Full wwPDB X-ray Structure Validation Report (i)

Dec 6, 2023 – 06:46 am GMT

PDB ID	:	2BOY
Title	:	Crystal structure of 3-ChloroCatechol 1,2-Dioxygenase from Rhodococcus Opacus 1CP
Authors	:	Ferraroni, M.; Solyanikova, I.P.; Kolomytseva, M.P.; Scozzafava, A.; Golovleva, L.A.; Briganti, F.
Deposited on	:	2005-04-15
Resolution	:	1.90 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:

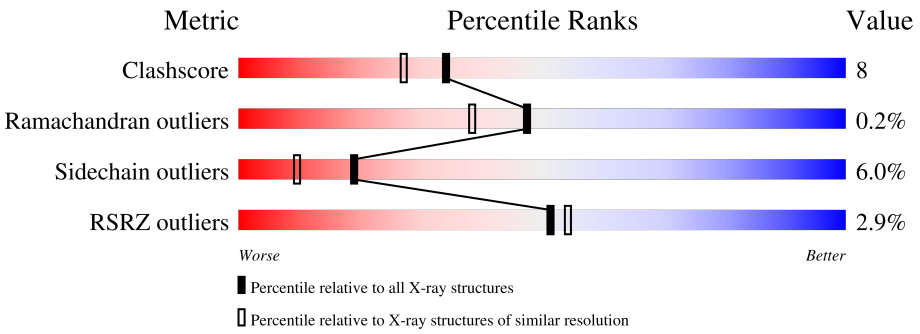
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.90 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))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	254	3% 86% 11% •
1	B	254	4% 85% 13% • •
1	C	254	2% 87% 9% • •
1	D	254	4% 85% 11% • •
1	E	254	3% 80% 16% • • •
1	F	254	2% 84% 11% • •

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Mol	Chain	Length	Quality of chain
1	G	254	3% 80% 15%
1	H	254	2% 77% 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
3	BHO	B	1256[B]	-	-	X	-
3	BHO	E	1256[A]	-	-	X	-
3	BHO	F	1256[B]	-	-	X	-
3	BHO	G	1256	-	X	-	-
3	BHO	H	1256[B]	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 17938 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 3-CHLOROCATECHOL 1,2-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	253	1990	1279	324	383	4	0	4	0
1	B	252	1967	1266	319	378	4	0	2	0
1	C	251	1973	1267	322	380	4	0	4	0
1	D	251	1975	1268	323	380	4	0	5	0
1	E	252	1973	1269	320	380	4	0	4	2
1	F	248	1952	1252	318	378	4	0	5	0
1	G	251	1952	1259	316	373	4	0	1	1
1	H	248	1924	1240	314	366	4	0	1	0

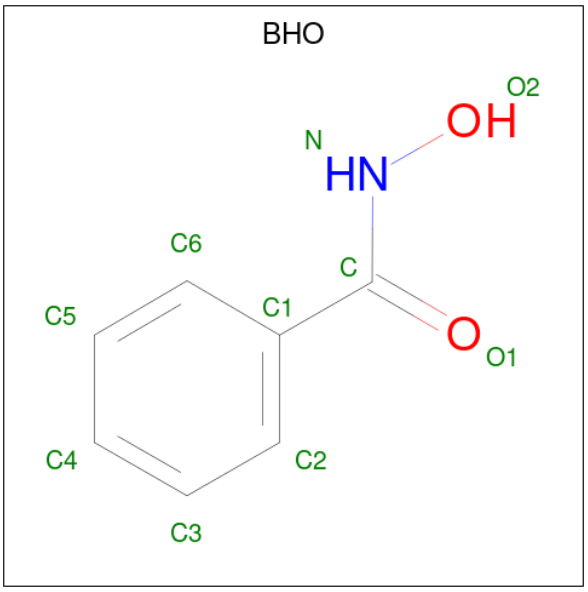
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	LYS	GLN	conflict	UNP Q8G9L3
B	44	LYS	GLN	conflict	UNP Q8G9L3
C	44	LYS	GLN	conflict	UNP Q8G9L3
D	44	LYS	GLN	conflict	UNP Q8G9L3
E	44	LYS	GLN	conflict	UNP Q8G9L3
F	44	LYS	GLN	conflict	UNP Q8G9L3
G	44	LYS	GLN	conflict	UNP Q8G9L3
H	44	LYS	GLN	conflict	UNP Q8G9L3

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0
2	E	1	1	1	0	0
2	F	1	1	1	0	0
2	G	1	1	1	0	0
2	H	1	1	1	0	0

- Molecule 3 is BENZHYDROXAMIC ACID (three-letter code: BHO) (formula: $C_7H_7NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	10	7	1	2	0	0
3	B	1	20	14	2	4	0	1
3	C	1	20	14	2	4	0	1
3	D	1	14	8	2	4	0	1

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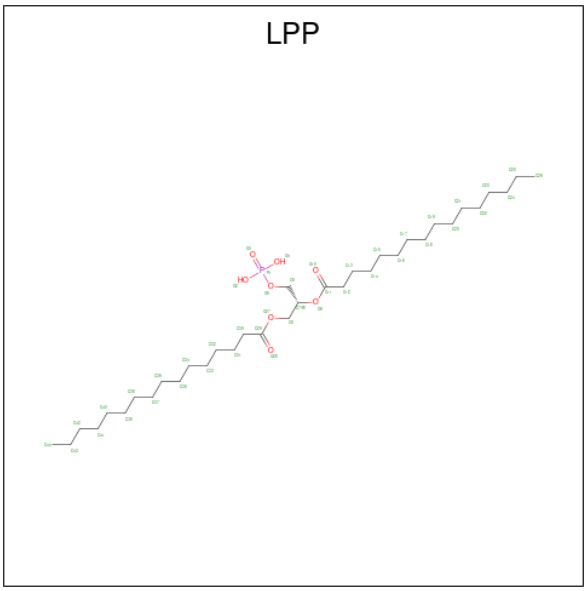
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	E	1	20	14	2	4	0	1
			Total	C	N	O		
3	F	1	20	14	2	4	0	1
			Total	C	N	O		
3	G	1	10	7	1	2	0	0
			Total	C	N	O		
3	H	1	20	14	2	4	0	1

- Molecule 4 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (three-letter code: LPP) (formula: $C_{35}H_{69}O_8P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
4	A	1	33	29	4		0	0
			Total	C	O			
4	B	1	33	29	4		0	0
			Total	C	O			
4	C	1	34	30	4		0	0
			Total	C	O	P		
4	D	1	36	30	5	1	0	0
			Total	C	O			
4	E	1	34	31	3		0	0
			Total	C	O			
4	F	1	34	31	3		0	0
			Total	C	O			
4	G	1	34	31	3		0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C O 36 32 4	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Mg 2 2	0	0
5	B	3	Total Mg 3 3	0	0
5	C	4	Total Mg 4 4	0	0
5	D	2	Total Mg 2 2	0	0
5	E	1	Total Mg 1 1	0	0
5	F	1	Total Mg 1 1	0	0
5	G	1	Total Mg 1 1	0	0
5	H	2	Total Mg 2 2	0	0

- Molecule 6 is water.

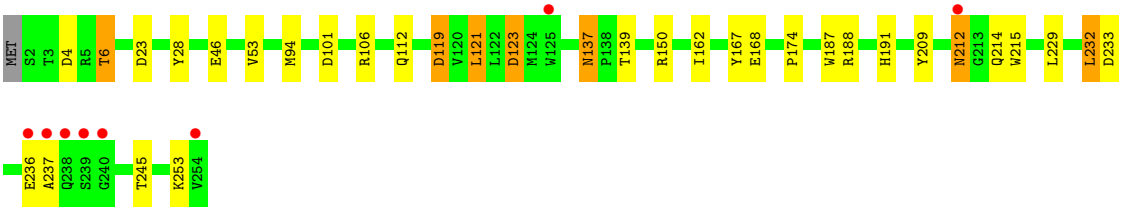
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	267	Total O 267 267	0	0
6	B	241	Total O 241 241	0	0
6	C	203	Total O 203 203	0	0
6	D	241	Total O 241 241	0	0
6	E	233	Total O 233 233	0	0
6	F	230	Total O 230 230	0	0
6	G	180	Total O 180 180	0	0
6	H	205	Total O 205 205	0	0

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.

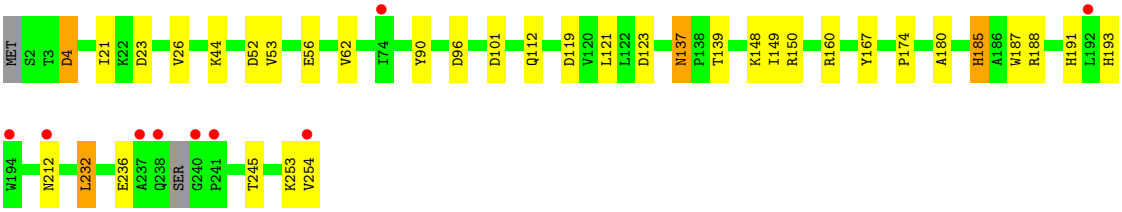
• Molecule 1: 3-CHLOROCATECHOL 1,2-DIOXYGENASE

Chain A:



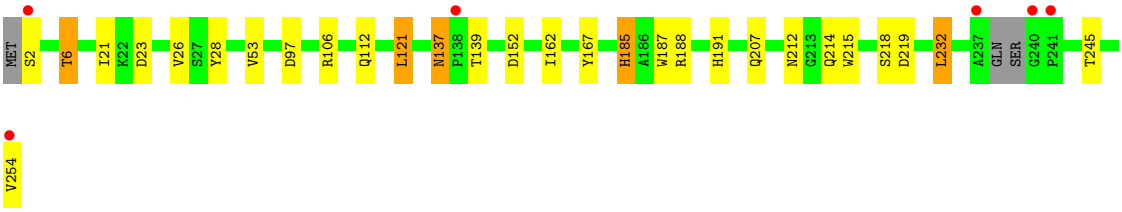
• Molecule 1: 3-CHLOROCATECHOL 1,2-DIOXYGENASE

Chain B:



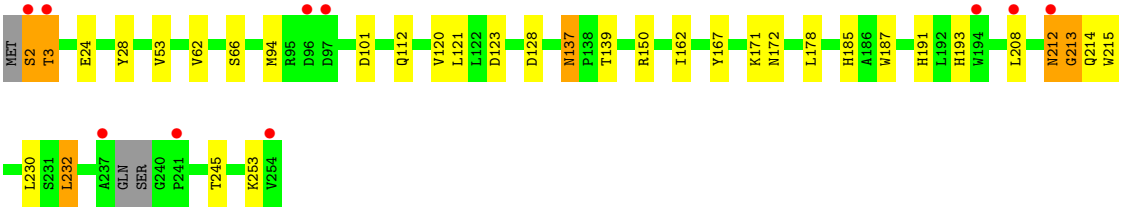
• Molecule 1: 3-CHLOROCATECHOL 1,2-DIOXYGENASE

Chain C:



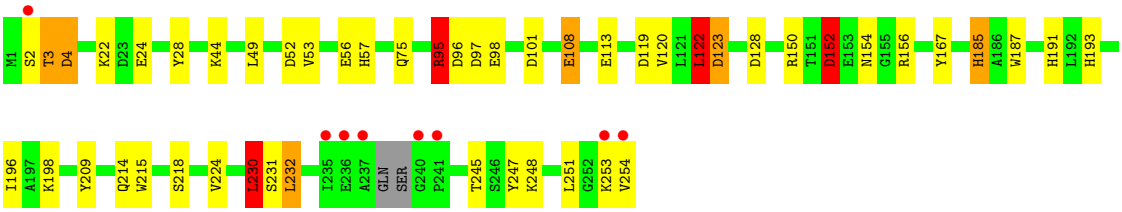
• Molecule 1: 3-CHLOROCATECHOL 1,2-DIOXYGENASE

Chain D:



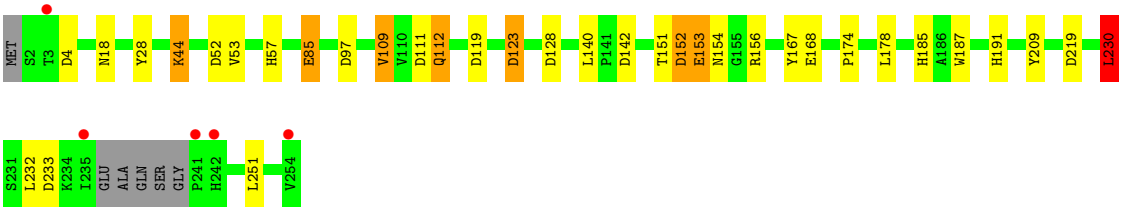
• Molecule 1: 3-CHLOROCATECHOL 1,2-DIOXYGENASE

Chain E:



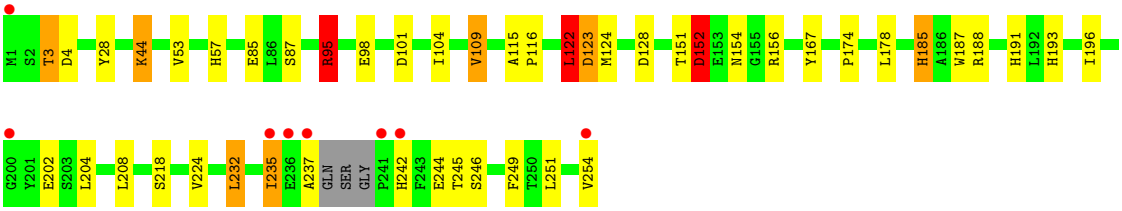
• Molecule 1: 3-CHLOROCATECHOL 1,2-DIOXYGENASE

Chain F:



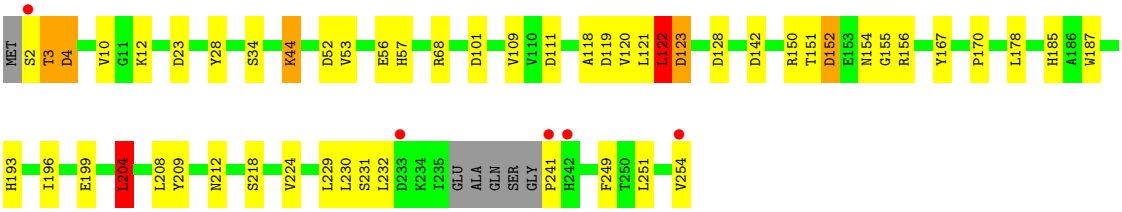
• Molecule 1: 3-CHLOROCATECHOL 1,2-DIOXYGENASE

Chain G:



• Molecule 1: 3-CHLOROCATECHOL 1,2-DIOXYGENASE

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	83.18Å 86.61Å 93.45Å 85.37° 66.53° 76.94°	Depositor
Resolution (Å)	84.51 – 1.90 28.12 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.2 (84.51-1.90) 93.0 (28.12-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.81 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.176 , 0.219 0.177 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	23.5	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.005 for -h,-k,-h+l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17938	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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: BHO, FE, LPP, MG

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	0.78	0/2061	0.89	7/2806 (0.2%)
1	B	0.79	0/2027	0.87	6/2763 (0.2%)
1	C	0.80	0/2043	0.87	5/2785 (0.2%)
1	D	0.77	0/2050	0.86	4/2792 (0.1%)
1	E	0.78	0/2044	0.90	13/2783 (0.5%)
1	F	0.76	0/2026	0.88	10/2760 (0.4%)
1	G	0.69	0/2007	0.88	8/2734 (0.3%)
1	H	0.75	0/1978	0.89	10/2696 (0.4%)
All	All	0.77	0/16236	0.88	63/22119 (0.3%)

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	D	0	1

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	95	ARG	NE-CZ-NH2	-11.84	114.38	120.30
1	E	122	LEU	CA-CB-CG	9.49	137.14	115.30
1	E	95	ARG	NE-CZ-NH1	8.55	124.58	120.30
1	G	95	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	E	128	ASP	CB-CG-OD2	7.95	125.46	118.30
1	G	122	LEU	CA-CB-CG	7.87	133.41	115.30
1	H	142	ASP	CB-CG-OD2	7.35	124.92	118.30
1	H	128	ASP	CB-CG-OD2	7.30	124.87	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	23	ASP	CB-CG-OD2	7.17	124.75	118.30
1	H	4	ASP	CB-CG-OD2	6.99	124.59	118.30
1	F	128	ASP	CB-CG-OD2	6.78	124.40	118.30
1	G	128	ASP	CB-CG-OD2	6.72	124.35	118.30
1	B	23	ASP	CB-CG-OD2	6.57	124.22	118.30
1	H	122	LEU	CA-CB-CG	6.54	130.35	115.30
1	D	123	ASP	CB-CG-OD2	6.53	124.17	118.30
1	E	152	ASP	CB-CG-OD2	6.43	124.09	118.30
1	E	101	ASP	CB-CG-OD2	6.38	124.04	118.30
1	A	4	ASP	CB-CG-OD2	6.37	124.03	118.30
1	F	123	ASP	CB-CG-OD2	6.32	123.98	118.30
1	C	121	LEU	CA-CB-CG	-6.31	100.78	115.30
1	H	152	ASP	CB-CG-OD2	6.28	123.95	118.30
1	B	123	ASP	CB-CG-OD2	6.28	123.95	118.30
1	G	4	ASP	CB-CG-OD2	6.26	123.94	118.30
1	B	4[A]	ASP	CB-CG-OD2	6.16	123.84	118.30
1	B	4[B]	ASP	CB-CG-OD2	6.16	123.84	118.30
1	F	233	ASP	CB-CG-OD2	6.10	123.79	118.30
1	G	95	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	F	4	ASP	CB-CG-OD2	6.01	123.71	118.30
1	F	230	LEU	CA-CB-CG	6.00	129.10	115.30
1	F	97	ASP	CB-CG-OD2	5.99	123.69	118.30
1	A	123	ASP	CB-CG-OD2	5.98	123.68	118.30
1	G	152	ASP	CB-CG-OD2	5.94	123.64	118.30
1	B	101	ASP	CB-CG-OD2	5.83	123.55	118.30
1	D	101	ASP	CB-CG-OD2	5.83	123.55	118.30
1	F	152	ASP	CB-CG-OD2	5.83	123.54	118.30
1	F	142	ASP	CB-CG-OD2	5.78	123.50	118.30
1	C	23	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	23	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	233	ASP	CB-CG-OD2	5.65	123.39	118.30
1	E	123	ASP	CB-CG-OD2	5.60	123.34	118.30
1	C	106	ARG	NE-CZ-NH1	-5.59	117.51	120.30
1	A	101	ASP	CB-CG-OD2	5.52	123.27	118.30
1	H	119	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	106	ARG	NE-CZ-NH1	-5.49	117.56	120.30
1	C	152	ASP	CB-CG-OD1	5.44	123.20	118.30
1	A	119	ASP	CB-CG-OD2	5.42	123.17	118.30
1	B	96	ASP	CB-CG-OD2	5.40	123.16	118.30
1	E	122	LEU	CB-CG-CD2	5.39	120.16	111.00
1	G	123	ASP	CB-CG-OD2	5.33	123.10	118.30
1	C	97	ASP	CB-CG-OD2	5.32	123.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	219	ASP	CB-CG-OD1	5.29	123.06	118.30
1	E	4	ASP	CB-CG-OD2	5.20	122.98	118.30
1	H	123	ASP	CB-CG-OD2	5.19	122.97	118.30
1	E	230	LEU	CA-CB-CG	5.17	127.20	115.30
1	F	52	ASP	CB-CG-OD2	5.15	122.94	118.30
1	E	97	ASP	CB-CG-OD2	5.13	122.92	118.30
1	G	101	ASP	CB-CG-OD2	5.12	122.91	118.30
1	D	213	GLY	N-CA-C	5.09	125.83	113.10
1	H	101	ASP	CB-CG-OD2	5.07	122.86	118.30
1	E	119	ASP	CB-CG-OD2	5.07	122.86	118.30
1	H	204	LEU	CB-CG-CD2	5.05	119.59	111.00
1	D	128	ASP	CB-CG-OD1	5.02	122.82	118.30
1	E	96	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	212	ASN	Peptide

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	1990	0	1906	27	0
1	B	1967	0	1862	29	0
1	C	1973	0	1868	27	0
1	D	1975	0	1885	27	0
1	E	1973	0	1889	43	0
1	F	1952	0	1847	25	0
1	G	1952	0	1860	31	0
1	H	1924	0	1828	49	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	10	0	6	3	0
3	B	20	0	14	9	0
3	C	20	0	11	3	0
3	D	14	0	1	2	0
3	E	20	0	12	8	0
3	F	20	0	11	4	0
3	G	10	0	6	3	0
3	H	20	0	13	14	0
4	A	33	0	47	0	0
4	B	33	0	47	1	0
4	C	34	0	49	0	0
4	D	36	0	51	0	0
4	E	34	0	55	0	0
4	F	34	0	55	2	0
4	G	34	0	55	1	0
4	H	36	0	57	1	0
5	A	2	0	0	0	0
5	B	3	0	0	0	0
5	C	4	0	0	0	0
5	D	2	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	2	0	0	0	0
6	A	267	0	0	3	0
6	B	241	0	0	7	0
6	C	203	0	0	2	0
6	D	241	0	0	7	0
6	E	233	0	0	8	0
6	F	230	0	0	6	0
6	G	180	0	0	4	0
6	H	205	0	0	8	0
All	All	17938	0	15435	266	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 (266) 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:H:167[B]:TYR:OH	3:H:1256[B]:BHO:C6	1.74	1.35
1:H:167[B]:TYR:OH	3:H:1256[B]:BHO:H6	1.06	1.19
1:C:167[B]:TYR:CE1	1:C:191:HIS:CE1	2.42	1.08
1:A:212:ASN:H	1:A:212:ASN:ND2	1.46	1.05
1:F:112:GLN:HG2	6:F:2136:HOH:O	1.56	1.04
1:C:167[B]:TYR:HE1	1:C:191:HIS:CE1	1.75	1.03
1:C:167[B]:TYR:CE1	1:C:191:HIS:HE1	1.79	0.99
1:E:185:HIS:HD2	1:E:187:TRP:H	1.11	0.99
1:E:185:HIS:HE1	1:E:218:SER:O	1.44	0.98
1:F:167[B]:TYR:CE2	1:F:191:HIS:CE1	2.52	0.97
1:D:185:HIS:HD2	1:D:187:TRP:H	1.13	0.96
1:G:185:HIS:HD2	1:G:187:TRP:H	1.13	0.95
1:E:185:HIS:CE1	1:E:218:SER:O	2.19	0.94
1:A:212:ASN:H	1:A:212:ASN:HD22	1.06	0.93
1:F:167[B]:TYR:CE2	1:F:191:HIS:HE1	1.85	0.93
1:H:167[B]:TYR:HH	3:H:1256[B]:BHO:H6	1.10	0.92
1:H:170:PRO:HD3	6:H:2155:HOH:O	1.69	0.92
1:B:44:LYS:HD3	1:B:174:PRO:HD3	1.51	0.92
1:F:191:HIS:CE1	6:F:2169:HOH:O	2.24	0.91
3:E:1256[A]:BHO:H2	3:E:1256[A]:BHO:O2	1.71	0.90
1:E:185:HIS:CD2	1:E:187:TRP:H	1.89	0.89
1:F:44:LYS:HE3	1:F:174:PRO:HD3	1.53	0.88
1:F:167[B]:TYR:HE2	1:F:191:HIS:CE1	1.90	0.88
1:H:167[B]:TYR:OH	3:H:1256[B]:BHO:C1	2.21	0.88
1:F:185:HIS:HD2	1:F:187:TRP:H	1.21	0.86
1:H:185:HIS:HD2	1:H:187:TRP:H	1.20	0.85
3:B:1256[B]:BHO:H6	3:B:1256[B]:BHO:O2	1.76	0.84
1:E:3:THR:HG23	6:E:2006:HOH:O	1.78	0.84
1:C:185:HIS:HD2	1:C:187:TRP:H	1.22	0.83
1:G:152:ASP:HB2	1:G:156:ARG:H	1.43	0.83
1:B:193:HIS:HE1	3:B:1256[B]:BHO:HN	1.23	0.83
1:G:167[B]:TYR:CE1	1:G:191:HIS:CE1	2.66	0.83
1:D:112:GLN:HE22	1:D:253:LYS:H	1.27	0.82
1:G:167[B]:TYR:CE1	1:G:191:HIS:HE1	1.97	0.82
1:A:212:ASN:ND2	1:A:212:ASN:N	2.27	0.82
1:H:167[B]:TYR:CZ	3:H:1256[B]:BHO:H6	2.14	0.81
1:H:170:PRO:CD	6:H:2155:HOH:O	2.24	0.81
1:A:112:GLN:HE22	1:A:253:LYS:H	1.29	0.80
1:F:109:VAL:HG13	1:F:151:THR:HG21	1.62	0.80
1:D:185:HIS:CD2	1:D:187:TRP:H	2.01	0.78
1:H:152:ASP:HB2	1:H:156:ARG:H	1.48	0.78
1:E:152:ASP:HB3	1:E:154:ASN:H	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:HIS:HD2	1:B:187:TRP:H	1.28	0.77
4:B:1257:LPP:HC7	6:B:2241:HOH:O	1.84	0.77
1:C:21:ILE:HA	1:C:26:VAL:HG13	1.67	0.77
1:G:152:ASP:HB3	1:G:154:ASN:H	1.47	0.77
1:G:185:HIS:CD2	1:G:187:TRP:H	2.01	0.76
1:E:198:LYS:CD	6:E:2132:HOH:O	2.34	0.76
1:A:112:GLN:NE2	1:A:253:LYS:H	1.82	0.76
1:D:112:GLN:NE2	1:D:253:LYS:H	1.83	0.75
1:E:152:ASP:HB2	1:E:156:ARG:H	1.50	0.75
1:F:152:ASP:HB3	1:F:154:ASN:H	1.53	0.74
1:C:185:HIS:CD2	1:C:187:TRP:H	2.05	0.73
1:B:167[A]:TYR:HB2	6:B:2141:HOH:O	1.89	0.73
1:F:152:ASP:HB2	1:F:156:ARG:H	1.54	0.73
1:B:21:ILE:HA	1:B:26:VAL:HG13	1.71	0.72
1:A:6:THR:HG22	6:A:2001:HOH:O	1.87	0.72
1:C:6:THR:HG22	6:C:2001:HOH:O	1.91	0.71
1:F:191:HIS:HE1	6:F:2169:HOH:O	1.62	0.71
1:A:212:ASN:HD22	1:A:212:ASN:N	1.87	0.70
1:A:137:ASN:C	1:A:137:ASN:HD22	1.95	0.70
1:B:193:HIS:CE1	3:B:1256[B]:BHO:HN	2.09	0.69
1:G:95:ARG:HD3	1:G:98:GLU:OE1	1.92	0.69
1:G:167[B]:TYR:HE1	1:G:191:HIS:CE1	2.07	0.69
1:E:122:LEU:HD13	1:E:196:ILE:HG12	1.75	0.69
3:B:1256[A]:BHO:O2	6:B:2240:HOH:O	2.09	0.69
1:H:185:HIS:HE1	1:H:218:SER:OG	1.77	0.68
1:E:95:ARG:HD3	1:E:98:GLU:OE1	1.94	0.68
1:E:185:HIS:HD2	1:E:187:TRP:N	1.91	0.67
1:C:53:VAL:HG23	3:C:1256[B]:BHO:H4	1.78	0.66
3:E:1256[A]:BHO:O2	3:E:1256[A]:BHO:C2	2.39	0.66
1:B:112:GLN:NE2	1:B:253:LYS:H	1.93	0.66
1:C:137:ASN:HD22	1:C:139:THR:H	1.42	0.66
1:D:24:GLU:OE2	1:H:12:LYS:NZ	2.29	0.65
1:H:185:HIS:CD2	1:H:187:TRP:H	2.10	0.65
1:G:109:VAL:HG13	1:G:151:THR:HG21	1.78	0.65
1:C:188[B]:ARG:HD2	1:C:219:ASP:OD1	1.97	0.64
1:D:172:ASN:HB3	6:D:2183:HOH:O	1.98	0.64
1:H:152:ASP:HB3	1:H:154:ASN:H	1.63	0.64
1:F:178:LEU:HD13	4:F:1257:LPP:H161	1.79	0.63
1:A:214:GLN:HG3	1:A:215:TRP:CD1	2.34	0.63
1:B:185:HIS:CD2	1:B:187:TRP:H	2.14	0.62
1:E:167[B]:TYR:CE2	1:E:191:HIS:HE1	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:TYR:CE1	1:B:149:ILE:HG23	2.35	0.62
1:D:137:ASN:C	1:D:137:ASN:HD22	2.03	0.62
1:D:137:ASN:HD22	1:D:139:THR:H	1.47	0.61
1:E:167[B]:TYR:CE2	1:E:191:HIS:CE1	2.88	0.61
1:G:44:LYS:HE2	1:G:174:PRO:HD3	1.82	0.61
1:H:44:LYS:N	1:H:44:LYS:HD2	2.16	0.61
1:E:167[B]:TYR:HE2	1:E:191:HIS:CE1	2.20	0.60
1:B:119:ASP:OD1	1:B:150:ARG:NH1	2.34	0.60
1:C:137:ASN:ND2	1:C:139:THR:H	1.99	0.60
1:C:2:SER:O	1:C:6:THR:HG23	2.02	0.60
1:C:185:HIS:CE1	1:C:218:SER:O	2.55	0.60
1:E:150:ARG:HD3	6:E:2154:HOH:O	2.02	0.59
1:B:150:ARG:NH2	6:B:2152:HOH:O	2.35	0.59
1:H:53:VAL:CG2	3:H:1256[A]:BHO:H4	2.31	0.59
1:A:121[A]:LEU:HD12	1:A:150:ARG:HG2	1.85	0.59
1:F:168:GLU:HG3	1:F:187:TRP:CE2	2.38	0.59
1:A:167[B]:TYR:CE2	1:A:191:HIS:CE1	2.91	0.59
1:H:167[B]:TYR:HH	3:H:1256[B]:BHO:C6	1.89	0.58
1:A:188:ARG:NH1	3:A:1256:BHO:O1	2.37	0.57
1:C:188[B]:ARG:NH2	1:C:207:GLN:OE1	2.38	0.57
1:E:193:HIS:HE1	3:E:1256[A]:BHO:HN	1.52	0.57
1:A:168:GLU:HG3	1:A:187:TRP:CE2	2.40	0.56
1:H:109:VAL:HG13	1:H:151:THR:HG21	1.88	0.56
1:C:53:VAL:CG2	3:C:1256[B]:BHO:H4	2.35	0.56
1:F:185:HIS:CD2	1:F:187:TRP:H	2.13	0.56
1:G:95:ARG:CD	1:G:98:GLU:OE1	2.54	0.56
1:H:53:VAL:HG22	3:H:1256[A]:BHO:H4	1.87	0.56
1:F:109:VAL:HG13	1:F:151:THR:CG2	2.33	0.55
1:F:111:ASP:HB2	6:F:2136:HOH:O	2.06	0.55
1:G:152:ASP:HB3	1:G:154:ASN:N	2.21	0.55
3:F:1256[B]:BHO:O2	3:F:1256[B]:BHO:H6	2.07	0.55
1:G:3:THR:CG2	6:G:2001:HOH:O	2.55	0.55
1:G:57:HIS:HD2	6:G:2059:HOH:O	1.89	0.55
1:H:111:ASP:HB2	6:H:2126:HOH:O	2.06	0.55
1:D:213:GLY:HA2	6:D:2212:HOH:O	2.07	0.55
1:A:94:MET:SD	1:A:162:ILE:HD12	2.46	0.54
1:B:112:GLN:HE22	1:B:253:LYS:H	1.53	0.54
1:B:160:ARG:HD3	6:B:2166:HOH:O	2.07	0.54
1:H:57:HIS:HD2	6:H:2072:HOH:O	1.90	0.54
1:E:120:VAL:HG12	1:E:122:LEU:HD22	1.89	0.54
1:H:121:LEU:HD13	6:H:2145:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:95:ARG:CD	1:E:98:GLU:OE1	2.55	0.54
1:A:53:VAL:HG23	3:A:1256:BHO:H4	1.89	0.54
1:H:34:SER:OG	4:H:1257:LPP:H161	2.08	0.53
1:D:214:GLN:HG2	1:D:215:TRP:CD1	2.44	0.53
1:E:22[B]:LYS:HG2	6:E:2026:HOH:O	2.08	0.53
1:A:112:GLN:HG2	6:A:2140:HOH:O	2.09	0.53
1:A:119:ASP:OD1	1:A:150:ARG:NH1	2.42	0.53
1:B:188:ARG:NH2	3:B:1256[A]:BHO:O1	2.41	0.53
1:E:108:GLU:HG3	1:E:248:LYS:CB	2.39	0.53
1:A:53:VAL:CG2	3:A:1256:BHO:H4	2.39	0.52
1:B:185:HIS:CD2	1:B:185:HIS:C	2.82	0.52
1:D:2:SER:OG	1:D:3:THR:N	2.39	0.52
1:E:214:GLN:HG2	1:E:215:TRP:CD1	2.45	0.52
1:H:185:HIS:CE1	1:H:218:SER:O	2.63	0.52
1:B:253:LYS:O	1:B:254:VAL:HB	2.10	0.52
1:C:188[B]:ARG:NH1	1:C:219:ASP:OD2	2.43	0.52
1:H:241:PRO:CA	6:H:2197:HOH:O	2.58	0.52
1:E:232:LEU:HD12	1:E:245:THR:HB	1.93	0.51
1:B:167[A]:TYR:CE2	1:B:191:HIS:CE1	2.99	0.51
1:G:104:ILE:HB	1:G:244:GLU:HG2	1.92	0.51
1:G:124:MET:HG2	1:G:193:HIS:O	2.09	0.51
1:A:167[B]:TYR:CE2	1:A:191:HIS:HE1	2.29	0.51
1:B:137:ASN:C	1:B:137:ASN:HD22	2.14	0.51
1:H:209:TYR:HB2	1:H:229:LEU:HD23	1.93	0.51
1:E:193:HIS:CE1	3:E:1256[A]:BHO:HN	2.30	0.50
1:E:167[B]:TYR:CD2	1:E:191:HIS:HE1	2.28	0.50
1:F:53:VAL:HG23	3:F:1256[B]:BHO:H4	1.94	0.50
1:H:68:ARG:NH1	1:H:254:VAL:HB	2.26	0.50
1:G:232:LEU:HD12	1:G:245:THR:HB	1.93	0.50
1:F:57:HIS:HD2	6:F:2075:HOH:O	1.95	0.49
1:A:112:GLN:NE2	6:A:2140:HOH:O	2.39	0.49
1:C:185:HIS:CD2	1:C:185:HIS:C	2.85	0.49
1:E:53:VAL:HG22	3:E:1256[B]:BHO:H4	1.95	0.49
1:E:57:HIS:HD2	6:E:2085:HOH:O	1.95	0.49
1:B:112:GLN:HG2	6:B:2128:HOH:O	2.12	0.49
1:E:53:VAL:HG23	3:E:1256[A]:BHO:H4	1.95	0.48
1:C:167[B]:TYR:CZ	1:C:191:HIS:CE1	2.97	0.48
1:E:53:VAL:CG2	3:E:1256[B]:BHO:H4	2.43	0.48
1:D:178:LEU:HD11	1:H:10:VAL:HG11	1.94	0.48
1:D:137:ASN:ND2	1:D:139:THR:H	2.09	0.48
1:F:53:VAL:CG2	3:F:1256[B]:BHO:H4	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:LEU:HD12	3:E:1256[A]:BHO:H4	1.96	0.48
1:D:167[A]:TYR:CE1	1:D:191:HIS:CE1	3.02	0.48
1:E:3:THR:CG2	6:E:2006:HOH:O	2.50	0.47
1:E:44:LYS:NZ	6:E:2060:HOH:O	2.46	0.47
1:G:185:HIS:CD2	1:G:185:HIS:C	2.88	0.47
1:B:137:ASN:HD22	1:B:139:THR:H	1.62	0.47
1:E:75:GLN:NE2	6:E:2102:HOH:O	2.43	0.47
1:D:112:GLN:NE2	6:D:2128:HOH:O	2.46	0.47
1:G:115:ALA:HA	1:G:116:PRO:HD2	1.72	0.47
1:G:53:VAL:CG2	3:G:1256:BHO:H4	2.45	0.47
1:A:137:ASN:HD22	1:A:139:THR:H	1.63	0.47
1:H:185:HIS:CE1	1:H:218:SER:OG	2.64	0.47
1:B:121:LEU:HD21	1:B:148:LYS:HB3	1.95	0.47
1:E:209:TYR:O	1:E:230:LEU:HB2	2.14	0.47
1:H:3:THR:HG22	1:H:4:ASP:N	2.30	0.47
1:C:112:GLN:HG3	6:C:2063:HOH:O	2.14	0.47
1:E:108:GLU:HG2	1:E:248:LYS:HA	1.96	0.47
1:B:53:VAL:HG23	3:B:1256[A]:BHO:H4	1.97	0.47
1:F:153:GLU:OE1	1:F:154:ASN:OD1	2.33	0.46
1:H:52:ASP:HA	1:H:56:GLU:HB2	1.97	0.46
1:D:212:ASN:C	6:D:2212:HOH:O	2.53	0.46
1:E:108:GLU:HG3	1:E:248:LYS:HG3	1.97	0.46
1:E:120:VAL:O	1:E:150:ARG:HA	2.14	0.46
1:G:202:GLU:HG3	1:G:254:VAL:OXT	2.15	0.46
1:H:151:THR:HB	1:H:155:GLY:HA2	1.96	0.46
3:B:1256[B]:BHO:O2	3:B:1256[B]:BHO:C6	2.45	0.46
1:A:137:ASN:ND2	1:A:139:THR:H	2.13	0.45
1:B:52:ASP:HA	1:B:56:GLU:HB2	1.98	0.45
1:C:167[B]:TYR:CZ	1:C:191:HIS:HE1	2.29	0.45
1:G:109:VAL:HB	1:G:249:PHE:HB2	1.98	0.45
1:E:185:HIS:CD2	1:E:185:HIS:C	2.90	0.45
1:C:21:ILE:HA	1:C:26:VAL:CG1	2.43	0.45
1:F:209:TYR:O	1:F:230:LEU:HB2	2.17	0.45
1:H:53:VAL:HG23	3:H:1256[A]:BHO:H4	1.97	0.45
1:B:53:VAL:HG23	3:B:1256[B]:BHO:H4	1.99	0.44
1:G:235:ILE:HD12	1:G:242:HIS:CE1	2.52	0.44
1:C:137:ASN:HD22	1:C:137:ASN:C	2.20	0.44
1:E:185:HIS:CE1	1:E:218:SER:OG	2.71	0.44
1:G:185:HIS:CE1	1:G:218:SER:O	2.71	0.44
1:B:53:VAL:CG2	3:B:1256[B]:BHO:H4	2.48	0.43
1:C:185:HIS:HE1	1:C:218:SER:O	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ASN:C	1:A:137:ASN:ND2	2.67	0.43
1:C:232:LEU:HD12	1:C:245:THR:HB	1.99	0.43
1:C:188[B]:ARG:HH11	1:C:219:ASP:CG	2.21	0.43
1:E:108:GLU:CG	1:E:248:LYS:HA	2.49	0.43
1:G:235:ILE:HD11	1:G:237:ALA:HB2	2.00	0.43
1:H:118:ALA:HA	1:H:152:ASP:O	2.17	0.43
1:D:213:GLY:CA	6:D:2212:HOH:O	2.66	0.43
1:H:196:ILE:HD12	1:H:204:LEU:HD13	1.99	0.43
1:B:112:GLN:NE2	6:B:2128:HOH:O	2.36	0.43
1:G:109:VAL:HG13	1:G:151:THR:CG2	2.46	0.43
1:H:109:VAL:HG13	1:H:151:THR:CG2	2.48	0.43
1:F:85[B]:GLU:OE2	6:F:2110:HOH:O	2.21	0.43
1:D:121:LEU:CG	6:D:2155:HOH:O	2.66	0.43
1:H:122:LEU:HD13	1:H:196:ILE:HG12	2.01	0.43
1:H:109:VAL:HB	1:H:249:PHE:HB2	2.01	0.43
1:E:108:GLU:HG3	1:E:248:LYS:CG	2.49	0.42
1:H:193:HIS:HE1	3:H:1256[B]:BHO:O1	2.02	0.42
1:D:193:HIS:HE1	3:D:1256[B]:BHO:O1	2.03	0.42
1:E:52:ASP:HA	1:E:56:GLU:HB2	2.01	0.42
1:F:18:ASN:HD22	1:F:18:ASN:HA	1.66	0.42
1:C:53:VAL:HG22	3:C:1256[A]:BHO:H4	2.01	0.42
1:G:53:VAL:HG23	3:G:1256:BHO:H4	2.00	0.42
4:G:1257:LPP:H122	4:G:1257:LPP:C29	2.49	0.42
1:G:167[B]:TYR:HB2	6:G:2113:HOH:O	2.18	0.42
1:H:170:PRO:HD2	6:H:2155:HOH:O	2.04	0.42
1:H:193:HIS:CE1	3:H:1256[B]:BHO:O1	2.72	0.42
1:F:185:HIS:CD2	1:F:185:HIS:C	2.93	0.42
1:C:214:GLN:HB3	1:C:215:TRP:CD1	2.55	0.42
1:D:121:LEU:HB3	6:D:2154:HOH:O	2.19	0.41
1:F:152:ASP:HB3	1:F:154:ASN:N	2.29	0.41
1:G:122:LEU:HD13	1:G:196:ILE:HG12	2.02	0.41
1:H:44:LYS:HZ2	1:H:44:LYS:HG3	1.43	0.41
1:H:44:LYS:HD3	6:H:2054:HOH:O	2.20	0.41
1:H:167[B]:TYR:OH	3:H:1256[B]:BHO:C	2.21	0.41
1:D:94:MET:SD	1:D:162:ILE:HD12	2.61	0.41
1:A:168:GLU:HG3	1:A:187:TRP:CD2	2.55	0.41
1:H:120:VAL:O	1:H:150:ARG:HA	2.20	0.41
1:A:232:LEU:HD12	1:A:245:THR:HB	2.02	0.41
1:B:167[A]:TYR:CE2	1:B:191:HIS:HE1	2.38	0.41
1:D:232:LEU:HD12	1:D:245:THR:HB	2.03	0.41
1:G:188:ARG:NH1	3:G:1256:BHO:O1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:53:VAL:CG2	3:H:1256[B]:BHO:H4	2.51	0.41
1:B:180:ALA:O	1:H:212:ASN:HB3	2.20	0.41
1:E:108:GLU:HG2	1:E:247:TYR:O	2.20	0.41
1:B:232:LEU:HD12	1:B:245:THR:HB	2.03	0.41
1:D:120:VAL:O	1:D:150:ARG:HA	2.20	0.41
1:D:167[A]:TYR:CZ	1:D:191:HIS:HE1	2.39	0.41
1:D:208:LEU:HD13	1:D:230:LEU:HD21	2.02	0.41
1:H:53:VAL:HG23	3:H:1256[B]:BHO:H4	2.02	0.41
1:A:46:GLU:CD	1:A:174:PRO:HD2	2.41	0.40
4:F:1257:LPP:H151	4:F:1257:LPP:H311	2.02	0.40
1:H:185:HIS:CD2	1:H:185:HIS:C	2.94	0.40
1:G:3:THR:HG23	6:G:2001:HOH:O	2.17	0.40
1:A:209:TYR:HB2	1:A:229:LEU:HD23	2.03	0.40
1:E:108:GLU:HG3	1:E:248:LYS:HB2	2.02	0.40
3:F:1256[B]:BHO:O2	3:F:1256[B]:BHO:C6	2.66	0.40
1:H:44:LYS:CB	1:H:44:LYS:HZ3	2.28	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	255/254 (100%)	248 (97%)	6 (2%)	1 (0%)	34 24
1	B	250/254 (98%)	247 (99%)	3 (1%)	0	100 100
1	C	251/254 (99%)	247 (98%)	4 (2%)	0	100 100
1	D	252/254 (99%)	248 (98%)	4 (2%)	0	100 100
1	E	252/254 (99%)	246 (98%)	5 (2%)	1 (0%)	34 24
1	F	249/254 (98%)	244 (98%)	5 (2%)	0	100 100
1	G	248/254 (98%)	243 (98%)	4 (2%)	1 (0%)	34 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	245/254 (96%)	239 (98%)	6 (2%)	0	100	100
All	All	2002/2032 (98%)	1962 (98%)	37 (2%)	3 (0%)	47	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	152	ASP
1	G	152	ASP
1	A	237	ALA

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	208/209 (100%)	199 (96%)	9 (4%)	29	19
1	B	200/209 (96%)	192 (96%)	8 (4%)	31	22
1	C	203/209 (97%)	194 (96%)	9 (4%)	28	19
1	D	206/209 (99%)	197 (96%)	9 (4%)	28	19
1	E	206/209 (99%)	188 (91%)	18 (9%)	10	4
1	F	203/209 (97%)	190 (94%)	13 (6%)	17	8
1	G	199/209 (95%)	181 (91%)	18 (9%)	9	3
1	H	196/209 (94%)	181 (92%)	15 (8%)	13	5
All	All	1621/1672 (97%)	1522 (94%)	99 (6%)	19	9

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	28	TYR
1	A	121[A]	LEU
1	A	121[B]	LEU
1	A	123	ASP

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Mol	Chain	Res	Type
1	A	137	ASN
1	A	212	ASN
1	A	232	LEU
1	A	236	GLU
1	B	4[A]	ASP
1	B	4[B]	ASP
1	B	62	VAL
1	B	137	ASN
1	B	185	HIS
1	B	212	ASN
1	B	232	LEU
1	B	236	GLU
1	C	6	THR
1	C	28	TYR
1	C	121	LEU
1	C	137	ASN
1	C	162	ILE
1	C	185	HIS
1	C	212	ASN
1	C	232	LEU
1	C	254	VAL
1	D	2	SER
1	D	3	THR
1	D	28	TYR
1	D	62	VAL
1	D	66[A]	SER
1	D	66[B]	SER
1	D	137	ASN
1	D	171	LYS
1	D	232	LEU
1	E	2	SER
1	E	3	THR
1	E	4	ASP
1	E	24	GLU
1	E	28	TYR
1	E	95	ARG
1	E	108	GLU
1	E	113	GLU
1	E	122	LEU
1	E	123	ASP
1	E	185	HIS
1	E	224	VAL

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Mol	Chain	Res	Type
1	E	230	LEU
1	E	231	SER
1	E	232	LEU
1	E	251	LEU
1	E	253	LYS
1	E	254	VAL
1	F	28	TYR
1	F	44	LYS
1	F	85[A]	GLU
1	F	85[B]	GLU
1	F	109	VAL
1	F	112	GLN
1	F	119	ASP
1	F	123	ASP
1	F	140	LEU
1	F	153	GLU
1	F	230	LEU
1	F	232	LEU
1	F	251	LEU
1	G	3	THR
1	G	28	TYR
1	G	44	LYS
1	G	85	GLU
1	G	87	SER
1	G	95	ARG
1	G	109	VAL
1	G	122	LEU
1	G	123	ASP
1	G	178	LEU
1	G	185	HIS
1	G	204	LEU
1	G	208	LEU
1	G	224	VAL
1	G	232	LEU
1	G	235	ILE
1	G	246	SER
1	G	251	LEU
1	H	2	SER
1	H	3	THR
1	H	28	TYR
1	H	44	LYS
1	H	122	LEU

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Mol	Chain	Res	Type
1	H	123	ASP
1	H	178	LEU
1	H	199	GLU
1	H	204	LEU
1	H	208	LEU
1	H	224	VAL
1	H	230	LEU
1	H	231	SER
1	H	232	LEU
1	H	251	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	137	ASN
1	A	212	ASN
1	B	112	GLN
1	B	137	ASN
1	B	185	HIS
1	B	214	GLN
1	C	137	ASN
1	C	185	HIS
1	D	112	GLN
1	D	137	ASN
1	D	185	HIS
1	D	214	GLN
1	E	18	ASN
1	E	57	HIS
1	E	67	ASN
1	E	75	GLN
1	E	154	ASN
1	E	185	HIS
1	F	18	ASN
1	F	57	HIS
1	F	67	ASN
1	F	185	HIS
1	G	8	ASN
1	G	18	ASN
1	G	57	HIS
1	G	67	ASN
1	G	185	HIS

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Mol	Chain	Res	Type
1	H	18	ASN
1	H	57	HIS
1	H	67	ASN
1	H	185	HIS
1	H	212	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 46 ligands modelled in this entry, 24 are monoatomic - leaving 22 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	LPP	E	1257	-	32,32,43	1.10	2 (6%)	31,31,48	0.87	1 (3%)
4	LPP	H	1257	-	34,34,43	1.05	2 (5%)	33,33,48	0.83	1 (3%)
3	BHO	G	1256	2	10,10,10	2.72	2 (20%)	12,12,12	1.65	5 (41%)
3	BHO	D	1256[A]	2	10,10,10	2.81	2 (20%)	12,12,12	1.27	1 (8%)
3	BHO	B	1256[B]	2	10,10,10	2.77	2 (20%)	12,12,12	1.11	3 (25%)
3	BHO	F	1256[A]	2	10,10,10	2.77	2 (20%)	12,12,12	1.37	1 (8%)
3	BHO	H	1256[B]	2	10,10,10	2.70	2 (20%)	12,12,12	1.37	2 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	BHO	E	1256[A]	-	10,10,10	2.59	2 (20%)	12,12,12	1.05	0
3	BHO	C	1256[A]	2	10,10,10	2.79	2 (20%)	12,12,12	1.09	1 (8%)
4	LPP	C	1257	-	33,33,43	1.27	2 (6%)	35,35,48	1.39	4 (11%)
3	BHO	A	1256	2	10,10,10	2.64	3 (30%)	12,12,12	2.36	3 (25%)
4	LPP	F	1257	-	32,32,43	1.05	2 (6%)	31,31,48	0.87	0
3	BHO	D	1256[B]	2	10,10,10	2.66	2 (20%)	12,12,12	1.75	3 (25%)
3	BHO	B	1256[A]	2	10,10,10	2.71	2 (20%)	12,12,12	1.41	2 (16%)
4	LPP	B	1257	-	32,32,43	1.27	2 (6%)	34,34,48	1.34	5 (14%)
3	BHO	F	1256[B]	2	10,10,10	2.49	2 (20%)	12,12,12	1.11	1 (8%)
4	LPP	D	1257	-	34,35,43	1.29	2 (5%)	36,37,48	1.19	3 (8%)
4	LPP	A	1257	-	32,32,43	1.31	2 (6%)	34,34,48	1.41	5 (14%)
3	BHO	H	1256[A]	2	10,10,10	2.65	2 (20%)	12,12,12	1.08	0
3	BHO	E	1256[B]	2	10,10,10	2.88	3 (30%)	12,12,12	1.19	0
4	LPP	G	1257	-	32,32,43	1.08	2 (6%)	31,31,48	0.83	0
3	BHO	C	1256[B]	2	10,10,10	2.55	2 (20%)	12,12,12	1.19	1 (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
4	LPP	E	1257	-	-	15/29/29/45	-
4	LPP	H	1257	-	-	17/31/31/45	-
3	BHO	G	1256	2	-	6/6/6/6	0/1/1/1
3	BHO	D	1256[A]	2	-	6/6/6/6	0/1/1/1
3	BHO	B	1256[B]	2	-	2/6/6/6	0/1/1/1
3	BHO	F	1256[A]	2	-	6/6/6/6	0/1/1/1
3	BHO	H	1256[B]	2	-	2/6/6/6	0/1/1/1
3	BHO	E	1256[A]	-	-	2/6/6/6	0/1/1/1
3	BHO	C	1256[A]	2	-	6/6/6/6	0/1/1/1
4	LPP	C	1257	-	-	18/34/34/45	-
3	BHO	A	1256	2	-	2/6/6/6	0/1/1/1
4	LPP	F	1257	-	-	18/29/29/45	-
3	BHO	D	1256[B]	2	-	2/6/6/6	0/1/1/1
3	BHO	B	1256[A]	2	-	2/6/6/6	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LPP	B	1257	-	-	17/33/33/45	-
3	BHO	F	1256[B]	2	-	2/6/6/6	0/1/1/1
4	LPP	D	1257	-	-	16/36/37/45	-
4	LPP	A	1257	-	-	15/33/33/45	-
3	BHO	H	1256[A]	2	-	6/6/6/6	0/1/1/1
3	BHO	E	1256[B]	2	-	6/6/6/6	0/1/1/1
4	LPP	G	1257	-	-	15/29/29/45	-
3	BHO	C	1256[B]	2	-	2/6/6/6	0/1/1/1

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1256[B]	BHO	O2-N	-6.48	1.23	1.40
3	F	1256[A]	BHO	O2-N	-6.44	1.23	1.40
3	C	1256[A]	BHO	O2-N	-6.30	1.24	1.40
3	D	1256[A]	BHO	C2-C1	6.21	1.49	1.39
3	D	1256[B]	BHO	C2-C1	6.21	1.49	1.39
3	D	1256[A]	BHO	O2-N	-6.18	1.24	1.40
3	A	1256	BHO	O2-N	-6.09	1.24	1.40
3	E	1256[B]	BHO	O2-N	-6.03	1.24	1.40
3	G	1256	BHO	O2-N	-5.99	1.24	1.40
3	H	1256[B]	BHO	C2-C1	5.98	1.49	1.39
3	E	1256[B]	BHO	C2-C1	5.98	1.49	1.39
3	B	1256[A]	BHO	O2-N	-5.91	1.25	1.40
3	C	1256[A]	BHO	C2-C1	5.91	1.49	1.39
3	B	1256[A]	BHO	C2-C1	5.79	1.49	1.39
3	H	1256[B]	BHO	O2-N	-5.79	1.25	1.40
3	H	1256[A]	BHO	O2-N	-5.78	1.25	1.40
3	H	1256[A]	BHO	C2-C1	5.78	1.49	1.39
3	C	1256[B]	BHO	C2-C1	5.73	1.49	1.39
3	E	1256[A]	BHO	C2-C1	5.73	1.49	1.39
3	E	1256[A]	BHO	O2-N	-5.61	1.25	1.40
3	F	1256[B]	BHO	C2-C1	5.59	1.48	1.39
3	F	1256[A]	BHO	C2-C1	5.59	1.48	1.39
3	G	1256	BHO	C2-C1	5.58	1.48	1.39
3	B	1256[B]	BHO	C2-C1	5.57	1.48	1.39
3	D	1256[B]	BHO	O2-N	-5.45	1.26	1.40
4	A	1257	LPP	O9-C11	5.36	1.49	1.34
3	F	1256[B]	BHO	O2-N	-5.36	1.26	1.40
3	C	1256[B]	BHO	O2-N	-5.33	1.26	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1257	LPP	O9-C11	5.26	1.49	1.34
4	D	1257	LPP	O27-C29	5.23	1.48	1.33
3	A	1256	BHO	C2-C1	5.14	1.48	1.39
4	D	1257	LPP	O9-C11	4.84	1.48	1.34
4	B	1257	LPP	O9-C11	4.84	1.48	1.34
4	E	1257	LPP	O9-C11	4.76	1.48	1.33
4	H	1257	LPP	O9-C11	4.59	1.46	1.33
4	G	1257	LPP	O9-C11	4.54	1.47	1.33
4	A	1257	LPP	O27-C29	4.51	1.46	1.33
4	C	1257	LPP	O27-C29	4.44	1.46	1.33
4	B	1257	LPP	O27-C29	4.43	1.46	1.33
4	F	1257	LPP	O9-C11	4.27	1.46	1.33
4	F	1257	LPP	O27-C29	-3.87	1.22	1.42
4	G	1257	LPP	O27-C29	-3.86	1.22	1.42
4	E	1257	LPP	O27-C29	-3.69	1.23	1.42
4	H	1257	LPP	O27-C29	-3.62	1.23	1.42
3	E	1256[B]	BHO	C-N	2.84	1.36	1.32
3	A	1256	BHO	O1-C	-2.03	1.19	1.23

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1256	BHO	C1-C-N	6.35	126.34	116.16
4	A	1257	LPP	O9-C11-C12	5.15	122.61	111.50
4	C	1257	LPP	O9-C11-C12	4.59	121.39	111.50
4	D	1257	LPP	O9-C11-C12	4.34	120.85	111.50
4	B	1257	LPP	O9-C11-C12	4.06	120.26	111.50
3	D	1256[B]	BHO	C1-C-N	3.34	121.51	116.16
3	B	1256[A]	BHO	C1-C-N	3.24	121.36	116.16
3	A	1256	BHO	O1-C-N	-3.23	116.91	122.94
4	B	1257	LPP	C7-O9-C11	-3.01	114.01	117.88
3	D	1256[B]	BHO	O1-C-C1	-2.98	115.61	120.94
4	C	1257	LPP	O27-C29-C30	2.92	121.08	111.91
4	A	1257	LPP	O27-C29-C30	2.92	121.08	111.91
3	H	1256[B]	BHO	C1-C-N	2.85	120.73	116.16
4	D	1257	LPP	O27-C29-C30	2.78	120.63	111.91
4	B	1257	LPP	O27-C29-C30	2.76	120.57	111.91
4	H	1257	LPP	O9-C11-C12	2.73	120.46	111.91
3	C	1256[B]	BHO	C1-C-N	2.68	120.47	116.16
3	D	1256[A]	BHO	C3-C2-C1	-2.50	117.38	120.34
3	D	1256[B]	BHO	C3-C2-C1	-2.50	117.38	120.34
3	G	1256	BHO	O2-N-C	2.50	125.80	119.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	1256[B]	BHO	O1-C-C1	-2.46	116.54	120.94
3	A	1256	BHO	O1-C-C1	-2.37	116.70	120.94
3	G	1256	BHO	C6-C1-C2	2.37	121.96	118.59
3	C	1256[A]	BHO	C3-C2-C1	-2.35	117.56	120.34
3	G	1256	BHO	C3-C2-C1	-2.32	117.60	120.34
4	A	1257	LPP	O9-C11-O10	-2.31	118.12	123.70
4	E	1257	LPP	O9-C11-C12	2.30	121.33	112.23
3	G	1256	BHO	C5-C4-C3	2.25	124.12	119.93
3	B	1256[A]	BHO	O1-C-C1	-2.24	116.94	120.94
3	B	1256[B]	BHO	C1-C-N	2.20	119.69	116.16
4	C	1257	LPP	O9-C7-C8	2.09	110.98	106.13
4	B	1257	LPP	O9-C7-C8	2.08	110.94	106.13
4	C	1257	LPP	O27-C29-O28	-2.07	118.37	123.59
4	B	1257	LPP	O27-C29-O28	-2.07	118.37	123.59
3	B	1256[B]	BHO	O1-C-N	-2.07	119.08	122.94
3	B	1256[B]	BHO	C3-C2-C1	-2.06	117.91	120.34
3	F	1256[B]	BHO	C1-C-N	2.04	119.44	116.16
4	A	1257	LPP	O9-C7-C8	2.03	110.83	106.13
4	A	1257	LPP	O27-C29-O28	-2.03	118.48	123.59
4	D	1257	LPP	O9-C11-O10	-2.01	118.84	123.70
3	G	1256	BHO	C1-C-N	2.01	119.38	116.16
3	F	1256[A]	BHO	C3-C2-C1	-2.00	117.97	120.34

There are no chirality outliers.

All (183) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1256	BHO	C1-C-N-O2
3	A	1256	BHO	O1-C-N-O2
3	B	1256[A]	BHO	C1-C-N-O2
3	B	1256[A]	BHO	O1-C-N-O2
3	B	1256[B]	BHO	C1-C-N-O2
3	B	1256[B]	BHO	O1-C-N-O2
3	C	1256[A]	BHO	N-C-C1-C2
3	C	1256[A]	BHO	N-C-C1-C6
3	C	1256[A]	BHO	C1-C-N-O2
3	C	1256[A]	BHO	O1-C-N-O2
3	C	1256[B]	BHO	C1-C-N-O2
3	C	1256[B]	BHO	O1-C-N-O2
3	D	1256[A]	BHO	N-C-C1-C2
3	D	1256[A]	BHO	N-C-C1-C6
3	D	1256[A]	BHO	C1-C-N-O2

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Mol	Chain	Res	Type	Atoms
3	D	1256[A]	BHO	O1-C-N-O2
3	D	1256[B]	BHO	C1-C-N-O2
3	D	1256[B]	BHO	O1-C-N-O2
3	E	1256[A]	BHO	C1-C-N-O2
3	E	1256[A]	BHO	O1-C-N-O2
3	E	1256[B]	BHO	N-C-C1-C2
3	E	1256[B]	BHO	N-C-C1-C6
3	E	1256[B]	BHO	C1-C-N-O2
3	E	1256[B]	BHO	O1-C-N-O2
3	F	1256[A]	BHO	N-C-C1-C2
3	F	1256[A]	BHO	N-C-C1-C6
3	F	1256[A]	BHO	C1-C-N-O2
3	F	1256[A]	BHO	O1-C-N-O2
3	F	1256[B]	BHO	C1-C-N-O2
3	F	1256[B]	BHO	O1-C-N-O2
3	G	1256	BHO	N-C-C1-C2
3	G	1256	BHO	N-C-C1-C6
3	G	1256	BHO	C1-C-N-O2
3	G	1256	BHO	O1-C-N-O2
3	H	1256[A]	BHO	N-C-C1-C2
3	H	1256[A]	BHO	N-C-C1-C6
3	H	1256[A]	BHO	C1-C-N-O2
3	H	1256[A]	BHO	O1-C-N-O2
3	H	1256[B]	BHO	C1-C-N-O2
3	H	1256[B]	BHO	O1-C-N-O2
4	A	1257	LPP	C6-C7-C8-O27
4	A	1257	LPP	O9-C7-C8-O27
4	A	1257	LPP	O10-C11-O9-C7
4	A	1257	LPP	C12-C11-O9-C7
4	B	1257	LPP	C6-C7-C8-O27
4	B	1257	LPP	O9-C7-C8-O27
4	C	1257	LPP	O10-C11-O9-C7
4	D	1257	LPP	C12-C11-O9-C7
4	E	1257	LPP	C12-C11-O9-C7
4	F	1257	LPP	C12-C11-O9-C7
4	G	1257	LPP	C12-C11-O9-C7
4	E	1257	LPP	O10-C11-O9-C7
3	C	1256[A]	BHO	O1-C-C1-C2
3	C	1256[A]	BHO	O1-C-C1-C6
3	H	1256[A]	BHO	O1-C-C1-C2
3	H	1256[A]	BHO	O1-C-C1-C6
4	G	1257	LPP	O10-C11-O9-C7

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Mol	Chain	Res	Type	Atoms
3	F	1256[A]	BHO	O1-C-C1-C6
3	D	1256[A]	BHO	O1-C-C1-C2
3	E	1256[B]	BHO	O1-C-C1-C2
3	F	1256[A]	BHO	O1-C-C1-C2
3	D	1256[A]	BHO	O1-C-C1-C6
4	C	1257	LPP	C12-C11-O9-C7
3	E	1256[B]	BHO	O1-C-C1-C6
4	F	1257	LPP	O10-C11-O9-C7
4	D	1257	LPP	O10-C11-O9-C7
3	G	1256	BHO	O1-C-C1-C2
4	B	1257	LPP	C30-C29-O27-C8
4	H	1257	LPP	C12-C11-O9-C7
4	B	1257	LPP	O28-C29-O27-C8
4	H	1257	LPP	O10-C11-O9-C7
3	G	1256	BHO	O1-C-C1-C6
4	A	1257	LPP	C29-C30-C31-C32
4	E	1257	LPP	C11-C12-C13-C14
4	F	1257	LPP	C11-C12-C13-C14
4	D	1257	LPP	C29-C30-C31-C32
4	B	1257	LPP	C12-C11-O9-C7
4	H	1257	LPP	C22-C23-C24-C25
4	B	1257	LPP	C31-C32-C33-C34
4	C	1257	LPP	C31-C32-C33-C34
4	H	1257	LPP	C16-C17-C18-C19
4	B	1257	LPP	O10-C11-O9-C7
4	D	1257	LPP	C36-C37-C38-C39
4	E	1257	LPP	C12-C13-C14-C15
4	F	1257	LPP	C16-C17-C18-C19
4	G	1257	LPP	C12-C13-C14-C15
4	F	1257	LPP	C19-C20-C21-C22
4	F	1257	LPP	C15-C16-C17-C18
4	G	1257	LPP	C31-C32-C33-C34
4	E	1257	LPP	C20-C21-C22-C23
4	H	1257	LPP	C19-C20-C21-C22
4	G	1257	LPP	C13-C14-C15-C16
4	C	1257	LPP	C16-C17-C18-C19
4	D	1257	LPP	C13-C14-C15-C16
4	H	1257	LPP	C15-C16-C17-C18
4	B	1257	LPP	C17-C18-C19-C20
4	G	1257	LPP	C14-C15-C16-C17
4	D	1257	LPP	C35-C36-C37-C38
4	F	1257	LPP	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
4	B	1257	LPP	C39-C40-C41-C42
4	H	1257	LPP	C17-C18-C19-C20
4	D	1257	LPP	C11-C12-C13-C14
4	D	1257	LPP	C18-C19-C20-C21
4	D	1257	LPP	C38-C39-C40-C41
4	G	1257	LPP	C11-C12-C13-C14
4	F	1257	LPP	C31-C32-C33-C34
4	F	1257	LPP	C14-C15-C16-C17
4	G	1257	LPP	C29-C30-C31-C32
4	G	1257	LPP	C19-C20-C21-C22
4	F	1257	LPP	C40-C41-C42-C43
4	E	1257	LPP	C29-C30-C31-C32
4	D	1257	LPP	C17-C18-C19-C20
4	F	1257	LPP	C12-C13-C14-C15
4	C	1257	LPP	C17-C18-C19-C20
4	C	1257	LPP	C36-C37-C38-C39
4	A	1257	LPP	C16-C17-C18-C19
4	A	1257	LPP	C39-C40-C41-C42
4	G	1257	LPP	C20-C21-C22-C23
4	F	1257	LPP	C29-C30-C31-C32
4	F	1257	LPP	C17-C18-C19-C20
4	E	1257	LPP	C17-C18-C19-C20
4	E	1257	LPP	C34-C35-C36-C37
4	F	1257	LPP	C41-C42-C43-C44
4	E	1257	LPP	C19-C20-C21-C22
4	H	1257	LPP	O27-C29-C30-C31
4	E	1257	LPP	C31-C32-C33-C34
4	G	1257	LPP	C36-C37-C38-C39
4	H	1257	LPP	C18-C19-C20-C21
4	C	1257	LPP	C13-C14-C15-C16
4	H	1257	LPP	C39-C40-C41-C42
4	A	1257	LPP	C15-C16-C17-C18
4	C	1257	LPP	C35-C36-C37-C38
4	B	1257	LPP	C35-C36-C37-C38
4	F	1257	LPP	C21-C22-C23-C24
4	D	1257	LPP	C6-C7-C8-O27
4	D	1257	LPP	C31-C32-C33-C34
4	E	1257	LPP	C38-C39-C40-C41
4	D	1257	LPP	O9-C7-C8-O27
4	A	1257	LPP	C36-C37-C38-C39
4	B	1257	LPP	O9-C11-C12-C13
4	H	1257	LPP	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
4	C	1257	LPP	C18-C19-C20-C21
4	D	1257	LPP	C12-C13-C14-C15
4	C	1257	LPP	C15-C16-C17-C18
4	A	1257	LPP	C35-C36-C37-C38
4	C	1257	LPP	C19-C20-C21-C22
4	G	1257	LPP	C17-C18-C19-C20
4	G	1257	LPP	C30-C31-C32-C33
4	G	1257	LPP	C41-C42-C43-C44
4	B	1257	LPP	C29-C30-C31-C32
4	D	1257	LPP	C34-C35-C36-C37
4	B	1257	LPP	C13-C14-C15-C16
4	H	1257	LPP	C34-C35-C36-C37
4	A	1257	LPP	C31-C32-C33-C34
4	C	1257	LPP	C14-C15-C16-C17
4	F	1257	LPP	C36-C37-C38-C39
4	H	1257	LPP	C12-C13-C14-C15
4	C	1257	LPP	C11-C12-C13-C14
4	B	1257	LPP	C16-C17-C18-C19
4	A	1257	LPP	C12-C13-C14-C15
4	C	1257	LPP	C30-C29-O27-C8
4	B	1257	LPP	C34-C35-C36-C37
4	H	1257	LPP	C29-C30-C31-C32
4	B	1257	LPP	C38-C39-C40-C41
4	D	1257	LPP	C39-C40-C41-C42
4	E	1257	LPP	C37-C38-C39-C40
4	H	1257	LPP	C14-C15-C16-C17
4	C	1257	LPP	O28-C29-O27-C8
4	E	1257	LPP	C18-C19-C20-C21
4	E	1257	LPP	C21-C22-C23-C24
4	C	1257	LPP	C34-C35-C36-C37
4	E	1257	LPP	O27-C29-C30-C31
4	F	1257	LPP	C33-C34-C35-C36
4	A	1257	LPP	C38-C39-C40-C41
4	H	1257	LPP	C20-C21-C22-C23
4	G	1257	LPP	C21-C22-C23-C24
4	A	1257	LPP	O9-C11-C12-C13
4	C	1257	LPP	O9-C11-C12-C13
4	F	1257	LPP	C18-C19-C20-C21
4	B	1257	LPP	O10-C11-C12-C13
4	A	1257	LPP	O10-C11-C12-C13
4	H	1257	LPP	C35-C36-C37-C38
4	C	1257	LPP	O10-C11-C12-C13

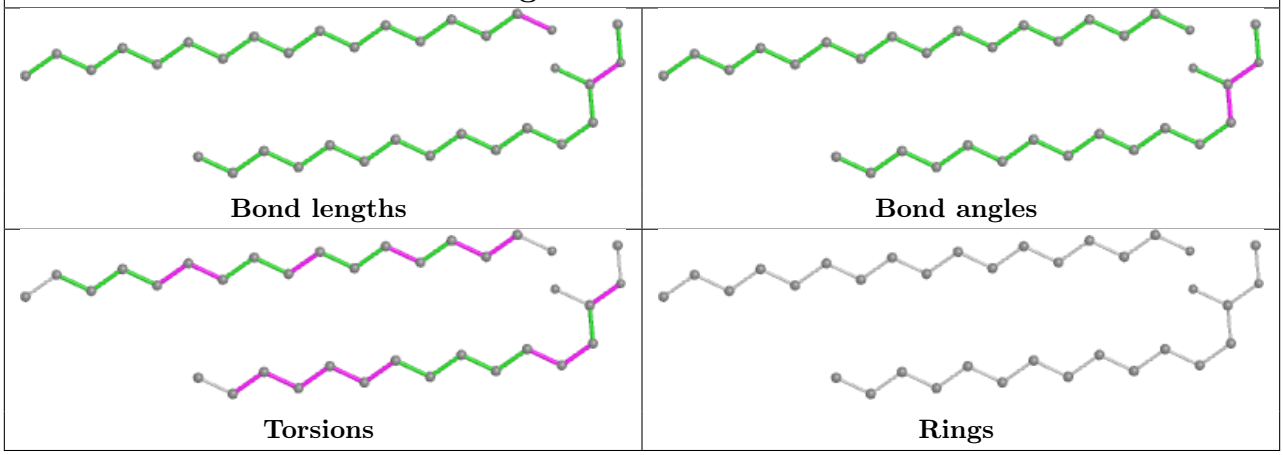
There are no ring outliers.

16 monomers are involved in 51 short contacts:

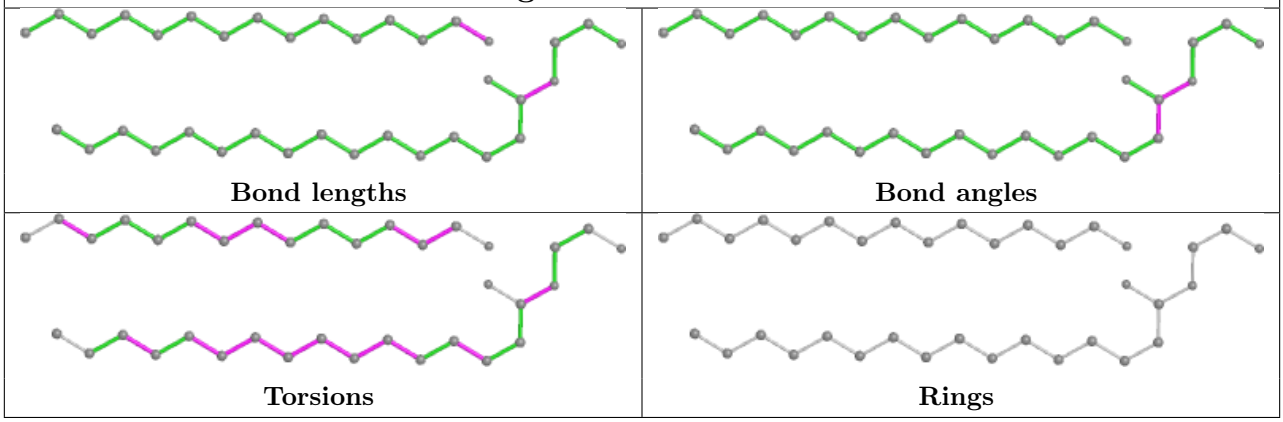
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1257	LPP	1	0
3	G	1256	BHO	3	0
3	B	1256[B]	BHO	6	0
3	H	1256[B]	BHO	11	0
3	E	1256[A]	BHO	6	0
3	C	1256[A]	BHO	1	0
3	A	1256	BHO	3	0
4	F	1257	LPP	2	0
3	D	1256[B]	BHO	2	0
3	B	1256[A]	BHO	3	0
4	B	1257	LPP	1	0
3	F	1256[B]	BHO	4	0
3	H	1256[A]	BHO	3	0
3	E	1256[B]	BHO	2	0
4	G	1257	LPP	1	0
3	C	1256[B]	BHO	2	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.

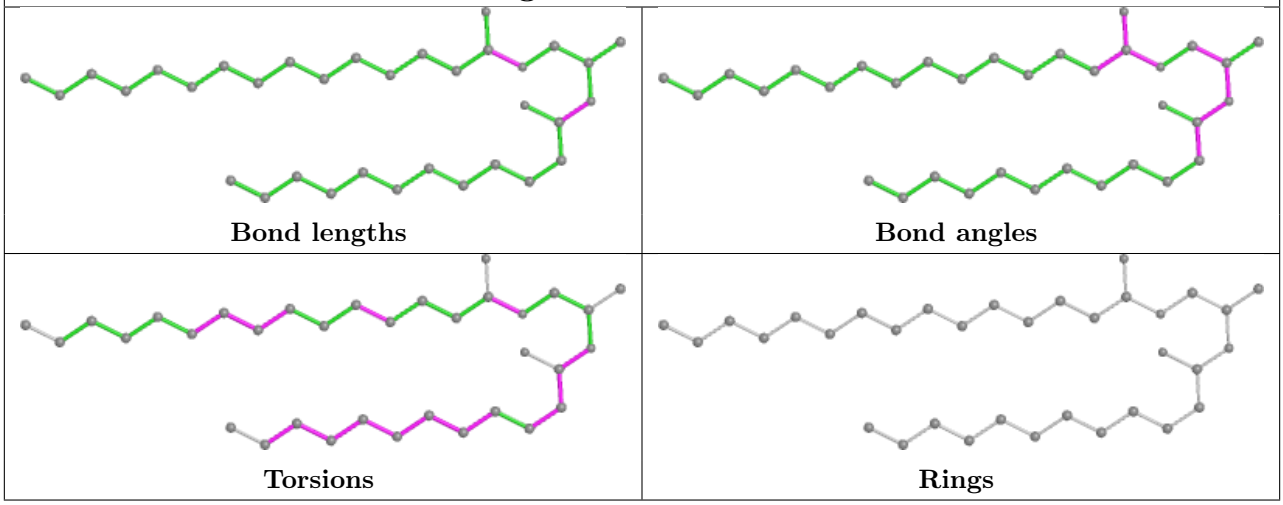
Ligand LPP E 1257



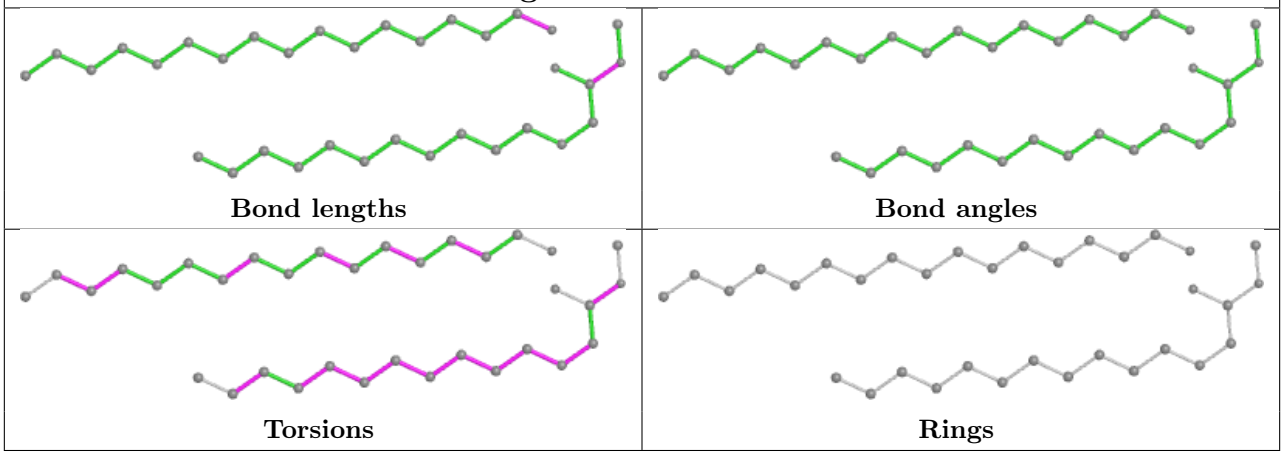
Ligand LPP H 1257



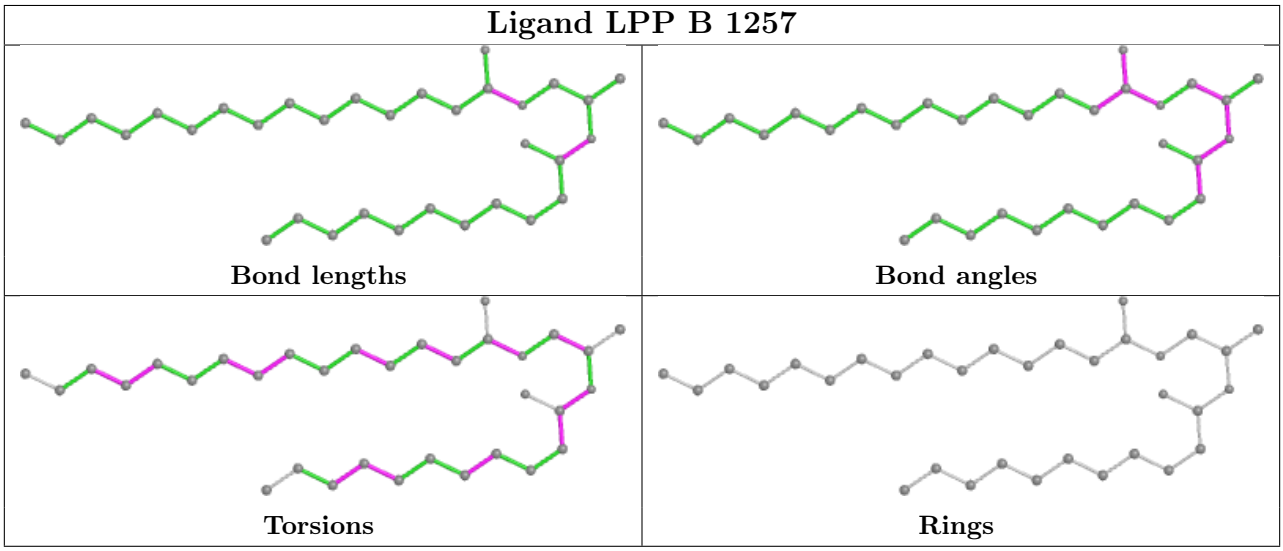
Ligand LPP C 1257



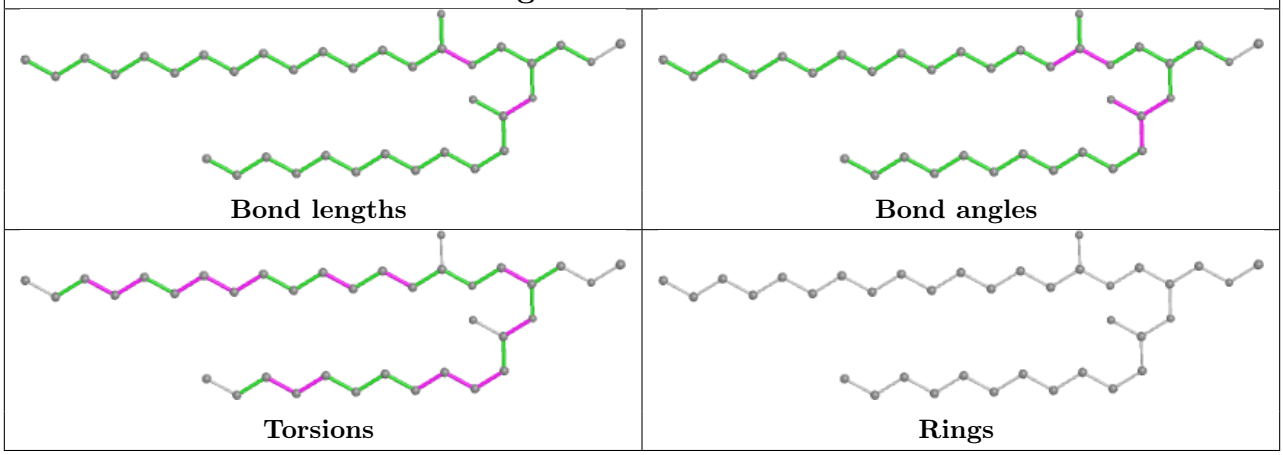
Ligand LPP F 1257



Ligand LPP B 1257



Ligand LPP D 1257



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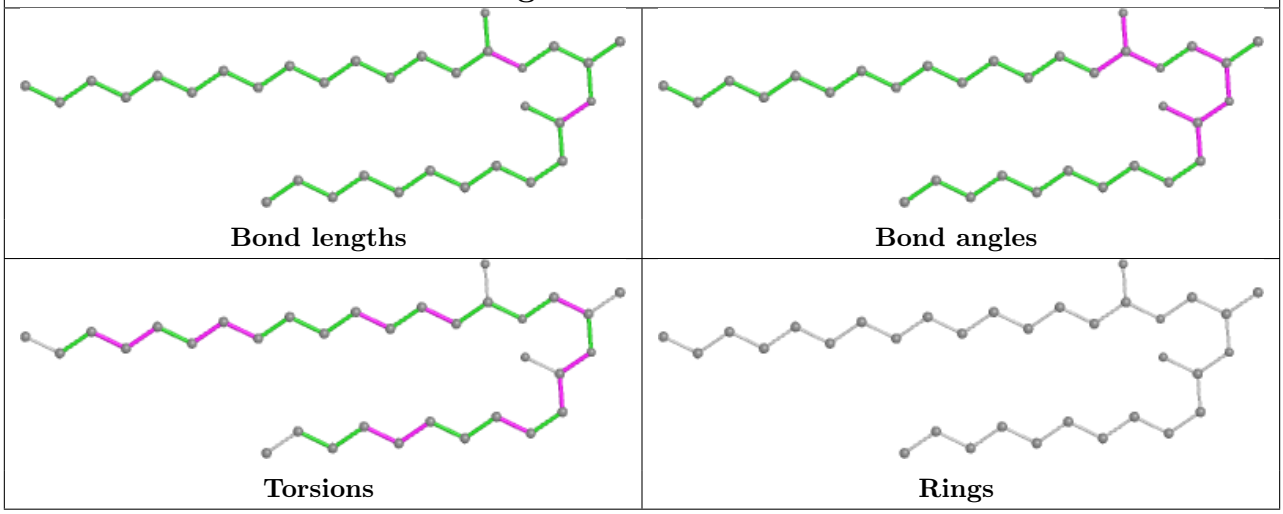
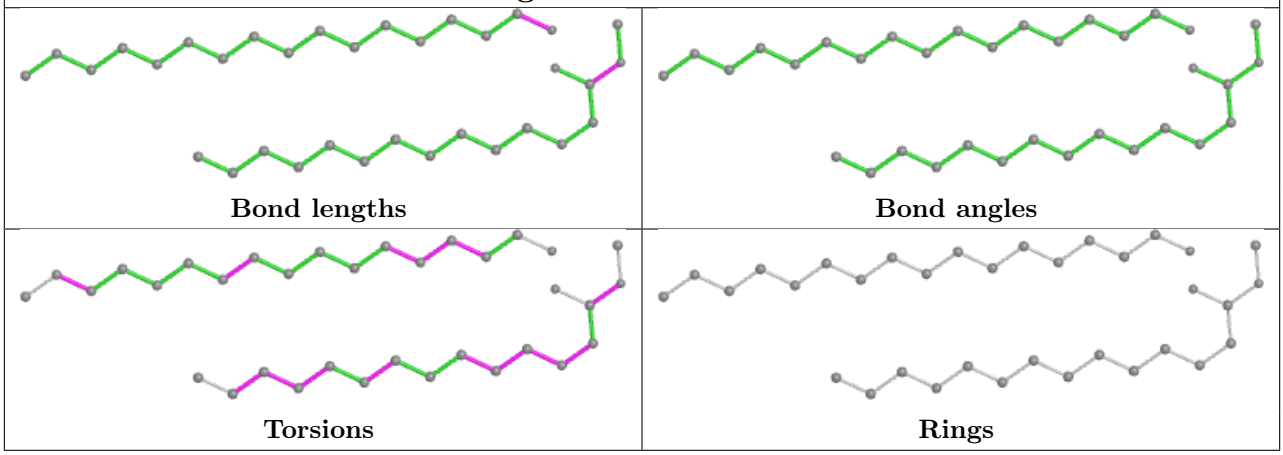


Ligand LPP G 1257



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	253/254 (99%)	-0.19	8 (3%)	47	50	16, 22, 38, 57	0
1	B	252/254 (99%)	-0.15	9 (3%)	42	45	17, 23, 36, 55	0
1	C	251/254 (98%)	-0.24	6 (2%)	59	62	17, 25, 38, 53	0
1	D	251/254 (98%)	-0.16	10 (3%)	38	41	17, 25, 40, 52	0
1	E	252/254 (99%)	-0.14	8 (3%)	47	50	18, 25, 42, 53	0
1	F	248/254 (97%)	-0.23	5 (2%)	65	68	16, 24, 43, 53	0
1	G	251/254 (98%)	-0.02	8 (3%)	47	50	19, 30, 47, 66	0
1	H	248/254 (97%)	-0.09	5 (2%)	65	68	18, 28, 43, 53	0
All	All	2006/2032 (98%)	-0.15	59 (2%)	51	54	16, 25, 42, 66	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	237	ALA	5.6
1	B	237	ALA	5.6
1	B	254	VAL	5.6
1	G	1	MET	5.3
1	E	237	ALA	5.1
1	F	254	VAL	5.1
1	C	240	GLY	4.8
1	A	237	ALA	4.7
1	F	3	THR	4.5
1	E	254	VAL	4.3
1	A	239	SER	4.3
1	B	240	GLY	4.0
1	C	241	PRO	4.0
1	B	238	GLN	4.0
1	G	254	VAL	3.8
1	E	241	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	241	PRO	3.7
1	C	2	SER	3.4
1	D	2	SER	3.4
1	D	237	ALA	3.3
1	G	242	HIS	3.3
1	A	212	ASN	3.1
1	B	241	PRO	3.0
1	D	96	ASP	3.0
1	H	2	SER	3.0
1	C	237	ALA	2.9
1	C	138	PRO	2.7
1	D	3	THR	2.7
1	D	254	VAL	2.7
1	H	242	HIS	2.6
1	B	212	ASN	2.6
1	F	241	PRO	2.6
1	E	240	GLY	2.6
1	F	242	HIS	2.6
1	A	238	GLN	2.5
1	G	236	GLU	2.5
1	A	240	GLY	2.5
1	G	235	ILE	2.5
1	A	254	VAL	2.5
1	D	97	ASP	2.5
1	F	235	ILE	2.4
1	D	212	ASN	2.4
1	E	236	GLU	2.3
1	A	236	GLU	2.3
1	G	200	GLY	2.3
1	C	254	VAL	2.3
1	H	254	VAL	2.3
1	E	235	ILE	2.2
1	H	241	PRO	2.2
1	B	74	ILE	2.2
1	E	2	SER	2.2
1	H	233	ASP	2.2
1	D	194	TRP	2.1
1	E	253	LYS	2.1
1	B	192	LEU	2.1
1	A	125	TRP	2.1
1	D	208	LEU	2.0
1	D	241	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	194	TRP	2.0

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, 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
4	LPP	D	1257	36/44	0.52	0.32	37,46,69,76	0
4	LPP	C	1257	34/44	0.60	0.29	40,45,64,65	0
4	LPP	E	1257	34/44	0.62	0.29	32,44,63,64	0
4	LPP	B	1257	33/44	0.65	0.26	35,43,64,64	0
4	LPP	H	1257	36/44	0.65	0.28	37,45,63,64	0
4	LPP	A	1257	33/44	0.68	0.23	38,42,58,58	0
5	MG	B	1258	1/1	0.69	0.11	54,54,54,54	0
5	MG	C	1260	1/1	0.71	0.13	51,51,51,51	0
4	LPP	F	1257	34/44	0.72	0.24	33,41,58,60	0
4	LPP	G	1257	34/44	0.73	0.22	35,44,58,61	0
5	MG	B	1260	1/1	0.81	0.10	52,52,52,52	0
5	MG	E	1258	1/1	0.82	0.13	53,53,53,53	0
5	MG	D	1258	1/1	0.83	0.14	47,47,47,47	0
5	MG	C	1261	1/1	0.84	0.10	53,53,53,53	0
3	BHO	G	1256	10/10	0.91	0.15	24,31,41,42	0
5	MG	A	1258	1/1	0.94	0.18	48,48,48,48	0
3	BHO	D	1256[B]	10/10	0.94	0.13	25,27,32,39	4
3	BHO	D	1256[A]	10/10	0.94	0.13	25,26,27,27	4
5	MG	C	1259	1/1	0.94	0.08	55,55,55,55	0
5	MG	G	1258	1/1	0.94	0.06	46,46,46,46	0
5	MG	H	1258	1/1	0.94	0.08	39,39,39,39	0
5	MG	F	1258	1/1	0.95	0.10	44,44,44,44	0

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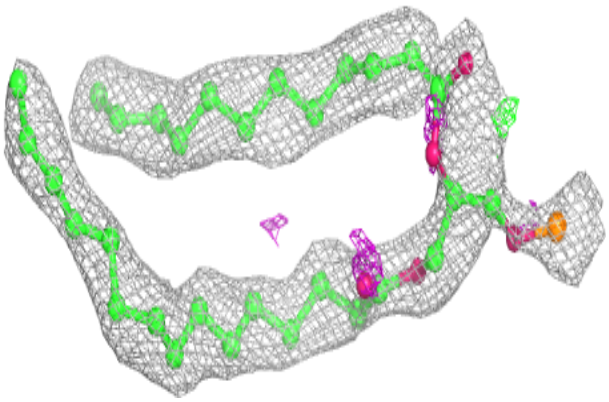
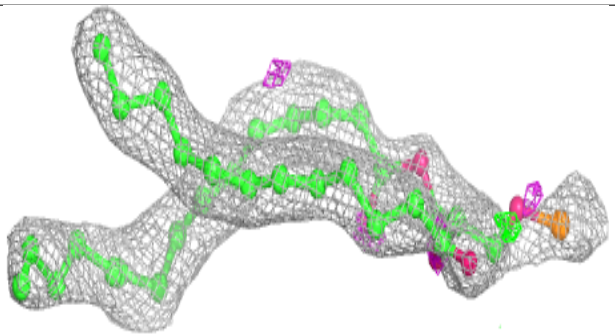
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BHO	F	1256[B]	10/10	0.95	0.14	24,27,29,29	10
3	BHO	F	1256[A]	10/10	0.95	0.14	20,26,27,29	10
5	MG	H	1259	1/1	0.95	0.14	40,40,40,40	0
5	MG	D	1259	1/1	0.96	0.13	43,43,43,43	0
3	BHO	A	1256	10/10	0.96	0.12	23,27,37,37	0
3	BHO	E	1256[A]	10/10	0.96	0.12	21,22,25,27	10
3	BHO	E	1256[B]	10/10	0.96	0.12	16,21,23,23	10
3	BHO	H	1256[A]	10/10	0.96	0.12	22,28,29,30	10
3	BHO	H	1256[B]	10/10	0.96	0.12	28,29,30,31	10
3	BHO	C	1256[B]	10/10	0.97	0.13	20,22,24,25	10
5	MG	C	1258	1/1	0.97	0.07	44,44,44,44	0
5	MG	A	1259	1/1	0.97	0.04	37,37,37,37	0
3	BHO	C	1256[A]	10/10	0.97	0.13	17,26,27,28	10
3	BHO	B	1256[A]	10/10	0.98	0.14	18,20,24,25	10
3	BHO	B	1256[B]	10/10	0.98	0.14	26,28,30,30	10
2	FE	H	1255	1/1	0.99	0.07	22,22,22,22	0
2	FE	B	1255	1/1	0.99	0.10	21,21,21,21	0
5	MG	B	1259	1/1	0.99	0.04	28,28,28,28	0
2	FE	E	1255	1/1	1.00	0.04	20,20,20,20	0
2	FE	F	1255	1/1	1.00	0.06	19,19,19,19	0
2	FE	G	1255	1/1	1.00	0.07	23,23,23,23	0
2	FE	A	1255	1/1	1.00	0.07	19,19,19,19	0
2	FE	C	1255	1/1	1.00	0.06	21,21,21,21	0
2	FE	D	1255	1/1	1.00	0.06	23,23,23,23	0

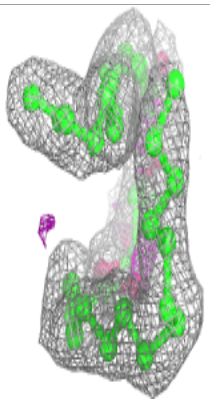
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LPP D 1257:

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

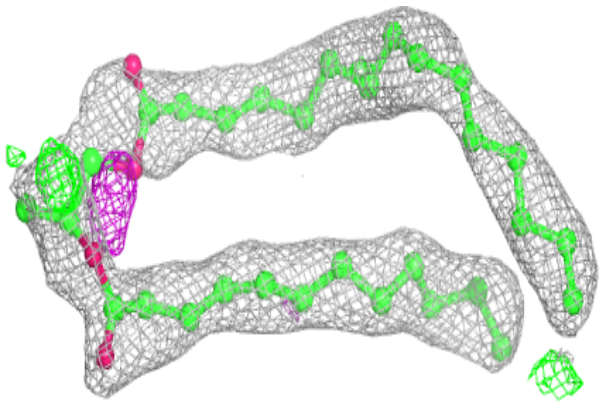


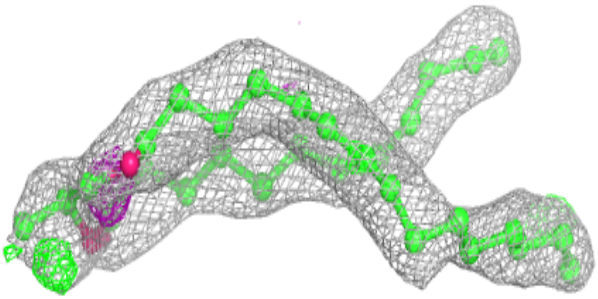


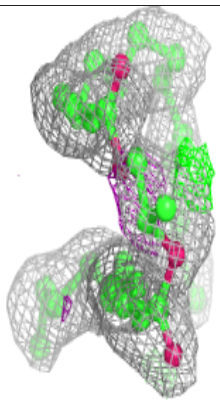


Electron density around LPP C 1257:

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

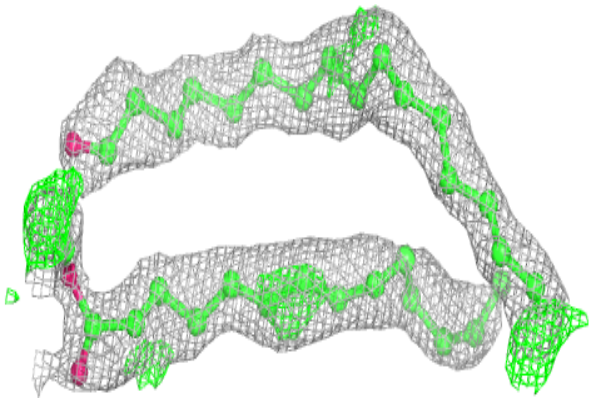


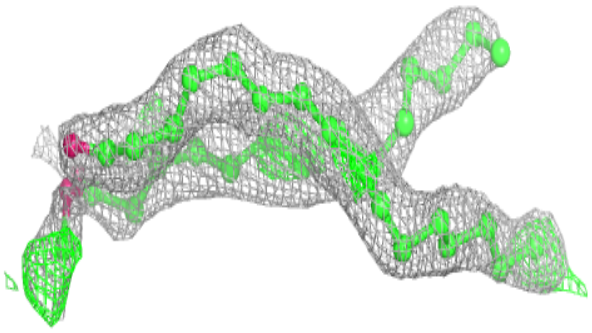


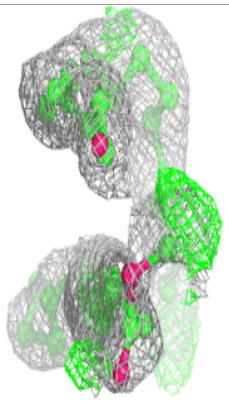


Electron density around LPP E 1257:

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

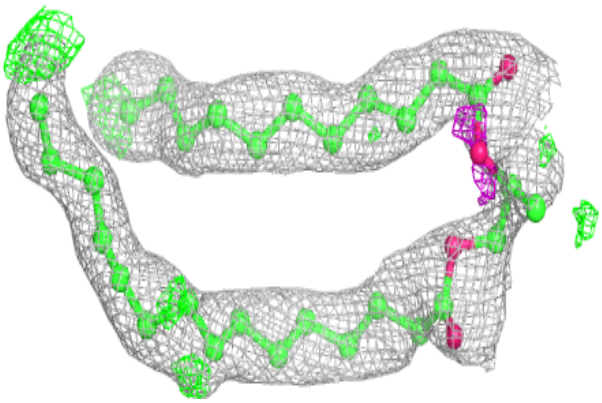


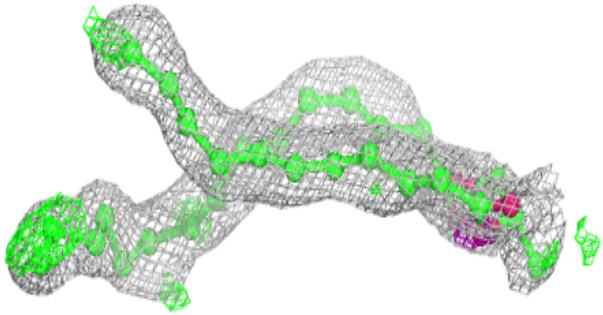


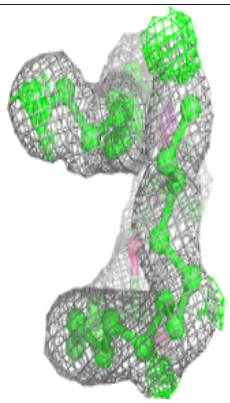


Electron density around LPP B 1257:

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

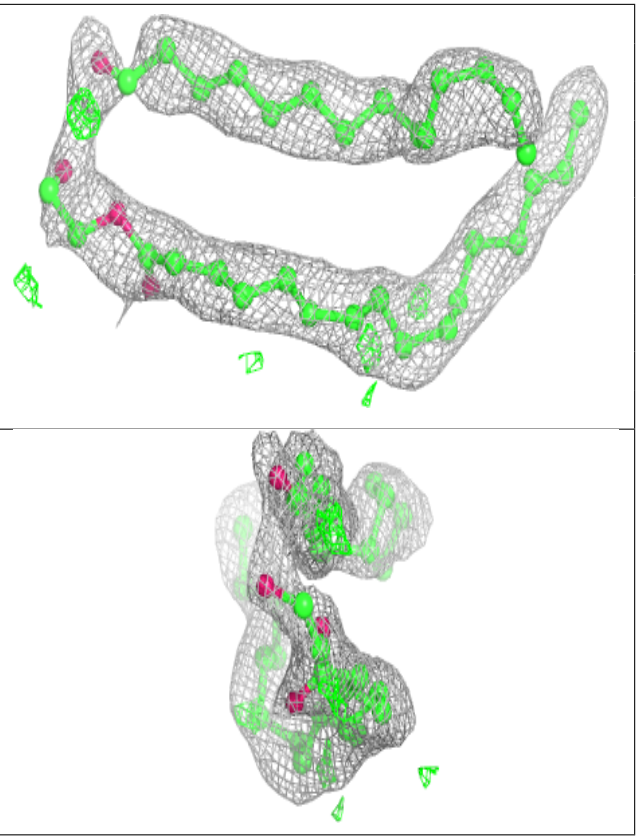






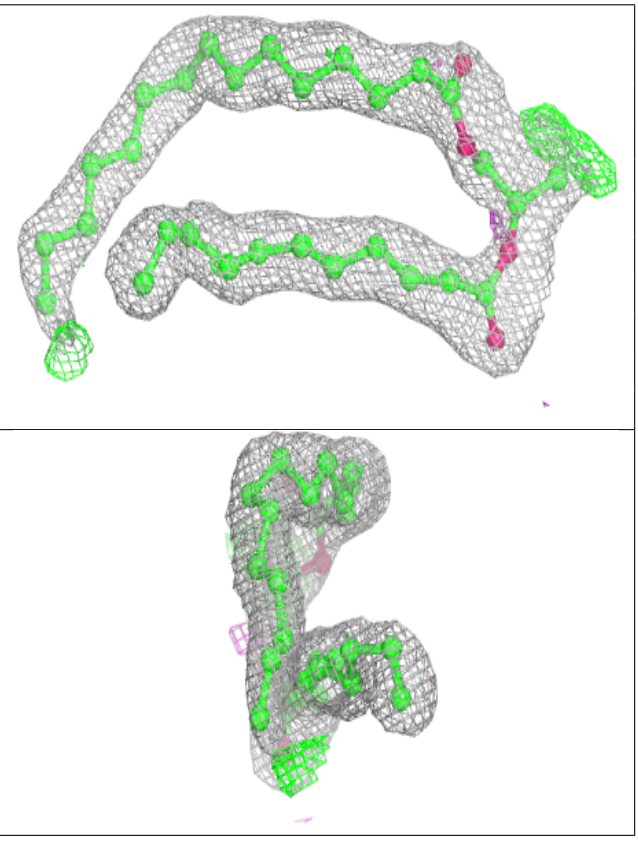
Electron density around LPP H 1257:

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



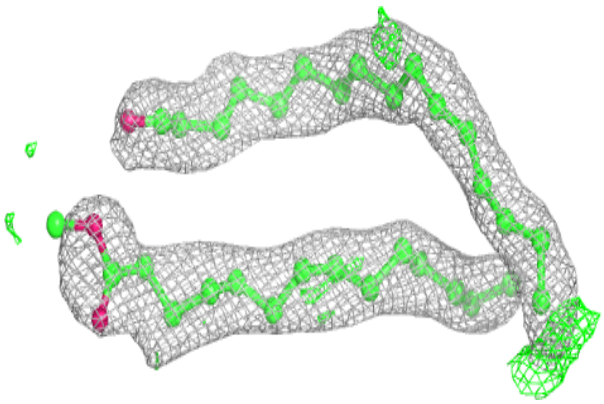
Electron density around LPP A 1257:

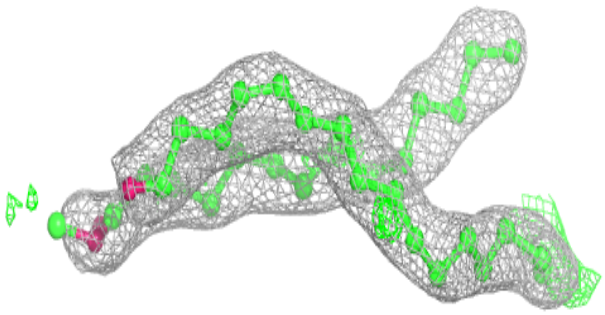
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

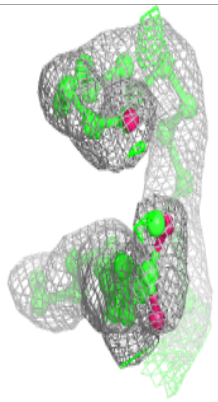


Electron density around LPP F 1257:

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

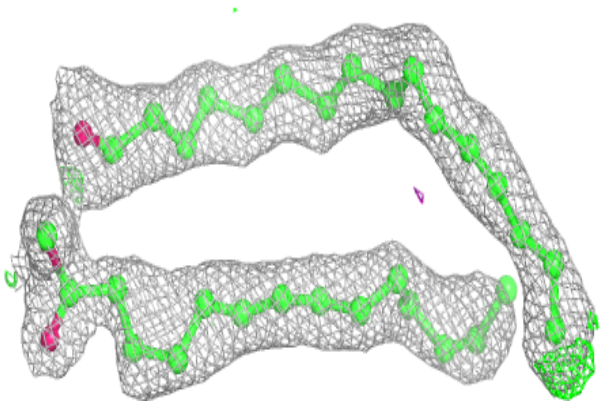


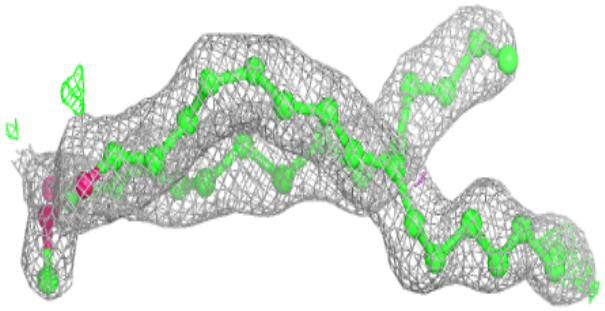


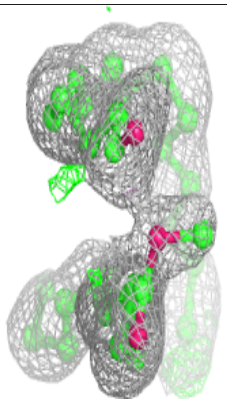


Electron density around LPP G 1257:

$2mF_o$-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.