Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2021 – 10:07 PM EST

PDB ID	:	3Q34
Title	:	The crystal structure of YceI-like family protein from Pseudomonas syringae
Authors	:	Zhang, Z.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2010-12-21
Resolution	:	1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

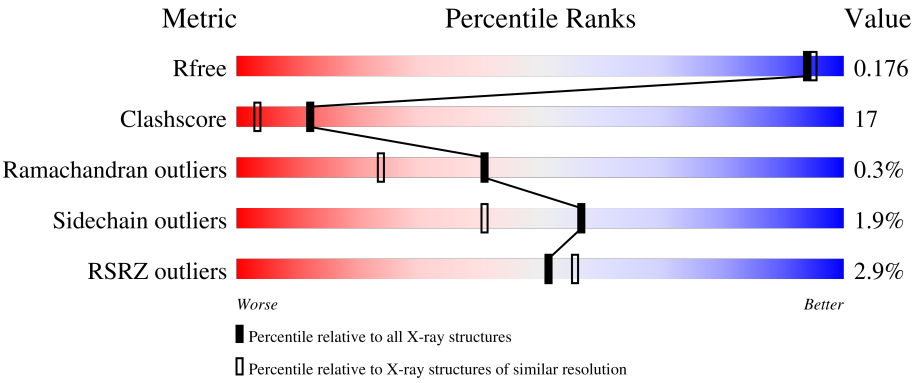
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	184	79% 15% 5%
1	B	184	71% 21% 8%
1	C	184	5% 74% 16% 7%
1	D	184	4% 81% 12% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UQ8	A	1	-	-	X	-
2	UQ8	B	2	-	-	X	-
2	UQ8	D	4	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6225 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 YceI-like family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	Se	0	4	0
			1384	878	247	257	2			
1	B	170	Total	C	N	O	Se	0	3	0
			1337	850	235	250	2			
1	C	171	Total	C	N	O	Se	0	5	0
			1370	873	240	255	2			
1	D	173	Total	C	N	O	Se	0	6	0
			1389	883	244	260	2			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MSE	-	expression tag	UNP Q48EL2
A	19	SER	-	expression tag	UNP Q48EL2
A	20	LEU	-	expression tag	UNP Q48EL2
A	194	GLU	-	expression tag	UNP Q48EL2
A	195	GLY	-	expression tag	UNP Q48EL2
A	196	HIS	-	expression tag	UNP Q48EL2
A	197	HIS	-	expression tag	UNP Q48EL2
A	198	HIS	-	expression tag	UNP Q48EL2
A	199	HIS	-	expression tag	UNP Q48EL2
A	200	HIS	-	expression tag	UNP Q48EL2
A	201	HIS	-	expression tag	UNP Q48EL2
B	18	MSE	-	expression tag	UNP Q48EL2
B	19	SER	-	expression tag	UNP Q48EL2
B	20	LEU	-	expression tag	UNP Q48EL2
B	194	GLU	-	expression tag	UNP Q48EL2
B	195	GLY	-	expression tag	UNP Q48EL2
B	196	HIS	-	expression tag	UNP Q48EL2
B	197	HIS	-	expression tag	UNP Q48EL2
B	198	HIS	-	expression tag	UNP Q48EL2
B	199	HIS	-	expression tag	UNP Q48EL2
B	200	HIS	-	expression tag	UNP Q48EL2

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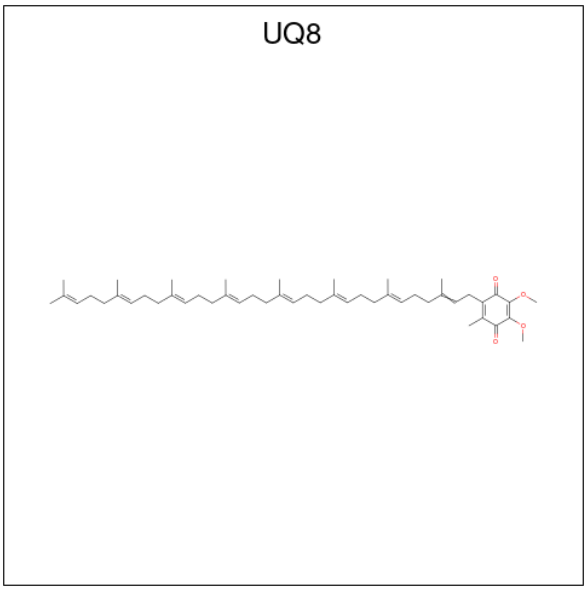
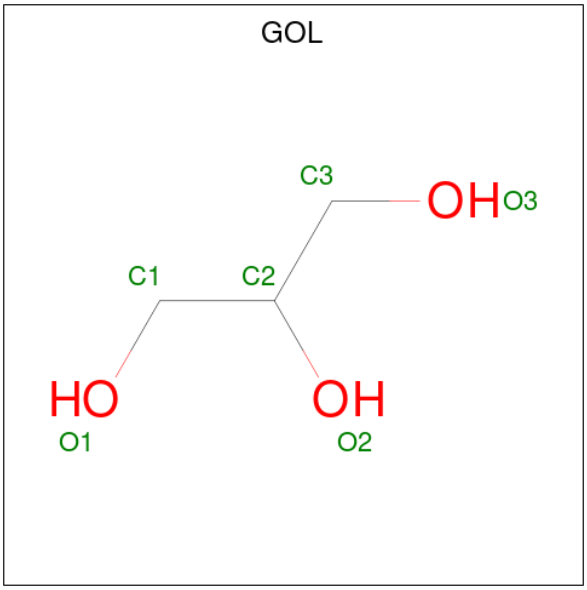
Chain	Residue	Modelled	Actual	Comment	Reference
B	201	HIS	-	expression tag	UNP Q48EL2
C	18	MSE	-	expression tag	UNP Q48EL2
C	19	SER	-	expression tag	UNP Q48EL2
C	20	LEU	-	expression tag	UNP Q48EL2
C	194	GLU	-	expression tag	UNP Q48EL2
C	195	GLY	-	expression tag	UNP Q48EL2
C	196	HIS	-	expression tag	UNP Q48EL2
C	197	HIS	-	expression tag	UNP Q48EL2
C	198	HIS	-	expression tag	UNP Q48EL2
C	199	HIS	-	expression tag	UNP Q48EL2
C	200	HIS	-	expression tag	UNP Q48EL2
C	201	HIS	-	expression tag	UNP Q48EL2
D	18	MSE	-	expression tag	UNP Q48EL2
D	19	SER	-	expression tag	UNP Q48EL2
D	20	LEU	-	expression tag	UNP Q48EL2
D	194	GLU	-	expression tag	UNP Q48EL2
D	195	GLY	-	expression tag	UNP Q48EL2
D	196	HIS	-	expression tag	UNP Q48EL2
D	197	HIS	-	expression tag	UNP Q48EL2
D	198	HIS	-	expression tag	UNP Q48EL2
D	199	HIS	-	expression tag	UNP Q48EL2
D	200	HIS	-	expression tag	UNP Q48EL2
D	201	HIS	-	expression tag	UNP Q48EL2

- Molecule 2 is Ubiquinone-8 (three-letter code: UQ8) (formula: $C_{49}H_{74}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 53 49 4	0	0
2	B	1	Total C O 53 49 4	0	0
2	C	1	Total C O 53 49 4	0	0
2	D	1	Total C O 53 49 4	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	147	Total O 147 147	0	0
4	B	125	Total O 125 125	0	0
4	C	122	Total O 122 122	0	0

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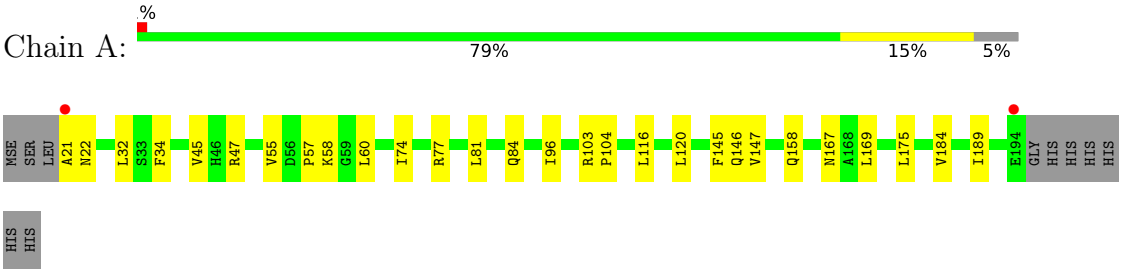
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	121	Total	O	0	0
			121	121		

3 Residue-property plots

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

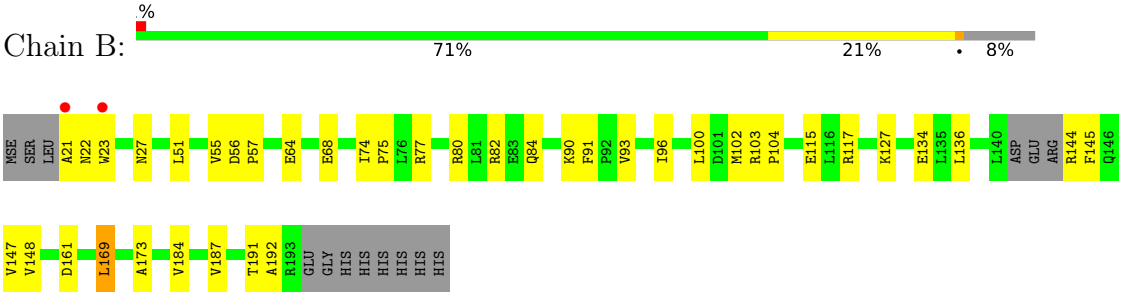
• Molecule 1: YceI-like family protein

Chain A:



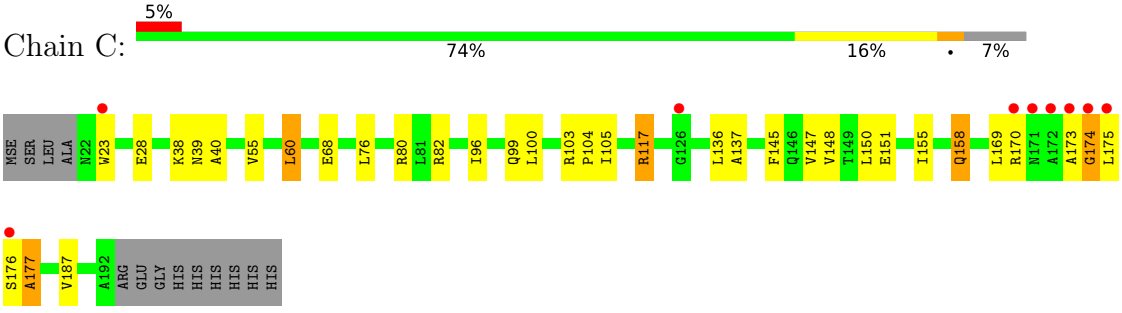
• Molecule 1: YceI-like family protein

Chain B:



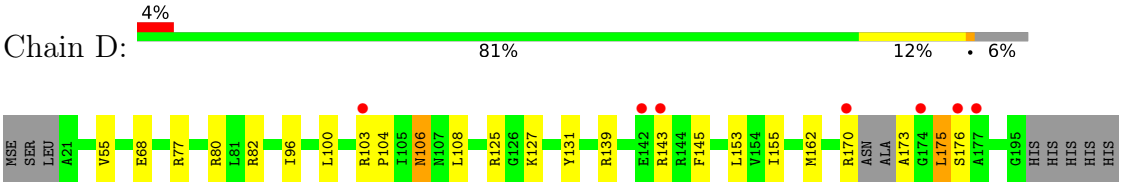
• Molecule 1: YceI-like family protein

Chain C:



• Molecule 1: YceI-like family protein

Chain D:



HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.65Å 103.36Å 63.19Å 90.00° 109.04° 90.00°	Depositor
Resolution (Å)	47.48 – 1.70 51.72 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.48-1.70) 99.5 (51.72-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 1.70Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.170 , 0.207 0.172 , 0.176	Depositor DCC
R_{free} test set	3650 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	17.0	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 47.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6225	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0616e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, UQ8

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	0.66	0/1419	0.78	0/1925
1	B	0.64	0/1367	0.79	0/1855
1	C	0.68	0/1408	0.81	1/1911 (0.1%)
1	D	0.70	0/1426	0.78	1/1931 (0.1%)
All	All	0.67	0/5620	0.79	2/7622 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	143	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	C	174	GLY	N-CA-C	5.04	125.70	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1384	0	1405	47	0
1	B	1337	0	1357	41	0
1	C	1370	0	1393	42	0
1	D	1389	0	1411	41	0
2	A	53	0	74	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	53	0	74	25	0
2	C	53	0	74	20	0
2	D	53	0	74	32	0
3	A	6	0	7	0	0
3	B	6	0	7	0	0
3	D	6	0	7	0	0
4	A	147	0	0	4	0
4	B	125	0	0	0	0
4	C	122	0	0	2	0
4	D	121	0	0	0	0
All	All	6225	0	5883	198	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 17.

All (198) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ALA:HB3	1:A:57:PRO:HG3	1.30	1.10
1:A:96:ILE:HD13	2:A:1:UQ8:H31	1.07	1.05
1:A:21:ALA:HB1	1:A:22:ASN:HA	1.42	1.01
1:B:184:VAL:HG11	2:B:2:UQ8:H27	1.40	0.99
1:B:96:ILE:HG12	2:B:2:UQ8:H28	0.99	0.98
1:D:100:LEU:HD13	2:D:4:UQ8:H45A	1.45	0.98
1:A:96:ILE:HD13	2:A:1:UQ8:C31	1.95	0.97
1:B:96:ILE:HG12	2:B:2:UQ8:C28	1.94	0.96
2:D:4:UQ8:H4MB	2:D:4:UQ8:H3MB	1.48	0.95
1:D:145[B]:PHE:CE2	2:D:4:UQ8:H46A	2.00	0.95
1:B:96:ILE:CG1	2:B:2:UQ8:H28	1.95	0.94
1:B:102:MSE:HE1	2:B:2:UQ8:H45A	1.48	0.94
1:D:100:LEU:CD1	2:D:4:UQ8:H45A	1.97	0.93
1:A:184:VAL:CG1	2:A:1:UQ8:H30	1.98	0.93
1:A:32:LEU:HD11	2:A:1:UQ8:H30	1.51	0.92
1:D:145[B]:PHE:HE2	2:D:4:UQ8:H46A	1.29	0.92
1:C:117:ARG:HH11	1:C:117:ARG:HB3	1.34	0.91
1:B:80:ARG:NH1	2:B:2:UQ8:O2	2.05	0.89
1:D:175:LEU:H	1:D:175:LEU:HD12	1.38	0.89
1:C:80:ARG:HD2	2:C:3:UQ8:O2	1.74	0.87
1:B:21:ALA:N	1:B:22:ASN:HA	1.91	0.85
1:A:96:ILE:CD1	2:A:1:UQ8:H31	2.01	0.85
1:D:175:LEU:HD21	2:D:4:UQ8:C7	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:UQ8:O4	2:B:2:UQ8:H3MA	1.75	0.83
2:D:4:UQ8:H4MB	2:D:4:UQ8:C3M	2.09	0.82
1:C:80:ARG:CZ	2:C:3:UQ8:H3MB	2.09	0.82
2:B:2:UQ8:H3MA	2:B:2:UQ8:C4M	2.10	0.82
1:D:77:ARG:HH11	2:D:4:UQ8:H10B	1.45	0.81
1:A:184:VAL:HG11	2:A:1:UQ8:H30	1.61	0.81
1:A:32:LEU:HD11	2:A:1:UQ8:C30	2.09	0.81
1:A:147:VAL:HG11	2:A:1:UQ8:H40B	1.62	0.80
1:D:100:LEU:HD21	2:D:4:UQ8:H43	1.64	0.79
1:D:125:ARG:HB2	1:D:162:MSE:HE3	1.62	0.78
1:D:175:LEU:HD21	2:D:4:UQ8:H7	1.65	0.77
1:D:175:LEU:HD12	1:D:175:LEU:N	2.02	0.75
1:A:21:ALA:HB3	1:A:57:PRO:CG	2.13	0.74
1:B:145:PHE:CD2	2:B:2:UQ8:H46	2.22	0.74
1:A:55:VAL:HG21	2:A:1:UQ8:H43	1.72	0.72
1:A:184:VAL:CG1	2:A:1:UQ8:C30	2.67	0.72
1:A:175:LEU:HD11	2:A:1:UQ8:H7A	1.72	0.72
1:D:173:ALA:O	1:D:175:LEU:HD12	1.89	0.72
1:D:173:ALA:HB3	1:D:175:LEU:HD11	1.72	0.71
1:A:184:VAL:HG12	2:A:1:UQ8:H30	1.71	0.71
1:A:58:LYS:HE3	4:A:221:HOH:O	1.89	0.71
1:D:175:LEU:H	1:D:175:LEU:CD1	2.04	0.70
1:A:184:VAL:HG12	2:A:1:UQ8:C30	2.20	0.70
1:D:77:ARG:HH11	2:D:4:UQ8:C10	2.04	0.69
1:C:117:ARG:HH11	1:C:117:ARG:CB	2.04	0.69
1:D:175:LEU:HD21	2:D:4:UQ8:H7A	1.72	0.69
1:D:77:ARG:HD2	2:D:4:UQ8:H10B	1.75	0.69
2:C:3:UQ8:H4MA	2:C:3:UQ8:O3	1.93	0.68
2:D:4:UQ8:C4M	2:D:4:UQ8:O3	2.42	0.68
1:D:100:LEU:HD22	2:D:4:UQ8:H45	1.76	0.67
1:B:80:ARG:HD2	2:B:2:UQ8:O2	1.95	0.66
1:B:77:ARG:HH11	2:B:2:UQ8:H10B	1.60	0.66
2:D:4:UQ8:H10	2:D:4:UQ8:O5	1.95	0.66
1:C:117:ARG:HB3	1:C:117:ARG:NH1	2.09	0.66
1:B:90:LYS:HG2	1:B:91:PHE:CE2	2.31	0.65
1:C:155:ILE:HD11	2:C:3:UQ8:H21	1.79	0.64
2:C:3:UQ8:O2	2:C:3:UQ8:H3MB	1.98	0.64
1:B:55:VAL:HG21	2:B:2:UQ8:H42A	1.79	0.64
1:C:60:LEU:HD23	1:C:99:GLN:NE2	2.13	0.64
1:C:76:LEU:HD23	1:C:80:ARG:HH21	1.63	0.64
1:C:105:ILE:HG23	1:C:145:PHE:CZ	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:VAL:HG21	2:B:2:UQ8:H41A	1.79	0.64
2:D:4:UQ8:C4M	2:D:4:UQ8:C3M	2.76	0.64
1:A:103:ARG:HB3	1:A:104:PRO:HD3	1.80	0.63
2:B:2:UQ8:C3M	2:B:2:UQ8:O4	2.46	0.63
1:D:55:VAL:HG21	2:D:4:UQ8:H46B	1.79	0.63
1:A:32:LEU:CD1	2:A:1:UQ8:C30	2.77	0.62
1:B:74:ILE:HG21	2:B:2:UQ8:H3MB	1.81	0.62
1:C:28:GLU:HG3	4:C:513:HOH:O	1.99	0.61
1:B:144:ARG:HG2	1:B:191:THR:HG22	1.82	0.61
1:D:103:ARG:HB2	1:D:104:PRO:HD3	1.81	0.61
1:D:131:TYR:HB3	1:D:153:LEU:HD11	1.82	0.61
1:C:60:LEU:HD13	4:C:248:HOH:O	2.01	0.61
1:A:167:ASN:ND2	4:A:481:HOH:O	2.33	0.61
1:B:147:VAL:CG2	2:B:2:UQ8:H41A	2.31	0.60
1:A:145:PHE:CB	2:A:1:UQ8:H46A	2.32	0.60
1:A:169:LEU:HD12	2:A:1:UQ8:H15	1.83	0.60
2:C:3:UQ8:O3	2:C:3:UQ8:C4M	2.49	0.60
1:C:23[B]:TRP:CZ3	2:C:3:UQ8:H46	2.37	0.59
1:D:100:LEU:HD11	2:D:4:UQ8:H45A	1.82	0.59
1:D:96:ILE:HD13	2:D:4:UQ8:H31	1.84	0.59
1:C:39:ASN:OD1	1:C:175:LEU:HB3	2.03	0.59
2:C:3:UQ8:C3M	2:C:3:UQ8:O2	2.50	0.58
1:D:173:ALA:C	1:D:175:LEU:HD12	2.23	0.58
1:B:21:ALA:N	1:B:22:ASN:CA	2.66	0.58
1:A:184:VAL:HG11	2:A:1:UQ8:C30	2.31	0.57
1:B:77:ARG:NH1	2:B:2:UQ8:H10B	2.19	0.57
1:D:170:ARG:HA	1:D:175:LEU:HD13	1.88	0.56
1:C:170:ARG:HD2	1:C:177:ALA:HA	1.88	0.56
2:D:4:UQ8:H4MA	2:D:4:UQ8:O3	2.05	0.56
1:C:76:LEU:CD2	1:C:80:ARG:HH21	2.18	0.56
1:B:96:ILE:HD12	1:B:96:ILE:N	2.22	0.54
1:D:77:ARG:NH1	2:D:4:UQ8:H10B	2.17	0.54
1:D:100:LEU:HD13	2:D:4:UQ8:C45	2.30	0.54
1:C:60:LEU:HD23	1:C:99:GLN:HE22	1.74	0.53
1:D:145[B]:PHE:CZ	2:D:4:UQ8:H46A	2.43	0.53
1:A:145:PHE:HB3	2:A:1:UQ8:H46A	1.91	0.53
1:B:68:GLU:HG3	1:B:82:ARG:HD3	1.92	0.52
1:C:173:ALA:O	1:C:175:LEU:HG	2.09	0.52
1:C:100:LEU:HD11	2:C:3:UQ8:H43	1.91	0.52
1:D:175:LEU:CD1	1:D:175:LEU:N	2.71	0.52
1:B:145:PHE:CD2	2:B:2:UQ8:C46	2.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:GLN:NE2	4:A:207:HOH:O	2.42	0.52
1:B:173:ALA:HB2	2:B:2:UQ8:C1	2.40	0.51
1:C:96:ILE:N	1:C:96:ILE:HD12	2.25	0.51
1:D:100:LEU:CD2	2:D:4:UQ8:H45	2.40	0.51
1:C:147:VAL:HG21	2:C:3:UQ8:C44	2.41	0.50
1:D:77:ARG:CD	2:D:4:UQ8:H10B	2.40	0.50
1:C:158:GLN:HE21	1:C:158:GLN:HA	1.76	0.50
1:B:84:GLN:HG2	1:B:169:LEU:HD23	1.92	0.50
1:A:120:LEU:CD2	2:A:1:UQ8:C35	2.90	0.50
1:B:64:GLU:HG3	1:B:93:VAL:CG1	2.41	0.50
1:B:27:ASN:ND2	1:B:51:LEU:H	2.10	0.49
1:B:21:ALA:HB3	1:B:23:TRP:CD1	2.46	0.49
1:A:120:LEU:CD2	2:A:1:UQ8:H35A	2.43	0.49
1:B:22:ASN:HD22	1:B:56:ASP:HA	1.77	0.49
1:D:155:ILE:C	1:D:155:ILE:HD12	2.33	0.49
1:C:103:ARG:HB3	1:C:104:PRO:HD3	1.94	0.48
1:C:80:ARG:CD	2:C:3:UQ8:O2	2.54	0.48
2:D:4:UQ8:H38	2:D:4:UQ8:H42	1.55	0.48
1:A:96:ILE:CD1	2:A:1:UQ8:C29	2.91	0.48
1:B:127:LYS:HE3	1:B:161:ASP:OD2	2.12	0.48
1:B:64:GLU:HG3	1:B:93:VAL:HG11	1.96	0.48
1:C:148[B]:VAL:HG13	1:C:187:VAL:HG22	1.95	0.48
1:B:21:ALA:HB2	1:B:23:TRP:NE1	2.29	0.48
1:B:117:ARG:HD3	1:B:134:GLU:OE1	2.14	0.47
1:B:21:ALA:CB	1:B:23:TRP:CD1	2.97	0.47
1:B:100:LEU:HD11	2:B:2:UQ8:C39	2.45	0.47
1:A:147:VAL:CG2	2:A:1:UQ8:H46	2.45	0.46
1:D:173:ALA:HB3	1:D:175:LEU:CD1	2.44	0.46
1:C:176:SER:O	1:C:177:ALA:HB2	2.16	0.46
1:C:100:LEU:HD11	2:C:3:UQ8:C43	2.46	0.46
1:C:170:ARG:CD	1:C:177:ALA:HA	2.45	0.46
2:D:4:UQ8:H42A	2:D:4:UQ8:H46	1.68	0.46
2:A:1:UQ8:H10	2:A:1:UQ8:O5	2.15	0.45
1:A:96:ILE:HD11	2:A:1:UQ8:C29	2.46	0.45
1:A:32:LEU:CD1	2:A:1:UQ8:H30	2.35	0.45
1:C:169:LEU:HD11	2:C:3:UQ8:H15A	1.98	0.45
1:D:125:ARG:HB2	1:D:162:MSE:CE	2.42	0.45
1:D:68:GLU:HG3	1:D:82:ARG:HD3	1.99	0.45
1:B:56:ASP:HB2	1:B:57:PRO:CD	2.47	0.45
1:A:34:PHE:CE1	2:A:1:UQ8:H18	2.51	0.44
1:A:21:ALA:CB	1:A:22:ASN:HA	2.23	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:LEU:CD1	2:D:4:UQ8:C45	2.84	0.44
1:D:106:ASN:O	1:D:139:ARG:NH2	2.46	0.44
1:A:184:VAL:HG21	2:A:1:UQ8:H23	1.99	0.44
1:B:173:ALA:HB2	2:B:2:UQ8:C6	2.47	0.44
2:B:2:UQ8:H3MA	2:B:2:UQ8:H4MA	1.95	0.44
1:A:22:ASN:OD1	1:A:57:PRO:HD3	2.17	0.44
2:B:2:UQ8:H10	2:B:2:UQ8:H7A	1.50	0.44
1:D:108:LEU:O	1:D:139:ARG:HD2	2.18	0.44
1:A:147:VAL:HG21	2:A:1:UQ8:H42A	1.99	0.44
1:C:137:ALA:HB1	1:C:145:PHE:HE2	1.82	0.44
1:A:45:VAL:HG11	1:C:151:GLU:HB3	2.00	0.44
1:C:23[B]:TRP:CZ3	2:C:3:UQ8:C46	3.00	0.44
2:C:3:UQ8:H25	2:C:3:UQ8:H22A	1.78	0.44
1:B:103:ARG:HB3	1:B:104:PRO:HD3	2.00	0.44
1:A:32:LEU:CD1	2:A:1:UQ8:H30B	2.48	0.43
1:C:23[B]:TRP:HB2	1:C:55:VAL:HB	1.99	0.43
1:A:81:LEU:HD23	1:A:169:LEU:HD11	2.00	0.43
1:B:21:ALA:HA	1:B:57:PRO:HG3	2.00	0.43
1:A:60:LEU:HD12	1:A:60:LEU:HA	1.78	0.43
1:C:23[B]:TRP:HZ3	2:C:3:UQ8:H46	1.82	0.43
1:A:96:ILE:HD11	2:A:1:UQ8:C28	2.49	0.42
2:B:2:UQ8:H12	2:B:2:UQ8:H15	1.41	0.42
1:A:96:ILE:CD1	2:A:1:UQ8:C31	2.79	0.42
1:C:148[A]:VAL:HG12	1:C:187:VAL:HG13	2.01	0.42
1:C:175:LEU:HD11	2:C:3:UQ8:H7A	2.01	0.42
1:B:148:VAL:HG12	1:B:187:VAL:HG13	2.01	0.42
1:A:158:GLN:NE2	4:A:336:HOH:O	2.52	0.42
1:C:39:ASN:HA	1:C:176:SER:HB2	2.01	0.42
1:C:136:LEU:HB3	1:C:148[A]:VAL:HG22	2.01	0.42
1:C:150:LEU:HD23	1:C:150:LEU:HA	1.90	0.42
1:D:127:LYS:HA	1:D:127:LYS:HD3	1.86	0.42
2:C:3:UQ8:H40	2:C:3:UQ8:H37	1.87	0.41
1:C:76:LEU:HD23	1:C:80:ARG:NH2	2.33	0.41
2:D:4:UQ8:C5	2:D:4:UQ8:H10	2.50	0.41
1:A:146:GLN:HA	1:A:189:ILE:HD13	2.02	0.41
1:C:68:GLU:HG3	1:C:82:ARG:HD3	2.02	0.41
1:A:120:LEU:CD2	2:A:1:UQ8:H35	2.51	0.41
1:D:125:ARG:HD3	1:D:162:MSE:HE2	2.01	0.41
2:A:1:UQ8:H7A	2:A:1:UQ8:H10	1.83	0.41
2:C:3:UQ8:H30	2:C:3:UQ8:H27A	1.93	0.41
1:B:115[A]:GLU:HG2	1:B:136:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1:UQ8:H37A	2:A:1:UQ8:H40	1.71	0.41
1:A:74:ILE:HD12	1:A:77:ARG:CZ	2.50	0.41
1:C:38:LYS:HD3	2:C:3:UQ8:C10	2.51	0.41
2:B:2:UQ8:H20	2:B:2:UQ8:H17A	1.78	0.41
1:C:39:ASN:O	1:C:40:ALA:HB3	2.21	0.41
2:A:1:UQ8:H32	2:A:1:UQ8:H35	1.72	0.41
1:B:21:ALA:CB	1:B:23:TRP:NE1	2.84	0.41
1:D:80:ARG:HD2	2:D:4:UQ8:O2	2.20	0.40
1:A:77:ARG:HH11	2:A:1:UQ8:H10B	1.86	0.40
1:B:23:TRP:CZ2	1:B:192:ALA:HB2	2.56	0.40
2:D:4:UQ8:H35	2:D:4:UQ8:H32A	1.61	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	176/184 (96%)	174 (99%)	2 (1%)	0	100 100
1	B	169/184 (92%)	168 (99%)	1 (1%)	0	100 100
1	C	174/184 (95%)	167 (96%)	5 (3%)	2 (1%)	14 3
1	D	175/184 (95%)	173 (99%)	2 (1%)	0	100 100
All	All	694/736 (94%)	682 (98%)	10 (1%)	2 (0%)	41 24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	174	GLY
1	C	177	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	153/156 (98%)	150 (98%)	3 (2%)	55	38
1	B	148/156 (95%)	146 (99%)	2 (1%)	67	53
1	C	153/156 (98%)	150 (98%)	3 (2%)	55	38
1	D	155/156 (99%)	152 (98%)	3 (2%)	57	41
All	All	609/624 (98%)	598 (98%)	11 (2%)	57	43

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	84	GLN
1	A	116	LEU
1	B	75	PRO
1	B	169	LEU
1	C	60	LEU
1	C	117	ARG
1	C	158	GLN
1	D	106	ASN
1	D	175	LEU
1	D	176	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	99	GLN
1	A	107	ASN
1	A	158	GLN
1	A	167	ASN
1	B	22	ASN
1	B	27	ASN
1	B	84	GLN

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Mol	Chain	Res	Type
1	B	99	GLN
1	B	107	ASN
1	B	158	GLN
1	B	167	ASN
1	C	84	GLN
1	C	99	GLN
1	C	107	ASN
1	C	158	GLN
1	D	97	ASN
1	D	99	GLN
1	D	158	GLN
1	D	167	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)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	UQ8	A	1	-	53,53,53	2.10	12 (22%)	64,67,67	2.56	26 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	A	3	-	5,5,5	1.99	1 (20%)	5,5,5	2.01	2 (40%)
2	UQ8	B	2	-	53,53,53	2.41	18 (33%)	64,67,67	3.15	31 (48%)
2	UQ8	C	3	-	53,53,53	2.10	12 (22%)	64,67,67	2.56	26 (40%)
3	GOL	B	1	-	5,5,5	2.03	1 (20%)	5,5,5	1.95	2 (40%)
3	GOL	D	2	-	5,5,5	2.20	1 (20%)	5,5,5	2.03	2 (40%)
2	UQ8	D	4	-	53,53,53	2.10	13 (24%)	64,67,67	2.56	26 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UQ8	A	1	-	-	21/51/75/75	0/1/1/1
3	GOL	A	3	-	-	1/4/4/4	-
2	UQ8	B	2	-	-	25/51/75/75	0/1/1/1
2	UQ8	C	3	-	-	23/51/75/75	0/1/1/1
3	GOL	B	1	-	-	2/4/4/4	-
3	GOL	D	2	-	-	2/4/4/4	-
2	UQ8	D	4	-	-	20/51/75/75	0/1/1/1

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	UQ8	O2-C2	7.92	1.40	1.23
2	A	1	UQ8	O2-C2	7.92	1.40	1.23
2	D	4	UQ8	O2-C2	7.91	1.40	1.23
2	B	2	UQ8	O2-C2	7.52	1.39	1.23
2	A	1	UQ8	O5-C5	7.41	1.39	1.23
2	C	3	UQ8	O5-C5	7.41	1.39	1.23
2	D	4	UQ8	O5-C5	7.37	1.39	1.23
2	B	2	UQ8	O5-C5	6.87	1.38	1.23
2	B	2	UQ8	C31-C29	5.15	1.62	1.51
3	D	2	GOL	C3-C2	-4.75	1.32	1.51
2	B	2	UQ8	C26-C24	4.60	1.60	1.51
3	B	1	GOL	C3-C2	-4.42	1.33	1.51
3	A	3	GOL	C3-C2	-4.17	1.34	1.51
2	B	2	UQ8	C28-C29	3.53	1.41	1.33
2	B	2	UQ8	C27-C28	3.34	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	UQ8	C4-C5	-3.33	1.39	1.48
2	C	3	UQ8	C4-C5	-3.10	1.39	1.48
2	A	1	UQ8	C4-C5	-3.08	1.40	1.48
2	D	4	UQ8	C4-C5	-3.06	1.40	1.48
2	B	2	UQ8	C21-C19	3.06	1.57	1.51
2	D	4	UQ8	C7-C8	3.02	1.55	1.50
2	B	2	UQ8	C36-C34	3.01	1.57	1.51
2	C	3	UQ8	C7-C8	3.00	1.55	1.50
2	B	2	UQ8	C32-C33	2.94	1.60	1.50
2	A	1	UQ8	C7-C8	2.94	1.54	1.50
2	B	2	UQ8	C33-C34	2.84	1.39	1.33
2	C	3	UQ8	C7-C6	2.77	1.56	1.51
2	A	1	UQ8	C7-C6	2.76	1.55	1.51
2	D	4	UQ8	C7-C6	2.71	1.55	1.51
2	B	2	UQ8	O3-C3M	-2.69	1.39	1.45
2	B	2	UQ8	O4-C4M	-2.63	1.39	1.45
2	C	3	UQ8	C31-C29	2.55	1.56	1.51
2	A	1	UQ8	C31-C29	2.55	1.56	1.51
2	D	4	UQ8	C31-C29	2.53	1.56	1.51
2	D	4	UQ8	C16-C14	2.46	1.56	1.51
2	C	3	UQ8	C16-C14	2.43	1.56	1.51
2	A	1	UQ8	C16-C14	2.43	1.56	1.51
2	B	2	UQ8	C3-C2	-2.38	1.42	1.48
2	B	2	UQ8	C22-C23	2.27	1.57	1.50
2	B	2	UQ8	C31-C32	2.26	1.61	1.53
2	A	1	UQ8	O4-C4M	-2.24	1.40	1.45
2	C	3	UQ8	O4-C4M	-2.24	1.40	1.45
2	D	4	UQ8	O4-C4M	-2.24	1.40	1.45
2	B	2	UQ8	C16-C14	2.21	1.55	1.51
2	B	2	UQ8	C7-C6	2.17	1.55	1.51
2	D	4	UQ8	C36-C34	2.10	1.55	1.51
2	C	3	UQ8	C36-C34	2.10	1.55	1.51
2	A	1	UQ8	O3-C3M	-2.09	1.40	1.45
2	A	1	UQ8	C36-C34	2.07	1.55	1.51
2	C	3	UQ8	O3-C3M	-2.06	1.40	1.45
2	D	4	UQ8	O3-C3M	-2.06	1.40	1.45
2	A	1	UQ8	C26-C24	2.04	1.55	1.51
2	C	3	UQ8	C26-C24	2.04	1.55	1.51
2	D	4	UQ8	C26-C24	2.04	1.55	1.51
2	D	4	UQ8	C12-C13	2.03	1.57	1.50
2	C	3	UQ8	C12-C13	2.03	1.57	1.50
2	A	1	UQ8	C12-C13	2.02	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	UQ8	C32-C33	2.00	1.56	1.50

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	UQ8	C35-C34-C36	-8.22	101.44	115.27
2	B	2	UQ8	C7-C8-C9	-6.54	115.91	126.79
2	B	2	UQ8	C15-C14-C13	-5.93	108.46	123.68
2	B	2	UQ8	C40-C39-C41	-5.90	105.35	115.27
2	B	2	UQ8	C26-C27-C28	5.84	131.06	111.88
2	D	4	UQ8	C7-C8-C9	-5.62	117.44	126.79
2	A	1	UQ8	C7-C8-C9	-5.60	117.46	126.79
2	C	3	UQ8	C7-C8-C9	-5.58	117.50	126.79
2	B	2	UQ8	C22-C21-C19	5.58	131.33	112.98
2	B	2	UQ8	C25-C24-C23	-5.48	109.61	123.68
2	B	2	UQ8	C32-C31-C29	5.37	130.64	112.98
2	B	2	UQ8	C27-C26-C24	4.93	129.19	112.98
2	B	2	UQ8	C10-C9-C8	-4.72	111.58	123.68
2	B	2	UQ8	C40-C39-C38	-4.70	111.62	123.68
2	B	2	UQ8	C11-C9-C8	-4.52	111.97	121.12
2	B	2	UQ8	C12-C13-C14	-4.46	116.91	127.66
2	B	2	UQ8	C20-C19-C21	4.45	122.76	115.27
2	B	2	UQ8	C20-C19-C18	-4.32	112.59	123.68
2	D	4	UQ8	C17-C18-C19	-4.12	117.74	127.66
2	C	3	UQ8	C12-C13-C14	-4.11	117.76	127.66
2	A	1	UQ8	C12-C13-C14	-4.11	117.77	127.66
2	D	4	UQ8	C12-C13-C14	-4.11	117.77	127.66
2	A	1	UQ8	C17-C18-C19	-4.10	117.78	127.66
2	C	3	UQ8	C17-C18-C19	-4.10	117.78	127.66
2	C	3	UQ8	C27-C28-C29	-4.08	117.83	127.66
2	A	1	UQ8	C27-C28-C29	-4.08	117.84	127.66
2	D	4	UQ8	C27-C28-C29	-4.08	117.84	127.66
2	A	1	UQ8	C22-C23-C24	-4.07	117.86	127.66
2	D	4	UQ8	C22-C23-C24	-4.06	117.87	127.66
2	C	3	UQ8	C22-C23-C24	-4.06	117.89	127.66
2	D	4	UQ8	C37-C38-C39	-4.05	117.90	127.66
2	D	4	UQ8	C32-C33-C34	-4.05	117.91	127.66
2	A	1	UQ8	C37-C38-C39	-4.04	117.94	127.66
2	C	3	UQ8	C32-C33-C34	-4.03	117.95	127.66
2	C	3	UQ8	C37-C38-C39	-4.03	117.96	127.66
2	A	1	UQ8	C32-C33-C34	-4.02	117.97	127.66
2	A	1	UQ8	C15-C14-C13	-3.97	113.50	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	4	UQ8	C15-C14-C13	-3.96	113.51	123.68
2	C	3	UQ8	C15-C14-C13	-3.95	113.53	123.68
2	A	1	UQ8	C30-C29-C28	-3.94	113.56	123.68
2	A	1	UQ8	C20-C19-C18	-3.94	113.58	123.68
2	A	1	UQ8	C25-C24-C23	-3.93	113.58	123.68
2	D	4	UQ8	C25-C24-C23	-3.93	113.59	123.68
2	C	3	UQ8	C20-C19-C18	-3.93	113.59	123.68
2	D	4	UQ8	C20-C19-C18	-3.93	113.60	123.68
2	D	4	UQ8	C30-C29-C28	-3.93	113.61	123.68
2	C	3	UQ8	C30-C29-C28	-3.92	113.62	123.68
2	C	3	UQ8	C25-C24-C23	-3.92	113.62	123.68
2	C	3	UQ8	C10-C9-C8	-3.91	113.64	123.68
2	A	1	UQ8	C10-C9-C8	-3.90	113.67	123.68
2	D	4	UQ8	C10-C9-C8	-3.90	113.67	123.68
2	A	1	UQ8	C35-C34-C33	-3.88	113.72	123.68
2	C	3	UQ8	C35-C34-C33	-3.88	113.73	123.68
2	D	4	UQ8	C35-C34-C33	-3.86	113.78	123.68
2	C	3	UQ8	C40-C39-C38	-3.82	113.87	123.68
2	A	1	UQ8	C40-C39-C38	-3.81	113.91	123.68
2	D	4	UQ8	C40-C39-C38	-3.80	113.94	123.68
2	C	3	UQ8	C41-C39-C38	-3.73	113.58	121.12
2	A	1	UQ8	C41-C39-C38	-3.72	113.58	121.12
2	D	4	UQ8	C41-C39-C38	-3.71	113.60	121.12
2	D	4	UQ8	C36-C34-C33	-3.61	113.81	121.12
2	C	3	UQ8	C36-C34-C33	-3.61	113.82	121.12
2	B	2	UQ8	C8-C7-C6	3.60	121.74	112.05
2	A	1	UQ8	C36-C34-C33	-3.58	113.86	121.12
2	C	3	UQ8	C31-C29-C28	-3.54	113.95	121.12
2	C	3	UQ8	C21-C19-C18	-3.52	113.99	121.12
2	A	1	UQ8	C31-C29-C28	-3.52	113.99	121.12
2	D	4	UQ8	C16-C14-C13	-3.52	113.99	121.12
2	A	1	UQ8	C26-C24-C23	-3.52	114.00	121.12
2	D	4	UQ8	C11-C9-C8	-3.51	114.00	121.12
2	D	4	UQ8	C31-C29-C28	-3.51	114.01	121.12
2	D	4	UQ8	C26-C24-C23	-3.51	114.01	121.12
2	C	3	UQ8	C26-C24-C23	-3.51	114.02	121.12
2	D	4	UQ8	C21-C19-C18	-3.51	114.02	121.12
2	C	3	UQ8	C16-C14-C13	-3.50	114.03	121.12
2	A	1	UQ8	C11-C9-C8	-3.50	114.03	121.12
2	B	2	UQ8	C16-C14-C13	-3.49	114.05	121.12
2	C	3	UQ8	C11-C9-C8	-3.49	114.05	121.12
2	A	1	UQ8	C16-C14-C13	-3.49	114.06	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	UQ8	C21-C19-C18	-3.49	114.06	121.12
2	B	2	UQ8	C31-C29-C28	3.43	128.05	121.12
2	B	2	UQ8	C35-C34-C33	-3.33	115.14	123.68
2	B	2	UQ8	C42-C41-C39	3.23	123.61	112.98
2	B	2	UQ8	C37-C36-C34	3.22	123.56	112.98
2	B	2	UQ8	C45-C44-C43	-3.14	113.57	122.65
2	C	3	UQ8	C46-C44-C43	-3.13	113.59	122.65
2	A	1	UQ8	C46-C44-C43	-3.12	113.62	122.65
2	D	4	UQ8	C46-C44-C43	-3.12	113.62	122.65
2	A	1	UQ8	C45-C44-C43	-3.08	113.73	122.65
2	C	3	UQ8	C45-C44-C43	-3.07	113.76	122.65
2	D	4	UQ8	C45-C44-C43	-3.07	113.78	122.65
2	B	2	UQ8	C30-C29-C28	-3.06	115.82	123.68
2	D	4	UQ8	C42-C43-C44	-2.96	117.63	127.75
2	C	3	UQ8	C42-C43-C44	-2.96	117.63	127.75
2	A	1	UQ8	C42-C43-C44	-2.96	117.63	127.75
2	B	2	UQ8	C17-C16-C14	2.90	122.50	112.98
3	A	3	GOL	C3-C2-C1	2.79	122.57	111.70
2	B	2	UQ8	C21-C19-C18	-2.69	115.67	121.12
2	D	4	UQ8	C1M-C1-C6	-2.69	120.01	124.40
2	B	2	UQ8	C15-C14-C16	2.69	119.79	115.27
2	A	1	UQ8	C1M-C1-C6	-2.66	120.05	124.40
2	B	2	UQ8	C46-C44-C43	-2.66	114.96	122.65
2	C	3	UQ8	C1M-C1-C6	-2.65	120.07	124.40
2	B	2	UQ8	C42-C43-C44	-2.54	119.08	127.75
3	D	2	GOL	O2-C2-C1	2.50	120.13	109.12
3	B	1	GOL	C3-C2-C1	2.49	121.40	111.70
2	B	2	UQ8	C31-C32-C33	2.48	120.02	111.88
3	A	3	GOL	O3-C3-C2	2.32	121.32	110.20
3	D	2	GOL	O1-C1-C2	2.29	121.17	110.20
2	D	4	UQ8	C8-C7-C6	2.27	118.16	112.05
2	A	1	UQ8	C8-C7-C6	2.26	118.13	112.05
2	C	3	UQ8	C8-C7-C6	2.24	118.08	112.05
2	B	2	UQ8	C41-C42-C43	2.21	119.16	111.88
2	B	2	UQ8	C21-C22-C23	2.05	118.62	111.88
3	B	1	GOL	O2-C2-C3	2.02	118.03	109.12

There are no chirality outliers.

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	UQ8	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
2	A	1	UQ8	C29-C31-C32-C33
2	A	1	UQ8	C30-C29-C31-C32
2	A	1	UQ8	C28-C29-C31-C32
2	A	1	UQ8	C27-C28-C29-C30
2	A	1	UQ8	C22-C23-C24-C26
2	A	1	UQ8	C15-C14-C16-C17
2	A	1	UQ8	C12-C13-C14-C16
2	A	1	UQ8	C12-C13-C14-C15
2	A	1	UQ8	C7-C8-C9-C10
2	B	2	UQ8	C32-C33-C34-C36
2	B	2	UQ8	C32-C33-C34-C35
2	B	2	UQ8	C27-C28-C29-C31
2	B	2	UQ8	C22-C23-C24-C26
2	B	2	UQ8	C20-C19-C21-C22
2	B	2	UQ8	C18-C19-C21-C22
2	B	2	UQ8	C12-C13-C14-C16
2	C	3	UQ8	C37-C38-C39-C40
2	C	3	UQ8	C22-C23-C24-C25
2	C	3	UQ8	C17-C18-C19-C20
2	C	3	UQ8	C12-C13-C14-C16
3	B	1	GOL	O1-C1-C2-C3
3	D	2	GOL	C1-C2-C3-O3
2	D	4	UQ8	C37-C38-C39-C40
2	D	4	UQ8	C22-C23-C24-C25
2	D	4	UQ8	C7-C8-C9-C10
2	A	1	UQ8	C42-C43-C44-C46
2	C	3	UQ8	C42-C43-C44-C45
2	A	1	UQ8	C38-C39-C41-C42
2	A	1	UQ8	C33-C34-C36-C37
2	D	4	UQ8	C13-C14-C16-C17
2	A	1	UQ8	C42-C43-C44-C45
2	B	2	UQ8	C42-C43-C44-C45
2	B	2	UQ8	C37-C38-C39-C40
2	B	2	UQ8	C27-C28-C29-C30
2	C	3	UQ8	C27-C28-C29-C30
2	C	3	UQ8	C7-C8-C9-C10
2	D	4	UQ8	C27-C28-C29-C30
2	D	4	UQ8	C17-C18-C19-C20
2	D	4	UQ8	C12-C13-C14-C15
2	C	3	UQ8	C17-C18-C19-C21
2	C	3	UQ8	C42-C43-C44-C46
2	D	4	UQ8	C42-C43-C44-C46

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Mol	Chain	Res	Type	Atoms
2	B	2	UQ8	C33-C34-C36-C37
2	A	1	UQ8	C39-C41-C42-C43
2	B	2	UQ8	C29-C31-C32-C33
2	B	2	UQ8	C24-C26-C27-C28
2	B	2	UQ8	C19-C21-C22-C23
2	B	2	UQ8	C14-C16-C17-C18
2	D	4	UQ8	C39-C41-C42-C43
2	D	4	UQ8	C34-C36-C37-C38
2	D	4	UQ8	C9-C11-C12-C13
2	B	2	UQ8	C7-C8-C9-C10
2	C	3	UQ8	C4-C3-O3-C3M
2	A	1	UQ8	C9-C11-C12-C13
2	A	1	UQ8	C12-C11-C9-C10
3	B	1	GOL	C1-C2-C3-O3
2	D	4	UQ8	C12-C11-C9-C8
2	C	3	UQ8	C12-C11-C9-C8
2	C	3	UQ8	C29-C31-C32-C33
2	B	2	UQ8	C5-C6-C7-C8
2	C	3	UQ8	C40-C39-C41-C42
2	D	4	UQ8	C40-C39-C41-C42
2	D	4	UQ8	C18-C19-C21-C22
2	C	3	UQ8	C35-C34-C36-C37
2	A	1	UQ8	C17-C18-C19-C21
2	C	3	UQ8	C2-C3-O3-C3M
3	D	2	GOL	O1-C1-C2-O2
2	B	2	UQ8	C12-C11-C9-C10
2	D	4	UQ8	C6-C7-C8-C9
2	B	2	UQ8	C1-C6-C7-C8
2	D	4	UQ8	C12-C11-C9-C10
2	B	2	UQ8	C25-C24-C26-C27
2	C	3	UQ8	C6-C7-C8-C9
2	A	1	UQ8	C37-C38-C39-C40
2	A	1	UQ8	C20-C19-C21-C22
2	C	3	UQ8	C28-C29-C31-C32
2	B	2	UQ8	C2-C3-O3-C3M
2	C	3	UQ8	C18-C19-C21-C22
2	B	2	UQ8	C40-C39-C41-C42
2	B	2	UQ8	C15-C14-C16-C17
2	C	3	UQ8	C38-C39-C41-C42
2	C	3	UQ8	C25-C24-C26-C27
2	C	3	UQ8	C15-C14-C16-C17
2	D	4	UQ8	C28-C29-C31-C32

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Mol	Chain	Res	Type	Atoms
2	B	2	UQ8	C38-C39-C41-C42
2	D	4	UQ8	C25-C24-C26-C27
2	B	2	UQ8	C3-C4-O4-C4M
2	D	4	UQ8	C5-C4-O4-C4M
2	A	1	UQ8	C25-C24-C26-C27
2	C	3	UQ8	C5-C4-O4-C4M
3	A	3	GOL	O1-C1-C2-O2
2	C	3	UQ8	C3-C4-O4-C4M
2	D	4	UQ8	C32-C33-C34-C35

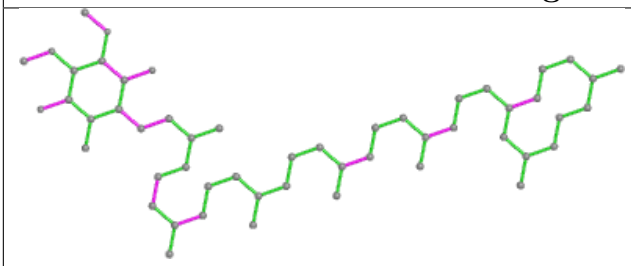
There are no ring outliers.

4 monomers are involved in 113 short contacts:

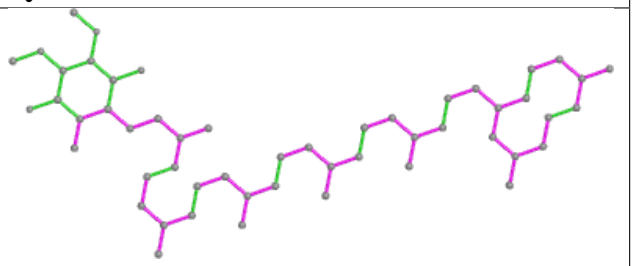
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	UQ8	36	0
2	B	2	UQ8	25	0
2	C	3	UQ8	20	0
2	D	4	UQ8	32	0

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.

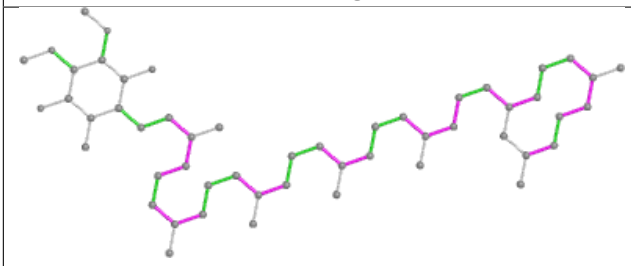
Ligand UQ8 A 1



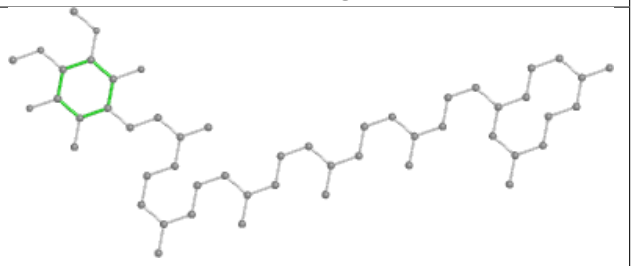
Bond lengths



Bond angles

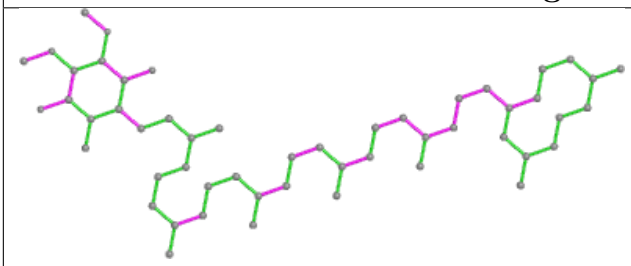


Torsions

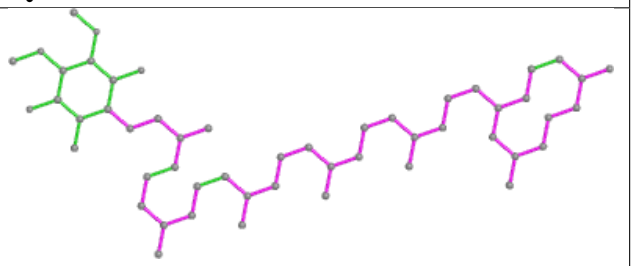


Rings

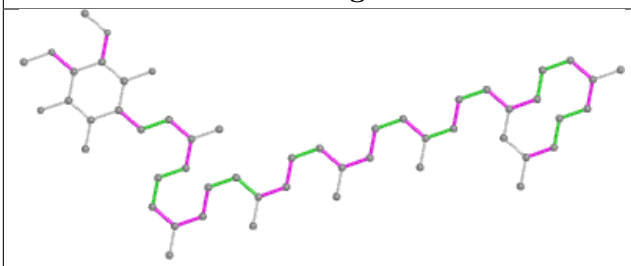
Ligand UQ8 B 2



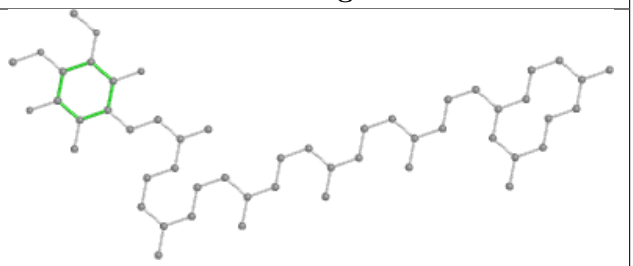
Bond lengths



Bond angles

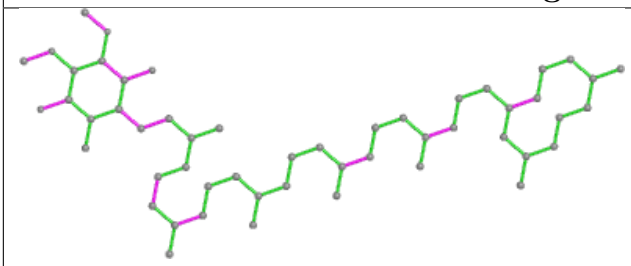


Torsions

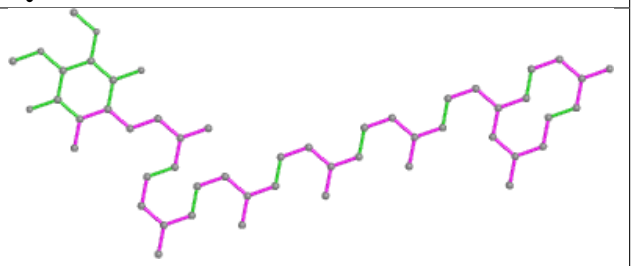


Rings

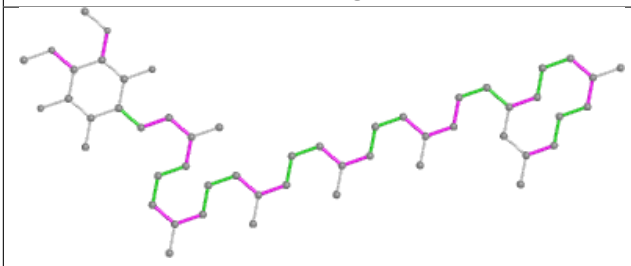
Ligand UQ8 C 3



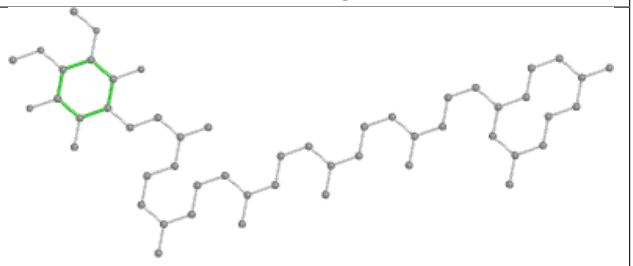
Bond lengths



Bond angles

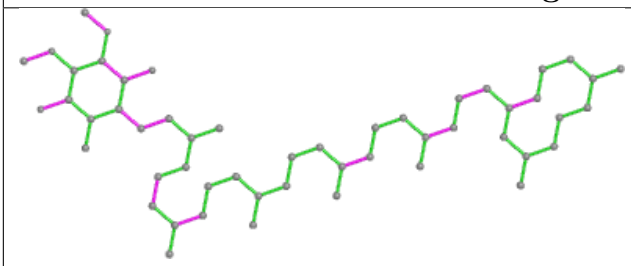


Torsions

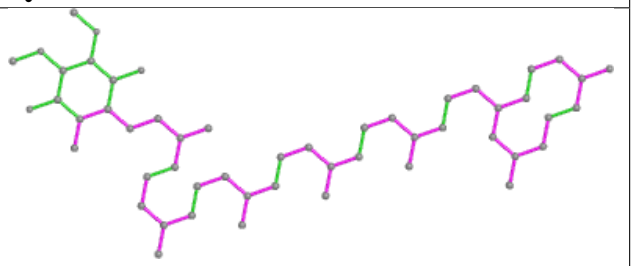


Rings

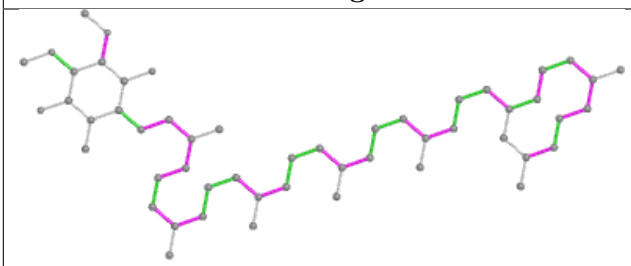
Ligand UQ8 D 4



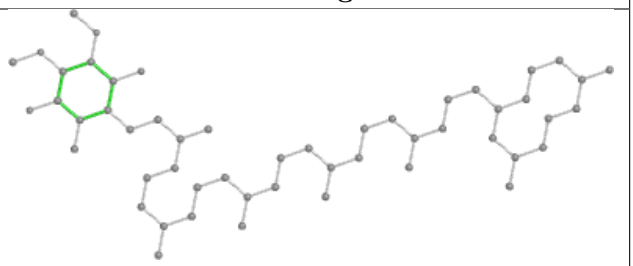
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	172/184 (93%)	-0.42	2 (1%)	79	82	9, 17, 26, 36	0
1	B	168/184 (91%)	-0.47	2 (1%)	79	82	10, 16, 26, 46	0
1	C	169/184 (91%)	-0.20	9 (5%)	26	29	10, 17, 36, 52	0
1	D	171/184 (92%)	-0.17	7 (4%)	37	41	10, 18, 37, 49	0
All	All	680/736 (92%)	-0.32	20 (2%)	51	56	9, 17, 33, 52	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	176	SER	5.6
1	B	21	ALA	4.6
1	C	174	GLY	4.4
1	D	143	ARG	4.3
1	C	176	SER	4.2
1	D	174	GLY	3.7
1	C	173	ALA	3.6
1	C	172	ALA	3.1
1	C	23[A]	TRP	2.9
1	D	103	ARG	2.8
1	D	170	ARG	2.7
1	C	171	ASN	2.6
1	B	23	TRP	2.4
1	C	170	ARG	2.4
1	C	175	LEU	2.3
1	A	21	ALA	2.3
1	D	177	ALA	2.2
1	C	126	GLY	2.2
1	D	142	GLU	2.2
1	A	194	GLU	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)

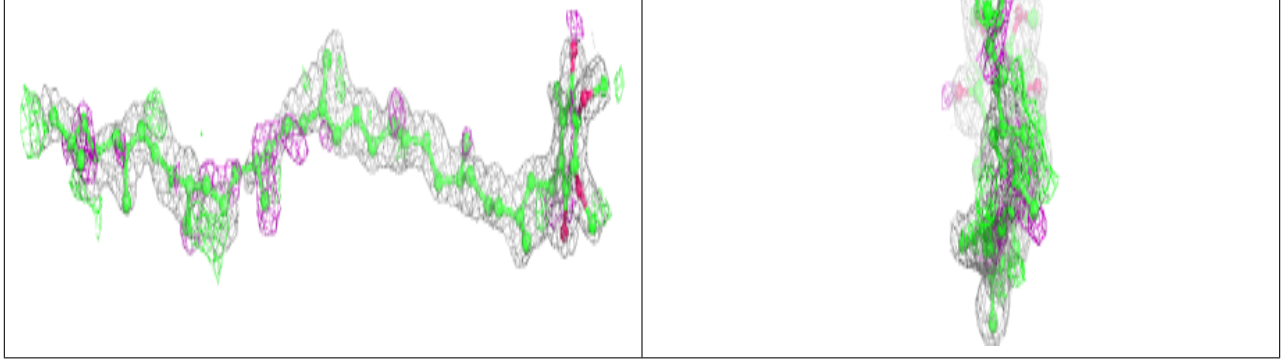
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	UQ8	A	1	53/53	0.71	0.27	19,30,38,39	0
2	UQ8	B	2	53/53	0.74	0.22	20,31,37,42	0
2	UQ8	C	3	53/53	0.78	0.17	21,29,38,41	0
2	UQ8	D	4	53/53	0.85	0.17	18,28,40,46	0
3	GOL	A	3	6/6	0.91	0.13	23,25,28,28	0
3	GOL	D	2	6/6	0.92	0.14	15,27,29,30	0
3	GOL	B	1	6/6	0.92	0.12	18,23,26,27	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.

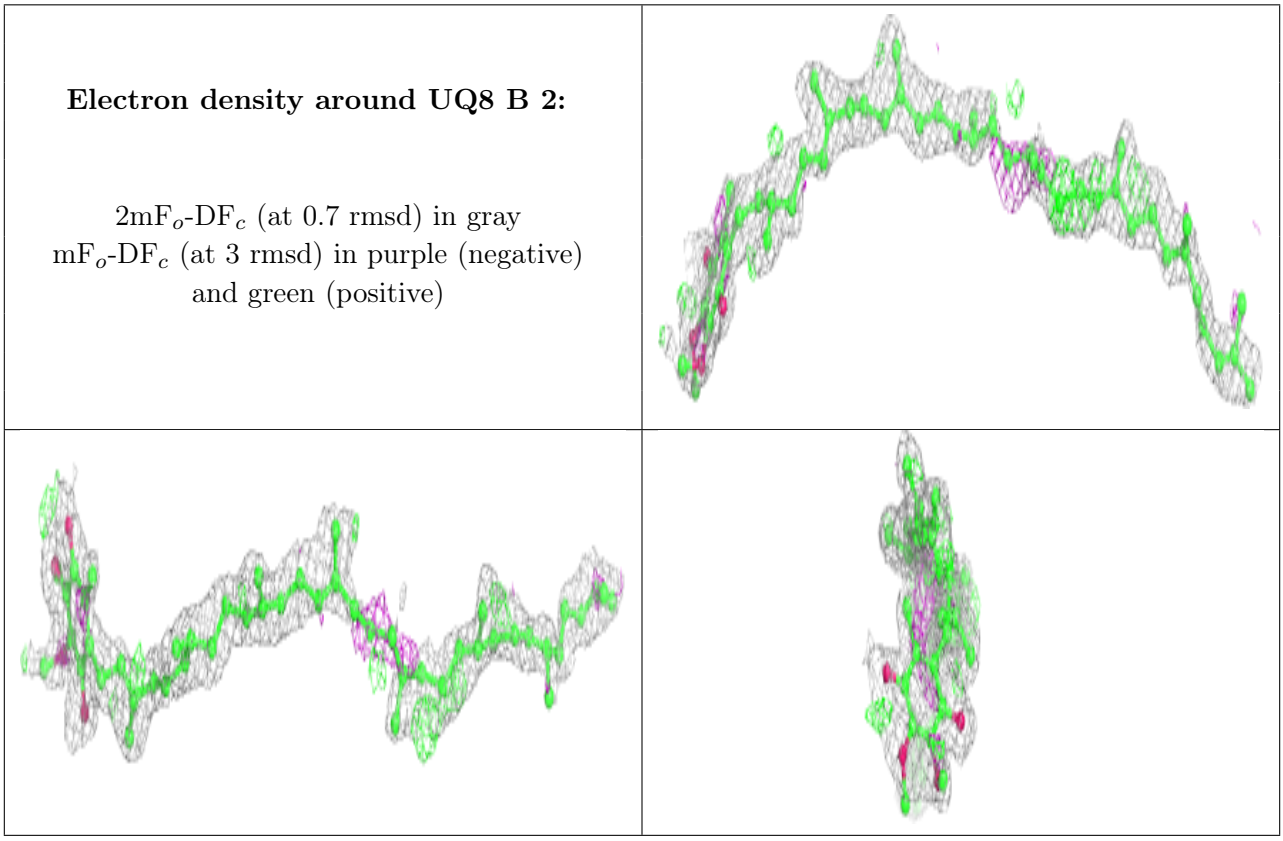
Electron density around UQ8 A 1:

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



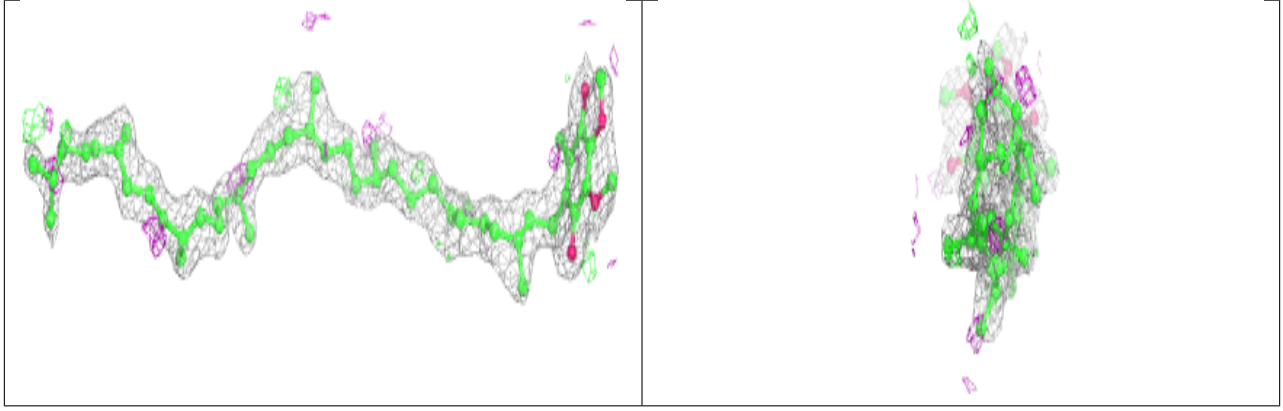
Electron density around UQ8 B 2:

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



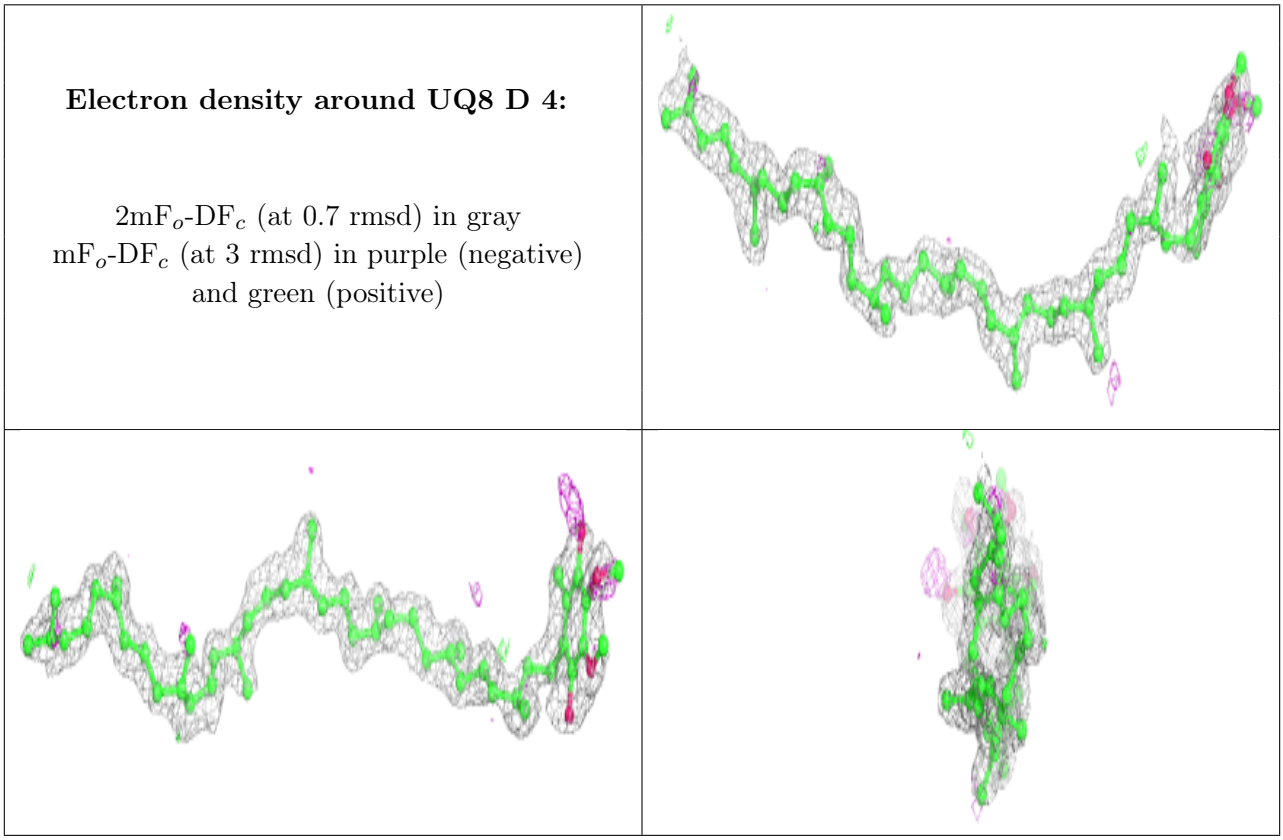
Electron density around UQ8 C 3:

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



Electron density around UQ8 D 4:

$2mF_o$-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.