Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2024 – 01:02 AM EST

PDB ID	:	3O6J
Title	:	Crystal Structure of 4-Chlorocatechol Dioxygenase from Rhodococcus opacus 1CP in complex with hydroxyquinol
Authors	:	Ferraroni, M.; Briganti, F.; Kolomitseva, M.; Golovleva, L.
Deposited on	:	2010-07-29
Resolution	:	2.90 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:

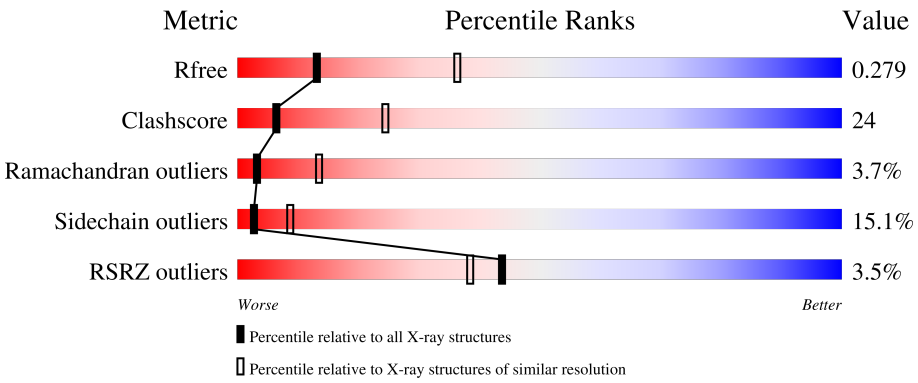
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.90 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))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	257	3% 58% 35% 6%
1	B	257	4% 43% 44% 12% •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4127 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.

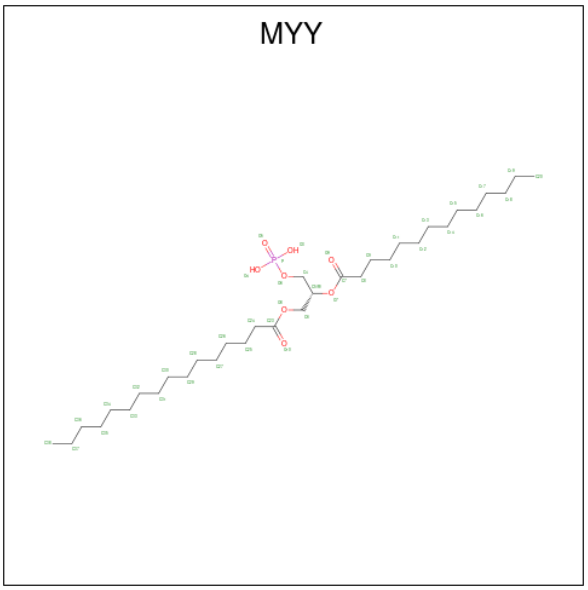
- Molecule 1 is a protein called Chlorocatechol 1,2-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	256	2027	1299	336	386	6	0	0	0
1	B	256	1988	1267	329	386	6	0	0	0

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

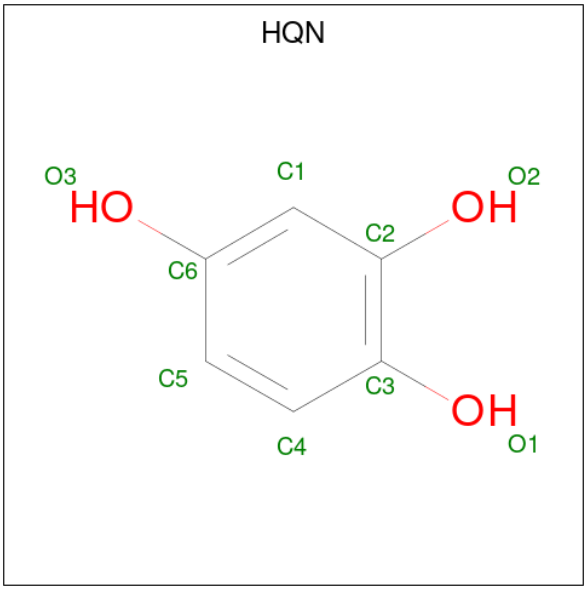
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
2	A	1	1	1	0	0
2	B	1	1	1	0	0

- Molecule 3 is (2R)-3-(PHOSPHONOOXY)-2-(TETRADECANOYLOXY)PROPYL PALMITATE (three-letter code: MYY) (formula: $C_{33}H_{65}O_8P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 36 32 4	0	0
3	B	1	Total C O P 38 32 5 1	0	0

- Molecule 4 is benzene-1,2,4-triol (three-letter code: HQN) (formula: $C_6H_6O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 9 6 3	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

- Molecule 6 is water.

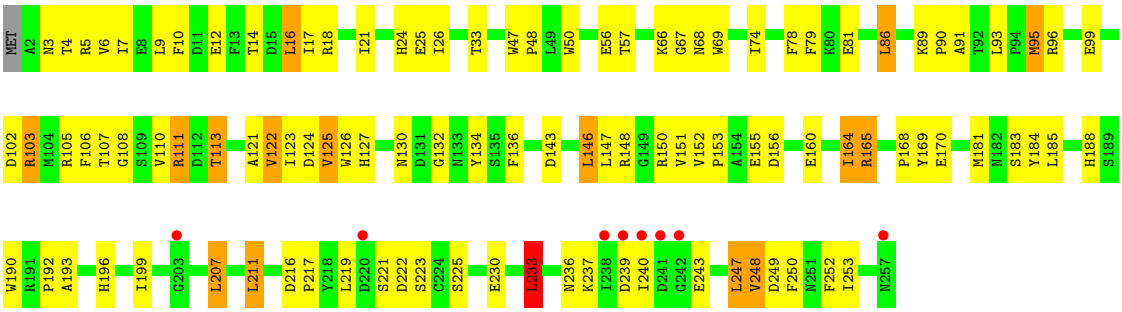
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	22	Total O 22 22	0	0
6	B	4	Total O 4 4	0	0

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.

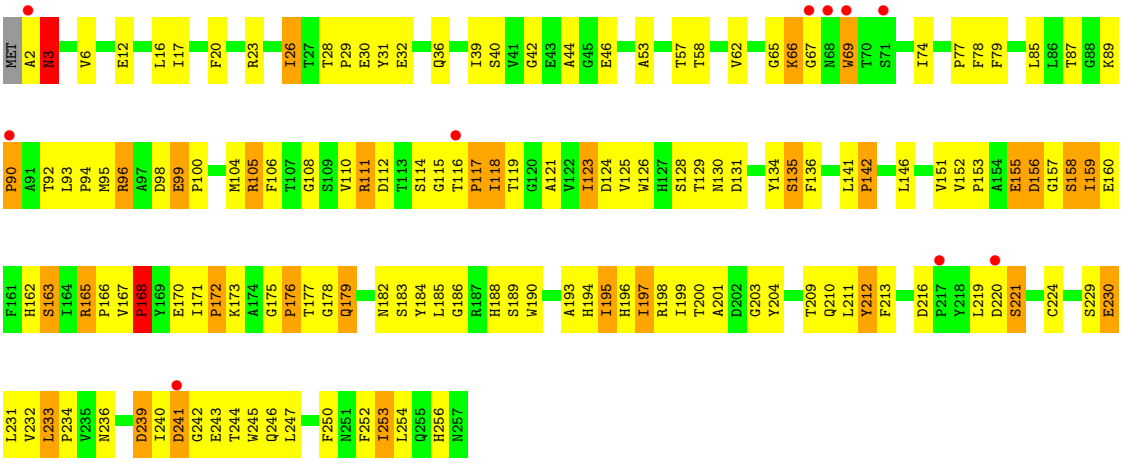
• Molecule 1: Chlorocatechol 1,2-dioxygenase

Chain A:



• Molecule 1: Chlorocatechol 1,2-dioxygenase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α, β, γ	90.18Å 90.18Å 305.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.90 34.78 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.90) 99.1 (34.78-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.21 (at 2.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.215 , 0.293 0.212 , 0.279	Depositor DCC
R_{free} test set	855 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	67.1	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4127	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% 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: MYY, CL, FE, HQN

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	0.96	1/2088 (0.0%)	0.99	7/2851 (0.2%)
1	B	0.78	0/2045	0.86	0/2796
All	All	0.88	1/4133 (0.0%)	0.93	7/5647 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	VAL	CA-CB	5.65	1.66	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	207	LEU	CA-CB-CG	5.40	127.71	115.30
1	A	105	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	16	LEU	CB-CG-CD2	-5.32	101.96	111.00
1	A	233	LEU	CA-CB-CG	5.18	127.20	115.30
1	A	95	MET	N-CA-CB	-5.14	101.34	110.60
1	A	211	LEU	CB-CG-CD1	5.09	119.66	111.00
1	A	165	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	89	LYS	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	2027	0	1929	86	0
1	B	1988	0	1855	115	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	36	0	56	1	0
3	B	38	0	58	4	0
4	A	9	0	4	2	0
5	A	1	0	0	0	0
6	A	22	0	0	8	0
6	B	4	0	0	1	0
All	All	4127	0	3902	192	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 24.

All (192) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:VAL:HG12	1:B:118:ILE:HD12	1.37	1.03
1:B:99:GLU:OE2	1:B:100:PRO:HD3	1.58	1.01
1:A:16:LEU:HD23	1:B:16:LEU:HD11	1.45	0.98
1:A:188:HIS:HD2	1:A:190:TRP:H	1.05	0.97
1:B:239:ASP:O	1:B:241:ASP:N	2.05	0.89
1:A:188:HIS:CD2	1:A:190:TRP:H	1.90	0.88
1:B:216:ASP:HB3	1:B:219:LEU:HG	1.57	0.86
1:B:162:HIS:HD1	1:B:245:TRP:HH2	1.20	0.85
1:B:135:SER:O	1:B:136:PHE:HB2	1.78	0.83
1:B:168:PRO:HD3	1:B:193:ALA:HB2	1.60	0.83
1:A:21:ILE:HA	1:A:26:ILE:HG13	1.59	0.82
1:B:99:GLU:OE2	1:B:100:PRO:CD	2.27	0.82
1:B:165:ARG:HG3	1:B:165:ARG:HH11	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:PHE:O	1:B:216:ASP:HB2	1.80	0.81
1:B:66:LYS:O	1:B:69:TRP:HZ3	1.65	0.79
1:B:36:GLN:HA	1:B:36:GLN:OE1	1.84	0.77
1:A:16:LEU:CD2	1:B:16:LEU:HD11	2.15	0.76
1:A:196:HIS:HE1	4:A:258:HQN:O2	1.61	0.76
1:B:110:VAL:CG1	1:B:118:ILE:HD12	2.12	0.76
1:A:123:ILE:HG13	1:A:199:ILE:HG12	1.69	0.74
1:B:165:ARG:HH11	1:B:165:ARG:CG	2.02	0.73
1:B:188:HIS:HD2	1:B:190:TRP:H	1.33	0.73
1:B:123:ILE:HG12	1:B:123:ILE:O	1.88	0.71
1:B:200:THR:HG22	1:B:201:ALA:N	2.07	0.69
1:A:95:MET:HG3	1:A:99:GLU:HG2	1.75	0.69
1:B:96:ARG:HG3	1:B:99:GLU:HG2	1.74	0.68
1:A:18:ARG:HD2	6:A:277:HOH:O	1.94	0.68
1:B:104:MET:HE1	1:B:166:PRO:HD3	1.76	0.68
1:A:193:ALA:HA	6:A:274:HOH:O	1.93	0.67
1:B:220:ASP:O	1:B:221:SER:HB3	1.95	0.67
1:A:184:TYR:CE2	3:B:303:MYY:O10	2.47	0.67
1:B:123:ILE:HB	1:B:199:ILE:HG13	1.77	0.66
1:B:89:LYS:CB	1:B:90:PRO:HD3	2.26	0.65
1:A:236:ASN:O	1:A:247:LEU:HB2	1.97	0.64
1:B:129:THR:C	1:B:131:ASP:H	2.00	0.63
1:A:108:GLY:HA3	1:A:250:PHE:O	1.99	0.62
1:B:42:GLY:O	1:B:44:ALA:O	2.16	0.62
1:B:152:VAL:HG13	1:B:153:PRO:HD2	1.82	0.61
1:B:166:PRO:HG2	1:B:195:ILE:HG22	1.82	0.60
1:A:66:LYS:NZ	1:A:230:GLU:OE2	2.27	0.60
1:B:66:LYS:O	1:B:69:TRP:CZ3	2.52	0.60
1:B:123:ILE:O	1:B:123:ILE:CG1	2.50	0.60
1:A:50:TRP:CH2	3:B:303:MYY:H332	2.38	0.59
1:A:96:ARG:HD3	1:A:99:GLU:OE1	2.02	0.59
1:A:25:GLU:HA	1:B:62:VAL:HG11	1.84	0.59
1:B:2:ALA:N	3:B:303:MYY:O7	2.36	0.58
1:A:107:THR:O	1:A:249:ASP:HA	2.02	0.58
1:B:175:GLY:O	1:B:178:GLY:N	2.36	0.58
1:B:95:MET:HB2	1:B:99:GLU:HG3	1.85	0.58
1:B:212:TYR:O	1:B:233:LEU:HB2	2.04	0.58
1:B:179:GLN:HA	1:B:179:GLN:NE2	2.19	0.58
1:A:24:HIS:HE1	1:B:12:GLU:OE1	1.87	0.57
1:B:46:GLU:OE2	1:B:177:THR:OG1	2.13	0.57
1:B:179:GLN:HA	1:B:179:GLN:HE21	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:VAL:HG21	1:A:150:ARG:HD3	1.87	0.56
1:A:233:LEU:HD11	1:A:250:PHE:HD2	1.70	0.56
1:A:56:GLU:CD	1:A:74:ILE:HB	2.26	0.56
1:A:192:PRO:HB3	1:A:216:ASP:OD2	2.04	0.56
1:B:129:THR:C	1:B:131:ASP:N	2.58	0.56
1:A:18:ARG:NE	6:A:277:HOH:O	2.39	0.56
1:A:111:ARG:NE	6:A:269:HOH:O	2.38	0.56
1:B:124:ASP:OD1	1:B:198:ARG:NH2	2.31	0.56
1:B:197:ILE:CG2	1:B:199:ILE:CD1	2.83	0.56
1:B:220:ASP:O	1:B:221:SER:CB	2.53	0.55
1:B:189:SER:OG	1:B:189:SER:O	2.25	0.55
1:B:197:ILE:CG2	1:B:199:ILE:HD11	2.36	0.55
1:B:153:PRO:HA	1:B:159:ILE:HG22	1.88	0.55
1:A:216:ASP:O	1:A:219:LEU:HB2	2.07	0.55
1:A:67:GLY:HA3	1:A:69:TRP:CZ2	2.42	0.54
1:A:10:PHE:CD1	1:B:185:LEU:HD11	2.43	0.54
1:A:156:ASP:C	1:A:156:ASP:OD2	2.45	0.54
1:B:195:ILE:HG13	1:B:197:ILE:CD1	2.38	0.53
1:B:93:LEU:HD12	1:B:163:SER:OG	2.07	0.53
1:A:18:ARG:CZ	6:A:277:HOH:O	2.56	0.53
1:A:18:ARG:CD	6:A:277:HOH:O	2.54	0.53
1:A:148:ARG:HD3	6:A:270:HOH:O	2.08	0.53
1:B:193:ALA:HB3	1:B:213:PHE:HD2	1.72	0.53
1:B:106:PHE:HZ	1:B:252:PHE:HE2	1.57	0.53
1:A:86:LEU:CD2	1:A:93:LEU:HD23	2.39	0.52
1:B:195:ILE:O	1:B:210:GLN:HA	2.09	0.52
1:B:104:MET:HG3	1:B:105:ARG:N	2.25	0.52
1:B:200:THR:CG2	1:B:201:ALA:N	2.72	0.52
1:A:86:LEU:HA	6:A:267:HOH:O	2.10	0.51
1:A:56:GLU:CG	1:A:74:ILE:HB	2.40	0.51
1:A:111:ARG:HH21	1:A:253:ILE:HD11	1.74	0.51
1:A:222:ASP:HB3	1:A:225:SER:HA	1.91	0.51
1:B:77:PRO:O	1:B:78:PHE:CD1	2.64	0.51
1:B:2:ALA:O	1:B:3:ASN:C	2.49	0.50
1:A:192:PRO:CB	1:A:216:ASP:OD2	2.59	0.50
1:B:119:THR:HG22	1:B:155:GLU:HA	1.93	0.50
1:B:197:ILE:HG23	1:B:199:ILE:HD11	1.93	0.50
1:A:68:ASN:ND2	1:A:113:THR:HG22	2.27	0.50
1:A:127:HIS:HE1	1:A:164:ILE:HD13	1.76	0.50
1:A:111:ARG:HH21	1:A:253:ILE:CD1	2.24	0.50
1:B:108:GLY:HA3	1:B:250:PHE:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:GLU:OE1	1:B:23:ARG:NH2	2.45	0.49
1:A:233:LEU:HD11	1:A:250:PHE:CD2	2.47	0.49
1:B:195:ILE:HG13	1:B:197:ILE:HD11	1.95	0.49
1:B:165:ARG:HD2	1:B:246:GLN:NE2	2.27	0.49
1:B:156:ASP:OD1	1:B:158:SER:N	2.41	0.48
1:A:106:PHE:C	1:A:106:PHE:CD1	2.86	0.48
1:A:181:MET:HA	1:A:185:LEU:HD12	1.94	0.48
1:B:2:ALA:N	3:B:303:MYY:O6	2.46	0.48
1:A:155:GLU:HG2	1:A:155:GLU:O	2.14	0.48
1:B:167:VAL:HB	1:B:168:PRO:HD2	1.95	0.48
1:A:47:TRP:HA	1:A:47:TRP:CE3	2.48	0.48
1:B:128:SER:HB3	1:B:134:TYR:CE2	2.49	0.48
1:B:111:ARG:O	1:B:253:ILE:HA	2.14	0.48
1:A:216:ASP:HB3	1:A:219:LEU:HD13	1.96	0.47
1:A:24:HIS:CE1	6:B:259:HOH:O	2.67	0.47
1:A:78:PHE:CD1	1:A:134:TYR:CD1	3.02	0.47
1:B:121:ALA:HB3	1:B:153:PRO:HG3	1.97	0.47
1:A:111:ARG:NH2	1:A:253:ILE:HD11	2.30	0.47
1:B:182:ASN:O	1:B:186:GLY:HA2	2.14	0.47
1:B:58:THR:O	1:B:62:VAL:HG23	2.14	0.46
1:A:9:LEU:HD13	1:B:26:ILE:HD11	1.97	0.46
1:B:126:TRP:CZ2	1:B:196:HIS:HB3	2.51	0.46
1:B:170:GLU:OE1	1:B:190:TRP:CZ2	2.69	0.46
1:B:195:ILE:CG1	1:B:197:ILE:HD11	2.45	0.46
1:B:229:SER:C	1:B:231:LEU:H	2.18	0.46
1:A:24:HIS:CE1	1:B:12:GLU:OE1	2.69	0.46
1:A:123:ILE:HD12	1:A:123:ILE:N	2.31	0.46
1:A:3:ASN:CG	1:A:6:VAL:HG23	2.37	0.46
1:B:39:ILE:O	1:B:40:SER:C	2.53	0.45
1:B:123:ILE:HG23	1:B:151:VAL:O	2.16	0.45
1:A:21:ILE:HG21	1:B:58:THR:HG22	1.97	0.45
1:A:169:TYR:CE2	4:A:258:HQN:H4	2.52	0.45
1:A:86:LEU:HD21	1:A:93:LEU:HD23	1.98	0.45
1:B:141:LEU:O	1:B:142:PRO:O	2.34	0.45
1:B:105:ARG:HB3	1:B:247:LEU:HD22	1.97	0.45
1:B:229:SER:O	1:B:232:VAL:HG12	2.17	0.45
1:B:53:ALA:O	1:B:224:CYS:HA	2.16	0.45
1:B:129:THR:O	1:B:131:ASP:N	2.50	0.45
1:A:151:VAL:HG12	1:A:152:VAL:N	2.31	0.45
1:B:152:VAL:CG1	1:B:153:PRO:HD2	2.45	0.45
1:A:103:ARG:HH21	1:A:243:GLU:CG	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:MET:HG2	1:A:99:GLU:CB	2.46	0.45
1:A:132:GLY:O	1:A:169:TYR:CE1	2.70	0.45
1:A:168:PRO:O	1:A:190:TRP:HZ3	2.00	0.44
1:B:28:THR:N	1:B:29:PRO:CD	2.80	0.44
1:B:111:ARG:C	1:B:118:ILE:HD11	2.38	0.44
1:A:188:HIS:HE1	1:A:221:SER:OG	2.00	0.44
1:A:233:LEU:HD23	1:A:248:VAL:HG22	1.99	0.44
1:A:233:LEU:CD1	1:A:250:PHE:HD2	2.30	0.44
1:A:110:VAL:HG12	1:A:252:PHE:HB2	1.99	0.44
3:A:304:MYY:H241	1:B:184:TYR:CG	2.53	0.44
1:B:171:ILE:O	1:B:189:SER:OG	2.23	0.44
1:B:194:HIS:HB3	1:B:212:TYR:CD2	2.53	0.44
1:B:229:SER:C	1:B:231:LEU:N	2.71	0.44
1:A:122:VAL:CG2	1:A:150:ARG:HD3	2.47	0.44
1:A:111:ARG:HE	1:A:111:ARG:HB2	1.60	0.43
1:B:254:LEU:HD23	1:B:254:LEU:HA	1.81	0.43
1:A:136:PHE:CD1	1:A:143:ASP:HB3	2.53	0.43
1:B:170:GLU:HG3	1:B:190:TRP:CE2	2.54	0.43
1:B:233:LEU:HA	1:B:234:PRO:HD3	1.91	0.43
1:A:3:ASN:O	1:A:7:ILE:N	2.51	0.43
1:A:56:GLU:HG2	1:A:74:ILE:HB	2.00	0.43
1:B:94:PRO:O	1:B:146:LEU:HA	2.19	0.43
1:A:3:ASN:HB3	1:A:6:VAL:CG2	2.49	0.43
1:B:92:THR:HG22	1:B:93:LEU:O	2.18	0.43
1:B:67:GLY:HA3	1:B:69:TRP:CZ3	2.54	0.43
1:B:165:ARG:CG	1:B:165:ARG:NH1	2.68	0.42
1:B:172:PRO:O	1:B:173:LYS:C	2.57	0.42
1:B:197:ILE:HG23	1:B:199:ILE:CD1	2.49	0.42
1:B:126:TRP:NE1	1:B:196:HIS:CD2	2.88	0.42
1:A:216:ASP:HA	1:A:217:PRO:HD2	1.61	0.42
1:A:96:ARG:CD	1:A:99:GLU:OE1	2.68	0.41
1:B:194:HIS:CD2	1:B:196:HIS:CE1	3.08	0.41
1:A:3:ASN:HB3	1:A:6:VAL:HB	2.01	0.41
1:A:16:LEU:O	1:A:17:ILE:C	2.56	0.41
1:B:17:ILE:O	1:B:20:PHE:N	2.53	0.41
1:B:126:TRP:CE2	1:B:196:HIS:HB2	2.54	0.41
1:A:121:ALA:O	1:A:153:PRO:HD3	2.20	0.41
1:A:10:PHE:O	1:A:14:THR:HG23	2.20	0.41
1:B:112:ASP:OD1	1:B:112:ASP:C	2.59	0.41
1:B:175:GLY:O	1:B:176:PRO:C	2.59	0.41
1:A:47:TRP:N	1:A:48:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LEU:O	1:A:147:LEU:C	2.56	0.41
1:B:98:ASP:O	1:B:99:GLU:C	2.58	0.41
1:B:115:GLY:O	1:B:117:PRO:HD3	2.21	0.41
1:A:79:PHE:HE2	1:A:81:GLU:HG2	1.85	0.41
1:A:106:PHE:O	1:A:160:GLU:HA	2.21	0.41
1:A:188:HIS:HD2	1:A:190:TRP:N	1.90	0.41
1:B:30:GLU:O	1:B:31:TYR:C	2.59	0.41
1:B:171:ILE:O	1:B:172:PRO:C	2.59	0.41
1:B:106:PHE:O	1:B:160:GLU:HA	2.21	0.41
1:B:209:THR:OG1	1:B:231:LEU:HD21	2.21	0.40
1:A:86:LEU:HB3	1:A:91:ALA:HB1	2.04	0.40
1:B:89:LYS:CB	1:B:90:PRO:CD	2.98	0.40
1:B:117:PRO:HB3	1:B:157:GLY:HA2	2.03	0.40
1:A:126:TRP:CD2	1:A:196:HIS:HB2	2.55	0.40
1:B:203:GLY:O	1:B:204:TYR:CD1	2.75	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	254/257 (99%)	227 (89%)	26 (10%)	1 (0%)	34 66
1	B	254/257 (99%)	192 (76%)	44 (17%)	18 (7%)	1 3
All	All	508/514 (99%)	419 (82%)	70 (14%)	19 (4%)	3 13

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3	ASN
1	B	66	LYS
1	B	221	SER

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Mol	Chain	Res	Type
1	B	230	GLU
1	B	240	ILE
1	B	241	ASP
1	B	256	HIS
1	B	65	GLY
1	B	142	PRO
1	B	243	GLU
1	B	69	TRP
1	B	130	ASN
1	B	135	SER
1	B	172	PRO
1	A	90	PRO
1	B	79	PHE
1	B	90	PRO
1	B	168	PRO
1	B	242	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	219/223 (98%)	192 (88%)	27 (12%)	4 14
1	B	212/223 (95%)	174 (82%)	38 (18%)	2 5
All	All	431/446 (97%)	366 (85%)	65 (15%)	3 9

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	5	ARG
1	A	33	THR
1	A	57	THR
1	A	86	LEU
1	A	102	ASP
1	A	103	ARG

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Mol	Chain	Res	Type
1	A	111	ARG
1	A	113	THR
1	A	122	VAL
1	A	124	ASP
1	A	125	VAL
1	A	130	ASN
1	A	146	LEU
1	A	164	ILE
1	A	165	ARG
1	A	170	GLU
1	A	183	SER
1	A	207	LEU
1	A	211	LEU
1	A	223	SER
1	A	233	LEU
1	A	237	LYS
1	A	239	ASP
1	A	240	ILE
1	A	247	LEU
1	A	248	VAL
1	B	3	ASN
1	B	6	VAL
1	B	26	ILE
1	B	32	GLU
1	B	57	THR
1	B	74	ILE
1	B	85	LEU
1	B	87	THR
1	B	96	ARG
1	B	99	GLU
1	B	105	ARG
1	B	111	ARG
1	B	114	SER
1	B	116	THR
1	B	117	PRO
1	B	118	ILE
1	B	123	ILE
1	B	125	VAL
1	B	155	GLU
1	B	156	ASP
1	B	158	SER
1	B	159	ILE

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Mol	Chain	Res	Type
1	B	163	SER
1	B	165	ARG
1	B	168	PRO
1	B	176	PRO
1	B	179	GLN
1	B	183	SER
1	B	195	ILE
1	B	197	ILE
1	B	211	LEU
1	B	212	TYR
1	B	230	GLU
1	B	233	LEU
1	B	236	ASN
1	B	239	ASP
1	B	244	THR
1	B	253	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	133	ASN
1	A	179	GLN
1	A	188	HIS
1	A	246	GLN
1	A	251	ASN
1	B	24	HIS
1	B	127	HIS
1	B	133	ASN
1	B	179	GLN
1	B	188	HIS
1	B	236	ASN
1	B	251	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 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	HQN	A	258	2	9,9,9	1.41	1 (11%)	12,12,12	0.95	0
3	MYY	B	303	-	36,37,41	1.42	2 (5%)	38,39,46	1.34	3 (7%)
3	MYY	A	304	-	35,35,41	1.43	4 (11%)	37,37,46	1.39	5 (13%)

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	HQN	A	258	2	-	-	0/1/1/1
3	MYY	B	303	-	-	26/38/39/43	-
3	MYY	A	304	-	-	21/36/36/43	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	304	MYY	O8-C23	5.40	1.49	1.33
3	B	303	MYY	O8-C23	5.39	1.49	1.33
3	A	304	MYY	O7-C7	5.01	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	303	MYY	O7-C7	4.97	1.48	1.34
4	A	258	HQN	C3-C2	3.78	1.46	1.40
3	A	304	MYY	C6-C5	2.53	1.56	1.50
3	A	304	MYY	C17-C16	2.26	1.64	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	303	MYY	O7-C7-C8	4.80	121.84	111.50
3	A	304	MYY	O7-C7-C8	3.99	120.10	111.50
3	B	303	MYY	O8-C23-C24	3.47	122.79	111.91
3	A	304	MYY	O7-C5-C6	3.08	113.27	106.13
3	A	304	MYY	O8-C6-C5	2.70	116.17	108.38
3	A	304	MYY	O7-C5-C4	2.61	113.90	107.93
3	B	303	MYY	O7-C7-O9	-2.52	117.62	123.70
3	A	304	MYY	O8-C23-C24	2.43	119.53	111.91

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	304	MYY	C4-C5-C6-O8
3	A	304	MYY	O7-C5-C6-O8
3	A	304	MYY	C4-C5-O7-C7
3	B	303	MYY	O9-C7-O7-C5
3	B	303	MYY	C8-C7-O7-C5
3	B	303	MYY	O10-C23-O8-C6
3	B	303	MYY	C24-C23-O8-C6
3	A	304	MYY	C8-C7-O7-C5
3	A	304	MYY	C23-C24-C25-C26
3	A	304	MYY	O9-C7-O7-C5
3	A	304	MYY	C15-C16-C17-C18
3	B	303	MYY	C15-C16-C17-C18
3	A	304	MYY	C12-C13-C14-C15
3	B	303	MYY	C25-C26-C27-C28
3	B	303	MYY	C24-C25-C26-C27
3	B	303	MYY	C26-C27-C28-C29
3	A	304	MYY	C14-C15-C16-C17
3	A	304	MYY	C10-C11-C12-C13
3	B	303	MYY	C30-C31-C32-C33
3	B	303	MYY	C29-C30-C31-C32
3	A	304	MYY	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
3	B	303	MYY	C7-C8-C9-C10
3	B	303	MYY	O6-C4-C5-O7
3	A	304	MYY	C33-C34-C35-C36
3	B	303	MYY	C34-C35-C36-C37
3	B	303	MYY	C4-C5-C6-O8
3	A	304	MYY	C30-C31-C32-C33
3	B	303	MYY	C35-C36-C37-C38
3	A	304	MYY	C24-C25-C26-C27
3	B	303	MYY	O6-C4-C5-C6
3	A	304	MYY	C28-C29-C30-C31
3	A	304	MYY	C7-C8-C9-C10
3	B	303	MYY	C9-C10-C11-C12
3	B	303	MYY	C23-C24-C25-C26
3	B	303	MYY	O7-C5-C6-O8
3	B	303	MYY	C16-C17-C18-C19
3	A	304	MYY	C31-C32-C33-C34
3	A	304	MYY	C25-C26-C27-C28
3	B	303	MYY	C10-C11-C12-C13
3	A	304	MYY	C5-C6-O8-C23
3	B	303	MYY	C12-C13-C14-C15
3	B	303	MYY	C28-C29-C30-C31
3	B	303	MYY	C14-C15-C16-C17
3	A	304	MYY	C29-C30-C31-C32
3	B	303	MYY	O7-C7-C8-C9
3	B	303	MYY	O9-C7-C8-C9
3	A	304	MYY	C32-C33-C34-C35

There are no ring outliers.

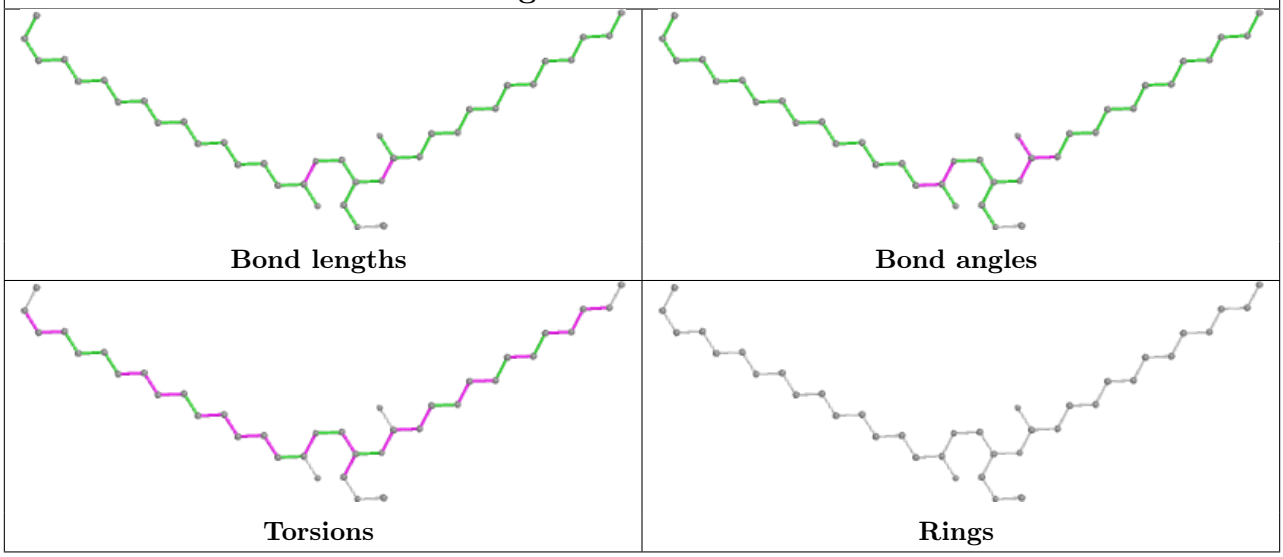
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	258	HQN	2	0
3	B	303	MYY	4	0
3	A	304	MYY	1	0

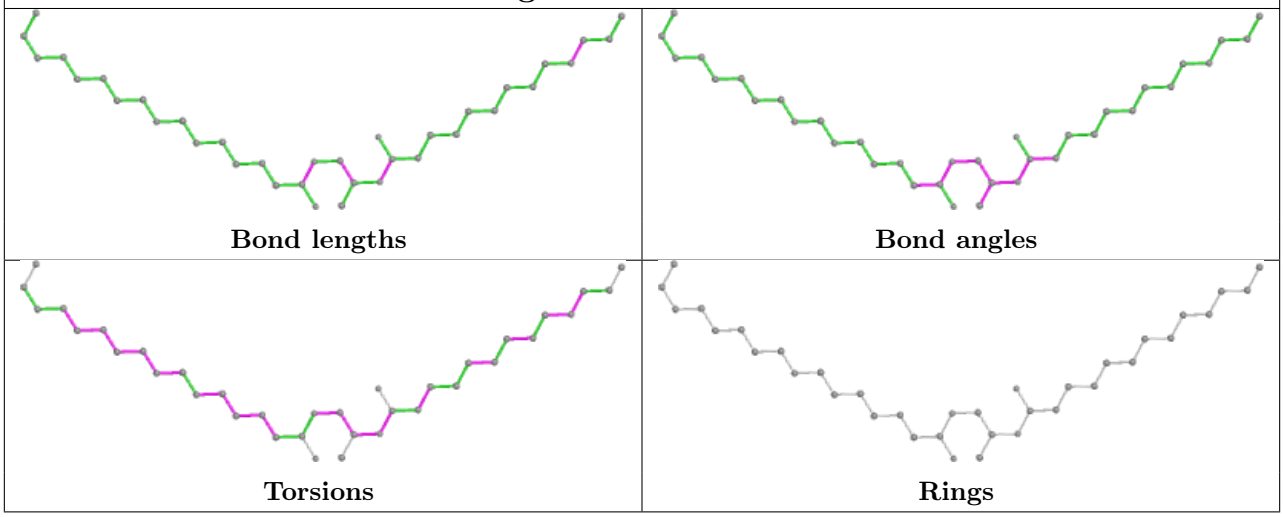
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand MYY B 303



Ligand MYY A 304



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	256/257 (99%)	-0.28	8 (3%)	49	44	30, 49, 65, 90	0
1	B	256/257 (99%)	0.05	10 (3%)	39	35	33, 76, 93, 107	0
All	All	512/514 (99%)	-0.12	18 (3%)	44	38	30, 59, 89, 107	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	67	GLY	5.1
1	A	238	ILE	4.4
1	A	241	ASP	4.0
1	A	239	ASP	3.9
1	A	242	GLY	3.8
1	B	68	ASN	3.7
1	A	240	ILE	3.5
1	B	69	TRP	2.8
1	A	220	ASP	2.6
1	B	2	ALA	2.6
1	B	217	PRO	2.5
1	B	116	THR	2.5
1	A	257	ASN	2.4
1	A	203	GLY	2.3
1	B	90	PRO	2.2
1	B	71	SER	2.2
1	B	220	ASP	2.1
1	B	241	ASP	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)

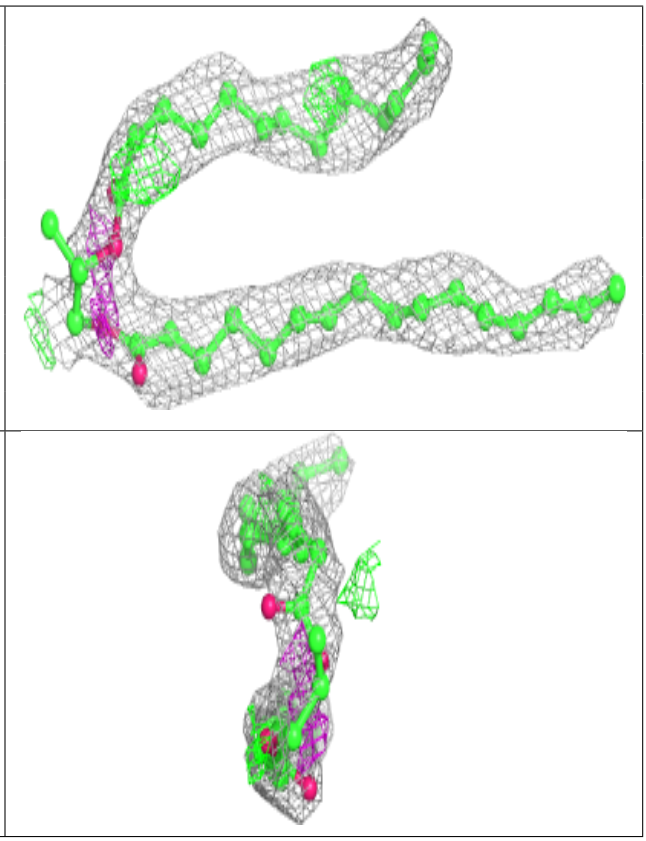
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MYY	A	304	36/42	0.78	0.32	48,58,85,88	0
3	MYY	B	303	38/42	0.81	0.32	42,65,87,92	0
5	CL	A	259	1/1	0.91	0.09	62,62,62,62	0
2	FE	B	301	1/1	0.97	0.18	67,67,67,67	0
4	HQN	A	258	9/9	0.98	0.21	58,64,66,66	0
2	FE	A	300	1/1	0.99	0.12	37,37,37,37	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.

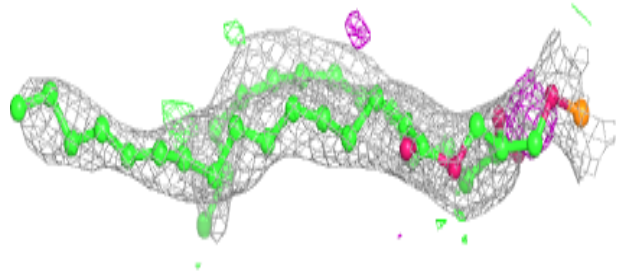
Electron density around MYY A 304:

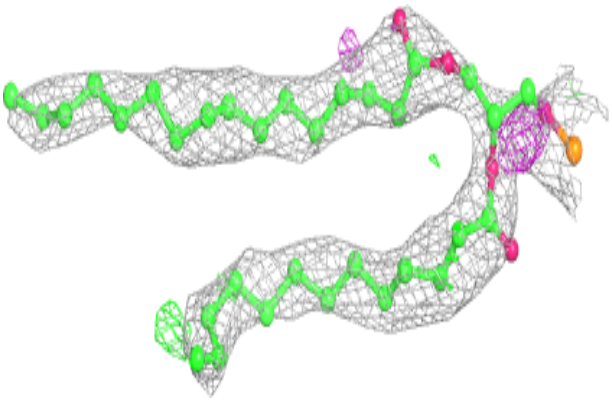
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

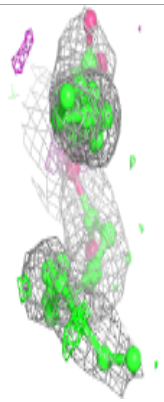


Electron density around MYY B 303:

$2mF_o$-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.