Full wwPDB X-ray Structure Validation Report (i)

Feb 17, 2024 – 11:22 AM EST

PDB ID	:	3SL4
Title	:	Crystal structure of the catalytic domain of PDE4D2 with compound 10D
Authors	:	Feil, S.F.
Deposited on	:	2011-06-24
Resolution	:	1.90 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:

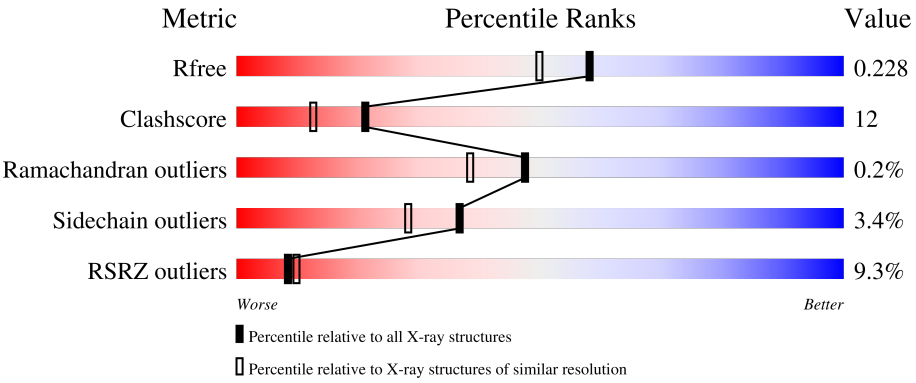
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	9% 75% 15% • 9%
1	B	361	7% 76% 13% • 10%
1	C	361	11% 71% 18% • 10%
1	D	361	6% 74% 14% • 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	A	21	-	-	X	-
3	EDO	A	443	-	-	X	-
3	EDO	B	15	-	-	X	-
3	EDO	B	16	-	-	X	-
3	EDO	B	18	-	-	X	-
3	EDO	D	21	-	-	X	-
3	EDO	D	5	-	-	X	-
4	DMS	D	23	-	-	X	-
4	DMS	D	8	-	-	X	-
5	PEG	D	12	-	-	X	-
5	PEG	D	16	-	-	X	X
5	PEG	D	441	-	-	X	-
6	PO4	A	20	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 11484 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.

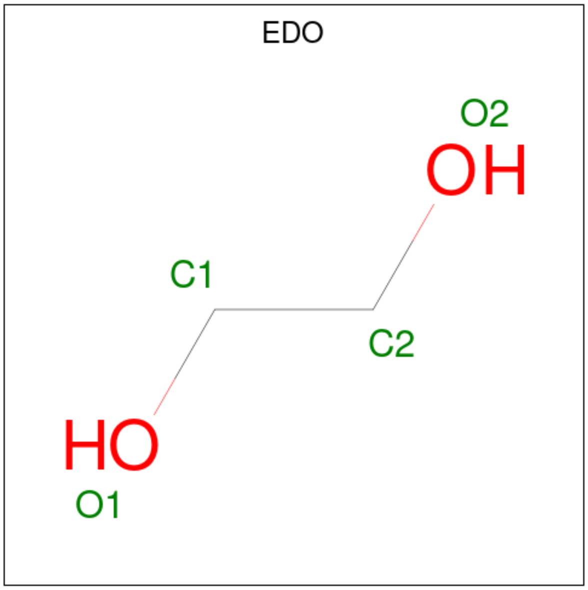
- Molecule 1 is a protein called cAMP-specific 3',5'-cyclic phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2658	1681	454	509	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	2	0
			2647	1672	452	508	15			
1	D	324	Total	C	N	O	S	0	2	0
			2636	1666	450	506	14			

- Molecule 2 is ZINC ION (three-letter code: 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 (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

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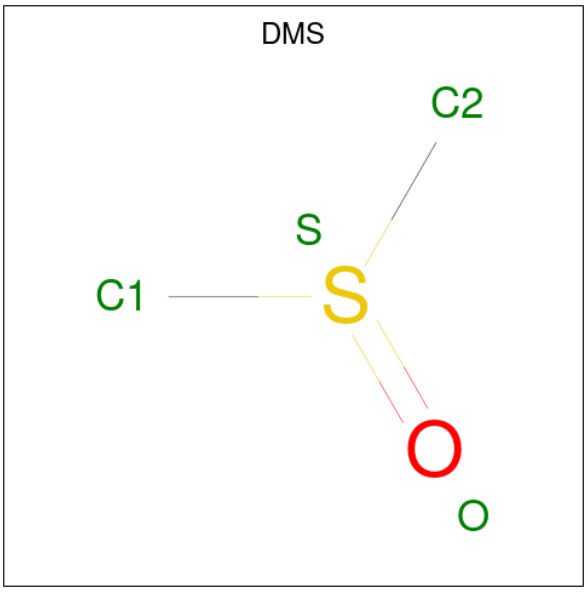
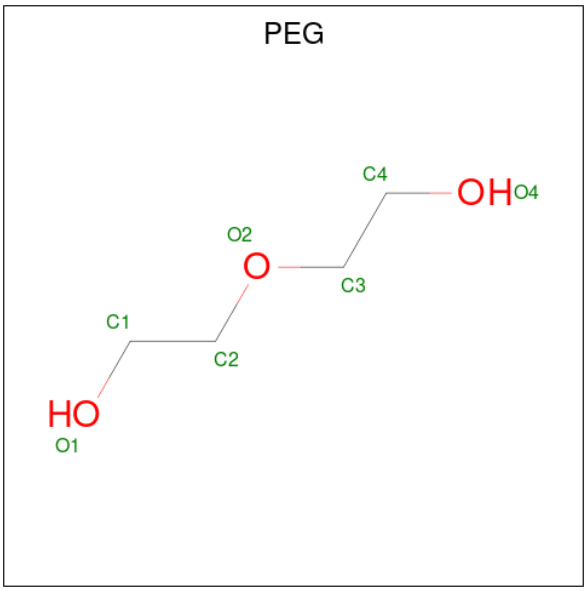
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0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

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



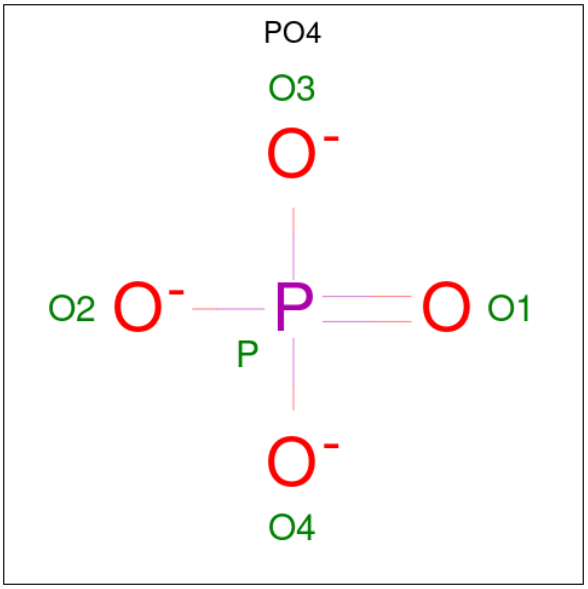
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O S 4 2 1 1	0	0
4	A	1	Total C O S 4 2 1 1	0	0
4	B	1	Total C O S 4 2 1 1	0	0
4	C	1	Total C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



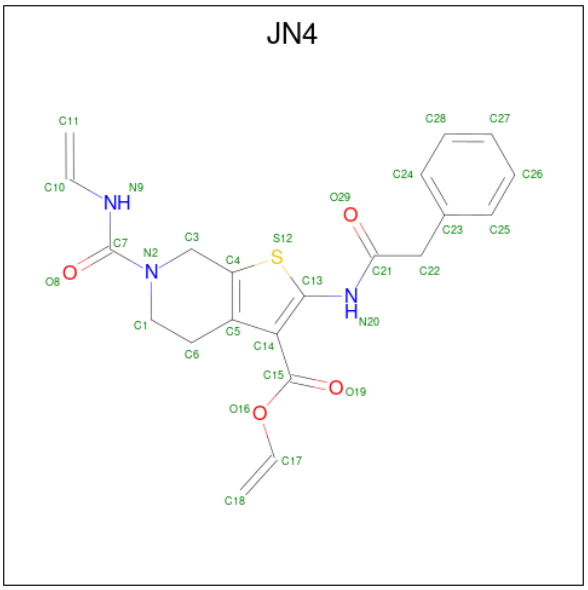
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



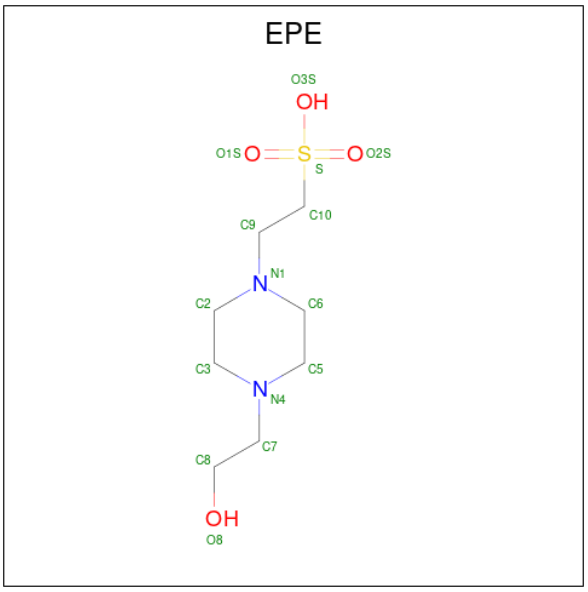
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O P 5 4 1	0	0
6	B	1	Total O P 5 4 1	0	0
6	C	1	Total O P 5 4 1	0	0
6	D	1	Total O P 5 4 1	0	0

- Molecule 7 is ethenyl 6-(ethenylcarbamoyl)-2-[(phenylacetyl)amino]-4,5,6,7-tetrahydrothieno[2,3-c]pyridine-3-carboxylate (three-letter code: JN4) (formula: $C_{21}H_{21}N_3O_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O S 29 21 3 4 1	0	0
7	B	1	Total C N O S 29 21 3 4 1	0	0
7	C	1	Total C N O S 29 21 3 4 1	0	0
7	D	1	Total C N O S 29 21 3 4 1	0	0

- Molecule 8 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
8	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
8	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

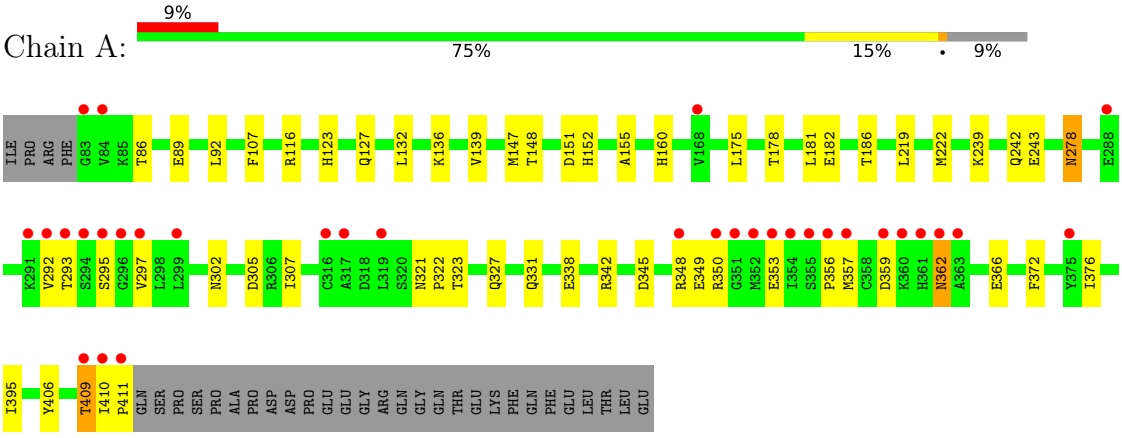
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	119	Total	O	0	0
			119	119		
9	B	121	Total	O	0	0
			121	121		
9	C	87	Total	O	0	0
			87	87		
9	D	140	Total	O	0	0
			140	140		

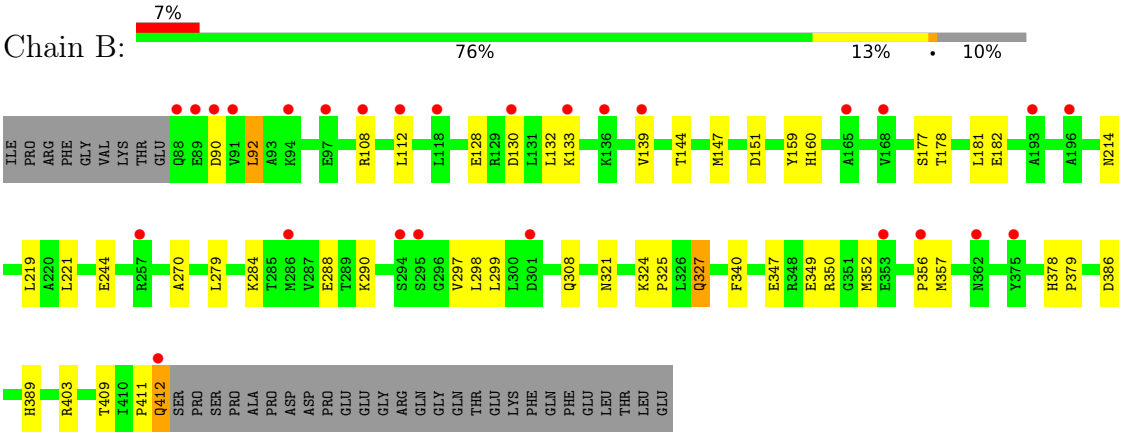
3 Residue-property plots (i)

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.

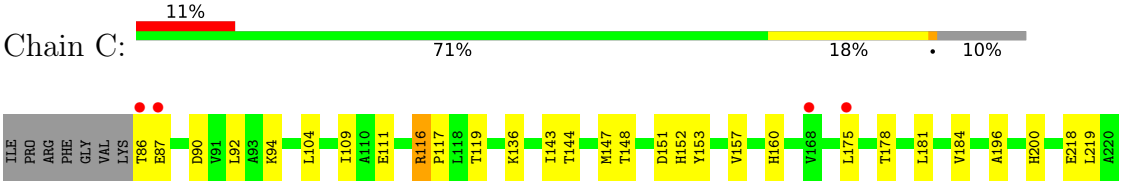
• Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

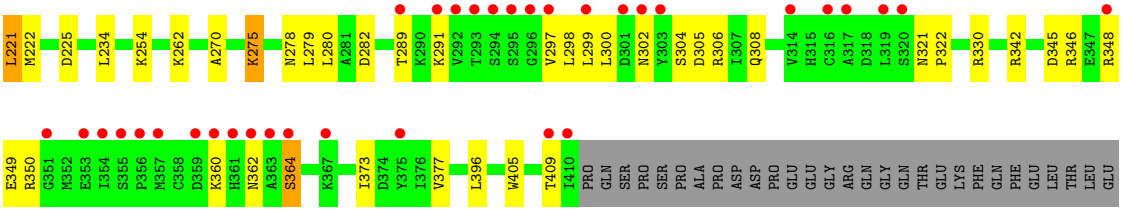


• Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

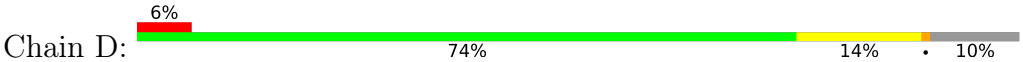


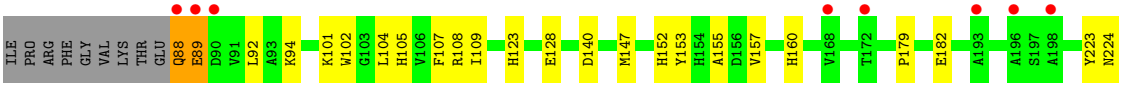
• Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

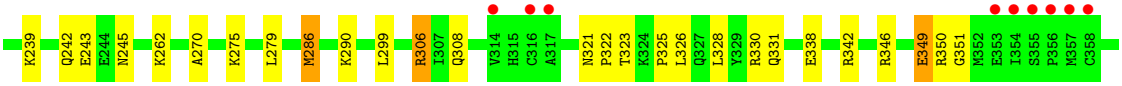


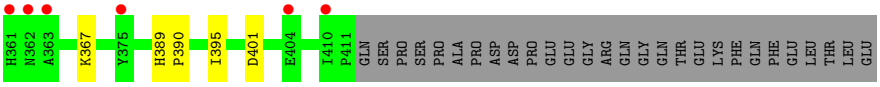


• Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	99.38Å 111.09Å 161.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.62 – 1.90 32.62 – 1.90	Depositor EDS
% Data completeness (in resolution range)	90.5 (32.62-1.90) 98.6 (32.62-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.59 (at 1.91Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, R_{free}	0.194 , 0.227 0.199 , 0.228	Depositor DCC
R_{free} test set	6946 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	27.5	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 56.5	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	0.95	EDS
Total number of atoms	11484	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, EDO, JN4, EPE, PO4, DMS, ZN

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	0.38	0/2712	0.51	0/3684
1	B	0.34	0/2685	0.48	0/3648
1	C	0.34	0/2700	0.48	0/3668
1	D	0.40	0/2690	0.52	1/3655 (0.0%)
All	All	0.36	0/10787	0.50	1/14655 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	306	ARG	NE-CZ-NH2	-5.11	117.75	120.30

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	2658	0	2616	67	0
1	B	2631	0	2586	47	0
1	C	2647	0	2598	59	0
1	D	2636	0	2585	87	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	64	0	96	22	0
3	B	44	0	66	19	0
3	C	40	0	60	13	0
3	D	56	0	84	23	0
4	A	8	0	12	1	0
4	B	4	0	6	0	0
4	C	4	0	6	0	0
4	D	16	0	24	16	0
5	A	7	0	10	1	0
5	D	28	0	40	20	0
6	A	5	0	0	3	0
6	B	5	0	0	1	0
6	C	5	0	0	1	0
6	D	5	0	0	1	0
7	A	29	0	21	2	0
7	B	29	0	21	2	0
7	C	29	0	21	4	0
7	D	29	0	21	3	0
8	B	15	0	17	0	0
8	C	15	0	17	2	0
9	A	119	0	0	6	0
9	B	121	0	0	10	0
9	C	87	0	0	5	0
9	D	140	0	0	9	0
All	All	11484	0	10907	265	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 (265) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ASN:HD22	3:B:15:EDO:H21	1.01	1.14
1:B:214:ASN:ND2	3:B:15:EDO:H21	1.78	0.96
1:C:157:VAL:HA	3:C:13:EDO:H11	1.52	0.89
7:D:442:JN4:C10	7:D:442:JN4:H1	2.03	0.86
1:D:102:TRP:H	5:D:12:PEG:C4	1.89	0.86
1:B:221:LEU:HG	9:B:483:HOH:O	1.75	0.85
1:A:132:LEU:HD22	1:A:139:VAL:HG12	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:5:EDO:H11	9:D:495:HOH:O	1.80	0.82
1:A:366:GLU:HG2	1:A:409:THR:HG23	1.63	0.81
1:D:102:TRP:H	5:D:12:PEG:H42	1.46	0.81
1:D:243:GLU:OE1	3:D:5:EDO:H21	1.82	0.79
1:D:275:LYS:HE2	9:D:443:HOH:O	1.81	0.79
1:A:148:THR:HG23	3:A:443:EDO:H22	1.65	0.79
1:D:152:HIS:HE1	3:D:5:EDO:H22	1.46	0.79
1:B:352:MET:HE2	3:B:15:EDO:H22	1.63	0.79
1:D:401:ASP:HB2	5:D:16:PEG:H41	1.64	0.78
1:D:331:GLN:HE22	4:D:23:DMS:H21	1.48	0.78
1:D:108:ARG:H	4:D:23:DMS:C1	1.97	0.77
1:C:151:ASP:HA	3:C:14:EDO:H21	1.65	0.76
1:A:239:LYS:HZ2	1:D:239:LYS:HZ1	1.30	0.76
1:A:362:ASN:H	1:A:362:ASN:HD22	1.32	0.74
1:D:286:MET:HG3	3:D:15:EDO:H11	1.69	0.74
1:C:345:ASP:O	1:C:349:GLU:HG3	1.87	0.73
1:D:306:ARG:NH2	9:D:508:HOH:O	2.19	0.72
1:B:177:SER:HA	3:B:16:EDO:H21	1.70	0.72
1:B:214:ASN:HD22	3:B:15:EDO:C2	1.92	0.72
1:C:111:GLU:OE1	8:C:7:EPE:H52	1.90	0.71
1:A:148:THR:HG23	3:A:443:EDO:C2	2.19	0.71
1:A:406:TYR:O	1:A:409:THR:HG22	1.89	0.70
1:D:223:TYR:HD1	3:D:21:EDO:H11	1.56	0.70
1:A:239:LYS:HZ2	1:D:239:LYS:NZ	1.89	0.70
1:B:412:GLN:HA	1:B:412:GLN:OE1	1.91	0.69
1:D:346:ARG:HH21	1:D:350:ARG:HH22	1.37	0.69
7:C:18:JN4:H18A	9:C:482:HOH:O	1.91	0.69
1:A:239:LYS:NZ	1:D:239:LYS:NZ	2.41	0.69
1:D:123:HIS:HD2	3:D:10:EDO:H22	1.58	0.69
1:C:116:ARG:NE	1:C:147[A]:MET:HE1	2.09	0.68
1:C:321[B]:ASN:HD22	7:C:18:JN4:C24	2.06	0.68
1:B:130:ASP:OD2	1:B:133:LYS:HB2	1.94	0.67
1:A:278:ASN:H	1:A:278:ASN:HD22	1.42	0.66
1:B:290:LYS:NZ	3:B:18:EDO:H21	2.09	0.66
1:D:108:ARG:H	4:D:23:DMS:H13	1.58	0.66
1:C:153:TYR:O	3:C:14:EDO:H12	1.95	0.66
1:D:105:HIS:HB3	4:D:23:DMS:H12	1.76	0.66
1:D:102:TRP:H	5:D:12:PEG:H41	1.60	0.66
1:C:178:THR:HB	3:C:440:EDO:H21	1.78	0.66
1:D:262:LYS:HG3	5:D:441:PEG:H32	1.76	0.66
1:A:152:HIS:HE1	3:A:443:EDO:H12	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ASN:H	1:A:278:ASN:ND2	1.92	0.65
1:C:116:ARG:CZ	1:C:147[A]:MET:HE1	2.26	0.65
1:A:372:PHE:CE1	1:A:376:ILE:HD12	2.31	0.65
1:A:132:LEU:CD2	1:A:139:VAL:HG12	2.25	0.65
1:A:366:GLU:HG2	1:A:409:THR:CG2	2.27	0.64
1:D:326:LEU:H	5:D:16:PEG:H21	1.63	0.64
1:A:123:HIS:CE1	1:A:127:GLN:HE21	2.16	0.64
1:A:362:ASN:HD22	1:A:362:ASN:N	1.93	0.63
1:B:178:THR:CG2	1:B:181:LEU:HD12	2.28	0.63
1:D:153:TYR:O	4:D:13:DMS:H23	1.99	0.63
1:C:218:GLU:O	1:C:222:MET:HG2	1.98	0.63
1:D:107:PHE:HB2	4:D:23:DMS:H13	1.79	0.63
1:C:364:SER:HB2	9:C:77:HOH:O	1.99	0.62
1:D:152:HIS:CE1	3:D:5:EDO:H22	2.33	0.62
1:B:178:THR:HG21	1:B:181:LEU:HD12	1.80	0.62
3:B:18:EDO:H22	9:B:527:HOH:O	2.00	0.62
1:D:101:LYS:HA	5:D:12:PEG:H42	1.82	0.61
1:A:350:ARG:HE	3:A:7:EDO:H11	1.64	0.61
1:A:152:HIS:HE1	3:A:443:EDO:C1	2.13	0.61
1:B:347:GLU:OE2	3:B:15:EDO:H12	2.00	0.61
1:A:345:ASP:O	1:A:348:ARG:HG2	2.00	0.61
3:D:21:EDO:H22	9:D:452:HOH:O	1.99	0.61
1:B:290:LYS:HZ3	3:B:18:EDO:H21	1.64	0.61
3:C:13:EDO:H21	9:C:507:HOH:O	2.01	0.61
1:D:102:TRP:N	5:D:12:PEG:H42	2.15	0.60
1:D:401:ASP:CB	5:D:16:PEG:H41	2.31	0.60
1:D:155:ALA:HA	3:D:17:EDO:H12	1.83	0.59
1:C:116:ARG:HG2	1:C:147[A]:MET:HE3	1.84	0.59
1:D:182:GLU:HB2	4:D:8:DMS:H13	1.84	0.59
1:C:262:LYS:NZ	3:C:11:EDO:H22	2.17	0.59
1:D:157:VAL:HA	5:D:19:PEG:H11	1.83	0.59
1:B:182:GLU:HA	3:B:16:EDO:H11	1.83	0.59
1:B:139:VAL:HG23	9:B:468:HOH:O	2.02	0.59
1:D:331:GLN:HE22	4:D:23:DMS:C2	2.16	0.59
1:C:119:THR:OG1	1:C:147[A]:MET:HE2	2.03	0.58
1:D:262:LYS:CG	5:D:441:PEG:H32	2.32	0.58
1:C:302:ASN:ND2	1:C:305:ASP:H	2.02	0.58
1:B:177:SER:CA	3:B:16:EDO:H21	2.33	0.58
1:B:409:THR:O	1:B:409:THR:HG22	2.03	0.58
1:B:352:MET:CE	3:B:15:EDO:H22	2.32	0.58
1:A:152:HIS:CE1	3:A:443:EDO:H12	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:MET:CG	3:D:15:EDO:H11	2.35	0.57
1:A:321:ASN:HD22	7:A:23:JN4:C25	2.18	0.57
1:D:108:ARG:N	4:D:23:DMS:H13	2.20	0.57
1:A:139:VAL:HG11	9:A:454:HOH:O	2.04	0.56
1:D:182:GLU:HB2	4:D:8:DMS:C1	2.35	0.56
1:D:275:LYS:HD2	3:D:14:EDO:H22	1.86	0.56
1:D:326:LEU:H	5:D:16:PEG:C2	2.17	0.56
1:B:182:GLU:HG3	3:B:16:EDO:H22	1.86	0.56
1:C:330:ARG:HD3	1:C:405:TRP:CH2	2.40	0.56
1:A:292:VAL:CG1	1:A:293:THR:N	2.69	0.56
1:B:132:LEU:HD22	1:B:139:VAL:HG22	1.88	0.56
1:D:331:GLN:NE2	4:D:23:DMS:H21	2.17	0.55
1:C:270:ALA:HB1	1:C:279:LEU:HD11	1.88	0.55
1:C:302:ASN:O	1:C:306:ARG:HG3	2.07	0.55
3:B:18:EDO:H12	9:B:527:HOH:O	2.07	0.55
1:D:346:ARG:HH21	1:D:350:ARG:NH2	2.05	0.55
1:D:108:ARG:H	4:D:23:DMS:H12	1.69	0.54
1:B:177:SER:C	3:B:16:EDO:H21	2.27	0.54
1:A:239:LYS:NZ	1:D:239:LYS:HZ3	2.05	0.54
1:B:284:LYS:O	1:B:288:GLU:HG3	2.07	0.54
1:C:234:LEU:HB3	3:D:20:EDO:H21	1.89	0.54
1:C:178:THR:CB	3:C:440:EDO:H21	2.37	0.53
1:D:326:LEU:HG	1:D:330:ARG:HD3	1.90	0.53
1:A:349:GLU:HB3	1:C:147[B]:MET:SD	2.49	0.53
1:D:346:ARG:HH11	5:D:19:PEG:C4	2.21	0.53
1:A:292:VAL:HG12	1:A:293:THR:N	2.22	0.53
1:B:327:GLN:HE21	1:B:327:GLN:HA	1.73	0.53
1:D:328:LEU:CD2	4:D:23:DMS:H22	2.38	0.53
1:A:86:THR:OG1	1:A:89:GLU:HG3	2.08	0.53
1:C:160:HIS:NE2	6:C:17:PO4:O2	2.42	0.53
7:B:21:JN4:H18A	9:B:526:HOH:O	2.08	0.53
1:A:356:PRO:C	1:A:357:MET:HG2	2.29	0.52
1:A:147:MET:SD	1:C:349:GLU:HB3	2.49	0.52
7:D:442:JN4:H18A	9:D:559:HOH:O	2.09	0.52
3:A:21:EDO:H12	1:D:242:GLN:HE22	1.75	0.51
1:C:321[A]:ASN:HB2	1:C:322:PRO:HD3	1.90	0.51
1:D:155:ALA:HA	3:D:17:EDO:C1	2.39	0.51
1:C:116:ARG:CG	1:C:147[A]:MET:HE3	2.40	0.51
3:D:21:EDO:H21	3:D:22:EDO:H12	1.92	0.51
1:C:282:ASP:HB3	1:C:308:GLN:NE2	2.25	0.51
1:C:225:ASP:OD2	5:D:441:PEG:H42	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:ALA:HB1	1:B:279:LEU:HD11	1.94	0.50
1:C:143:ILE:O	1:C:147[B]:MET:HG3	2.11	0.50
1:B:350:ARG:HB3	9:B:477:HOH:O	2.10	0.50
1:D:308:GLN:HG3	9:D:470:HOH:O	2.10	0.50
1:D:325:PRO:HA	5:D:16:PEG:H21	1.93	0.50
1:A:155:ALA:HA	3:A:17:EDO:C2	2.42	0.50
1:D:262:LYS:CB	5:D:441:PEG:H32	2.41	0.50
1:C:181:LEU:HD21	1:C:298:LEU:HD12	1.92	0.50
1:A:239:LYS:HZ1	1:D:239:LYS:HZ3	1.59	0.49
1:A:350:ARG:HE	3:A:7:EDO:C1	2.25	0.49
1:C:321[B]:ASN:HB2	1:C:322:PRO:HD3	1.95	0.49
1:C:196:ALA:O	1:C:200:HIS:HB3	2.12	0.49
1:B:389:HIS:O	3:B:18:EDO:O2	2.29	0.49
1:C:409:THR:HG22	1:C:409:THR:O	2.13	0.49
5:D:19:PEG:H21	9:D:476:HOH:O	2.12	0.49
1:C:147[A]:MET:HE2	1:C:147[A]:MET:HA	1.94	0.49
1:C:304:SER:O	1:C:308:GLN:HB2	2.13	0.49
1:B:244:GLU:OE2	1:C:254:LYS:HE2	2.13	0.48
1:A:349:GLU:HB3	1:C:147[B]:MET:CE	2.43	0.48
1:A:356:PRO:O	1:A:357:MET:HG2	2.13	0.48
1:A:362:ASN:N	1:A:362:ASN:ND2	2.61	0.48
1:C:221:LEU:HD13	1:C:221:LEU:O	2.13	0.48
1:A:123:HIS:HE1	1:A:127:GLN:HE21	1.60	0.48
9:B:494:HOH:O	1:D:147:MET:HE1	2.13	0.48
1:D:88:GLN:NE2	1:D:89:GLU:HG2	2.29	0.47
1:C:104:LEU:HD11	1:C:109:ILE:HD11	1.95	0.47
1:A:278:ASN:ND2	1:A:278:ASN:N	2.60	0.47
7:D:442:JN4:C10	7:D:442:JN4:C1	2.86	0.47
1:A:242:GLN:OE1	1:D:242:GLN:OE1	2.31	0.47
3:A:443:EDO:H21	9:C:73:HOH:O	2.15	0.47
1:B:411:PRO:O	1:B:412:GLN:CB	2.63	0.47
1:A:239:LYS:HE3	3:A:21:EDO:O1	2.14	0.47
1:B:178:THR:CG2	1:B:181:LEU:HB2	2.44	0.47
1:C:348:ARG:HH22	1:C:360:LYS:HE2	1.79	0.47
1:D:123:HIS:CD2	3:D:10:EDO:H22	2.45	0.47
1:A:243:GLU:OE1	3:A:443:EDO:H21	2.14	0.47
1:A:342:ARG:HD2	9:A:506:HOH:O	2.14	0.47
1:D:123:HIS:HD2	3:D:10:EDO:C2	2.28	0.47
1:D:224:ASN:OD1	3:D:20:EDO:H11	2.15	0.47
3:A:21:EDO:C1	1:D:242:GLN:HE22	2.28	0.47
1:C:136:LYS:HE2	3:C:5:EDO:O1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:THR:HG23	1:D:350:ARG:HB2	1.96	0.46
1:D:140[B]:ASP:OD1	9:D:479:HOH:O	2.20	0.46
1:C:289:THR:O	1:C:289:THR:HG22	2.16	0.46
3:A:19:EDO:H22	9:A:463:HOH:O	2.14	0.46
1:B:92:LEU:HD23	1:B:112:LEU:HB2	1.97	0.46
1:D:104:LEU:HD11	1:D:109:ILE:HD11	1.98	0.46
1:D:179:PRO:HA	4:D:8:DMS:C1	2.45	0.46
1:A:147:MET:HE3	1:C:350:ARG:HG2	1.98	0.46
1:A:160:HIS:NE2	6:A:20:PO4:P	2.89	0.46
1:A:327:GLN:O	1:A:331:GLN:HG3	2.15	0.46
7:A:23:JN4:H18A	9:A:444:HOH:O	2.15	0.45
1:B:159:TYR:CE1	7:B:21:JN4:H24	2.51	0.45
1:C:94:LYS:HA	1:C:94:LYS:HD2	1.82	0.45
6:A:20:PO4:P	9:A:486:HOH:O	2.74	0.45
1:B:160:HIS:NE2	6:B:20:PO4:P	2.90	0.45
1:B:411:PRO:O	1:B:412:GLN:HB2	2.16	0.45
1:B:108:ARG:NH1	1:B:112:LEU:HD21	2.32	0.45
1:B:147:MET:HE3	1:D:350:ARG:HB3	1.99	0.45
1:D:152:HIS:HE1	3:D:5:EDO:C2	2.23	0.45
3:B:16:EDO:H12	9:B:459:HOH:O	2.16	0.45
1:B:352:MET:HE1	3:B:15:EDO:H11	1.98	0.44
1:D:104:LEU:HD11	1:D:109:ILE:CD1	2.47	0.44
1:D:128:GLU:CG	3:D:18:EDO:H21	2.47	0.44
1:C:275:LYS:CD	3:C:12:EDO:H21	2.47	0.44
1:D:321:ASN:HB2	1:D:322:PRO:HD3	1.99	0.44
1:A:178:THR:HG22	1:A:181:LEU:HD12	1.99	0.44
1:D:401:ASP:CB	5:D:16:PEG:C4	2.95	0.44
1:C:275:LYS:HD3	3:C:12:EDO:H21	2.00	0.44
1:D:179:PRO:HA	4:D:8:DMS:H13	1.99	0.44
1:A:107:PHE:HB2	4:A:442:DMS:H21	1.99	0.44
1:A:151:ASP:O	5:A:440:PEG:H12	2.16	0.44
8:C:7:EPE:H101	8:C:7:EPE:H22	1.60	0.44
1:D:290:LYS:HA	3:D:15:EDO:H21	2.00	0.44
1:D:323:THR:HB	1:D:395:ILE:HG23	1.98	0.44
3:A:7:EDO:H22	1:C:148:THR:HA	1.99	0.43
1:B:108:ARG:CZ	1:B:112:LEU:HD21	2.48	0.43
1:D:223:TYR:CD1	3:D:21:EDO:H11	2.46	0.43
3:A:9:EDO:H11	9:A:482:HOH:O	2.17	0.43
1:D:101:LYS:CA	5:D:12:PEG:H42	2.46	0.43
3:A:21:EDO:H22	1:D:242:GLN:HE22	1.84	0.43
1:C:116:ARG:N	1:C:117:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:HIS:HE1	3:C:8:EDO:O1	2.02	0.43
1:D:102:TRP:HB2	5:D:12:PEG:H41	2.00	0.43
1:C:175:LEU:HD23	3:C:440:EDO:H22	2.00	0.42
1:A:175:LEU:HD23	3:A:10:EDO:H12	2.00	0.42
1:A:292:VAL:CG1	1:A:293:THR:H	2.30	0.42
1:D:270:ALA:HB1	1:D:279:LEU:HD11	2.02	0.42
1:A:136:LYS:N	1:A:136:LYS:HD2	2.35	0.42
1:A:160:HIS:NE2	6:A:20:PO4:O4	2.52	0.42
1:A:293:THR:O	1:A:293:THR:HG23	2.19	0.42
1:B:349:GLU:HG3	1:D:147:MET:SD	2.60	0.42
1:C:104:LEU:HD12	9:C:472:HOH:O	2.20	0.42
1:C:291:LYS:O	1:C:299:LEU:HB3	2.20	0.42
1:C:373:ILE:HA	1:C:377:VAL:HB	2.01	0.42
1:A:321:ASN:HB2	1:A:322:PRO:HD3	2.02	0.42
1:B:324:LYS:HB3	1:B:325:PRO:HD2	2.01	0.42
1:B:178:THR:HG23	1:B:181:LEU:HB2	2.01	0.42
1:B:340:PHE:CE1	3:B:4:EDO:H12	2.55	0.42
1:C:116:ARG:CG	1:C:147[A]:MET:CE	2.98	0.42
1:A:410:ILE:HA	1:A:411:PRO:HD3	1.93	0.41
1:D:346:ARG:O	1:D:350:ARG:HG2	2.20	0.41
1:C:144:THR:HA	1:C:147[B]:MET:HE2	2.02	0.41
3:D:21:EDO:H12	9:D:468:HOH:O	2.20	0.41
1:D:160:HIS:NE2	6:D:24:PO4:O1	2.54	0.41
1:A:178:THR:HB	3:A:10:EDO:H21	2.02	0.41
1:D:299:LEU:C	1:D:299:LEU:HD13	2.40	0.41
1:A:338:GLU:O	1:A:342:ARG:HG3	2.19	0.41
1:C:184:VAL:HG11	1:C:300:LEU:HD12	2.03	0.41
1:D:349:GLU:C	1:D:351:GLY:H	2.24	0.41
1:A:293:THR:HG22	1:A:297:VAL:O	2.20	0.41
1:A:359:ASP:CG	1:A:362:ASN:HD21	2.24	0.41
1:C:278:ASN:ND2	1:C:278:ASN:H	2.19	0.41
1:C:321[B]:ASN:HD22	7:C:18:JN4:C23	2.33	0.41
1:A:186:THR:OG1	3:A:18:EDO:H21	2.21	0.41
1:B:151:ASP:OD1	1:D:350:ARG:NH2	2.54	0.41
1:B:356:PRO:C	1:B:357:MET:HG2	2.41	0.41
1:B:378:HIS:HB3	1:B:379:PRO:HD3	2.03	0.41
1:D:128:GLU:HG3	3:D:18:EDO:H21	2.03	0.41
1:D:328:LEU:HD23	4:D:23:DMS:C2	2.49	0.41
1:D:338:GLU:O	1:D:342:ARG:HG2	2.20	0.41
1:D:346:ARG:NH2	1:D:350:ARG:HH22	2.13	0.41
1:D:389:HIS:HA	1:D:390:PRO:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:THR:O	1:A:295:SER:N	2.47	0.41
1:A:323:THR:HB	1:A:395:ILE:HG23	2.03	0.40
1:B:297:VAL:HA	9:B:56:HOH:O	2.20	0.40
1:A:186:THR:HG21	3:A:18:EDO:H21	2.02	0.40
1:A:350:ARG:HG2	1:C:144:THR:HG23	2.03	0.40
1:B:221:LEU:HD12	9:B:78:HOH:O	2.21	0.40
1:A:148:THR:HG23	3:A:443:EDO:H21	2.00	0.40
1:A:302:ASN:ND2	1:A:305:ASP:H	2.19	0.40
1:A:307:ILE:HD12	1:A:307:ILE:HA	1.90	0.40
1:C:342:ARG:HD3	3:C:13:EDO:H12	2.03	0.40
7:C:18:JN4:O29	7:C:18:JN4:S12	2.80	0.40
1:D:286:MET:HE2	1:D:286:MET:HB2	1.95	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	327/361 (91%)	319 (98%)	8 (2%)	0	100	100
1	B	323/361 (90%)	316 (98%)	7 (2%)	0	100	100
1	C	325/361 (90%)	317 (98%)	7 (2%)	1 (0%)	41	31
1	D	324/361 (90%)	315 (97%)	8 (2%)	1 (0%)	41	31
All	All	1299/1444 (90%)	1267 (98%)	30 (2%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	87	GLU
1	D	349	GLU

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%)	291 (97%)	9 (3%)	41	33
1	B	297/329 (90%)	285 (96%)	12 (4%)	31	22
1	C	299/329 (91%)	286 (96%)	13 (4%)	29	19
1	D	298/329 (91%)	291 (98%)	7 (2%)	50	45
All	All	1194/1316 (91%)	1153 (97%)	41 (3%)	37	28

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	LEU
1	A	116	ARG
1	A	182	GLU
1	A	219	LEU
1	A	222	MET
1	A	278	ASN
1	A	353	GLU
1	A	362	ASN
1	A	409	THR
1	B	90	ASP
1	B	92	LEU
1	B	128	GLU
1	B	219	LEU
1	B	298	LEU
1	B	299	LEU
1	B	308	GLN
1	B	321	ASN
1	B	327	GLN
1	B	386	ASP
1	B	403	ARG
1	B	412	GLN
1	C	86	THR
1	C	90	ASP
1	C	92	LEU

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Mol	Chain	Res	Type
1	C	116	ARG
1	C	219	LEU
1	C	221	LEU
1	C	275	LYS
1	C	280	LEU
1	C	297	VAL
1	C	346	ARG
1	C	362	ASN
1	C	364	SER
1	C	396	LEU
1	D	88	GLN
1	D	89	GLU
1	D	92	LEU
1	D	94	LYS
1	D	245	ASN
1	D	286	MET
1	D	367	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	A	152	HIS
1	A	216	ASN
1	A	245	ASN
1	A	278	ASN
1	A	302	ASN
1	A	308	GLN
1	A	321	ASN
1	A	331	GLN
1	A	362	ASN
1	A	407	GLN
1	B	88	GLN
1	B	123	HIS
1	B	210	GLN
1	B	214	ASN
1	B	245	ASN
1	B	327	GLN
1	B	362	ASN
1	C	105	HIS
1	C	152	HIS
1	C	245	ASN

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Mol	Chain	Res	Type
1	C	278	ASN
1	C	302	ASN
1	C	308	GLN
1	D	88	GLN
1	D	105	HIS
1	D	123	HIS
1	D	245	ASN
1	D	250	GLN
1	D	278	ASN
1	D	331	GLN
1	D	389	HIS

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 82 ligands modelled in this entry, 8 are monoatomic - leaving 74 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	B	17	-	3,3,3	0.46	0	2,2,2	0.41	0
3	EDO	D	20	-	3,3,3	0.62	0	2,2,2	0.12	0
3	EDO	A	443	-	3,3,3	0.46	0	2,2,2	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	DMS	A	442	-	3,3,3	2.45	1 (33%)	3,3,3	0.40	0
3	EDO	A	13	-	3,3,3	0.39	0	2,2,2	0.53	0
7	JN4	D	442	-	28,31,31	4.24	12 (42%)	25,42,42	1.42	5 (20%)
3	EDO	D	18	-	3,3,3	0.49	0	2,2,2	0.27	0
8	EPE	C	7	-	15,15,15	0.78	1 (6%)	18,20,20	2.06	5 (27%)
3	EDO	C	5	-	3,3,3	0.40	0	2,2,2	0.44	0
3	EDO	B	13	-	3,3,3	0.52	0	2,2,2	0.38	0
7	JN4	A	23	-	28,31,31	4.30	12 (42%)	25,42,42	1.74	4 (16%)
3	EDO	C	15	-	3,3,3	0.46	0	2,2,2	0.36	0
3	EDO	B	4	-	3,3,3	0.48	0	2,2,2	0.44	0
3	EDO	B	11	-	3,3,3	0.47	0	2,2,2	0.65	0
3	EDO	D	5	-	3,3,3	0.42	0	2,2,2	0.50	0
3	EDO	B	19	-	3,3,3	0.42	0	2,2,2	0.44	0
3	EDO	D	6	-	3,3,3	0.54	0	2,2,2	0.31	0
3	EDO	A	17	-	3,3,3	0.44	0	2,2,2	0.58	0
3	EDO	A	5	-	3,3,3	0.49	0	2,2,2	0.33	0
3	EDO	A	11	-	3,3,3	0.48	0	2,2,2	0.43	0
4	DMS	A	6	-	3,3,3	2.71	1 (33%)	3,3,3	0.53	0
5	PEG	D	12	-	6,6,6	0.50	0	5,5,5	0.47	0
3	EDO	D	10	-	3,3,3	0.52	0	2,2,2	0.33	0
3	EDO	A	10	-	3,3,3	0.44	0	2,2,2	0.41	0
3	EDO	A	4	-	3,3,3	0.43	0	2,2,2	0.45	0
5	PEG	D	16	-	6,6,6	0.48	0	5,5,5	0.50	0
3	EDO	A	19	-	3,3,3	0.50	0	2,2,2	0.19	0
3	EDO	D	440	-	3,3,3	0.56	0	2,2,2	0.27	0
4	DMS	D	23	-	3,3,3	2.58	1 (33%)	3,3,3	0.47	0
7	JN4	C	18	-	28,31,31	4.38	12 (42%)	25,42,42	1.30	3 (12%)
3	EDO	A	18	-	3,3,3	0.51	0	2,2,2	0.31	0
3	EDO	C	8	-	3,3,3	0.52	0	2,2,2	0.53	0
3	EDO	D	4	-	3,3,3	0.53	0	2,2,2	0.18	0
5	PEG	D	19	-	6,6,6	0.47	0	5,5,5	0.25	0
3	EDO	D	14	-	3,3,3	0.53	0	2,2,2	0.25	0
3	EDO	D	22	-	3,3,3	0.53	0	2,2,2	0.16	0
3	EDO	D	11	-	3,3,3	0.54	0	2,2,2	0.17	0
4	DMS	B	7	-	3,3,3	2.66	1 (33%)	3,3,3	0.52	0
7	JN4	B	21	-	28,31,31	4.27	12 (42%)	25,42,42	1.39	3 (12%)
3	EDO	B	16	-	3,3,3	0.38	0	2,2,2	0.44	0
3	EDO	A	15	-	3,3,3	0.52	0	2,2,2	0.31	0
3	EDO	B	15	-	3,3,3	0.55	0	2,2,2	0.06	0
3	EDO	C	13	-	3,3,3	0.53	0	2,2,2	0.21	0
3	EDO	C	6	-	3,3,3	0.49	0	2,2,2	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	D	7	-	3,3,3	0.42	0	2,2,2	0.39	0
3	EDO	D	15	-	3,3,3	0.50	0	2,2,2	0.34	0
4	DMS	D	13	-	3,3,3	2.73	1 (33%)	3,3,3	0.60	0
5	PEG	D	441	-	6,6,6	0.58	0	5,5,5	0.50	0
6	PO4	C	17	2	4,4,4	0.67	0	6,6,6	0.77	0
3	EDO	B	10	-	3,3,3	0.46	0	2,2,2	0.72	0
3	EDO	C	11	-	3,3,3	0.50	0	2,2,2	0.32	0
3	EDO	A	16	-	3,3,3	0.42	0	2,2,2	0.57	0
3	EDO	A	21	-	3,3,3	0.46	0	2,2,2	0.40	0
3	EDO	A	9	-	3,3,3	0.56	0	2,2,2	0.24	0
3	EDO	D	17	-	3,3,3	0.50	0	2,2,2	0.44	0
4	DMS	D	8	-	3,3,3	2.68	1 (33%)	3,3,3	0.42	0
6	PO4	D	24	2	4,4,4	0.79	0	6,6,6	0.71	0
8	EPE	B	6	-	15,15,15	0.95	1 (6%)	18,20,20	1.86	6 (33%)
3	EDO	C	440	-	3,3,3	0.44	0	2,2,2	0.37	0
3	EDO	C	12	-	3,3,3	0.51	0	2,2,2	0.27	0
4	DMS	D	9	-	3,3,3	2.62	1 (33%)	3,3,3	0.46	0
3	EDO	B	18	-	3,3,3	0.52	0	2,2,2	0.04	0
3	EDO	C	14	-	3,3,3	0.49	0	2,2,2	0.20	0
5	PEG	A	440	-	6,6,6	0.45	0	5,5,5	0.46	0
3	EDO	D	21	-	3,3,3	0.52	0	2,2,2	0.08	0
3	EDO	C	4	-	3,3,3	0.49	0	2,2,2	0.26	0
6	PO4	A	20	2	4,4,4	0.88	0	6,6,6	0.56	0
4	DMS	C	10	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
6	PO4	B	20	2	4,4,4	0.84	0	6,6,6	0.72	0
3	EDO	A	7	-	3,3,3	0.45	0	2,2,2	0.46	0
3	EDO	B	8	-	3,3,3	0.41	0	2,2,2	0.50	0
3	EDO	A	441	-	3,3,3	0.53	0	2,2,2	0.32	0
3	EDO	A	14	-	3,3,3	0.41	0	2,2,2	0.49	0
3	EDO	B	9	-	3,3,3	0.50	0	2,2,2	0.25	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	B	17	-	-	0/1/1/1	-
3	EDO	D	20	-	-	1/1/1/1	-
3	EDO	A	443	-	-	1/1/1/1	-
3	EDO	A	13	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	JN4	D	442	-	-	4/18/31/31	0/3/3/3
3	EDO	D	18	-	-	0/1/1/1	-
8	EPE	C	7	-	-	2/9/19/19	0/1/1/1
3	EDO	C	5	-	-	0/1/1/1	-
3	EDO	B	13	-	-	0/1/1/1	-
7	JN4	A	23	-	-	2/18/31/31	0/3/3/3
3	EDO	C	15	-	-	1/1/1/1	-
3	EDO	B	4	-	-	0/1/1/1	-
3	EDO	B	11	-	-	1/1/1/1	-
3	EDO	D	5	-	-	0/1/1/1	-
3	EDO	B	19	-	-	1/1/1/1	-
3	EDO	D	6	-	-	0/1/1/1	-
3	EDO	A	17	-	-	1/1/1/1	-
3	EDO	A	5	-	-	0/1/1/1	-
3	EDO	A	11	-	-	1/1/1/1	-
5	PEG	D	12	-	-	3/4/4/4	-
3	EDO	D	10	-	-	1/1/1/1	-
3	EDO	A	10	-	-	1/1/1/1	-
3	EDO	A	4	-	-	0/1/1/1	-
5	PEG	D	16	-	-	3/4/4/4	-
3	EDO	A	19	-	-	0/1/1/1	-
3	EDO	D	440	-	-	1/1/1/1	-
7	JN4	C	18	-	-	3/18/31/31	0/3/3/3
3	EDO	A	18	-	-	1/1/1/1	-
3	EDO	C	8	-	-	0/1/1/1	-
3	EDO	D	4	-	-	0/1/1/1	-
5	PEG	D	19	-	-	4/4/4/4	-
3	EDO	D	14	-	-	0/1/1/1	-
3	EDO	D	22	-	-	0/1/1/1	-
3	EDO	D	11	-	-	1/1/1/1	-
7	JN4	B	21	-	-	2/18/31/31	0/3/3/3
3	EDO	B	16	-	-	0/1/1/1	-
3	EDO	A	15	-	-	0/1/1/1	-
3	EDO	B	15	-	-	0/1/1/1	-
3	EDO	C	13	-	-	0/1/1/1	-
3	EDO	C	6	-	-	0/1/1/1	-
3	EDO	D	7	-	-	1/1/1/1	-
3	EDO	D	15	-	-	0/1/1/1	-
5	PEG	D	441	-	-	2/4/4/4	-
3	EDO	B	10	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	11	-	-	1/1/1/1	-
3	EDO	A	16	-	-	0/1/1/1	-
3	EDO	A	21	-	-	1/1/1/1	-
3	EDO	A	9	-	-	0/1/1/1	-
3	EDO	D	17	-	-	0/1/1/1	-
8	EPE	B	6	-	-	3/9/19/19	0/1/1/1
3	EDO	C	440	-	-	0/1/1/1	-
3	EDO	C	12	-	-	1/1/1/1	-
5	PEG	A	440	-	-	1/4/4/4	-
3	EDO	B	18	-	-	1/1/1/1	-
3	EDO	C	14	-	-	0/1/1/1	-
3	EDO	D	21	-	-	0/1/1/1	-
3	EDO	C	4	-	-	0/1/1/1	-
3	EDO	A	7	-	-	1/1/1/1	-
3	EDO	B	8	-	-	0/1/1/1	-
3	EDO	A	441	-	-	1/1/1/1	-
3	EDO	A	14	-	-	0/1/1/1	-
3	EDO	B	9	-	-	0/1/1/1	-

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	18	JN4	C14-C5	16.64	1.70	1.39
7	A	23	JN4	C14-C5	16.43	1.69	1.39
7	B	21	JN4	C14-C5	16.28	1.69	1.39
7	D	442	JN4	C14-C5	16.14	1.69	1.39
7	C	18	JN4	C13-S12	-9.62	1.57	1.72
7	B	21	JN4	C13-S12	-9.34	1.57	1.72
7	D	442	JN4	C13-S12	-8.95	1.58	1.72
7	A	23	JN4	C13-S12	-8.61	1.59	1.72
7	A	23	JN4	C14-C13	6.12	1.54	1.41
7	C	18	JN4	C14-C13	5.94	1.53	1.41
7	D	442	JN4	C14-C13	5.85	1.53	1.41
7	B	21	JN4	C14-C13	5.79	1.53	1.41
7	D	442	JN4	C10-N9	5.01	1.44	1.32
7	C	18	JN4	C10-N9	4.92	1.44	1.32
7	A	23	JN4	C10-N9	4.84	1.44	1.32
7	B	21	JN4	C10-N9	4.70	1.43	1.32
4	D	13	DMS	O-S	4.60	1.81	1.50
4	A	6	DMS	O-S	4.54	1.80	1.50
4	D	8	DMS	O-S	4.50	1.80	1.50
4	C	10	DMS	O-S	4.49	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	7	DMS	O-S	4.46	1.80	1.50
4	D	9	DMS	O-S	4.40	1.80	1.50
4	D	23	DMS	O-S	4.40	1.80	1.50
7	B	21	JN4	C7-N2	4.36	1.44	1.36
7	D	442	JN4	C7-N2	4.21	1.44	1.36
7	C	18	JN4	C7-N2	4.20	1.44	1.36
7	A	23	JN4	C7-N2	4.12	1.44	1.36
4	A	442	DMS	O-S	4.10	1.77	1.50
7	A	23	JN4	C21-N20	3.97	1.44	1.35
7	A	23	JN4	C18-C17	3.84	1.49	1.30
7	C	18	JN4	C18-C17	3.84	1.49	1.30
7	B	21	JN4	C18-C17	3.83	1.49	1.30
7	D	442	JN4	C11-C10	3.82	1.49	1.29
7	D	442	JN4	C18-C17	3.82	1.49	1.30
7	B	21	JN4	C11-C10	3.80	1.49	1.29
7	C	18	JN4	C21-N20	3.79	1.44	1.35
7	A	23	JN4	C11-C10	3.79	1.49	1.29
7	C	18	JN4	C11-C10	3.76	1.49	1.29
7	C	18	JN4	C25-C23	3.74	1.46	1.38
7	B	21	JN4	C21-N20	3.70	1.43	1.35
7	A	23	JN4	C25-C23	3.66	1.46	1.38
7	D	442	JN4	C21-N20	3.55	1.43	1.35
7	D	442	JN4	C25-C23	3.51	1.46	1.38
7	B	21	JN4	C25-C23	3.38	1.46	1.38
8	B	6	EPE	C10-S	3.25	1.82	1.77
7	A	23	JN4	C28-C24	3.10	1.45	1.38
7	A	23	JN4	C3-C4	3.07	1.55	1.51
7	B	21	JN4	C28-C24	2.99	1.45	1.38
7	C	18	JN4	C28-C24	2.95	1.45	1.38
7	D	442	JN4	C28-C24	2.94	1.45	1.38
7	C	18	JN4	C3-C4	2.85	1.54	1.51
8	C	7	EPE	C10-S	2.52	1.81	1.77
7	D	442	JN4	C7-N9	2.47	1.45	1.39
7	D	442	JN4	C3-C4	2.31	1.54	1.51
7	A	23	JN4	C7-N9	2.11	1.44	1.39
7	B	21	JN4	C3-C4	2.10	1.54	1.51
7	B	21	JN4	C7-N9	2.04	1.44	1.39
7	C	18	JN4	C7-N9	2.01	1.44	1.39

All (26) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	23	JN4	C6-C1-N2	5.66	116.70	110.04
7	B	21	JN4	C6-C1-N2	4.48	115.32	110.04
8	C	7	EPE	C5-N4-C3	4.07	117.98	108.83
8	C	7	EPE	O3S-S-C10	4.05	112.33	105.77
7	A	23	JN4	C1-C6-C5	3.71	117.73	111.63
8	B	6	EPE	C7-N4-C3	3.56	120.34	111.23
7	D	442	JN4	C6-C1-N2	3.52	114.18	110.04
8	C	7	EPE	C7-N4-C3	3.49	120.16	111.23
8	B	6	EPE	O1S-S-C10	3.47	111.09	106.92
8	C	7	EPE	C7-N4-C5	3.46	120.08	111.23
7	A	23	JN4	C4-C3-N2	3.42	116.31	112.72
7	D	442	JN4	O8-C7-N2	-3.34	117.09	121.78
7	C	18	JN4	C6-C1-N2	3.27	113.90	110.04
7	B	21	JN4	C1-C6-C5	3.21	116.91	111.63
8	B	6	EPE	C5-N4-C3	3.15	115.92	108.83
7	C	18	JN4	C1-C6-C5	3.11	116.75	111.63
7	C	18	JN4	O29-C21-N20	-2.96	118.23	123.63
8	B	6	EPE	C7-N4-C5	2.95	118.78	111.23
8	B	6	EPE	O3S-S-C10	2.90	110.47	105.77
7	D	442	JN4	C1-C6-C5	2.66	116.01	111.63
7	B	21	JN4	O29-C21-N20	-2.45	119.16	123.63
7	A	23	JN4	O29-C21-N20	-2.43	119.19	123.63
8	C	7	EPE	O1S-S-C10	2.17	109.53	106.92
7	D	442	JN4	O29-C21-N20	-2.14	119.72	123.63
7	D	442	JN4	O8-C7-N9	-2.13	118.01	121.91
8	B	6	EPE	C6-N1-C2	2.05	113.44	108.83

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	442	JN4	N2-C7-N9-C10
8	B	6	EPE	C10-C9-N1-C2
8	C	7	EPE	S-C10-C9-N1
5	A	440	PEG	O2-C3-C4-O4
5	D	12	PEG	O2-C3-C4-O4
7	D	442	JN4	O8-C7-N9-C10
3	A	11	EDO	O1-C1-C2-O2
3	A	18	EDO	O1-C1-C2-O2
3	D	440	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	D	7	EDO	O1-C1-C2-O2
3	D	11	EDO	O1-C1-C2-O2
5	D	12	PEG	O1-C1-C2-O2
5	D	19	PEG	O1-C1-C2-O2
3	A	13	EDO	O1-C1-C2-O2
3	B	19	EDO	O1-C1-C2-O2
3	C	11	EDO	O1-C1-C2-O2
3	C	12	EDO	O1-C1-C2-O2
3	D	20	EDO	O1-C1-C2-O2
7	D	442	JN4	N20-C21-C22-C23
8	B	6	EPE	C10-C9-N1-C6
5	D	19	PEG	O2-C3-C4-O4
3	A	441	EDO	O1-C1-C2-O2
5	D	16	PEG	O2-C3-C4-O4
5	D	12	PEG	C1-C2-O2-C3
7	C	18	JN4	N20-C21-C22-C23
3	A	10	EDO	O1-C1-C2-O2
3	B	10	EDO	O1-C1-C2-O2
3	C	15	EDO	O1-C1-C2-O2
3	D	10	EDO	O1-C1-C2-O2
5	D	441	PEG	C1-C2-O2-C3
7	C	18	JN4	O29-C21-N20-C13
7	A	23	JN4	N20-C21-C22-C23
7	B	21	JN4	N20-C21-C22-C23
5	D	19	PEG	C4-C3-O2-C2
3	A	17	EDO	O1-C1-C2-O2
3	B	18	EDO	O1-C1-C2-O2
7	C	18	JN4	O29-C21-C22-C23
7	D	442	JN4	N9-C7-N2-C1
3	A	443	EDO	O1-C1-C2-O2
5	D	16	PEG	C1-C2-O2-C3
5	D	441	PEG	O2-C3-C4-O4
5	D	19	PEG	C1-C2-O2-C3
3	A	7	EDO	O1-C1-C2-O2
3	A	21	EDO	O1-C1-C2-O2
3	B	11	EDO	O1-C1-C2-O2
8	B	6	EPE	N4-C7-C8-O8
7	A	23	JN4	O29-C21-C22-C23
7	B	21	JN4	O29-C21-C22-C23
8	C	7	EPE	C10-C9-N1-C2
5	D	16	PEG	C4-C3-O2-C2

There are no ring outliers.

46 monomers are involved in 134 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	20	EDO	2	0
3	A	443	EDO	8	0
4	A	442	DMS	1	0
7	D	442	JN4	3	0
3	D	18	EDO	2	0
8	C	7	EPE	2	0
3	C	5	EDO	1	0
7	A	23	JN4	2	0
3	B	4	EDO	1	0
3	D	5	EDO	5	0
3	A	17	EDO	1	0
5	D	12	PEG	7	0
3	D	10	EDO	3	0
3	A	10	EDO	2	0
5	D	16	PEG	6	0
3	A	19	EDO	1	0
4	D	23	DMS	11	0
7	C	18	JN4	4	0
3	A	18	EDO	2	0
3	C	8	EDO	1	0
5	D	19	PEG	3	0
3	D	14	EDO	1	0
3	D	22	EDO	1	0
7	B	21	JN4	2	0
3	B	16	EDO	6	0
3	B	15	EDO	7	0
3	C	13	EDO	3	0
3	D	15	EDO	3	0
4	D	13	DMS	1	0
5	D	441	PEG	4	0
6	C	17	PO4	1	0
3	C	11	EDO	1	0
3	A	21	EDO	4	0
3	A	9	EDO	1	0
3	D	17	EDO	2	0
4	D	8	DMS	4	0
6	D	24	PO4	1	0
3	C	440	EDO	3	0
3	C	12	EDO	2	0
3	B	18	EDO	5	0
3	C	14	EDO	2	0
5	A	440	PEG	1	0

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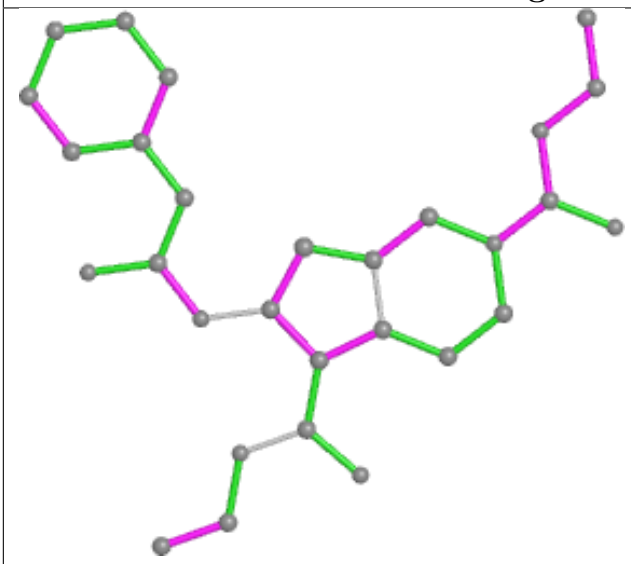
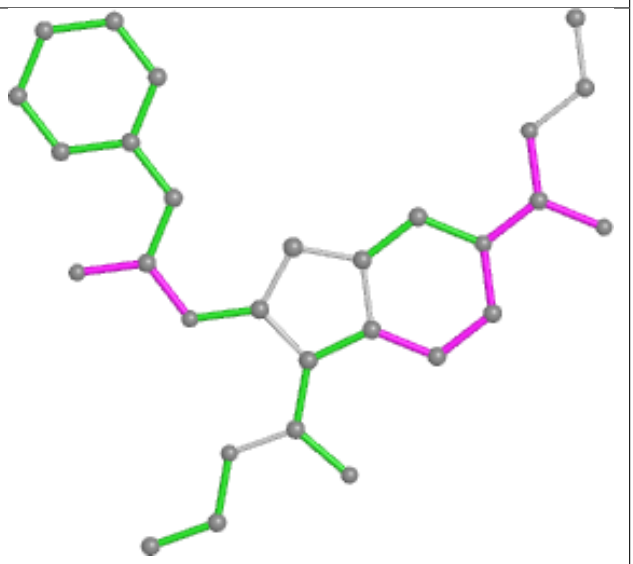
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	21	EDO	5	0
6	A	20	PO4	3	0
6	B	20	PO4	1	0
3	A	7	EDO	3	0

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.

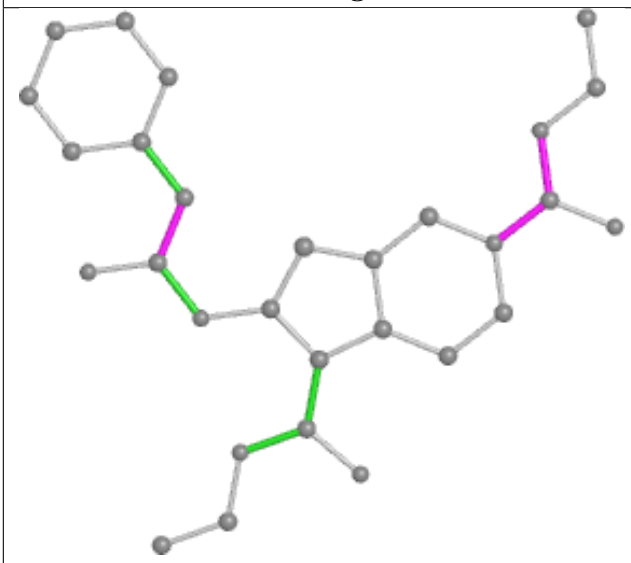
Ligand JN4 D 442



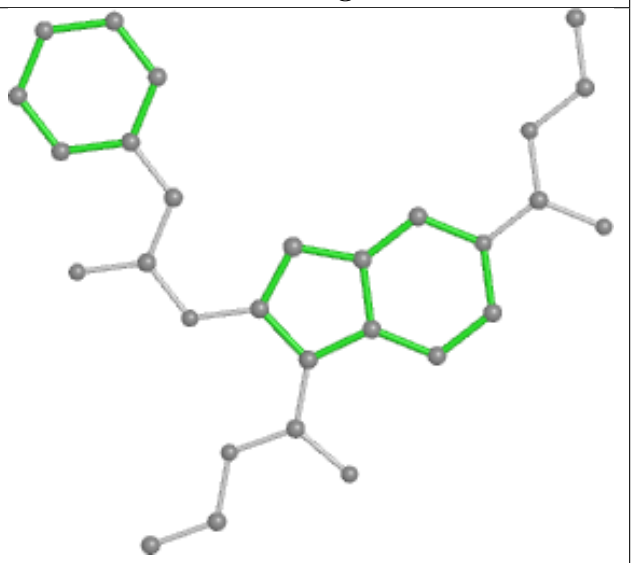
Bond lengths



Bond angles

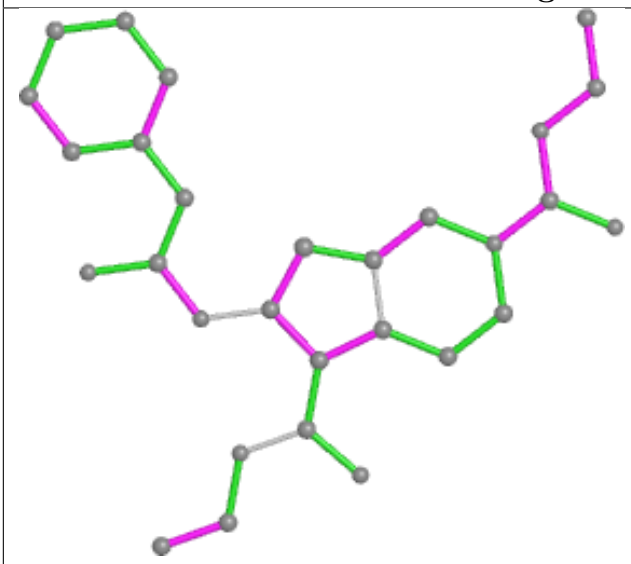


Torsions

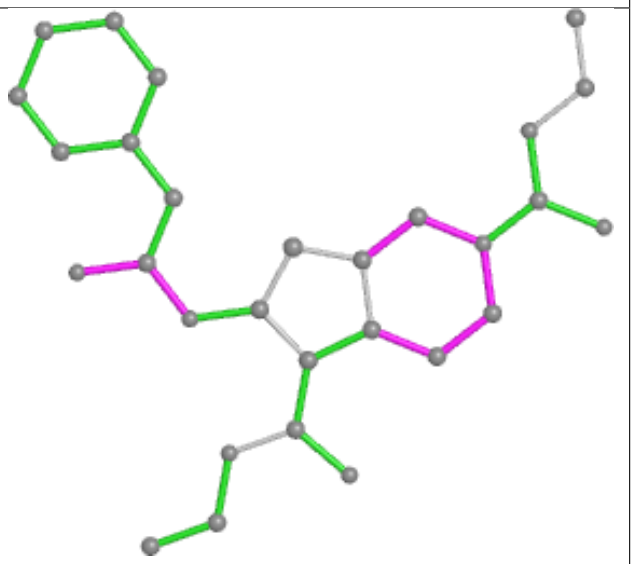


Rings

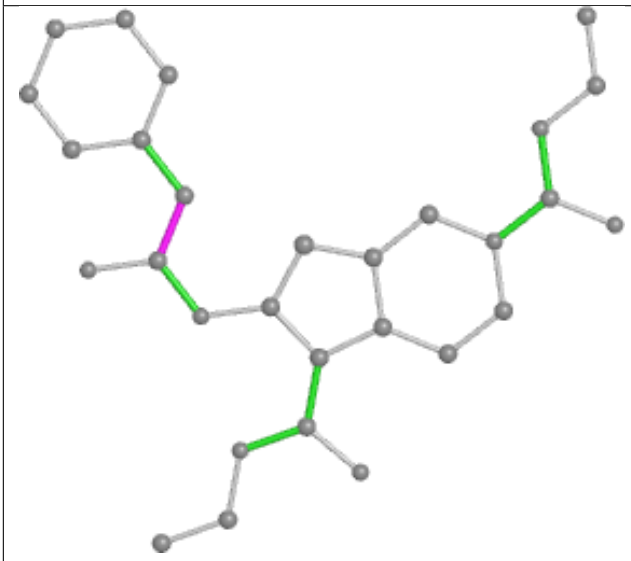
Ligand JN4 A 23



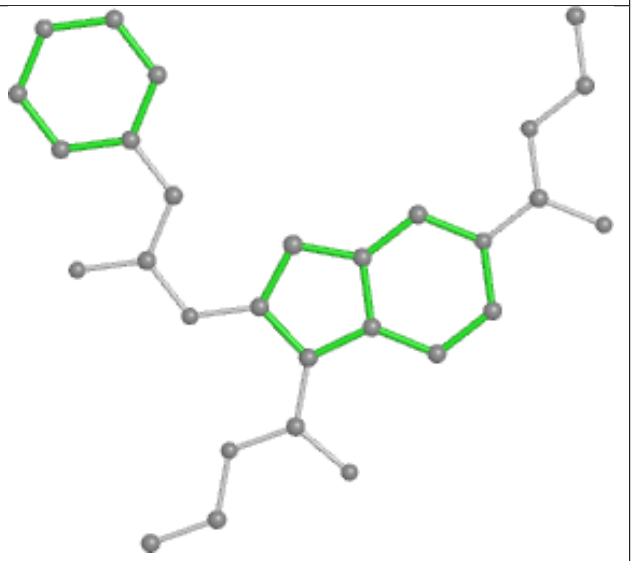
Bond lengths



Bond angles

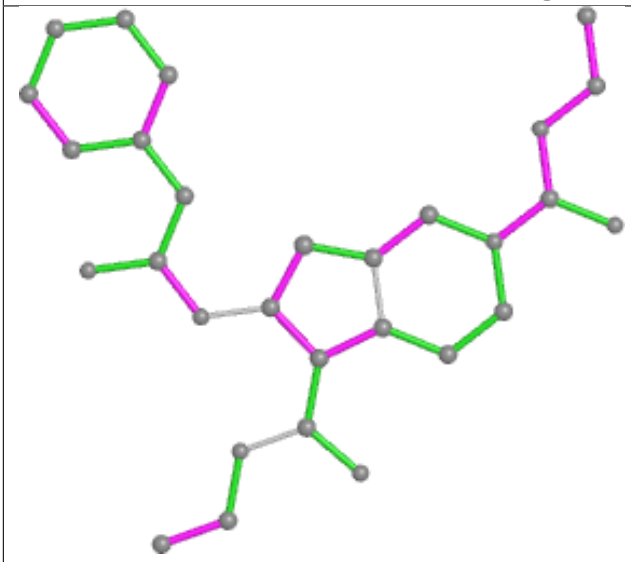


Torsions

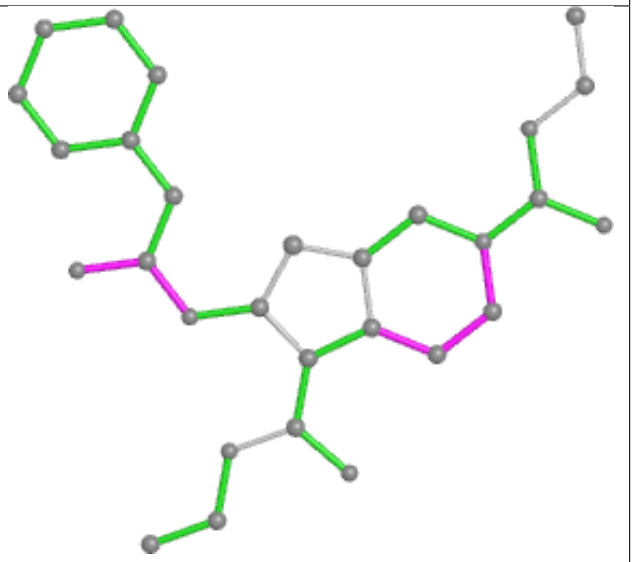


Rings

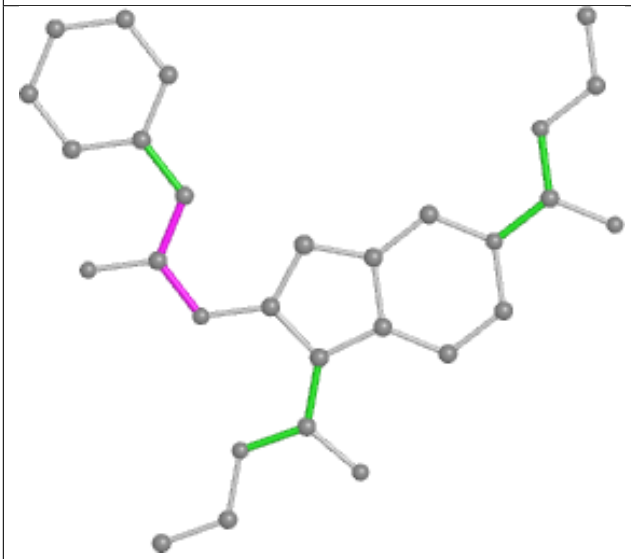
Ligand JN4 C 18



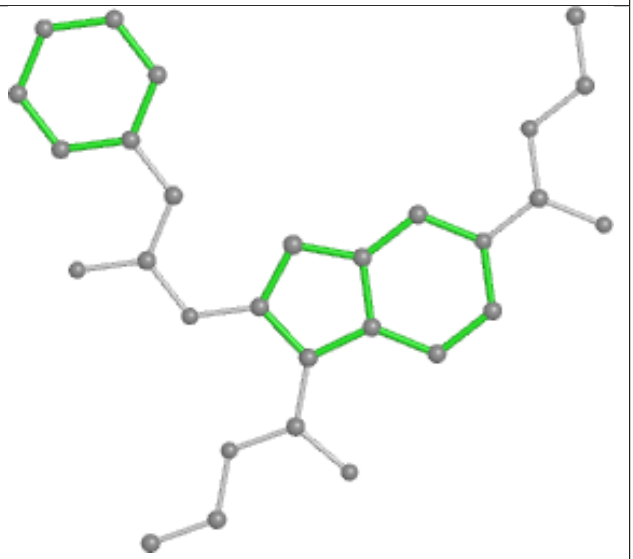
Bond lengths



Bond angles

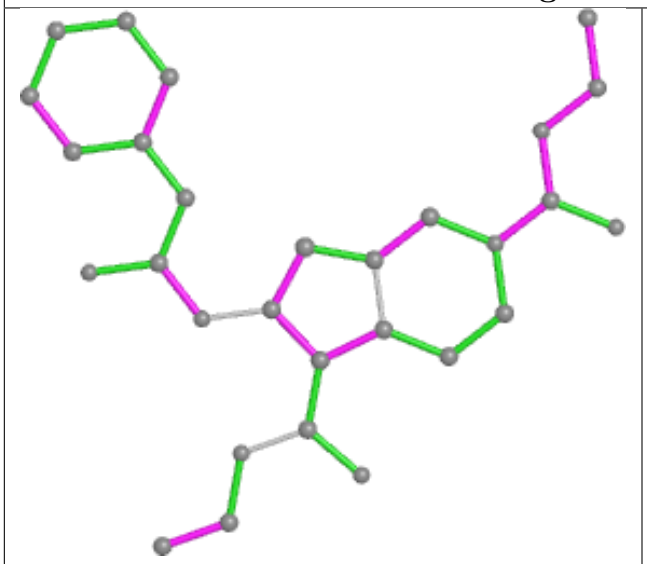


Torsions

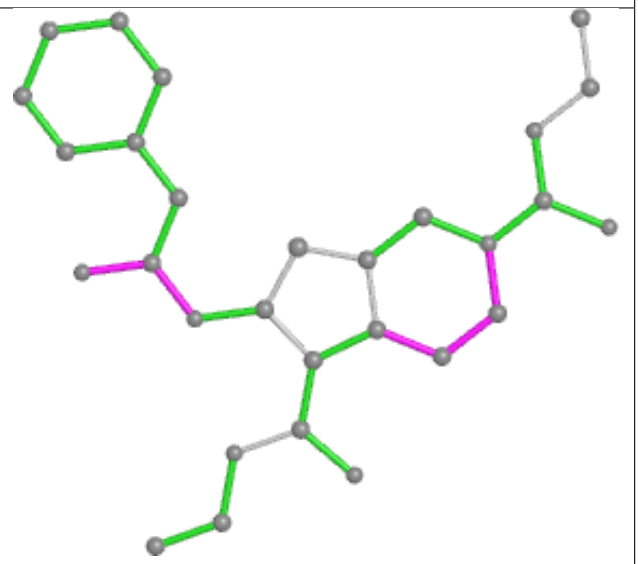


Rings

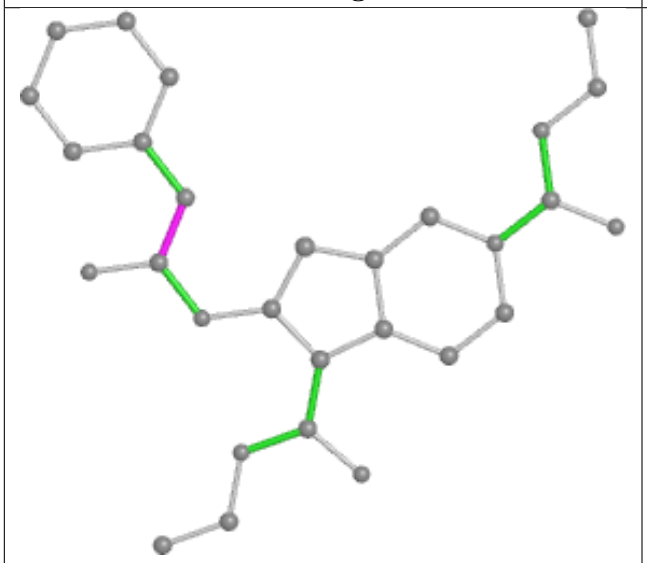
Ligand JN4 B 21



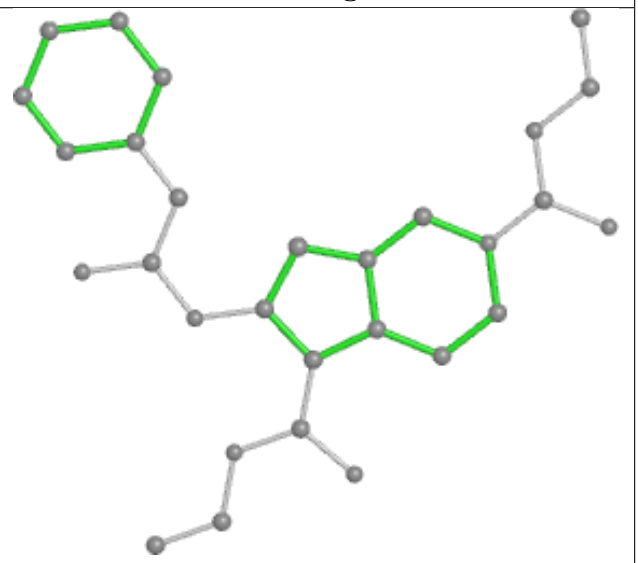
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	329/361 (91%)	0.49	33 (10%) 7 8	14, 28, 58, 86	0
1	B	325/361 (90%)	0.45	27 (8%) 11 13	17, 34, 50, 79	0
1	C	325/361 (90%)	0.58	38 (11%) 4 5	17, 32, 62, 81	0
1	D	324/361 (89%)	0.30	23 (7%) 16 17	14, 24, 50, 69	0
All	All	1303/1444 (90%)	0.45	121 (9%) 8 10	14, 29, 56, 86	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	356	PRO	7.2
1	C	294	SER	7.2
1	C	351	GLY	5.5
1	D	362	ASN	5.4
1	A	293	THR	5.4
1	C	353	GLU	5.2
1	A	296	GLY	5.2
1	D	354	ILE	5.1
1	A	295	SER	5.0
1	A	361	HIS	5.0
1	C	295	SER	5.0
1	C	362	ASN	4.9
1	A	356	PRO	4.9
1	A	294	SER	4.8
1	C	363	ALA	4.8
1	C	354	ILE	4.7
1	A	362	ASN	4.7
1	A	411	PRO	4.5
1	A	353	GLU	4.5
1	C	87	GLU	4.5
1	A	363	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	354	ILE	4.4
1	C	293	THR	4.3
1	B	88	GLN	4.3
1	C	361	HIS	4.3
1	A	375	TYR	4.2
1	C	297	VAL	4.2
1	D	363	ALA	4.1
1	A	410	ILE	4.0
1	D	357	MET	3.9
1	D	361	HIS	3.9
1	B	90	ASP	3.9
1	A	357	MET	3.8
1	D	356	PRO	3.8
1	D	355	SER	3.8
1	C	357	MET	3.7
1	A	299	LEU	3.7
1	B	94	LYS	3.6
1	C	296	GLY	3.6
1	A	84	VAL	3.6
1	B	108	ARG	3.6
1	C	375	TYR	3.6
1	B	412	GLN	3.5
1	D	375	TYR	3.4
1	C	410	ILE	3.4
1	D	353	GLU	3.3
1	A	297	VAL	3.3
1	C	292	VAL	3.3
1	A	352	MET	3.3
1	D	90	ASP	3.2
1	C	86	THR	3.2
1	C	289	THR	3.2
1	B	91	VAL	3.2
1	C	168	VAL	3.2
1	C	409	THR	3.2
1	A	317	ALA	3.2
1	C	291	LYS	3.2
1	B	139	VAL	3.1
1	B	133	LYS	3.1
1	A	359	ASP	3.1
1	C	319	LEU	3.0
1	A	83	GLY	2.9
1	A	355	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	196	ALA	2.8
1	C	301	ASP	2.7
1	D	88	GLN	2.7
1	A	316	CYS	2.7
1	C	355	SER	2.7
1	B	168	VAL	2.7
1	C	316	CYS	2.7
1	D	89	GLU	2.6
1	C	299	LEU	2.6
1	C	317	ALA	2.6
1	B	301	ASP	2.6
1	D	314	VAL	2.6
1	B	130	ASP	2.6
1	D	198	ALA	2.6
1	B	362	ASN	2.6
1	D	193	ALA	2.5
1	A	351	GLY	2.5
1	C	348	ARG	2.5
1	A	168	VAL	2.5
1	A	291	LYS	2.5
1	B	257	ARG	2.5
1	A	348	ARG	2.5
1	B	356	PRO	2.4
1	C	302	ASN	2.4
1	B	136	LYS	2.4
1	C	359	ASP	2.3
1	C	320	SER	2.3
1	D	317	ALA	2.3
1	C	364	SER	2.3
1	B	89	GLU	2.3
1	A	350	ARG	2.3
1	B	196	ALA	2.3
1	A	360	LYS	2.3
1	B	286	MET	2.2
1	C	314	VAL	2.2
1	B	118	LEU	2.2
1	C	367	LYS	2.2
1	D	168	VAL	2.2
1	B	353	GLU	2.2
1	C	175	LEU	2.1
1	B	193	ALA	2.1
1	D	172	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	410	ILE	2.1
1	B	295	SER	2.1
1	B	375	TYR	2.1
1	B	165	ALA	2.1
1	B	294	SER	2.1
1	C	303	TYR	2.1
1	A	409	THR	2.1
1	A	292	VAL	2.1
1	B	97	GLU	2.0
1	D	404	GLU	2.0
1	A	319	LEU	2.0
1	B	112	LEU	2.0
1	C	360	LYS	2.0
1	D	316	CYS	2.0
1	D	358	CYS	2.0
1	A	288	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PEG	D	16	7/7	0.65	0.40	36,43,47,55	0
3	EDO	C	13	4/4	0.74	0.37	27,33,40,48	0
3	EDO	A	443	4/4	0.76	0.22	26,33,41,42	0
5	PEG	A	440	7/7	0.77	0.30	31,38,41,43	0
3	EDO	D	10	4/4	0.77	0.17	38,45,47,49	0
3	EDO	A	16	4/4	0.79	0.26	34,37,44,45	0
3	EDO	A	9	4/4	0.80	0.27	38,40,45,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	D	20	4/4	0.80	0.26	32,33,40,40	0
3	EDO	C	15	4/4	0.80	0.27	33,37,39,46	0
3	EDO	D	6	4/4	0.80	0.30	39,44,47,52	0
3	EDO	D	18	4/4	0.81	0.24	41,43,44,47	0
3	EDO	D	14	4/4	0.81	0.23	39,40,50,51	0
3	EDO	A	15	4/4	0.82	0.21	41,44,45,46	0
5	PEG	D	12	7/7	0.82	0.21	26,32,46,50	0
3	EDO	C	14	4/4	0.82	0.21	33,35,40,43	0
7	JN4	A	23	29/29	0.82	0.23	32,43,77,82	0
3	EDO	B	9	4/4	0.83	0.14	31,38,38,39	0
5	PEG	D	19	7/7	0.84	0.29	34,42,48,51	0
5	PEG	D	441	7/7	0.84	0.18	16,34,35,36	0
3	EDO	C	8	4/4	0.85	0.20	35,38,39,40	0
3	EDO	C	11	4/4	0.85	0.15	38,43,44,46	0
4	DMS	D	8	4/4	0.85	0.32	37,47,52,62	0
3	EDO	A	19	4/4	0.86	0.26	47,50,50,55	0
3	EDO	A	17	4/4	0.86	0.23	34,36,38,43	0
3	EDO	B	4	4/4	0.86	0.16	34,44,44,47	0
3	EDO	B	18	4/4	0.87	0.23	33,37,39,42	0
3	EDO	B	8	4/4	0.87	0.20	37,41,46,53	0
3	EDO	B	13	4/4	0.87	0.17	35,41,44,49	0
3	EDO	D	440	4/4	0.87	0.17	21,25,29,33	0
7	JN4	D	442	29/29	0.87	0.17	28,40,63,67	0
3	EDO	D	15	4/4	0.88	0.27	37,39,39,53	0
3	EDO	C	12	4/4	0.88	0.18	40,45,47,52	0
3	EDO	A	441	4/4	0.88	0.28	33,39,44,45	0
3	EDO	A	5	4/4	0.88	0.13	42,43,46,48	0
6	PO4	B	20	5/5	0.88	0.21	24,24,26,31	2
4	DMS	D	23	4/4	0.88	0.21	20,39,43,45	0
3	EDO	B	17	4/4	0.88	0.25	44,47,52,55	0
3	EDO	A	11	4/4	0.89	0.25	33,34,42,43	0
3	EDO	B	15	4/4	0.89	0.37	29,36,39,44	0
3	EDO	D	22	4/4	0.89	0.34	28,37,38,43	0
4	DMS	B	7	4/4	0.89	0.29	40,44,50,61	0
3	EDO	A	10	4/4	0.89	0.18	36,38,40,42	0
4	DMS	D	9	4/4	0.89	0.22	34,42,43,59	0
4	DMS	D	13	4/4	0.89	0.25	34,35,42,53	0
3	EDO	D	17	4/4	0.89	0.20	28,29,37,44	0
8	EPE	B	6	15/15	0.89	0.28	43,54,60,62	0
3	EDO	A	7	4/4	0.90	0.12	39,42,43,45	0
3	EDO	D	11	4/4	0.90	0.18	38,40,44,45	0
3	EDO	D	21	4/4	0.90	0.33	29,30,31,37	0

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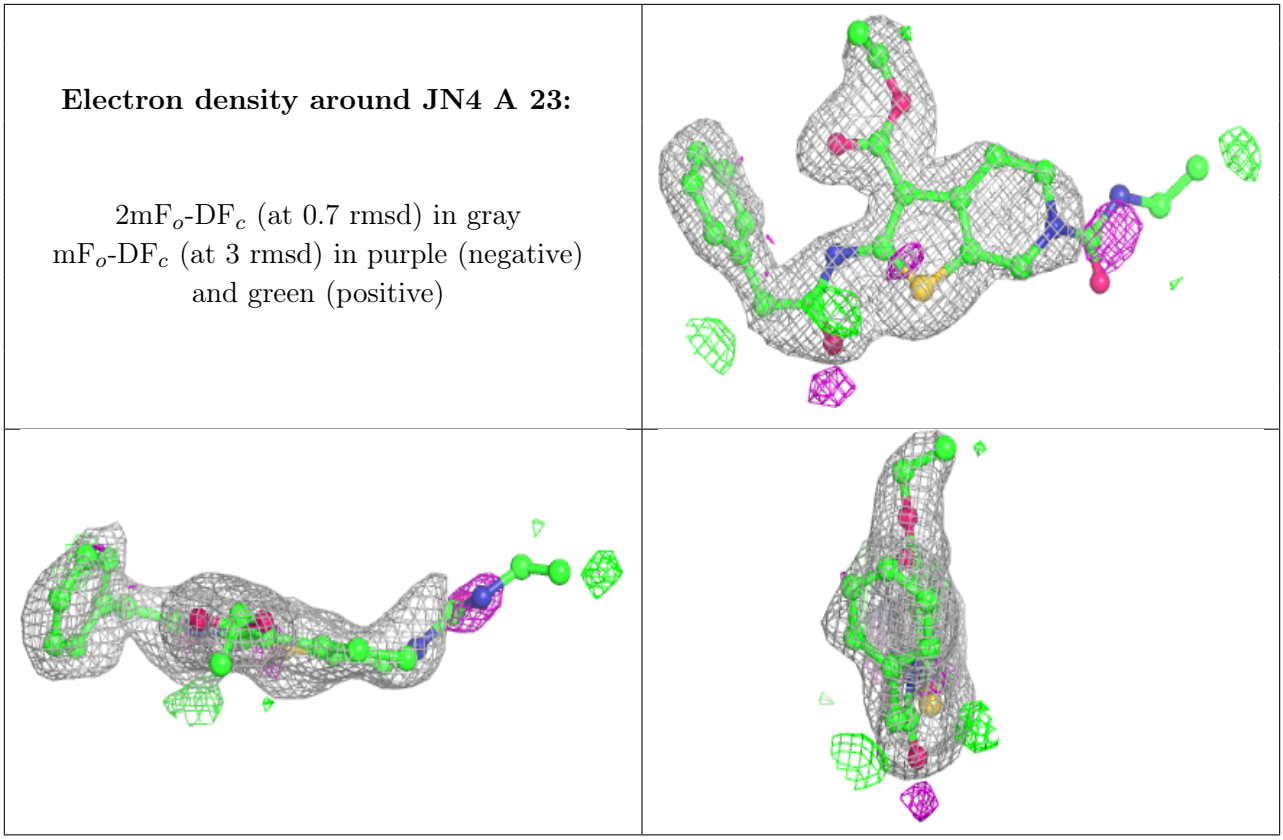
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	D	5	4/4	0.90	0.17	24,35,37,41	0
7	JN4	C	18	29/29	0.90	0.17	32,40,57,65	0
3	EDO	C	5	4/4	0.90	0.18	38,40,41,44	0
3	EDO	B	10	4/4	0.90	0.13	32,33,41,48	0
6	PO4	A	20	5/5	0.91	0.21	20,22,29,32	1
3	EDO	B	11	4/4	0.91	0.26	39,40,42,43	0
3	EDO	C	6	4/4	0.91	0.13	39,39,41,46	0
3	EDO	C	440	4/4	0.91	0.14	43,43,44,49	0
3	EDO	A	18	4/4	0.91	0.22	21,38,41,44	0
4	DMS	A	6	4/4	0.91	0.30	42,43,44,55	0
7	JN4	B	21	29/29	0.92	0.14	29,35,56,64	0
3	EDO	B	19	4/4	0.92	0.44	35,36,39,40	0
3	EDO	C	4	4/4	0.92	0.13	36,40,43,51	0
4	DMS	C	10	4/4	0.92	0.15	36,42,51,60	0
8	EPE	C	7	15/15	0.92	0.23	34,50,68,71	0
3	EDO	A	4	4/4	0.93	0.11	25,26,30,31	0
3	EDO	A	21	4/4	0.93	0.35	37,38,40,44	0
6	PO4	D	24	5/5	0.93	0.18	22,22,25,25	3
3	EDO	B	16	4/4	0.94	0.32	37,39,40,45	0
3	EDO	A	14	4/4	0.94	0.10	24,30,30,37	0
6	PO4	C	17	5/5	0.94	0.19	22,22,30,35	1
3	EDO	D	7	4/4	0.94	0.11	28,29,32,37	0
3	EDO	A	13	4/4	0.94	0.13	25,30,38,42	0
4	DMS	A	442	4/4	0.95	0.19	34,41,44,50	0
3	EDO	D	4	4/4	0.95	0.10	23,24,27,31	0
2	ZN	B	2	1/1	0.98	0.08	27,27,27,27	1
2	ZN	C	2	1/1	0.99	0.08	24,24,24,24	1
2	ZN	D	2	1/1	0.99	0.07	24,24,24,24	1
2	ZN	B	1	1/1	0.99	0.07	25,25,25,25	0
2	ZN	A	2	1/1	0.99	0.08	25,25,25,25	1
2	ZN	C	1	1/1	1.00	0.10	24,24,24,24	0
2	ZN	A	1	1/1	1.00	0.10	22,22,22,22	0
2	ZN	D	1	1/1	1.00	0.09	21,21,21,21	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.

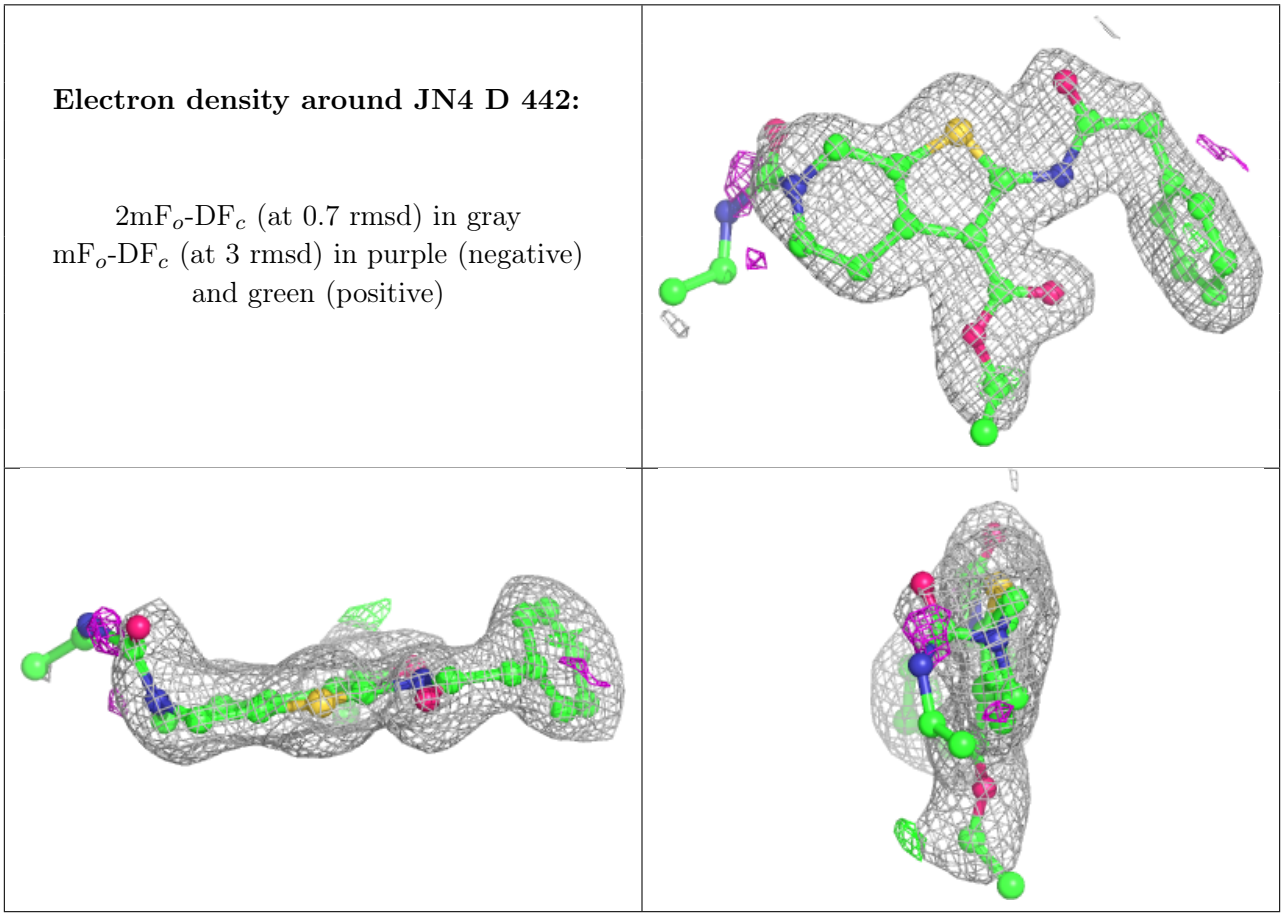
Electron density around JN4 A 23:

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



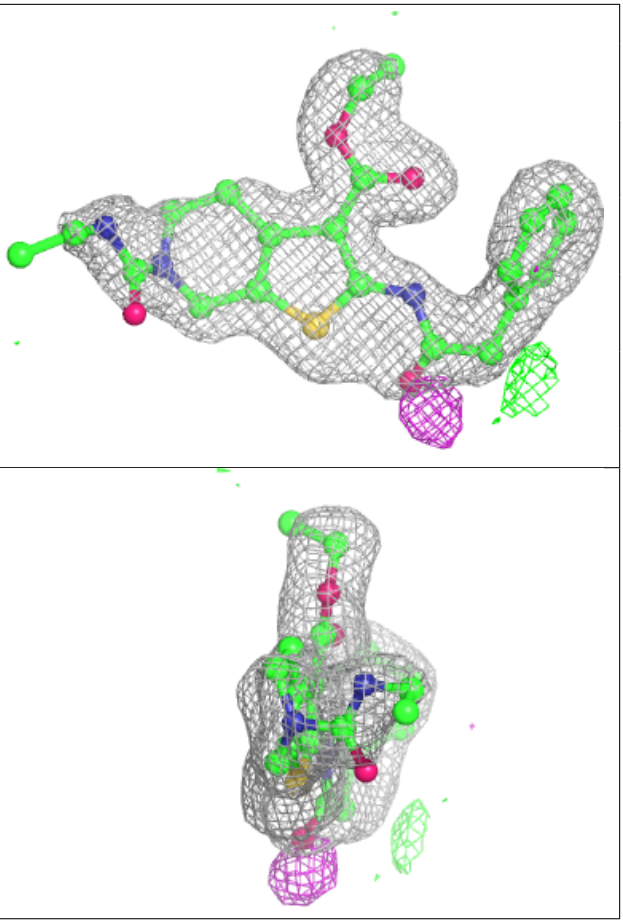
Electron density around JN4 D 442:

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



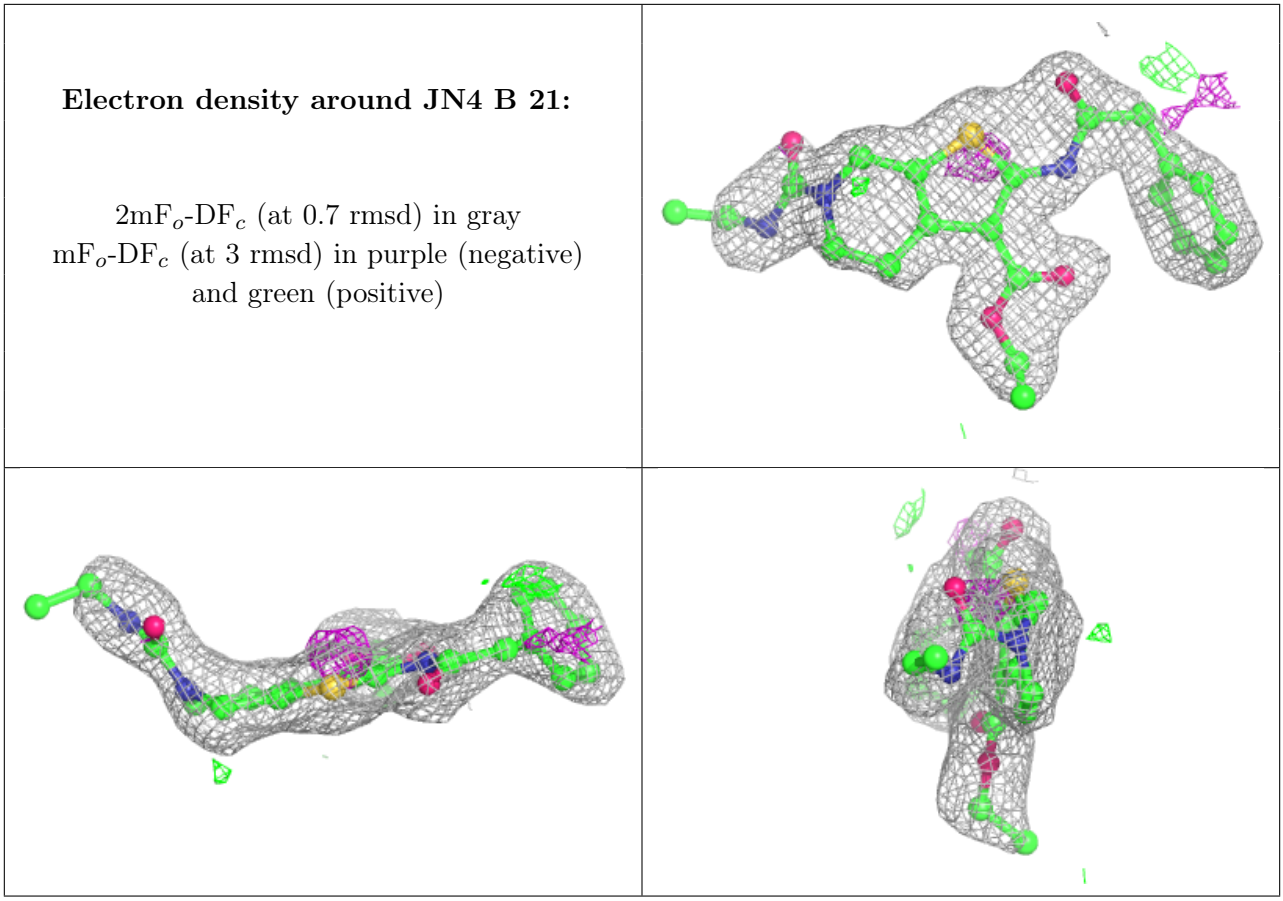
Electron density around JN4 C 18:

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



Electron density around JN4 B 21:

$2mF_o$-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

There are no such residues in this entry.