



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:50 PM UTC

PDB ID : 8QD3 / pdb_00008qd3
Title : Ayglp in complex with 1,3,6,8-Tetrahydroxynaphthalene
Authors : Schmalhofer, M.; Vagstad, A.L.; Zhou, Q.; Bode, H.B.; Groll, M.
Deposited on : 2023-08-28
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

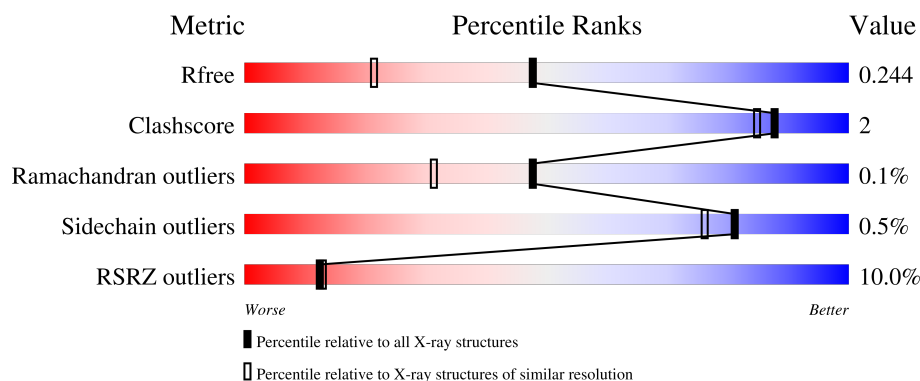
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 $\leq 5\%$. 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	423	8% 88% 6% 6%
1	B	423	11% 91% • 6%
1	C	423	10% 89% 5% 6%
1	D	423	9% 91% • 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
3	PGE	C	1002	-	-	X	-
5	EDO	C	1003	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13718 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 Pigment biosynthesis protein yellowish-green 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	5	0
			3138	2015	538	576	9			
1	B	398	Total	C	N	O	S	0	4	0
			3129	2004	541	575	9			
1	C	398	Total	C	N	O	S	0	4	0
			3098	1990	527	572	9			
1	D	398	Total	C	N	O	S	0	5	0
			3122	2002	536	575	9			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	initiating methionine	UNP Q9UVV1
A	-15	ARG	-	expression tag	UNP Q9UVV1
A	-14	GLY	-	expression tag	UNP Q9UVV1
A	-13	SER	-	expression tag	UNP Q9UVV1
A	-12	HIS	-	expression tag	UNP Q9UVV1
A	-11	HIS	-	expression tag	UNP Q9UVV1
A	-10	HIS	-	expression tag	UNP Q9UVV1
A	-9	HIS	-	expression tag	UNP Q9UVV1
A	-8	HIS	-	expression tag	UNP Q9UVV1
A	-7	HIS	-	expression tag	UNP Q9UVV1
A	-6	GLU	-	expression tag	UNP Q9UVV1
A	-5	ASN	-	expression tag	UNP Q9UVV1
A	-4	LEU	-	expression tag	UNP Q9UVV1
A	-3	TYR	-	expression tag	UNP Q9UVV1
A	-2	PHE	-	expression tag	UNP Q9UVV1
A	-1	GLN	-	expression tag	UNP Q9UVV1
A	0	GLY	-	expression tag	UNP Q9UVV1
A	1	SER	-	expression tag	UNP Q9UVV1
B	-16	MET	-	initiating methionine	UNP Q9UVV1
B	-15	ARG	-	expression tag	UNP Q9UVV1
B	-14	GLY	-	expression tag	UNP Q9UVV1

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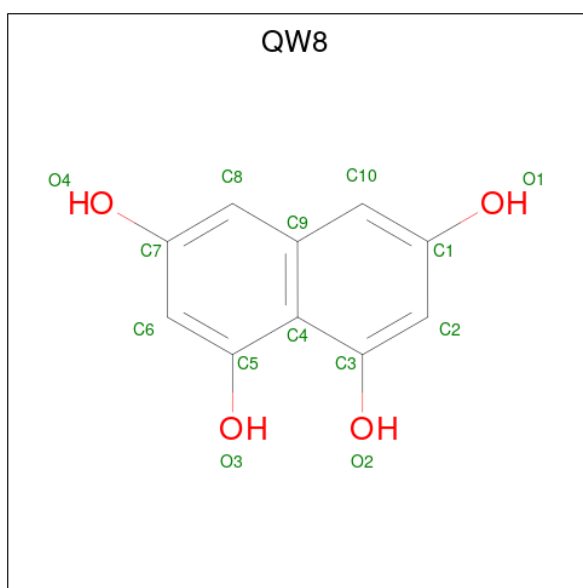
Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	SER	-	expression tag	UNP Q9UVV1
B	-12	HIS	-	expression tag	UNP Q9UVV1
B	-11	HIS	-	expression tag	UNP Q9UVV1
B	-10	HIS	-	expression tag	UNP Q9UVV1
B	-9	HIS	-	expression tag	UNP Q9UVV1
B	-8	HIS	-	expression tag	UNP Q9UVV1
B	-7	HIS	-	expression tag	UNP Q9UVV1
B	-6	GLU	-	expression tag	UNP Q9UVV1
B	-5	ASN	-	expression tag	UNP Q9UVV1
B	-4	LEU	-	expression tag	UNP Q9UVV1
B	-3	TYR	-	expression tag	UNP Q9UVV1
B	-2	PHE	-	expression tag	UNP Q9UVV1
B	-1	GLN	-	expression tag	UNP Q9UVV1
B	0	GLY	-	expression tag	UNP Q9UVV1
B	1	SER	-	expression tag	UNP Q9UVV1
C	-16	MET	-	initiating methionine	UNP Q9UVV1
C	-15	ARG	-	expression tag	UNP Q9UVV1
C	-14	GLY	-	expression tag	UNP Q9UVV1
C	-13	SER	-	expression tag	UNP Q9UVV1
C	-12	HIS	-	expression tag	UNP Q9UVV1
C	-11	HIS	-	expression tag	UNP Q9UVV1
C	-10	HIS	-	expression tag	UNP Q9UVV1
C	-9	HIS	-	expression tag	UNP Q9UVV1
C	-8	HIS	-	expression tag	UNP Q9UVV1
C	-7	HIS	-	expression tag	UNP Q9UVV1
C	-6	GLU	-	expression tag	UNP Q9UVV1
C	-5	ASN	-	expression tag	UNP Q9UVV1
C	-4	LEU	-	expression tag	UNP Q9UVV1
C	-3	TYR	-	expression tag	UNP Q9UVV1
C	-2	PHE	-	expression tag	UNP Q9UVV1
C	-1	GLN	-	expression tag	UNP Q9UVV1
C	0	GLY	-	expression tag	UNP Q9UVV1
C	1	SER	-	expression tag	UNP Q9UVV1
D	-16	MET	-	initiating methionine	UNP Q9UVV1
D	-15	ARG	-	expression tag	UNP Q9UVV1
D	-14	GLY	-	expression tag	UNP Q9UVV1
D	-13	SER	-	expression tag	UNP Q9UVV1
D	-12	HIS	-	expression tag	UNP Q9UVV1
D	-11	HIS	-	expression tag	UNP Q9UVV1
D	-10	HIS	-	expression tag	UNP Q9UVV1
D	-9	HIS	-	expression tag	UNP Q9UVV1
D	-8	HIS	-	expression tag	UNP Q9UVV1

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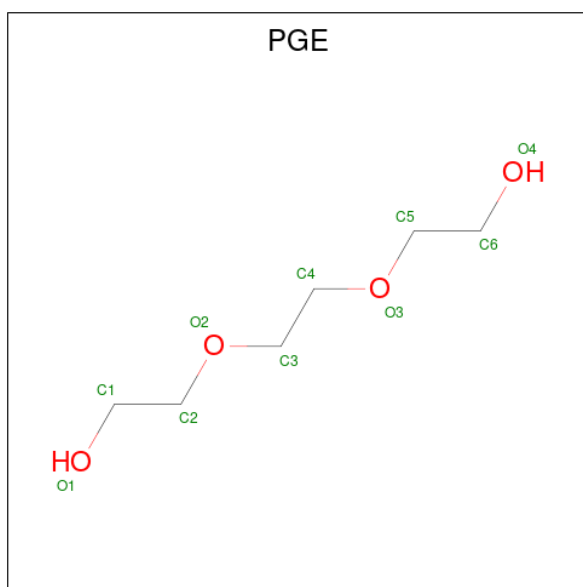
Chain	Residue	Modelled	Actual	Comment	Reference
D	-7	HIS	-	expression tag	UNP Q9UVV1
D	-6	GLU	-	expression tag	UNP Q9UVV1
D	-5	ASN	-	expression tag	UNP Q9UVV1
D	-4	LEU	-	expression tag	UNP Q9UVV1
D	-3	TYR	-	expression tag	UNP Q9UVV1
D	-2	PHE	-	expression tag	UNP Q9UVV1
D	-1	GLN	-	expression tag	UNP Q9UVV1
D	0	GLY	-	expression tag	UNP Q9UVV1
D	1	SER	-	expression tag	UNP Q9UVV1

- Molecule 2 is naphthalene-1,3,6,8-tetrol (CCD ID: QW8) (formula: $C_{10}H_8O_4$) (labeled as "Ligand of Interest" by depositor).



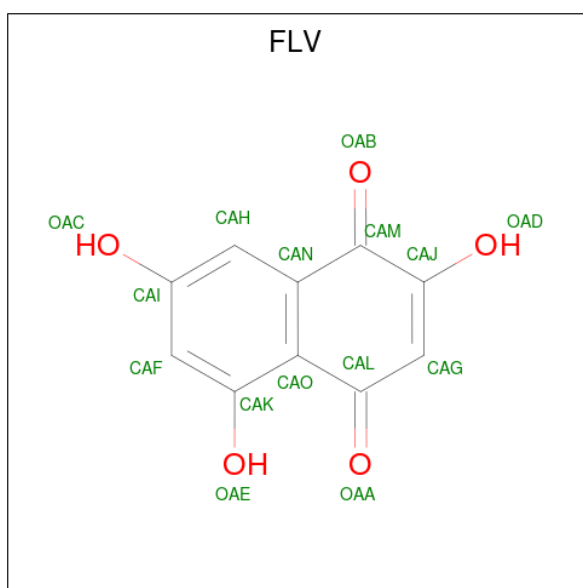
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	1
			14	10	4		
2	B	1	Total	C	O	0	1
			14	10	4		
2	C	1	Total	C	O	0	1
			14	10	4		
2	D	1	Total	C	O	0	1
			14	10	4		

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is FLAVIOLIN (CCD ID: FLV) (formula: $C_{10}H_6O_5$).



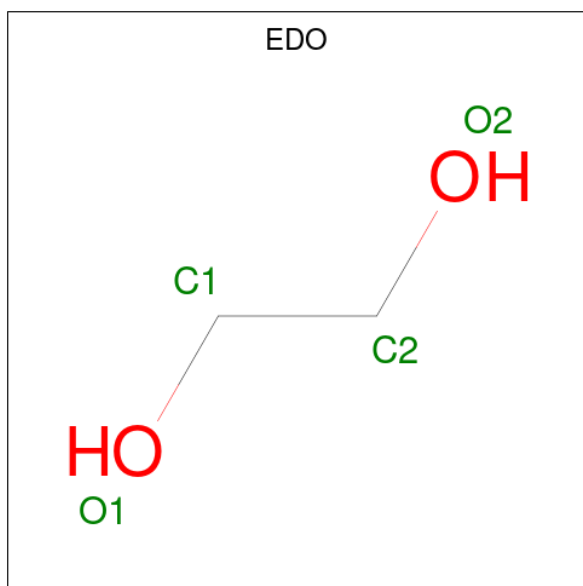
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			15	10	5		
4	A	1	Total	C	O	0	1
			15	10	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	1
			15	10	5		
4	B	1	Total	C	O	0	1
			15	10	5		
4	C	1	Total	C	O	0	1
			15	10	5		
4	C	1	Total	C	O	0	1
			15	10	5		
4	D	1	Total	C	O	0	1
			15	10	5		
4	D	1	Total	C	O	0	1
			15	10	5		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		

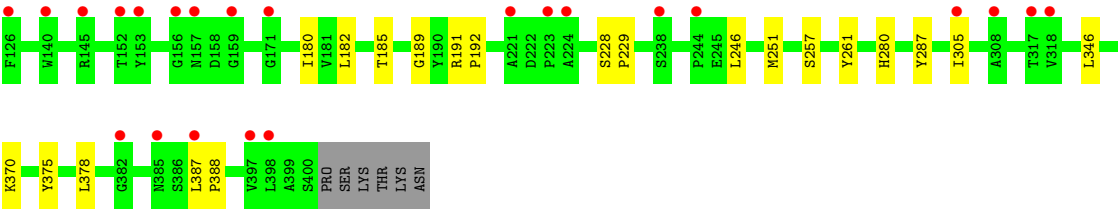
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	276	Total	O	0	0
			276	276		

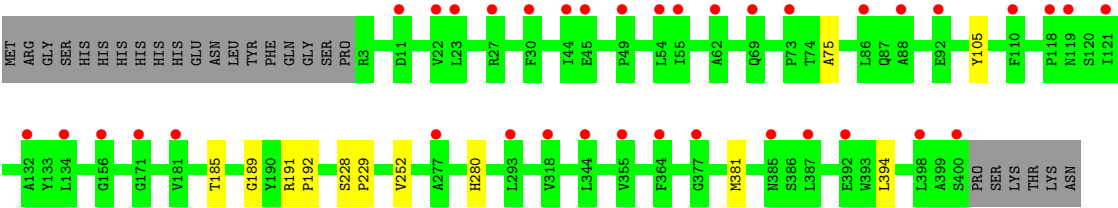
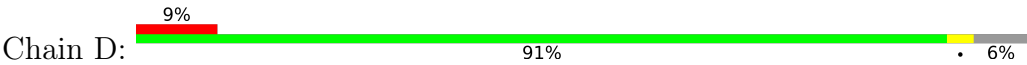
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	259	Total 259	O 259	0	0
6	C	236	Total 236	O 236	0	0
6	D	256	Total 256	O 256	0	0



● Molecule 1: Pigment biosynthesis protein yellowish-green 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.48Å 107.44Å 92.72Å 90.00° 90.16° 90.00°	Depositor
Resolution (Å)	46.48 – 1.70 46.48 – 1.70	Depositor EDS
% Data completeness (in resolution range)	93.9 (46.48-1.70) 99.2 (46.48-1.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.196 , 0.221 0.217 , 0.244	Depositor DCC
R_{free} test set	9218 reflections (3.95%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.59$, $\langle L^2 \rangle = 0.44$	Xtriage
Estimated twinning fraction	0.077 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13718	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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 47.78 % 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 9.4519e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: EDO, QW8, PGE, FLV

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	1.00	0/3244	1.38	0/4430
1	B	1.00	0/3229	1.39	0/4410
1	C	1.01	0/3200	1.39	0/4375
1	D	1.00	0/3227	1.38	0/4410
All	All	1.00	0/12900	1.38	0/17625

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3138	0	3042	16	0
1	B	3129	0	3010	14	0
1	C	3098	0	2966	17	0
1	D	3122	0	3007	5	0
2	A	14	0	0	0	0
2	B	14	0	0	0	0
2	C	14	0	0	0	0
2	D	14	0	0	0	0
3	A	10	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	10	0	14	7	0
4	A	30	0	6	0	0
4	B	30	0	6	0	0
4	C	30	0	6	0	0
4	D	30	0	6	0	0
5	B	4	0	6	0	0
5	C	4	0	6	6	0
6	A	276	0	0	0	0
6	B	259	0	0	4	0
6	C	236	0	0	4	0
6	D	256	0	0	0	0
All	All	13718	0	12089	50	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 2.

All (50) 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:371[A]:GLU:HG2	1:B:371[A]:GLU:CG	1.70	1.20
1:A:371[A]:GLU:HG2	1:B:371[A]:GLU:HG3	1.26	1.07
1:A:371[A]:GLU:CG	1:B:371[A]:GLU:HG2	1.97	0.93
1:B:187:LEU:HD11	6:B:1103:HOH:O	1.69	0.93
1:A:371[A]:GLU:CG	1:B:371[A]:GLU:CG	2.48	0.92
1:A:371[A]:GLU:HG2	1:B:371[A]:GLU:HG2	1.53	0.90
1:B:308:ALA:C	6:B:1103:HOH:O	2.31	0.73
1:A:371[A]:GLU:HG3	1:B:371[A]:GLU:HG2	1.72	0.69
1:C:287:TYR:OH	3:C:1002:PGE:H1	1.99	0.63
1:B:360:CYS:SG	6:B:1158:HOH:O	2.49	0.61
1:D:228:SER:N	1:D:229:PRO:HD2	2.22	0.55
1:A:233:TRP:O	1:A:237:LEU:HG	2.10	0.52
1:A:185:THR:HB	1:A:189:GLY:O	2.11	0.51
1:C:305:ILE:HD11	5:C:1003:EDO:C1	2.41	0.51
1:B:228:SER:N	1:B:229:PRO:HD2	2.25	0.51
1:D:252:VAL:HG11	1:D:394:LEU:CD2	2.42	0.50
1:C:387:LEU:HB2	1:C:388:PRO:HD3	1.93	0.50
1:C:228:SER:N	1:C:229:PRO:HD2	2.26	0.50
1:A:228:SER:N	1:A:229:PRO:HD2	2.26	0.49
1:B:191:ARG:N	1:B:192:PRO:CD	2.77	0.47
1:C:375:TYR:HB3	1:C:378:LEU:HD12	1.97	0.47
1:C:257:SER:OG	3:C:1002:PGE:O4	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:SER:HA	6:B:1123:HOH:O	2.14	0.47
1:C:305:ILE:HD11	5:C:1003:EDO:H11	1.97	0.46
1:A:182:LEU:HB2	1:A:251:MET:HE3	1.98	0.46
1:A:191:ARG:N	1:A:192:PRO:CD	2.79	0.46
1:C:191:ARG:N	1:C:192:PRO:CD	2.79	0.46
3:C:1002:PGE:H32	6:C:1174:HOH:O	2.15	0.45
1:D:191:ARG:N	1:D:192:PRO:CD	2.79	0.45
1:C:180:ILE:HD11	1:C:246:LEU:HB3	1.97	0.45
1:C:75:ALA:HB1	1:C:105:TYR:CZ	2.51	0.45
5:C:1003:EDO:H21	6:C:1143:HOH:O	2.16	0.45
1:C:185:THR:HB	1:C:189:GLY:O	2.17	0.45
1:C:346:LEU:HD12	6:C:1101:HOH:O	2.17	0.44
3:C:1002:PGE:O4	5:C:1003:EDO:H21	2.18	0.43
1:C:261:TYR:CB	3:C:1002:PGE:H2	2.50	0.42
1:A:75:ALA:HB1	1:A:105:TYR:CZ	2.55	0.42
1:C:182:LEU:HB2	1:C:251:MET:HE3	2.01	0.42
1:B:182:LEU:HB2	1:B:251:MET:HE3	2.00	0.42
1:D:185:THR:HB	1:D:189:GLY:O	2.20	0.42
1:B:387:LEU:HB2	1:B:388:PRO:HD3	2.02	0.41
1:A:72:LEU:N	1:A:73:PRO:CD	2.84	0.41
1:A:48:GLU:HB3	1:A:49:PRO:HD3	2.03	0.41
1:A:301:TYR:CG	1:A:302:PRO:HD2	2.56	0.41
1:C:305:ILE:HD11	5:C:1003:EDO:H12	2.02	0.41
3:C:1002:PGE:O4	5:C:1003:EDO:C1	2.68	0.41
1:D:75:ALA:HB1	1:D:105:TYR:CZ	2.55	0.41
1:A:279:ALA:HB3	1:A:346:LEU:HD23	2.03	0.40
1:C:370:LYS:HB3	6:C:1101:HOH:O	2.22	0.40
1:C:261:TYR:CD1	3:C:1002:PGE:H22	2.56	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	401/423 (95%)	383 (96%)	17 (4%)	1 (0%)	43	28
1	B	400/423 (95%)	383 (96%)	17 (4%)	0	100	100
1	C	400/423 (95%)	384 (96%)	16 (4%)	0	100	100
1	D	401/423 (95%)	384 (96%)	16 (4%)	1 (0%)	43	28
All	All	1602/1692 (95%)	1534 (96%)	66 (4%)	2 (0%)	48	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	381	MET
1	D	381	MET

5.3.2 Protein sidechains ⓘ

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	328/354 (93%)	325 (99%)	3 (1%)	70	62
1	B	324/354 (92%)	322 (99%)	2 (1%)	78	72
1	C	318/354 (90%)	317 (100%)	1 (0%)	86	83
1	D	324/354 (92%)	323 (100%)	1 (0%)	86	83
All	All	1294/1416 (91%)	1287 (100%)	7 (0%)	81	76

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ASP
1	A	174	GLN
1	A	280	HIS
1	B	41	ASP
1	B	280	HIS
1	C	280	HIS
1	D	280	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	B	69	GLN
1	B	161	HIS
1	C	53	HIS
1	D	53	HIS
1	D	157	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 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	$\# Z > 2$
4	FLV	C	1005[C]	-	16,16,16	0.36	0	22,24,24	0.62	0
4	FLV	D	1002[B]	-	16,16,16	0.35	0	22,24,24	0.59	0
3	PGE	A	1002	-	9,9,9	0.17	0	8,8,8	0.15	0
5	EDO	B	1002	-	3,3,3	0.08	0	2,2,2	0.25	0
2	QW8	D	1001[A]	-	15,15,15	0.42	0	22,22,22	0.47	0
5	EDO	C	1003	-	3,3,3	0.09	0	2,2,2	0.21	0
4	FLV	A	1004[C]	-	16,16,16	0.35	0	22,24,24	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FLV	B	1003[B]	-	16,16,16	0.36	0	22,24,24	0.59	0
4	FLV	D	1003[C]	-	16,16,16	0.35	0	22,24,24	0.54	0
4	FLV	A	1003[B]	-	16,16,16	0.35	0	22,24,24	0.59	0
4	FLV	C	1004[B]	-	16,16,16	0.37	0	22,24,24	0.55	0
2	QW8	B	1001[A]	-	15,15,15	0.42	0	22,22,22	0.50	0
2	QW8	A	1001[A]	-	15,15,15	0.42	0	22,22,22	0.46	0
4	FLV	B	1004[C]	-	16,16,16	0.36	0	22,24,24	0.61	0
3	PGE	C	1002	-	9,9,9	0.13	0	8,8,8	0.16	0
2	QW8	C	1001[A]	-	15,15,15	0.40	0	22,22,22	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FLV	C	1005[C]	-	-	-	0/2/2/2
2	QW8	C	1001[A]	-	-	-	0/2/2/2
4	FLV	D	1002[B]	-	-	-	0/2/2/2
3	PGE	A	1002	-	-	4/7/7/7	-
5	EDO	C	1003	-	-	1/1/1/1	-
2	QW8	D	1001[A]	-	-	-	0/2/2/2
4	FLV	A	1004[C]	-	-	-	0/2/2/2
4	FLV	B	1003[B]	-	-	-	0/2/2/2
4	FLV	D	1003[C]	-	-	-	0/2/2/2
4	FLV	A	1003[B]	-	-	-	0/2/2/2
4	FLV	C	1004[B]	-	-	-	0/2/2/2
2	QW8	B	1001[A]	-	-	-	0/2/2/2
2	QW8	A	1001[A]	-	-	-	0/2/2/2
4	FLV	B	1004[C]	-	-	-	0/2/2/2
3	PGE	C	1002	-	-	4/7/7/7	-
5	EDO	B	1002	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1002	PGE	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
3	C	1002	PGE	O3-C5-C6-O4
3	A	1002	PGE	C4-C3-O2-C2
3	C	1002	PGE	C6-C5-O3-C4
3	C	1002	PGE	C1-C2-O2-C3
5	C	1003	EDO	O1-C1-C2-O2
3	A	1002	PGE	O3-C5-C6-O4
3	A	1002	PGE	O2-C3-C4-O3
3	A	1002	PGE	C6-C5-O3-C4

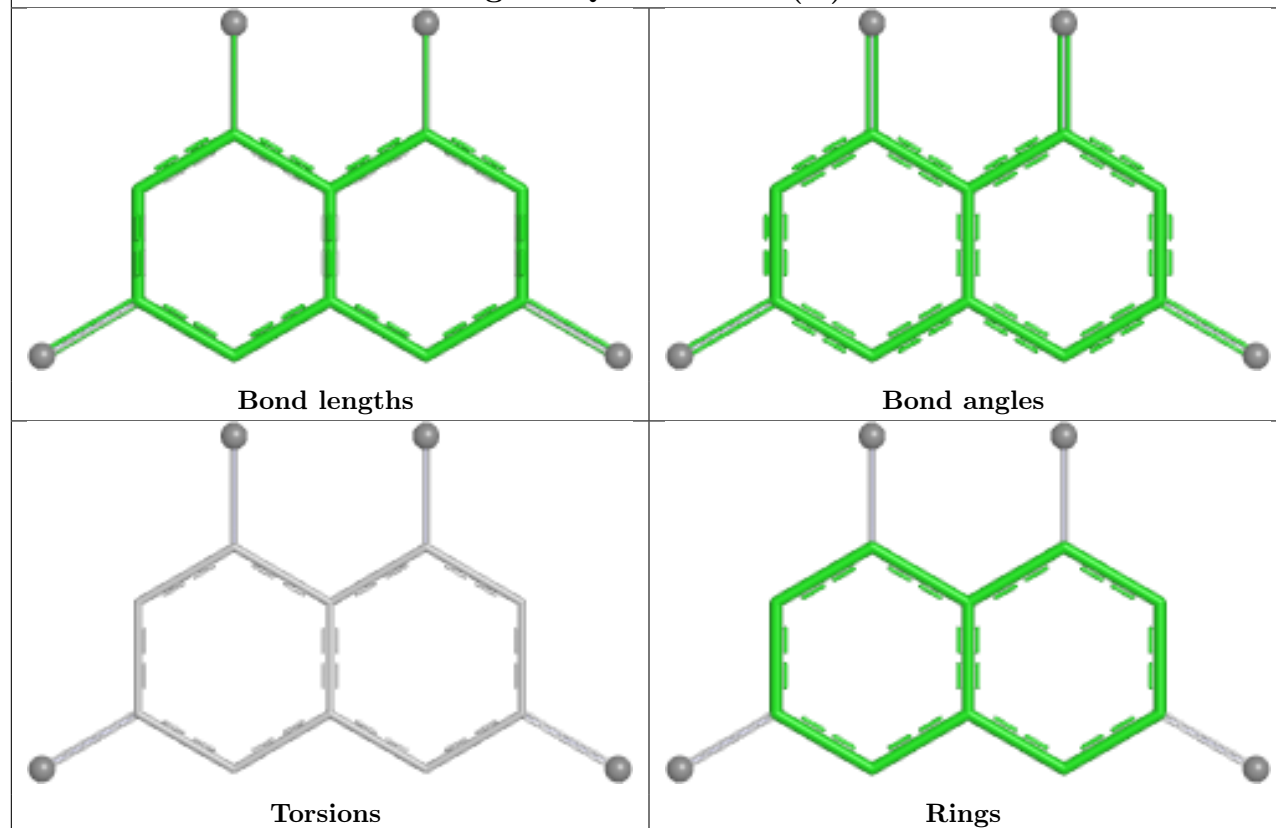
There are no ring outliers.

2 monomers are involved in 11 short contacts:

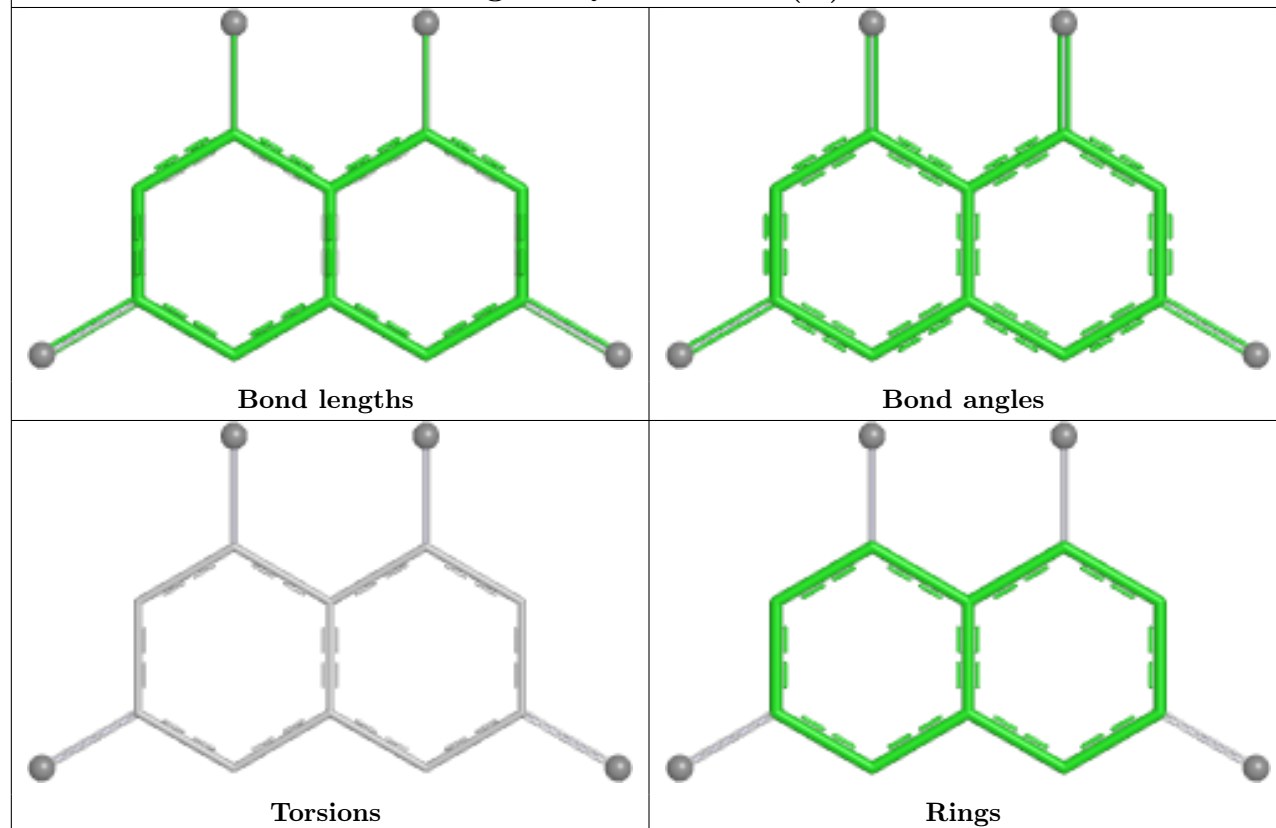
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1003	EDO	6	0
3	C	1002	PGE	7	0

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 than 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.

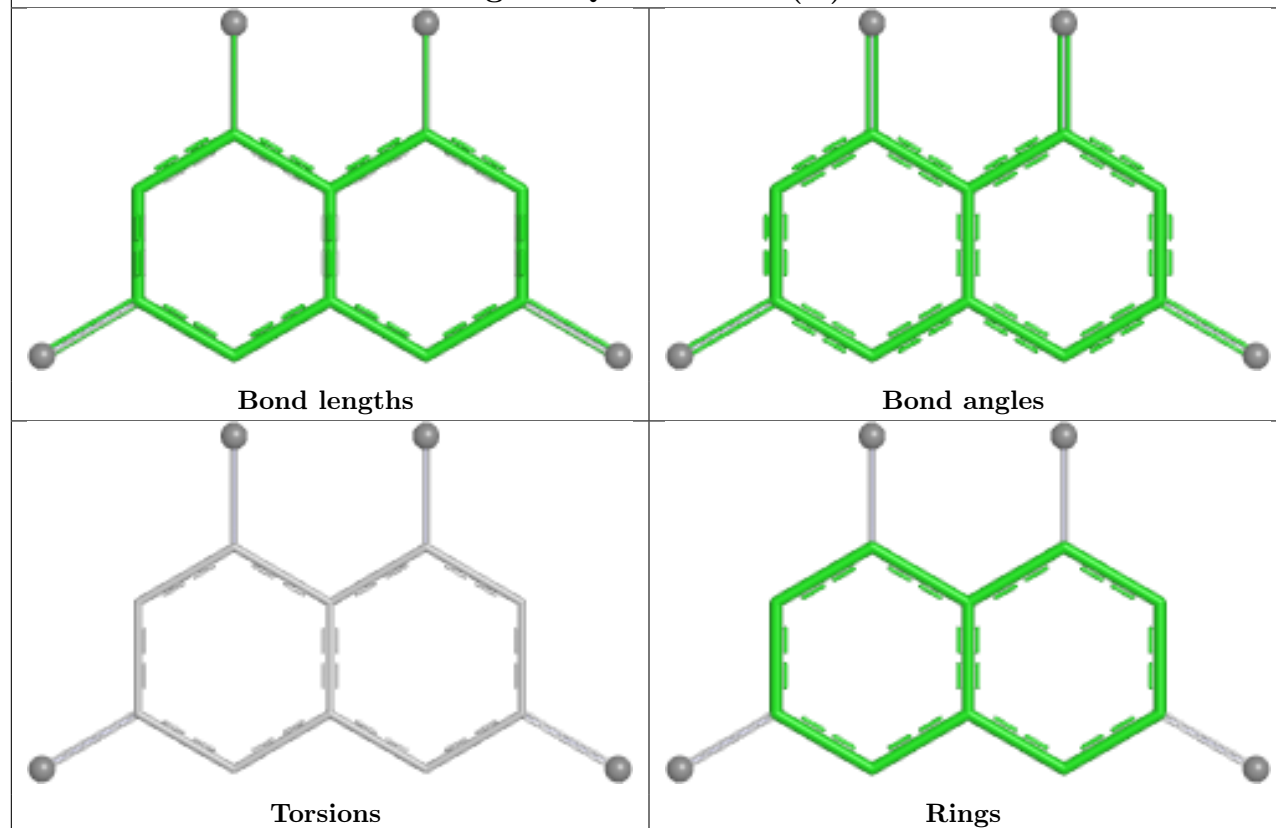
Ligand QW8 D 1001 (A)



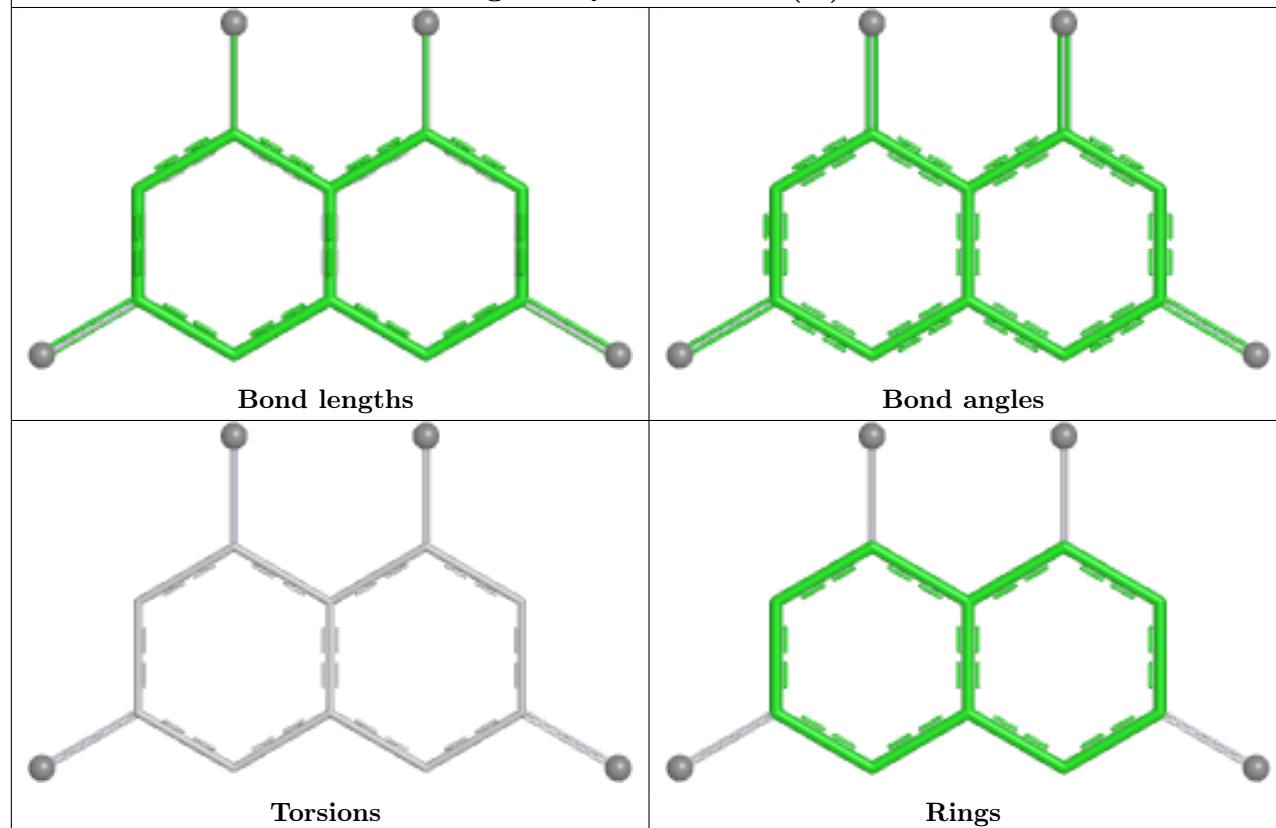
Ligand QW8 B 1001 (A)



Ligand QW8 A 1001 (A)



Ligand QW8 C 1001 (A)



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, 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	398/423 (94%)	0.92	34 (8%) 16 17	8, 20, 29, 35	5 (1%)
1	B	398/423 (94%)	1.11	46 (11%) 9 9	8, 22, 33, 38	4 (1%)
1	C	398/423 (94%)	1.11	42 (10%) 11 11	9, 22, 31, 38	4 (1%)
1	D	398/423 (94%)	0.95	37 (9%) 14 15	13, 21, 29, 38	5 (1%)
All	All	1592/1692 (94%)	1.02	159 (9%) 12 13	8, 21, 31, 38	18 (1%)

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	400	SER	4.9
1	C	30	PHE	4.3
1	B	399	ALA	4.1
1	A	30	PHE	4.0
1	B	80	GLU	4.0
1	B	30	PHE	3.7
1	A	399	ALA	3.6
1	C	387	LEU	3.6
1	A	121	ILE	3.6
1	D	55	ILE	3.3
1	C	86	LEU	3.3
1	C	124	VAL	3.3
1	B	175	SER	3.3
1	C	51	PHE	3.3
1	B	69	GLN	3.2
1	B	400	SER	3.2
1	D	377	GLY	3.2
1	C	156	GLY	3.1
1	C	56	SER	3.1
1	C	62	ALA	3.0
1	C	159	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	93	GLU	3.0
1	D	45	GLU	3.0
1	B	11	ASP	3.0
1	B	155	THR	2.9
1	D	134	LEU	2.9
1	B	274	LEU	2.9
1	A	387	LEU	2.9
1	A	320	GLU	2.9
1	C	45	GLU	2.9
1	D	30	PHE	2.8
1	A	175	SER	2.8
1	D	73	PRO	2.8
1	A	119	ASN	2.8
1	B	333	GLU	2.8
1	B	355	VAL	2.8
1	C	59	ILE	2.8
1	B	3	ARG	2.7
1	B	253	VAL	2.7
1	D	11	ASP	2.7
1	A	118	PRO	2.7
1	C	119	ASN	2.7
1	B	55	ILE	2.7
1	C	69	GLN	2.6
1	C	152	THR	2.6
1	A	237	LEU	2.6
1	B	325	ALA	2.6
1	D	119	ASN	2.6
1	D	54	LEU	2.6
1	B	252	VAL	2.6
1	D	22	VAL	2.6
1	A	94	ALA	2.6
1	B	140	TRP	2.6
1	D	49	PRO	2.6
1	A	69	GLN	2.5
1	A	87	GLN	2.5
1	A	154	ARG	2.5
1	D	27[A]	ARG	2.5
1	A	115	ILE	2.5
1	B	156	GLY	2.5
1	C	116	THR	2.5
1	B	110	PHE	2.5
1	A	153	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	384	PRO	2.5
1	B	22	VAL	2.5
1	B	104	VAL	2.5
1	B	226	PRO	2.5
1	A	116	THR	2.5
1	B	199	HIS	2.5
1	A	327	LYS	2.5
1	B	52	ASN	2.5
1	A	131	GLN	2.5
1	D	110	PHE	2.5
1	D	364	PHE	2.5
1	C	221	ALA	2.5
1	C	244	PRO	2.5
1	D	293	LEU	2.4
1	D	118	PRO	2.4
1	B	308	ALA	2.4
1	C	308	ALA	2.4
1	B	144	ILE	2.4
1	B	27[A]	ARG	2.4
1	A	377	GLY	2.4
1	C	157	ASN	2.4
1	A	272	ASP	2.4
1	D	88	ALA	2.4
1	A	156	GLY	2.3
1	B	157	ASN	2.3
1	D	400	SER	2.3
1	B	49	PRO	2.3
1	C	82	ALA	2.3
1	C	88	ALA	2.3
1	D	121	ILE	2.3
1	B	36	VAL	2.3
1	C	385	ASN	2.3
1	B	26	SER	2.3
1	B	24	TRP	2.3
1	B	283	GLY	2.3
1	C	117	LYS	2.3
1	B	224	ALA	2.3
1	B	78	LEU	2.3
1	D	86	LEU	2.3
1	A	93	GLU	2.3
1	B	43	SER	2.3
1	D	44	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	355	VAL	2.3
1	D	69	GLN	2.2
1	C	145	ARG	2.2
1	C	78	LEU	2.2
1	C	238	SER	2.2
1	C	382	GLY	2.2
1	D	171	GLY	2.2
1	A	315	TYR	2.2
1	B	301	TYR	2.2
1	C	305	ILE	2.2
1	B	103	VAL	2.2
1	C	397	VAL	2.2
1	A	140	TRP	2.2
1	A	26	SER	2.2
1	B	23	LEU	2.2
1	D	23	LEU	2.2
1	D	387	LEU	2.2
1	D	318	VAL	2.2
1	C	224	ALA	2.2
1	D	132	ALA	2.2
1	D	398	LEU	2.2
1	C	126	PHE	2.2
1	D	385	ASN	2.2
1	C	67	TYR	2.2
1	D	92	GLU	2.1
1	B	102	ALA	2.1
1	C	140	TRP	2.1
1	A	176	ASN	2.1
1	B	10	PHE	2.1
1	A	45	GLU	2.1
1	A	59	ILE	2.1
1	C	121	ILE	2.1
1	C	153	TYR	2.1
1	C	85	ALA	2.1
1	B	152	THR	2.1
1	D	62	ALA	2.1
1	D	277	ALA	2.1
1	C	398	LEU	2.1
1	B	118	PRO	2.1
1	A	9	LYS	2.1
1	B	303	PHE	2.1
1	C	44	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	392	GLU	2.0
1	B	318	VAL	2.0
1	C	318	VAL	2.0
1	D	344	LEU	2.0
1	C	317	THR	2.0
1	C	223	PRO	2.0
1	C	171	GLY	2.0
1	D	156	GLY	2.0
1	A	85	ALA	2.0
1	A	224	ALA	2.0
1	A	236	VAL	2.0
1	D	181	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	FLV	A	1004[C]	15/15	0.53	0.17	27,28,28,28	15
4	FLV	D	1003[C]	15/15	0.65	0.21	25,26,27,27	15
4	FLV	C	1005[C]	15/15	0.66	0.13	22,24,24,25	15
4	FLV	B	1004[C]	15/15	0.66	0.17	25,26,26,28	15
4	FLV	D	1002[B]	15/15	0.68	0.18	23,24,24,25	15
3	PGE	A	1002	10/10	0.70	0.19	32,33,34,34	0
4	FLV	C	1004[B]	15/15	0.74	0.12	24,25,25,27	15
3	PGE	C	1002	10/10	0.75	0.16	22,26,30,30	0
5	EDO	B	1002	4/4	0.80	0.16	22,23,25,27	0
4	FLV	B	1003[B]	15/15	0.83	0.16	26,26,27,28	15
2	QW8	D	1001[A]	14/14	0.85	0.13	20,22,22,23	14

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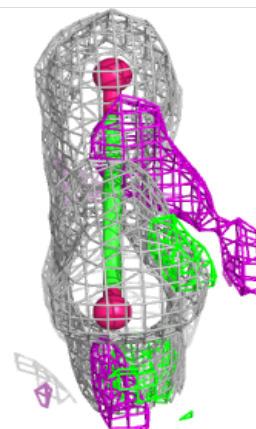
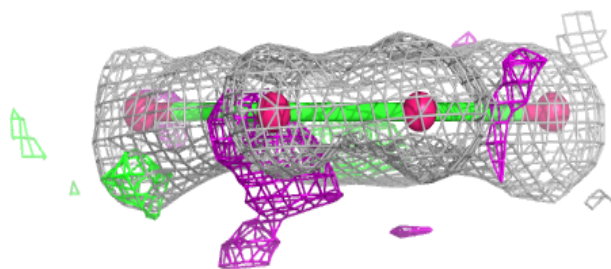
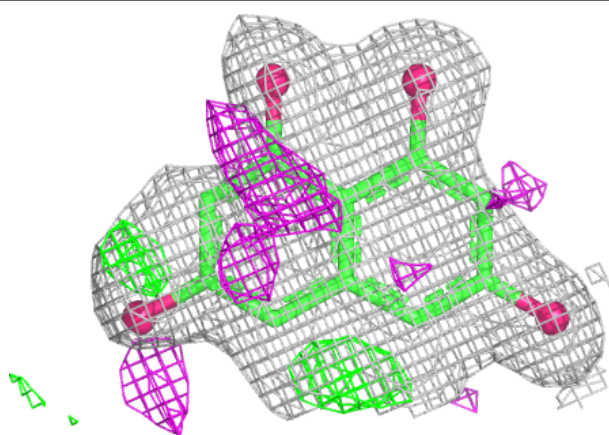
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FLV	A	1003[B]	15/15	0.85	0.11	24,24,25,25	15
5	EDO	C	1003	4/4	0.87	0.23	25,26,26,27	0
2	QW8	C	1001[A]	14/14	0.88	0.11	25,26,28,31	14
2	QW8	B	1001[A]	14/14	0.91	0.10	21,22,23,25	14
2	QW8	A	1001[A]	14/14	0.94	0.08	19,20,21,21	14

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.

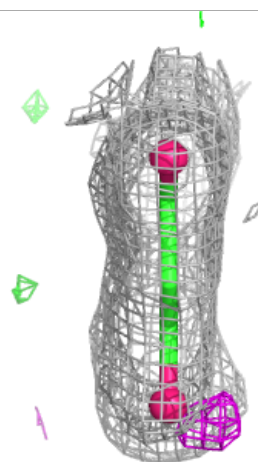
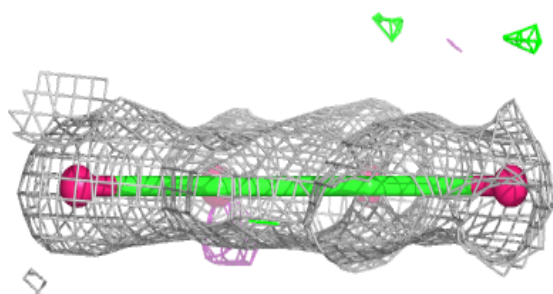
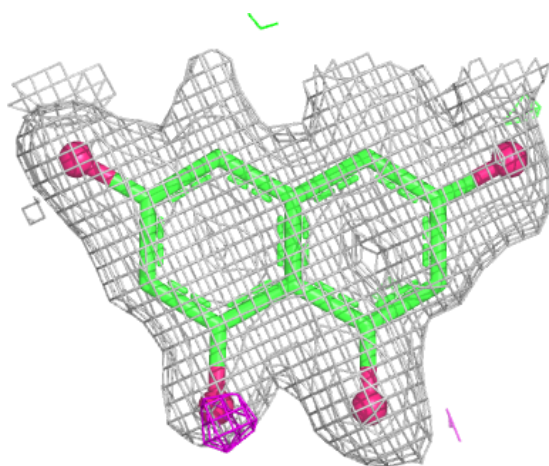
Electron density around QW8 D 1001 (A):

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



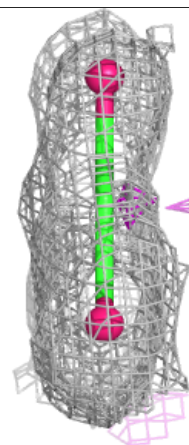
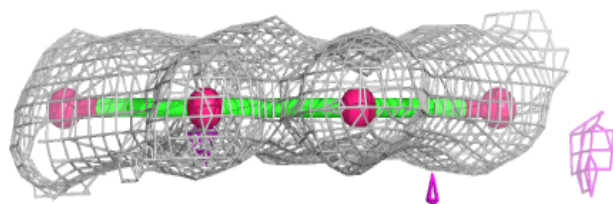
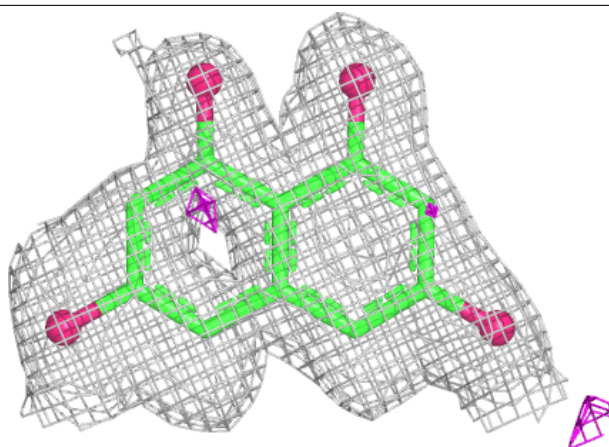
Electron density around QW8 C 1001 (A):

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



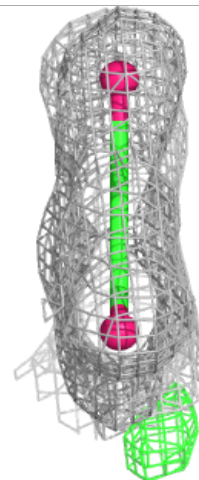
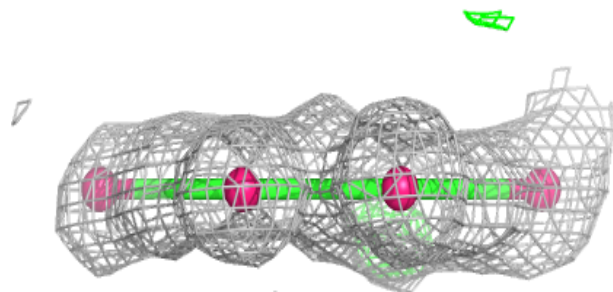
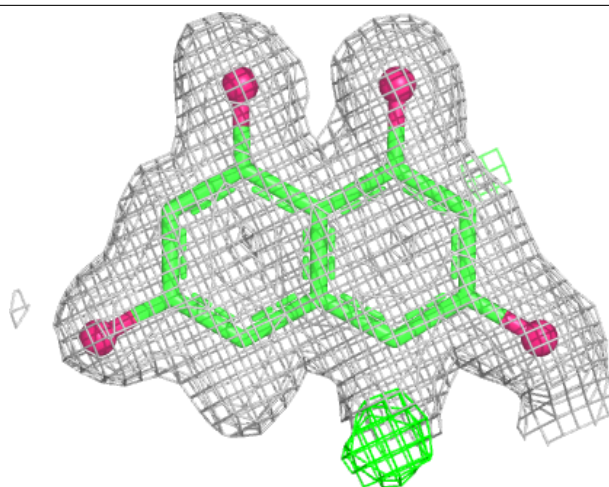
Electron density around QW8 B 1001 (A):

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



Electron density around QW8 A 1001 (A):

$2mF_o-DF_c$ (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.