Full wwPDB X-ray Structure Validation Report (i)

Feb 17, 2024 – 01:22 PM EST

PDB ID	:	3SL6
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 (i) symbol.

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

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

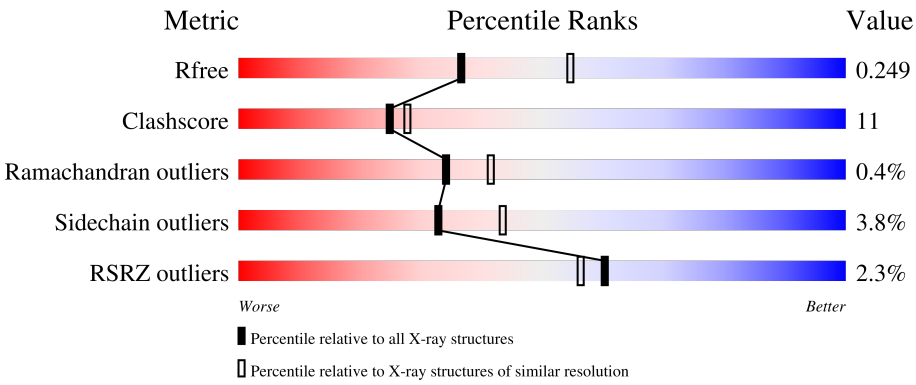
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.44 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}	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (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 <=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% 73% 16% • 9%
1	B	361	2% 66% 22% • 10%
1	C	361	2% 68% 20% • 10%
1	D	361	% 72% 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	X
3	EDO	D	3	-	-	X	-

2 Entry composition (i)

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.

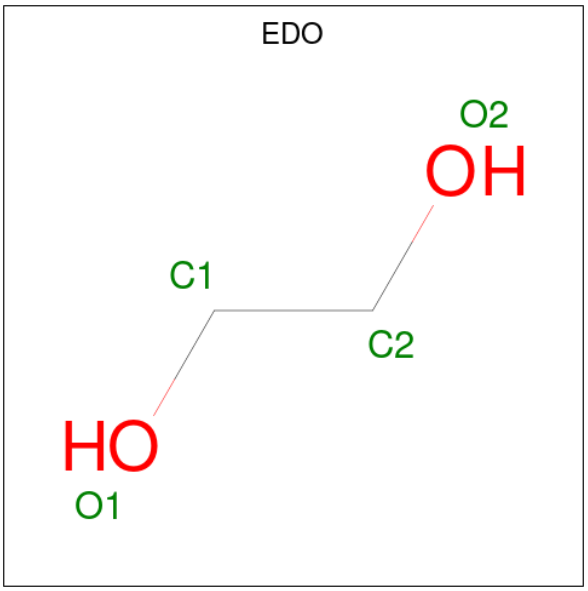
- Molecule 1 is a protein called cAMP-specific 3',5'-cyclic phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	327	2657	1680	455	508	14	0	1	0
1	B	325	2631	1664	450	503	14	0	0	0
1	C	325	2631	1663	449	505	14	0	0	0
1	D	324	2632	1665	451	502	14	0	1	0

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

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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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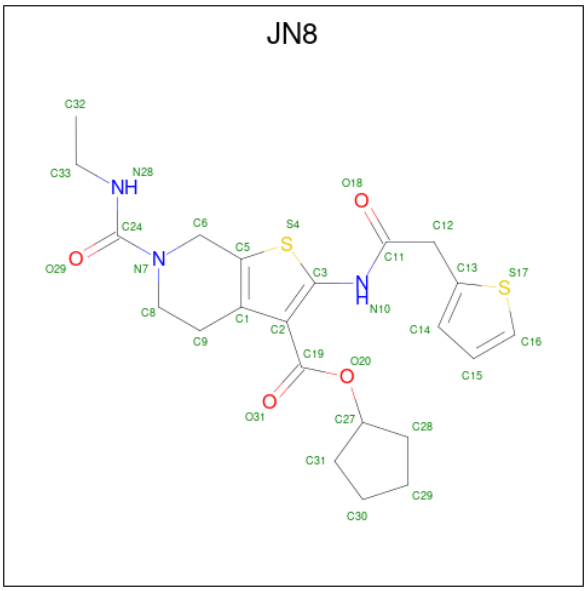
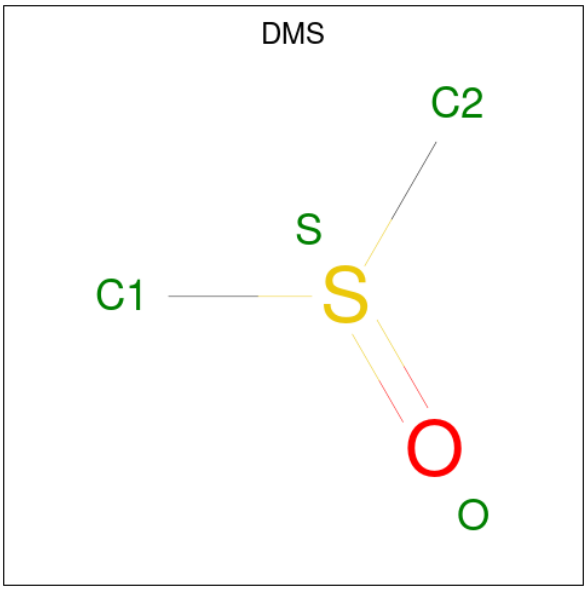
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	C	1	4	2	2	0	0
			Total	C	O		
3	C	1	4	2	2	0	0
			Total	C	O		
3	C	1	4	2	2	0	0
			Total	C	O		
3	C	1	4	2	2	0	0
			Total	C	O		
3	C	1	4	2	2	0	0
			Total	C	O		
3	D	1	4	2	2	0	0
			Total	C	O		
3	D	1	4	2	2	0	0
			Total	C	O		
3	D	1	4	2	2	0	0
			Total	C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

- Molecule 4 is cyclopentyl 6-(ethylcarbamoyl)-2-[(thiophen-2-ylacetyl)amino]-4,5,6,7-tetrahydrothieno[2,3-c]pyridine-3-carboxylate (three-letter code: JN8) (formula: $C_{22}H_{27}N_3O_4S_2$).



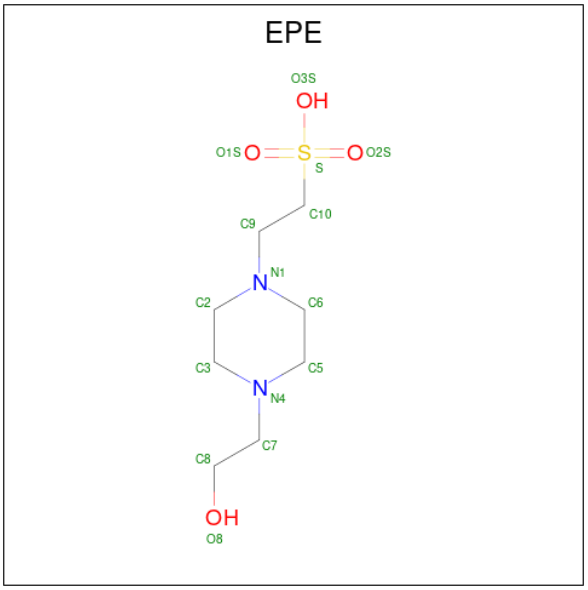
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	31	22	3	4	2	0	0
			Total	C	N	O	S		
4	B	1	31	22	3	4	2	0	0
			Total	C	N	O	S		
4	C	1	31	22	3	4	2	0	0
			Total	C	N	O	S		
4	D	1	31	22	3	4	2	0	0

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

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



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

- Molecule 7 is water.

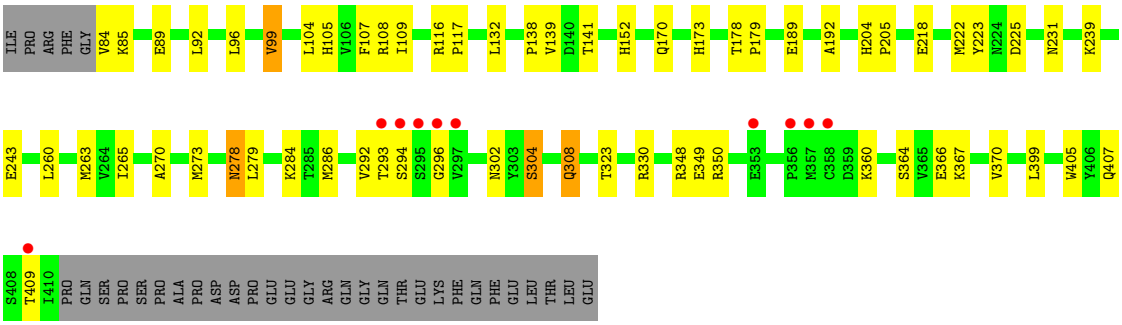
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	64	64	64	0	0
			Total	O		
7	B	47	47	47	0	0
			Total	O		
7	C	36	36	36	0	0
			Total	O		
7	D	73	73	73	0	0

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.

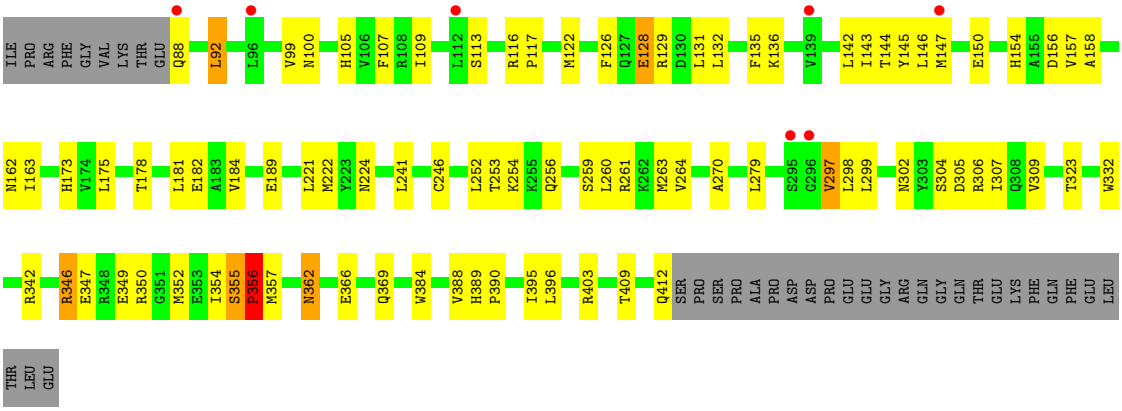
• Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain A:



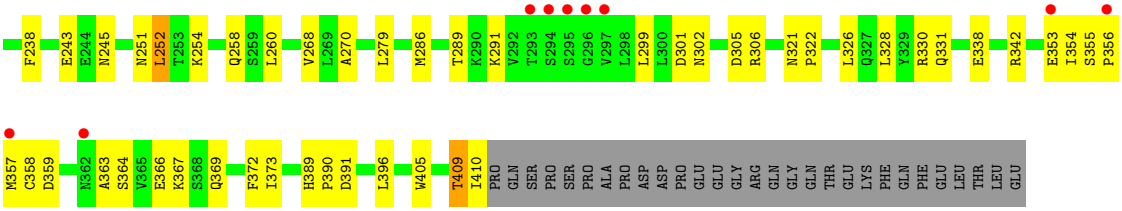
• Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain B:



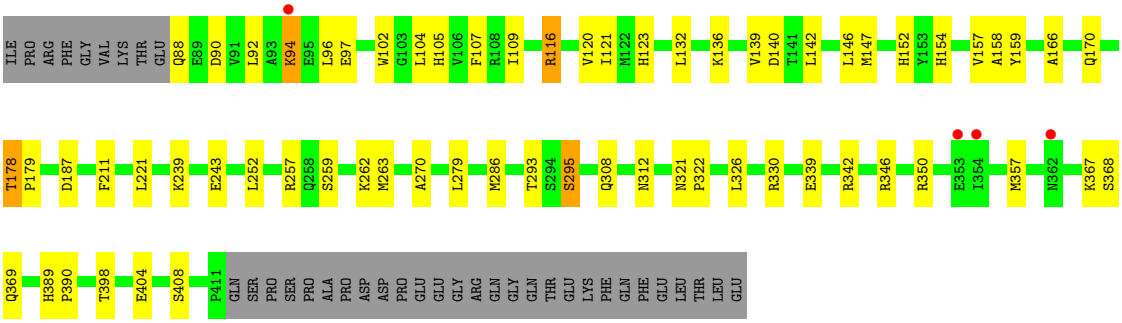
• Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain C:



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

Chain D:



4 Data and refinement statistics (i)

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 67.36 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.0 (65.19-2.44) 99.5 (67.36-2.44)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.23 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, R_{free}	0.198 , 0.256 0.192 , 0.249	Depositor DCC
R_{free} test set	3381 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)	0.35 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	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.*

[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: JN8, EPE, ZN, DMS, EDO

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	0.42	0/2711	0.55	0/3682
1	B	0.39	0/2685	0.53	0/3648
1	C	0.37	0/2684	0.52	0/3646
1	D	0.44	0/2687	0.56	0/3651
All	All	0.40	0/10767	0.54	0/14627

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	2657	0	2612	43	0
1	B	2631	0	2586	76	0
1	C	2631	0	2584	50	0
1	D	2632	0	2584	61	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	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	232	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 11.

All (232) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:286:MET:HE1	1:C:305:ASP:HA	1.82	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
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:A:348:ARG:C	1:A:350:ARG:H	2.07	0.56
1:D:142:LEU:O	1:D:146:LEU:HG	2.04	0.56
1:D:308:GLN:HE21	1:D:312:ASN:ND2	2.03	0.56
1:B:350:ARG:NH1	7:B:22:HOH:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:273:MET:HE2	4:A:440:JN8:HN28	1.71	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: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: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:B:354:ILE:C	1:B:356:PRO:HD3	2.30	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:A:225:ASP:CG	1:B:261:ARG:HH21	2.13	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
1:A:265:ILE:HD13	1:B:224:ASN:O	2.12	0.50
1:B:355:SER:C	1:B:357:MET:H	2.15	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:182:GLU:HG2	3:B:5:EDO:H11	1.93	0.49
1:A:270:ALA:HB1	1:A:279:LEU:HD11	1.94	0.49
1:B:163:ILE:HG22	1:B:332:TRP:HH2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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:D:104:LEU:HD11	1:D:109:ILE:HD11	1.96	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:154:HIS:N	1:B:154:HIS:CD2	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:348:ARG:C	1:A:350:ARG:N	2.70	0.45
1:C:179:PRO:HD2	1:C:391:ASP:CG	2.37	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:135:PHE:O	1:B:136:LYS:HB2	2.18	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: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
1:A:348:ARG:O	1:A:350:ARG:N	2.51	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:347:GLU:HG2	1:B:352:MET:HE1	2.00	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:366:GLU:H	1:C:366:GLU:CD	2.19	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:D:367:LYS:C	1:D:367:LYS:HD3	2.38	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:C:389:HIS:CE1	1:C:390:PRO:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:211:PHE:CD1	1:D:211:PHE:C	2.92	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
1:B:128:GLU:HG3	1:B:129:ARG:N	2.32	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:132:LEU:HD21	1:B:142:LEU:CD2	2.45	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)

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	326/361 (90%)	312 (96%)	12 (4%)	2 (1%)	25	29
1	B	323/361 (90%)	300 (93%)	21 (6%)	2 (1%)	25	29
1	C	323/361 (90%)	305 (94%)	17 (5%)	1 (0%)	41	49
1	D	323/361 (90%)	313 (97%)	10 (3%)	0	100	100
All	All	1295/1444 (90%)	1230 (95%)	60 (5%)	5 (0%)	34	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	356	PRO
1	A	294	SER
1	A	349	GLU
1	C	353	GLU
1	B	355	SER

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	300/329 (91%)	290 (97%)	10 (3%)	38	49
1	B	297/329 (90%)	284 (96%)	13 (4%)	28	37
1	C	297/329 (90%)	282 (95%)	15 (5%)	24	31
1	D	297/329 (90%)	290 (98%)	7 (2%)	49	61
All	All	1191/1316 (90%)	1146 (96%)	45 (4%)	33	43

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	VAL
1	A	92	LEU
1	A	99	VAL
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	B	92	LEU
1	B	128	GLU
1	B	221	LEU
1	B	252	LEU
1	B	259	SER
1	B	297	VAL
1	B	298	LEU
1	B	299	LEU
1	B	346	ARG
1	B	356	PRO
1	B	362	ASN
1	B	396	LEU
1	B	403	ARG
1	C	86	THR

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Mol	Chain	Res	Type
1	C	90	ASP
1	C	92	LEU
1	C	116	ARG
1	C	132	LEU
1	C	139	VAL
1	C	147	MET
1	C	178	THR
1	C	245	ASN
1	C	252	LEU
1	C	258	GLN
1	C	289	THR
1	C	301	ASP
1	C	396	LEU
1	C	409	THR
1	D	92	LEU
1	D	94	LYS
1	D	116	ARG
1	D	136	LYS
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 (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	A	224	ASN
1	A	245	ASN
1	A	258	GLN
1	A	278	ASN
1	A	302	ASN
1	A	331	GLN
1	A	361	HIS
1	A	407	GLN
1	B	231	ASN
1	B	245	ASN
1	B	308	GLN
1	B	327	GLN
1	B	362	ASN
1	B	389	HIS
1	C	245	ASN
1	C	258	GLN

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Mol	Chain	Res	Type
1	C	308	GLN
1	C	331	GLN
1	C	393	GLN
1	D	123	HIS
1	D	127	GLN
1	D	152	HIS
1	D	245	ASN
1	D	278	ASN
1	D	312	ASN
1	D	321	ASN
1	D	393	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 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	D	5	-	3,3,3	0.55	0	2,2,2	0.19	0
3	EDO	A	5	-	3,3,3	0.56	0	2,2,2	0.11	0
3	EDO	D	11	-	3,3,3	0.60	0	2,2,2	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	EDO	D	440	-	3,3,3	0.46	0	2,2,2	0.11	0
3	EDO	A	2	-	3,3,3	0.51	0	2,2,2	0.22	0
4	JN8	A	440	-	32,34,34	2.27	9 (28%)	31,47,47	2.72	5 (16%)
3	EDO	C	440	-	3,3,3	0.47	0	2,2,2	0.31	0
3	EDO	A	4	-	3,3,3	0.53	0	2,2,2	0.25	0
3	EDO	D	7	-	3,3,3	0.59	0	2,2,2	0.25	0
6	EPE	C	2	-	15,15,15	1.04	1 (6%)	18,20,20	1.77	6 (33%)
3	EDO	A	6	-	3,3,3	0.54	0	2,2,2	0.15	0
3	EDO	D	3	-	3,3,3	0.38	0	2,2,2	0.81	0
3	EDO	D	10	-	3,3,3	0.63	0	2,2,2	0.14	0
3	EDO	A	441	-	3,3,3	0.43	0	2,2,2	0.42	0
3	EDO	A	9	-	3,3,3	0.45	0	2,2,2	0.76	0
3	EDO	C	5	-	3,3,3	0.55	0	2,2,2	0.26	0
3	EDO	D	6	-	3,3,3	0.52	0	2,2,2	0.41	0
3	EDO	D	8	-	3,3,3	0.68	0	2,2,2	0.12	0
3	EDO	D	9	-	3,3,3	0.52	0	2,2,2	0.11	0
3	EDO	C	7	-	3,3,3	0.57	0	2,2,2	0.30	0
3	EDO	C	3	-	3,3,3	0.61	0	2,2,2	0.24	0
3	EDO	D	4	-	3,3,3	0.59	0	2,2,2	0.19	0
3	EDO	A	442	-	3,3,3	0.61	0	2,2,2	0.26	0
3	EDO	A	7	-	3,3,3	0.61	0	2,2,2	0.18	0
3	EDO	A	8	-	3,3,3	0.56	0	2,2,2	0.23	0
4	JN8	C	441	-	32,34,34	2.33	9 (28%)	31,47,47	1.57	5 (16%)
4	JN8	B	440	-	32,34,34	2.38	10 (31%)	31,47,47	1.98	8 (25%)
3	EDO	C	8	-	3,3,3	0.57	0	2,2,2	0.06	0
3	EDO	C	9	-	3,3,3	0.57	0	2,2,2	0.23	0
3	EDO	C	4	-	3,3,3	0.40	0	2,2,2	0.52	0
3	EDO	B	4	-	3,3,3	0.59	0	2,2,2	0.10	0
5	DMS	B	14	-	3,3,3	2.68	1 (33%)	3,3,3	0.61	0
4	JN8	D	15	-	32,34,34	2.31	11 (34%)	31,47,47	2.57	9 (29%)
3	EDO	B	6	-	3,3,3	0.57	0	2,2,2	0.10	0
3	EDO	D	2	-	3,3,3	0.48	0	2,2,2	0.44	0
3	EDO	B	5	-	3,3,3	0.56	0	2,2,2	0.15	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	D	5	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	5	-	-	1/1/1/1	-
3	EDO	D	11	-	-	0/1/1/1	-
3	EDO	D	440	-	-	1/1/1/1	-
3	EDO	A	2	-	-	0/1/1/1	-
4	JN8	A	440	-	-	4/19/39/39	0/4/4/4
3	EDO	C	440	-	-	1/1/1/1	-
3	EDO	A	4	-	-	0/1/1/1	-
3	EDO	D	7	-	-	1/1/1/1	-
6	EPE	C	2	-	-	5/9/19/19	0/1/1/1
3	EDO	A	6	-	-	0/1/1/1	-
3	EDO	D	3	-	-	1/1/1/1	-
3	EDO	D	10	-	-	0/1/1/1	-
3	EDO	A	441	-	-	0/1/1/1	-
3	EDO	A	9	-	-	0/1/1/1	-
3	EDO	C	5	-	-	0/1/1/1	-
3	EDO	D	6	-	-	1/1/1/1	-
3	EDO	D	8	-	-	1/1/1/1	-
3	EDO	D	9	-	-	0/1/1/1	-
3	EDO	C	7	-	-	1/1/1/1	-
3	EDO	C	3	-	-	0/1/1/1	-
3	EDO	D	4	-	-	0/1/1/1	-
3	EDO	A	442	-	-	0/1/1/1	-
3	EDO	A	7	-	-	0/1/1/1	-
3	EDO	A	8	-	-	0/1/1/1	-
4	JN8	C	441	-	-	4/19/39/39	0/4/4/4
4	JN8	B	440	-	-	4/19/39/39	0/4/4/4
3	EDO	C	8	-	-	0/1/1/1	-
3	EDO	C	9	-	-	1/1/1/1	-
3	EDO	C	4	-	-	1/1/1/1	-
3	EDO	B	4	-	-	0/1/1/1	-
4	JN8	D	15	-	-	5/19/39/39	0/4/4/4
3	EDO	B	6	-	-	0/1/1/1	-
3	EDO	D	2	-	-	1/1/1/1	-
3	EDO	B	5	-	-	0/1/1/1	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	440	JN8	C2-C1	7.92	1.54	1.39
4	D	15	JN8	C2-C1	7.84	1.53	1.39
4	C	441	JN8	C2-C1	7.77	1.53	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	440	JN8	C2-C1	7.67	1.53	1.39
4	B	440	JN8	C24-N7	6.16	1.47	1.36
4	C	441	JN8	C24-N7	6.05	1.47	1.36
4	A	440	JN8	C24-N7	5.72	1.47	1.36
4	D	15	JN8	C24-N7	5.26	1.46	1.36
5	B	14	DMS	O-S	4.47	1.80	1.50
4	A	440	JN8	C11-N10	4.14	1.44	1.35
4	C	441	JN8	C11-N10	4.02	1.44	1.35
4	D	15	JN8	C11-N10	3.95	1.44	1.35
4	B	440	JN8	O20-C19	-3.78	1.27	1.34
4	B	440	JN8	C11-N10	3.73	1.43	1.35
6	C	2	EPE	C10-S	3.52	1.82	1.77
4	D	15	JN8	C12-C13	-3.48	1.48	1.51
4	B	440	JN8	C6-C5	-3.35	1.48	1.51
4	C	441	JN8	O20-C19	-3.28	1.28	1.34
4	D	15	JN8	O20-C19	-3.19	1.28	1.34
4	A	440	JN8	O20-C19	-3.17	1.28	1.34
4	D	15	JN8	C6-C5	-2.89	1.48	1.51
4	B	440	JN8	O20-C27	-2.81	1.39	1.46
4	C	441	JN8	C2-C3	2.76	1.47	1.41
4	C	441	JN8	C24-N28	2.69	1.46	1.34
4	C	441	JN8	C15-C16	2.65	1.42	1.34
4	B	440	JN8	C24-N28	2.62	1.46	1.34
4	A	440	JN8	C24-N28	2.62	1.46	1.34
4	A	440	JN8	C15-C16	2.59	1.42	1.34
4	D	15	JN8	C24-N28	2.58	1.45	1.34
4	D	15	JN8	C6-N7	-2.53	1.42	1.46
4	A	440	JN8	C2-C3	2.40	1.46	1.41
4	A	440	JN8	C6-C5	-2.32	1.49	1.51
4	B	440	JN8	C6-N7	-2.25	1.43	1.46
4	B	440	JN8	C15-C16	2.24	1.41	1.34
4	C	441	JN8	O20-C27	-2.24	1.41	1.46
4	D	15	JN8	C15-C16	2.20	1.41	1.34
4	D	15	JN8	O20-C27	-2.19	1.41	1.46
4	C	441	JN8	C6-C5	-2.18	1.49	1.51
4	B	440	JN8	C2-C3	2.17	1.46	1.41
4	D	15	JN8	C2-C3	2.11	1.46	1.41
4	A	440	JN8	O20-C27	-2.10	1.41	1.46

All (33) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	440	JN8	N28-C24-N7	11.69	123.29	117.67
4	D	15	JN8	N28-C24-N7	9.53	122.25	117.67
4	B	440	JN8	C5-C6-N7	-7.03	105.36	112.72
4	D	15	JN8	C5-C6-N7	-6.34	106.09	112.72
4	A	440	JN8	C5-C6-N7	-4.84	107.66	112.72
4	A	440	JN8	C27-O20-C19	4.83	125.88	117.56
4	C	441	JN8	C5-C6-N7	-4.10	108.43	112.72
4	B	440	JN8	C15-C16-S17	-4.04	109.70	112.98
6	C	2	EPE	O1S-S-C10	3.89	111.60	106.92
4	D	15	JN8	C27-O20-C19	3.77	124.06	117.56
4	B	440	JN8	N28-C24-N7	3.63	119.41	117.67
4	C	441	JN8	N28-C24-N7	3.56	119.38	117.67
4	D	15	JN8	C15-C16-S17	-3.18	110.40	112.98
4	A	440	JN8	O29-C24-N7	-3.13	117.39	121.78
6	C	2	EPE	C7-N4-C5	3.05	119.02	111.23
4	D	15	JN8	C13-C12-C11	-2.93	107.56	113.39
4	C	441	JN8	C15-C16-S17	-2.90	110.63	112.98
4	C	441	JN8	C13-C12-C11	-2.84	107.74	113.39
6	C	2	EPE	C5-N4-C3	2.76	115.03	108.83
6	C	2	EPE	O2S-S-C10	2.70	110.17	106.92
4	B	440	JN8	C9-C8-N7	2.68	113.20	110.04
4	C	441	JN8	C27-O20-C19	2.63	122.08	117.56
4	D	15	JN8	O29-C24-N7	-2.55	118.20	121.78
6	C	2	EPE	C7-N4-C3	2.45	117.51	111.23
4	D	15	JN8	O20-C19-C2	2.42	119.47	113.33
4	B	440	JN8	C27-O20-C19	2.26	121.46	117.56
4	D	15	JN8	C3-N10-C11	-2.25	119.44	124.36
4	B	440	JN8	O18-C11-N10	-2.17	119.66	123.63
4	B	440	JN8	C12-C11-N10	2.14	119.20	114.77
4	A	440	JN8	C15-C16-S17	-2.09	111.29	112.98
4	B	440	JN8	O20-C19-O31	-2.06	120.17	123.53
4	D	15	JN8	C8-C9-C1	-2.03	108.29	111.63
6	C	2	EPE	C9-N1-C2	-2.02	106.06	111.23

There are no chirality outliers.

All (33) 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

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Mol	Chain	Res	Type	Atoms
4	C	441	JN8	C28-C27-O20-C19
4	D	15	JN8	C31-C27-O20-C19
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	C	441	JN8	O31-C19-O20-C27
4	D	15	JN8	C32-C33-N28-C24
3	C	4	EDO	O1-C1-C2-O2
3	C	7	EDO	O1-C1-C2-O2
3	D	2	EDO	O1-C1-C2-O2
6	C	2	EPE	S-C10-C9-N1
6	C	2	EPE	C8-C7-N4-C3
3	A	5	EDO	O1-C1-C2-O2
3	D	440	EDO	O1-C1-C2-O2
3	D	8	EDO	O1-C1-C2-O2
4	A	440	JN8	N10-C11-C12-C13
4	D	15	JN8	O18-C11-C12-C13
3	D	3	EDO	O1-C1-C2-O2
3	D	7	EDO	O1-C1-C2-O2
4	B	440	JN8	O18-C11-C12-C13
4	B	440	JN8	N10-C11-C12-C13
3	C	440	EDO	O1-C1-C2-O2
3	C	9	EDO	O1-C1-C2-O2
3	D	6	EDO	O1-C1-C2-O2
4	C	441	JN8	N10-C11-C12-C13
4	C	441	JN8	O18-C11-C12-C13
4	B	440	JN8	C28-C27-O20-C19
4	D	15	JN8	N10-C11-C12-C13
4	B	440	JN8	O31-C19-O20-C27

There are no ring outliers.

23 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	5	EDO	2	0
3	A	5	EDO	1	0
3	D	11	EDO	4	0
3	D	440	EDO	1	0
3	A	2	EDO	1	0
4	A	440	JN8	3	0

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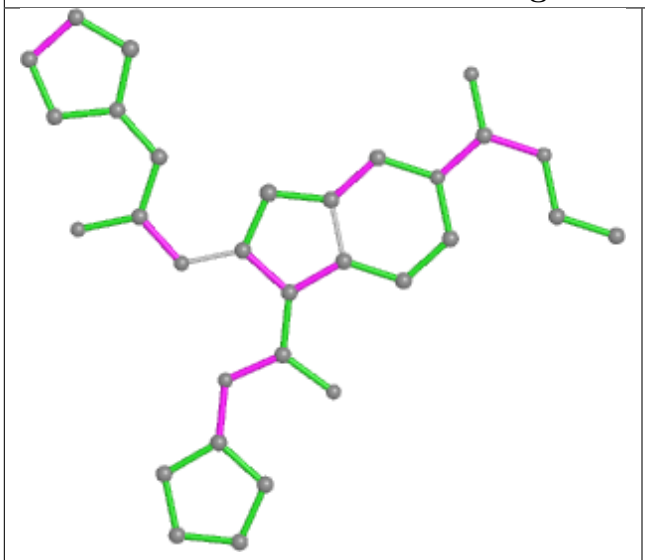
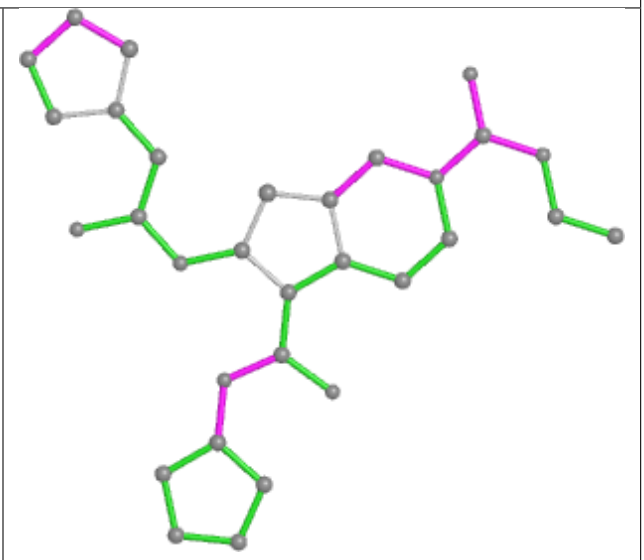
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	440	EDO	1	0
3	D	7	EDO	1	0
6	C	2	EPE	3	0
3	D	3	EDO	5	0
3	D	10	EDO	2	0
3	D	8	EDO	1	0
3	D	9	EDO	2	0
3	C	7	EDO	2	0
3	C	3	EDO	2	0
3	D	4	EDO	2	0
3	A	442	EDO	3	0
4	C	441	JN8	2	0
4	B	440	JN8	2	0
3	C	8	EDO	2	0
3	C	4	EDO	1	0
4	D	15	JN8	4	0
3	B	5	EDO	4	0

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.

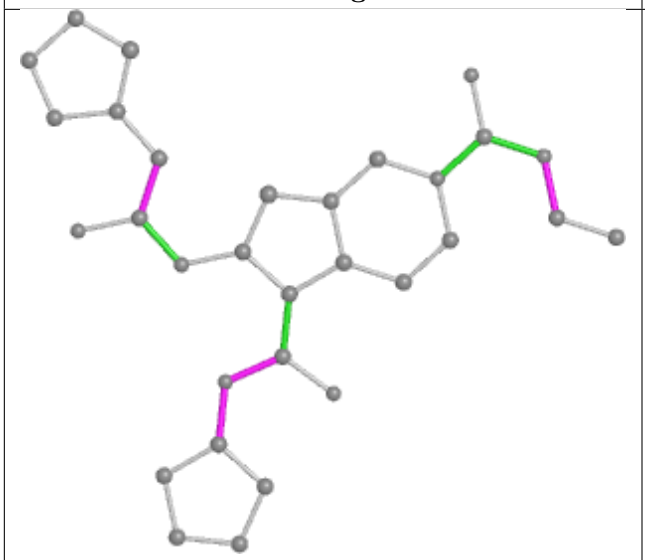
Ligand JN8 A 440



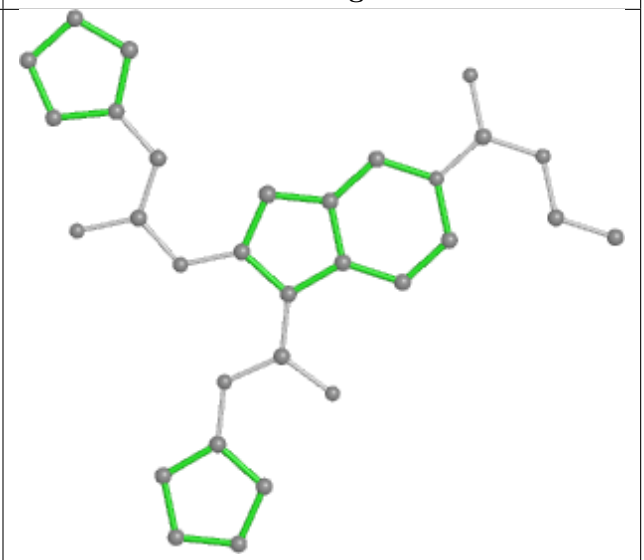
Bond lengths



Bond angles

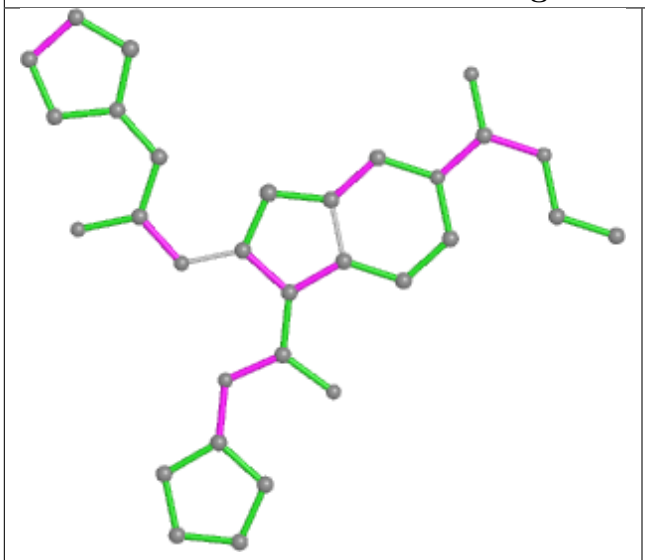


Torsions

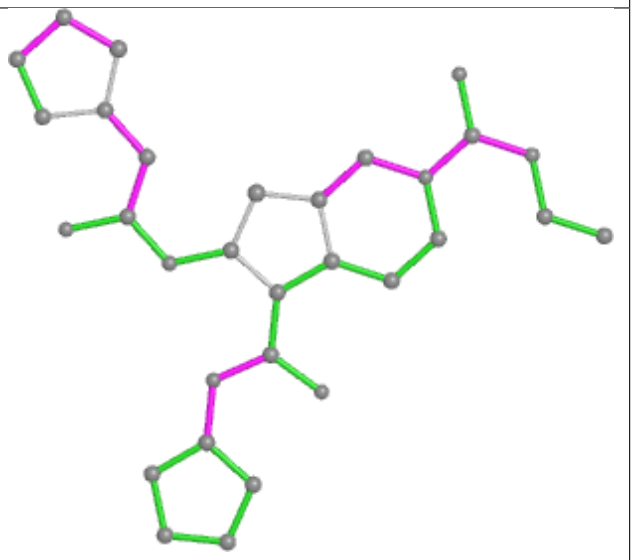


Rings

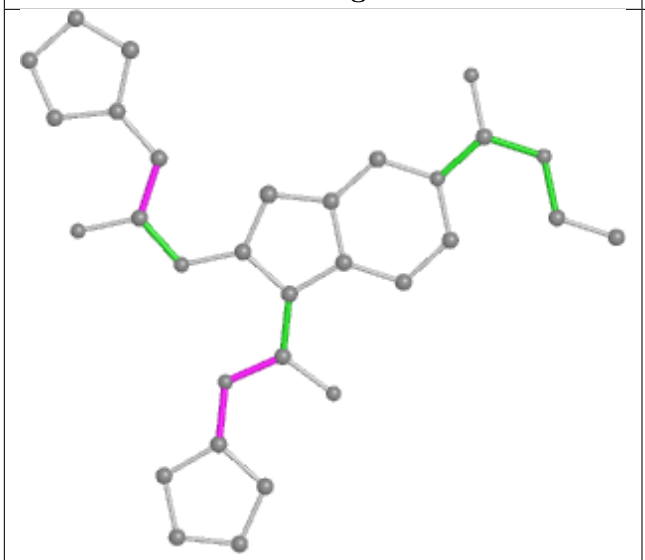
Ligand JN8 C 441



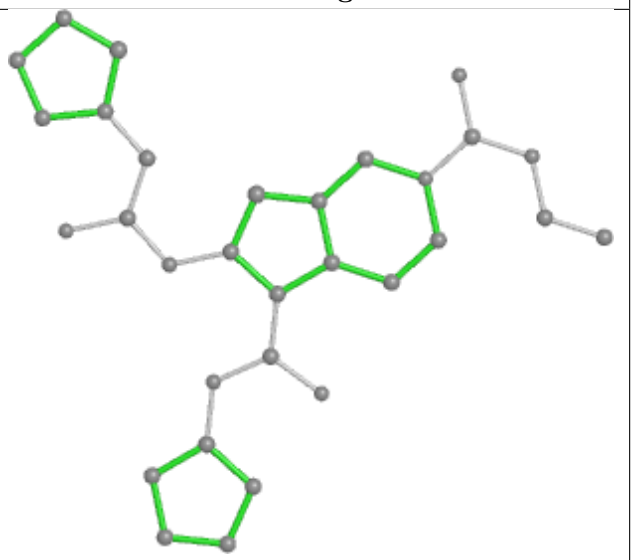
Bond lengths



Bond angles

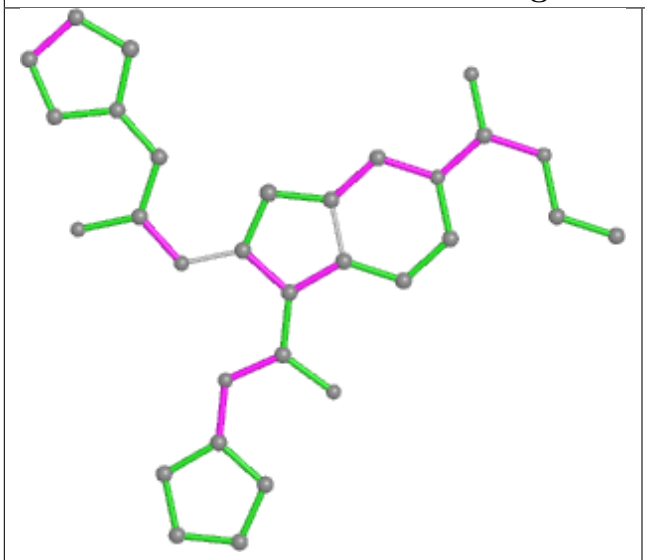


Torsions

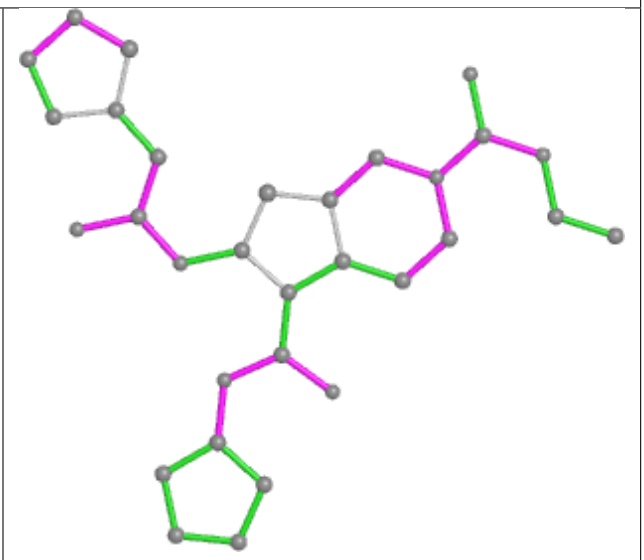


Rings

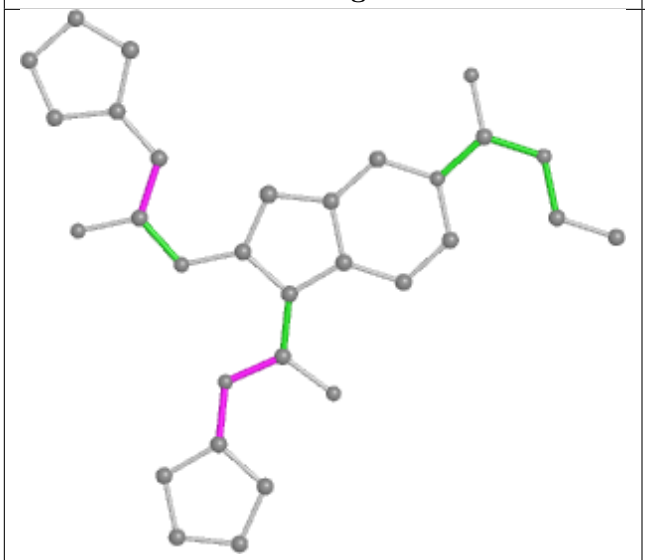
Ligand JN8 B 440



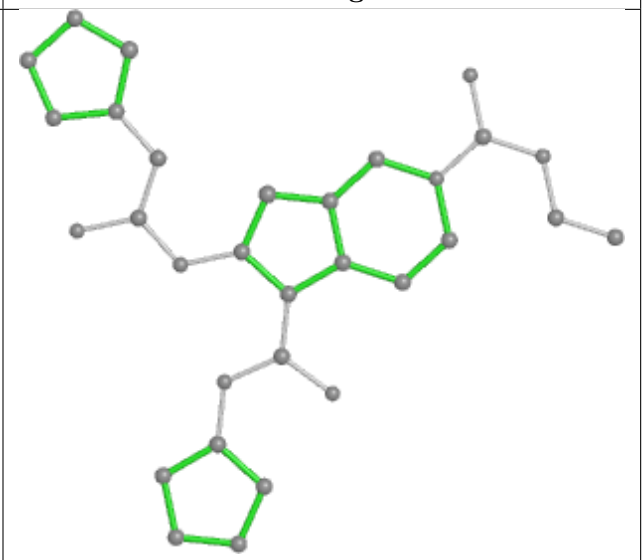
Bond lengths



Bond angles

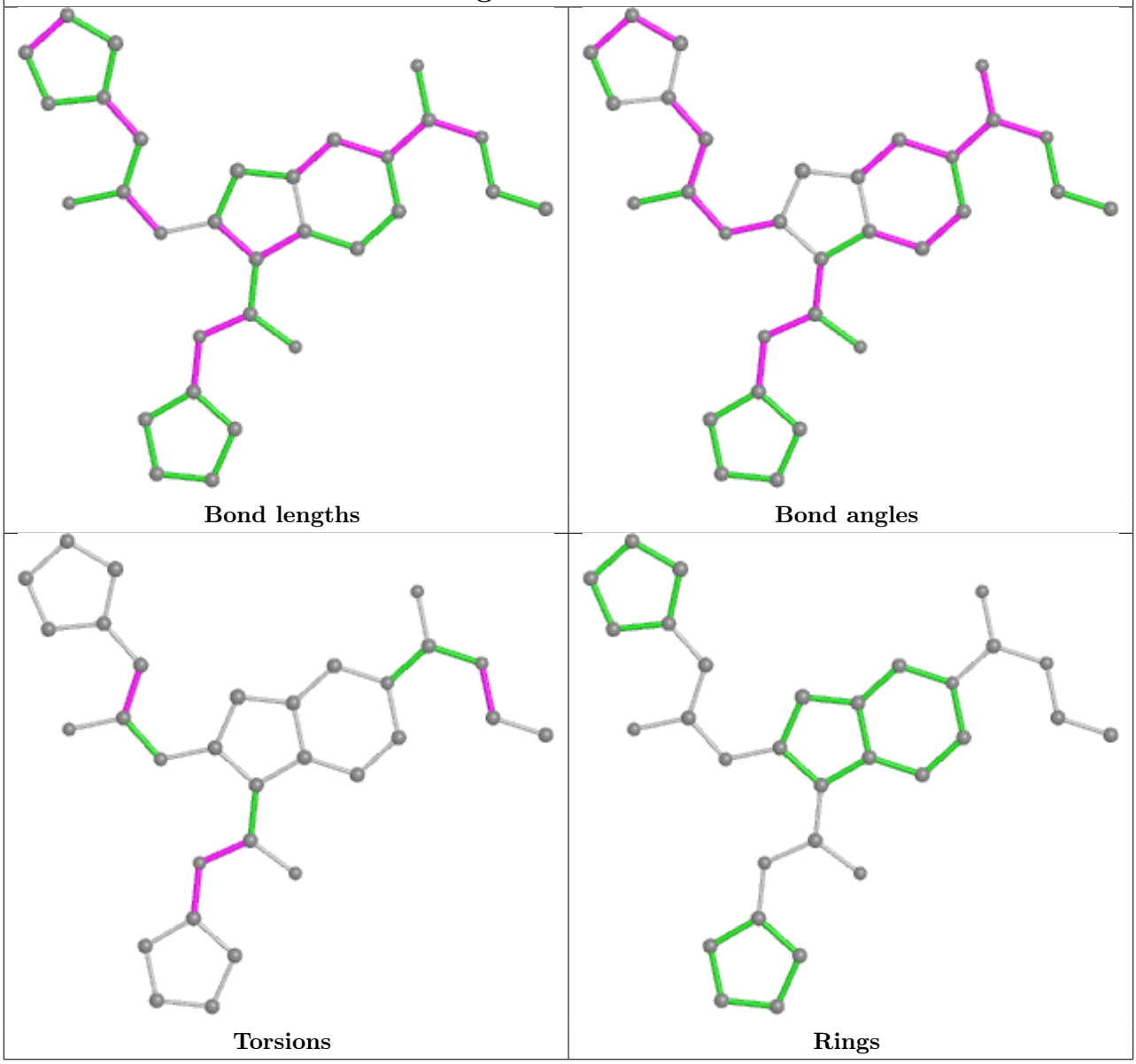


Torsions



Rings

Ligand JN8 D 15



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	327/361 (90%)	0.17	10 (3%)	49	45	23, 37, 73, 111	0
1	B	325/361 (90%)	0.21	7 (2%)	62	58	26, 48, 69, 103	0
1	C	325/361 (90%)	0.18	9 (2%)	53	49	28, 46, 79, 104	0
1	D	324/361 (89%)	0.09	4 (1%)	79	77	23, 35, 65, 90	0
All	All	1301/1444 (90%)	0.16	30 (2%)	60	56	23, 42, 71, 111	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	296	GLY	7.9
1	C	295	SER	6.9
1	A	295	SER	6.4
1	A	297	VAL	5.6
1	C	296	GLY	5.3
1	C	297	VAL	4.8
1	A	357	MET	4.4
1	C	353	GLU	4.4
1	A	294	SER	4.1
1	A	353	GLU	4.0
1	C	294	SER	3.8
1	A	356	PRO	3.3
1	A	293	THR	3.3
1	D	362	ASN	3.1
1	C	293	THR	2.8
1	A	409	THR	2.8
1	B	88	GLN	2.7
1	B	96	LEU	2.4
1	B	139	VAL	2.3
1	C	356	PRO	2.3
1	D	94	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	354	ILE	2.2
1	A	358	CYS	2.2
1	C	362	ASN	2.2
1	C	357	MET	2.2
1	B	296	GLY	2.2
1	B	295	SER	2.2
1	D	353	GLU	2.1
1	B	147	MET	2.1
1	B	112	LEU	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	C	7	4/4	0.62	0.27	46,53,55,56	0
3	EDO	B	5	4/4	0.74	0.29	50,55,56,57	0
3	EDO	A	8	4/4	0.74	0.23	52,52,53,58	0
3	EDO	D	10	4/4	0.75	0.23	46,48,49,49	0
3	EDO	C	8	4/4	0.77	0.34	49,53,54,60	0
3	EDO	D	11	4/4	0.79	0.44	44,49,54,57	0
3	EDO	D	4	4/4	0.80	0.29	40,48,51,56	0
3	EDO	B	6	4/4	0.81	0.22	53,56,56,59	0
3	EDO	A	7	4/4	0.81	0.20	47,48,51,54	0
3	EDO	D	5	4/4	0.82	0.19	47,48,50,55	0
3	EDO	D	8	4/4	0.82	0.27	42,46,48,49	0
3	EDO	A	5	4/4	0.84	0.17	47,48,50,51	0
3	EDO	C	3	4/4	0.85	0.20	41,44,48,53	0
3	EDO	B	4	4/4	0.85	0.46	51,53,59,61	0

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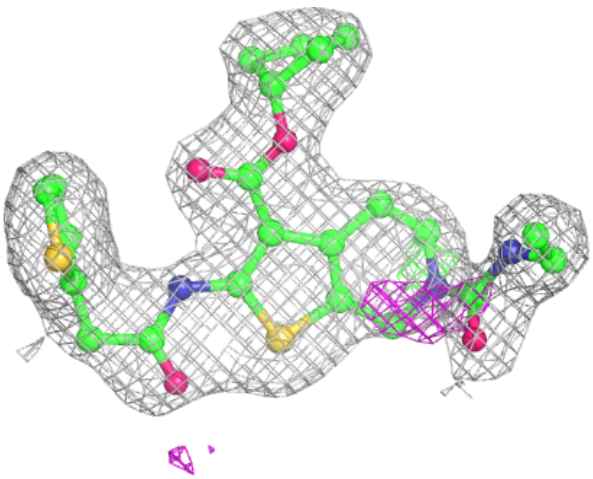
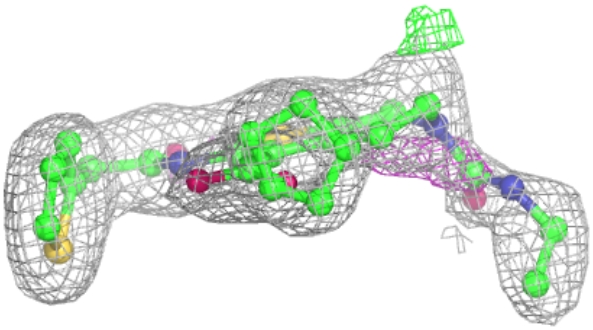
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DMS	B	14	4/4	0.85	0.19	69,69,75,80	0
4	JN8	C	441	31/31	0.90	0.19	34,48,63,67	0
3	EDO	A	2	4/4	0.90	0.15	49,53,55,57	0
3	EDO	C	9	4/4	0.91	0.17	50,52,52,55	0
3	EDO	D	3	4/4	0.92	0.40	29,30,38,39	0
3	EDO	D	6	4/4	0.92	0.16	38,39,40,46	0
3	EDO	C	5	4/4	0.92	0.19	42,44,47,48	0
4	JN8	D	15	31/31	0.92	0.17	27,48,64,75	0
3	EDO	D	9	4/4	0.92	0.26	31,35,38,40	0
4	JN8	B	440	31/31	0.93	0.19	29,39,55,60	0
3	EDO	D	440	4/4	0.93	0.21	34,35,38,39	0
3	EDO	A	6	4/4	0.93	0.19	33,40,41,42	0
4	JN8	A	440	31/31	0.93	0.26	36,49,72,78	0
6	EPE	C	2	15/15	0.93	0.26	47,68,82,83	0
3	EDO	A	4	4/4	0.94	0.17	39,43,45,47	0
3	EDO	D	2	4/4	0.94	0.17	34,40,40,42	0
3	EDO	A	442	4/4	0.95	0.25	37,39,40,43	0
3	EDO	D	7	4/4	0.95	0.13	35,39,39,41	0
3	EDO	C	440	4/4	0.95	0.23	54,55,56,59	0
3	EDO	C	4	4/4	0.95	0.18	49,50,53,54	0
3	EDO	A	441	4/4	0.96	0.15	27,31,32,34	0
3	EDO	A	9	4/4	0.97	0.23	32,34,38,48	0
2	ZN	B	8	1/1	0.97	0.12	64,64,64,64	0
2	ZN	C	10	1/1	0.97	0.13	65,65,65,65	0
2	ZN	A	10	1/1	0.99	0.15	35,35,35,35	0
2	ZN	A	11	1/1	0.99	0.09	54,54,54,54	0
2	ZN	C	11	1/1	0.99	0.16	40,40,40,40	0
2	ZN	D	12	1/1	0.99	0.12	59,59,59,59	0
2	ZN	B	7	1/1	0.99	0.16	43,43,43,43	0
2	ZN	D	13	1/1	1.00	0.15	37,37,37,37	0

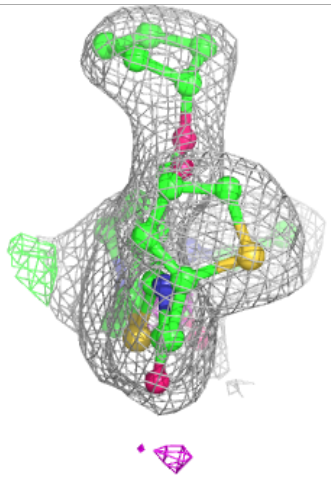
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

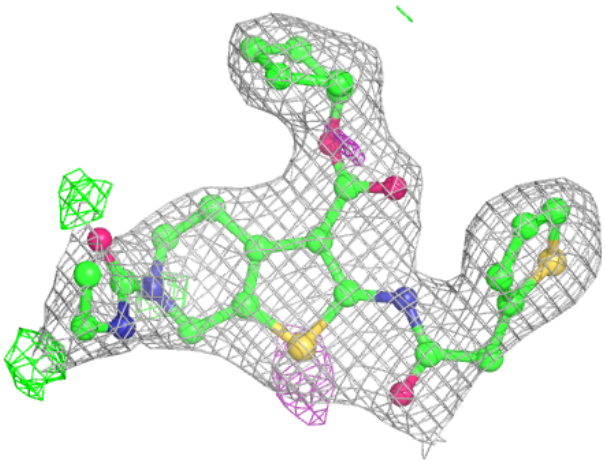


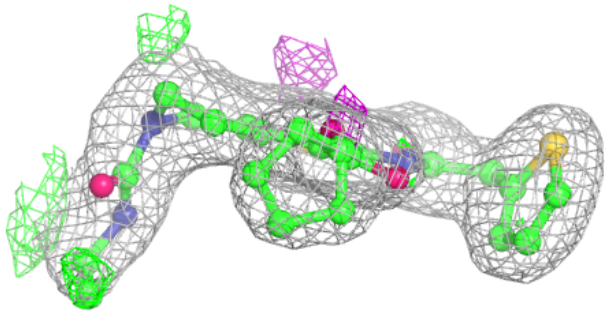


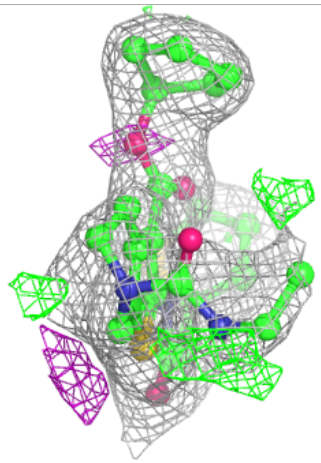


Electron density around JN8 D 15:

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

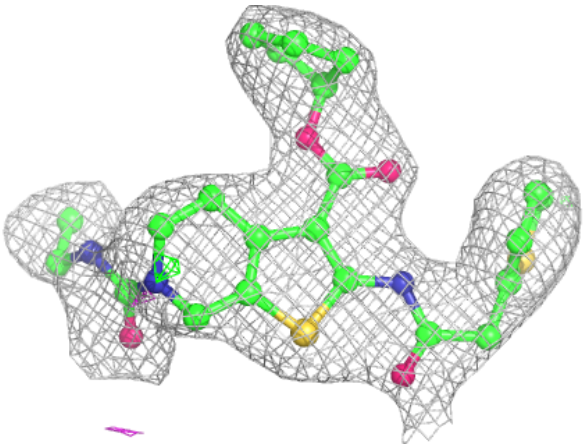


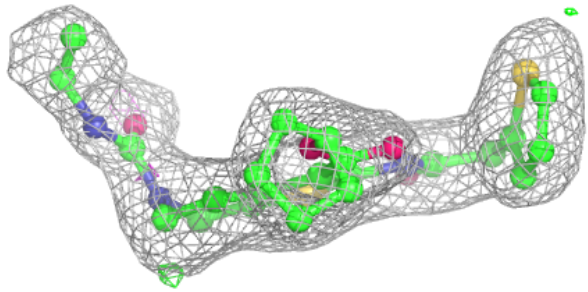


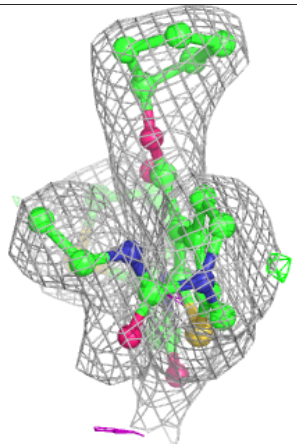


Electron density around JN8 B 440:

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

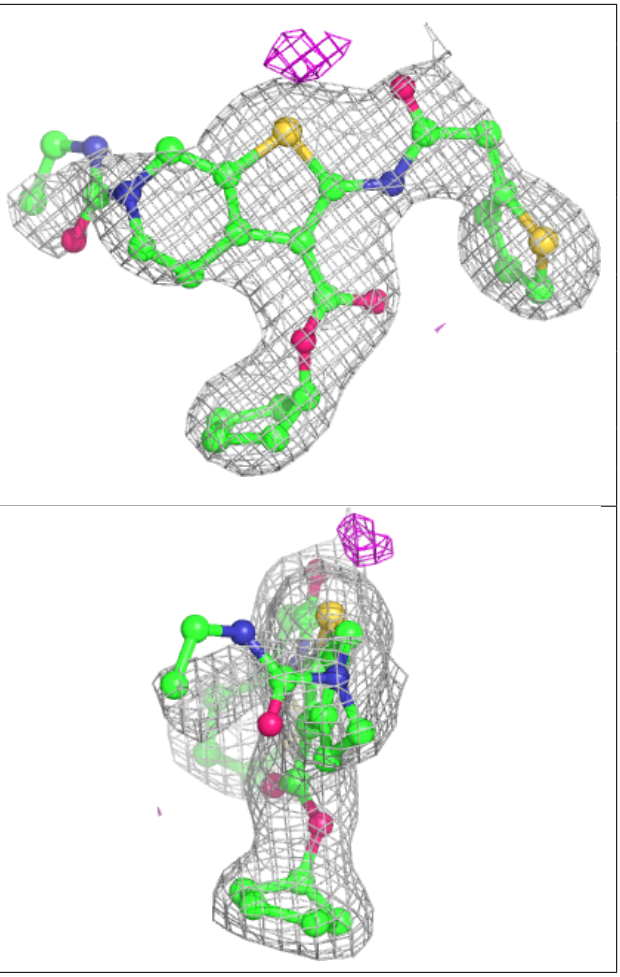






Electron density around JN8 A 440:

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



6.5 Other polymers (i)

There are no such residues in this entry.