



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:31 PM UTC

PDB ID : 3SL6 / pdb_00003sl6
Title : Crystal structure of the catalytic domain of PDE4D2 with compound 12c
Authors : Feil, S.F.
Deposited on : 2011-06-24
Resolution : 2.44 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

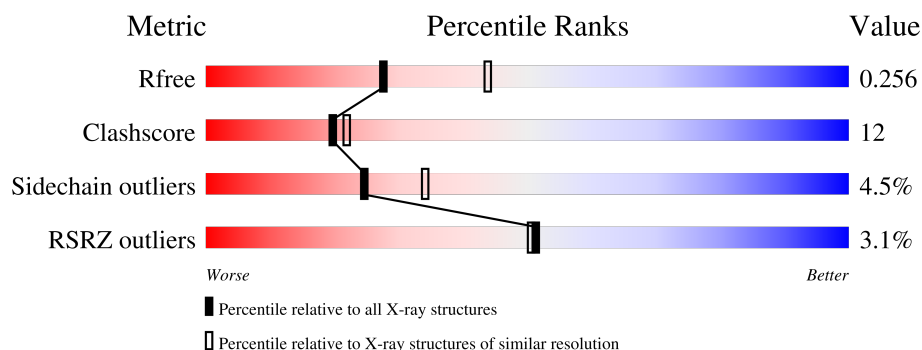
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	361	3% 72% 17% • 9%
1	B	361	3% 64% 24% • 10%
1	C	361	3% 68% 20% • 10%
1	D	361	2% 71% 17% • 10%

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	EDO	B	5	-	-	X	-
3	EDO	D	11	-	-	X	-
3	EDO	D	3	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11042 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
1	A	327	Total	C	N	O	S	0	1	0
			2657	1680	455	508	14			
1	B	325	Total	C	N	O	S	0	0	0
			2631	1664	450	503	14			
1	C	325	Total	C	N	O	S	0	0	0
			2631	1663	449	505	14			
1	D	324	Total	C	N	O	S	0	1	0
			2632	1665	451	502	14			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



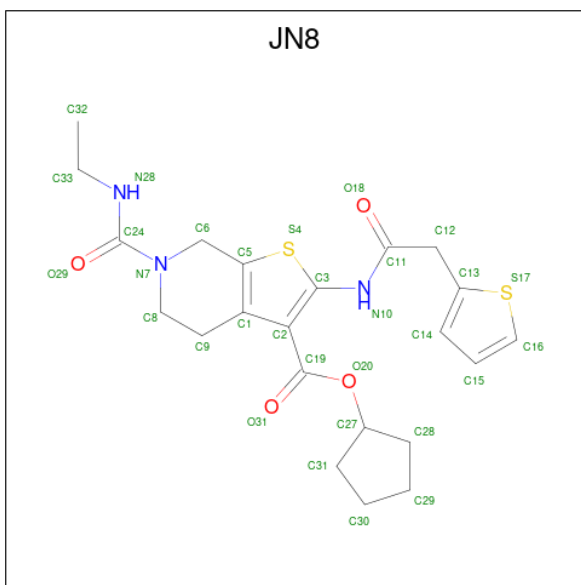
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total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

Continued on next page...

Continued from previous page...

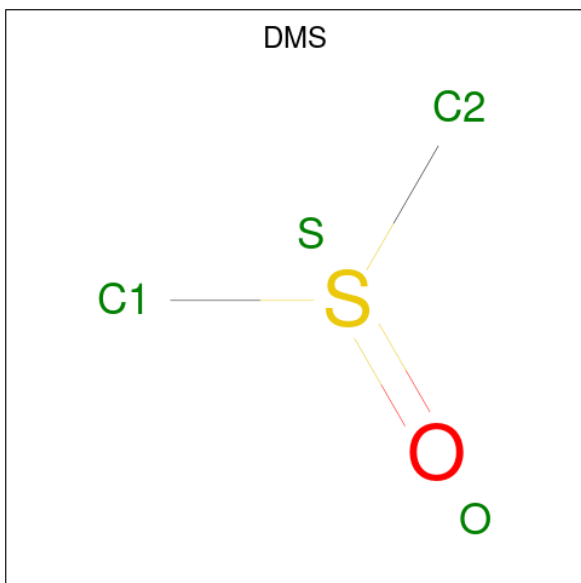
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is cyclopentyl 6-(ethylcarbamoyl)-2-[(thiophen-2-ylacetyl)amino]-4,5,6,7-tetrahydrothieno[2,3-c]pyridine-3-carboxylate (CCD ID: JN8) (formula: C₂₂H₂₇N₃O₄S₂).



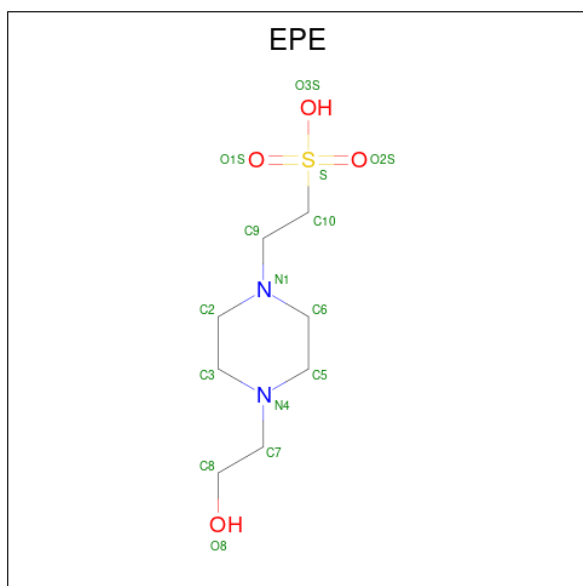
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			31	22	3	4	2		
4	B	1	Total	C	N	O	S	0	0
			31	22	3	4	2		
4	C	1	Total	C	N	O	S	0	0
			31	22	3	4	2		
4	D	1	Total	C	N	O	S	0	0
			31	22	3	4	2		

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



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

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).

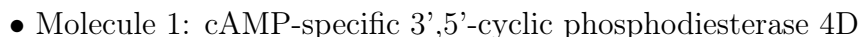
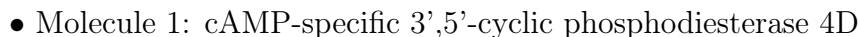


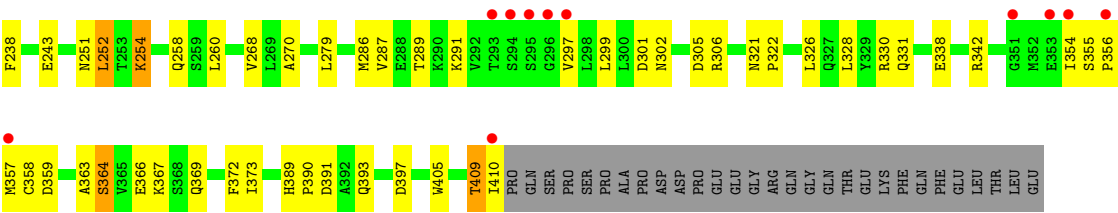
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 7 is water.

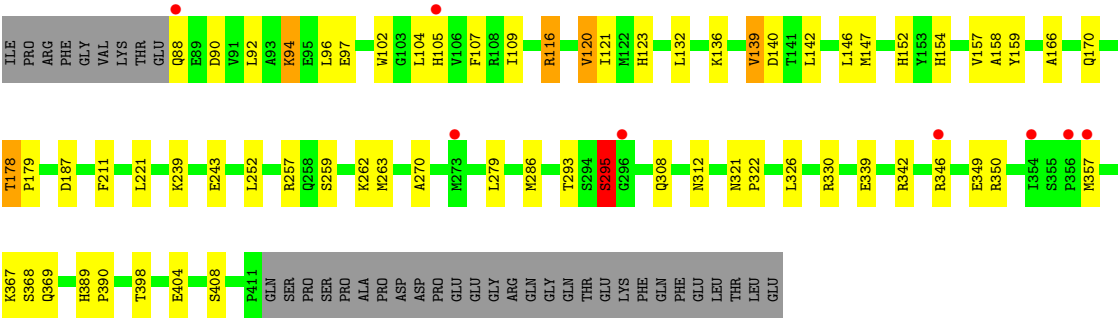
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	64	Total	O	0	0
			64	64		
7	B	47	Total	O	0	0
			47	47		
7	C	36	Total	O	0	0
			36	36		
7	D	73	Total	O	0	0
			73	73		

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





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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.54Å 111.20Å 160.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.19 – 2.44 65.19 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.0 (65.19-2.44) 99.5 (65.19-2.44)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.23 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, R_{free}	0.198 , 0.256 (Not available) , 0.256	Depositor DCC
R_{free} test set	3382 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11042	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DMS, EDO, JN8, ZN, EPE

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	0.51	0/2711	0.80	1/3682 (0.0%)
1	B	0.49	0/2685	0.81	3/3648 (0.1%)
1	C	0.48	0/2684	0.81	2/3646 (0.1%)
1	D	0.55	0/2687	0.82	1/3651 (0.0%)
All	All	0.51	0/10767	0.81	7/14627 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	357	MET	N-CA-C	-7.47	104.41	113.97
1	C	178	THR	CA-C-N	6.85	126.10	118.97
1	C	178	THR	C-N-CA	6.85	126.10	118.97
1	B	355	SER	CA-C-N	6.75	128.27	119.84
1	B	355	SER	C-N-CA	6.75	128.27	119.84
1	D	295	SER	N-CA-C	-6.18	102.81	110.41
1	A	99	VAL	CB-CA-C	-5.70	104.58	112.04

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	2657	0	2612	46	0
1	B	2631	0	2586	84	0
1	C	2631	0	2584	55	0
1	D	2632	0	2584	63	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	36	0	54	5	0
3	B	12	0	18	4	0
3	C	28	0	42	8	0
3	D	44	0	66	20	0
4	A	31	0	27	3	0
4	B	31	0	27	2	0
4	C	31	0	27	2	0
4	D	31	0	27	4	0
5	B	4	0	6	2	0
6	C	15	0	17	3	0
7	A	64	0	0	2	0
7	B	47	0	0	2	0
7	C	36	0	0	0	0
7	D	73	0	0	5	0
All	All	11042	0	10677	248	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 12.

All (248) 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:D:152:HIS:HE1	3:D:3:EDO:H22	1.14	1.10
1:D:140:ASP:HB3	7:D:484:HOH:O	1.53	1.05
1:D:116:ARG:HG2	1:D:116:ARG:HH11	1.20	1.04
1:B:182:GLU:O	1:B:297:VAL:HG21	1.63	0.98
1:D:116:ARG:HE	1:D:147:MET:HG2	1.28	0.96
1:D:152:HIS:CE1	3:D:3:EDO:H22	2.01	0.93
1:D:187:ASP:HB2	3:D:4:EDO:H12	1.52	0.92
1:B:105:HIS:CE1	1:B:107:PHE:HB2	2.07	0.89
1:A:132:LEU:HD22	1:A:139:VAL:HG12	1.58	0.83
1:B:158:ALA:H	1:B:342:ARG:HH22	1.25	0.83
1:D:157:VAL:HA	3:D:11:EDO:H22	1.61	0.82
1:D:152:HIS:HE1	3:D:3:EDO:C2	1.90	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:GLN:HG3	1:D:90:ASP:H	1.46	0.80
1:A:105[A]:HIS:HD2	1:A:108:ARG:H	1.26	0.80
1:B:105:HIS:HE1	1:B:107:PHE:HB2	1.45	0.78
7:A:474:HOH:O	1:B:222:MET:HG2	1.83	0.78
1:D:116:ARG:HH11	1:D:116:ARG:CG	1.99	0.75
1:A:96:LEU:O	1:A:99:VAL:HG22	1.90	0.72
1:B:362:ASN:N	1:B:362:ASN:HD22	1.85	0.72
1:D:326:LEU:H	3:D:10:EDO:H22	1.54	0.72
1:D:116:ARG:HG2	1:D:116:ARG:NH1	1.95	0.72
1:B:270:ALA:HB1	1:B:279:LEU:HD11	1.72	0.71
1:D:179:PRO:HG2	3:D:7:EDO:H11	1.72	0.70
1:B:132:LEU:HD21	1:B:142:LEU:HD22	1.72	0.70
1:C:225:ASP:OD2	3:D:9:EDO:H12	1.94	0.68
1:B:158:ALA:N	1:B:342:ARG:HH22	1.91	0.67
1:B:158:ALA:H	1:B:342:ARG:NH2	1.94	0.66
1:D:158:ALA:H	3:D:11:EDO:H12	1.60	0.66
1:D:339:GLU:HA	3:D:11:EDO:H11	1.77	0.65
1:C:364:SER:HB2	1:C:367:LYS:HE3	1.78	0.64
1:D:398:THR:HG23	3:D:10:EDO:H11	1.79	0.64
1:A:225:ASP:OD1	1:B:261:ARG:NH2	2.30	0.64
1:A:243:GLU:OE1	3:A:442:EDO:H21	1.98	0.63
1:A:152:HIS:HE1	3:A:442:EDO:H22	1.64	0.63
1:C:369:GLN:OE1	4:C:441:JN8:H15	1.99	0.63
1:D:105[A]:HIS:HE1	1:D:107:PHE:HB2	1.63	0.63
1:B:354:ILE:HG22	1:B:355:SER:N	2.14	0.62
1:B:178:THR:CG2	1:B:181:LEU:HD12	2.28	0.62
1:D:105[A]:HIS:CE1	1:D:107:PHE:HB2	2.33	0.62
1:D:96:LEU:HD11	1:D:120:VAL:HG13	1.81	0.62
1:D:321:ASN:HB2	1:D:322:PRO:HD3	1.82	0.61
1:A:348:ARG:C	1:A:350:ARG:H	2.07	0.61
1:B:302:ASN:O	1:B:306:ARG:HG3	2.01	0.61
3:C:8:EDO:H21	1:D:221:LEU:O	2.01	0.60
1:B:178:THR:HG21	1:B:181:LEU:HD12	1.82	0.60
1:B:355:SER:O	1:B:357:MET:N	2.33	0.60
1:B:126:PHE:HA	1:B:131:LEU:HD12	1.83	0.59
1:B:129:ARG:HE	1:B:173:HIS:CE1	2.19	0.59
1:C:409:THR:O	1:C:410:ILE:HG13	2.01	0.59
1:B:354:ILE:HG22	1:B:355:SER:H	1.66	0.59
1:D:178:THR:OG1	3:D:440:EDO:H21	2.02	0.58
1:C:326:LEU:HD21	1:C:405:TRP:CE2	2.38	0.58
1:C:330:ARG:HD3	1:C:405:TRP:CH2	2.39	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:CD2	1:A:139:VAL:HG12	2.33	0.58
1:D:243:GLU:OE1	3:D:3:EDO:H21	2.03	0.57
1:B:109:ILE:O	1:B:113:SER:HB2	2.04	0.57
1:D:123:HIS:HD2	3:D:5:EDO:H21	1.69	0.57
1:D:142:LEU:O	1:D:146:LEU:HG	2.04	0.56
1:B:354:ILE:C	1:B:356:PRO:HD3	2.30	0.56
1:D:308:GLN:HE21	1:D:312:ASN:ND2	2.03	0.56
1:A:225:ASP:CG	1:B:261:ARG:HH21	2.13	0.56
1:B:350:ARG:NH1	7:B:22:HOH:O	2.39	0.56
1:D:321:ASN:ND2	1:D:321:ASN:H	2.03	0.56
1:B:323:THR:HB	1:B:395:ILE:HG23	1.88	0.56
1:A:178:THR:OG1	3:A:5:EDO:H12	2.06	0.55
1:A:278:ASN:ND2	1:A:278:ASN:H	2.04	0.55
1:A:302:ASN:HD22	1:A:304:SER:HB2	1.71	0.55
1:B:355:SER:C	1:B:357:MET:H	2.15	0.55
1:B:369:GLN:OE1	4:B:440:JN8:H15	2.07	0.54
1:B:366:GLU:HG2	1:B:409:THR:HG22	1.88	0.54
1:C:364:SER:CB	1:C:367:LYS:HE3	2.38	0.53
1:C:286:MET:HE1	1:C:305:ASP:HA	1.89	0.53
1:B:178:THR:HG23	1:B:181:LEU:HB2	1.89	0.53
1:C:291:LYS:HB2	1:C:299:LEU:HB3	1.90	0.53
1:A:105[A]:HIS:CD2	1:A:108:ARG:H	2.17	0.53
1:B:99:VAL:HG13	1:B:100:ASN:OD1	2.09	0.53
1:D:342:ARG:HD3	7:D:480:HOH:O	2.08	0.53
1:D:346:ARG:HH21	1:D:350:ARG:HH22	1.56	0.53
1:B:362:ASN:N	1:B:362:ASN:ND2	2.56	0.52
1:B:384:TRP:O	1:B:388:VAL:HG22	2.09	0.52
1:C:243:GLU:OE1	3:C:3:EDO:H12	2.08	0.52
1:C:354:ILE:HG12	1:C:354:ILE:O	2.09	0.52
1:C:302:ASN:O	1:C:306:ARG:HG3	2.09	0.52
1:A:105[A]:HIS:NE2	1:A:107:PHE:HB2	2.23	0.52
1:B:143:ILE:O	1:B:147:MET:HG2	2.09	0.52
1:B:366:GLU:HG2	1:B:409:THR:CG2	2.39	0.52
1:C:152:HIS:HE1	3:C:3:EDO:H11	1.75	0.52
1:C:372:PHE:HE2	4:C:441:JN8:H14	1.75	0.52
1:A:302:ASN:ND2	1:A:304:SER:HB2	2.25	0.51
1:A:104:LEU:HD11	1:A:109:ILE:HD11	1.92	0.51
1:A:192:ALA:HB2	1:A:260:LEU:HD12	1.91	0.51
1:C:270:ALA:HB1	1:C:279:LEU:HD11	1.93	0.51
1:B:305:ASP:O	1:B:309:VAL:HG23	2.11	0.50
1:B:92:LEU:HD21	1:B:109:ILE:HG23	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ILE:HD13	1:B:224:ASN:O	2.12	0.50
1:D:123:HIS:CD2	3:D:5:EDO:H21	2.47	0.50
1:B:342:ARG:NH2	7:B:466:HOH:O	2.45	0.50
1:A:366:GLU:HG2	1:A:409:THR:CG2	2.41	0.50
1:B:105:HIS:H	5:B:14:DMS:H23	1.77	0.50
1:B:182:GLU:HG2	3:B:5:EDO:H11	1.93	0.49
1:C:179:PRO:HD2	1:C:391:ASP:CG	2.37	0.49
1:A:270:ALA:HB1	1:A:279:LEU:HD11	1.94	0.49
1:A:348:ARG:C	1:A:350:ARG:N	2.70	0.49
1:B:163:ILE:HG22	1:B:332:TRP:HH2	1.78	0.49
1:A:273:MET:HE2	4:A:440:JN8:HN28	1.76	0.49
1:C:291:LYS:O	1:C:299:LEU:HB3	2.11	0.49
4:D:15:JN8:S4	4:D:15:JN8:O18	2.70	0.49
1:B:412:GLN:O	1:B:412:GLN:HG2	2.13	0.49
4:A:440:JN8:O29	4:A:440:JN8:H32A	2.13	0.49
1:A:366:GLU:HG2	1:A:409:THR:HB	1.95	0.49
1:C:369:GLN:O	1:C:373:ILE:HG13	2.13	0.49
1:D:132:LEU:HD22	1:D:139:VAL:HG12	1.95	0.49
1:B:182:GLU:HA	3:B:5:EDO:H11	1.94	0.48
1:C:366:GLU:H	1:C:366:GLU:CD	2.19	0.48
1:B:109:ILE:O	1:B:113:SER:CB	2.62	0.48
1:B:182:GLU:HA	3:B:5:EDO:C1	2.44	0.48
1:A:323:THR:HG22	1:A:399:LEU:HB2	1.95	0.48
1:B:189:GLU:HG2	1:B:263:MET:SD	2.54	0.48
1:D:367:LYS:C	1:D:367:LYS:HD3	2.38	0.48
1:B:182:GLU:HA	3:B:5:EDO:C2	2.44	0.48
1:B:389:HIS:CD2	1:B:390:PRO:HA	2.49	0.48
1:A:223:TYR:CE1	1:A:231:ASN:HB3	2.49	0.48
1:A:364:SER:HB2	1:A:367:LYS:HB2	1.96	0.48
1:D:158:ALA:H	3:D:11:EDO:C1	2.27	0.48
1:B:409:THR:HG22	1:B:409:THR:O	2.13	0.47
4:B:440:JN8:O18	4:B:440:JN8:S4	2.72	0.47
1:C:356:PRO:O	1:C:357:MET:HB2	2.14	0.47
1:D:152:HIS:CE1	3:D:3:EDO:C2	2.80	0.47
1:B:122:MET:HB2	1:B:146:LEU:HD13	1.97	0.47
1:C:359:ASP:O	1:C:363:ALA:HB2	2.14	0.47
1:D:211:PHE:CD1	1:D:211:PHE:C	2.92	0.47
1:D:321:ASN:H	1:D:321:ASN:HD22	1.62	0.47
1:A:152:HIS:CE1	3:A:442:EDO:H22	2.48	0.47
1:D:159:TYR:HB3	1:D:339:GLU:OE1	2.14	0.47
1:D:262:LYS:HB2	3:D:9:EDO:H21	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:440:JN8:O29	4:A:440:JN8:C32	2.61	0.47
1:B:346:ARG:O	1:B:350:ARG:HG3	2.15	0.47
1:B:150:GLU:HG3	1:B:162:ASN:HB2	1.96	0.47
1:C:234:LEU:HD21	1:C:268:VAL:HB	1.96	0.47
1:C:104:LEU:HD11	1:C:109:ILE:HD11	1.97	0.47
1:B:105:HIS:N	5:B:14:DMS:H23	2.31	0.46
1:D:104:LEU:HD11	1:D:109:ILE:HD11	1.96	0.46
1:D:286:MET:HE3	1:D:308:GLN:OE1	2.15	0.46
1:B:88:GLN:HA	1:B:88:GLN:OE1	2.15	0.46
1:B:254:LYS:HB2	1:B:254:LYS:HE3	1.62	0.46
1:D:326:LEU:O	1:D:330:ARG:HG3	2.14	0.46
1:C:96:LEU:HD23	1:C:109:ILE:HD13	1.96	0.46
1:D:408:SER:HB3	7:D:464:HOH:O	2.16	0.46
1:A:330:ARG:HD3	1:A:405:TRP:CH2	2.51	0.46
1:C:331:GLN:HE22	6:C:2:EPE:H101	1.81	0.46
1:B:147:MET:HE3	1:D:349:GLU:HB3	1.97	0.46
1:B:154:HIS:N	1:B:154:HIS:CD2	2.83	0.46
1:C:99:VAL:HG13	1:C:100:ASN:OD1	2.16	0.46
1:C:116:ARG:N	1:C:117:PRO:CD	2.79	0.46
1:C:192:ALA:HB2	1:C:260:LEU:HD12	1.98	0.45
1:D:94:LYS:O	1:D:97:GLU:HB2	2.16	0.45
1:D:252:LEU:HB2	1:D:257:ARG:HG3	1.98	0.45
1:A:286:MET:SD	1:A:308:GLN:OE1	2.74	0.45
1:B:211:PHE:CD2	1:B:352:MET:HE1	2.50	0.45
4:D:15:JN8:O29	4:D:15:JN8:H32A	2.16	0.45
1:C:160:HIS:HD2	1:C:201:ASP:OD2	2.00	0.45
1:C:328:LEU:HD23	6:C:2:EPE:O3S	2.17	0.45
1:D:259:SER:O	1:D:263:MET:HG3	2.17	0.45
1:D:369:GLN:OE1	4:D:15:JN8:H15	2.17	0.45
1:C:178:THR:OG1	3:C:440:EDO:H11	2.17	0.45
1:A:218:GLU:OE2	3:A:2:EDO:H22	2.16	0.45
1:A:360:LYS:HE2	1:A:360:LYS:HB3	1.69	0.45
1:B:154:HIS:HB2	1:B:157:VAL:HG23	1.99	0.45
1:C:254:LYS:H	3:C:7:EDO:H22	1.82	0.45
1:A:170:GLN:O	1:A:173:HIS:HB3	2.17	0.44
1:B:303:TYR:O	1:B:304:SER:C	2.60	0.44
1:B:354:ILE:CG2	1:B:355:SER:N	2.80	0.44
1:A:116:ARG:N	1:A:117:PRO:CD	2.80	0.44
1:A:321:ASN:HD22	1:A:332:TRP:CG	2.36	0.44
1:D:104:LEU:HD22	1:D:170:GLN:HG3	1.99	0.44
1:C:364:SER:HB2	1:C:367:LYS:HB2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ARG:O	1:A:350:ARG:N	2.51	0.44
1:B:135:PHE:O	1:B:136:LYS:HB2	2.18	0.44
1:B:260:LEU:O	1:B:264:VAL:HG23	2.17	0.44
1:B:304:SER:O	1:B:307:ILE:HG22	2.18	0.44
1:B:354:ILE:CG2	1:B:355:SER:H	2.30	0.44
1:C:238:PHE:HD2	3:C:8:EDO:H12	1.82	0.44
1:C:321:ASN:HB2	1:C:322:PRO:HD3	1.99	0.43
6:C:2:EPE:H81	6:C:2:EPE:H31	1.81	0.43
1:A:105[A]:HIS:HD2	1:A:108:ARG:N	2.04	0.43
1:C:251:ASN:O	3:C:4:EDO:H12	2.18	0.43
1:D:293:THR:O	1:D:295:SER:O	2.36	0.43
1:A:292:VAL:HG11	1:A:296:GLY:HA2	2.00	0.43
1:B:145:TYR:CE1	1:B:241:LEU:HD23	2.53	0.43
1:A:189:GLU:HG2	1:A:263:MET:SD	2.58	0.43
1:B:354:ILE:C	1:B:356:PRO:CD	2.91	0.43
1:C:389:HIS:CE1	1:C:390:PRO:HB3	2.54	0.43
1:A:85:LYS:HB2	1:A:89:GLU:HB2	2.01	0.43
1:C:142:LEU:O	1:C:146:LEU:HG	2.18	0.43
1:D:104:LEU:HD11	1:D:109:ILE:CD1	2.49	0.43
1:A:370:VAL:HG11	1:A:407:GLN:HE21	1.84	0.42
1:C:355:SER:O	1:C:358:CYS:HB2	2.19	0.42
1:C:143:ILE:O	1:C:147:MET:HG3	2.20	0.42
1:D:308:GLN:HE21	1:D:312:ASN:HD22	1.64	0.42
1:A:204:HIS:HA	1:A:205:PRO:HD3	1.85	0.42
1:D:286:MET:CE	1:D:308:GLN:OE1	2.67	0.42
1:D:404:GLU:HG2	7:D:487:HOH:O	2.18	0.42
1:B:354:ILE:HB	1:B:356:PRO:HD3	2.01	0.42
1:D:270:ALA:HB1	1:D:279:LEU:HD11	2.02	0.42
7:A:474:HOH:O	1:B:222:MET:CG	2.56	0.42
1:C:135:PHE:HB3	1:C:252:LEU:HD21	2.01	0.42
1:B:154:HIS:HB3	1:B:156:ASP:OD1	2.19	0.42
1:C:254:LYS:HB3	3:C:7:EDO:H22	2.02	0.42
1:A:138:PRO:HB2	1:A:141:THR:OG1	2.19	0.42
1:B:178:THR:CG2	1:B:181:LEU:HB2	2.49	0.42
1:D:132:LEU:CD2	1:D:139:VAL:HG12	2.50	0.42
1:A:222:MET:HE1	1:B:222:MET:SD	2.60	0.42
1:B:116:ARG:N	1:B:117:PRO:CD	2.83	0.41
1:B:144:THR:HG22	1:B:246:CYS:SG	2.60	0.41
1:B:175:LEU:HD23	1:B:175:LEU:HA	1.85	0.41
1:C:204:HIS:HA	1:C:205:PRO:HD3	1.94	0.41
1:C:286:MET:HE3	1:C:286:MET:HB2	1.91	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:ILE:O	1:C:355:SER:C	2.63	0.41
1:D:121:ILE:HD12	1:D:166:ALA:HB1	2.02	0.41
1:B:349:GLU:HB3	1:D:147:MET:SD	2.60	0.41
1:A:279:LEU:HD23	1:A:279:LEU:HA	1.88	0.41
1:C:181:LEU:O	1:C:184:VAL:HG23	2.21	0.41
1:C:221:LEU:HD13	1:C:221:LEU:O	2.20	0.41
1:C:279:LEU:HD23	1:C:279:LEU:HA	1.86	0.41
1:D:102:TRP:HB2	3:D:8:EDO:H11	2.03	0.41
1:B:389:HIS:HA	1:B:390:PRO:HA	1.74	0.41
1:B:260:LEU:O	1:B:260:LEU:HG	2.21	0.41
1:B:142:LEU:O	1:B:146:LEU:HG	2.20	0.41
1:C:252:LEU:HD23	1:C:252:LEU:N	2.36	0.41
1:C:338:GLU:O	1:C:342:ARG:HG3	2.20	0.41
1:D:187:ASP:HB2	3:D:4:EDO:C1	2.38	0.41
1:B:253:THR:OG1	1:B:256:GLN:HB2	2.21	0.41
1:D:154:HIS:CD2	1:D:154:HIS:N	2.87	0.41
1:A:178:THR:HA	1:A:179:PRO:HD3	1.96	0.40
1:B:286:MET:HE2	1:B:286:MET:HB3	1.93	0.40
1:C:179:PRO:C	1:C:181:LEU:H	2.29	0.40
1:C:393:GLN:HE21	1:C:397:ASP:CG	2.30	0.40
1:D:389:HIS:HA	1:D:390:PRO:HA	1.82	0.40
1:B:181:LEU:O	1:B:184:VAL:HG23	2.21	0.40
1:B:179:PRO:HA	1:B:182:GLU:CD	2.46	0.40
1:C:86:THR:O	1:C:87:GLU:C	2.65	0.40
1:C:204:HIS:ND1	1:C:205:PRO:HD2	2.36	0.40
1:D:239:LYS:HG3	7:D:490:HOH:O	2.21	0.40
1:A:223:TYR:O	1:A:224:ASN:C	2.65	0.40
1:B:132:LEU:HD21	1:B:142:LEU:CD2	2.45	0.40
1:B:238:PHE:O	1:B:239:LYS:C	2.64	0.40
1:C:326:LEU:HD21	1:C:405:TRP:CD2	2.55	0.40
1:D:368:SER:HB3	4:D:15:JN8:H29A	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	288/329 (88%)	275 (96%)	13 (4%)	24	34
1	B	297/329 (90%)	282 (95%)	15 (5%)	21	29
1	C	297/329 (90%)	281 (95%)	16 (5%)	20	27
1	D	297/329 (90%)	288 (97%)	9 (3%)	36	48
All	All	1179/1316 (90%)	1126 (96%)	53 (4%)	24	34

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	VAL
1	A	85	LYS
1	A	92	LEU
1	A	99	VAL
1	A	219	LEU
1	A	222	MET
1	A	239	LYS
1	A	278	ASN
1	A	284	LYS
1	A	293	THR
1	A	304	SER
1	A	308	GLN
1	A	353	GLU
1	B	92	LEU
1	B	128	GLU
1	B	219	LEU
1	B	221	LEU
1	B	252	LEU
1	B	254	LYS
1	B	259	SER
1	B	288	GLU
1	B	297	VAL
1	B	298	LEU
1	B	299	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	346	ARG
1	B	356	PRO
1	B	362	ASN
1	B	396	LEU
1	C	86	THR
1	C	87	GLU
1	C	92	LEU
1	C	132	LEU
1	C	139	VAL
1	C	147	MET
1	C	178	THR
1	C	252	LEU
1	C	254	LYS
1	C	258	GLN
1	C	287	VAL
1	C	289	THR
1	C	297	VAL
1	C	301	ASP
1	C	364	SER
1	C	409	THR
1	D	92	LEU
1	D	94	LYS
1	D	116	ARG
1	D	120	VAL
1	D	136	LYS
1	D	139	VAL
1	D	178	THR
1	D	295	SER
1	D	357	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	A	216	ASN
1	A	224	ASN
1	A	245	ASN
1	A	278	ASN
1	A	302	ASN
1	A	361	HIS
1	A	389	HIS
1	A	407	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	245	ASN
1	B	250	GLN
1	B	308	GLN
1	B	327	GLN
1	B	343	GLN
1	B	362	ASN
1	C	152	HIS
1	C	210	GLN
1	C	245	ASN
1	C	250	GLN
1	C	258	GLN
1	C	308	GLN
1	C	312	ASN
1	C	331	GLN
1	C	393	GLN
1	D	123	HIS
1	D	127	GLN
1	D	152	HIS
1	D	210	GLN
1	D	216	ASN
1	D	224	ASN
1	D	245	ASN
1	D	250	GLN
1	D	258	GLN
1	D	278	ASN
1	D	312	ASN
1	D	321	ASN
1	D	393	GLN

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

Of 44 ligands modelled in this entry, 8 are monoatomic - leaving 36 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
3	EDO	C	7	-	3,3,3	0.54	0	2,2,2	0.31	0
3	EDO	D	11	-	3,3,3	0.56	0	2,2,2	0.09	0
3	EDO	A	5	-	3,3,3	0.53	0	2,2,2	0.16	0
3	EDO	C	3	-	3,3,3	0.58	0	2,2,2	0.26	0
3	EDO	D	8	-	3,3,3	0.65	0	2,2,2	0.06	0
3	EDO	C	8	-	3,3,3	0.54	0	2,2,2	0.10	0
3	EDO	D	3	-	3,3,3	0.35	0	2,2,2	0.83	0
4	JN8	D	15	-	34,34,34	2.24	11 (32%)	46,47,47	2.43	15 (32%)
3	EDO	C	9	-	3,3,3	0.54	0	2,2,2	0.28	0
3	EDO	D	2	-	3,3,3	0.44	0	2,2,2	0.48	0
3	EDO	A	7	-	3,3,3	0.58	0	2,2,2	0.23	0
3	EDO	A	2	-	3,3,3	0.47	0	2,2,2	0.26	0
6	EPE	C	2	-	15,15,15	1.04	1 (6%)	19,20,20	1.61	5 (26%)
3	EDO	A	9	-	3,3,3	0.42	0	2,2,2	0.78	0
3	EDO	A	4	-	3,3,3	0.50	0	2,2,2	0.29	0
3	EDO	A	441	-	3,3,3	0.40	0	2,2,2	0.46	0
3	EDO	D	440	-	3,3,3	0.44	0	2,2,2	0.17	0
3	EDO	D	5	-	3,3,3	0.52	0	2,2,2	0.24	0
3	EDO	C	440	-	3,3,3	0.44	0	2,2,2	0.35	0
3	EDO	D	6	-	3,3,3	0.48	0	2,2,2	0.45	0
3	EDO	D	9	-	3,3,3	0.48	0	2,2,2	0.09	0
4	JN8	B	440	-	34,34,34	2.32	12 (35%)	46,47,47	1.94	13 (28%)
3	EDO	C	5	-	3,3,3	0.52	0	2,2,2	0.31	0
4	JN8	C	441	-	34,34,34	2.34	11 (32%)	46,47,47	1.92	10 (21%)
3	EDO	A	8	-	3,3,3	0.53	0	2,2,2	0.28	0
5	DMS	B	14	-	3,3,3	2.74	1 (33%)	3,3,3	0.63	0
3	EDO	A	442	-	3,3,3	0.58	0	2,2,2	0.30	0
3	EDO	B	4	-	3,3,3	0.55	0	2,2,2	0.14	0
4	JN8	A	440	-	34,34,34	2.24	11 (32%)	46,47,47	2.39	13 (28%)
3	EDO	B	6	-	3,3,3	0.54	0	2,2,2	0.16	0
3	EDO	B	5	-	3,3,3	0.52	0	2,2,2	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	D	10	-	3,3,3	0.60	0	2,2,2	0.19	0
3	EDO	D	4	-	3,3,3	0.56	0	2,2,2	0.23	0
3	EDO	C	4	-	3,3,3	0.37	0	2,2,2	0.55	0
3	EDO	D	7	-	3,3,3	0.56	0	2,2,2	0.28	0
3	EDO	A	6	-	3,3,3	0.51	0	2,2,2	0.18	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
3	EDO	C	7	-	-	1/1/1/1	-
3	EDO	D	11	-	-	0/1/1/1	-
3	EDO	A	5	-	-	1/1/1/1	-
3	EDO	C	3	-	-	0/1/1/1	-
3	EDO	D	8	-	-	1/1/1/1	-
3	EDO	C	8	-	-	0/1/1/1	-
3	EDO	D	3	-	-	1/1/1/1	-
4	JN8	D	15	-	-	4/23/39/39	0/4/4/4
3	EDO	C	9	-	-	1/1/1/1	-
3	EDO	D	2	-	-	1/1/1/1	-
3	EDO	A	7	-	-	0/1/1/1	-
3	EDO	A	2	-	-	0/1/1/1	-
6	EPE	C	2	-	-	5/9/19/19	0/1/1/1
3	EDO	A	9	-	-	0/1/1/1	-
3	EDO	A	4	-	-	0/1/1/1	-
3	EDO	A	441	-	-	0/1/1/1	-
3	EDO	D	440	-	-	1/1/1/1	-
3	EDO	D	5	-	-	0/1/1/1	-
3	EDO	C	440	-	-	1/1/1/1	-
3	EDO	D	6	-	-	1/1/1/1	-
3	EDO	D	9	-	-	0/1/1/1	-
4	JN8	B	440	-	-	2/23/39/39	0/4/4/4
3	EDO	C	5	-	-	0/1/1/1	-
4	JN8	C	441	-	-	3/23/39/39	0/4/4/4
3	EDO	A	8	-	-	0/1/1/1	-
3	EDO	A	442	-	-	0/1/1/1	-
3	EDO	B	4	-	-	0/1/1/1	-
4	JN8	A	440	-	-	3/23/39/39	0/4/4/4
3	EDO	B	6	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	5	-	-	0/1/1/1	-
3	EDO	D	10	-	-	0/1/1/1	-
3	EDO	D	4	-	-	0/1/1/1	-
3	EDO	C	4	-	-	1/1/1/1	-
3	EDO	D	7	-	-	1/1/1/1	-
3	EDO	A	6	-	-	0/1/1/1	-

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	440	JN8	C24-N7	6.56	1.47	1.36
4	C	441	JN8	C24-N7	6.45	1.47	1.36
4	A	440	JN8	C24-N7	6.09	1.47	1.36
4	D	15	JN8	C24-N7	5.60	1.46	1.36
4	C	441	JN8	C3-N10	4.92	1.44	1.38
4	B	440	JN8	C2-C1	4.82	1.54	1.44
4	D	15	JN8	C2-C1	4.75	1.53	1.44
4	C	441	JN8	C2-C1	4.69	1.53	1.44
4	A	440	JN8	C2-C1	4.60	1.53	1.44
5	B	14	DMS	O-S	4.58	1.80	1.50
4	C	441	JN8	C2-C3	4.38	1.47	1.39
4	D	15	JN8	C3-N10	4.33	1.44	1.38
4	D	15	JN8	C5-C1	4.17	1.41	1.36
4	A	440	JN8	C11-N10	4.16	1.44	1.37
4	B	440	JN8	C3-N10	4.12	1.43	1.38
4	C	441	JN8	C11-N10	4.02	1.44	1.37
4	A	440	JN8	C2-C3	3.96	1.46	1.39
4	A	440	JN8	C5-C1	3.94	1.40	1.36
4	D	15	JN8	C11-N10	3.94	1.44	1.37
4	A	440	JN8	C3-N10	3.92	1.43	1.38
4	B	440	JN8	C5-C1	3.84	1.40	1.36
4	B	440	JN8	C2-C3	3.69	1.46	1.39
4	B	440	JN8	C11-N10	3.67	1.43	1.37
4	C	441	JN8	C5-C1	3.65	1.40	1.36
4	D	15	JN8	C2-C3	3.62	1.46	1.39
6	C	2	EPE	C10-S	3.51	1.82	1.77
4	B	440	JN8	O20-C19	-3.40	1.27	1.34
4	C	441	JN8	O31-C19	3.17	1.27	1.21
4	B	440	JN8	O20-C27	-2.99	1.39	1.46
4	C	441	JN8	O20-C19	-2.93	1.28	1.34
4	C	441	JN8	C24-N28	2.93	1.46	1.34
4	D	15	JN8	O20-C19	-2.86	1.28	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	440	JN8	C24-N28	2.85	1.46	1.34
4	A	440	JN8	C24-N28	2.84	1.46	1.34
4	A	440	JN8	O20-C19	-2.83	1.28	1.34
4	D	15	JN8	C24-N28	2.81	1.45	1.34
4	D	15	JN8	O31-C19	2.78	1.27	1.21
4	B	440	JN8	O31-C19	2.78	1.27	1.21
4	A	440	JN8	O31-C19	2.72	1.27	1.21
4	B	440	JN8	C6-C5	-2.57	1.48	1.50
4	D	15	JN8	C6-N7	-2.57	1.42	1.46
4	C	441	JN8	O20-C27	-2.38	1.41	1.46
4	D	15	JN8	O20-C27	-2.34	1.41	1.46
4	B	440	JN8	C6-N7	-2.26	1.43	1.46
4	A	440	JN8	O20-C27	-2.23	1.41	1.46
4	C	441	JN8	C15-C16	2.23	1.42	1.34
4	A	440	JN8	C15-C16	2.16	1.42	1.34

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	440	JN8	N28-C24-N7	9.29	123.29	117.66
4	C	441	JN8	C5-S4-C3	7.77	95.10	91.14
4	D	15	JN8	N28-C24-N7	7.57	122.25	117.66
4	D	15	JN8	C5-S4-C3	6.71	94.56	91.14
4	A	440	JN8	C27-O20-C19	6.10	125.88	117.35
4	B	440	JN8	C5-S4-C3	6.09	94.24	91.14
4	A	440	JN8	C5-S4-C3	5.31	93.84	91.14
4	D	15	JN8	C27-O20-C19	4.80	124.06	117.35
4	D	15	JN8	C11-N10-C3	-4.38	119.44	124.87
4	A	440	JN8	C19-C2-C3	4.13	126.21	120.09
4	B	440	JN8	C5-C6-N7	-4.04	105.36	109.22
4	D	15	JN8	O31-C19-C2	-3.91	117.52	124.60
4	C	441	JN8	C19-C2-C3	3.64	125.48	120.09
4	B	440	JN8	C11-N10-C3	-3.57	120.43	124.87
4	D	15	JN8	O20-C19-C2	3.53	119.47	112.21
4	B	440	JN8	C12-C11-N10	3.42	119.20	115.14
4	C	441	JN8	C27-O20-C19	3.38	122.08	117.35
4	D	15	JN8	C6-C5-C1	3.28	127.40	125.21
4	D	15	JN8	C5-C6-N7	-3.28	106.09	109.22
6	C	2	EPE	O1S-S-C10	3.22	111.60	106.73
4	B	440	JN8	C2-C1-C5	-3.19	109.67	112.08
4	A	440	JN8	S4-C3-N10	3.11	126.76	122.95
4	D	15	JN8	C9-C1-C5	-3.09	118.16	121.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	441	JN8	C12-C11-N10	3.07	118.78	115.14
4	A	440	JN8	O29-C24-N7	-3.07	117.39	121.67
4	D	15	JN8	C6-C5-S4	-3.05	119.15	121.91
4	C	441	JN8	C2-C1-C5	-3.02	109.81	112.08
4	B	440	JN8	C27-O20-C19	2.94	121.46	117.35
6	C	2	EPE	C7-N4-C5	2.92	119.02	111.24
4	B	440	JN8	N28-C24-N7	2.90	119.41	117.66
6	C	2	EPE	C5-N4-C3	2.87	115.03	108.84
4	C	441	JN8	N28-C24-N7	2.84	119.38	117.66
4	B	440	JN8	C19-C2-C3	2.84	124.29	120.09
4	D	15	JN8	C9-C1-C2	2.79	131.62	127.16
4	C	441	JN8	C9-C1-C2	2.77	131.58	127.16
4	A	440	JN8	C12-C11-N10	2.75	118.41	115.14
4	C	441	JN8	C9-C1-C5	-2.66	118.61	121.39
4	A	440	JN8	C2-C3-N10	-2.64	121.98	124.61
4	B	440	JN8	C9-C1-C2	2.56	131.24	127.16
4	D	15	JN8	O29-C24-N7	-2.48	118.20	121.67
4	D	15	JN8	C2-C1-C5	-2.48	110.21	112.08
4	D	15	JN8	C12-C11-N10	2.48	118.08	115.14
4	A	440	JN8	O31-C19-C2	-2.47	120.12	124.60
4	B	440	JN8	O20-C19-C2	2.46	117.26	112.21
4	A	440	JN8	C9-C1-C5	-2.44	118.84	121.39
6	C	2	EPE	C7-N4-C3	2.35	117.51	111.24
4	B	440	JN8	S4-C3-N10	2.33	125.80	122.95
4	C	441	JN8	O31-C19-C2	-2.29	120.45	124.60
6	C	2	EPE	O2S-S-C10	2.27	110.17	106.73
4	B	440	JN8	C9-C1-C5	-2.22	119.07	121.39
4	A	440	JN8	C9-C1-C2	2.15	130.59	127.16
4	A	440	JN8	O20-C19-C2	2.07	116.46	112.21
4	C	441	JN8	C2-C3-S4	-2.06	109.92	112.62
4	A	440	JN8	C2-C1-C5	-2.03	110.55	112.08
4	B	440	JN8	C6-C5-S4	-2.02	120.08	121.91
4	D	15	JN8	C19-C2-C3	2.01	123.07	120.09

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	440	JN8	C28-C27-O20-C19
4	A	440	JN8	C32-C33-N28-C24
4	C	441	JN8	C28-C27-O20-C19
4	D	15	JN8	C31-C27-O20-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	C	2	EPE	C9-C10-S-O1S
6	C	2	EPE	C9-C10-S-O2S
6	C	2	EPE	C9-C10-S-O3S
4	A	440	JN8	O31-C19-O20-C27
4	D	15	JN8	O31-C19-O20-C27
4	D	15	JN8	C32-C33-N28-C24
3	C	7	EDO	O1-C1-C2-O2
4	C	441	JN8	O31-C19-O20-C27
6	C	2	EPE	S-C10-C9-N1
3	C	4	EDO	O1-C1-C2-O2
3	D	2	EDO	O1-C1-C2-O2
3	D	440	EDO	O1-C1-C2-O2
6	C	2	EPE	C8-C7-N4-C3
4	D	15	JN8	O18-C11-C12-C13
3	A	5	EDO	O1-C1-C2-O2
3	D	8	EDO	O1-C1-C2-O2
3	C	440	EDO	O1-C1-C2-O2
3	C	9	EDO	O1-C1-C2-O2
3	D	3	EDO	O1-C1-C2-O2
3	D	6	EDO	O1-C1-C2-O2
3	D	7	EDO	O1-C1-C2-O2
4	B	440	JN8	O18-C11-C12-C13
4	C	441	JN8	O18-C11-C12-C13
4	B	440	JN8	C28-C27-O20-C19

There are no ring outliers.

24 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	7	EDO	2	0
3	D	11	EDO	4	0
3	A	5	EDO	1	0
3	C	3	EDO	2	0
3	D	8	EDO	1	0
3	C	8	EDO	2	0
3	D	3	EDO	5	0
4	D	15	JN8	4	0
3	A	2	EDO	1	0
6	C	2	EPE	3	0
3	D	440	EDO	1	0
3	D	5	EDO	2	0
3	C	440	EDO	1	0

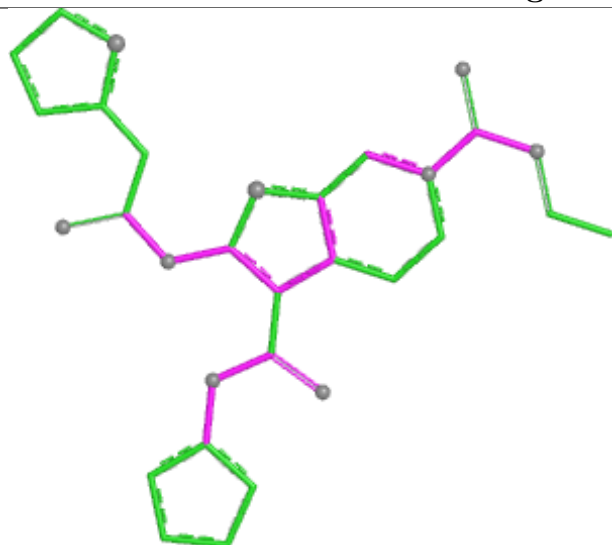
Continued on next page...

Continued from previous page...

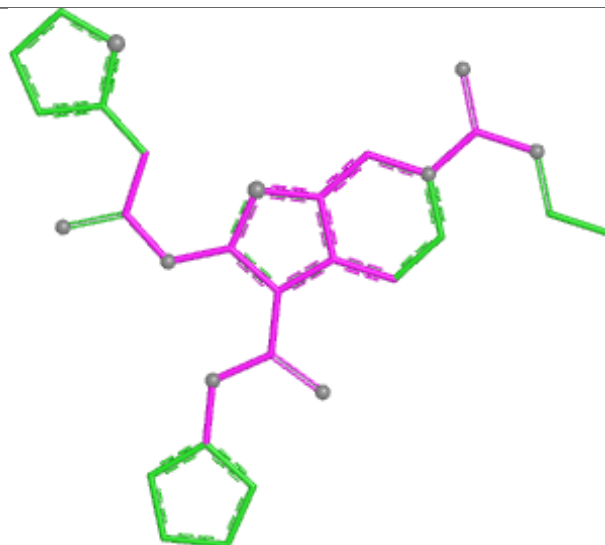
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	9	EDO	2	0
4	B	440	JN8	2	0
4	C	441	JN8	2	0
5	B	14	DMS	2	0
3	A	442	EDO	3	0
4	A	440	JN8	3	0
3	B	5	EDO	4	0
3	D	10	EDO	2	0
3	D	4	EDO	2	0
3	C	4	EDO	1	0
3	D	7	EDO	1	0

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 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.

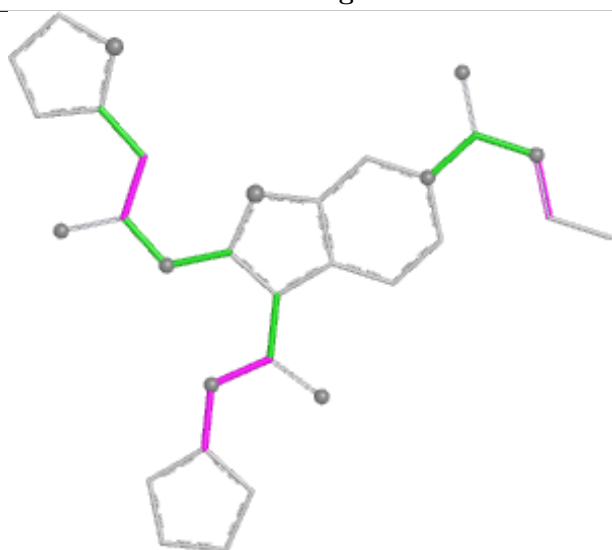
Ligand JN8 D 15



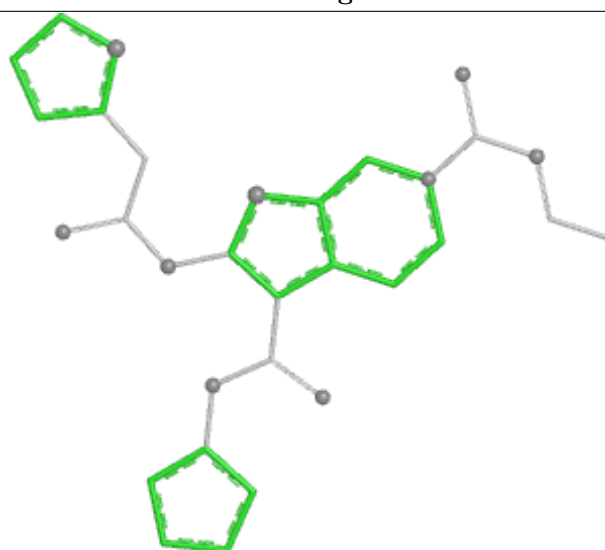
Bond lengths



Bond angles

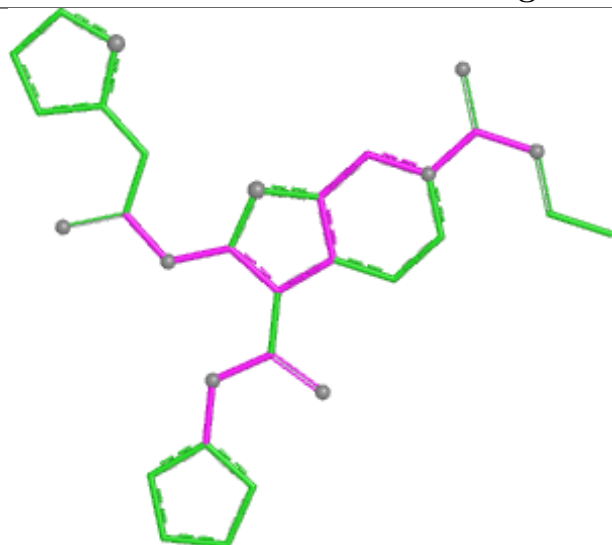


Torsions

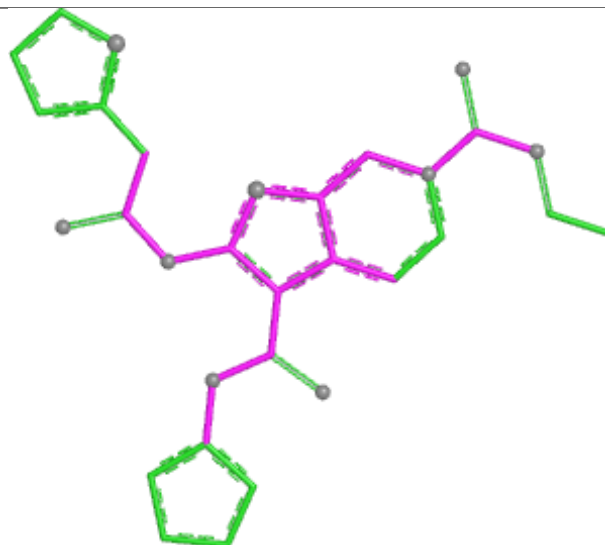


Rings

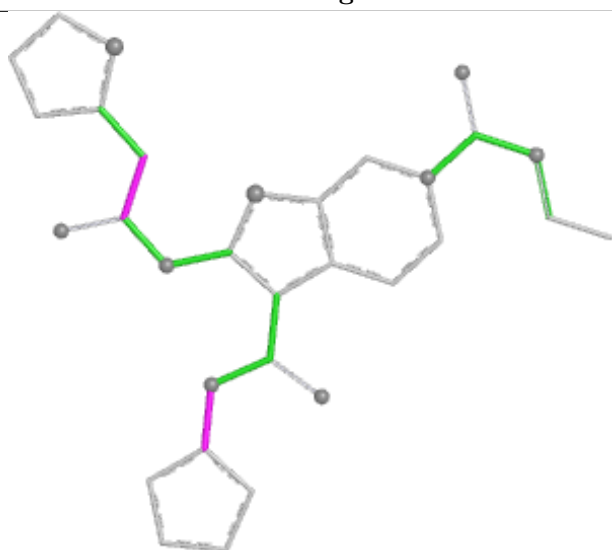
Ligand JN8 B 440



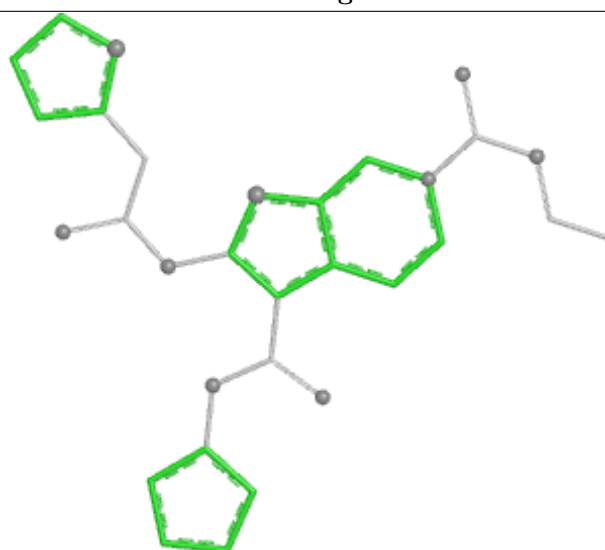
Bond lengths



Bond angles

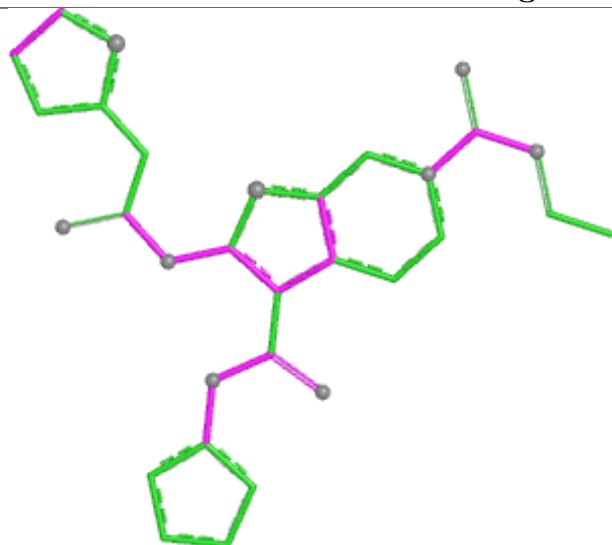


Torsions

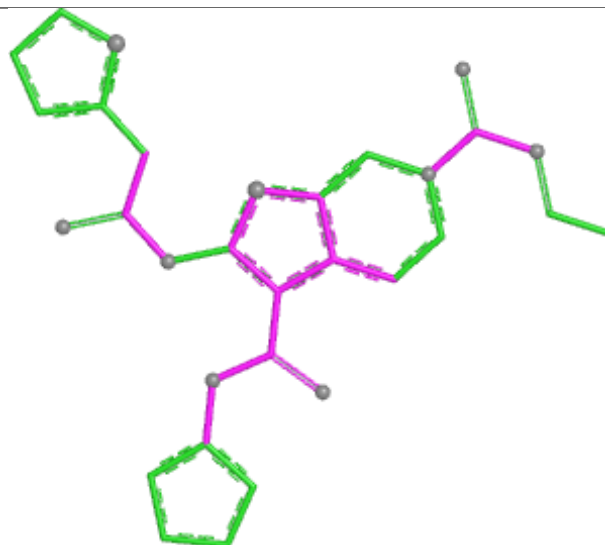


Rings

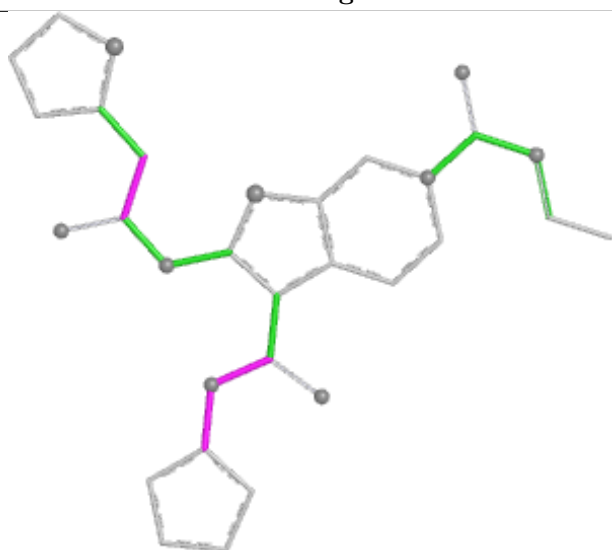
Ligand JN8 C 441



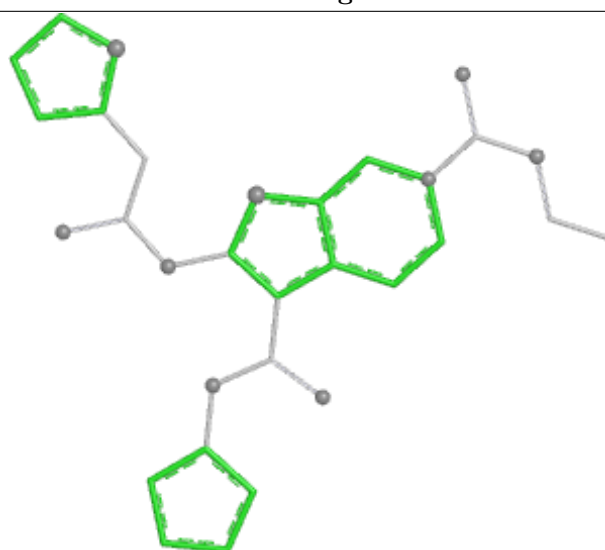
Bond lengths



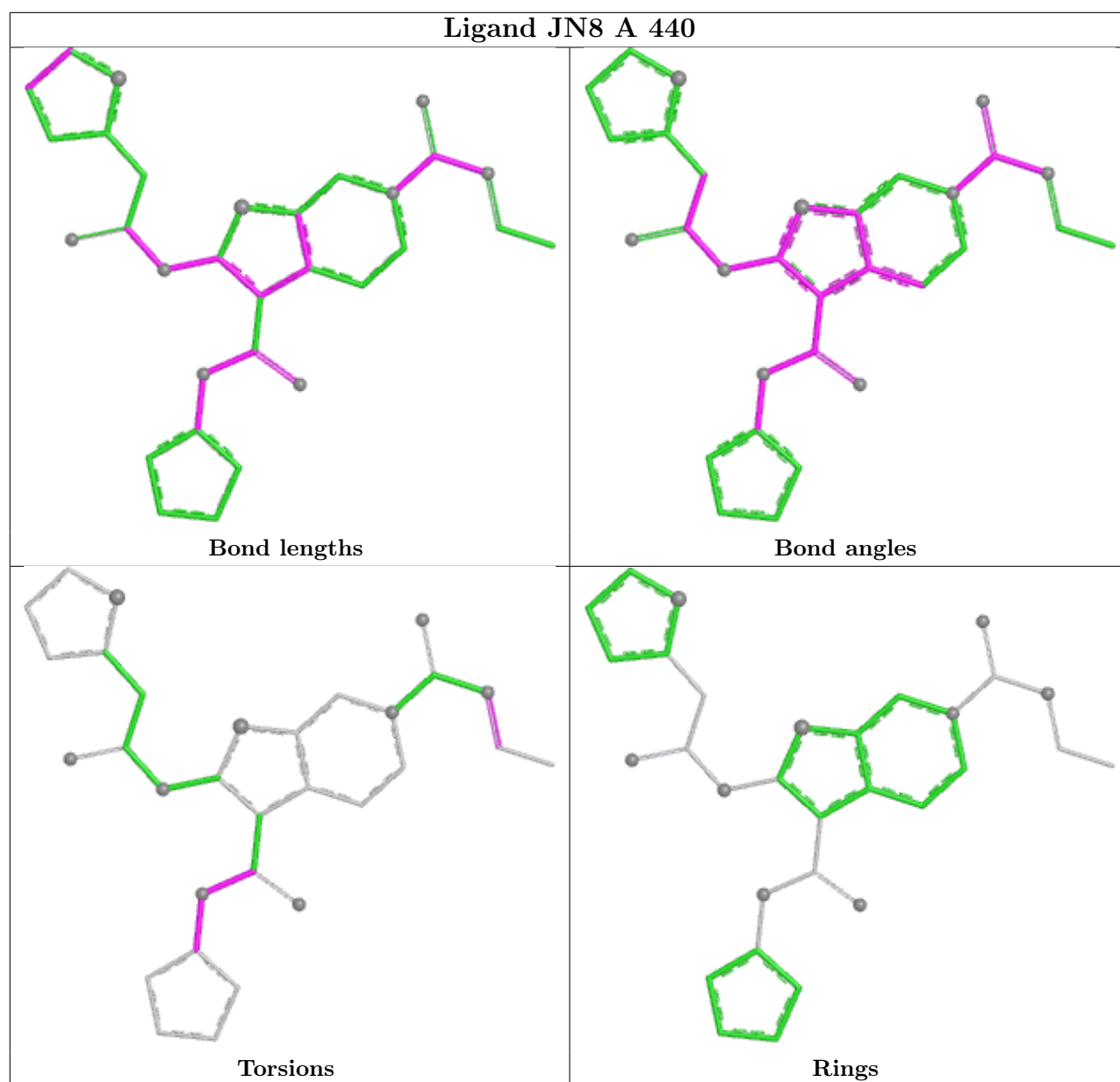
Bond angles



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, 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	327/361 (90%)	-0.03	11 (3%) 48 46	16, 37, 73, 111	1 (0%)
1	B	325/361 (90%)	0.36	10 (3%) 51 50	26, 48, 69, 103	0
1	C	325/361 (90%)	0.24	11 (3%) 48 46	28, 46, 79, 104	0
1	D	324/361 (89%)	-0.07	8 (2%) 58 59	15, 35, 65, 90	1 (0%)
All	All	1301/1444 (90%)	0.12	40 (3%) 51 50	15, 42, 71, 111	2 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	351	GLY	5.2
1	C	353	GLU	4.4
1	B	356	PRO	4.1
1	C	357	MET	3.7
1	C	354	ILE	3.7
1	C	356	PRO	3.6
1	A	296	GLY	3.6
1	A	357	MET	3.5
1	A	293	THR	3.4
1	B	251	ASN	3.3
1	B	295	SER	3.3
1	D	356	PRO	3.3
1	C	296	GLY	3.2
1	A	294	SER	3.0
1	D	357	MET	3.0
1	A	295	SER	3.0
1	B	296	GLY	3.0
1	C	410	ILE	2.9
1	A	297	VAL	2.9
1	D	354	ILE	2.8
1	A	356	PRO	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	294	SER	2.7
1	B	351	GLY	2.5
1	B	93	ALA	2.5
1	D	105[A]	HIS	2.4
1	C	293	THR	2.4
1	A	361	HIS	2.4
1	A	409	THR	2.4
1	A	105[A]	HIS	2.3
1	D	346	ARG	2.3
1	D	88	GLN	2.2
1	C	297	VAL	2.2
1	B	88	GLN	2.2
1	D	296	GLY	2.2
1	B	412	GLN	2.1
1	B	136	LYS	2.1
1	A	299	LEU	2.0
1	B	133	LYS	2.0
1	C	295	SER	2.0
1	D	273	MET	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
3	EDO	B	6	4/4	0.74	0.19	53,56,56,59	0
3	EDO	B	5	4/4	0.75	0.19	50,55,56,57	0
3	EDO	C	7	4/4	0.75	0.21	46,53,55,56	0
5	DMS	B	14	4/4	0.76	0.21	69,69,75,80	0

Continued on next page...

Continued from previous page...

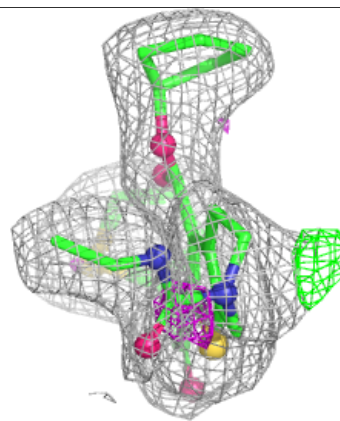
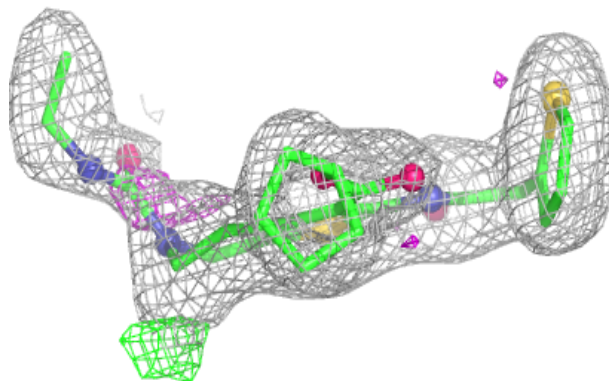
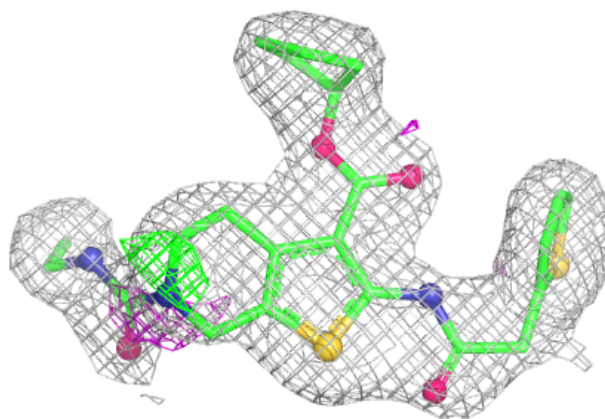
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	D	10	4/4	0.80	0.18	46,48,49,49	0
3	EDO	A	8	4/4	0.80	0.16	52,52,53,58	0
3	EDO	A	7	4/4	0.81	0.18	47,48,51,54	0
3	EDO	C	8	4/4	0.83	0.21	49,53,54,60	0
3	EDO	D	5	4/4	0.83	0.15	47,48,50,55	0
6	EPE	C	2	15/15	0.85	0.16	47,68,82,83	0
3	EDO	C	9	4/4	0.87	0.13	50,52,52,55	0
3	EDO	D	4	4/4	0.87	0.15	40,48,51,56	0
3	EDO	C	3	4/4	0.88	0.12	41,44,48,53	0
3	EDO	A	2	4/4	0.88	0.14	49,53,55,57	0
3	EDO	A	5	4/4	0.88	0.12	47,48,50,51	0
3	EDO	D	3	4/4	0.89	0.29	29,30,38,39	0
3	EDO	D	11	4/4	0.89	0.22	44,49,54,57	0
3	EDO	C	440	4/4	0.90	0.12	54,55,56,59	0
3	EDO	B	4	4/4	0.91	0.19	51,53,59,61	0
4	JN8	C	441	31/31	0.91	0.12	34,48,63,67	0
4	JN8	D	15	31/31	0.91	0.11	27,48,64,75	0
3	EDO	D	6	4/4	0.91	0.13	38,39,40,46	0
3	EDO	A	6	4/4	0.91	0.11	33,40,41,42	0
3	EDO	A	442	4/4	0.92	0.12	37,39,40,43	0
3	EDO	D	8	4/4	0.92	0.12	42,46,48,49	0
3	EDO	A	4	4/4	0.92	0.12	39,43,45,47	0
3	EDO	C	4	4/4	0.92	0.11	49,50,53,54	0
3	EDO	D	9	4/4	0.93	0.17	31,35,38,40	0
4	JN8	A	440	31/31	0.93	0.11	36,49,72,78	0
4	JN8	B	440	31/31	0.94	0.10	29,39,55,60	0
3	EDO	A	9	4/4	0.94	0.10	32,34,38,48	0
3	EDO	C	5	4/4	0.94	0.10	42,44,47,48	0
3	EDO	A	441	4/4	0.94	0.07	27,31,32,34	0
3	EDO	D	440	4/4	0.94	0.14	34,35,38,39	0
3	EDO	D	2	4/4	0.96	0.06	34,40,40,42	0
3	EDO	D	7	4/4	0.96	0.07	35,39,39,41	0
2	ZN	B	8	1/1	0.97	0.05	64,64,64,64	0
2	ZN	C	10	1/1	0.97	0.06	65,65,65,65	0
2	ZN	A	11	1/1	0.98	0.04	54,54,54,54	0
2	ZN	B	7	1/1	0.98	0.05	43,43,43,43	0
2	ZN	D	12	1/1	0.98	0.04	59,59,59,59	0
2	ZN	C	11	1/1	0.99	0.05	40,40,40,40	0
2	ZN	A	10	1/1	0.99	0.04	35,35,35,35	0
2	ZN	D	13	1/1	0.99	0.04	37,37,37,37	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

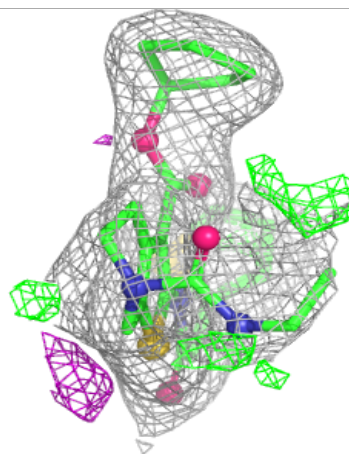
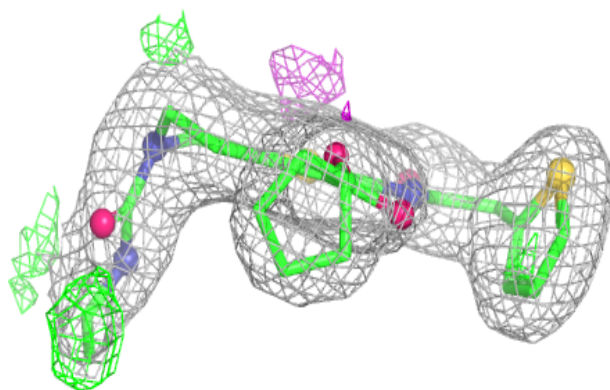
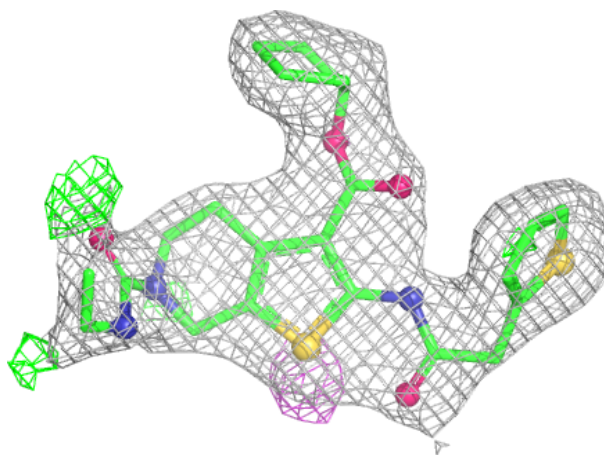
Electron density around JN8 C 441:

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



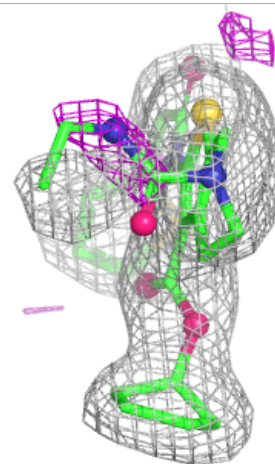
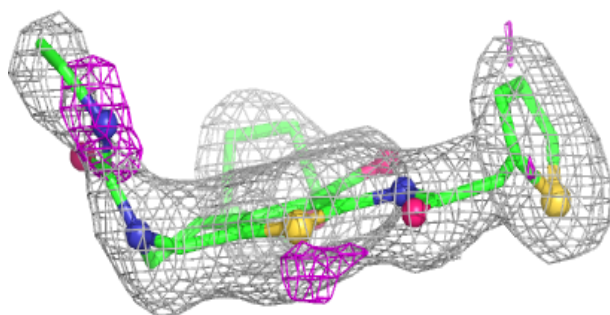
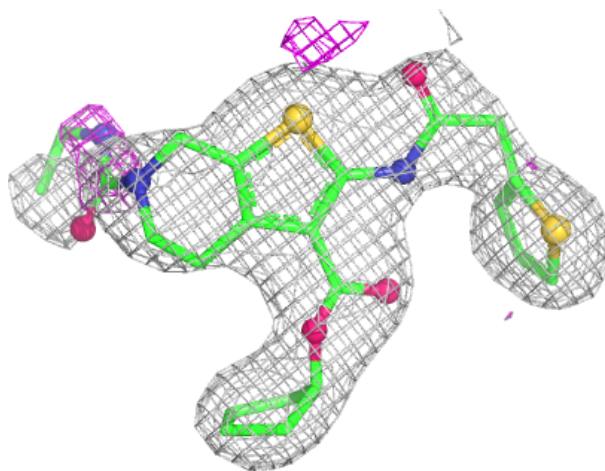
Electron density around JN8 D 15:

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



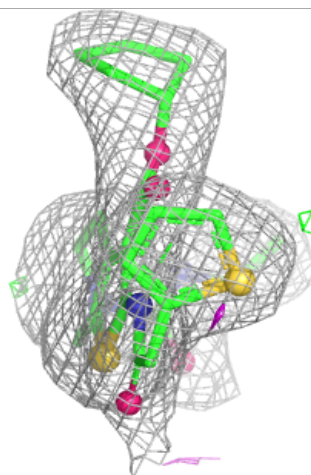
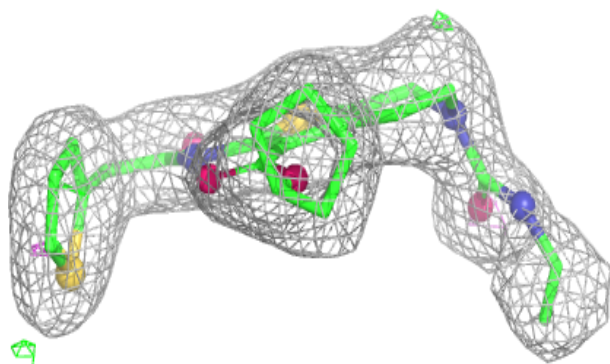
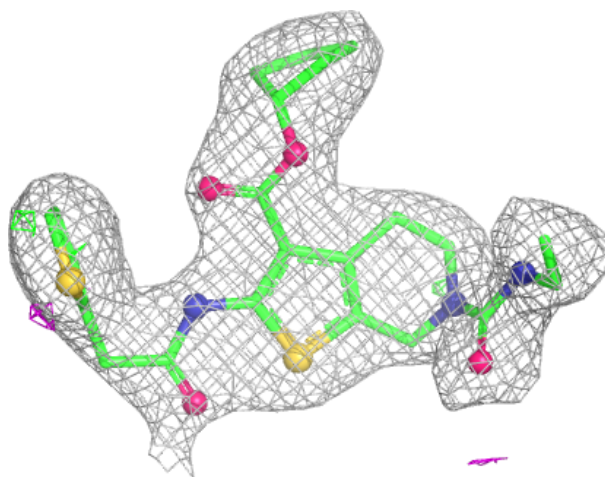
Electron density around JN8 A 440:

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



Electron density around JN8 B 440:

$2mF_o-DF_c$ (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.