Full wwPDB X-ray Structure Validation Report (i)

Jan 3, 2024 – 07:57 pm GMT

PDB ID	:	5K32
Title	:	PDE4D crystal structure in complex with small molecule inhibitor
Authors	:	Segarra, V.; Hernandez, B.; Roberts, R.; Gracia, J.; Soler, M.; Bonin, I.; Aymami, J.
Deposited on	:	2016-05-19
Resolution	:	1.99 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

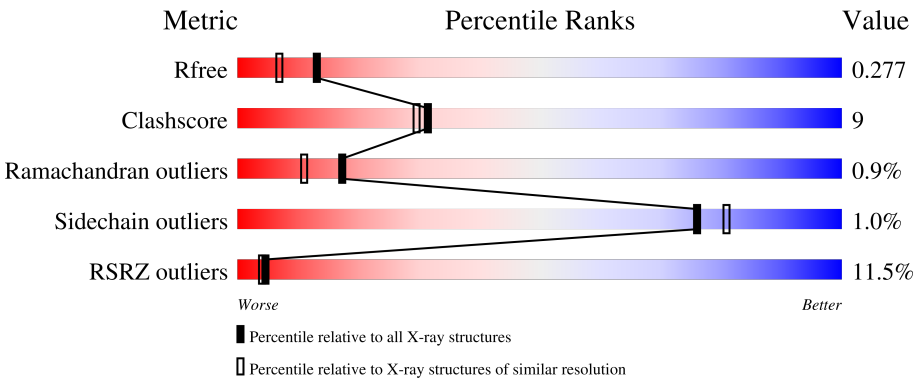
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	325	13% 76% 21% ••
1	B	325	10% 80% 17% ••

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
5	EDO	B	1019	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5879 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 cAMP-specific 3',5'-cyclic phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	322	2617	1656	447	499	15	4	2	0
1	B	321	2607	1651	446	496	14	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	87	ALA	-	expression tag	UNP Q08499
B	87	ALA	-	expression tag	UNP Q08499

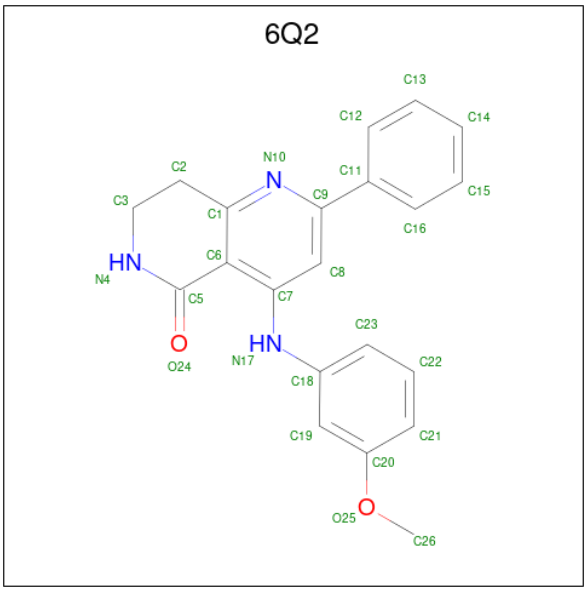
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

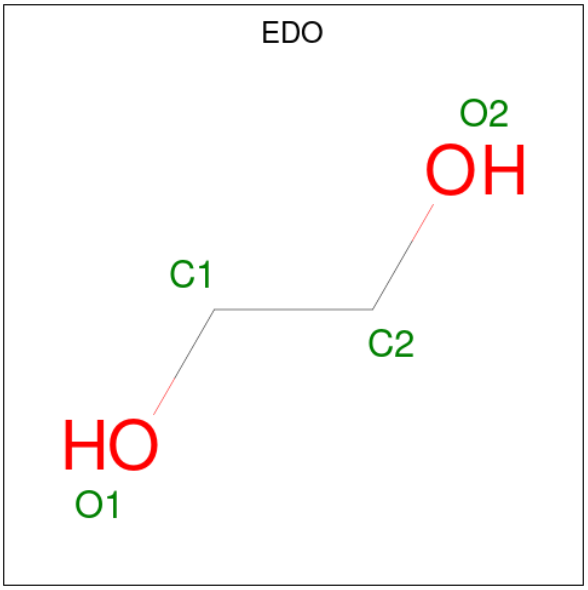
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0
3	B	1	1	1	0	0

- Molecule 4 is 4-[(3-methoxyphenyl)amino]-2-phenyl-7,8-dihydro-1,6-naphthyridin-5(6H)-one (three-letter code: 6Q2) (formula: $C_{21}H_{19}N_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	26	21	3	2	0	0
			Total	C	N	O		
4	B	1	26	21	3	2	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

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

- Molecule 6 is water.

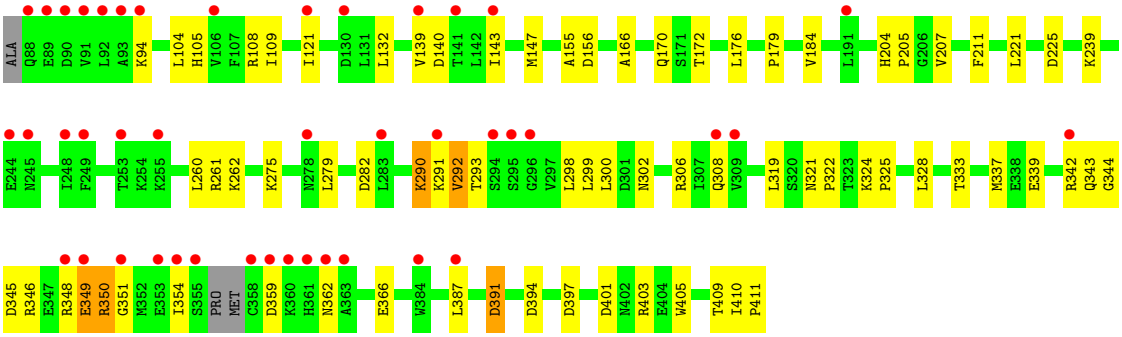
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	236	236	236	0	0
			Total	O		
6	B	235	235	235	0	0

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.

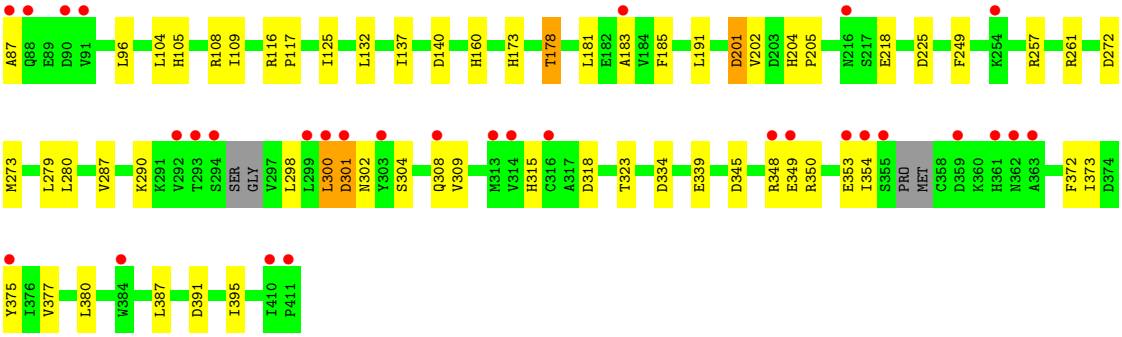
• Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain A:



• Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	59.97Å 79.74Å 163.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.99 19.42 – 1.99	Depositor EDS
% Data completeness (in resolution range)	94.5 (20.00-1.99) 94.5 (19.42-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.220 , 0.281 0.213 , 0.277	Depositor DCC
R_{free} test set	2627 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	29.3	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 60.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5879	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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: EDO, ZN, 6Q2, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.96	0/2674	0.91	5/3630 (0.1%)
1	B	1.04	1/2660 (0.0%)	0.95	10/3611 (0.3%)
All	All	1.00	1/5334 (0.0%)	0.93	15/7241 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	202	VAL	CB-CG1	6.59	1.66	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	319	LEU	CB-CG-CD1	-7.64	98.01	111.00
1	B	201	ASP	CB-CG-OD1	6.95	124.55	118.30
1	B	261	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	B	225	ASP	CB-CG-OD1	6.55	124.19	118.30
1	B	334	ASP	CB-CG-OD1	6.40	124.06	118.30
1	A	279	LEU	CA-CB-CG	5.96	129.01	115.30
1	B	391	ASP	CB-CG-OD1	5.80	123.52	118.30
1	B	318	ASP	CB-CG-OD1	5.74	123.46	118.30
1	A	403	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	B	272	ASP	CB-CG-OD1	5.46	123.21	118.30
1	B	345	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	A	391	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	397	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	B	279	LEU	CA-CB-CG	5.25	127.37	115.30
1	B	96	LEU	CB-CG-CD1	-5.01	102.47	111.00

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	2617	0	2574	54	0
1	B	2607	0	2565	40	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	26	0	0	0	0
4	B	26	0	0	0	0
5	A	64	0	96	12	0
5	B	64	0	96	12	0
6	A	236	0	0	5	0
6	B	235	0	0	5	0
All	All	5879	0	5331	96	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 9.

All (96) 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:183:ALA:HA	5:B:1019:EDO:H22	1.48	0.94
1:A:155:ALA:HA	5:A:1007:EDO:H11	1.50	0.89
1:A:401:ASP:OD2	6:A:1101:HOH:O	1.93	0.86
1:A:299:LEU:CD1	5:A:1016:EDO:H11	2.09	0.82
1:A:94:LYS:HB2	6:A:1253:HOH:O	1.86	0.76
1:A:299:LEU:HD11	5:A:1016:EDO:H11	1.67	0.75
1:B:105:HIS:HB3	1:B:108:ARG:HD2	1.73	0.71
1:A:348:ARG:HG2	1:A:354:ILE:HG12	1.70	0.70
1:B:300:LEU:HA	1:B:301:ASP:CB	2.23	0.69
1:A:184:VAL:HG11	1:A:300:LEU:HD12	1.75	0.69
1:B:375:TYR:HE1	5:B:1010:EDO:H12	1.57	0.68
1:A:339:GLU:OE2	5:A:1010:EDO:H21	1.94	0.68
1:A:179:PRO:HB2	1:A:391:ASP:OD2	1.94	0.67
5:B:1016:EDO:H22	6:B:1303:HOH:O	1.96	0.66
5:B:1019:EDO:H12	6:B:1116:HOH:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:LEU:CD1	5:A:1016:EDO:C1	2.75	0.63
1:A:105:HIS:HB3	1:A:108:ARG:HD3	1.80	0.63
1:B:300:LEU:HA	1:B:301:ASP:HB2	1.80	0.62
1:B:372:PHE:HA	5:B:1012:EDO:H21	1.81	0.61
5:B:1016:EDO:C2	6:B:1303:HOH:O	2.49	0.61
1:B:132:LEU:HD23	1:B:137:ILE:HB	1.83	0.60
1:A:291:LYS:O	1:A:292:VAL:HG22	2.02	0.59
1:B:373:ILE:HA	1:B:377:VAL:HB	1.86	0.58
1:B:375:TYR:CE1	5:B:1010:EDO:H12	2.39	0.58
1:A:261:ARG:NH1	6:A:1106:HOH:O	2.36	0.57
1:B:185:PHE:HZ	1:B:309:VAL:CG1	2.17	0.57
1:B:201:ASP:O	1:B:204:HIS:HB2	2.05	0.57
1:B:287:VAL:O	1:B:290:LYS:HB2	2.03	0.57
1:A:298:LEU:HD11	1:A:387:LEU:HG	1.87	0.56
1:B:191:LEU:HD21	1:B:249:PHE:HE1	1.72	0.55
1:A:121:ILE:HD12	1:A:166:ALA:HB1	1.88	0.55
1:B:183:ALA:CA	5:B:1019:EDO:H22	2.32	0.55
1:B:191:LEU:HD21	1:B:249:PHE:CE1	2.44	0.53
1:A:239:LYS:NZ	1:B:218:GLU:OE2	2.42	0.53
1:B:185:PHE:O	5:B:1019:EDO:H21	2.09	0.53
1:A:325:PRO:HD2	1:A:328:LEU:HD12	1.91	0.53
1:A:349:GLU:C	1:A:351:GLY:H	2.13	0.52
1:B:257:ARG:HB3	5:B:1006:EDO:H11	1.91	0.51
1:B:125:ILE:HD13	1:B:173:HIS:HB2	1.92	0.51
1:A:104:LEU:HD22	1:A:170:GLN:HG3	1.93	0.50
1:A:348:ARG:NH2	1:A:359:ASP:OD1	2.44	0.50
1:B:125:ILE:HD13	1:B:173:HIS:CB	2.42	0.50
1:A:156:ASP:O	1:A:342:ARG:NH2	2.44	0.50
1:B:301:ASP:OD2	1:B:302:ASN:ND2	2.44	0.50
1:A:349:GLU:O	1:A:351:GLY:N	2.45	0.49
1:A:290:LYS:NZ	6:A:1102:HOH:O	2.28	0.49
1:B:218:GLU:OE2	6:B:1101:HOH:O	2.20	0.49
1:A:205:PRO:HB3	5:A:1012:EDO:H21	1.95	0.49
1:A:324:LYS:HB3	1:A:325:PRO:HD2	1.95	0.49
1:B:160:HIS:HD2	1:B:201:ASP:OD2	1.96	0.49
1:A:207:VAL:HG21	1:A:211:PHE:CD1	2.48	0.48
1:B:298:LEU:HD11	1:B:387:LEU:HG	1.96	0.48
1:A:282:ASP:HB3	1:A:308:GLN:HE21	1.78	0.48
1:B:304:SER:O	1:B:308:GLN:HG3	2.14	0.48
1:B:348:ARG:C	1:B:350:ARG:H	2.17	0.48
1:A:321:ASN:N	1:A:322:PRO:CD	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:ASP:HB2	6:A:1266:HOH:O	2.13	0.48
1:A:204:HIS:CE1	5:A:1010:EDO:H12	2.50	0.47
1:A:204:HIS:HE1	5:A:1010:EDO:H12	1.79	0.47
1:A:155:ALA:CA	5:A:1007:EDO:H11	2.35	0.47
1:B:116:ARG:N	1:B:117:PRO:CD	2.78	0.46
1:A:333:THR:O	1:A:337:MET:HG2	2.15	0.46
1:B:185:PHE:HZ	1:B:309:VAL:HG11	1.81	0.46
1:A:293:THR:CG2	1:A:299:LEU:HD21	2.46	0.46
1:A:346:ARG:O	1:A:350:ARG:HD2	2.16	0.46
1:B:87:ALA:N	6:B:1122:HOH:O	2.49	0.45
1:B:300:LEU:HA	1:B:301:ASP:HB3	1.98	0.45
1:A:260:LEU:C	1:A:260:LEU:HD23	2.37	0.45
1:B:348:ARG:HB2	1:B:354:ILE:HD11	1.99	0.45
1:A:345:ASP:O	1:A:349:GLU:HB2	2.16	0.44
1:A:172:THR:HG22	1:A:176:LEU:HD12	2.00	0.44
1:B:323:THR:HB	1:B:395:ILE:HG23	1.99	0.44
1:B:178:THR:CG2	1:B:181:LEU:HG	2.47	0.44
1:A:302:ASN:O	1:A:306:ARG:HG3	2.18	0.44
1:A:359:ASP:OD2	1:A:362:ASN:HB2	2.16	0.44
1:A:410:ILE:HA	1:A:411:PRO:HD3	1.88	0.44
1:B:353:GLU:HG2	1:B:354:ILE:N	2.33	0.44
1:A:139:VAL:HG13	1:A:140:ASP:N	2.32	0.43
1:A:207:VAL:HA	1:A:343:GLN:OE1	2.19	0.43
1:A:324:LYS:HB3	1:A:325:PRO:CD	2.48	0.43
1:B:205:PRO:HD3	5:B:1015:EDO:H11	2.01	0.43
1:A:143:ILE:O	1:A:147[B]:MET:HG2	2.19	0.43
1:B:273:MET:SD	1:B:315:HIS:HE1	2.41	0.42
1:B:104:LEU:HD11	1:B:109:ILE:HD11	2.01	0.42
1:A:139:VAL:CG1	1:A:140:ASP:N	2.83	0.42
1:B:300:LEU:CA	1:B:301:ASP:CB	2.95	0.42
1:A:344:GLY:O	1:A:348:ARG:HG3	2.20	0.42
1:A:405:TRP:HH2	5:A:1017:EDO:H21	1.84	0.41
1:A:300:LEU:O	1:A:306:ARG:NH1	2.49	0.41
1:A:366:GLU:HG2	1:A:409:THR:OG1	2.21	0.41
1:B:339:GLU:OE2	5:B:1011:EDO:H21	2.21	0.41
1:A:105:HIS:O	1:A:109:ILE:HD12	2.21	0.41
1:A:184:VAL:CG1	1:A:300:LEU:HD12	2.48	0.40
1:A:275:LYS:HE2	5:A:1019:EDO:H12	2.03	0.40
1:B:280:LEU:HD13	1:B:380:LEU:HA	2.01	0.40
1:A:262:LYS:HG3	5:A:1004:EDO:H22	2.01	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	320/325 (98%)	299 (93%)	17 (5%)	4 (1%)	12 6
1	B	316/325 (97%)	306 (97%)	8 (2%)	2 (1%)	25 19
All	All	636/650 (98%)	605 (95%)	25 (4%)	6 (1%)	17 11

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	349	GLU
1	A	350	ARG
1	B	301	ASP
1	A	292	VAL
1	B	349	GLU
1	A	225	ASP

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	296/296 (100%)	293 (99%)	3 (1%)	76 81
1	B	294/296 (99%)	291 (99%)	3 (1%)	76 81
All	All	590/592 (100%)	584 (99%)	6 (1%)	76 81

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	LEU
1	A	221	LEU
1	A	290	LYS
1	B	140	ASP
1	B	178	THR
1	B	300	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	369	GLN
1	B	105	HIS
1	B	369	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 38 ligands modelled in this entry, 4 are monoatomic - leaving 34 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	$\#\|Z\| > 2$
5	EDO	A	1017	-	3,3,3	0.59	0	2,2,2	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	6Q2	B	1003	-	28,29,29	1.48	6 (21%)	37,40,40	1.49	6 (16%)
5	EDO	A	1014	-	3,3,3	0.57	0	2,2,2	0.30	0
5	EDO	B	1011	-	3,3,3	0.57	0	2,2,2	0.36	0
5	EDO	B	1019	-	3,3,3	0.38	0	2,2,2	0.47	0
5	EDO	A	1010	-	3,3,3	0.56	0	2,2,2	0.40	0
5	EDO	B	1017	-	3,3,3	0.72	0	2,2,2	0.21	0
4	6Q2	A	1003	-	28,29,29	0.99	1 (3%)	37,40,40	1.41	4 (10%)
5	EDO	A	1006	-	3,3,3	0.50	0	2,2,2	1.07	0
5	EDO	B	1005	-	3,3,3	0.55	0	2,2,2	0.69	0
5	EDO	B	1009	-	3,3,3	0.56	0	2,2,2	0.79	0
5	EDO	B	1006	-	3,3,3	0.59	0	2,2,2	0.08	0
5	EDO	B	1008	-	3,3,3	0.50	0	2,2,2	0.37	0
5	EDO	B	1010	-	3,3,3	0.37	0	2,2,2	0.69	0
5	EDO	B	1018	-	3,3,3	0.56	0	2,2,2	0.32	0
5	EDO	B	1004	-	3,3,3	0.53	0	2,2,2	0.18	0
5	EDO	A	1008	-	3,3,3	0.31	0	2,2,2	0.57	0
5	EDO	A	1007	-	3,3,3	0.31	0	2,2,2	0.76	0
5	EDO	B	1015	-	3,3,3	0.65	0	2,2,2	0.15	0
5	EDO	B	1016	-	3,3,3	0.59	0	2,2,2	0.24	0
5	EDO	B	1007	-	3,3,3	0.76	0	2,2,2	0.56	0
5	EDO	A	1009	-	3,3,3	0.56	0	2,2,2	0.78	0
5	EDO	A	1018	-	3,3,3	0.76	0	2,2,2	0.49	0
5	EDO	A	1004	-	3,3,3	0.58	0	2,2,2	0.12	0
5	EDO	A	1012	-	3,3,3	0.56	0	2,2,2	0.10	0
5	EDO	B	1013	-	3,3,3	0.47	0	2,2,2	0.29	0
5	EDO	B	1014	-	3,3,3	0.40	0	2,2,2	0.57	0
5	EDO	A	1015	-	3,3,3	0.39	0	2,2,2	0.63	0
5	EDO	A	1016	-	3,3,3	0.64	0	2,2,2	0.41	0
5	EDO	B	1012	-	3,3,3	0.66	0	2,2,2	0.26	0
5	EDO	A	1005	-	3,3,3	0.37	0	2,2,2	0.50	0
5	EDO	A	1011	-	3,3,3	0.63	0	2,2,2	0.27	0
5	EDO	A	1013	-	3,3,3	0.51	0	2,2,2	0.39	0
5	EDO	A	1019	-	3,3,3	0.60	0	2,2,2	0.39	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
5	EDO	A	1017	-	-	1/1/1/1	-
4	6Q2	B	1003	-	-	4/10/20/20	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	1014	-	-	1/1/1/1	-
5	EDO	B	1011	-	-	1/1/1/1	-
5	EDO	B	1019	-	-	1/1/1/1	-
5	EDO	A	1010	-	-	1/1/1/1	-
5	EDO	B	1017	-	-	1/1/1/1	-
4	6Q2	A	1003	-	-	0/10/20/20	0/4/4/4
5	EDO	A	1006	-	-	1/1/1/1	-
5	EDO	B	1005	-	-	0/1/1/1	-
5	EDO	B	1009	-	-	1/1/1/1	-
5	EDO	B	1006	-	-	0/1/1/1	-
5	EDO	B	1008	-	-	1/1/1/1	-
5	EDO	B	1010	-	-	1/1/1/1	-
5	EDO	B	1018	-	-	1/1/1/1	-
5	EDO	B	1004	-	-	0/1/1/1	-
5	EDO	A	1008	-	-	1/1/1/1	-
5	EDO	A	1007	-	-	1/1/1/1	-
5	EDO	B	1015	-	-	1/1/1/1	-
5	EDO	B	1016	-	-	1/1/1/1	-
5	EDO	B	1007	-	-	1/1/1/1	-
5	EDO	A	1009	-	-	0/1/1/1	-
5	EDO	A	1018	-	-	1/1/1/1	-
5	EDO	A	1004	-	-	1/1/1/1	-
5	EDO	A	1012	-	-	1/1/1/1	-
5	EDO	B	1013	-	-	0/1/1/1	-
5	EDO	B	1014	-	-	1/1/1/1	-
5	EDO	A	1015	-	-	1/1/1/1	-
5	EDO	A	1016	-	-	1/1/1/1	-
5	EDO	B	1012	-	-	1/1/1/1	-
5	EDO	A	1005	-	-	0/1/1/1	-
5	EDO	A	1011	-	-	1/1/1/1	-
5	EDO	A	1013	-	-	0/1/1/1	-
5	EDO	A	1019	-	-	1/1/1/1	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1003	6Q2	C19-C20	3.25	1.44	1.38
4	A	1003	6Q2	C6-C1	-2.89	1.37	1.41
4	B	1003	6Q2	C6-C5	2.80	1.52	1.47
4	B	1003	6Q2	C19-C18	2.63	1.43	1.39
4	B	1003	6Q2	C1-N10	2.28	1.38	1.34
4	B	1003	6Q2	C6-C1	-2.26	1.38	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1003	6Q2	C9-N10	2.09	1.38	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1003	6Q2	O24-C5-C6	-3.61	116.42	123.98
4	B	1003	6Q2	C2-C1-N10	3.41	120.40	115.85
4	A	1003	6Q2	C2-C1-N10	3.23	120.17	115.85
4	A	1003	6Q2	C26-O25-C20	3.04	124.11	117.51
4	B	1003	6Q2	C8-C9-N10	-2.97	118.82	122.35
4	B	1003	6Q2	O24-C5-C6	-2.66	118.40	123.98
4	B	1003	6Q2	C9-N10-C1	2.63	120.64	118.35
4	B	1003	6Q2	C23-C18-C19	-2.35	116.86	119.65
4	A	1003	6Q2	C6-C1-N10	-2.31	120.27	122.83
4	B	1003	6Q2	C26-O25-C20	2.11	122.08	117.51

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1014	EDO	O1-C1-C2-O2
5	A	1006	EDO	O1-C1-C2-O2
5	A	1010	EDO	O1-C1-C2-O2
5	A	1011	EDO	O1-C1-C2-O2
5	A	1016	EDO	O1-C1-C2-O2
5	A	1018	EDO	O1-C1-C2-O2
5	B	1009	EDO	O1-C1-C2-O2
5	B	1011	EDO	O1-C1-C2-O2
5	B	1012	EDO	O1-C1-C2-O2
5	B	1014	EDO	O1-C1-C2-O2
5	B	1016	EDO	O1-C1-C2-O2
4	B	1003	6Q2	C16-C11-C9-N10
5	A	1004	EDO	O1-C1-C2-O2
5	B	1007	EDO	O1-C1-C2-O2
4	B	1003	6Q2	C16-C11-C9-C8
5	A	1008	EDO	O1-C1-C2-O2
5	B	1018	EDO	O1-C1-C2-O2
5	B	1019	EDO	O1-C1-C2-O2
4	B	1003	6Q2	C12-C11-C9-N10
5	A	1012	EDO	O1-C1-C2-O2
4	B	1003	6Q2	C12-C11-C9-C8
5	A	1015	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	1019	EDO	O1-C1-C2-O2
5	A	1017	EDO	O1-C1-C2-O2
5	B	1015	EDO	O1-C1-C2-O2
5	A	1007	EDO	O1-C1-C2-O2
5	B	1010	EDO	O1-C1-C2-O2
5	B	1017	EDO	O1-C1-C2-O2
5	B	1008	EDO	O1-C1-C2-O2

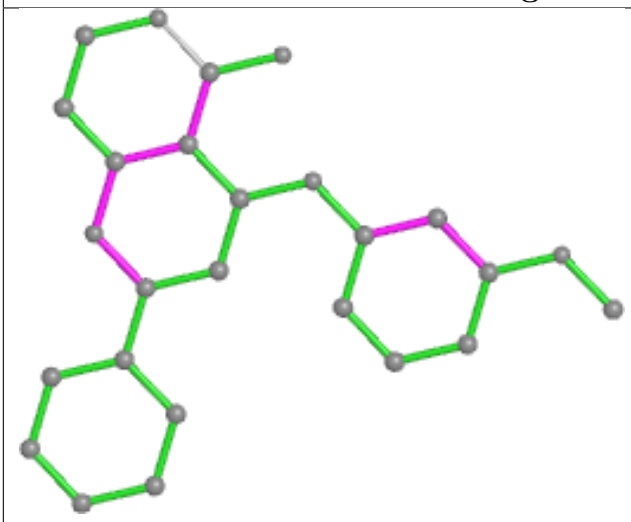
There are no ring outliers.

14 monomers are involved in 24 short contacts:

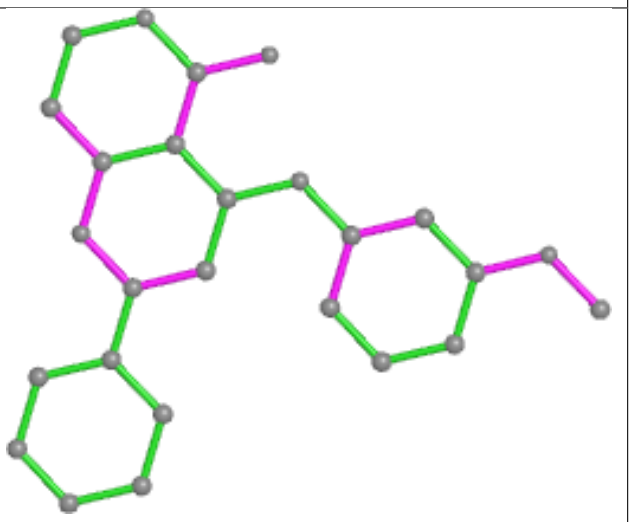
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1017	EDO	1	0
5	B	1011	EDO	1	0
5	B	1019	EDO	4	0
5	A	1010	EDO	3	0
5	B	1006	EDO	1	0
5	B	1010	EDO	2	0
5	A	1007	EDO	2	0
5	B	1015	EDO	1	0
5	B	1016	EDO	2	0
5	A	1004	EDO	1	0
5	A	1012	EDO	1	0
5	A	1016	EDO	3	0
5	B	1012	EDO	1	0
5	A	1019	EDO	1	0

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.

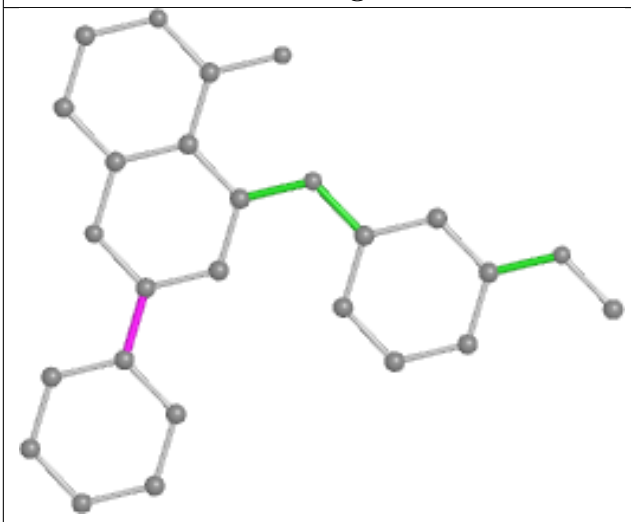
Ligand 6Q2 B 1003



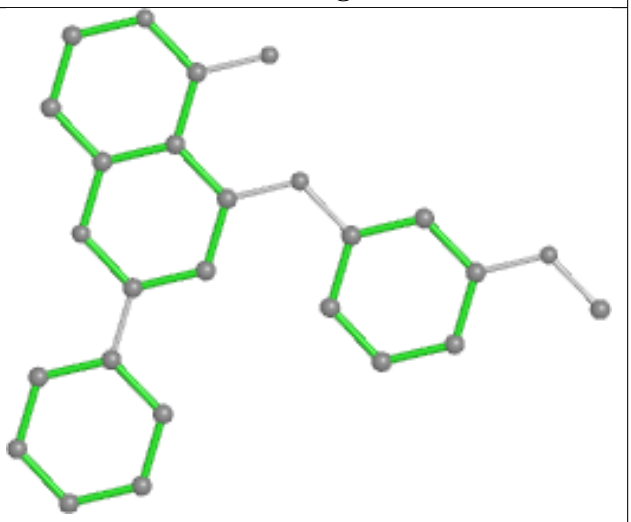
Bond lengths



Bond angles

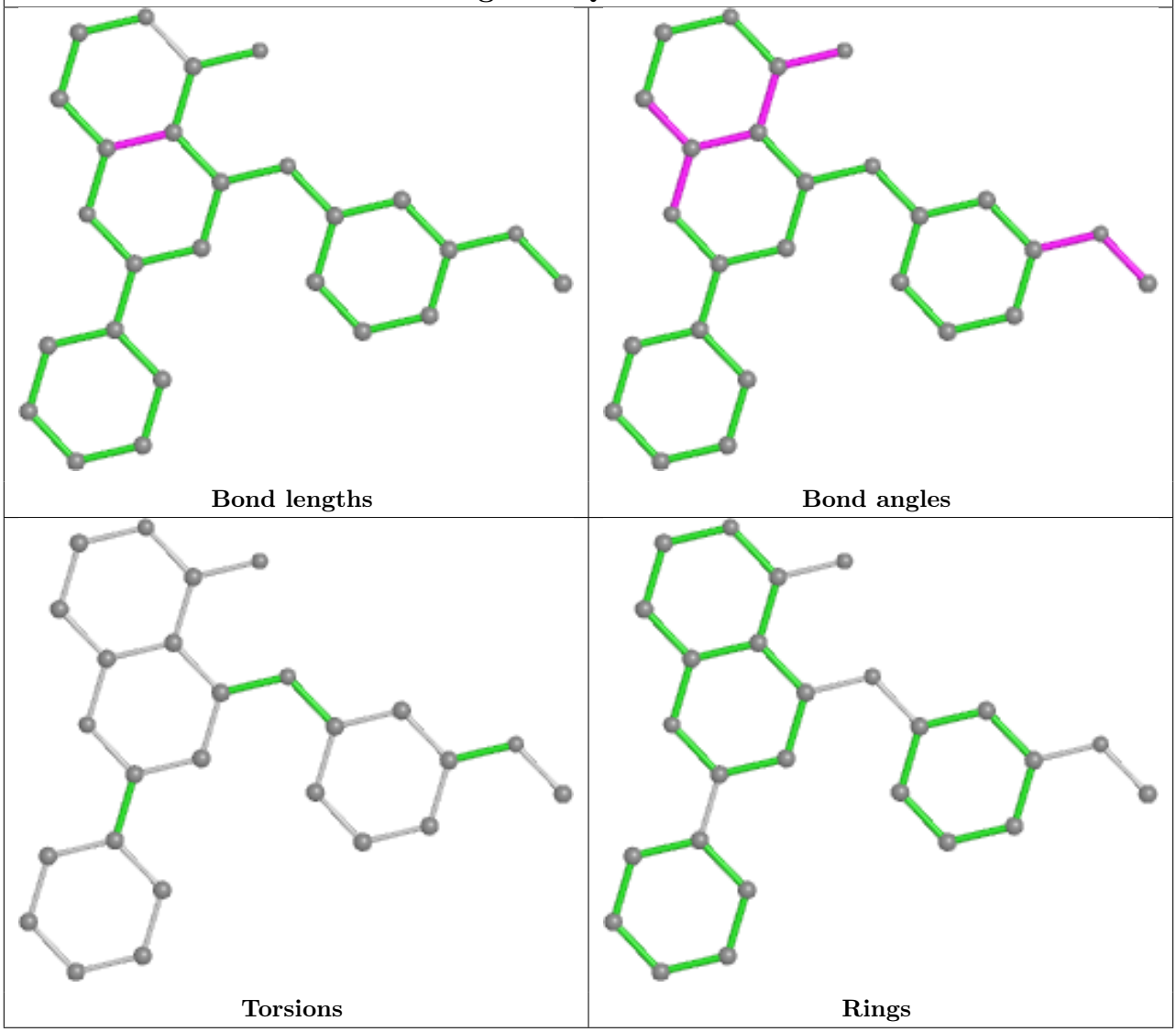


Torsions



Rings

Ligand 6Q2 A 1003



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	322/325 (99%)	0.81	43 (13%)	3	2	18, 29, 48, 61	1 (0%)
1	B	321/325 (98%)	0.55	31 (9%)	7	7	15, 25, 48, 56	0
All	All	643/650 (98%)	0.68	74 (11%)	4	4	15, 27, 48, 61	1 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	362	ASN	7.7
1	A	363	ALA	7.3
1	B	87	ALA	6.5
1	B	362	ASN	6.0
1	A	358	CYS	5.6
1	A	348	ARG	5.2
1	B	361	HIS	5.2
1	A	353	GLU	5.1
1	B	363	ALA	5.0
1	A	354	ILE	5.0
1	A	361	HIS	4.7
1	A	296	GLY	4.4
1	A	283	LEU	3.9
1	A	342	ARG	3.8
1	A	359	ASP	3.7
1	B	348	ARG	3.7
1	B	359	ASP	3.6
1	A	91	VAL	3.5
1	B	301	ASP	3.4
1	A	249	PHE	3.4
1	A	90	ASP	3.3
1	A	294	SER	3.2
1	B	90	ASP	3.2
1	B	353	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	410	ILE	3.2
1	A	255	LYS	3.1
1	A	89	GLU	3.1
1	A	93	ALA	3.0
1	A	387	LEU	3.0
1	B	303	TYR	2.9
1	A	130	ASP	2.9
1	B	293	THR	2.9
1	A	291	LYS	2.9
1	A	308	GLN	2.8
1	B	299	LEU	2.8
1	A	244	GLU	2.8
1	B	355	SER	2.8
1	B	292	VAL	2.8
1	B	300	LEU	2.8
1	A	121	ILE	2.7
1	B	384	TRP	2.7
1	A	191	LEU	2.7
1	A	88	GLN	2.7
1	B	294	SER	2.7
1	B	375	TYR	2.7
1	A	106	VAL	2.7
1	A	248	ILE	2.6
1	A	295	SER	2.6
1	A	139	VAL	2.6
1	B	354	ILE	2.6
1	A	92	LEU	2.5
1	B	183	ALA	2.5
1	A	278	ASN	2.5
1	B	91	VAL	2.5
1	A	309	VAL	2.4
1	B	216	ASN	2.4
1	A	355	SER	2.4
1	A	349	GLU	2.4
1	A	94	LYS	2.4
1	B	316	CYS	2.4
1	B	88	GLN	2.4
1	A	245	ASN	2.3
1	A	384	TRP	2.3
1	B	411	PRO	2.3
1	B	308	GLN	2.3
1	B	254	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	360	LYS	2.3
1	B	349	GLU	2.2
1	B	314	VAL	2.1
1	A	143	ILE	2.1
1	A	351	GLY	2.1
1	B	313	MET	2.1
1	A	141	THR	2.0
1	A	253	THR	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
5	EDO	B	1017	4/4	0.55	0.23	46,47,47,49	0
5	EDO	A	1010	4/4	0.65	0.33	35,37,39,44	0
5	EDO	A	1015	4/4	0.66	0.37	44,45,47,49	0
5	EDO	A	1007	4/4	0.70	0.30	35,36,36,38	0
5	EDO	B	1015	4/4	0.71	0.18	42,44,45,48	0
5	EDO	B	1016	4/4	0.71	0.17	41,43,45,48	0
5	EDO	A	1019	4/4	0.71	0.19	41,42,42,44	0
5	EDO	B	1011	4/4	0.73	0.25	30,38,38,44	0
5	EDO	A	1018	4/4	0.76	0.28	38,40,41,41	0
5	EDO	B	1006	4/4	0.78	0.23	33,40,42,46	0
5	EDO	A	1014	4/4	0.81	0.17	40,41,43,45	0
5	EDO	A	1012	4/4	0.81	0.15	41,42,45,46	0
5	EDO	A	1013	4/4	0.81	0.12	54,54,54,56	0
5	EDO	B	1018	4/4	0.81	0.17	50,51,52,53	0
5	EDO	A	1011	4/4	0.82	0.11	35,38,39,41	0

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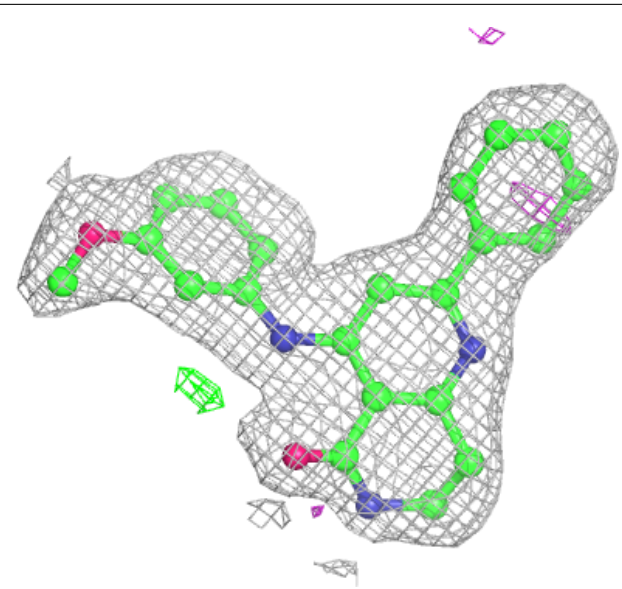
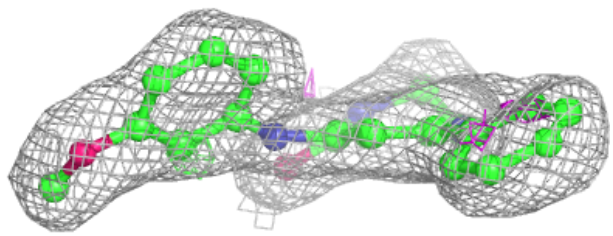
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	A	1016	4/4	0.82	0.19	40,43,43,45	0
5	EDO	B	1004	4/4	0.82	0.16	32,33,35,36	0
5	EDO	B	1009	4/4	0.84	0.20	42,45,46,46	0
5	EDO	B	1010	4/4	0.85	0.29	37,38,39,40	0
4	6Q2	A	1003	26/26	0.85	0.15	21,27,32,34	0
5	EDO	A	1009	4/4	0.86	0.21	34,36,40,44	0
5	EDO	B	1012	4/4	0.87	0.21	44,44,46,49	0
5	EDO	B	1019	4/4	0.87	0.20	41,43,43,44	0
5	EDO	A	1005	4/4	0.88	0.14	42,43,44,45	0
5	EDO	B	1014	4/4	0.89	0.15	52,53,54,54	0
5	EDO	A	1017	4/4	0.90	0.14	38,41,41,42	0
5	EDO	B	1013	4/4	0.90	0.15	51,52,52,53	0
5	EDO	A	1006	4/4	0.91	0.28	29,37,37,37	0
4	6Q2	B	1003	26/26	0.91	0.10	21,25,31,34	0
5	EDO	B	1007	4/4	0.92	0.11	27,30,31,31	0
5	EDO	B	1005	4/4	0.92	0.11	26,28,32,33	0
5	EDO	A	1004	4/4	0.93	0.11	42,42,43,45	0
5	EDO	A	1008	4/4	0.93	0.10	37,38,39,40	0
5	EDO	B	1008	4/4	0.94	0.14	28,30,31,34	0
3	MG	B	1002	1/1	0.94	0.11	17,17,17,17	0
3	MG	A	1002	1/1	0.99	0.20	18,18,18,18	0
2	ZN	A	1001	1/1	0.99	0.04	26,26,26,26	0
2	ZN	B	1001	1/1	1.00	0.03	24,24,24,24	0

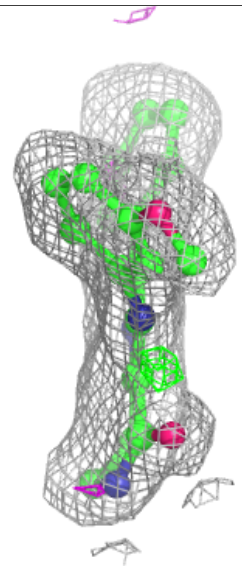
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 6Q2 A 1003:

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

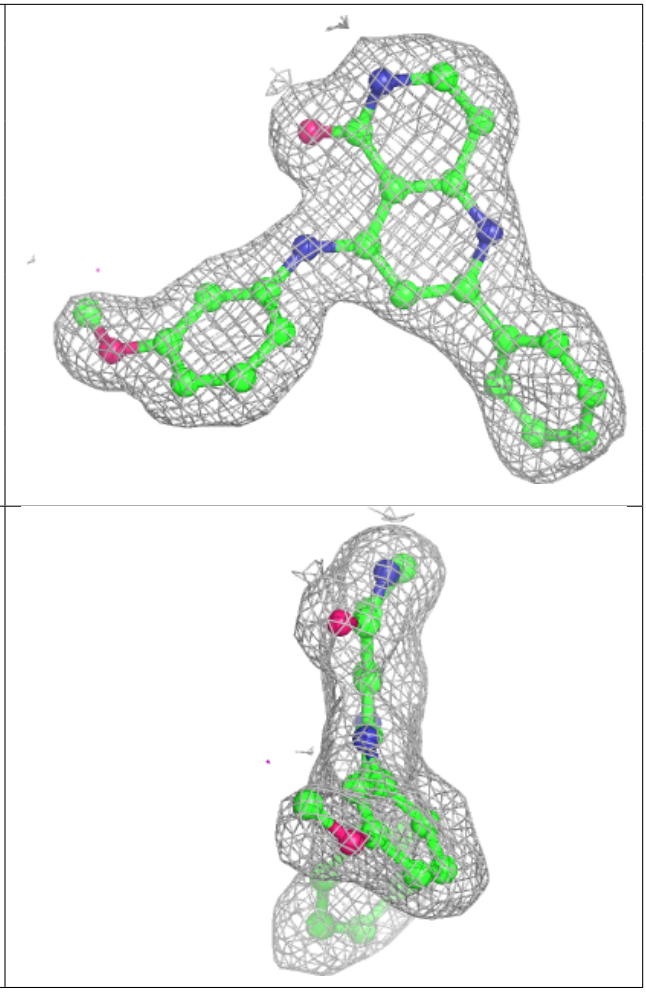






Electron density around 6Q2 B 1003:

$2mF_o$-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.