Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2023 – 09:11 PM EDT

PDB ID	:	2PX6
Title	:	Crystal structure of the thioesterase domain of human fatty acid synthase inhibited by Orlistat
Authors	:	Pemble IV, C.W.; Johnson, L.C.; Kridel, S.J.; Lowther, W.T.
Deposited on	:	2007-05-14
Resolution	:	2.30 Å(reported)

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	:	2.35
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)	:	2.35

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 2.30 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.
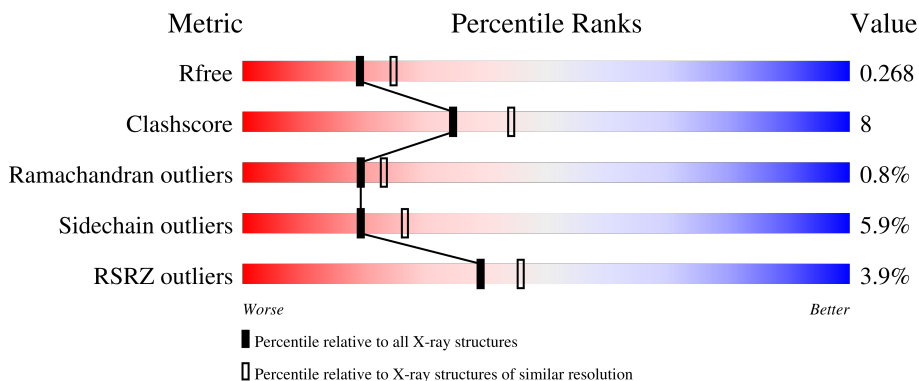
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	316	4% / 64% / 14% · / 20%
1	B	316	2% / 67% / 14% · / 17%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4143 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 Thioesterase domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			1970	1248	339	373	10			
1	B	263	Total	C	N	O	S	0	0	0
			2041	1290	352	389	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2196	GLY	-	cloning artifact	UNP P49327
A	2197	SER	-	cloning artifact	UNP P49327
A	2198	HIS	-	cloning artifact	UNP P49327
A	2199	ASN	-	cloning artifact	UNP P49327
B	2196	GLY	-	cloning artifact	UNP P49327
B	2197	SER	-	cloning artifact	UNP P49327
B	2198	HIS	-	cloning artifact	UNP P49327
B	2199	ASN	-	cloning artifact	UNP P49327

- Molecule 2 is (2S,3S,5S)-5-[(N-FORMYL-L-LEUCYL)OXY]-2-HEXYL-3-HYDROXYHEX ADECANOIC ACID (three-letter code: DH9) (formula: $C_{29}H_{55}NO_6$).
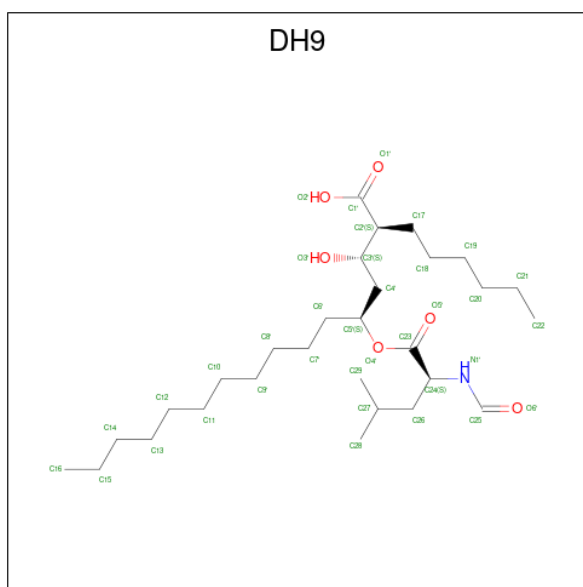
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			35	29	1	5		
2	B	1	Total	C	N	O	0	0
			36	29	1	6		

- Molecule 3 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).
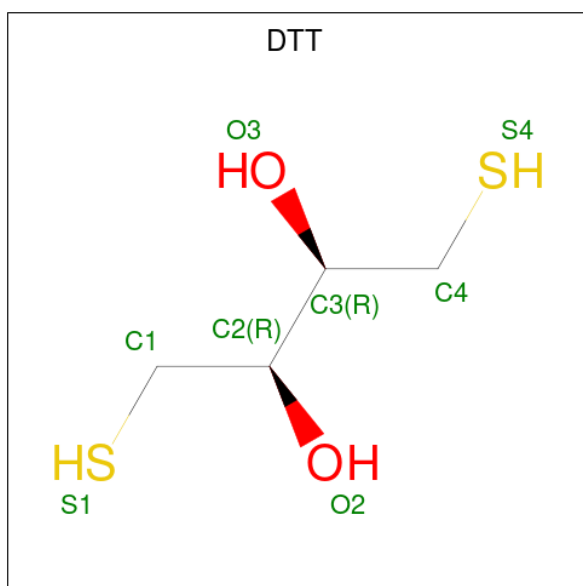
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	S	0	0
			8	4	2	2		

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total 26	O 26	0	0
4	B	27	Total 27	O 27	0	0

3 Residue-property plots ⓘ

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: Thioesterase domain

Chain A:

• Molecule 1: Thioesterase domain

Chain B:
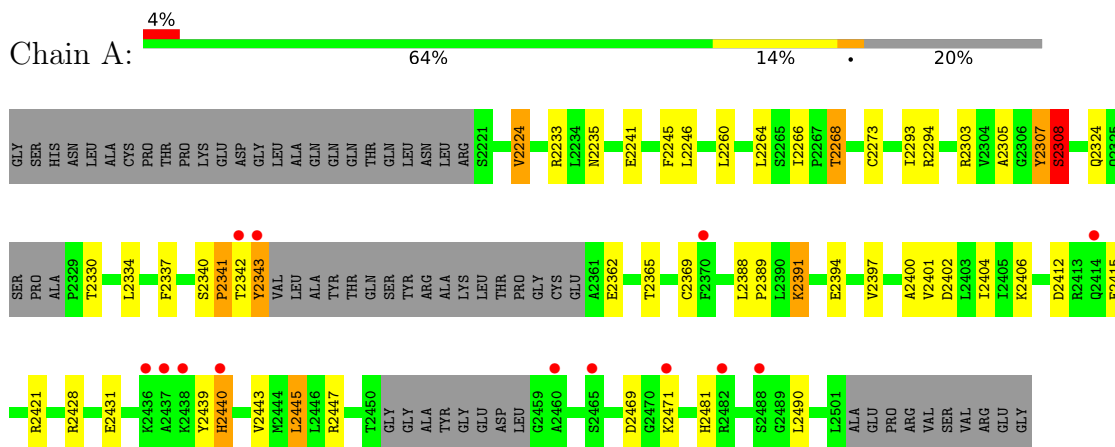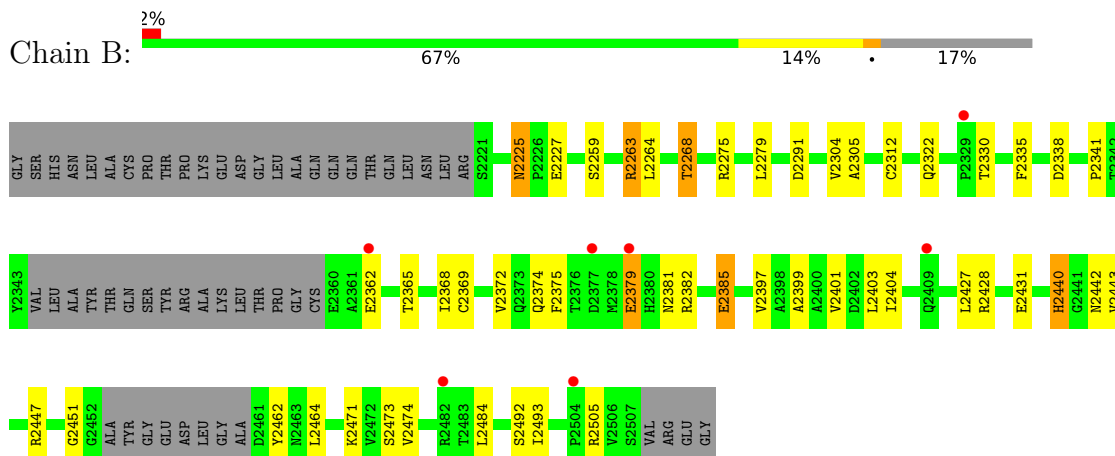
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	41.86Å 94.32Å 69.72Å 90.00° 95.82° 90.00°	Depositor
Resolution (Å)	39.01 – 2.30 39.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.0 (39.01-2.30) 96.0 (39.00-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.47 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.225 , 0.273 0.218 , 0.268	Depositor DCC
R_{free} test set	1184 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	36.8	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 48.6	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4143	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.98% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: DTT, DH9

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	0.71	2/2010 (0.1%)	0.72	5/2722 (0.2%)
1	B	0.61	3/2084 (0.1%)	0.63	0/2826
All	All	0.66	5/4094 (0.1%)	0.68	5/5548 (0.1%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2440	HIS	C-N	-21.63	0.94	1.33
1	B	2440	HIS	CA-CB	-8.69	1.34	1.53
1	B	2440	HIS	C-O	-8.47	1.07	1.23
1	B	2440	HIS	CA-C	-5.69	1.38	1.52
1	A	2439	TYR	C-N	-5.10	1.22	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2307	TYR	O-C-N	-10.92	105.23	122.70
1	A	2307	TYR	C-N-CA	10.47	147.88	121.70
1	A	2307	TYR	CA-C-N	7.47	133.64	117.20
1	A	2308	SER	O-C-N	-7.36	110.92	122.70
1	A	2440	HIS	O-C-N	-5.40	114.02	123.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2308	SER	Mainchain

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	1970	0	1939	38	0
1	B	2041	0	2008	34	0
2	A	35	0	54	3	0
2	B	36	0	54	3	0
3	B	8	0	10	0	0
4	A	26	0	0	1	0
4	B	27	0	0	2	0
All	All	4143	0	4065	68	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.

All (68) 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:2484:LEU:HD23	1:B:2493:ILE:HD11	1.42	1.02
1:B:2484:LEU:CD2	1:B:2493:ILE:HD11	1.98	0.94
1:A:2428:ARG:NH1	1:B:2291:ASP:OD1	2.13	0.82
1:B:2484:LEU:HD23	1:B:2493:ILE:CD1	2.09	0.82
1:A:2428:ARG:NH1	1:B:2291:ASP:OD2	2.20	0.74
1:A:2246:LEU:HD23	1:A:2305:ALA:HB3	1.67	0.73
1:A:2428:ARG:NH1	1:B:2291:ASP:CG	2.42	0.73
1:A:2428:ARG:HH12	1:B:2291:ASP:CG	1.94	0.71
1:B:2381:ASN:O	1:B:2385:GLU:HB3	1.91	0.70
1:A:2264:LEU:HB3	1:A:2266:ILE:HG22	1.75	0.69
1:B:2322:GLN:HE22	1:B:2440:HIS:H	1.43	0.67
1:B:2264:LEU:HD13	1:B:2268:THR:HG21	1.79	0.64
1:B:2484:LEU:CD2	1:B:2493:ILE:CD1	2.73	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2340:SER:O	1:A:2342:THR:N	2.31	0.61
1:B:2365:THR:O	1:B:2369:CYS:HB2	2.01	0.60
1:A:2440:HIS:ND1	1:A:2469:ASP:OD2	2.32	0.60
1:B:2259:SER:O	1:B:2263:ARG:HG2	2.02	0.59
1:A:2481:HIS:CE1	2:A:3000:DH9:H181	2.39	0.58
1:A:2264:LEU:HD12	1:A:2268:THR:HG21	1.86	0.57
1:B:2264:LEU:CD1	1:B:2268:THR:HG21	2.35	0.57
1:A:2402:ASP:O	1:A:2406:LYS:HG3	2.03	0.57
1:B:2225:ASN:HD22	1:B:2227:GLU:H	1.50	0.57
1:B:2484:LEU:HD21	1:B:2493:ILE:HD11	1.84	0.56
1:A:2428:ARG:NH2	4:A:20:HOH:O	2.34	0.55
1:B:2427:LEU:HD13	2:B:61:DH9:H132	1.89	0.54
1:A:2343:TYR:OH	2:A:3000:DH9:H2'	2.08	0.53
1:B:2338:ASP:HB2	1:B:2484:LEU:HD13	1.91	0.52
1:A:2340:SER:HB2	1:A:2341:PRO:HD2	1.91	0.52
1:B:2227:GLU:OE2	1:B:2275:ARG:NH2	2.43	0.52
1:B:2399:ALA:O	1:B:2403:LEU:HG	2.09	0.51
1:A:2412:ASP:OD2	1:A:2415:GLU:HG3	2.11	0.51
1:B:2338:ASP:HB2	1:B:2484:LEU:CD1	2.41	0.51
1:A:2394:GLU:OE1	1:A:2421:ARG:HD3	2.11	0.50
1:A:2397:VAL:O	1:A:2401:VAL:HG23	2.12	0.50
1:A:2233:ARG:HD2	1:A:2235:ASN:O	2.11	0.50
1:A:2388:LEU:N	1:A:2389:PRO:HD2	2.26	0.50
1:A:2245:PHE:CD2	1:A:2293:ILE:HG12	2.47	0.49
1:A:2260:LEU:HA	1:A:2490:LEU:HD11	1.95	0.49
1:A:2264:LEU:CD1	1:A:2268:THR:HG21	2.41	0.49
1:A:2445:LEU:HD13	1:A:2447:ARG:HG2	1.94	0.49
1:A:2264:LEU:HB3	1:A:2266:ILE:CG2	2.41	0.49
1:A:2241:GLU:HG3	1:A:2303:ARG:HH12	1.77	0.48
1:B:2225:ASN:ND2	1:B:2227:GLU:H	2.11	0.48
1:A:2342:THR:HG23	1:A:2343:TYR:HA	1.96	0.48
1:B:2397:VAL:O	1:B:2401:VAL:HG23	2.14	0.47
1:A:2391:LYS:HD3	1:B:2227:GLU:HG3	1.96	0.47
1:B:2431:GLU:HG2	2:B:61:DH9:H223	1.97	0.46
1:A:2481:HIS:NE2	2:A:3000:DH9:H181	2.29	0.46
1:B:2341:PRO:HG3	1:B:2464:LEU:HD23	1.97	0.46
1:A:2343:TYR:CD1	1:A:2343:TYR:N	2.83	0.46
1:A:2334:LEU:HD23	1:A:2443:VAL:HG22	1.97	0.45
1:A:2342:THR:CG2	1:A:2343:TYR:HA	2.47	0.45
1:A:2365:THR:O	1:A:2369:CYS:HB2	2.17	0.44
1:B:2368:ILE:O	1:B:2372:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2442:ASN:O	4:B:22:HOH:O	2.21	0.43
1:A:2224:VAL:HG21	1:A:2273:CYS:O	2.19	0.43
1:A:2294:ARG:HH21	1:A:2324:GLN:HE22	1.66	0.43
1:B:2447:ARG:HD3	1:B:2462:TYR:CE2	2.54	0.43
2:B:61:DH9:H4'1	2:B:61:DH9:H7'1	1.93	0.42
1:B:2225:ASN:HD22	1:B:2225:ASN:C	2.22	0.42
1:A:2235:ASN:ND2	1:A:2268:THR:HG23	2.34	0.42
1:A:2294:ARG:NH2	1:A:2324:GLN:HE22	2.18	0.42
1:A:2400:ALA:O	1:A:2404:ILE:HG13	2.19	0.42
1:B:2428:ARG:NH1	4:B:19:HOH:O	2.45	0.41
1:A:2307:TYR:HA	1:A:2337:PHE:HB2	2.01	0.41
1:B:2375:PHE:HB3	1:B:2404:ILE:HG23	2.02	0.41
1:B:2305:ALA:HA	1:B:2335:PHE:O	2.20	0.41
1:B:2379:GLU:H	1:B:2379:GLU:HG2	1.67	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	245/316 (78%)	235 (96%)	7 (3%)	3 (1%)	13	14
1	B	257/316 (81%)	246 (96%)	10 (4%)	1 (0%)	34	42
All	All	502/632 (79%)	481 (96%)	17 (3%)	4 (1%)	19	23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2341	PRO
1	A	2471	LYS
1	B	2451	GLY
1	A	2308	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	215/264 (81%)	207 (96%)	8 (4%)	34	48
1	B	223/264 (84%)	205 (92%)	18 (8%)	11	15
All	All	438/528 (83%)	412 (94%)	26 (6%)	19	27

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2224	VAL
1	A	2268	THR
1	A	2330	THR
1	A	2343	TYR
1	A	2362	GLU
1	A	2391	LYS
1	A	2431	GLU
1	A	2445	LEU
1	B	2225	ASN
1	B	2263	ARG
1	B	2268	THR
1	B	2279	LEU
1	B	2304	VAL
1	B	2312	CYS
1	B	2330	THR
1	B	2362	GLU
1	B	2374	GLN
1	B	2379	GLU
1	B	2382	ARG
1	B	2385	GLU
1	B	2443	VAL
1	B	2471	LYS
1	B	2473	SER
1	B	2474	VAL
1	B	2492	SER
1	B	2505	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2320	GLN
1	A	2324	GLN
1	A	2325	GLN
1	A	2373	GLN
1	A	2381	ASN
1	A	2432	GLN
1	A	2466	GLN
1	B	2225	ASN
1	B	2322	GLN
1	B	2409	GLN
1	B	2442	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 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	$\#|Z| > 2$
3	DTT	B	71	-	7,7,7	0.57	0	4,8,8	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	DH9	A	3000	1	34,34,35	1.31	4 (11%)	34,39,41	1.66	5 (14%)
2	DH9	B	61	-	35,35,35	0.88	2 (5%)	36,41,41	0.99	2 (5%)

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	DTT	B	71	-	-	0/8/8/8	-
2	DH9	A	3000	1	-	22/42/42/44	-
2	DH9	B	61	-	-	19/44/44/44	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3000	DH9	C2'-C1'	4.59	1.57	1.50
2	A	3000	DH9	C4'-C5'	2.71	1.58	1.52
2	B	61	DH9	C2'-C1'	2.40	1.55	1.51
2	A	3000	DH9	C17-C2'	2.24	1.57	1.53
2	B	61	DH9	C24-N1'	2.09	1.48	1.45
2	A	3000	DH9	C24-N1'	2.03	1.48	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	3000	DH9	O4'-C23-C24	4.82	122.90	111.35
2	A	3000	DH9	O4'-C5'-C4'	4.52	116.04	107.54
2	A	3000	DH9	C5'-O4'-C23	-3.62	111.76	117.69
2	B	61	DH9	O4'-C23-C24	3.31	119.28	111.35
2	A	3000	DH9	O4'-C23-O5'	-3.20	117.96	123.94
2	B	61	DH9	O1'-C1'-C2'	-2.24	117.33	122.95
2	A	3000	DH9	O4'-C5'-C6'	2.11	113.17	107.10

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3000	DH9	C18-C17-C2'-C1'
2	A	3000	DH9	C18-C17-C2'-C3'

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Mol	Chain	Res	Type	Atoms
2	A	3000	DH9	O1'-C1'-C2'-C17
2	A	3000	DH9	C2'-C3'-C4'-C5'
2	A	3000	DH9	O3'-C3'-C4'-C5'
2	A	3000	DH9	C23-C24-C26-C27
2	A	3000	DH9	O6'-C25-N1'-C24
2	B	61	DH9	C18-C17-C2'-C1'
2	B	61	DH9	O1'-C1'-C2'-C17
2	A	3000	DH9	N1'-C24-C26-C27
2	B	61	DH9	C24-C26-C27-C29
2	B	61	DH9	C11-C10-C9'-C8'
2	B	61	DH9	C12-C13-C14-C15
2	B	61	DH9	C17-C18-C19-C20
2	A	3000	DH9	C18-C19-C20-C21
2	A	3000	DH9	C11-C12-C13-C14
2	B	61	DH9	C24-C26-C27-C28
2	A	3000	DH9	C10-C11-C12-C13
2	A	3000	DH9	C9'-C10-C11-C12
2	B	61	DH9	C10-C11-C12-C13
2	A	3000	DH9	O4'-C23-C24-N1'
2	A	3000	DH9	O5'-C23-C24-N1'
2	B	61	DH9	C7'-C8'-C9'-C10
2	A	3000	DH9	C3'-C4'-C5'-C6'
2	B	61	DH9	C13-C14-C15-C16
2	A	3000	DH9	C7'-C8'-C9'-C10
2	A	3000	DH9	C19-C20-C21-C22
2	B	61	DH9	C18-C19-C20-C21
2	B	61	DH9	C6'-C7'-C8'-C9'
2	B	61	DH9	C17-C2'-C3'-C4'
2	A	3000	DH9	O4'-C23-C24-C26
2	B	61	DH9	C1'-C2'-C3'-C4'
2	B	61	DH9	O2'-C1'-C2'-C17
2	B	61	DH9	C1'-C2'-C3'-O3'
2	B	61	DH9	C19-C20-C21-C22
2	A	3000	DH9	O5'-C23-C24-C26
2	A	3000	DH9	C13-C14-C15-C16
2	A	3000	DH9	C3'-C4'-C5'-O4'
2	A	3000	DH9	C5'-C6'-C7'-C8'
2	B	61	DH9	C17-C2'-C3'-O3'
2	B	61	DH9	C11-C12-C13-C14

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3000	DH9	3	0
2	B	61	DH9	3	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 DH9 A 3000
Bond lengths   Bond angles
Torsions   Rings

Ligand DH9 B 61

Bond lengths

Bond angles

Torsions

Rings
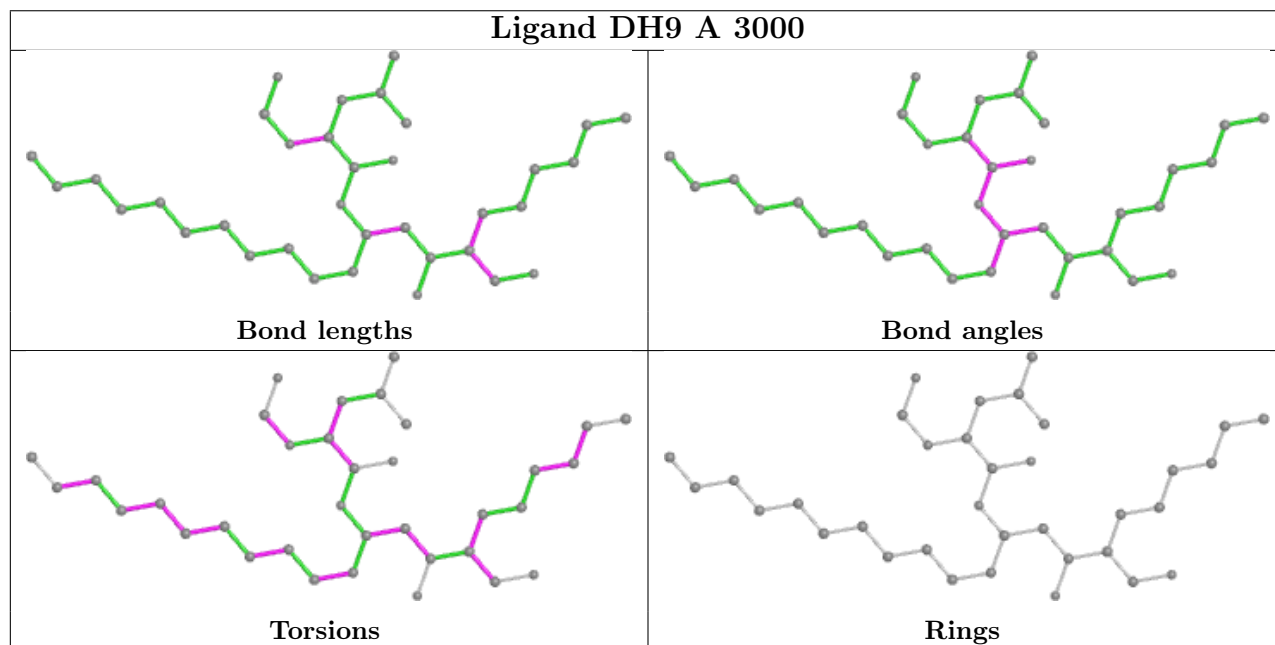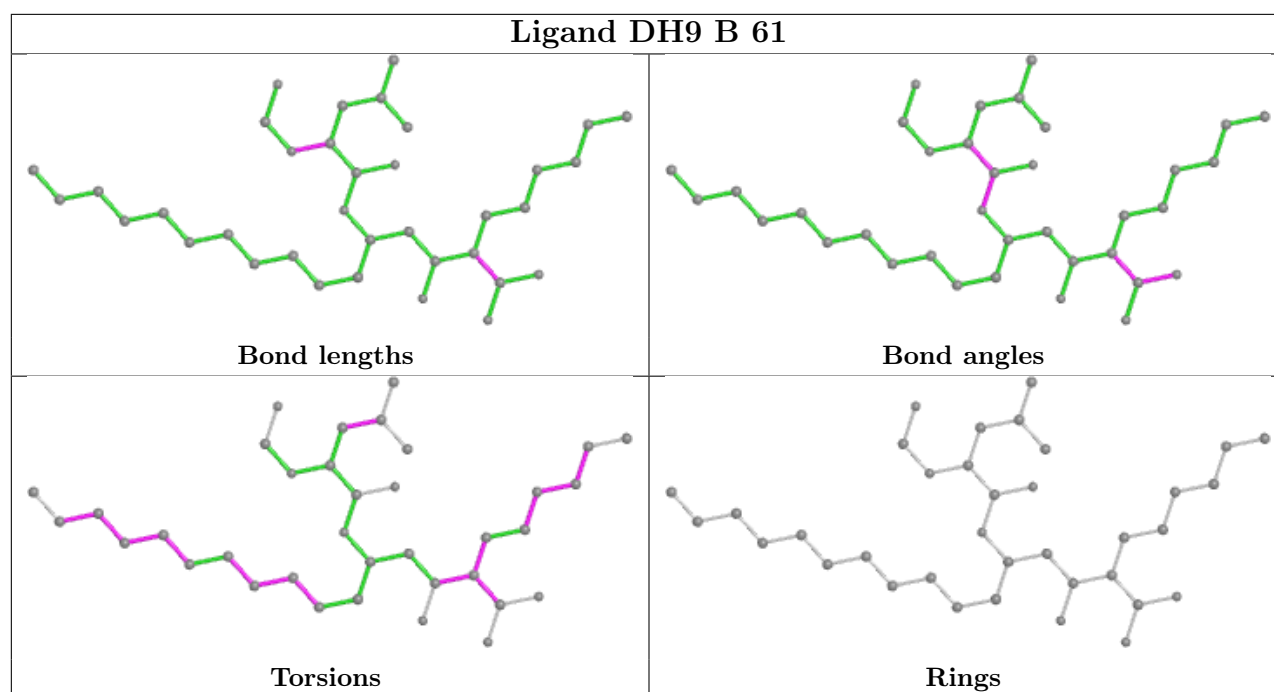
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2440:HIS	C	2441:GLY	N	0.94

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, 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(Å²)	Q<0.9
1	A	253/316 (80%)	0.27	13 (5%)	28	35	20, 35, 60, 69	0
1	B	263/316 (83%)	0.21	7 (2%)	54	62	16, 35, 53, 68	0
All	All	516/632 (81%)	0.24	20 (3%)	39	46	16, 35, 57, 69	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2460	ALA	4.5
1	B	2379	GLU	4.5
1	A	2343	TYR	3.8
1	B	2377	ASP	3.7
1	A	2465	SER	3.7
1	A	2471	LYS	3.0
1	A	2440	HIS	2.9
1	A	2342	THR	2.6
1	A	2414	GLN	2.4
1	A	2488	SER	2.4
1	A	2438	LYS	2.3
1	B	2504	PRO	2.2
1	B	2409	GLN	2.2
1	B	2329	PRO	2.2
1	A	2437	ALA	2.2
1	A	2436	LYS	2.1
1	A	2482	ARG	2.1
1	A	2370	PHE	2.1
1	B	2482	ARG	2.1
1	B	2362	GLU	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 monosaccharides in this entry.
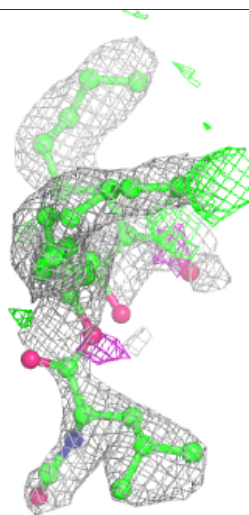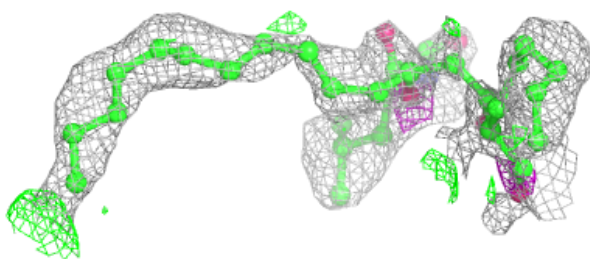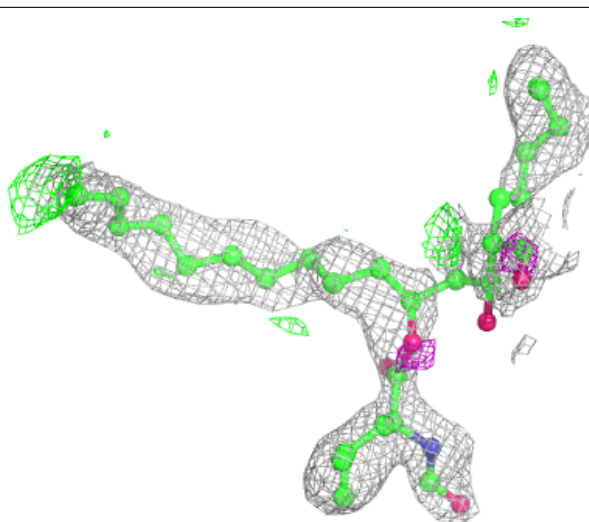
6.4 Ligands ⓘ

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.
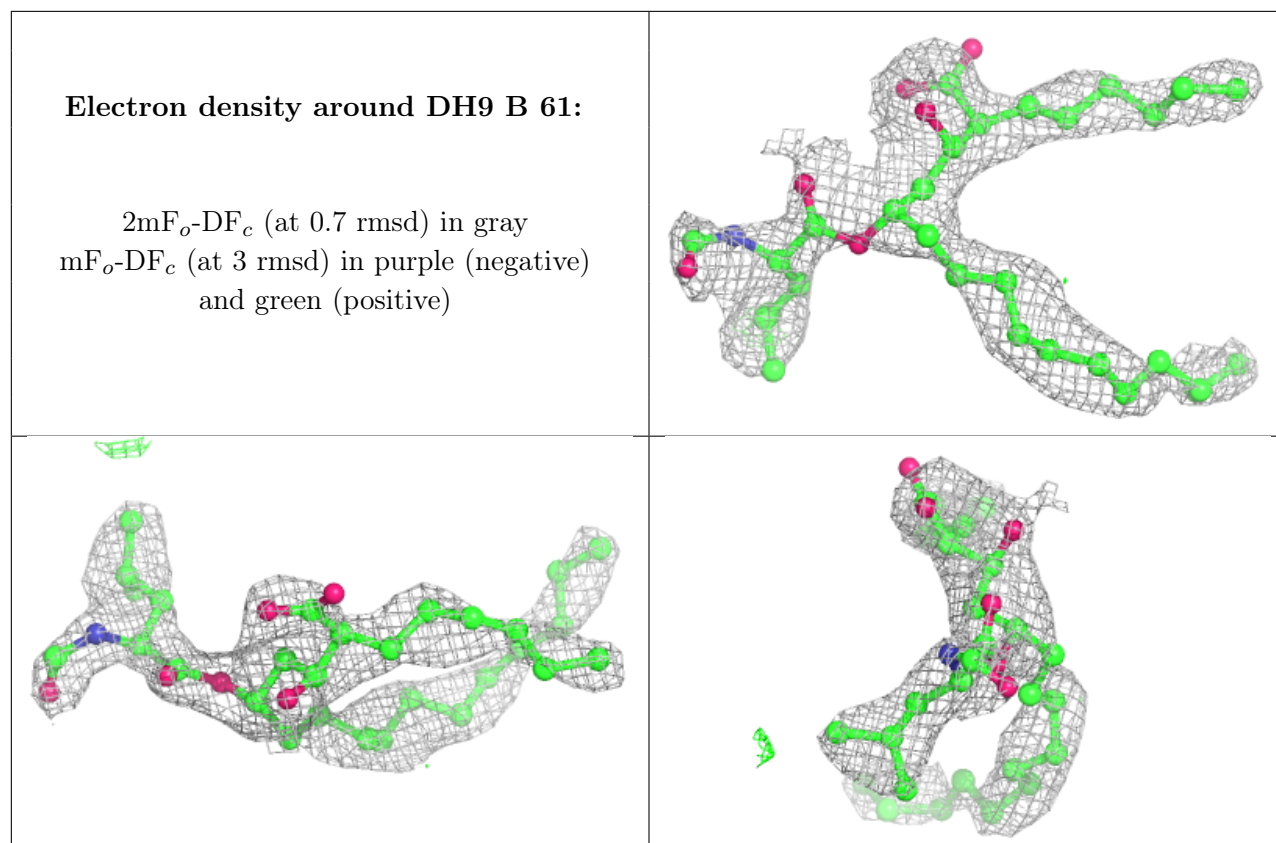
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	DH9	A	3000	35/36	0.56	0.32	50,61,65,67	0
2	DH9	B	61	36/36	0.71	0.28	61,67,71,72	0
3	DTT	B	71	8/8	0.97	0.13	22,23,25,26	0

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 DH9 A 3000:

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

Electron density around DH9 B 61:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.