Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 05:20 AM JST

PDB ID	:	5GIX / pdb_00005gix
Title	:	Human serum albumin-Palmitic acid-Fe(Hn3piT)Cl2
Authors	:	Yang, F.; Qi, J.; Wang, T.
Deposited on	:	2016-06-25
Resolution	:	2.80 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 (i) 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 (i)) were used in the production of this report:

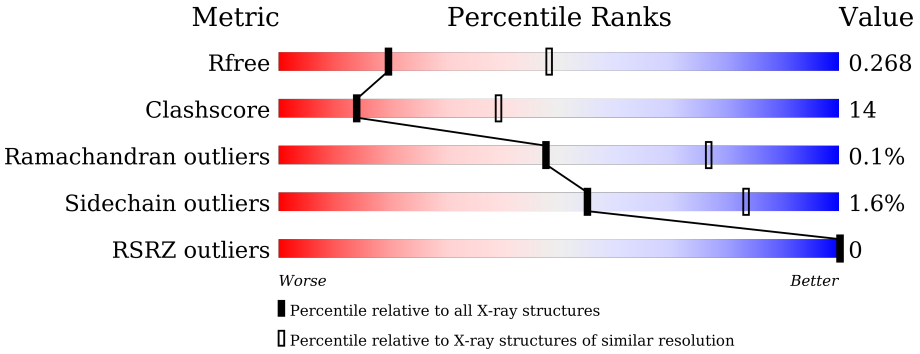
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	581	69% 30% •
1	B	581	69% 31% •

2 Entry composition (i)

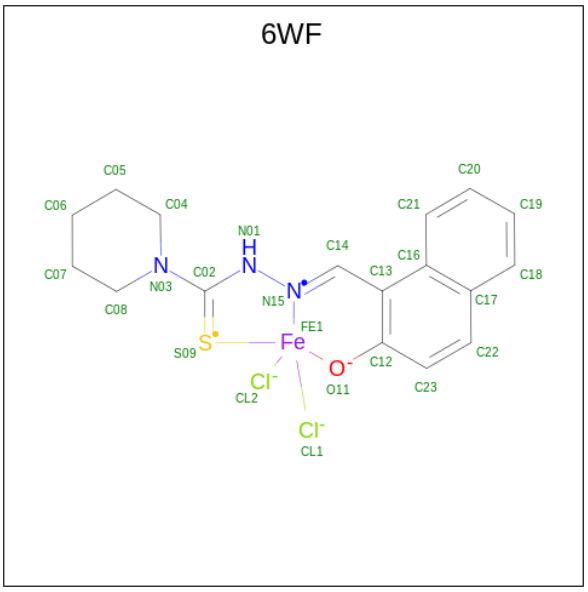
There are 4 unique types of molecules in this entry. The entry contains 9498 atoms, of which 36 are hydrogens and 0 are deuteriums.

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 Serum albumin.

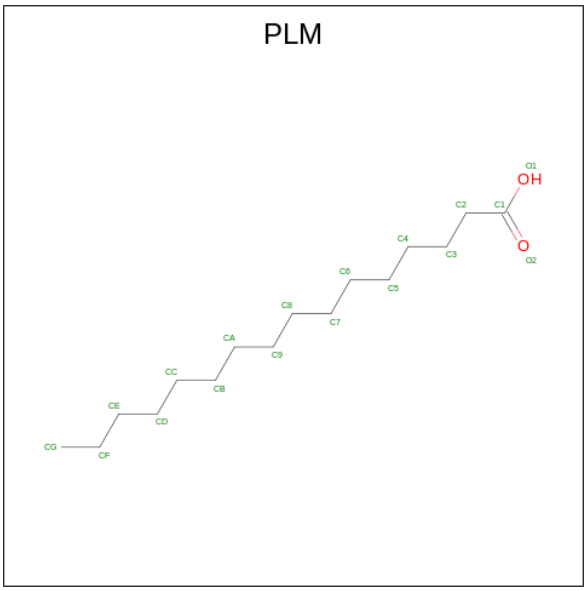
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	581	4606	2909	776	880	41	0	0	0
1	B	581	4606	2909	776	880	41	0	0	0

- Molecule 2 is 14-piperidin-1-yl-11-oxa-13$l^{3}-thia-15,16$l^{4}-diaza-12$l^{3}-ferratetracyclo[8.7.0.0^{2,7}.0^{12,16}]heptadeca-1(10),2(7),3,5,8,13,16-heptaene (CCD ID: 6WF) (formula: $C_{17}H_{18}Cl_2FeN_3OS$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	Fe	H	N	O	S		
2	A	1	41	17	1	18	3	1	1	0	0
2	B	1	41	17	1	18	3	1	1	0	0

- Molecule 3 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	13	11	2	0	0
			Total	C	O		
3	A	1	18	16	2	0	0
			Total	C	O		
3	A	1	17	15	2	0	0
			Total	C	O		
3	A	1	18	16	2	0	0
			Total	C	O		
3	A	1	17	15	2	0	0
			Total	C	O		
3	A	1	18	16	2	0	0
			Total	C	O		
3	B	1	13	11	2	0	0
			Total	C	O		
3	B	1	18	16	2	0	0
			Total	C	O		
3	B	1	17	15	2	0	0
			Total	C	O		
3	B	1	18	16	2	0	0
			Total	C	O		
3	B	1	17	15	2	0	0
			Total	C	O		
3	B	1	18	16	2	0	0

- Molecule 4 is water.

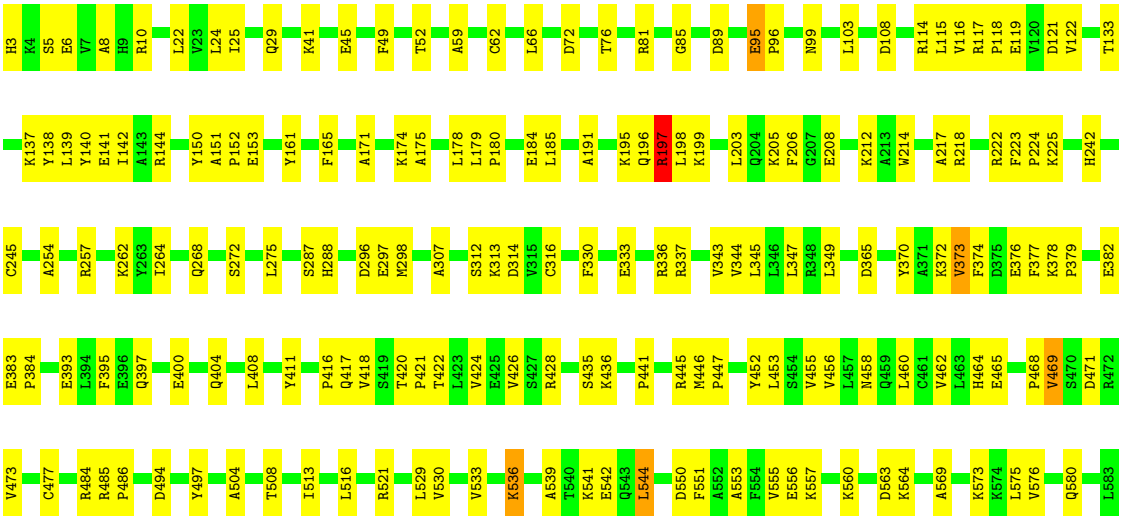
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	2	2	2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

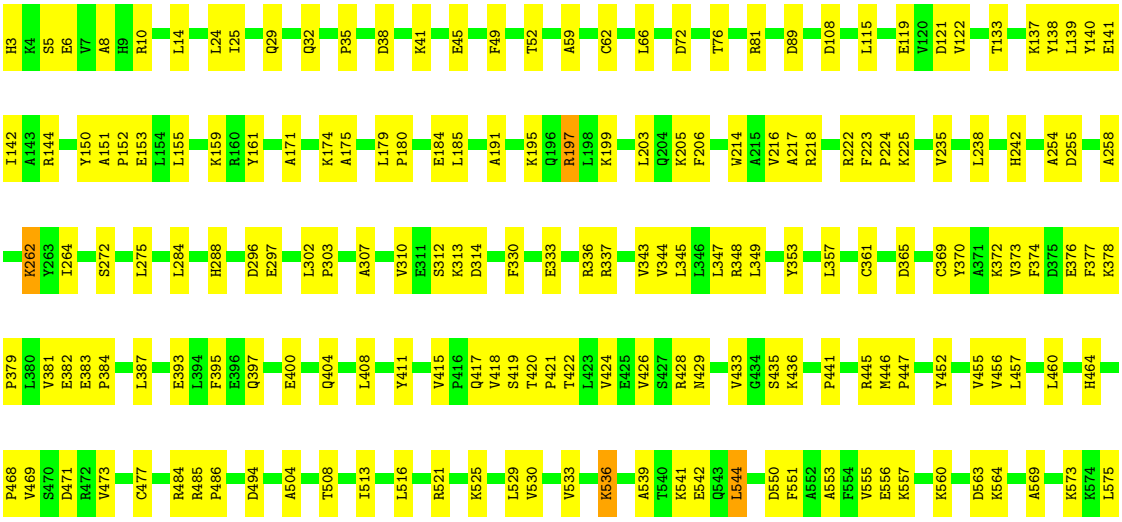
- Molecule 1: Serum albumin

Chain A:



- Molecule 1: Serum albumin

Chain B:



V576
Q580
L583

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	38.47Å 94.55Å 96.11Å 104.90° 89.90° 100.86°	Depositor
Resolution (Å)	27.13 – 2.80 27.13 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.6 (27.13-2.80) 95.4 (27.13-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	14.54 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.209 , 0.268 0.215 , 0.268	Depositor DCC
R_{free} test set	1995 reflections (6.31%)	wwPDB-VP
Wilson B-factor (Å^2)	55.1	Xtriage
Anisotropy	0.566	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 21.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.258 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9498	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 6WF, PLM

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	0.42	0/4696	0.76	9/6339 (0.1%)
1	B	0.29	0/4696	0.74	4/6339 (0.1%)
All	All	0.36	0/9392	0.75	13/12678 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	365	ASP	CA-C-N	6.81	126.78	119.28
1	A	365	ASP	C-N-CA	6.81	126.78	119.28
1	A	95	GLU	N-CA-C	-6.36	101.75	109.83
1	B	365	ASP	CA-C-N	5.91	125.78	119.28
1	B	365	ASP	C-N-CA	5.91	125.78	119.28
1	A	536	LYS	CA-C-N	5.51	125.60	119.87
1	A	536	LYS	C-N-CA	5.51	125.60	119.87
1	B	536	LYS	CA-C-N	5.13	125.21	119.87
1	B	536	LYS	C-N-CA	5.13	125.21	119.87
1	A	197	ARG	N-CA-C	-5.04	105.79	111.28
1	A	298	MET	CA-C-N	5.03	125.03	119.90
1	A	298	MET	C-N-CA	5.03	125.03	119.90
1	A	373	VAL	N-CA-C	5.02	115.45	110.23

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	4606	0	4501	129	0
1	B	4606	0	4499	130	0
2	A	23	18	0	6	0
2	B	23	18	0	8	0
3	A	101	0	163	16	0
3	B	101	0	163	18	0
4	A	2	0	0	0	0
All	All	9462	36	9326	271	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 14.

All (271) 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)
2:B:601:6WF:C13	2:B:601:6WF:C14	1.75	1.59
2:A:601:6WF:N15	2:A:601:6WF:N01	1.77	1.30
2:B:601:6WF:N01	2:B:601:6WF:N15	1.81	1.28
1:A:242:HIS:NE2	2:A:601:6WF:S09	2.25	1.05
1:B:199:LYS:NZ	2:B:601:6WF:S09	2.30	1.03
1:A:460:LEU:HD21	3:A:605:PLM:HC2	1.50	0.92
1:A:242:HIS:CD2	2:A:601:6WF:S09	2.67	0.88
1:B:460:LEU:HD21	3:B:605:PLM:HC2	1.54	0.86
1:A:222:ARG:HH11	1:A:222:ARG:HG3	1.43	0.84
1:B:222:ARG:HG3	1:B:222:ARG:HH11	1.43	0.83
1:B:418:VAL:HG21	3:B:605:PLM:HD2	1.62	0.80
1:A:316:CYS:SG	1:A:370:TYR:OH	2.40	0.80
1:B:59:ALA:HB3	1:B:62:CYS:SG	2.22	0.80
2:A:601:6WF:N15	2:A:601:6WF:C02	2.40	0.79
1:B:119:GLU:HB2	1:B:122:VAL:HG23	1.68	0.76
1:A:59:ALA:HB3	1:A:62:CYS:SG	2.26	0.75
2:B:601:6WF:N15	2:B:601:6WF:C02	2.50	0.74
2:B:601:6WF:S09	2:B:601:6WF:FE1	1.79	0.74
1:A:138:TYR:O	1:A:142:ILE:HG12	1.87	0.73
1:A:138:TYR:HB3	3:A:602:PLM:H81	1.69	0.72
3:B:604:PLM:H81	3:B:605:PLM:H22	1.72	0.71
1:A:191:ALA:O	1:A:195:LYS:HG3	1.91	0.71
1:A:198:LEU:HD12	1:A:198:LEU:O	1.90	0.70
2:B:601:6WF:N15	2:B:601:6WF:S09	2.66	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:HD11	1:A:141:GLU:HB3	1.74	0.69
1:B:138:TYR:O	1:B:142:ILE:HG12	1.93	0.69
1:B:151:ALA:HB3	1:B:152:PRO:HD3	1.73	0.68
1:A:119:GLU:HB2	1:A:122:VAL:HG23	1.75	0.67
1:A:424:VAL:O	1:A:428:ARG:HG3	1.94	0.67
1:B:108:ASP:OD2	1:B:197:ARG:NH1	2.27	0.67
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.77	0.66
1:B:310:VAL:HG13	1:B:370:TYR:HB3	1.77	0.65
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.78	0.65
1:A:153:GLU:OE2	1:A:288:HIS:ND1	2.29	0.65
1:B:224:PRO:HD2	1:B:296:ASP:HB3	1.78	0.64
1:A:138:TYR:CB	3:A:602:PLM:H81	2.27	0.64
1:B:417:GLN:NE2	1:B:494:ASP:OD2	2.31	0.63
1:A:117:ARG:HG3	3:A:602:PLM:H32	1.80	0.63
1:A:138:TYR:CD2	3:A:602:PLM:H61	2.34	0.63
1:A:417:GLN:NE2	1:A:494:ASP:OD2	2.30	0.63
1:B:41:LYS:O	1:B:45:GLU:HG3	1.99	0.62
1:B:424:VAL:O	1:B:428:ARG:HG3	1.99	0.62
1:A:161:TYR:CD1	1:A:185:LEU:HD23	2.35	0.61
1:A:222:ARG:HG3	1:A:222:ARG:NH1	2.15	0.61
1:A:10:ARG:HG3	1:A:66:LEU:HD11	1.83	0.61
1:A:72:ASP:O	1:A:76:THR:HG23	1.99	0.61
1:A:225:LYS:HE3	1:A:297:GLU:O	2.01	0.60
1:B:284:LEU:HD12	3:B:603:PLM:H31	1.83	0.60
1:A:81:ARG:NH2	1:A:89:ASP:OD1	2.35	0.59
1:B:485:ARG:HB3	1:B:486:PRO:HD3	1.85	0.59
1:B:115:LEU:HD11	1:B:141:GLU:HB3	1.83	0.59
1:B:10:ARG:HG3	1:B:66:LEU:HD11	1.85	0.59
1:B:372:LYS:O	1:B:376:GLU:HG3	2.03	0.59
1:B:457:LEU:HD21	3:B:605:PLM:H51	1.86	0.58
1:B:72:ASP:O	1:B:76:THR:HG23	2.03	0.58
1:A:408:LEU:HD23	1:A:529:LEU:HD23	1.86	0.58
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.86	0.58
1:A:95:GLU:OE2	1:A:99:ASN:HB2	2.03	0.57
1:B:6:GLU:HB3	1:B:66:LEU:HG	1.86	0.57
1:B:216:VAL:HG22	1:B:235:VAL:HG21	1.85	0.57
1:B:436:LYS:HE2	1:B:452:TYR:OH	2.05	0.57
1:A:422:THR:O	1:A:426:VAL:HG13	2.04	0.57
1:B:383:GLU:HB3	1:B:384:PRO:HD3	1.87	0.57
1:A:41:LYS:O	1:A:45:GLU:HG3	2.04	0.57
1:B:551:PHE:CD1	3:B:606:PLM:H91	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:TYR:HB3	3:B:605:PLM:HA1	1.87	0.57
1:A:108:ASP:OD2	1:A:197:ARG:NH1	2.38	0.56
1:B:225:LYS:HE3	1:B:297:GLU:O	2.06	0.56
1:A:464:HIS:CD2	1:A:468:PRO:HA	2.40	0.56
1:B:254:ALA:HB1	3:B:603:PLM:H42	1.85	0.56
1:A:25:ILE:O	1:A:29:GLN:HG3	2.05	0.56
1:B:5:SER:HB3	1:B:8:ALA:HB3	1.87	0.56
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.88	0.56
1:B:418:VAL:HG22	3:B:605:PLM:HF2	1.88	0.56
1:A:117:ARG:HG3	3:A:602:PLM:C3	2.36	0.56
1:B:25:ILE:O	1:B:29:GLN:HG3	2.05	0.55
1:B:191:ALA:O	1:B:195:LYS:HG3	2.07	0.55
1:A:569:ALA:O	1:A:573:LYS:HG3	2.07	0.55
1:B:138:TYR:HB3	3:B:602:PLM:HA1	1.88	0.55
1:B:137:LYS:O	1:B:141:GLU:HG2	2.07	0.55
1:B:155:LEU:HD23	1:B:284:LEU:HD21	1.89	0.55
1:B:161:TYR:CD1	1:B:185:LEU:HD23	2.43	0.54
1:B:214:TRP:CH2	1:B:218:ARG:HD2	2.42	0.54
1:A:418:VAL:HG22	3:A:605:PLM:HF2	1.89	0.54
1:B:81:ARG:NH2	1:B:89:ASP:OD1	2.40	0.54
1:B:473:VAL:HG11	3:B:605:PLM:HF1	1.90	0.54
2:B:601:6WF:C13	2:B:601:6WF:N15	2.65	0.54
1:A:563:ASP:OD1	1:A:564:LYS:N	2.41	0.54
1:B:14:LEU:HD11	3:B:603:PLM:H72	1.90	0.54
1:A:420:THR:HB	1:A:421:PRO:HD3	1.90	0.53
1:B:370:TYR:O	1:B:373:VAL:HB	2.08	0.53
1:B:175:ALA:O	1:B:179:LEU:HB2	2.06	0.53
1:A:5:SER:HB3	1:A:8:ALA:HB3	1.90	0.53
1:A:460:LEU:HG	3:A:605:PLM:HE2	1.89	0.53
1:B:238:LEU:HD22	1:B:242:HIS:CE1	2.43	0.53
1:B:378:LYS:N	1:B:379:PRO:HD2	2.24	0.53
1:B:441:PRO:O	1:B:445:ARG:HG3	2.08	0.53
1:A:411:TYR:HB3	3:A:605:PLM:HA1	1.91	0.53
1:B:446:MET:N	1:B:447:PRO:HD2	2.24	0.53
1:B:420:THR:HB	1:B:421:PRO:HD3	1.91	0.53
1:A:137:LYS:O	1:A:141:GLU:HG2	2.09	0.52
1:A:539:ALA:HB1	1:A:544:LEU:HD13	1.90	0.52
1:A:441:PRO:O	1:A:445:ARG:HG3	2.09	0.52
1:B:216:VAL:CG2	1:B:235:VAL:HG21	2.40	0.52
1:A:214:TRP:CH2	1:A:218:ARG:HD2	2.45	0.52
1:B:457:LEU:HD21	3:B:605:PLM:H62	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:ASP:OD1	1:B:564:LYS:N	2.43	0.52
1:B:504:ALA:O	1:B:508:THR:OG1	2.26	0.52
1:A:378:LYS:N	1:A:379:PRO:HD2	2.25	0.52
1:A:539:ALA:CB	1:A:544:LEU:HD13	2.41	0.51
1:B:550:ASP:HB3	1:B:575:LEU:HD11	1.92	0.51
1:A:446:MET:N	1:A:447:PRO:HD2	2.25	0.51
1:A:372:LYS:O	1:A:376:GLU:HG3	2.11	0.51
1:B:464:HIS:CD2	1:B:468:PRO:HA	2.46	0.51
1:A:264:ILE:CG2	1:A:275:LEU:HD21	2.41	0.50
1:A:393:GLU:O	1:A:397:GLN:HG3	2.11	0.50
1:B:426:VAL:HG11	1:B:460:LEU:HD13	1.93	0.50
1:A:49:PHE:O	1:A:52:THR:HB	2.10	0.50
1:A:95:GLU:HG3	1:A:96:PRO:HA	1.92	0.50
1:B:378:LYS:HE3	1:B:382:GLU:OE2	2.11	0.50
1:A:344:VAL:HA	1:A:347:LEU:HD12	1.93	0.50
1:A:370:TYR:O	1:A:373:VAL:HB	2.11	0.50
1:A:551:PHE:CD1	3:A:606:PLM:H82	2.47	0.50
1:B:49:PHE:O	1:B:52:THR:HB	2.11	0.50
1:A:66:LEU:HD22	3:A:603:PLM:HF2	1.94	0.49
1:A:208:GLU:O	1:A:212:LYS:HG3	2.12	0.49
1:A:550:ASP:HB3	1:A:575:LEU:CD1	2.42	0.49
1:A:556:GLU:O	1:A:560:LYS:HB2	2.11	0.49
1:B:529:LEU:O	1:B:533:VAL:HG23	2.12	0.49
1:B:264:ILE:CG2	1:B:275:LEU:HD21	2.42	0.49
1:B:550:ASP:HB3	1:B:575:LEU:CD1	2.41	0.49
3:A:604:PLM:HA1	3:A:605:PLM:H21	1.95	0.49
1:B:150:TYR:CD2	1:B:152:PRO:HD2	2.48	0.49
1:A:198:LEU:HD12	1:A:198:LEU:C	2.35	0.49
1:A:504:ALA:O	1:A:508:THR:OG1	2.24	0.49
1:B:408:LEU:HD11	1:B:530:VAL:CG2	2.42	0.49
1:B:422:THR:O	1:B:426:VAL:HG13	2.12	0.48
1:A:217:ALA:HB3	1:A:343:VAL:HG13	1.94	0.48
1:A:307:ALA:O	1:A:312:SER:HB2	2.12	0.48
1:B:140:TYR:O	1:B:144:ARG:HG2	2.13	0.48
1:B:205:LYS:HD3	1:B:206:PHE:CE2	2.48	0.48
1:A:553:ALA:O	1:A:557:LYS:HG3	2.13	0.48
1:A:426:VAL:HG11	1:A:460:LEU:HD13	1.95	0.48
1:B:393:GLU:O	1:B:397:GLN:HG3	2.14	0.48
1:A:383:GLU:HB3	1:A:384:PRO:CD	2.43	0.48
1:A:436:LYS:HE2	1:A:452:TYR:OH	2.12	0.48
1:B:333:GLU:HA	1:B:336:ARG:HD3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:ARG:NH2	1:B:521:ARG:HB2	2.29	0.48
1:B:539:ALA:CB	1:B:544:LEU:HD13	2.43	0.48
1:A:378:LYS:HE3	1:A:382:GLU:OE2	2.12	0.48
1:B:569:ALA:O	1:B:573:LYS:HG3	2.14	0.48
1:B:383:GLU:HB3	1:B:384:PRO:CD	2.44	0.47
1:A:313:LYS:HG2	1:A:314:ASP:H	1.80	0.47
1:A:452:TYR:O	1:A:455:VAL:HG22	2.14	0.47
1:A:150:TYR:CD2	1:A:152:PRO:HD2	2.50	0.47
1:B:556:GLU:O	1:B:560:LYS:HB2	2.14	0.47
1:A:400:GLU:O	1:A:404:GLN:HG3	2.13	0.47
1:A:408:LEU:HD11	1:A:530:VAL:CG2	2.44	0.47
1:B:217:ALA:HB3	1:B:343:VAL:HG13	1.97	0.47
1:B:222:ARG:HG3	1:B:222:ARG:NH1	2.17	0.47
1:B:452:TYR:O	1:B:455:VAL:HG22	2.14	0.47
1:B:576:VAL:O	1:B:580:GLN:HG3	2.15	0.47
1:B:477:CYS:O	1:B:484:ARG:NH2	2.48	0.47
1:A:175:ALA:O	1:A:179:LEU:HB2	2.14	0.47
1:B:313:LYS:HG2	1:B:314:ASP:H	1.80	0.46
1:B:35:PRO:HG2	1:B:38:ASP:CG	2.40	0.46
1:A:108:ASP:CG	1:A:197:ARG:HH12	2.23	0.46
1:A:223:PHE:CD1	1:A:272:SER:HB2	2.50	0.46
1:A:541:LYS:HE3	1:A:542:GLU:OE2	2.15	0.46
1:A:576:VAL:O	1:A:580:GLN:HG3	2.15	0.46
1:A:171:ALA:O	1:A:174:LYS:HG2	2.14	0.46
1:A:180:PRO:O	1:A:184:GLU:HG3	2.16	0.46
1:A:556:GLU:O	1:A:560:LYS:HE3	2.15	0.46
1:B:400:GLU:O	1:B:404:GLN:HG3	2.15	0.46
1:B:153:GLU:OE2	1:B:288:HIS:ND1	2.40	0.46
1:A:257:ARG:NH1	1:A:287:SER:OG	2.48	0.46
1:B:258:ALA:O	1:B:262:LYS:HB2	2.16	0.46
1:B:307:ALA:O	1:B:312:SER:HB2	2.15	0.46
1:B:330:PHE:HZ	1:B:377:PHE:CE2	2.34	0.46
1:A:462:VAL:O	1:A:465:GLU:HB3	2.16	0.45
1:B:199:LYS:HD3	1:B:242:HIS:CD2	2.51	0.45
1:A:133:THR:O	1:A:137:LYS:HB2	2.15	0.45
1:B:138:TYR:CE2	3:B:602:PLM:H51	2.51	0.45
1:B:525:LYS:HG2	1:B:551:PHE:HE2	1.82	0.45
1:B:161:TYR:CD1	3:B:602:PLM:H72	2.52	0.45
1:B:302:LEU:HA	1:B:303:PRO:HD3	1.82	0.45
1:B:513:ILE:HA	1:B:516:LEU:HD12	1.98	0.45
1:A:395:PHE:CZ	1:A:435:SER:HA	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:ARG:NH2	1:A:521:ARG:HB2	2.32	0.45
1:A:205:LYS:HD3	1:A:206:PHE:CE2	2.52	0.45
1:A:416:PRO:HB2	1:A:497:TYR:CD1	2.52	0.45
1:A:513:ILE:O	1:A:521:ARG:NH2	2.50	0.45
1:B:344:VAL:O	1:B:348:ARG:HG3	2.16	0.45
1:A:453:LEU:CD1	3:A:604:PLM:H62	2.47	0.45
1:B:337:ARG:HG3	1:B:337:ARG:HH11	1.82	0.44
1:B:377:PHE:O	1:B:381:VAL:HG23	2.16	0.44
1:A:373:VAL:HG12	1:A:374:PHE:N	2.31	0.44
1:B:180:PRO:O	1:B:184:GLU:HG3	2.18	0.44
1:B:408:LEU:HD23	1:B:529:LEU:HD23	1.98	0.44
1:B:464:HIS:CE1	1:B:473:VAL:HB	2.52	0.44
1:A:196:GLN:HG3	2:A:601:6WF:C07	2.47	0.44
1:B:238:LEU:HD23	1:B:238:LEU:HA	1.80	0.44
1:A:529:LEU:O	1:A:533:VAL:HG23	2.17	0.44
1:B:108:ASP:CG	1:B:197:ARG:HH12	2.25	0.44
1:B:171:ALA:O	1:B:174:LYS:HG2	2.17	0.44
1:A:115:LEU:HD11	1:A:141:GLU:CB	2.44	0.44
1:B:238:LEU:HD22	1:B:242:HIS:HE1	1.81	0.44
1:B:387:LEU:HD13	3:B:604:PLM:H71	2.00	0.44
1:B:471:ASP:OD1	1:B:471:ASP:N	2.46	0.44
1:A:550:ASP:HB3	1:A:575:LEU:HD11	1.99	0.44
1:A:140:TYR:O	1:A:144:ARG:HG2	2.18	0.43
1:B:373:VAL:HG12	1:B:374:PHE:N	2.32	0.43
1:B:419:SER:OG	1:B:421:PRO:HD2	2.18	0.43
1:A:464:HIS:CE1	1:A:473:VAL:HB	2.53	0.43
1:A:455:VAL:HG23	1:A:456:VAL:N	2.34	0.43
1:B:155:LEU:HG	1:B:159:LYS:HE2	2.00	0.43
1:B:369:CYS:HA	1:B:372:LYS:CG	2.49	0.43
1:A:103:LEU:HA	1:A:103:LEU:HD23	1.83	0.43
1:A:333:GLU:HA	1:A:336:ARG:HD3	2.00	0.43
1:B:395:PHE:CZ	1:B:435:SER:HA	2.52	0.43
1:B:455:VAL:HG23	1:B:456:VAL:N	2.33	0.43
1:A:337:ARG:HG3	1:A:337:ARG:HH11	1.83	0.43
1:A:471:ASP:OD1	1:A:471:ASP:N	2.46	0.43
1:A:161:TYR:CE1	1:A:185:LEU:HD23	2.52	0.43
1:B:539:ALA:HB1	1:B:544:LEU:HD13	2.01	0.43
1:B:133:THR:O	1:B:137:LYS:HB2	2.17	0.43
1:A:268:GLN:HG3	1:A:275:LEU:HB3	2.01	0.43
1:A:551:PHE:O	1:A:555:VAL:HG23	2.19	0.43
1:B:357:LEU:O	1:B:361:CYS:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ALA:HB1	3:A:603:PLM:H42	2.01	0.42
1:B:541:LYS:HE3	1:B:542:GLU:OE2	2.17	0.42
1:A:343:VAL:O	1:A:347:LEU:HG	2.18	0.42
1:A:426:VAL:HG11	1:A:460:LEU:CD1	2.48	0.42
1:B:553:ALA:O	1:B:557:LYS:HG3	2.19	0.42
2:B:601:6WF:C14	2:B:601:6WF:C16	2.74	0.42
1:A:245:CYS:HB3	2:A:601:6WF:C06	2.49	0.42
1:B:24:LEU:HD23	1:B:139:LEU:HD23	2.01	0.42
1:A:6:GLU:HB3	1:A:66:LEU:HG	2.01	0.42
1:B:372:LYS:H	1:B:372:LYS:HG2	1.68	0.42
1:A:114:ARG:NH1	1:A:116:VAL:HG12	2.34	0.42
1:B:429:ASN:O	1:B:433:VAL:HG23	2.20	0.42
3:B:604:PLM:H61	3:B:604:PLM:H92	1.81	0.42
1:A:117:ARG:HA	1:A:118:PRO:HD3	1.90	0.41
1:B:369:CYS:HA	1:B:372:LYS:HG3	2.02	0.41
1:A:417:GLN:HB2	1:A:469:VAL:CG1	2.49	0.41
1:A:418:VAL:HG21	3:A:605:PLM:HD2	2.01	0.41
1:B:345:LEU:O	1:B:349:LEU:HG	2.20	0.41
1:B:551:PHE:O	1:B:555:VAL:HG23	2.21	0.41
1:A:22:LEU:HD13	3:A:603:PLM:H72	2.03	0.41
1:B:222:ARG:NH1	1:B:222:ARG:CG	2.81	0.41
1:B:353:TYR:CZ	1:B:357:LEU:HD11	2.56	0.41
1:B:10:ARG:NH2	1:B:255:ASP:OD1	2.54	0.41
1:B:138:TYR:CB	3:B:602:PLM:HA1	2.50	0.41
1:B:223:PHE:CD1	1:B:272:SER:HB2	2.56	0.41
1:A:330:PHE:HZ	1:A:377:PHE:CE2	2.39	0.41
1:A:513:ILE:HA	1:A:516:LEU:HD12	2.01	0.41
1:B:343:VAL:O	1:B:347:LEU:HG	2.20	0.41
1:A:165:PHE:CE1	1:A:178:LEU:HD21	2.56	0.41
1:A:345:LEU:O	1:A:349:LEU:HG	2.21	0.41
1:A:416:PRO:HB2	1:A:497:TYR:CE1	2.56	0.41
1:A:477:CYS:O	1:A:484:ARG:NH2	2.54	0.41
1:B:32:GLN:H	1:B:32:GLN:HG3	1.71	0.41
1:A:458:ASN:O	1:A:462:VAL:HG23	2.21	0.40
1:B:415:VAL:HG12	1:B:418:VAL:HG23	2.03	0.40
1:A:24:LEU:HD23	1:A:139:LEU:HD23	2.04	0.40
1:B:417:GLN:H	1:B:417:GLN:CD	2.29	0.40
1:A:373:VAL:HA	1:A:376:GLU:OE1	2.22	0.40
1:B:203:LEU:HD23	1:B:203:LEU:O	2.20	0.40
1:A:119:GLU:HB2	1:A:122:VAL:CG2	2.47	0.40
1:A:417:GLN:H	1:A:417:GLN:CD	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:VAL:HA	1:B:347:LEU:HD12	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	579/581 (100%)	565 (98%)	13 (2%)	1 (0%)	43	72
1	B	579/581 (100%)	565 (98%)	14 (2%)	0	100	100
All	All	1158/1162 (100%)	1130 (98%)	27 (2%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	GLY

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	503/509 (99%)	494 (98%)	9 (2%)	51	82
1	B	503/509 (99%)	496 (99%)	7 (1%)	59	85
All	All	1006/1018 (99%)	990 (98%)	16 (2%)	55	83

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	121	ASP
1	A	197	ARG
1	A	199	LYS
1	A	203	LEU
1	A	262	LYS
1	A	469	VAL
1	A	536	LYS
1	A	544	LEU
1	B	3	HIS
1	B	121	ASP
1	B	197	ARG
1	B	262	LYS
1	B	469	VAL
1	B	536	LYS
1	B	544	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	B	3	HIS
1	B	67	HIS
1	B	391	ASN
1	B	404	GLN

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)

14 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	PLM	A	604	-	16,16,17	0.47	0	16,16,17	0.77	0
3	PLM	B	603	-	17,17,17	0.44	0	17,17,17	0.75	1 (5%)
3	PLM	A	603	-	17,17,17	0.48	0	17,17,17	0.73	0
3	PLM	B	604	-	16,16,17	0.48	0	16,16,17	0.78	0
3	PLM	B	605	-	17,17,17	0.47	0	17,17,17	0.73	0
3	PLM	A	607	-	17,17,17	0.46	0	17,17,17	0.73	0
3	PLM	A	602	1	12,12,17	0.58	0	12,12,17	0.78	0
2	6WF	B	601	1	23,27,29	6.57	11 (47%)	30,39,46	5.88	11 (36%)
3	PLM	B	602	-	12,12,17	0.56	0	12,12,17	0.82	0
3	PLM	B	606	-	16,16,17	0.48	0	16,16,17	0.71	0
3	PLM	B	607	1	17,17,17	0.46	0	17,17,17	0.74	0
2	6WF	A	601	1	23,27,29	6.02	12 (52%)	30,39,46	7.54	9 (30%)
3	PLM	A	606	-	16,16,17	0.47	0	16,16,17	0.77	0
3	PLM	A	605	-	17,17,17	0.46	0	17,17,17	0.71	0

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	PLM	A	604	-	-	7/14/14/15	-
3	PLM	B	603	-	-	8/15/15/15	-
3	PLM	A	603	-	-	9/15/15/15	-
3	PLM	B	604	-	-	10/14/14/15	-
3	PLM	B	605	-	-	8/15/15/15	-
3	PLM	A	607	-	-	8/15/15/15	-
3	PLM	A	602	1	-	5/10/10/15	-
2	6WF	B	601	1	-	3/4/32/40	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLM	B	602	-	-	8/10/10/15	-
3	PLM	B	606	-	-	8/14/14/15	-
3	PLM	B	607	1	-	7/15/15/15	-
2	6WF	A	601	1	-	3/4/32/40	0/5/5/5
3	PLM	A	606	-	-	9/14/14/15	-
3	PLM	A	605	-	-	6/15/15/15	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	6WF	N01-N15	16.08	1.81	1.37
2	A	601	6WF	N01-N15	14.71	1.77	1.37
2	B	601	6WF	C13-C14	14.25	1.75	1.43
2	B	601	6WF	C02-N01	13.84	1.58	1.35
2	A	601	6WF	C13-C14	12.70	1.71	1.43
2	A	601	6WF	C02-N01	10.84	1.53	1.35
2	B	601	6WF	C13-C12	9.12	1.60	1.41
2	A	601	6WF	C13-C12	8.97	1.59	1.41
2	A	601	6WF	C02-S09	8.47	1.85	1.70
2	B	601	6WF	O11-C12	8.42	1.44	1.32
2	A	601	6WF	O11-C12	8.24	1.43	1.32
2	B	601	6WF	C02-S09	8.13	1.84	1.70
2	A	601	6WF	C02-N03	6.14	1.44	1.33
2	B	601	6WF	C02-N03	6.12	1.44	1.33
2	B	601	6WF	C22-C17	5.98	1.56	1.41
2	B	601	6WF	C22-C23	5.14	1.47	1.36
2	A	601	6WF	C22-C17	4.73	1.53	1.41
2	A	601	6WF	C22-C23	4.63	1.46	1.36
2	A	601	6WF	C13-C16	-3.07	1.39	1.45
2	A	601	6WF	C16-C17	-2.80	1.37	1.43
2	A	601	6WF	C23-C12	-2.03	1.35	1.39
2	B	601	6WF	C20-C21	2.01	1.41	1.36
2	B	601	6WF	C19-C18	2.00	1.41	1.36

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	6WF	S09-C02-N01	-29.77	88.12	120.97
2	A	601	6WF	C02-N01-N15	-25.49	92.74	119.36
2	B	601	6WF	C02-N01-N15	-23.48	94.83	119.36
2	B	601	6WF	S09-C02-N01	-18.21	100.87	120.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	6WF	C04-N03-C02	-7.40	108.58	123.33
2	A	601	6WF	C14-N15-N01	7.08	128.48	115.36
2	A	601	6WF	C04-N03-C02	-6.34	110.69	123.33
2	B	601	6WF	C14-N15-N01	5.61	125.76	115.36
2	A	601	6WF	C08-N03-C02	-4.71	113.95	123.33
2	A	601	6WF	C12-C13-C16	4.41	124.51	119.60
2	B	601	6WF	C08-N03-C02	-3.67	116.02	123.33
2	B	601	6WF	N01-C02-N03	-3.27	112.16	117.53
2	A	601	6WF	C05-C04-N03	3.04	116.65	110.66
2	B	601	6WF	O11-C12-C13	-2.85	119.46	124.36
2	A	601	6WF	C16-C13-C14	-2.70	115.02	119.32
2	B	601	6WF	C21-C16-C13	-2.57	120.13	123.42
2	A	601	6WF	C21-C16-C17	2.36	120.94	117.89
2	B	601	6WF	C21-C16-C17	2.23	120.77	117.89
2	B	601	6WF	O11-C12-C23	2.09	121.78	118.66
2	B	601	6WF	C12-C13-C16	2.07	121.90	119.60
3	B	603	PLM	O1-C1-C2	2.07	120.67	114.03

There are no chirality outliers.

All (99) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	6WF	N01-C02-N03-C04
2	A	601	6WF	N01-C02-N03-C08
2	A	601	6WF	S09-C02-N03-C04
2	B	601	6WF	N01-C02-N03-C04
2	B	601	6WF	N01-C02-N03-C08
2	B	601	6WF	S09-C02-N03-C04
3	A	602	PLM	C1-C2-C3-C4
3	A	603	PLM	C1-C2-C3-C4
3	B	603	PLM	C1-C2-C3-C4
3	A	607	PLM	C1-C2-C3-C4
3	B	605	PLM	C1-C2-C3-C4
3	B	606	PLM	C1-C2-C3-C4
3	A	606	PLM	CA-CB-CC-CD
3	B	605	PLM	C4-C5-C6-C7
3	B	602	PLM	C5-C6-C7-C8
3	B	603	PLM	C2-C3-C4-C5
3	B	603	PLM	C9-CA-CB-CC
3	A	605	PLM	C4-C5-C6-C7
3	B	602	PLM	C4-C5-C6-C7
3	A	607	PLM	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	A	606	PLM	C6-C7-C8-C9
3	B	604	PLM	CA-CB-CC-CD
3	B	602	PLM	C1-C2-C3-C4
3	A	603	PLM	C7-C8-C9-CA
3	A	603	PLM	CA-CB-CC-CD
3	B	603	PLM	CA-CB-CC-CD
3	A	606	PLM	C8-C9-CA-CB
3	B	607	PLM	C5-C6-C7-C8
3	A	603	PLM	C3-C4-C5-C6
3	A	604	PLM	CA-CB-CC-CD
3	A	603	PLM	C6-C7-C8-C9
3	B	602	PLM	C3-C4-C5-C6
3	B	607	PLM	CC-CD-CE-CF
3	B	602	PLM	C2-C3-C4-C5
3	A	607	PLM	C5-C6-C7-C8
3	B	604	PLM	CB-CC-CD-CE
3	B	606	PLM	C5-C6-C7-C8
3	A	607	PLM	CC-CD-CE-CF
3	A	602	PLM	C2-C3-C4-C5
3	A	607	PLM	C4-C5-C6-C7
3	B	605	PLM	C3-C4-C5-C6
3	B	606	PLM	C8-C9-CA-CB
3	A	603	PLM	C5-C6-C7-C8
3	A	606	PLM	C5-C6-C7-C8
3	B	604	PLM	CC-CD-CE-CF
3	A	606	PLM	C2-C3-C4-C5
3	B	606	PLM	CB-CC-CD-CE
3	B	607	PLM	C2-C3-C4-C5
3	A	602	PLM	C8-C9-CA-CB
3	B	605	PLM	C9-CA-CB-CC
3	A	606	PLM	CB-CC-CD-CE
3	B	605	PLM	C2-C3-C4-C5
3	A	606	PLM	C9-CA-CB-CC
3	A	603	PLM	CB-CC-CD-CE
3	A	604	PLM	C5-C6-C7-C8
3	B	606	PLM	C6-C7-C8-C9
3	A	604	PLM	C2-C3-C4-C5
3	B	606	PLM	C4-C5-C6-C7
3	B	607	PLM	C1-C2-C3-C4
3	A	604	PLM	C3-C4-C5-C6
3	B	604	PLM	C6-C7-C8-C9
3	B	604	PLM	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	A	604	PLM	CB-CC-CD-CE
3	A	603	PLM	C4-C5-C6-C7
3	B	606	PLM	O1-C1-C2-C3
3	A	605	PLM	C9-CA-CB-CC
3	B	606	PLM	O2-C1-C2-C3
3	A	605	PLM	C8-C9-CA-CB
3	B	604	PLM	C7-C8-C9-CA
3	A	607	PLM	C3-C4-C5-C6
3	A	605	PLM	O1-C1-C2-C3
3	A	605	PLM	O2-C1-C2-C3
3	B	604	PLM	O1-C1-C2-C3
3	A	607	PLM	O1-C1-C2-C3
3	A	605	PLM	CA-CB-CC-CD
3	A	607	PLM	O2-C1-C2-C3
3	B	604	PLM	O2-C1-C2-C3
3	B	603	PLM	CB-CC-CD-CE
3	B	607	PLM	C9-CA-CB-CC
3	B	607	PLM	O2-C1-C2-C3
3	B	603	PLM	O1-C1-C2-C3
3	B	603	PLM	C5-C6-C7-C8
3	A	603	PLM	C9-CA-CB-CC
3	B	602	PLM	O1-C1-C2-C3
3	B	602	PLM	O2-C1-C2-C3
3	B	603	PLM	O2-C1-C2-C3
3	A	602	PLM	O1-C1-C2-C3
3	B	604	PLM	C9-CA-CB-CC
3	A	604	PLM	O1-C1-C2-C3
3	B	605	PLM	O1-C1-C2-C3
3	B	605	PLM	O2-C1-C2-C3
3	A	602	PLM	O2-C1-C2-C3
3	A	606	PLM	O1-C1-C2-C3
3	A	604	PLM	O2-C1-C2-C3
3	B	607	PLM	O1-C1-C2-C3
3	B	602	PLM	C6-C7-C8-C9
3	A	606	PLM	O2-C1-C2-C3
3	B	604	PLM	C1-C2-C3-C4
3	B	605	PLM	C6-C7-C8-C9

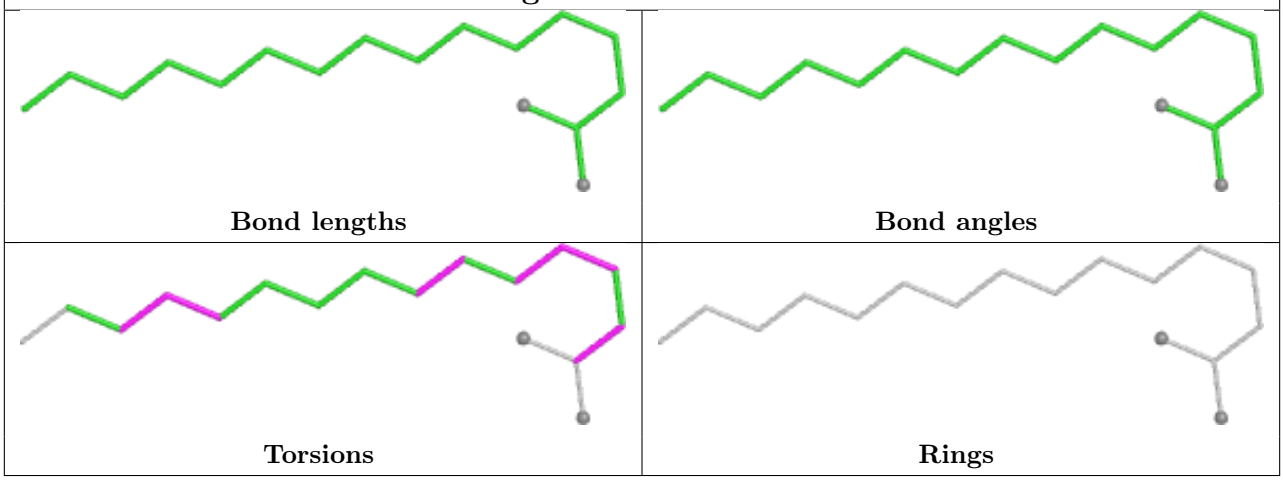
There are no ring outliers.

12 monomers are involved in 48 short contacts:

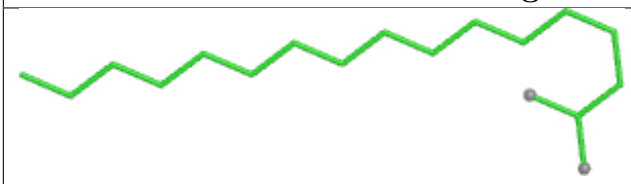
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	604	PLM	2	0
3	B	603	PLM	3	0
3	A	603	PLM	3	0
3	B	604	PLM	3	0
3	B	605	PLM	8	0
3	A	602	PLM	5	0
2	B	601	6WF	8	0
3	B	602	PLM	4	0
3	B	606	PLM	1	0
2	A	601	6WF	6	0
3	A	606	PLM	1	0
3	A	605	PLM	6	0

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.

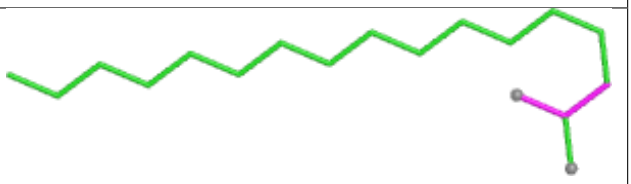
Ligand PLM A 604



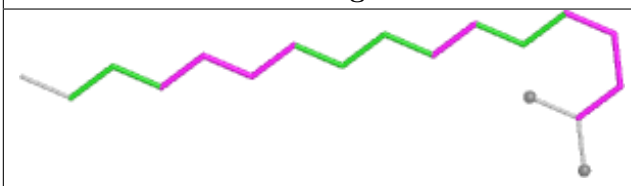
Ligand PLM B 603



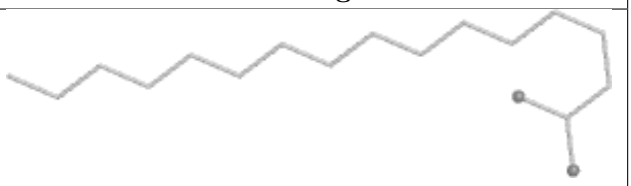
Bond lengths



Bond angles



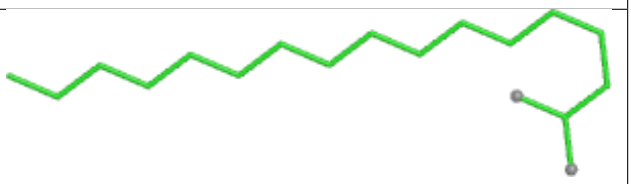
Torsions



Rings

Ligand PLM A 603

Bond lengths



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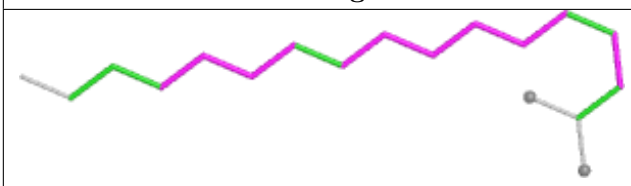

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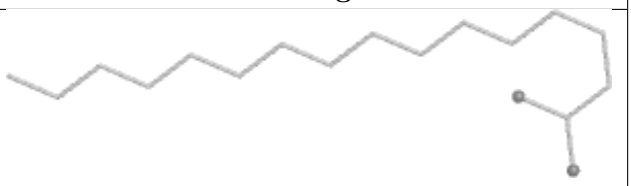
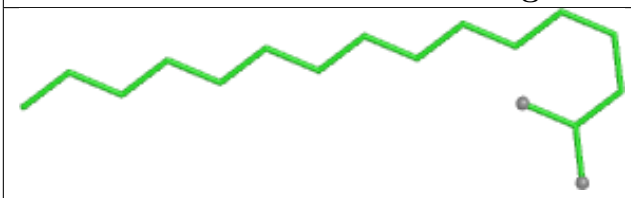
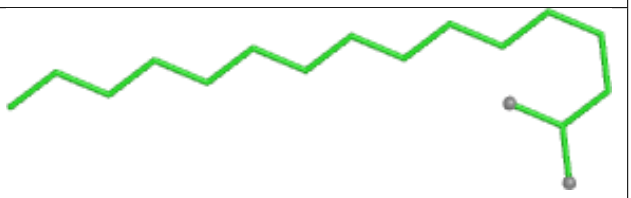


Rings

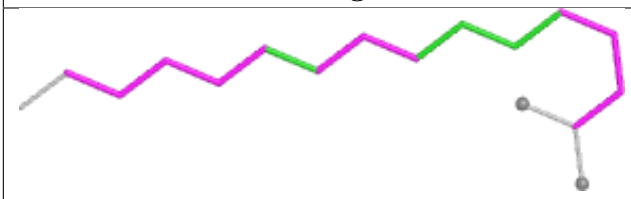
Ligand PLM B 604



Bond lengths



Bond angles



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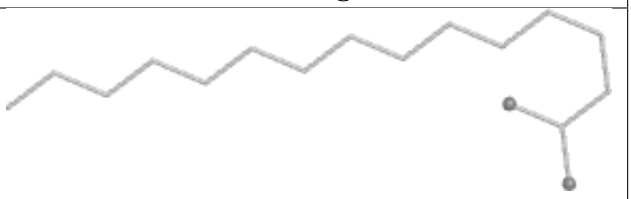
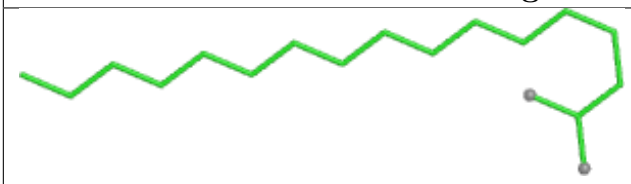


Rings

Ligand PLM B 605



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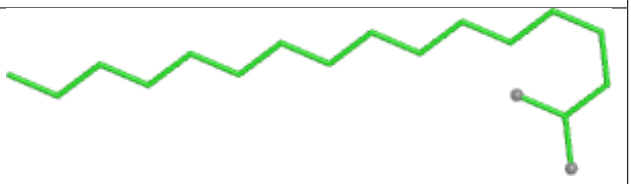
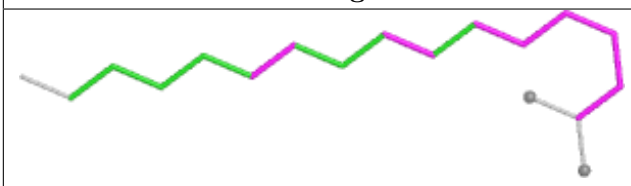


Bond angles



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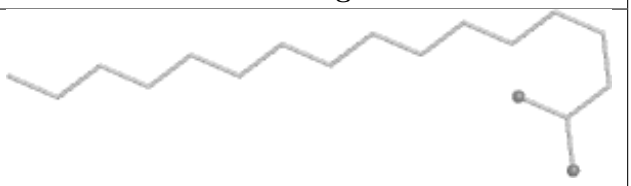
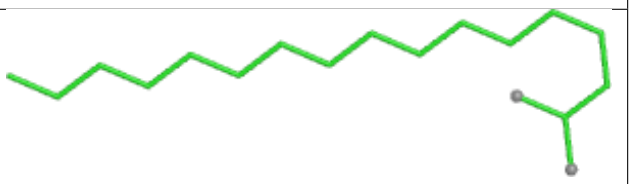


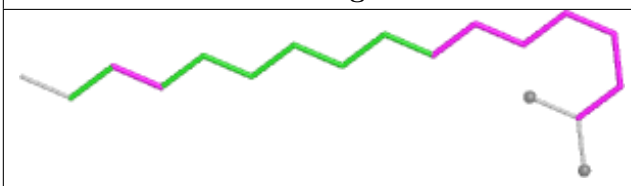
Rings

Ligand PLM A 607

Bond lengths



Bond angles



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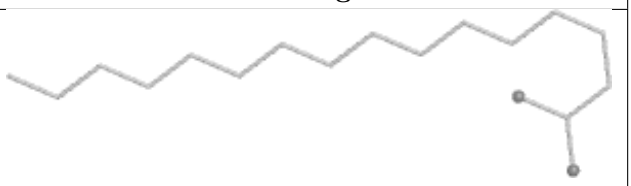
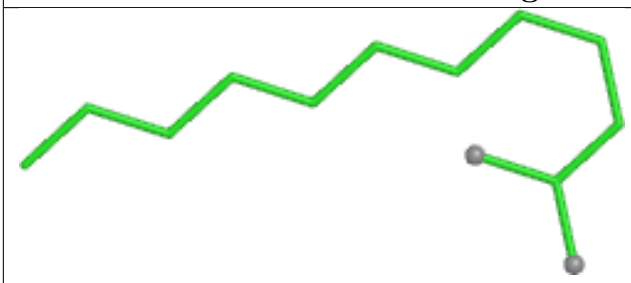


Rings

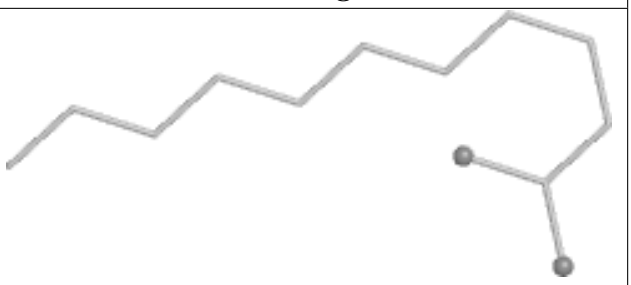
Ligand PLM A 602



Bond lengths

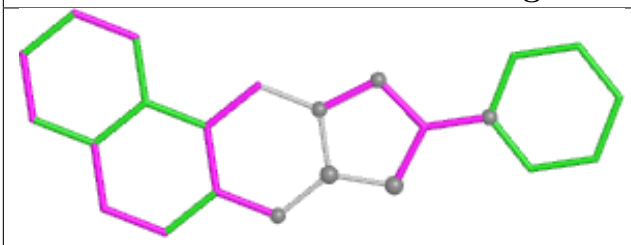
Bond angles

Torsions

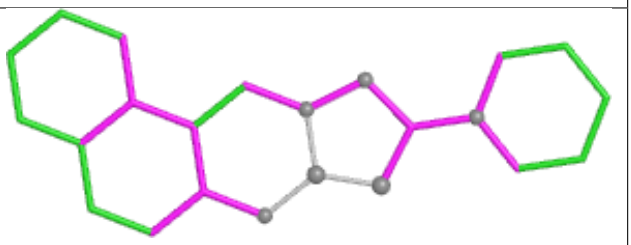


Rings

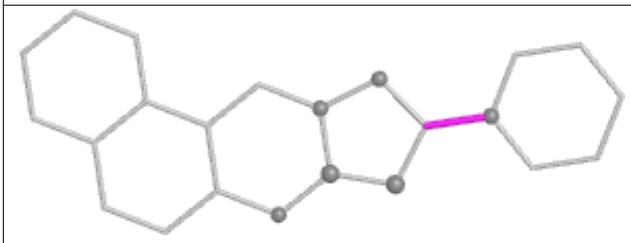
Ligand 6WF B 601



Bond lengths



Bond angles



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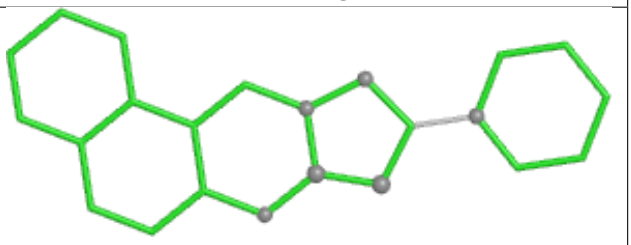
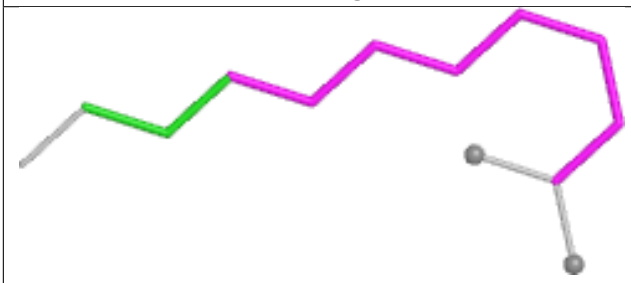


Rings

Ligand PLM B 602

Bond lengths

Bond angles



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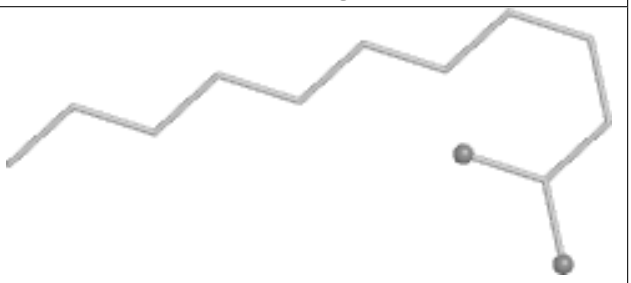

Rings

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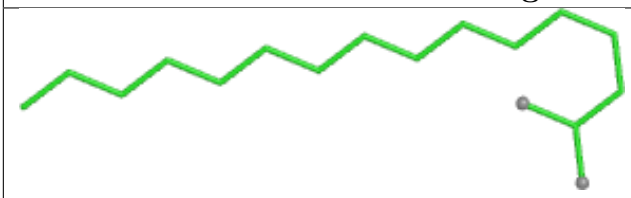

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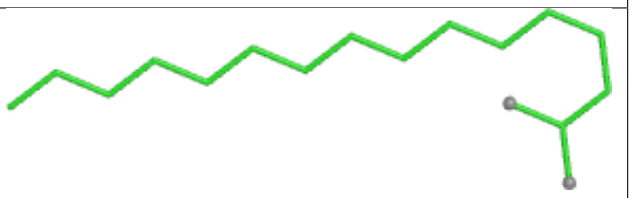

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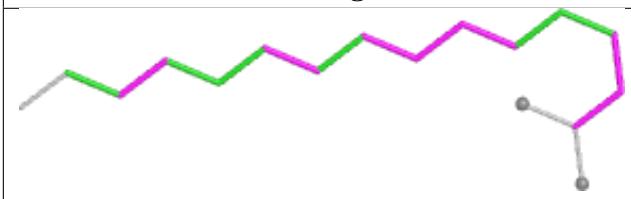

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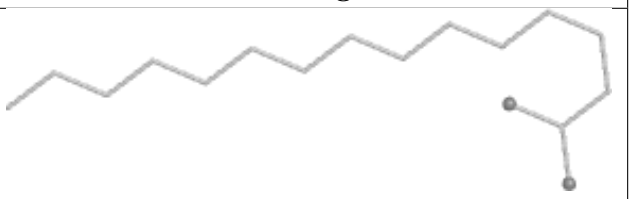

Rings

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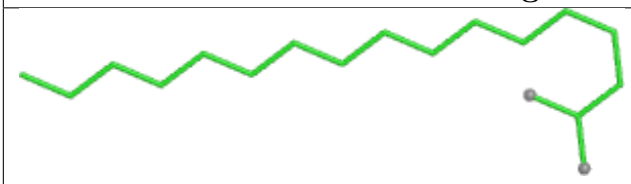
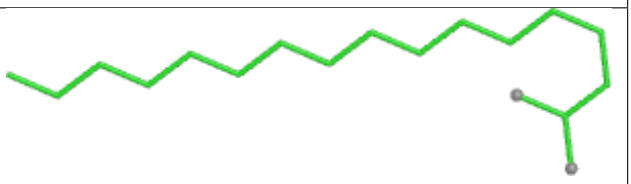
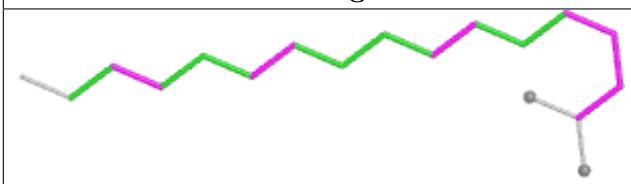


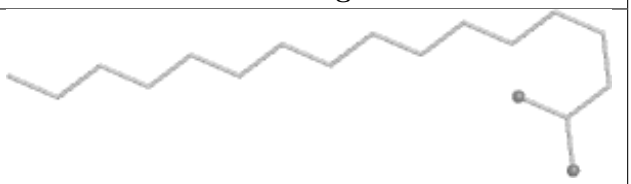
Bond lengths



Bond angles

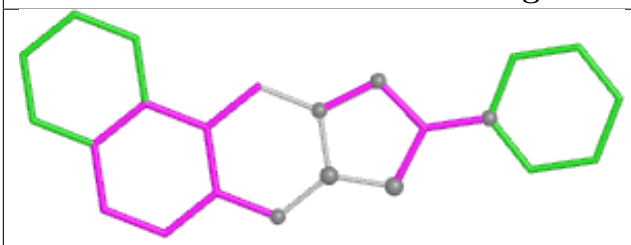


Torsions

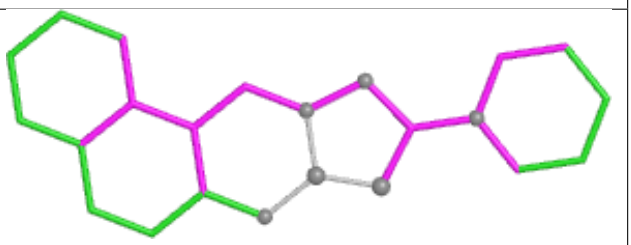


Rings

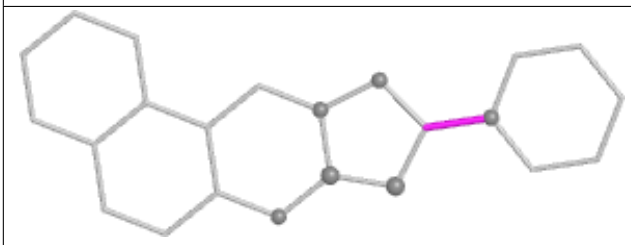
Ligand 6WF A 601



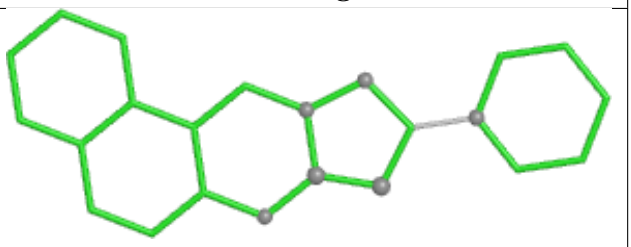
Bond lengths



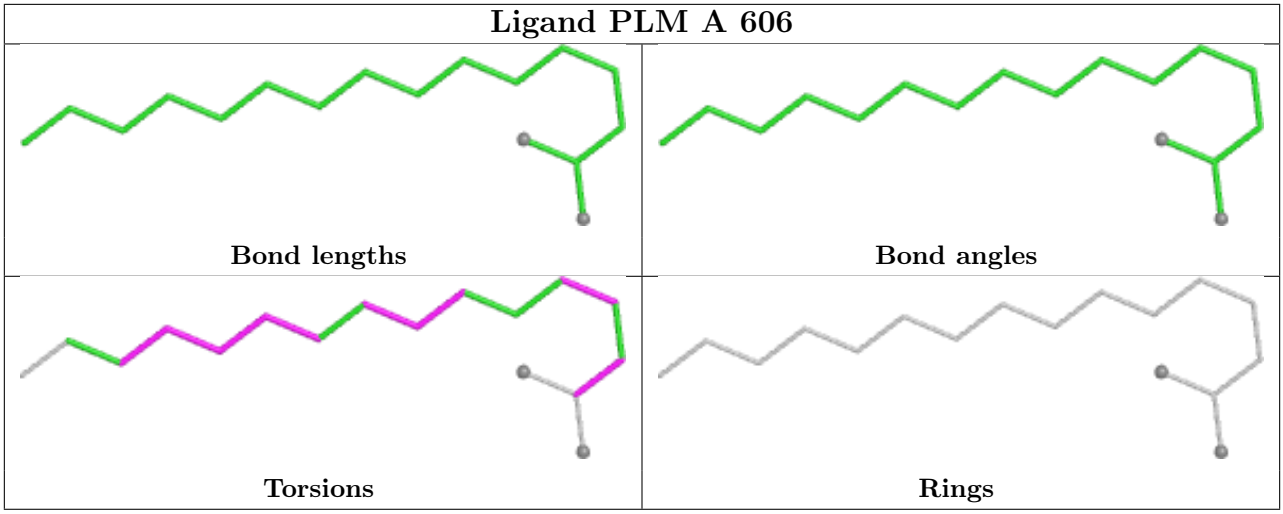
Bond angles

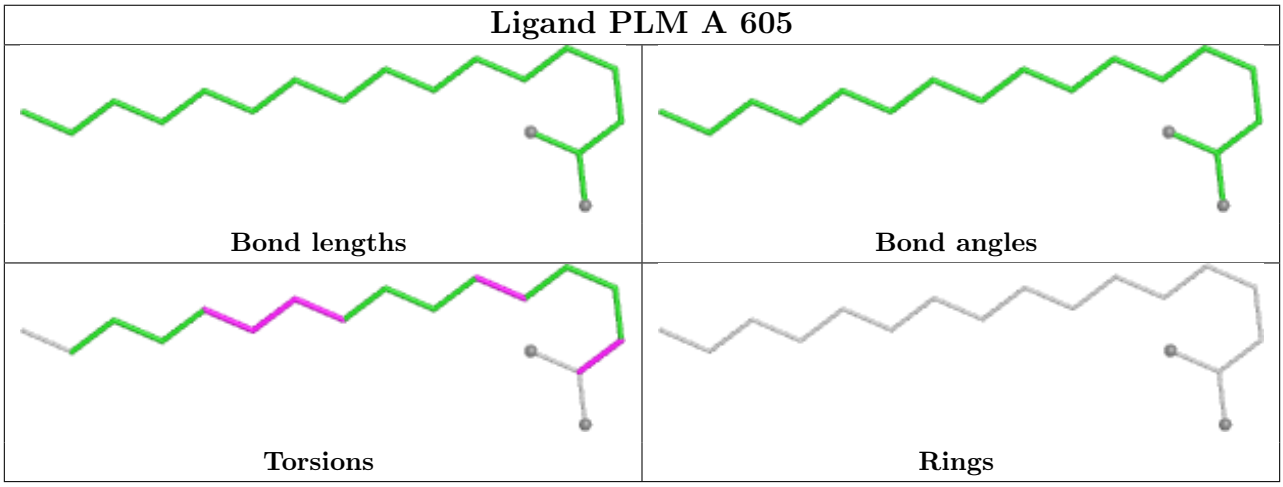


Torsions



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 (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	581/581 (100%)	-1.31	0	100	100	32, 58, 99, 168	0
1	B	581/581 (100%)	-1.26	0	100	100	39, 67, 106, 149	0
All	All	1162/1162 (100%)	-1.29	0	100	100	32, 62, 102, 168	0

There are no RSRZ outliers to report.

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
3	PLM	B	602	13/18	0.97	0.08	95,105,113,114	0
3	PLM	A	605	18/18	0.98	0.07	65,81,89,91	0
3	PLM	A	606	17/18	0.98	0.06	40,49,66,74	0
3	PLM	A	602	13/18	0.98	0.07	84,90,96,96	0
3	PLM	A	604	17/18	0.99	0.05	51,59,66,66	0
2	6WF	B	601	23/25	0.99	0.04	44,64,88,202	0
2	6WF	A	601	23/25	0.99	0.04	39,54,96,223	0

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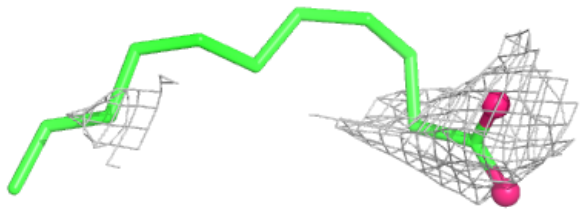
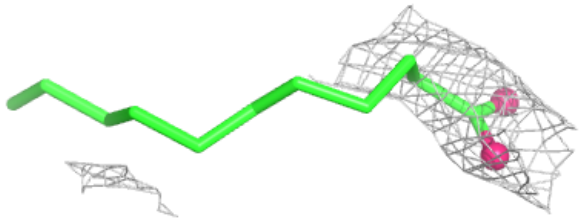
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PLM	A	607	18/18	0.99	0.06	44,59,108,111	0
3	PLM	A	603	18/18	0.99	0.05	60,67,80,84	0
3	PLM	B	603	18/18	0.99	0.06	58,66,80,81	0
3	PLM	B	604	17/18	0.99	0.04	51,63,72,72	0
3	PLM	B	605	18/18	0.99	0.05	68,82,95,95	0
3	PLM	B	606	17/18	0.99	0.05	57,60,68,72	0
3	PLM	B	607	18/18	0.99	0.05	33,51,92,93	0

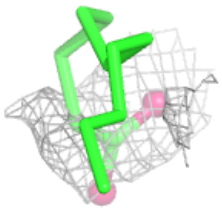
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PLM B 602:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

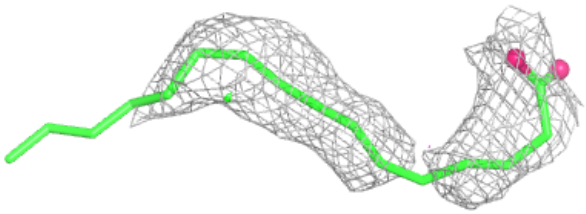


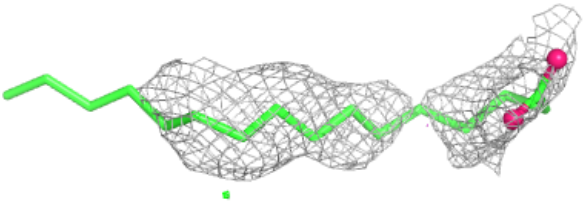


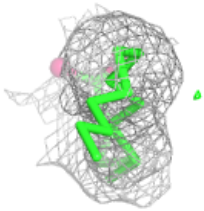


Electron density around PLM A 605:

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

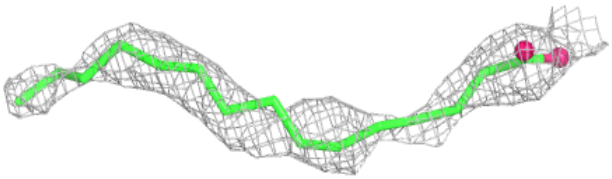


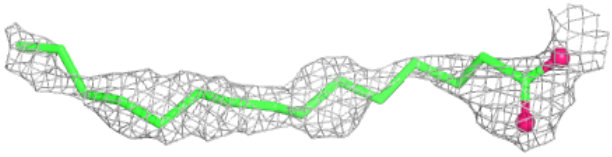


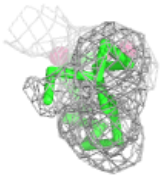


Electron density around PLM A 606:

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

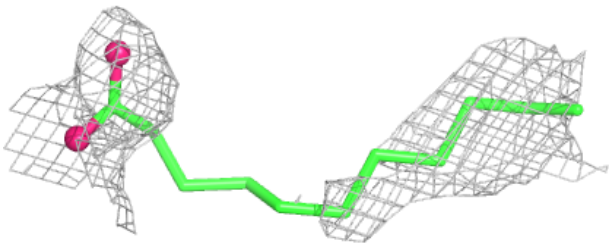


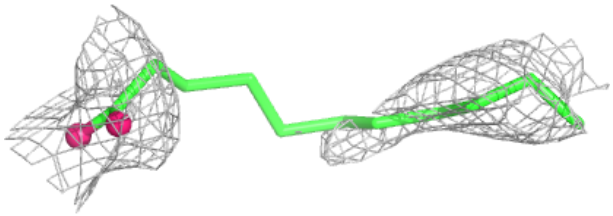


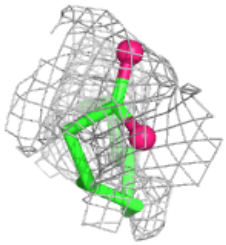


Electron density around PLM A 602:

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

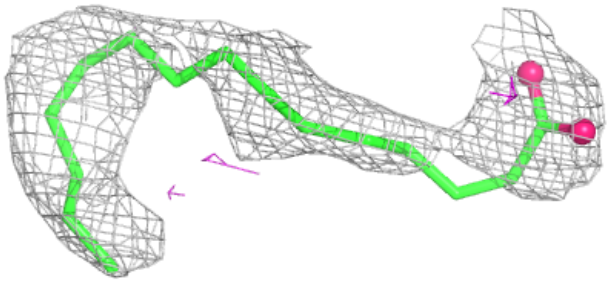


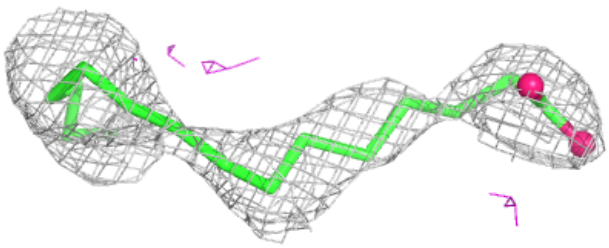


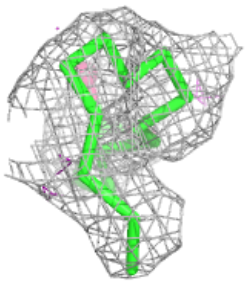


Electron density around PLM A 604:

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

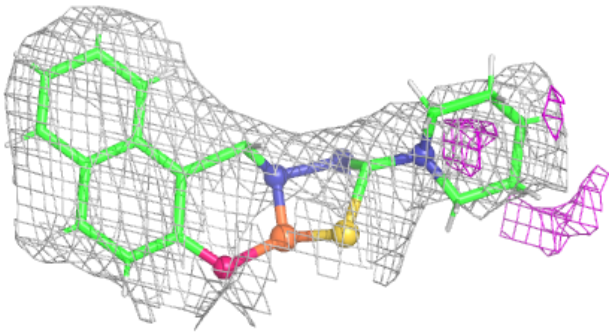


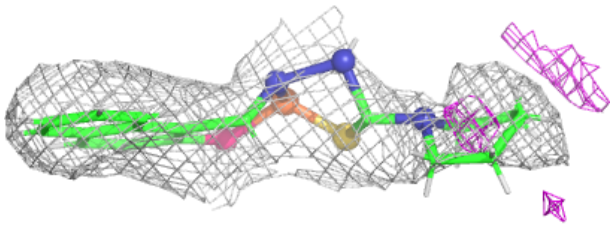


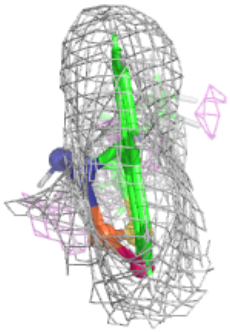


Electron density around 6WF B 601:

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

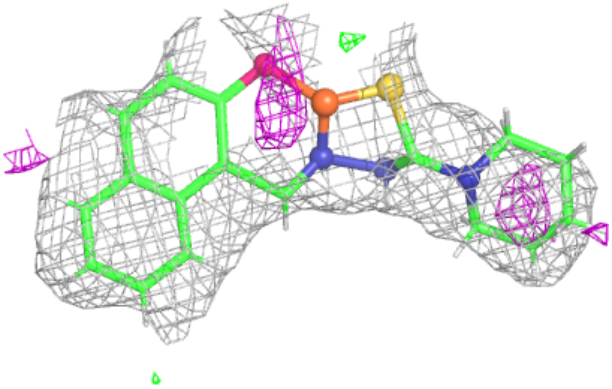


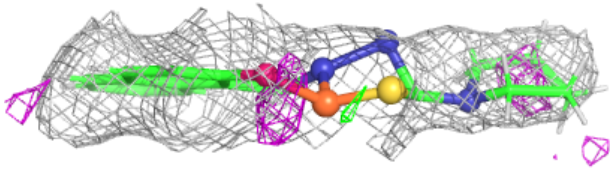


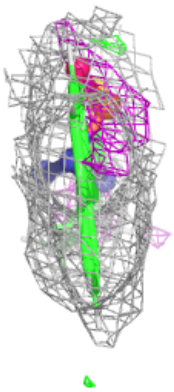


Electron density around 6WF A 601:

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

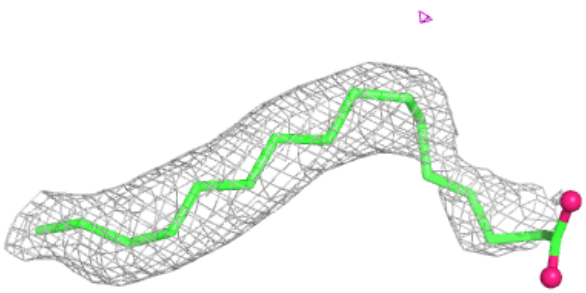


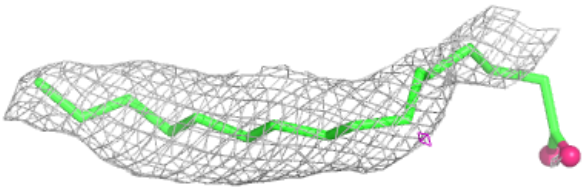


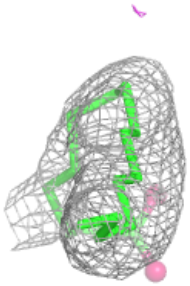


Electron density around PLM A 607:

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

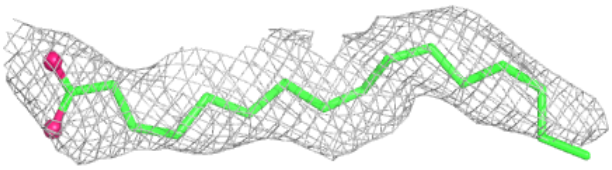


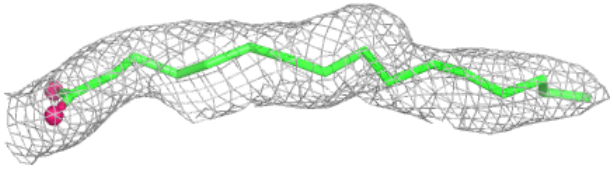


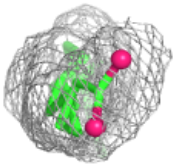


Electron density around PLM A 603:

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

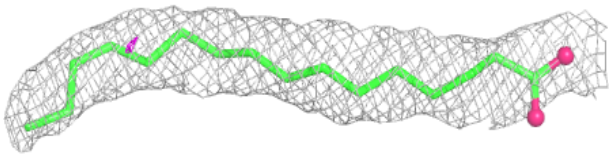


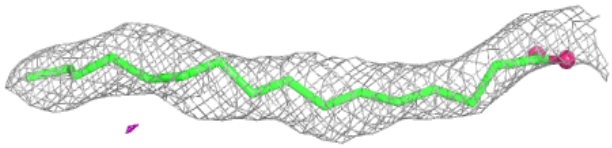


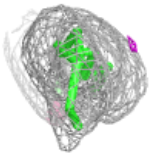


Electron density around PLM B 603:

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







Electron density around PLM B 604:

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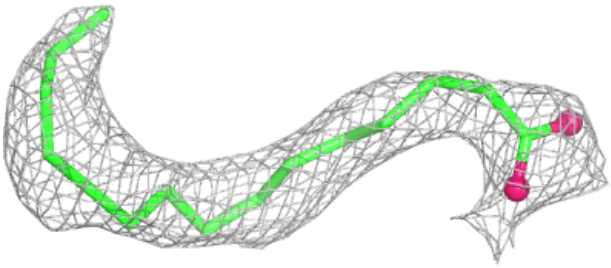
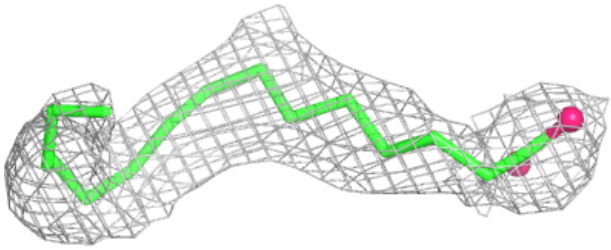
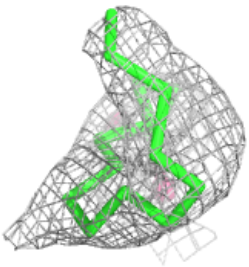
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

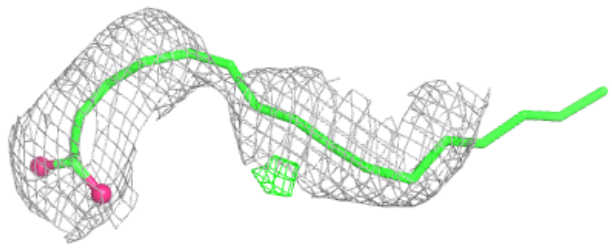


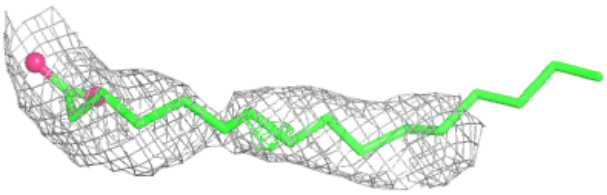


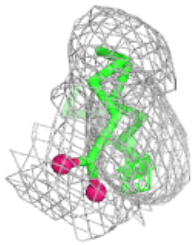


Electron density around PLM B 605:

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

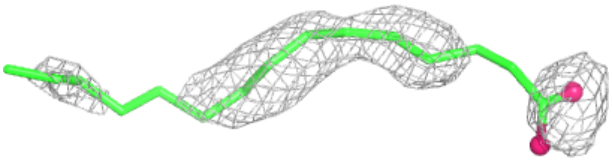


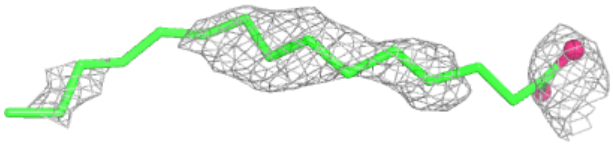


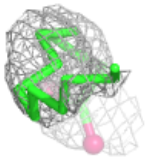


Electron density around PLM B 606:

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

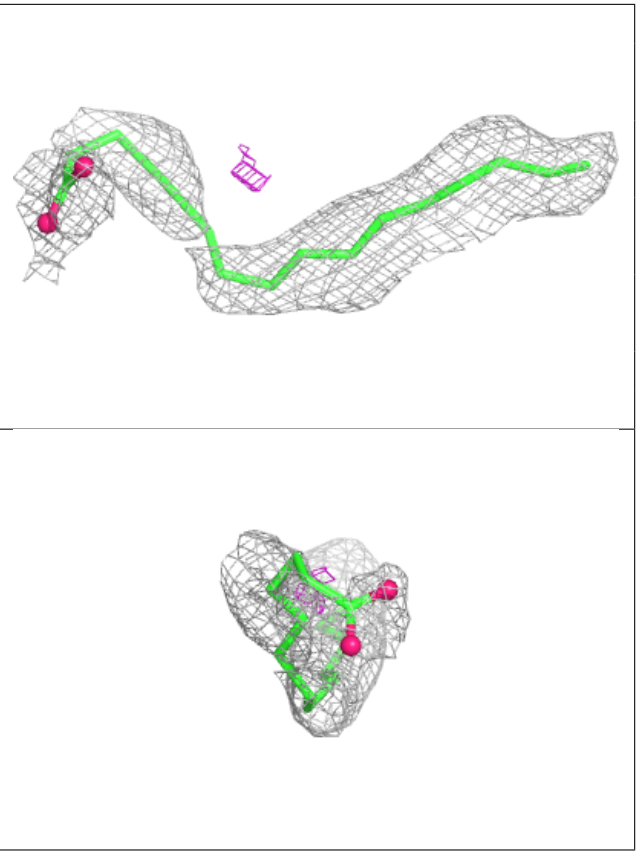






Electron density around PLM B 607:

$2mF_o$-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.