-	expression tag	UNP A0QWG5
D	12	SER	-	expression tag	UNP A0QWG5
D	305	SER	-	expression tag	UNP A0QWG5
D	306	ARG	-	expression tag	UNP A0QWG5
D	307	HIS	-	expression tag	UNP A0QWG5
D	308	HIS	-	expression tag	UNP A0QWG5
D	309	HIS	-	expression tag	UNP A0QWG5
D	310	HIS	-	expression tag	UNP A0QWG5
D	311	HIS	-	expression tag	UNP A0QWG5

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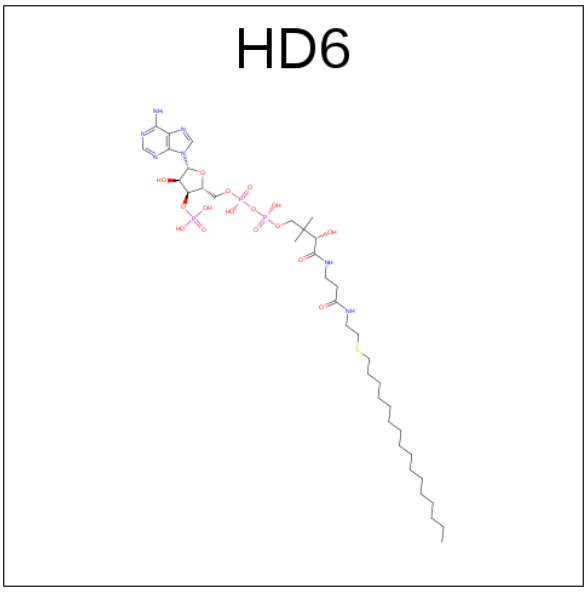
Chain	Residue	Modelled	Actual	Comment	Reference
D	312	HIS	-	expression tag	UNP A0QWG5

- Molecule 2 is [[(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-4-oxidanyl-3-phosphonooxy-oxolan-2-yl]methoxy-oxidanyl-phosphoryl] [(3 {S})-4-[[3-(2-hexadecylsulfanylethylamino)-3-oxidanylidene-propyl]amino]-2,2-dimethyl-3-oxidanyl-4-oxidanylidene-butyl] hydrogen phosphate (three-letter code: HD6) (formula: $C_{37}H_{68}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O P S 64 37 7 16 3 1	0	0
2	B	1	Total C N O S 26 22 2 1 1	0	0
2	C	1	Total C N O P S 42 27 2 10 2 1	0	0
2	D	1	Total C N O P S 42 27 2 10 2 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total O 8 8	0	0
3	B	8	Total O 8 8	0	0
3	C	4	Total O 4 4	0	0

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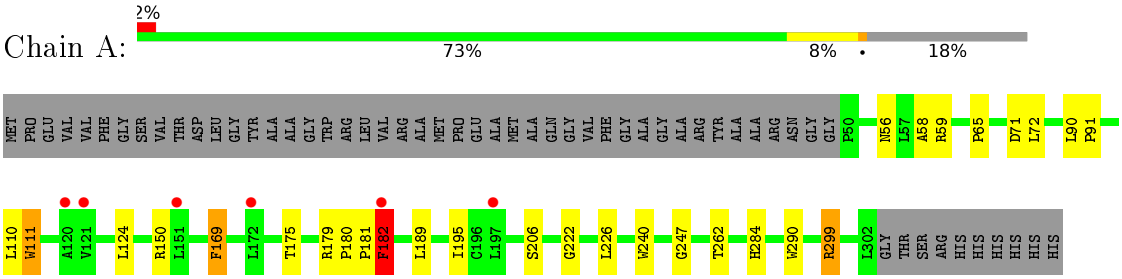
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	3	Total O 3 3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

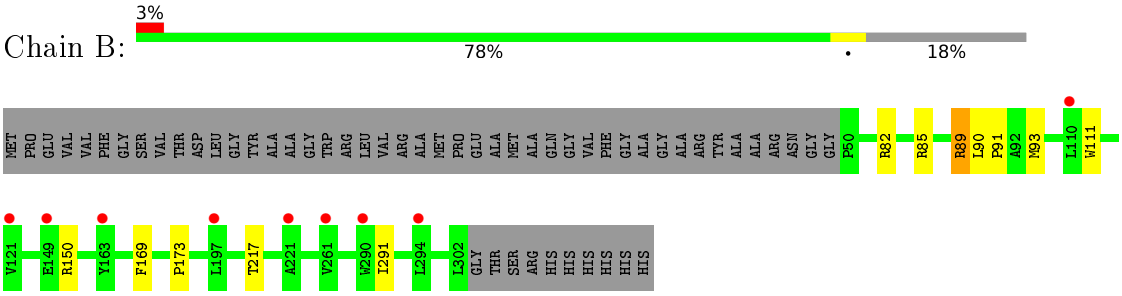
- Molecule 1: Phosphatidylinositol mannoside acyltransferase

Chain A:



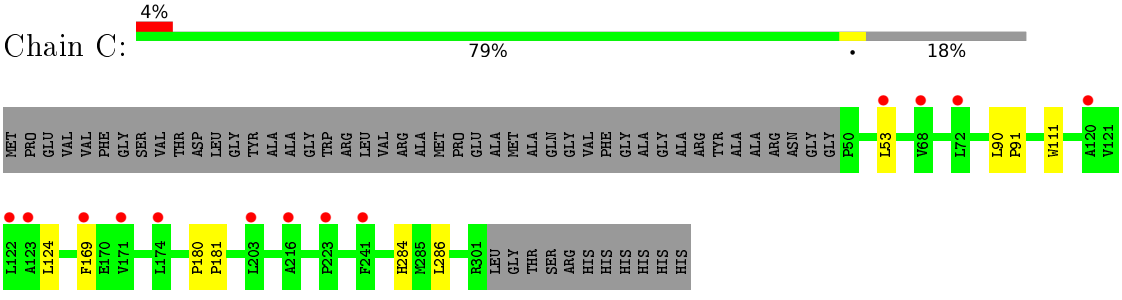
- Molecule 1: Phosphatidylinositol mannoside acyltransferase

Chain B:



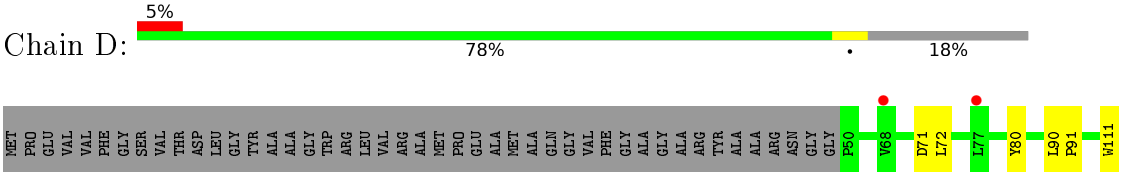
- Molecule 1: Phosphatidylinositol mannoside acyltransferase

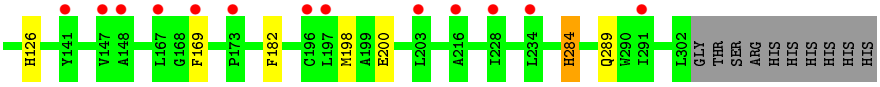
Chain C:



- Molecule 1: Phosphatidylinositol mannoside acyltransferase

Chain D:




H126
Y141
Y147
A148
L167
G168
F169
P173
F182
C196
L197
M198
A199
E200
L203
A216
I228
L234
H284
Q289
W290
I291
L302
GLY
THR
SER
ARG
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.08Å 80.27Å 97.38Å 90.00° 110.92° 90.00°	Depositor
Resolution (Å)	47.12 – 3.28 47.12 – 3.28	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.12-3.28) 99.1 (47.12-3.28)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.264 , 0.306 0.261 , 0.305	Depositor DCC
R_{free} test set	931 reflections (5.20%)	DCC
Wilson B-factor (Å^2)	103.6	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 71.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	1 of 17931 reflections (0.006%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7597	wwPDB-VP
Average B, all atoms (Å^2)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: HD6

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	0.27	0/1973	0.55	0/2701
1	B	0.27	0/1953	0.57	1/2674 (0.0%)
1	C	0.27	0/1867	0.52	0/2568
1	D	0.26	0/1825	0.50	0/2519
All	All	0.27	0/7618	0.54	1/10462 (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	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	89	ARG	NE-CZ-NH1	-5.24	117.68	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	182	PHE	Mainchain

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	1918	0	1790	18	0
1	B	1899	0	1755	6	0
1	C	1812	0	1615	4	0
1	D	1771	0	1508	7	0
2	A	64	0	0	1	0
2	B	26	0	0	0	0
2	C	42	0	0	0	0
2	D	42	0	0	1	0
3	A	8	0	0	1	0
3	B	8	0	0	0	0
3	C	4	0	0	0	0
3	D	3	0	0	0	0
All	All	7597	0	6668	35	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 2.

All (35) 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:206:SER:OG	2:A:401:HD6:OAU	2.11	0.68
1:D:200:GLU:O	1:D:289:GLN:NE2	2.29	0.66
1:A:179:ARG:HG2	1:A:180:PRO:HD2	1.79	0.64
1:A:182:PHE:CE1	1:A:226:LEU:HD12	2.39	0.58
1:A:110:LEU:HD12	1:A:111:TRP:CE3	2.40	0.56
1:A:179:ARG:HG2	1:A:180:PRO:CD	2.40	0.51
1:A:222:GLY:O	1:A:226:LEU:HD13	2.10	0.51
1:A:299:ARG:NH2	3:A:502:HOH:O	2.44	0.50
1:C:53:LEU:HB2	1:C:286:LEU:HA	1.94	0.49
1:A:56:ASN:O	1:A:59:ARG:HB2	2.13	0.49
1:A:150:ARG:HD2	1:A:175:THR:O	2.16	0.46
1:B:89:ARG:NH2	1:B:93:MET:SD	2.90	0.45
1:D:182:PHE:CB	2:D:401:HD6:CAW	2.95	0.44
1:A:182:PHE:CD2	1:A:182:PHE:O	2.70	0.44
1:A:169:PHE:CD1	1:A:169:PHE:N	2.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ALA:HB2	1:A:65:PRO:HA	2.00	0.43
1:C:90:LEU:HB3	1:C:91:PRO:HD3	2.00	0.43
1:D:80:TYR:HB2	1:D:284:HIS:HB3	2.00	0.43
1:B:150:ARG:NH2	1:B:173:PRO:CB	2.81	0.43
1:B:169:PHE:N	1:B:169:PHE:CD1	2.84	0.43
1:C:169:PHE:N	1:C:169:PHE:CD1	2.85	0.43
1:B:90:LEU:HB3	1:B:91:PRO:HD3	2.01	0.43
1:A:90:LEU:HB3	1:A:91:PRO:HD3	2.00	0.43
1:D:169:PHE:N	1:D:169:PHE:CD1	2.87	0.43
1:A:71:ASP:OD2	1:A:72:LEU:N	2.52	0.42
1:A:59:ARG:HG3	1:A:290:TRP:CE3	2.55	0.42
1:A:189:LEU:HD21	1:A:195:ILE:HG12	2.02	0.41
1:B:82:ARG:HA	1:B:85:ARG:HG2	2.02	0.41
1:A:180:PRO:HA	1:A:181:PRO:HD3	1.89	0.41
1:B:217:THR:HA	1:B:291:ILE:HG13	2.03	0.41
1:C:180:PRO:HA	1:C:181:PRO:HD3	2.00	0.41
1:D:71:ASP:OD1	1:D:72:LEU:N	2.54	0.41
1:D:126:HIS:CE1	1:D:198:MET:HB3	2.56	0.41
1:A:240:TRP:CE2	1:A:247:GLY:HA3	2.56	0.40
1:D:90:LEU:HB3	1:D:91:PRO:HD3	2.03	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	251/308 (82%)	249 (99%)	2 (1%)	0	100	100
1	B	251/308 (82%)	249 (99%)	2 (1%)	0	100	100
1	C	250/308 (81%)	247 (99%)	3 (1%)	0	100	100
1	D	251/308 (82%)	249 (99%)	2 (1%)	0	100	100
All	All	1003/1232 (81%)	994 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	182/241 (76%)	175 (96%)	7 (4%)	40 76
1	B	177/241 (73%)	176 (99%)	1 (1%)	90 96
1	C	157/241 (65%)	154 (98%)	3 (2%)	65 87
1	D	148/241 (61%)	146 (99%)	2 (1%)	74 90
All	All	664/964 (69%)	651 (98%)	13 (2%)	63 86

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	TRP
1	A	124	LEU
1	A	169	PHE
1	A	182	PHE
1	A	262	THR
1	A	284	HIS
1	A	299	ARG
1	B	111	TRP
1	C	111	TRP
1	C	124	LEU
1	C	284	HIS
1	D	111	TRP
1	D	284	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

4 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	HD6	A	401	-	57,66,66	1.11	4 (7%)	66,91,91	2.28	4 (6%)
2	HD6	B	401	-	25,25,66	1.33	1 (4%)	25,25,91	1.33	1 (4%)
2	HD6	C	401	-	36,41,66	0.71	0	41,52,91	0.97	1 (2%)
2	HD6	D	401	-	36,41,66	0.73	0	41,52,91	0.94	1 (2%)

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	HD6	A	401	-	-	0/60/80/80	0/3/3/3
2	HD6	B	401	-	-	0/24/24/80	0/0/0/3
2	HD6	C	401	-	-	0/49/49/80	0/0/0/3
2	HD6	D	401	-	-	0/49/49/80	0/0/0/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	HD6	CBZ-NBY	-6.09	1.34	1.47
2	A	401	HD6	C5-C4	-3.03	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	HD6	PAM-OAK	-2.21	1.47	1.54
2	A	401	HD6	C2-N1	3.09	1.39	1.33
2	A	401	HD6	C2-N3	4.00	1.39	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	HD6	N3-C2-N1	-12.87	118.76	128.87
2	A	401	HD6	CCJ-OCK-CCL	-11.02	97.96	109.64
2	A	401	HD6	OCK-CCJ-CAQ	-2.39	99.38	104.89
2	A	401	HD6	N6-C6-N1	2.03	121.92	118.52
2	D	401	HD6	OAS-PCG-OAR	2.75	119.59	110.63
2	C	401	HD6	OAS-PCG-OAR	2.76	119.63	110.63
2	B	401	HD6	CBZ-NBY-CBX	5.16	122.02	111.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	HD6	1	0
2	D	401	HD6	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	253/308 (82%)	0.24	6 (2%)	62	53	61, 94, 123, 148	0
1	B	253/308 (82%)	0.25	9 (3%)	46	37	62, 97, 133, 144	0
1	C	252/308 (81%)	0.39	13 (5%)	31	23	86, 123, 161, 182	0
1	D	253/308 (82%)	0.31	15 (5%)	26	19	100, 131, 156, 182	0
All	All	1011/1232 (82%)	0.30	43 (4%)	39	30	61, 112, 154, 182	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	197	LEU	4.5
1	A	151	LEU	3.3
1	A	197	LEU	3.3
1	D	228	ILE	3.2
1	D	148	ALA	3.1
1	C	122	LEU	3.1
1	D	169	PHE	3.0
1	C	174	LEU	2.9
1	D	173	PRO	2.8
1	C	53	LEU	2.8
1	D	77	LEU	2.8
1	D	141	TYR	2.7
1	C	68	VAL	2.7
1	C	216	ALA	2.7
1	C	171	VAL	2.7
1	D	68	VAL	2.7
1	B	163	TYR	2.6
1	C	169	PHE	2.6
1	B	294	LEU	2.5
1	D	234	LEU	2.5
1	C	123	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	241	PHE	2.4
1	D	167	LEU	2.4
1	A	182	PHE	2.4
1	B	121	VAL	2.4
1	C	72	LEU	2.3
1	A	121	VAL	2.3
1	B	261	VAL	2.3
1	C	203	LEU	2.3
1	C	120	ALA	2.3
1	B	221	ALA	2.3
1	B	149	GLU	2.2
1	D	216	ALA	2.2
1	D	203	LEU	2.2
1	D	196	CYS	2.2
1	D	147	VAL	2.1
1	A	120	ALA	2.1
1	B	197	LEU	2.1
1	B	110	LEU	2.1
1	A	172	LEU	2.1
1	C	223	PRO	2.1
1	B	290	TRP	2.0
1	D	291	ILE	2.0

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	HD6	B	401	26/64	0.85	1.07	9.55	82,108,122,125	0
2	HD6	C	401	42/64	0.76	0.87	5.04	97,149,182,191	0
2	HD6	D	401	42/64	0.68	0.96	4.79	104,154,189,190	0
2	HD6	A	401	64/64	0.73	0.54	2.24	83,146,176,180	0

6.5 Other polymers (i)

There are no such residues in this entry.