Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 02:44 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
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:

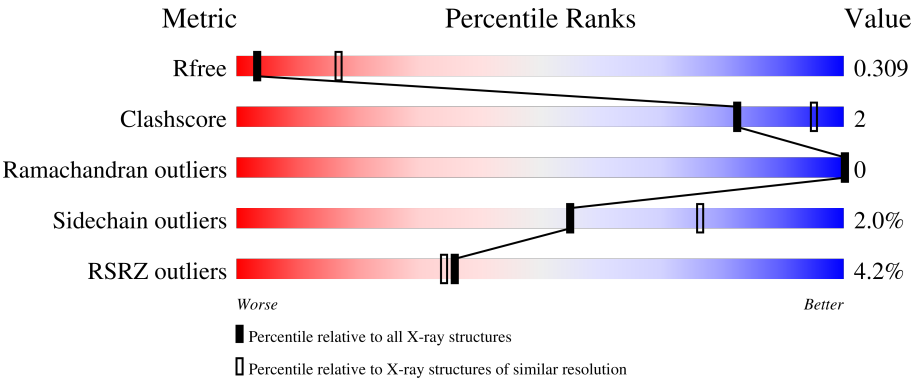
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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}	130704	1177 (3.32-3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)

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	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 criteria:

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

2 Entry composition (i)

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

Continued on next page...

Continued from previous page...

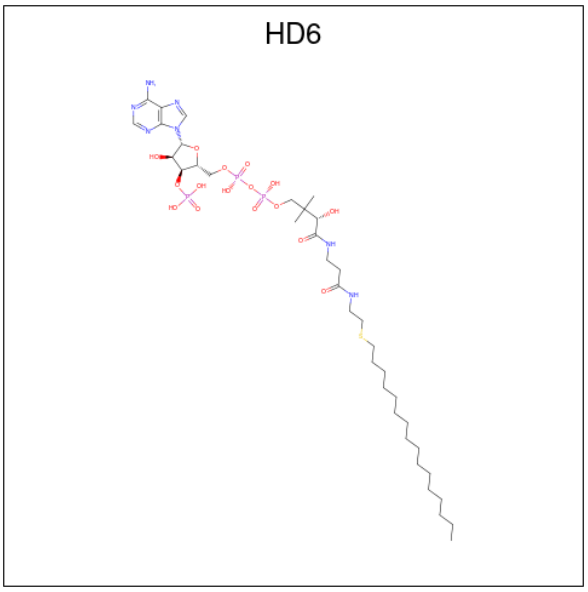
Chain	Residue	Modelled	Actual	Comment	Reference
B	10	PHE	-	expression tag	UNP A0QWG5
B	11	GLY	-	expression tag	UNP A0QWG5
B	12	SER	-	expression tag	UNP A0QWG5
B	305	SER	-	expression tag	UNP A0QWG5
B	306	ARG	-	expression tag	UNP A0QWG5
B	307	HIS	-	expression tag	UNP A0QWG5
B	308	HIS	-	expression tag	UNP 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

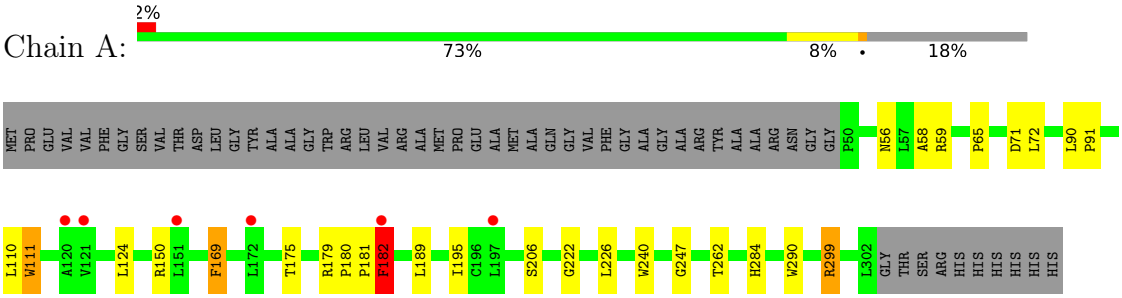
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	3	Total O 3 3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, 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.

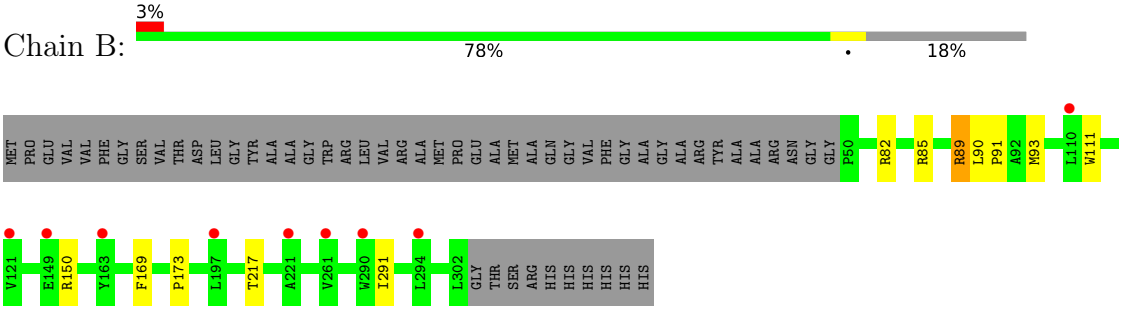
• Molecule 1: Phosphatidylinositol mannoside acyltransferase

Chain A:



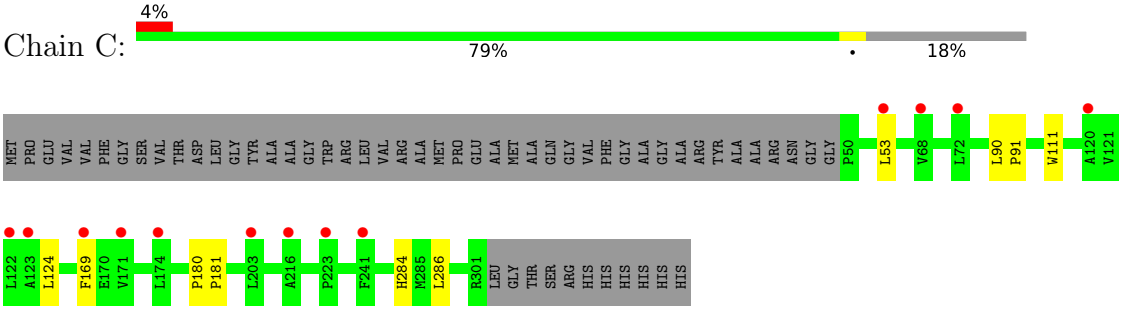
• Molecule 1: Phosphatidylinositol mannoside acyltransferase

Chain B:



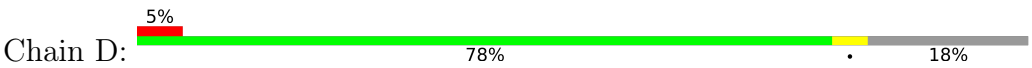
• Molecule 1: Phosphatidylinositol mannoside acyltransferase

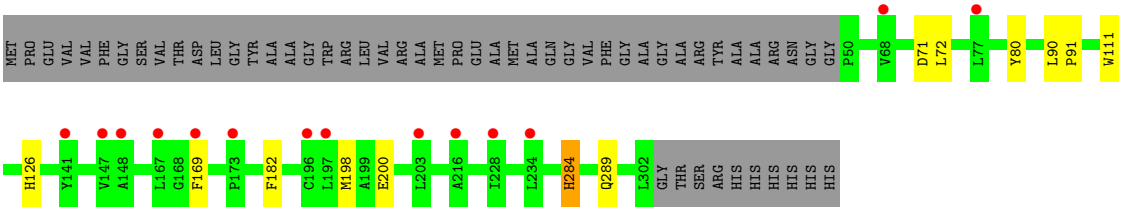
Chain C:



• Molecule 1: Phosphatidylinositol mannoside acyltransferase

Chain D:




MET PRO GLU VAL VAL PHE GLY SER VAL THR ASP LEU GLY TYR ALA ALA GLY TRP ARG LEU VAL ARG ALA MET PRO GLU ALA MET ALA GLN GLY VAL PHE GLY ALA GLY ALA ARG TYR ALA ALA ARG ASN GLY GLY
P50 V68 D71 L72 L77 Y80 L90 P91 W111
H126 Y141 V147 A148 L167 G168 F169 P173 F182 C196 L197 M198 A199 E200 L203 A216 I228 L234 H284 Q289 L302 GLY THR SER ARG HIS 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 1.9_1692	Depositor
R, R_{free}	0.264 , 0.306 0.267 , 0.309	Depositor DCC
R_{free} test set	932 reflections (5.20%)	wwPDB-VP
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 , 74.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 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: 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:O	1:A:182:PHE:CD2	2.70	0.44
1:A:58:ALA:HB2	1:A:65:PRO:HA	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:PHE:CD1	1:A:169:PHE:N	2.84	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:CD1	1:C:169:PHE:N	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%)	33	62
1	B	177/241 (73%)	176 (99%)	1 (1%)	86	91
1	C	157/241 (65%)	154 (98%)	3 (2%)	57	77
1	D	148/241 (61%)	146 (99%)	2 (1%)	67	82
All	All	664/964 (69%)	651 (98%)	13 (2%)	55	76

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

Sometimes 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 monosaccharides 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	C	401	-	36,41,66	0.67	0	47,52,91	1.10	2 (4%)
2	HD6	B	401	-	25,25,66	0.87	1 (4%)	25,25,91	1.10	1 (4%)
2	HD6	D	401	-	36,41,66	0.69	0	47,52,91	1.03	2 (4%)
2	HD6	A	401	-	58,66,66	1.15	4 (6%)	69,91,91	1.30	6 (8%)

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	C	401	-	-	14/49/49/80	-
2	HD6	B	401	-	-	10/24/24/80	-
2	HD6	D	401	-	-	19/49/49/80	-
2	HD6	A	401	-	-	27/60/80/80	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	HD6	C2-N3	4.42	1.39	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	HD6	CBZ-NBY	-3.37	1.34	1.47
2	A	401	HD6	C2-N1	3.19	1.39	1.33
2	A	401	HD6	C5-C4	-2.74	1.33	1.40
2	A	401	HD6	C6-C5	-2.62	1.33	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	HD6	N3-C2-N1	-6.34	118.76	128.68
2	C	401	HD6	PCE-OCF-PCG	-4.24	118.27	132.83
2	B	401	HD6	CBZ-NBY-CBX	3.49	122.02	111.95
2	D	401	HD6	PCE-OCF-PCG	-3.40	121.17	132.83
2	A	401	HD6	OCK-CCL-CAP	-3.24	102.18	106.93
2	A	401	HD6	PCG-OCF-PCE	-2.75	123.39	132.83
2	A	401	HD6	C5-C6-N6	-2.61	116.39	120.35
2	A	401	HD6	OCK-CCJ-CAQ	-2.56	99.38	104.87
2	C	401	HD6	OAS-PCG-OAR	2.28	119.63	110.68
2	D	401	HD6	OAS-PCG-OAR	2.28	119.59	110.68
2	A	401	HD6	CBX-CBW-CBV	-2.12	108.82	112.36

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	HD6	NBY-CBZ-CCA-OAX
2	A	401	HD6	NBY-CBZ-CCA-CCB
2	A	401	HD6	OAY-CBZ-CCA-OAX
2	A	401	HD6	OAY-CBZ-CCA-CCB
2	A	401	HD6	CCC-OCD-PCE-OAT
2	A	401	HD6	CCI-OCH-PCG-OCF
2	A	401	HD6	CCI-OCH-PCG-OAR
2	A	401	HD6	CCI-OCH-PCG-OAS
2	A	401	HD6	OCH-CCI-CCJ-OCK
2	C	401	HD6	SBR-CBS-CBT-NBU
2	C	401	HD6	CBV-CBW-CBX-NBY
2	C	401	HD6	OAY-CBZ-CCA-OAX
2	C	401	HD6	CCC-OCD-PCE-OAT
2	D	401	HD6	CBV-CBW-CBX-NBY
2	D	401	HD6	NBY-CBZ-CCA-OAX
2	D	401	HD6	NBY-CBZ-CCA-CCB
2	D	401	HD6	OAY-CBZ-CCA-CCB
2	D	401	HD6	CCA-CCB-CCC-OCD

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	401	HD6	CAW-CCB-CCC-OCD
2	D	401	HD6	PCE-OCF-PCG-OCH
2	A	401	HD6	CBW-CBV-NBU-CBT
2	B	401	HD6	CBW-CBV-NBU-CBT
2	C	401	HD6	CBW-CBV-NBU-CBT
2	D	401	HD6	CBW-CBV-NBU-CBT
2	A	401	HD6	OCH-CCI-CCJ-CAQ
2	A	401	HD6	OAZ-CBV-NBU-CBT
2	B	401	HD6	OAZ-CBV-NBU-CBT
2	C	401	HD6	OAZ-CBV-NBU-CBT
2	D	401	HD6	OAZ-CBV-NBU-CBT
2	C	401	HD6	CBN-CBO-CBP-CBQ
2	A	401	HD6	CAP-CAQ-OAN-PAM
2	B	401	HD6	CBJ-CBK-CBL-CBM
2	D	401	HD6	CAV-CCB-CCC-OCD
2	B	401	HD6	CBK-CBL-CBM-CBN
2	C	401	HD6	CBF-CBG-CBH-CBI
2	C	401	HD6	CBE-CBF-CBG-CBH
2	A	401	HD6	CCJ-CAQ-OAN-PAM
2	D	401	HD6	SBR-CBS-CBT-NBU
2	B	401	HD6	CBO-CBP-CBQ-SBR
2	C	401	HD6	CBG-CBH-CBI-CBJ
2	B	401	HD6	CBW-CBX-NBY-CBZ
2	D	401	HD6	CBF-CBG-CBH-CBI
2	C	401	HD6	CBI-CBJ-CBK-CBL
2	A	401	HD6	CBI-CBJ-CBK-CBL
2	A	401	HD6	CBB-CBC-CBD-CBE
2	D	401	HD6	OAY-CBZ-CCA-OAX
2	C	401	HD6	CBK-CBL-CBM-CBN
2	D	401	HD6	CBB-CBC-CBD-CBE
2	D	401	HD6	CBK-CBL-CBM-CBN
2	A	401	HD6	CCJ-CCI-OCH-PCG
2	D	401	HD6	CBO-CBP-CBQ-SBR
2	B	401	HD6	CBB-CBC-CBD-CBE
2	A	401	HD6	CCC-OCD-PCE-OCF
2	A	401	HD6	CAQ-OAN-PAM-OAK
2	A	401	HD6	PCG-OCF-PCE-OAU
2	C	401	HD6	CCB-CCC-OCD-PCE
2	A	401	HD6	CBL-CBM-CBN-CBO
2	D	401	HD6	CBI-CBJ-CBK-CBL
2	A	401	HD6	CCC-OCD-PCE-OAU
2	C	401	HD6	CBM-CBN-CBO-CBP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	401	HD6	CBP-CBQ-SBR-CBS
2	A	401	HD6	CBS-CBT-NBU-CBV
2	B	401	HD6	CBI-CBJ-CBK-CBL
2	A	401	HD6	CBT-CBS-SBR-CBQ
2	D	401	HD6	CBT-CBS-SBR-CBQ
2	A	401	HD6	CBH-CBI-CBJ-CBK
2	D	401	HD6	CBD-CBE-CBF-CBG
2	A	401	HD6	CBV-CBW-CBX-NBY
2	B	401	HD6	CBN-CBO-CBP-CBQ
2	A	401	HD6	PCG-OCF-PCE-OAT

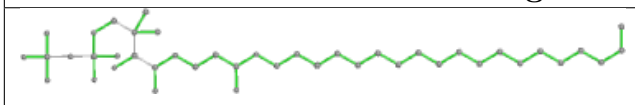
There are no ring outliers.

2 monomers are involved in 2 short contacts:

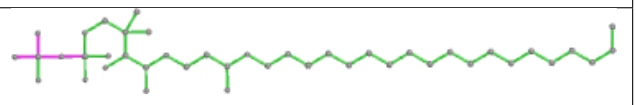
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	HD6	1	0
2	A	401	HD6	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand HD6 C 401



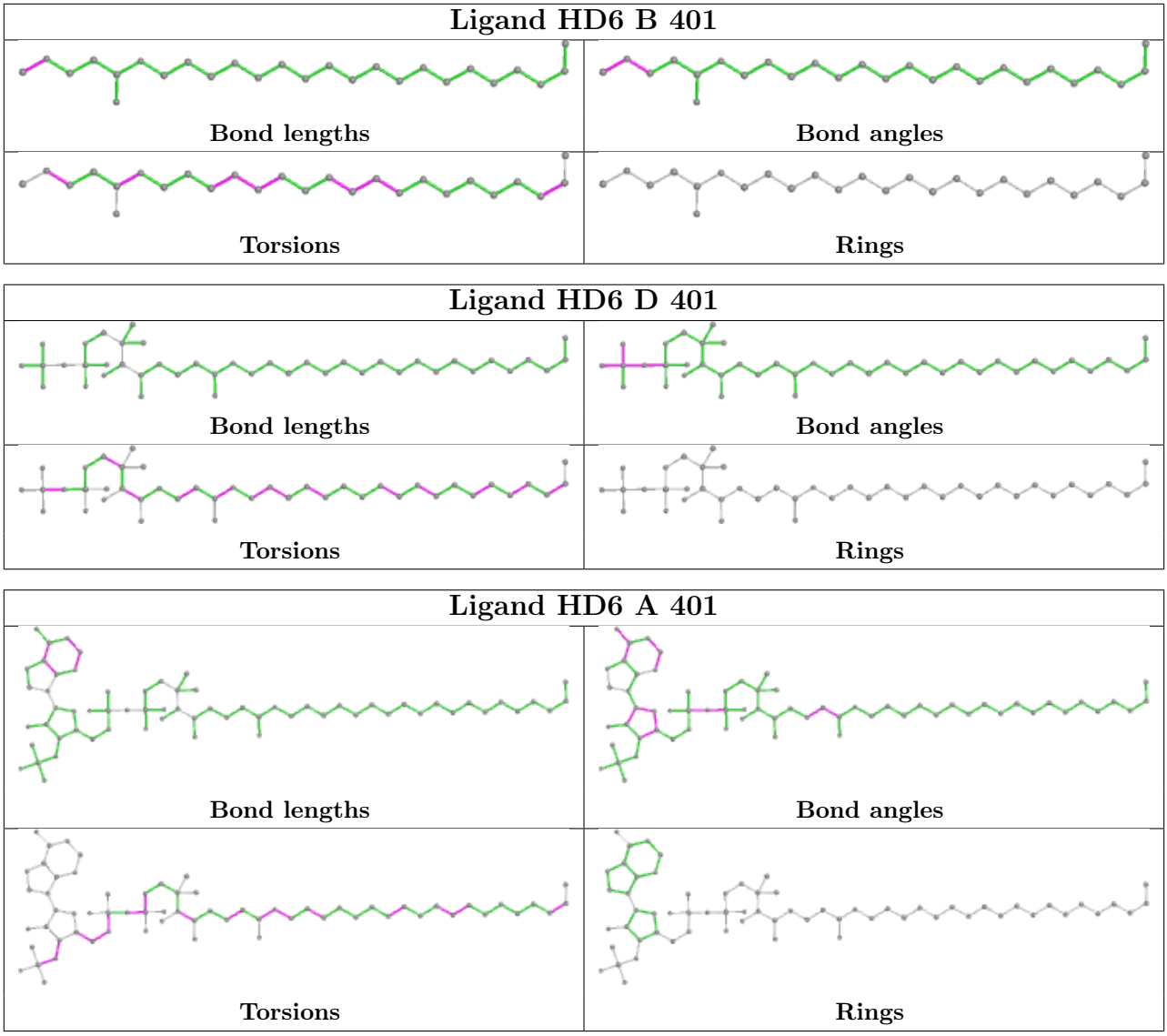
Bond lengths



Bond angles

Torsions

Rings



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%)	0.25	6 (2%)	59 55	61, 94, 123, 148	0
1	B	253/308 (82%)	0.26	9 (3%)	42 40	62, 97, 133, 144	0
1	C	252/308 (81%)	0.40	13 (5%)	27 25	86, 123, 161, 182	0
1	D	253/308 (82%)	0.32	14 (5%)	25 24	100, 131, 156, 182	0
All	All	1011/1232 (82%)	0.31	42 (4%)	36 34	61, 112, 154, 182	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	197	LEU	4.5
1	A	151	LEU	3.4
1	A	197	LEU	3.4
1	D	228	ILE	3.2
1	C	122	LEU	3.1
1	D	148	ALA	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	C	68	VAL	2.8
1	D	141	TYR	2.7
1	C	216	ALA	2.7
1	D	68	VAL	2.7
1	B	163	TYR	2.7
1	C	171	VAL	2.7
1	C	169	PHE	2.6
1	B	294	LEU	2.6
1	D	234	LEU	2.5
1	C	241	PHE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	167	LEU	2.4
1	A	182	PHE	2.4
1	C	123	ALA	2.4
1	B	121	VAL	2.4
1	A	121	VAL	2.4
1	B	261	VAL	2.4
1	C	72	LEU	2.4
1	C	203	LEU	2.3
1	B	221	ALA	2.3
1	C	120	ALA	2.3
1	D	216	ALA	2.2
1	A	120	ALA	2.2
1	D	203	LEU	2.2
1	B	197	LEU	2.1
1	B	149	GLU	2.1
1	D	147	VAL	2.1
1	D	196	CYS	2.1
1	A	172	LEU	2.1
1	B	110	LEU	2.1
1	C	223	PRO	2.1
1	B	290	TRP	2.1

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, 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	HD6	D	401	42/64	0.68	0.96	104,154,189,190	0
2	HD6	A	401	64/64	0.72	0.55	83,146,176,180	0

Continued on next page...

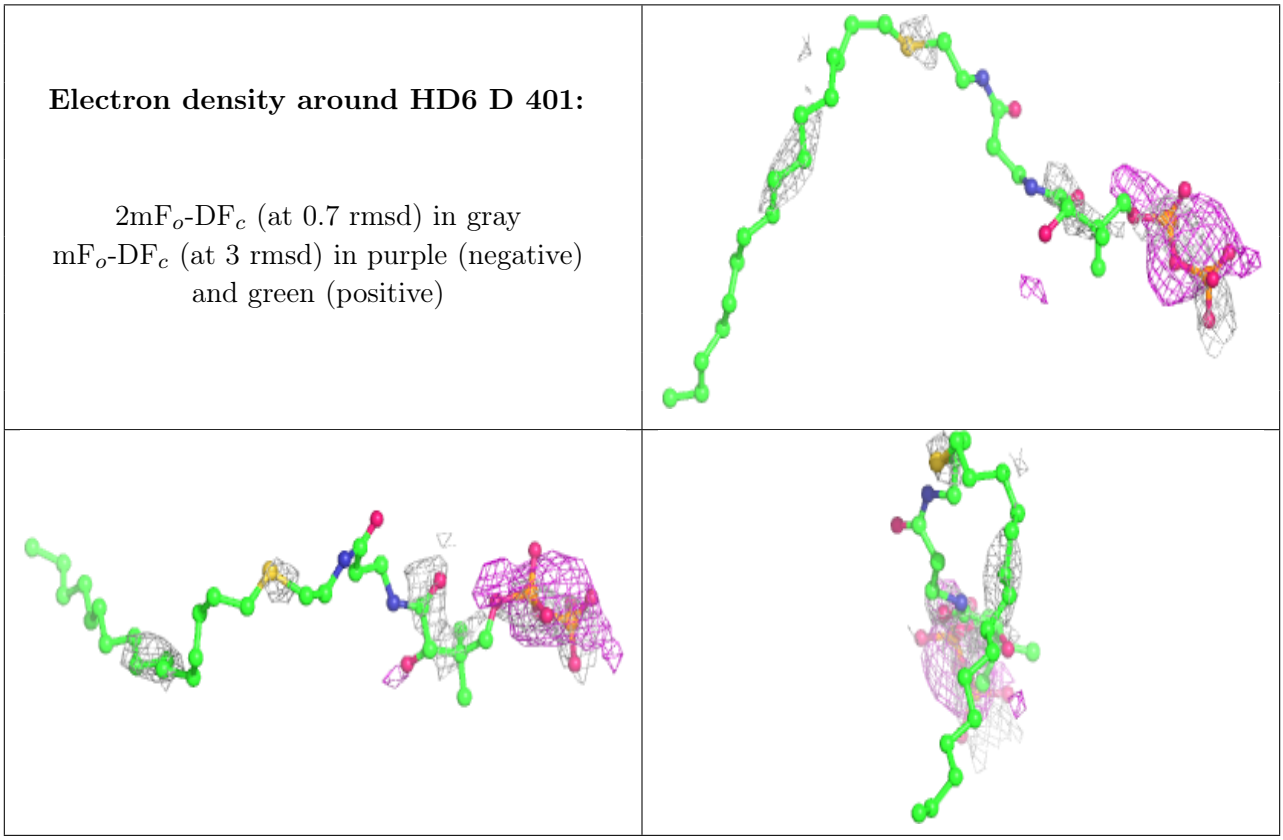
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HD6	C	401	42/64	0.76	0.87	97,149,182,191	0
2	HD6	B	401	26/64	0.84	1.08	82,108,122,125	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

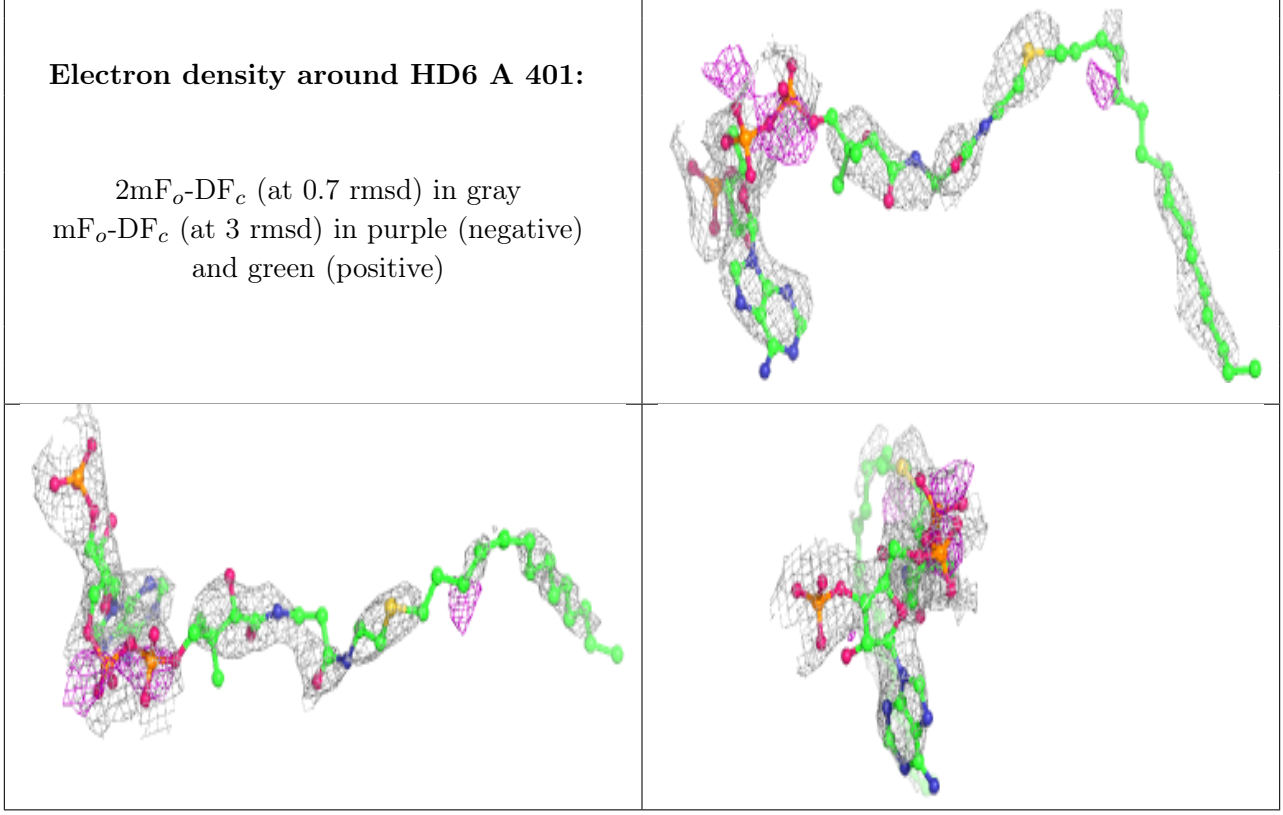
Electron density around HD6 D 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



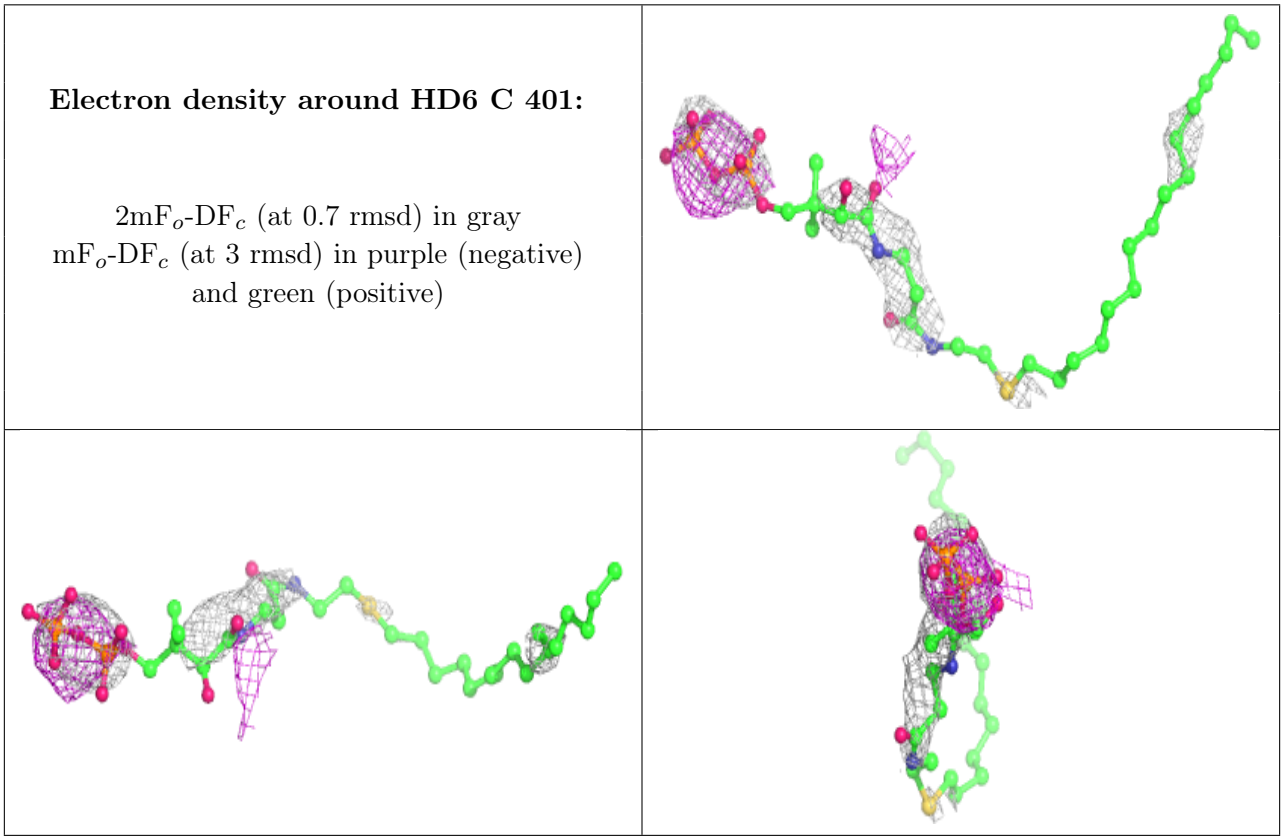
Electron density around HD6 A 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



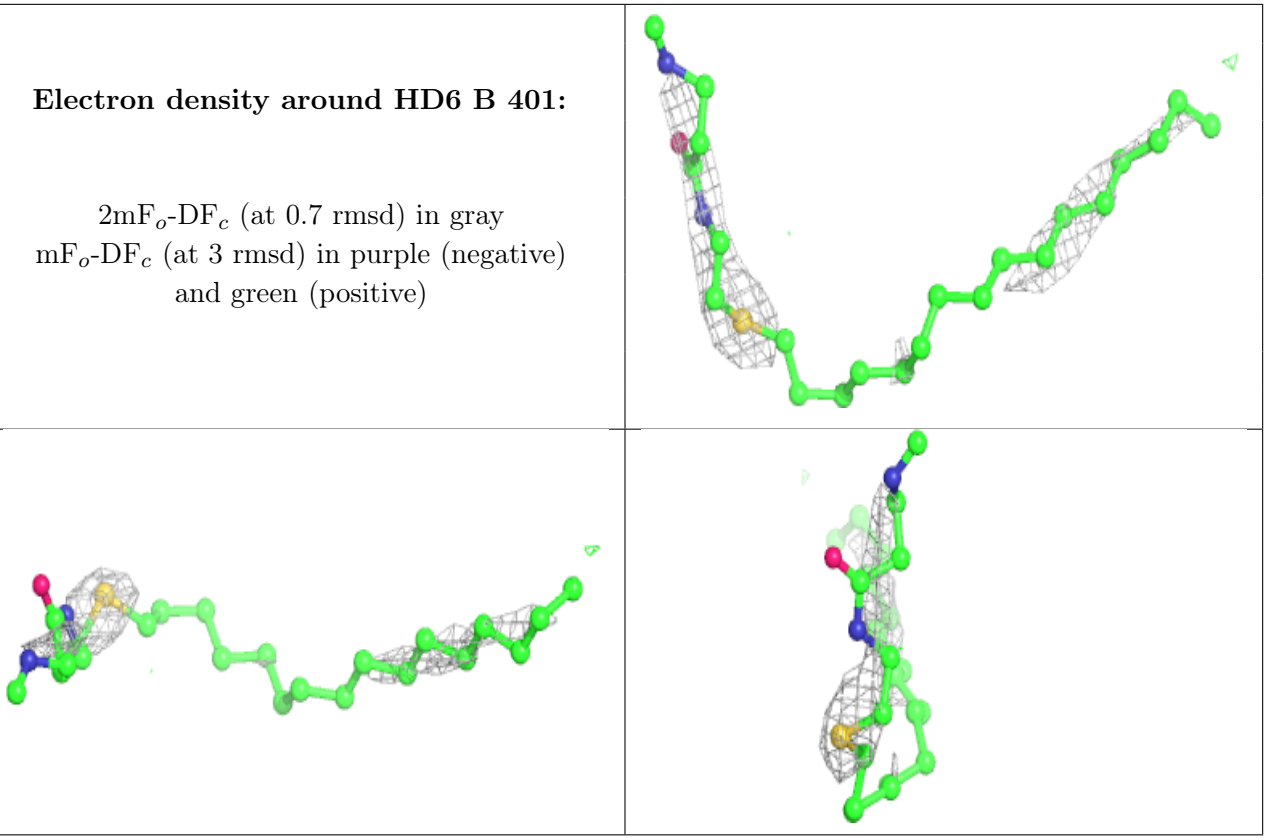
Electron density around HD6 C 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around HD6 B 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.