



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 10:45 pm BST

PDB ID : 3SL8
Title : Crystal structure of the catalytic domain of PDE4D2 with compound 10o
Authors : Feil, S.F.
Deposited on : 2011-06-24
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

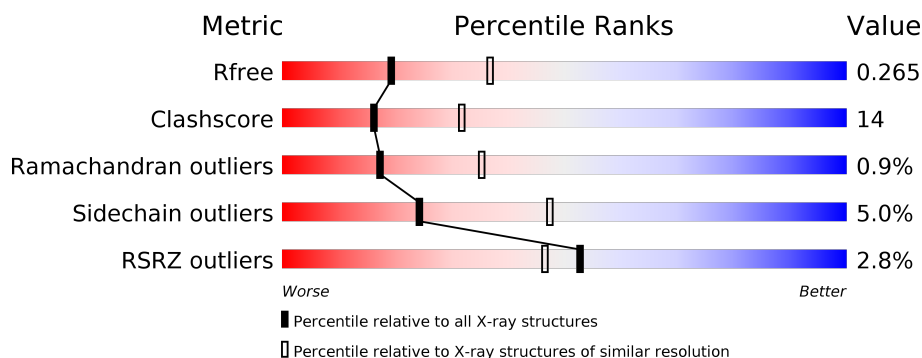
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	361	<div> <div>3%</div> <div> <div></div> <div>63%</div> <div>25%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	361	<div> <div>%</div> <div> <div></div> <div>59%</div> <div>28%</div> <div>•</div> <div>10%</div> </div> </div>
1	C	361	<div> <div>4%</div> <div> <div></div> <div>62%</div> <div>25%</div> <div>•</div> <div>10%</div> </div> </div>
1	D	361	<div> <div>2%</div> <div> <div></div> <div>66%</div> <div>21%</div> <div>•</div> <div>10%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	13	-	-	X	-
2	EDO	B	8	-	-	X	-
2	EDO	D	13	-	-	X	-
2	EDO	D	7	-	-	X	-
4	PEG	D	5	-	X	-	-
5	JN7	A	18	-	-	X	-

2 Entry composition [i](#)

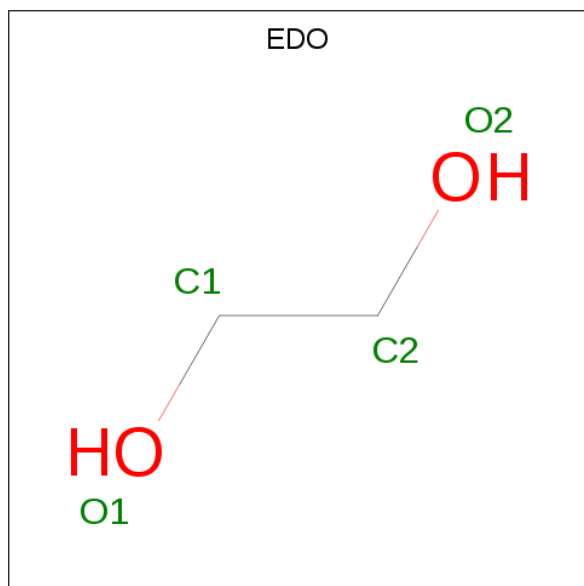
There are 8 unique types of molecules in this entry. The entry contains 11046 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	1	0
			2653	1679	453	507	14			
1	B	324	Total	C	N	O	S	0	1	0
			2628	1663	448	503	14			
1	C	324	Total	C	N	O	S	0	0	0
			2623	1657	448	504	14			
1	D	324	Total	C	N	O	S	0	0	0
			2622	1659	448	501	14			

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

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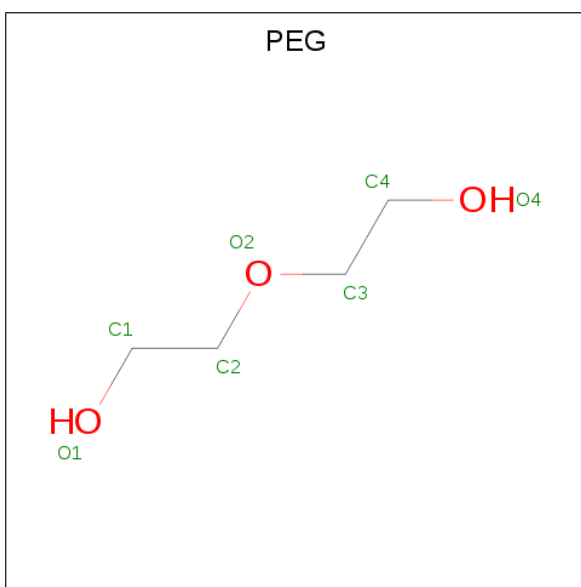
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

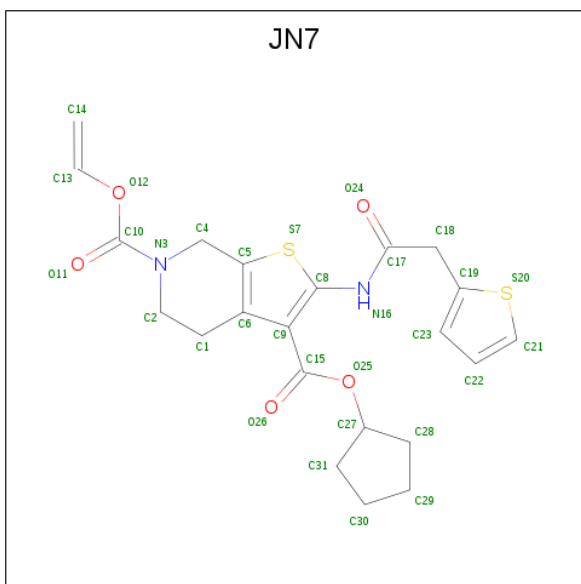
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Zn	0	0
			2	2		
3	A	2	Total	Zn	0	0
			2	2		
3	D	2	Total	Zn	0	0
			2	2		
3	C	2	Total	Zn	0	0
			2	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 5 is 3-cyclopentyl 6-ethenyl 2-[(thiophen-2-ylacetyl)amino]-4,7-dihydrothieno[2,3-c]pyridine-3,6(5H)-dicarboxylate (three-letter code: JN7) (formula: C₂₂H₂₄N₂O₅S₂).



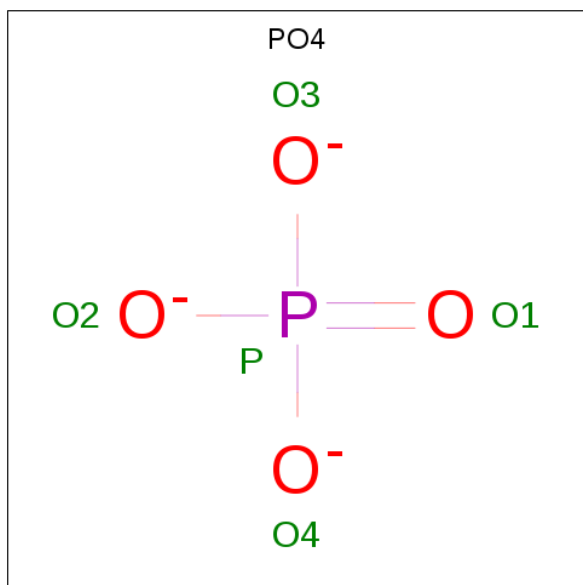
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			31	22	2	5	2		

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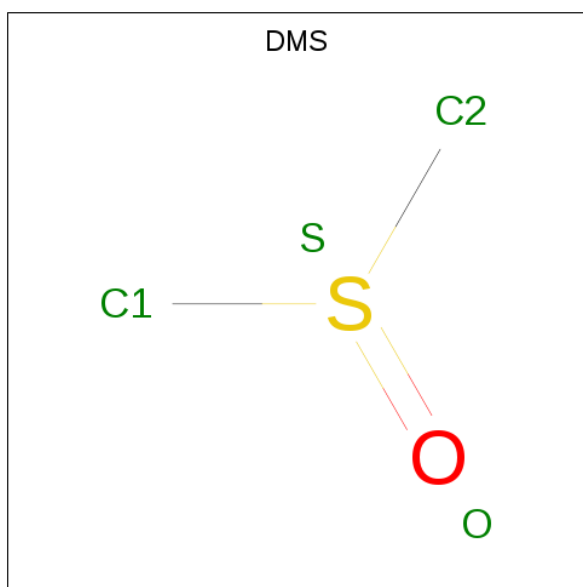
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			31	22	2	5	2		
5	C	1	Total	C	N	O	S	0	0
			31	22	2	5	2		
5	D	1	Total	C	N	O	S	0	0
			31	22	2	5	2		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

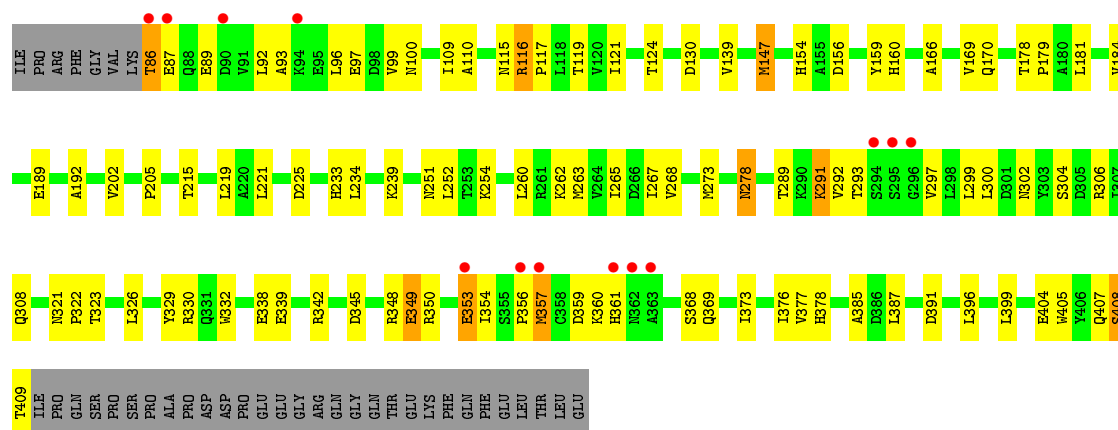
- Molecule 7 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



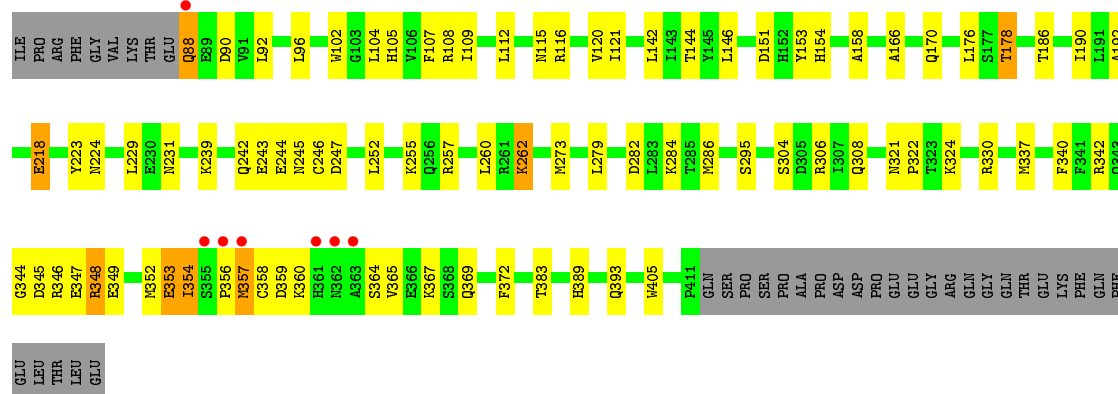
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	O	S	0	0
			4	2	1	1		
7	D	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	72	Total	O	0	0
			72	72		
8	B	46	Total	O	0	0
			46	46		
8	C	39	Total	O	0	0
			39	39		
8	D	79	Total	O	0	0
			79	79		



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.14Å 111.65Å 161.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.76 – 2.60 19.76 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.8 (19.76-2.60) 95.8 (19.76-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 2.59Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, R_{free}	0.196 , 0.273 0.189 , 0.265	Depositor DCC
R_{free} test set	2672 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 61.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11046	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, JN7, PO4, EDO, DMS, PEG

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	0.43	0/2709	0.59	0/3678
1	B	0.40	0/2685	0.55	0/3648
1	C	0.39	0/2676	0.55	0/3635
1	D	0.45	0/2676	0.59	0/3636
All	All	0.42	0/10746	0.57	0/14597

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	2653	0	2619	74	0
1	B	2628	0	2584	87	0
1	C	2623	0	2573	87	0
1	D	2622	0	2578	64	0
2	A	52	0	78	9	0
2	B	8	0	12	6	0
2	C	12	0	18	4	0
2	D	48	0	72	15	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	7	0	10	2	0
4	D	7	0	10	3	0
5	A	31	0	24	11	0
5	B	31	0	24	5	0
5	C	31	0	24	8	0
5	D	31	0	24	3	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
7	C	4	0	6	1	0
7	D	4	0	6	1	0
8	A	72	0	0	3	0
8	B	46	0	0	3	0
8	C	39	0	0	0	0
8	D	79	0	0	3	0
All	All	11046	0	10662	309	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 14.

All (309) 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:C:273:MET:HE2	5:C:1:JN7:H14	1.48	0.94
1:A:105:HIS:HD2	1:A:108:ARG:H	1.17	0.92
1:A:338:GLU:O	1:A:342:ARG:HG2	1.69	0.92
1:C:273:MET:CE	5:C:1:JN7:H14	2.03	0.87
1:B:137:ILE:HG21	1:B:142:LEU:HD13	1.56	0.85
1:B:352:MET:HG2	2:B:6:EDO:H12	1.61	0.81
5:A:18:JN7:H1A	5:A:18:JN7:H27	1.63	0.81
1:C:302:ASN:O	1:C:306:ARG:HG3	1.80	0.81
1:C:265:ILE:HD13	1:D:224:ASN:HB3	1.63	0.78
5:A:18:JN7:C1	5:A:18:JN7:H27	2.14	0.78
1:D:243:GLU:HB3	2:D:7:EDO:H22	1.67	0.77
1:A:105:HIS:CD2	1:A:108:ARG:H	2.03	0.75
1:B:355:SER:HB2	1:B:358:CYS:HB2	1.68	0.75
1:A:278:ASN:ND2	1:A:278:ASN:H	1.85	0.75
1:A:364:SER:HB3	1:A:367:LYS:HD2	1.68	0.75
1:B:178:THR:HG22	1:B:181:LEU:HD12	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ASN:HD22	1:A:278:ASN:H	1.34	0.72
1:D:345:ASP:O	1:D:349:GLU:HB2	1.89	0.72
1:D:369:GLN:OE1	5:D:1:JN7:H22	1.89	0.72
1:A:403:ARG:NH1	1:A:407:GLN:HG3	2.05	0.72
1:D:282:ASP:HB3	1:D:308:GLN:NE2	2.06	0.71
1:D:273:MET:HG3	5:D:1:JN7:H4A	1.70	0.71
1:A:147:MET:SD	1:C:349:GLU:HB3	2.31	0.70
1:C:353:GLU:H	1:C:353:GLU:CD	1.92	0.70
1:A:366:GLU:HG2	1:A:409:THR:CG2	2.21	0.70
1:C:321:ASN:HB2	1:C:322:PRO:HD3	1.73	0.70
1:B:372:PHE:HE2	5:B:1:JN7:H23	1.57	0.70
1:B:389:HIS:CD2	1:B:390:PRO:HA	2.26	0.70
1:A:121:ILE:HD12	1:A:166:ALA:HB1	1.74	0.69
1:A:178:THR:HG22	1:A:181:LEU:HD12	1.75	0.69
1:A:192:ALA:HB2	1:A:260:LEU:HD12	1.74	0.69
1:B:369:GLN:OE1	5:B:1:JN7:H22	1.93	0.68
1:B:253:THR:OG1	1:B:256:GLN:HG3	1.94	0.68
1:C:189:GLU:OE2	1:C:306:ARG:NH1	2.26	0.68
1:B:105:HIS:CE1	1:B:107:PHE:HB2	2.29	0.68
2:A:13:EDO:H22	1:C:350:ARG:HD3	1.75	0.67
1:A:225:ASP:CG	1:B:261:ARG:HH21	1.98	0.67
1:D:244:GLU:HB3	2:D:7:EDO:O1	1.95	0.67
1:C:192:ALA:HB2	1:C:260:LEU:HD12	1.78	0.66
2:A:13:EDO:C2	1:C:350:ARG:HD3	2.26	0.66
1:A:376:ILE:HD11	5:A:18:JN7:C13	2.25	0.66
1:C:181:LEU:O	1:C:184:VAL:HG23	1.97	0.65
1:B:182:GLU:O	1:B:297:VAL:HG21	1.96	0.65
1:D:96:LEU:HD11	1:D:120:VAL:CG1	2.27	0.64
1:A:409:THR:O	1:A:410:ILE:HG13	1.97	0.64
1:C:369:GLN:O	1:C:373:ILE:HG13	1.98	0.63
1:B:215:THR:HG22	2:D:7:EDO:H11	1.80	0.62
1:A:366:GLU:HG2	1:A:409:THR:HG21	1.80	0.62
1:D:246:CYS:SG	2:D:7:EDO:H21	2.40	0.62
1:B:178:THR:CG2	1:B:181:LEU:HD12	2.30	0.61
1:D:245:ASN:HA	2:D:13:EDO:H21	1.81	0.61
1:B:158:ALA:CB	2:B:8:EDO:H22	2.31	0.61
1:A:333:THR:HA	5:A:18:JN7:H22	1.81	0.61
5:A:18:JN7:C6	5:A:18:JN7:H27	2.31	0.61
1:D:356:PRO:O	1:D:357:MET:HB3	2.01	0.60
1:B:352:MET:CG	2:B:6:EDO:H12	2.31	0.60
1:B:141:THR:HG21	1:B:250:GLN:HE22	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:MET:O	1:C:267:ILE:HG13	2.02	0.59
1:C:376:ILE:HG12	5:C:1:JN7:H14A	1.84	0.59
1:B:355:SER:HB2	1:B:358:CYS:CB	2.32	0.59
1:C:262:LYS:NZ	2:C:3:EDO:H12	2.17	0.59
1:A:329:TYR:HE1	5:A:18:JN7:H21	1.67	0.59
1:C:262:LYS:HZ2	2:C:3:EDO:H12	1.68	0.59
1:C:110:ALA:HA	1:C:117:PRO:HG3	1.84	0.59
1:C:116:ARG:N	1:C:117:PRO:HD3	2.18	0.59
1:D:342:ARG:O	1:D:346:ARG:HG2	2.03	0.58
1:A:355:SER:HB2	1:A:358:CYS:HB2	1.86	0.58
1:A:364:SER:CB	1:A:367:LYS:HD2	2.33	0.57
1:C:93:ALA:O	1:C:97:GLU:HG3	2.03	0.57
1:A:218:GLU:HG3	1:C:239:LYS:HE2	1.86	0.57
1:C:99:VAL:HG12	1:C:100:ASN:OD1	2.04	0.57
1:C:323:THR:HG22	1:C:399:LEU:HD13	1.87	0.57
1:D:96:LEU:HD11	1:D:120:VAL:HG11	1.86	0.57
1:C:304:SER:O	1:C:308:GLN:HG3	2.03	0.57
1:D:344:GLY:HA3	1:D:358:CYS:O	2.04	0.57
1:C:369:GLN:OE1	5:C:1:JN7:H22	2.05	0.57
1:D:239:LYS:NZ	1:D:242:GLN:OE1	2.37	0.56
1:C:300:LEU:HB3	1:C:306:ARG:HG2	1.87	0.56
1:C:289:THR:O	1:C:289:THR:HG22	2.06	0.56
1:C:192:ALA:HB2	1:C:260:LEU:CD1	2.36	0.55
1:C:322:PRO:HB3	1:C:329:TYR:CZ	2.41	0.55
1:C:368:SER:HB3	5:C:1:JN7:H31	1.89	0.55
5:A:18:JN7:C27	5:A:18:JN7:H1A	2.36	0.55
1:A:409:THR:HG22	1:A:409:THR:O	2.07	0.55
1:B:125:ILE:O	1:B:128:GLU:HB3	2.07	0.55
1:A:234:LEU:HD21	1:A:268:VAL:HB	1.88	0.54
1:C:338:GLU:HG2	1:C:342:ARG:HD2	1.89	0.54
1:B:346:ARG:HD2	8:D:459:HOH:O	2.08	0.54
1:A:286:MET:HE1	1:A:305:ASP:HB3	1.89	0.54
1:B:366:GLU:HG2	1:B:409:THR:HG22	1.90	0.54
1:D:356:PRO:O	1:D:357:MET:CB	2.55	0.54
1:A:327:GLN:O	1:A:331:GLN:HG3	2.08	0.54
1:A:383:THR:O	1:A:386:ASP:HB2	2.08	0.54
1:B:367:LYS:HG3	1:B:410:ILE:HD13	1.88	0.54
1:B:323:THR:HG22	1:B:399:LEU:HB2	1.90	0.53
2:A:13:EDO:H12	1:C:215:THR:HB	1.91	0.53
1:C:251:ASN:O	2:C:440:EDO:H21	2.09	0.53
1:A:330:ARG:HD3	1:A:405:TRP:CH2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ASP:O	1:A:349:GLU:HG3	2.09	0.53
1:B:154:HIS:CD2	1:B:154:HIS:N	2.76	0.53
1:B:263:MET:O	1:B:267:ILE:HG13	2.09	0.52
1:C:154:HIS:HB3	1:C:156:ASP:OD1	2.09	0.52
1:A:138:PRO:HA	4:A:12:PEG:H41	1.92	0.52
1:D:245:ASN:ND2	2:D:13:EDO:O1	2.38	0.52
1:C:376:ILE:HG12	5:C:1:JN7:C14	2.40	0.52
1:B:116:ARG:NE	1:B:147:MET:SD	2.79	0.52
1:B:158:ALA:HB3	2:B:8:EDO:H22	1.91	0.52
1:B:145:TYR:CD2	1:B:145:TYR:C	2.83	0.52
1:D:347:GLU:HA	1:D:352:MET:HG3	1.91	0.52
1:D:262:LYS:HA	4:D:5:PEG:H12	1.91	0.52
1:B:247:ASP:O	1:B:249:PHE:N	2.43	0.51
1:D:337:MET:HG3	1:D:365:VAL:HG22	1.92	0.51
1:B:138:PRO:HG2	1:B:250:GLN:OE1	2.10	0.51
1:C:115:ASN:O	1:C:116:ARG:HD2	2.11	0.51
1:C:159:TYR:OH	5:C:1:JN7:H18	2.10	0.51
1:C:179:PRO:HD2	1:C:391:ASP:CG	2.31	0.51
1:C:356:PRO:O	1:C:357:MET:HB2	2.11	0.51
1:C:121:ILE:HD12	1:C:166:ALA:HB1	1.93	0.51
1:B:355:SER:HB2	1:B:358:CYS:SG	2.50	0.51
5:A:18:JN7:H1	5:A:18:JN7:H31A	1.93	0.51
1:D:192:ALA:HB2	1:D:260:LEU:HD12	1.92	0.51
1:B:239:LYS:NZ	1:D:218:GLU:HG3	2.26	0.51
1:A:101:LYS:NZ	8:A:468:HOH:O	2.43	0.50
1:B:123:HIS:CE1	1:B:127:GLN:HE21	2.29	0.50
1:B:372:PHE:CE2	5:B:1:JN7:H23	2.41	0.50
1:B:192:ALA:HB2	1:B:260:LEU:HD12	1.94	0.50
1:B:366:GLU:HG2	1:B:409:THR:CG2	2.42	0.50
1:B:132:LEU:HD22	1:B:139:VAL:HG13	1.94	0.50
1:C:99:VAL:HG21	1:C:124:THR:HG21	1.94	0.50
1:D:142:LEU:O	1:D:146:LEU:HG	2.12	0.50
1:C:86:THR:OG1	1:C:87:GLU:N	2.44	0.49
1:A:154:HIS:HB3	1:A:156:ASP:OD1	2.12	0.49
1:A:273:MET:HE2	5:A:18:JN7:O11	2.12	0.49
1:A:86:THR:HB	2:A:17:EDO:H21	1.93	0.49
1:B:105:HIS:HE1	1:B:107:PHE:HB2	1.76	0.49
1:B:354:ILE:N	1:B:354:ILE:HD12	2.27	0.49
1:C:373:ILE:HA	1:C:377:VAL:HB	1.94	0.49
1:D:284:LYS:HG2	2:D:12:EDO:H22	1.93	0.49
1:A:221:LEU:HD12	8:B:463:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:LEU:O	1:B:146:LEU:HG	2.13	0.49
1:C:234:LEU:HD21	1:C:268:VAL:HB	1.94	0.49
1:B:300:LEU:HB3	1:B:306:ARG:HG2	1.94	0.49
1:A:348:ARG:C	1:A:350:ARG:H	2.16	0.49
1:A:236:VAL:O	1:A:240:LEU:HG	2.13	0.49
1:D:102:TRP:CE2	1:D:324:LYS:HE2	2.48	0.49
1:A:354:ILE:HG21	1:A:359:ASP:OD2	2.13	0.49
1:C:345:ASP:OD1	1:C:348:ARG:NH2	2.47	0.48
1:B:143:ILE:O	1:B:147:MET:HG2	2.14	0.48
1:B:207:VAL:HA	1:B:343:GLN:OE1	2.13	0.48
1:D:151:ASP:O	2:D:9:EDO:H11	2.13	0.48
1:B:247:ASP:O	1:B:247:ASP:OD1	2.31	0.48
1:C:169:VAL:HG12	1:C:170:GLN:N	2.27	0.48
1:D:105:HIS:CE1	1:D:107:PHE:HB2	2.48	0.48
1:D:330:ARG:HD3	1:D:405:TRP:CZ3	2.48	0.48
1:A:184:VAL:HG22	1:A:297:VAL:HG13	1.95	0.48
1:D:247:ASP:H	2:D:13:EDO:C2	2.26	0.48
1:B:137:ILE:CG2	1:B:142:LEU:HD13	2.37	0.48
1:D:108:ARG:O	1:D:112:LEU:HG	2.14	0.48
1:D:186:THR:O	1:D:190:ILE:HG13	2.14	0.48
1:D:354:ILE:HG21	1:D:359:ASP:HB2	1.96	0.48
1:D:229:LEU:HA	1:D:229:LEU:HD23	1.70	0.48
1:D:154:HIS:N	1:D:154:HIS:CD2	2.82	0.47
1:B:291:LYS:HB2	1:B:299:LEU:HD12	1.95	0.47
1:B:129:ARG:HE	1:B:173:HIS:CE1	2.32	0.47
1:C:353:GLU:N	1:C:353:GLU:CD	2.65	0.47
1:C:184:VAL:CG1	1:C:300:LEU:HD12	2.44	0.47
1:D:389:HIS:HD2	8:D:62:HOH:O	1.97	0.47
1:B:104:LEU:HD12	8:B:14:HOH:O	2.15	0.47
1:D:96:LEU:HD23	1:D:109:ILE:HD12	1.96	0.47
1:B:359:ASP:O	1:B:363:ALA:HB2	2.15	0.47
1:D:262:LYS:NZ	4:D:5:PEG:O2	2.45	0.47
1:B:368:SER:HB3	5:B:1:JN7:H31	1.96	0.47
1:B:244:GLU:OE2	1:C:254:LYS:HE2	2.14	0.47
1:A:360:LYS:O	1:A:361:HIS:HB2	2.14	0.47
1:D:176:LEU:HD13	1:D:190:ILE:HG23	1.97	0.47
1:D:245:ASN:CA	2:D:13:EDO:H21	2.45	0.47
1:A:86:THR:HG23	1:A:89:GLU:OE1	2.15	0.46
1:A:201:ASP:O	1:A:204:HIS:HB2	2.16	0.46
1:C:116:ARG:HG2	1:C:147:MET:HE1	1.95	0.46
1:B:132:LEU:HD23	1:B:137:ILE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:ASN:HD22	1:C:304:SER:HB3	1.80	0.46
1:B:376:ILE:HG13	5:B:1:JN7:H13	1.96	0.46
1:B:223:TYR:CE1	1:B:231:ASN:HB3	2.50	0.46
1:B:110:ALA:HA	1:B:117:PRO:HD3	1.97	0.46
1:C:86:THR:HG23	1:C:89:GLU:HG3	1.98	0.46
1:B:108:ARG:NH1	1:B:112:LEU:HD21	2.31	0.46
1:C:116:ARG:CG	1:C:147:MET:HE1	2.45	0.46
1:C:354:ILE:HD11	1:C:359:ASP:HA	1.98	0.46
1:A:117:PRO:HD2	1:A:150:GLU:OE2	2.15	0.45
1:B:189:GLU:HG2	1:B:263:MET:SD	2.55	0.45
1:B:298:LEU:HD23	1:B:298:LEU:HA	1.74	0.45
1:B:158:ALA:HB2	2:B:8:EDO:H22	1.97	0.45
1:B:94:LYS:O	1:B:97:GLU:HG3	2.17	0.45
1:D:88:GLN:CB	1:D:90:ASP:OD1	2.63	0.45
1:B:130:ASP:OD2	1:B:133:LYS:HB3	2.16	0.45
1:B:329:TYR:CE2	1:B:406:TYR:CE2	3.05	0.45
1:D:372:PHE:HE2	5:D:1:JN7:H23	1.80	0.45
1:B:145:TYR:CE1	1:B:241:LEU:HD23	2.51	0.45
1:B:338:GLU:O	1:B:342:ARG:HG2	2.16	0.45
2:A:13:EDO:H12	1:C:215:THR:CB	2.47	0.45
1:C:160:HIS:ND1	1:C:339:GLU:OE2	2.43	0.45
1:D:383:THR:HG23	2:D:12:EDO:H11	1.97	0.45
1:C:385:ALA:C	1:C:387:LEU:H	2.19	0.45
1:A:278:ASN:ND2	1:A:278:ASN:N	2.57	0.45
1:B:116:ARG:HA	1:B:150:GLU:OE2	2.17	0.45
1:C:119:THR:OG1	1:C:147:MET:HE3	2.17	0.45
1:C:291:LYS:HB2	1:C:299:LEU:HB3	1.99	0.45
1:B:154:HIS:NE2	1:B:203:ASP:OD1	2.34	0.45
1:C:273:MET:HE1	5:C:1:JN7:H14	1.91	0.45
1:D:247:ASP:H	2:D:13:EDO:H22	1.81	0.45
1:B:396:LEU:O	1:B:400:GLU:OE2	2.35	0.45
1:C:184:VAL:HG11	1:C:300:LEU:HD12	1.99	0.45
1:A:133:LYS:O	1:A:136:LYS:HD2	2.18	0.44
1:A:254:LYS:HE3	1:A:258:GLN:CD	2.37	0.44
1:C:278:ASN:H	1:C:278:ASN:ND2	2.15	0.44
1:C:348:ARG:HH11	1:C:354:ILE:HD12	1.82	0.44
2:A:13:EDO:H21	1:C:350:ARG:HD3	1.99	0.44
1:C:181:LEU:C	1:C:184:VAL:HG23	2.37	0.44
1:C:326:LEU:HD21	1:C:405:TRP:CE2	2.52	0.44
1:D:306:ARG:NH2	8:D:47:HOH:O	2.49	0.44
1:D:96:LEU:CD2	1:D:109:ILE:HD12	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:ASP:N	1:C:156:ASP:OD1	2.45	0.44
1:A:403:ARG:HD3	1:A:403:ARG:C	2.37	0.44
1:D:252:LEU:HB2	1:D:257:ARG:HG3	2.00	0.44
1:A:179:PRO:HD2	1:A:391:ASP:CG	2.38	0.44
1:D:178:THR:OG1	2:D:4:EDO:H22	2.17	0.44
1:D:340:PHE:O	1:D:358:CYS:HB3	2.18	0.44
1:C:225:ASP:OD2	4:D:5:PEG:H11	2.17	0.44
1:A:296:GLY:O	1:A:297:VAL:HG23	2.17	0.44
1:C:262:LYS:HG3	2:C:3:EDO:H21	2.00	0.44
2:A:13:EDO:H21	1:C:350:ARG:HH11	1.83	0.44
1:B:279:LEU:HD22	1:B:312:ASN:ND2	2.33	0.44
1:C:360:LYS:HD2	1:C:361:HIS:CE1	2.53	0.43
1:D:304:SER:O	1:D:308:GLN:HG3	2.18	0.43
1:D:321:ASN:HB2	1:D:322:PRO:HD3	2.00	0.43
1:A:369:GLN:OE1	5:A:18:JN7:H21	2.18	0.43
1:A:389:HIS:HA	1:A:390:PRO:HA	1.62	0.43
1:A:108:ARG:NH2	1:A:112:LEU:HD21	2.34	0.43
1:A:136:LYS:HA	4:A:12:PEG:H12	1.99	0.43
1:A:245:ASN:ND2	8:A:445:HOH:O	2.50	0.43
1:B:338:GLU:HG2	2:B:8:EDO:H12	2.00	0.43
1:C:110:ALA:CA	1:C:117:PRO:HG3	2.49	0.43
1:A:324:LYS:NZ	8:A:53:HOH:O	2.40	0.43
1:B:299:LEU:HD13	1:B:299:LEU:O	2.17	0.43
1:C:360:LYS:HG3	1:C:361:HIS:ND1	2.33	0.43
1:B:355:SER:HB3	1:B:356:PRO:HD2	2.01	0.43
1:C:321:ASN:HD22	1:C:332:TRP:HB3	1.83	0.43
1:B:305:ASP:HA	1:B:308:GLN:HE21	1.84	0.43
1:B:324:LYS:HB3	1:B:325:PRO:HD2	2.00	0.43
1:A:324:LYS:HA	1:A:324:LYS:HD2	1.86	0.43
1:A:223:TYR:CE1	1:A:231:ASN:HB3	2.54	0.42
1:A:105:HIS:HD2	1:A:108:ARG:N	2.00	0.42
1:B:116:ARG:HD3	1:B:150:GLU:OE1	2.18	0.42
1:C:329:TYR:OH	1:C:373:ILE:HD11	2.19	0.42
1:D:353:GLU:O	1:D:354:ILE:C	2.57	0.42
1:C:326:LEU:HD21	1:C:405:TRP:CD2	2.53	0.42
1:A:355:SER:HB2	1:A:358:CYS:SG	2.60	0.42
1:C:348:ARG:HH22	1:C:360:LYS:HE3	1.84	0.42
1:C:407:GLN:O	1:C:409:THR:N	2.46	0.42
1:D:104:LEU:HD22	1:D:170:GLN:HG3	2.01	0.42
1:C:265:ILE:HD13	1:D:224:ASN:CB	2.40	0.42
1:A:293:THR:O	1:A:294:SER:O	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:LEU:HD22	1:A:312:ASN:ND2	2.35	0.42
1:D:348:ARG:HG3	1:D:354:ILE:HD11	2.02	0.42
1:A:116:ARG:O	1:A:120:VAL:HG22	2.19	0.42
1:B:247:ASP:C	1:B:249:PHE:H	2.23	0.42
1:D:223:TYR:CE1	1:D:231:ASN:HB3	2.54	0.42
1:A:159:TYR:OH	5:A:18:JN7:H18	2.20	0.41
1:A:243:GLU:OE1	2:A:440:EDO:H11	2.20	0.41
1:A:378:HIS:N	1:A:379:PRO:CD	2.83	0.41
1:B:254:LYS:HB2	1:B:254:LYS:HE3	1.77	0.41
1:B:261:ARG:NH1	8:B:463:HOH:O	2.51	0.41
1:C:96:LEU:HD23	1:C:109:ILE:HD13	2.02	0.41
1:B:350:ARG:NH1	2:D:7:EDO:O2	2.53	0.41
1:A:376:ILE:O	1:A:379:PRO:HD2	2.21	0.41
1:D:158:ALA:H	1:D:342:ARG:HH12	1.69	0.41
1:C:254:LYS:NZ	1:C:254:LYS:HB2	2.35	0.41
1:A:376:ILE:C	1:A:379:PRO:HD2	2.41	0.41
1:B:135:PHE:O	1:B:136:LYS:HB2	2.21	0.41
1:A:225:ASP:OD1	1:B:261:ARG:NH2	2.51	0.41
1:B:250:GLN:HE21	1:B:250:GLN:HB3	1.60	0.41
1:B:409:THR:O	1:B:409:THR:HG22	2.20	0.41
1:C:116:ARG:NH1	7:C:7:DMS:H23	2.36	0.41
1:D:115:ASN:HD21	7:D:14:DMS:C1	2.34	0.41
1:D:279:LEU:HD23	1:D:279:LEU:HA	1.90	0.41
1:A:105:HIS:NE2	1:A:107:PHE:HB2	2.36	0.41
1:A:302:ASN:ND2	1:A:304:SER:HB2	2.36	0.41
1:A:350:ARG:C	1:A:352:MET:H	2.24	0.41
1:B:175:LEU:HA	1:B:175:LEU:HD23	1.81	0.41
1:B:378:HIS:HB3	1:B:379:PRO:HD3	2.02	0.41
1:D:144:THR:HG22	1:D:246:CYS:SG	2.61	0.41
1:C:404:GLU:OE2	1:C:404:GLU:HA	2.21	0.41
1:D:96:LEU:CD1	1:D:120:VAL:CG1	2.97	0.41
1:D:345:ASP:OD1	1:D:360:LYS:HE2	2.20	0.41
1:A:370:VAL:HG11	1:A:407:GLN:NE2	2.36	0.41
1:B:353:GLU:HA	1:B:353:GLU:OE2	2.20	0.41
1:C:202:VAL:O	1:C:233:HIS:ND1	2.51	0.41
1:B:116:ARG:N	1:B:117:PRO:CD	2.84	0.41
1:B:283:LEU:HG	1:B:383:THR:HG22	2.03	0.40
1:D:88:GLN:HB2	1:D:90:ASP:OD1	2.21	0.40
1:C:330:ARG:HD3	1:C:405:TRP:CH2	2.56	0.40
1:D:121:ILE:HD12	1:D:166:ALA:HB1	2.03	0.40
1:A:196:ALA:O	1:A:200:HIS:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:440:EDO:O1	1:C:350:ARG:NH1	2.42	0.40
1:A:239[B]:LYS:HE3	1:A:239[B]:LYS:HB2	1.85	0.40
1:A:347:GLU:CD	1:A:355:SER:HG	2.24	0.40
1:B:389:HIS:HA	1:B:390:PRO:HA	1.84	0.40
1:C:378:HIS:HA	1:C:399:LEU:HD21	2.03	0.40
1:D:153:TYR:O	2:D:9:EDO:H21	2.21	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%)	304 (93%)	19 (6%)	3 (1%)	17	35
1	B	323/361 (90%)	292 (90%)	27 (8%)	4 (1%)	13	27
1	C	322/361 (89%)	299 (93%)	20 (6%)	3 (1%)	17	35
1	D	322/361 (89%)	306 (95%)	14 (4%)	2 (1%)	25	47
All	All	1293/1444 (90%)	1201 (93%)	80 (6%)	12 (1%)	17	35

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	SER
1	A	349	GLU
1	B	248	ILE
1	D	357	MET
1	C	293	THR
1	B	252	LEU
1	B	293	THR
1	B	352	MET
1	C	408	SER

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Mol	Chain	Res	Type
1	C	349	GLU
1	D	354	ILE
1	A	356	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	300/329 (91%)	288 (96%)	12 (4%)	31	57
1	B	297/329 (90%)	283 (95%)	14 (5%)	26	50
1	C	296/329 (90%)	277 (94%)	19 (6%)	17	35
1	D	296/329 (90%)	282 (95%)	14 (5%)	26	50
All	All	1189/1316 (90%)	1130 (95%)	59 (5%)	24	47

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	VAL
1	A	92	LEU
1	A	108	ARG
1	A	116	ARG
1	A	130	ASP
1	A	219	LEU
1	A	278	ASN
1	A	286	MET
1	A	342	ARG
1	A	353	GLU
1	A	354	ILE
1	A	359	ASP
1	B	92	LEU
1	B	99	VAL
1	B	139	VAL
1	B	178	THR
1	B	187	ASP
1	B	221	LEU

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Mol	Chain	Res	Type
1	B	250	GLN
1	B	252	LEU
1	B	297	VAL
1	B	298	LEU
1	B	364	SER
1	B	396	LEU
1	B	400	GLU
1	B	412	GLN
1	C	86	THR
1	C	92	LEU
1	C	116	ARG
1	C	130	ASP
1	C	139	VAL
1	C	147	MET
1	C	178	THR
1	C	205	PRO
1	C	219	LEU
1	C	221	LEU
1	C	252	LEU
1	C	278	ASN
1	C	291	LYS
1	C	292	VAL
1	C	297	VAL
1	C	353	GLU
1	C	357	MET
1	C	396	LEU
1	C	408	SER
1	D	88	GLN
1	D	92	LEU
1	D	116	ARG
1	D	178	THR
1	D	218	GLU
1	D	255	LYS
1	D	262	LYS
1	D	286	MET
1	D	295	SER
1	D	348	ARG
1	D	353	GLU
1	D	364	SER
1	D	367	LYS
1	D	393	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	A	245	ASN
1	A	258	GLN
1	A	278	ASN
1	A	312	ASN
1	A	407	GLN
1	B	123	HIS
1	B	245	ASN
1	B	250	GLN
1	B	308	GLN
1	B	389	HIS
1	C	210	GLN
1	C	214	ASN
1	C	245	ASN
1	C	250	GLN
1	C	278	ASN
1	D	123	HIS
1	D	127	GLN
1	D	245	ASN
1	D	250	GLN
1	D	258	GLN
1	D	308	GLN
1	D	389	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 48 ligands modelled in this entry, 8 are monoatomic - leaving 40 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
4	PEG	A	12	-	6,6,6	0.58	0	5,5,5	1.53	1 (20%)
2	EDO	D	12	-	3,3,3	0.57	0	2,2,2	0.25	0
7	DMS	C	7	-	3,3,3	2.73	1 (33%)	3,3,3	0.83	0
2	EDO	C	2	-	3,3,3	0.62	0	2,2,2	0.09	0
2	EDO	A	11	-	3,3,3	0.41	0	2,2,2	0.47	0
2	EDO	A	1	-	3,3,3	0.52	0	2,2,2	0.28	0
2	EDO	A	17	-	3,3,3	0.54	0	2,2,2	0.16	0
2	EDO	D	7	-	3,3,3	0.44	0	2,2,2	0.43	0
6	PO4	C	6	-	4,4,4	0.94	0	6,6,6	0.73	0
2	EDO	C	440	-	3,3,3	0.45	0	2,2,2	0.40	0
7	DMS	D	14	-	3,3,3	2.72	1 (33%)	3,3,3	0.71	0
2	EDO	D	8	-	3,3,3	0.58	0	2,2,2	0.22	0
6	PO4	B	4	3	4,4,4	0.82	0	6,6,6	0.46	0
2	EDO	D	13	-	3,3,3	0.61	0	2,2,2	0.22	0
2	EDO	A	7	-	3,3,3	0.54	0	2,2,2	0.34	0
2	EDO	B	8	-	3,3,3	0.55	0	2,2,2	0.10	0
2	EDO	A	16	-	3,3,3	0.38	0	2,2,2	0.67	0
2	EDO	A	5	-	3,3,3	0.48	0	2,2,2	0.26	0
2	EDO	D	11	-	3,3,3	0.55	0	2,2,2	0.39	0
2	EDO	D	15	-	3,3,3	0.48	0	2,2,2	0.40	0
2	EDO	A	440	-	3,3,3	0.38	0	2,2,2	0.46	0
2	EDO	D	10	-	3,3,3	0.48	0	2,2,2	0.42	0
2	EDO	A	8	-	3,3,3	0.48	0	2,2,2	0.44	0
2	EDO	A	6	-	3,3,3	0.53	0	2,2,2	0.23	0
2	EDO	A	9	-	3,3,3	0.57	0	2,2,2	0.10	0
2	EDO	A	14	-	3,3,3	0.54	0	2,2,2	0.11	0
2	EDO	B	6	-	3,3,3	0.58	0	2,2,2	0.18	0
4	PEG	D	5	-	6,6,6	0.40	0	5,5,5	1.89	3 (60%)
2	EDO	C	3	-	3,3,3	0.49	0	2,2,2	0.34	0
5	JN7	D	1	-	32,34,34	4.62	17 (53%)	28,47,47	2.24	7 (25%)
5	JN7	A	18	-	32,34,34	4.72	16 (50%)	28,47,47	2.23	7 (25%)
2	EDO	D	9	-	3,3,3	0.57	0	2,2,2	0.18	0
2	EDO	D	3	-	3,3,3	0.61	0	2,2,2	0.15	0
2	EDO	A	13	-	3,3,3	0.51	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	D	441	-	3,3,3	0.56	0	2,2,2	0.12	0
5	JN7	C	1	-	32,34,34	4.63	16 (50%)	28,47,47	1.87	5 (17%)
2	EDO	D	2	-	3,3,3	0.53	0	2,2,2	0.26	0
2	EDO	A	15	-	3,3,3	0.54	0	2,2,2	0.25	0
5	JN7	B	1	-	32,34,34	4.58	15 (46%)	28,47,47	2.01	7 (25%)
2	EDO	D	4	-	3,3,3	0.43	0	2,2,2	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	A	12	-	-	2/4/4/4	-
2	EDO	D	12	-	-	1/1/1/1	-
2	EDO	C	2	-	-	1/1/1/1	-
2	EDO	A	11	-	-	1/1/1/1	-
2	EDO	A	1	-	-	0/1/1/1	-
2	EDO	A	17	-	-	0/1/1/1	-
2	EDO	D	7	-	-	1/1/1/1	-
2	EDO	C	440	-	-	1/1/1/1	-
2	EDO	D	8	-	-	1/1/1/1	-
2	EDO	D	13	-	-	0/1/1/1	-
2	EDO	A	7	-	-	1/1/1/1	-
2	EDO	B	8	-	-	0/1/1/1	-
2	EDO	A	16	-	-	0/1/1/1	-
2	EDO	A	5	-	-	0/1/1/1	-
2	EDO	D	11	-	-	0/1/1/1	-
2	EDO	A	8	-	-	0/1/1/1	-
2	EDO	A	440	-	-	1/1/1/1	-
2	EDO	D	10	-	-	1/1/1/1	-
2	EDO	D	15	-	-	1/1/1/1	-
2	EDO	A	6	-	-	0/1/1/1	-
2	EDO	A	9	-	-	0/1/1/1	-
2	EDO	A	14	-	-	0/1/1/1	-
2	EDO	B	6	-	-	0/1/1/1	-
4	PEG	D	5	-	-	3/4/4/4	-
2	EDO	C	3	-	-	1/1/1/1	-
5	JN7	D	1	-	-	7/18/39/39	0/4/4/4
5	JN7	A	18	-	-	6/18/39/39	0/4/4/4
2	EDO	D	9	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	D	3	-	-	1/1/1/1	-
2	EDO	A	13	-	-	1/1/1/1	-
2	EDO	D	441	-	-	0/1/1/1	-
5	JN7	C	1	-	-	5/18/39/39	0/4/4/4
2	EDO	D	2	-	-	1/1/1/1	-
2	EDO	A	15	-	-	1/1/1/1	-
5	JN7	B	1	-	-	5/18/39/39	0/4/4/4
2	EDO	D	4	-	-	0/1/1/1	-

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	18	JN7	C9-C6	17.21	1.71	1.39
5	D	1	JN7	C9-C6	16.69	1.70	1.39
5	C	1	JN7	C9-C6	16.41	1.69	1.39
5	B	1	JN7	C9-C6	16.27	1.69	1.39
5	A	18	JN7	C22-C23	7.90	1.65	1.39
5	B	1	JN7	C22-C23	7.70	1.64	1.39
5	D	1	JN7	C22-C23	7.63	1.64	1.39
5	C	1	JN7	C22-C23	7.53	1.63	1.39
5	C	1	JN7	O12-C10	-7.43	1.27	1.37
5	B	1	JN7	O12-C10	-7.27	1.27	1.37
5	A	18	JN7	O12-C10	-7.25	1.28	1.37
5	C	1	JN7	C5-S7	-7.14	1.60	1.74
5	A	18	JN7	C5-S7	-7.09	1.60	1.74
5	D	1	JN7	O12-C10	-6.94	1.28	1.37
5	C	1	JN7	C23-C19	6.92	1.55	1.37
5	A	18	JN7	C23-C19	6.87	1.55	1.37
5	B	1	JN7	C5-S7	-6.65	1.61	1.74
5	D	1	JN7	C23-C19	6.47	1.54	1.37
5	D	1	JN7	C5-S7	-6.40	1.62	1.74
5	B	1	JN7	C23-C19	6.38	1.54	1.37
5	B	1	JN7	C10-N3	6.28	1.45	1.35
5	A	18	JN7	C10-N3	6.26	1.45	1.35
5	A	18	JN7	C22-C21	6.24	1.54	1.34
5	C	1	JN7	C22-C21	6.12	1.53	1.34
5	B	1	JN7	C22-C21	6.11	1.53	1.34
5	D	1	JN7	C22-C21	5.94	1.53	1.34
5	D	1	JN7	C10-N3	5.94	1.45	1.35
5	C	1	JN7	C10-N3	5.50	1.44	1.35
5	D	1	JN7	C19-S20	-4.93	1.63	1.73
5	C	1	JN7	C19-S20	-4.80	1.63	1.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	7	DMS	O-S	4.56	1.81	1.50
7	D	14	DMS	O-S	4.54	1.80	1.50
5	B	1	JN7	C9-C8	4.40	1.50	1.41
5	A	18	JN7	C9-C8	4.34	1.50	1.41
5	B	1	JN7	C19-S20	-4.27	1.64	1.73
5	A	18	JN7	C17-N16	4.23	1.45	1.35
5	D	1	JN7	O11-C10	4.07	1.27	1.21
5	B	1	JN7	O25-C15	-4.06	1.26	1.34
5	D	1	JN7	C14-C13	4.06	1.51	1.30
5	A	18	JN7	O11-C10	4.02	1.27	1.21
5	D	1	JN7	O25-C15	-3.98	1.26	1.34
5	C	1	JN7	C9-C8	3.97	1.49	1.41
5	B	1	JN7	C14-C13	3.95	1.50	1.30
5	C	1	JN7	O25-C15	-3.94	1.26	1.34
5	C	1	JN7	C14-C13	3.93	1.50	1.30
5	B	1	JN7	O11-C10	3.92	1.27	1.21
5	A	18	JN7	C14-C13	3.89	1.50	1.30
5	A	18	JN7	C19-S20	-3.87	1.65	1.73
5	C	1	JN7	C17-N16	3.79	1.44	1.35
5	D	1	JN7	C17-N16	3.74	1.43	1.35
5	B	1	JN7	O25-C27	-3.69	1.37	1.46
5	B	1	JN7	C17-N16	3.66	1.43	1.35
5	C	1	JN7	O25-C27	-3.58	1.37	1.46
5	C	1	JN7	O11-C10	3.56	1.26	1.21
5	D	1	JN7	O25-C27	-3.53	1.37	1.46
5	D	1	JN7	C9-C8	3.50	1.48	1.41
5	A	18	JN7	O25-C15	-3.23	1.28	1.34
5	A	18	JN7	O25-C27	-2.96	1.39	1.46
5	D	1	JN7	C18-C19	-2.51	1.49	1.51
5	C	1	JN7	C8-S7	-2.36	1.68	1.72
5	C	1	JN7	C1-C6	2.29	1.55	1.51
5	A	18	JN7	C1-C6	2.28	1.55	1.51
5	D	1	JN7	C2-C1	2.26	1.56	1.51
5	D	1	JN7	C1-C6	2.24	1.55	1.51
5	A	18	JN7	C2-C1	2.11	1.55	1.51
5	B	1	JN7	C1-C6	2.04	1.54	1.51

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1	JN7	C22-C21-S20	-7.29	107.06	112.98
5	D	1	JN7	C22-C21-S20	-7.25	107.10	112.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1	JN7	C22-C21-S20	-5.88	108.21	112.98
5	A	18	JN7	C22-C21-S20	-5.34	108.64	112.98
5	D	1	JN7	C1-C2-N3	5.26	116.24	110.04
5	A	18	JN7	O25-C15-C9	5.05	126.19	113.33
5	A	18	JN7	O25-C15-O26	-4.68	115.89	123.53
5	A	18	JN7	C27-O25-C15	4.44	125.21	117.56
5	C	1	JN7	C27-O25-C15	4.30	124.96	117.56
5	D	1	JN7	O11-C10-N3	-3.51	118.46	124.32
5	B	1	JN7	O11-C10-N3	-3.42	118.59	124.32
5	D	1	JN7	O24-C17-N16	-3.25	117.70	123.63
5	B	1	JN7	C5-C4-N3	-3.18	109.39	112.72
5	C	1	JN7	O24-C17-N16	-2.90	118.34	123.63
5	C	1	JN7	O11-C10-N3	-2.88	119.50	124.32
5	A	18	JN7	C5-C4-N3	-2.67	109.93	112.72
5	B	1	JN7	C27-O25-C15	2.45	121.78	117.56
5	B	1	JN7	O25-C15-O26	-2.44	119.55	123.53
5	D	1	JN7	C27-O25-C15	2.38	121.66	117.56
4	D	5	PEG	O2-C2-C1	2.29	120.14	110.07
4	A	12	PEG	O2-C3-C4	2.22	119.84	110.07
4	D	5	PEG	C3-O2-C2	2.22	122.92	113.29
5	A	18	JN7	O11-C10-N3	-2.19	120.65	124.32
5	B	1	JN7	O12-C10-O11	-2.18	118.37	122.09
5	A	18	JN7	C1-C2-N3	2.18	112.61	110.04
5	C	1	JN7	C5-C4-N3	-2.12	110.50	112.72
4	D	5	PEG	O2-C3-C4	2.11	119.35	110.07
5	B	1	JN7	C6-C9-C15	-2.10	121.18	126.02
5	D	1	JN7	C8-N16-C17	-2.07	119.83	124.36
5	D	1	JN7	C2-C1-C6	2.03	114.97	111.63

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1	JN7	O11-C10-N3-C2
5	D	1	JN7	O12-C10-N3-C2
5	D	1	JN7	O11-C10-N3-C4
5	D	1	JN7	O12-C10-N3-C4
5	D	1	JN7	C31-C27-O25-C15
5	A	18	JN7	C9-C15-O25-C27
5	A	18	JN7	O26-C15-O25-C27
5	B	1	JN7	O12-C10-N3-C2
4	A	12	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
5	B	1	JN7	O11-C10-N3-C2
2	C	2	EDO	O1-C1-C2-O2
2	D	2	EDO	O1-C1-C2-O2
5	C	1	JN7	O24-C17-C18-C19
4	D	5	PEG	O1-C1-C2-O2
5	D	1	JN7	O26-C15-O25-C27
5	D	1	JN7	O24-C17-C18-C19
2	D	8	EDO	O1-C1-C2-O2
2	D	15	EDO	O1-C1-C2-O2
2	A	11	EDO	O1-C1-C2-O2
2	A	15	EDO	O1-C1-C2-O2
2	A	440	EDO	O1-C1-C2-O2
5	A	18	JN7	O11-C10-N3-C2
2	A	7	EDO	O1-C1-C2-O2
2	C	3	EDO	O1-C1-C2-O2
2	A	13	EDO	O1-C1-C2-O2
4	D	5	PEG	O2-C3-C4-O4
5	B	1	JN7	O24-C17-C18-C19
5	A	18	JN7	C28-C27-O25-C15
5	C	1	JN7	C31-C27-O25-C15
5	B	1	JN7	C28-C27-O25-C15
5	B	1	JN7	C31-C27-O25-C15
4	A	12	PEG	C1-C2-O2-C3
4	D	5	PEG	C4-C3-O2-C2
5	C	1	JN7	C28-C27-O25-C15
2	D	12	EDO	O1-C1-C2-O2
2	D	7	EDO	O1-C1-C2-O2
2	C	440	EDO	O1-C1-C2-O2
2	D	10	EDO	O1-C1-C2-O2
2	D	3	EDO	O1-C1-C2-O2
5	A	18	JN7	O24-C17-C18-C19
5	C	1	JN7	N16-C17-C18-C19
5	C	1	JN7	O25-C15-C9-C6
5	A	18	JN7	O24-C17-N16-C8

There are no ring outliers.

20 monomers are involved in 68 short contacts:

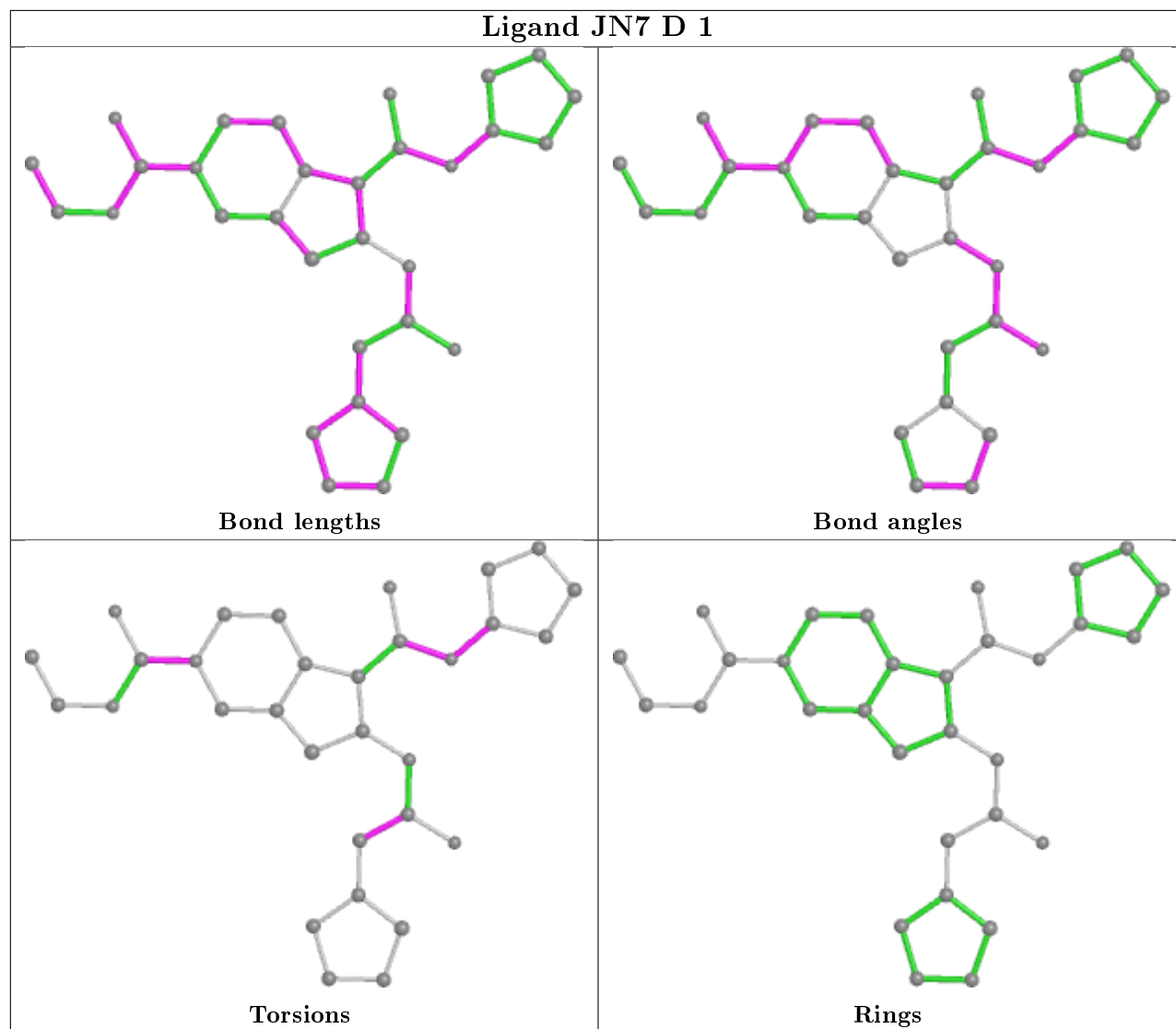
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	12	PEG	2	0
2	D	12	EDO	2	0
7	C	7	DMS	1	0

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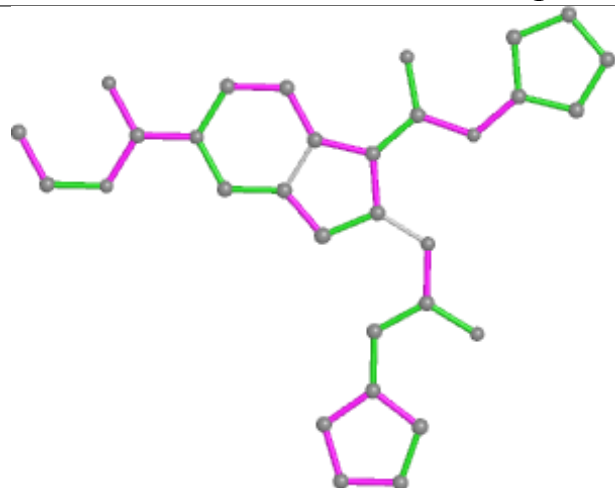
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	17	EDO	1	0
2	D	7	EDO	5	0
2	C	440	EDO	1	0
7	D	14	DMS	1	0
2	D	13	EDO	5	0
2	B	8	EDO	4	0
2	A	440	EDO	2	0
2	B	6	EDO	2	0
4	D	5	PEG	3	0
2	C	3	EDO	3	0
5	D	1	JN7	3	0
5	A	18	JN7	11	0
2	D	9	EDO	2	0
2	A	13	EDO	6	0
5	C	1	JN7	8	0
5	B	1	JN7	5	0
2	D	4	EDO	1	0

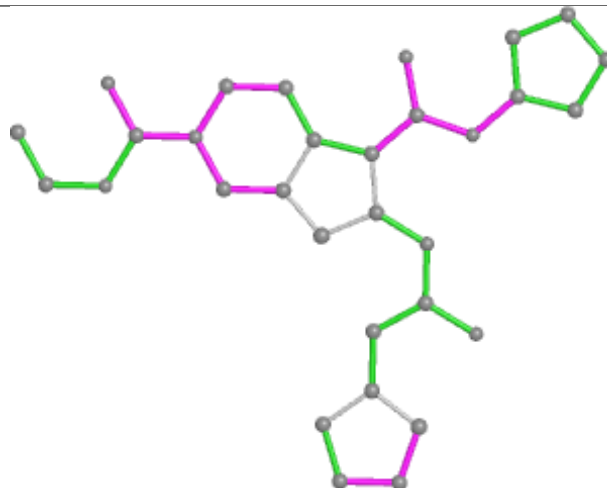
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



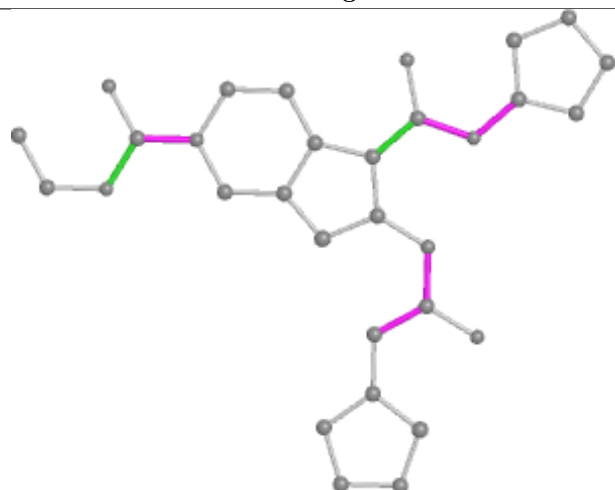
Ligand JN7 A 18



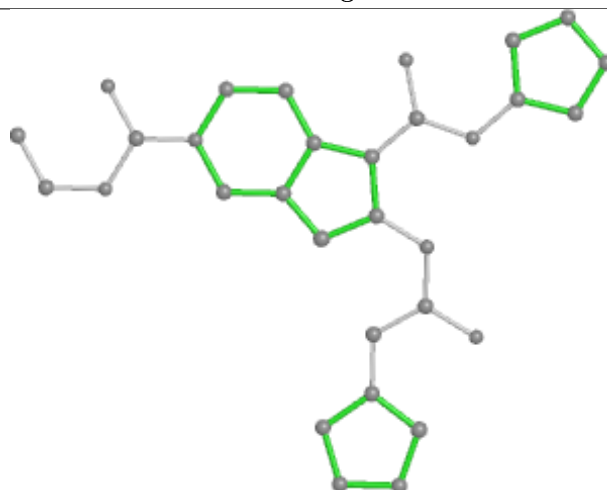
Bond lengths



Bond angles

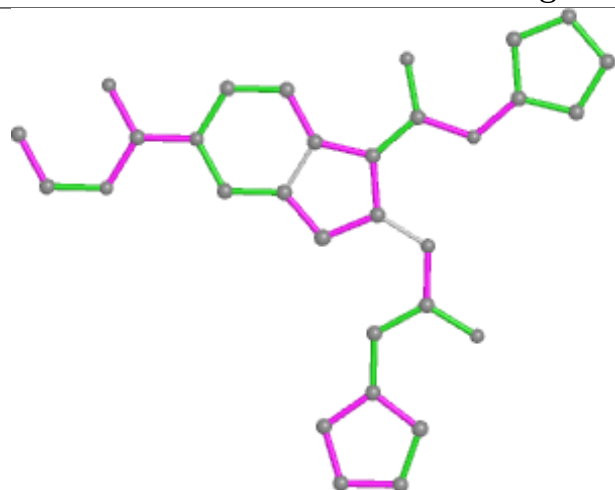


Torsions

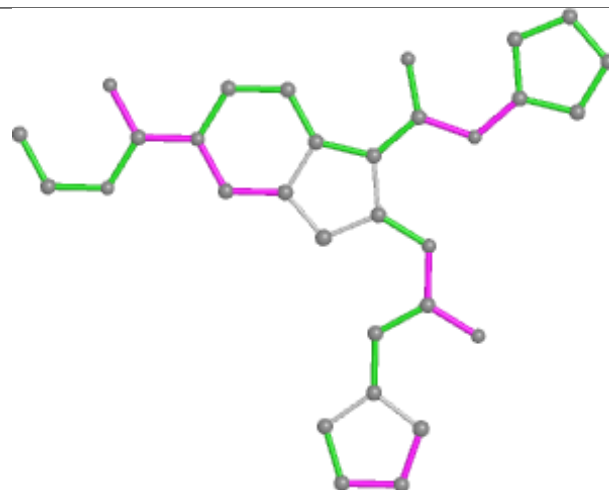


Rings

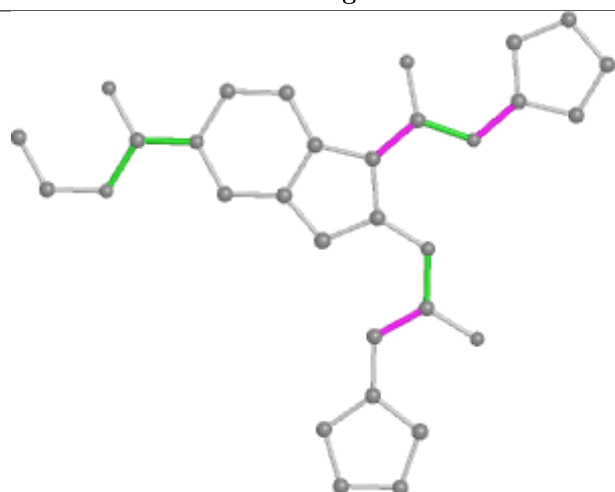
Ligand JN7 C 1



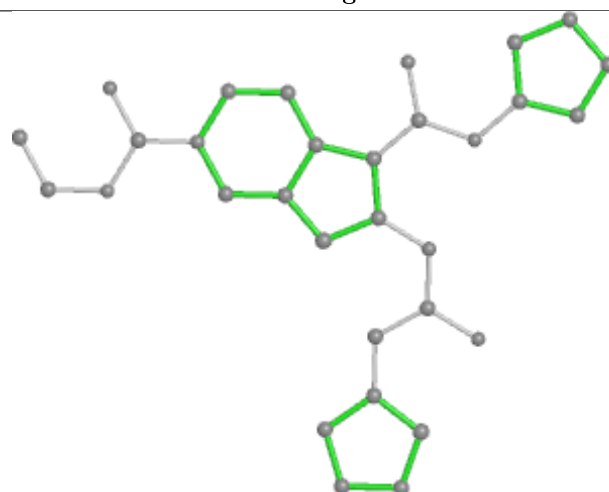
Bond lengths



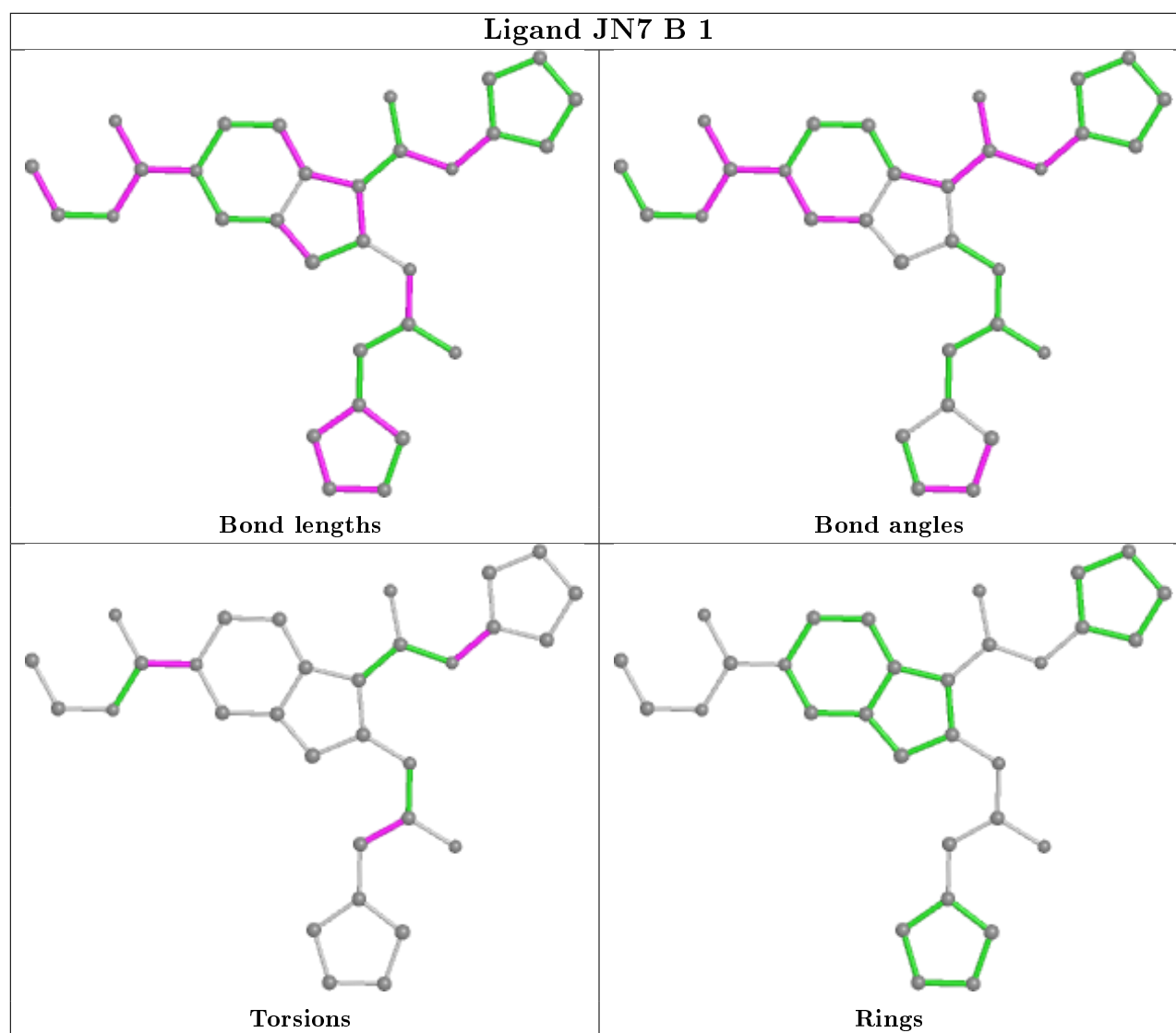
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	327/361 (90%)	-0.27	12 (3%) 41 34	21, 37, 74, 99	0
1	B	324/361 (89%)	-0.11	4 (1%) 79 76	24, 48, 67, 85	0
1	C	324/361 (89%)	-0.21	13 (4%) 38 31	26, 44, 72, 88	0
1	D	324/361 (89%)	-0.35	7 (2%) 62 56	21, 34, 62, 85	0
All	All	1299/1444 (89%)	-0.24	36 (2%) 53 46	21, 41, 69, 99	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	86	THR	4.4
1	D	362	ASN	4.4
1	C	353	GLU	4.2
1	C	356	PRO	3.9
1	C	362	ASN	3.9
1	A	357	MET	3.8
1	A	295	SER	3.8
1	B	90	ASP	3.7
1	C	295	SER	3.6
1	D	356	PRO	3.5
1	A	353	GLU	3.4
1	A	293	THR	3.4
1	C	361	HIS	3.3
1	A	294	SER	3.2
1	A	362	ASN	3.2
1	A	361	HIS	3.1
1	C	87	GLU	3.0
1	A	296	GLY	2.9
1	C	296	GLY	2.8
1	A	356	PRO	2.8
1	B	294	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	361	HIS	2.6
1	C	294	SER	2.6
1	C	357	MET	2.6
1	A	354	ILE	2.5
1	B	361	HIS	2.4
1	D	357	MET	2.4
1	A	410	ILE	2.3
1	C	363	ALA	2.3
1	D	88	GLN	2.2
1	C	94	LYS	2.2
1	A	359	ASP	2.1
1	B	322	PRO	2.0
1	D	363	ALA	2.0
1	C	90	ASP	2.0
1	D	355	SER	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 carbohydrates 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(\AA^2)	Q<0.9
2	EDO	A	15	4/4	0.80	0.29	47,47,48,56	0
4	PEG	D	5	7/7	0.83	0.29	36,39,47,48	0
2	EDO	D	12	4/4	0.84	0.28	48,51,54,55	0
5	JN7	A	18	31/31	0.84	0.29	47,66,86,91	0
2	EDO	D	2	4/4	0.85	0.24	38,42,50,54	0
5	JN7	B	1	31/31	0.87	0.21	38,52,61,66	0
2	EDO	B	6	4/4	0.88	0.35	39,40,41,49	0
7	DMS	C	7	4/4	0.88	0.26	43,45,51,64	0

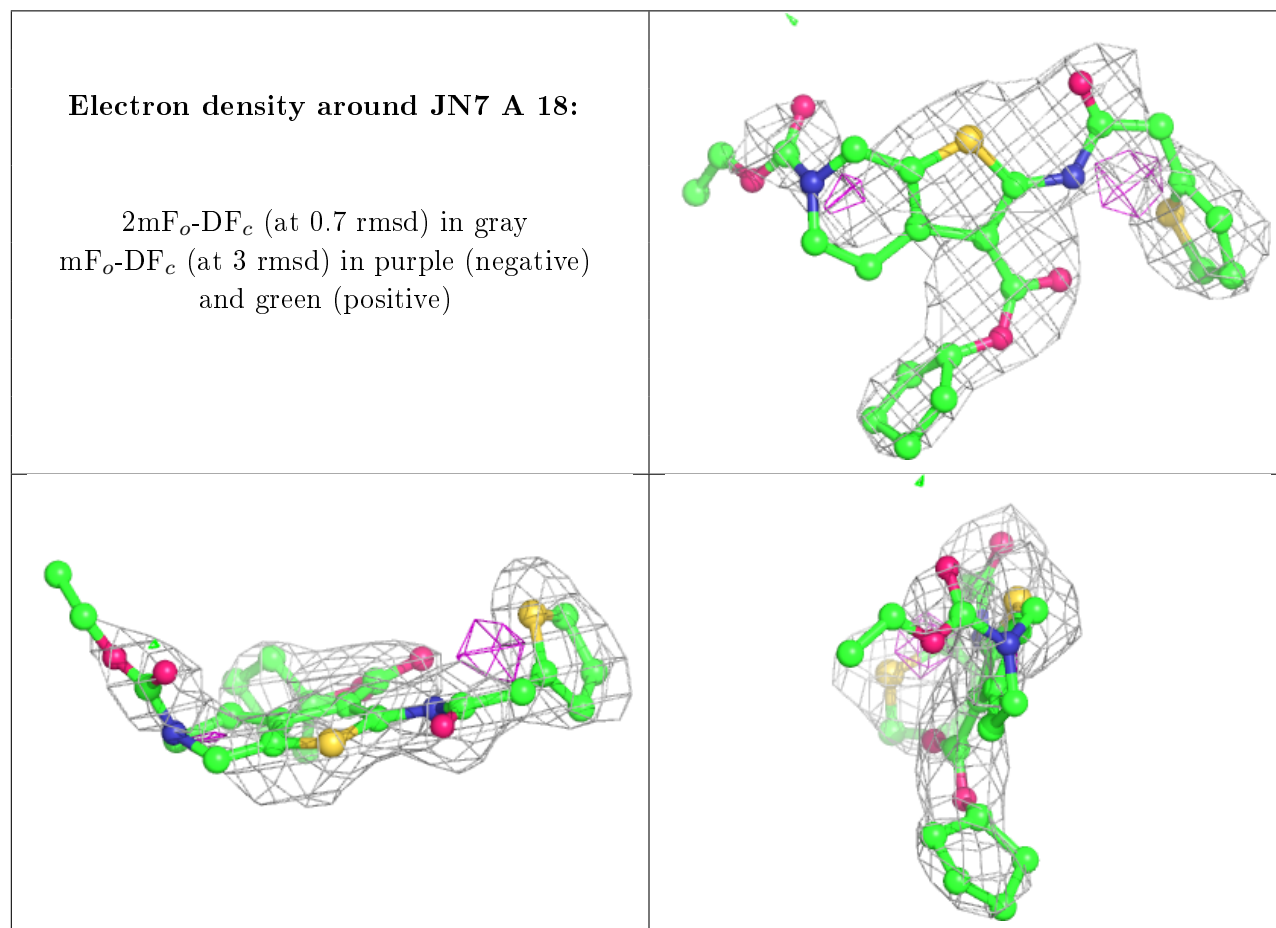
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	D	11	4/4	0.88	0.16	43,43,44,51	0
2	EDO	D	9	4/4	0.88	0.23	36,41,41,46	0
2	EDO	D	15	4/4	0.88	0.31	48,49,49,51	0
2	EDO	A	9	4/4	0.88	0.23	34,37,42,44	0
2	EDO	D	13	4/4	0.89	0.43	38,40,41,44	0
2	EDO	D	441	4/4	0.89	0.24	44,44,44,46	0
2	EDO	D	3	4/4	0.90	0.23	36,37,42,50	0
5	JN7	D	1	31/31	0.90	0.18	32,53,68,69	0
2	EDO	A	7	4/4	0.90	0.21	44,49,53,54	0
2	EDO	D	8	4/4	0.90	0.25	31,36,37,38	0
2	EDO	C	2	4/4	0.91	0.23	39,40,44,45	0
2	EDO	B	8	4/4	0.91	0.38	40,46,51,57	0
2	EDO	C	3	4/4	0.91	0.19	43,45,48,49	0
5	JN7	C	1	31/31	0.91	0.20	36,48,61,66	0
2	EDO	D	10	4/4	0.91	0.38	35,40,44,54	0
2	EDO	A	16	4/4	0.91	0.30	40,41,42,49	0
4	PEG	A	12	7/7	0.92	0.35	37,39,46,47	0
2	EDO	A	14	4/4	0.93	0.18	50,52,57,59	0
7	DMS	D	14	4/4	0.93	0.30	35,47,51,60	0
2	EDO	A	17	4/4	0.94	0.35	44,52,54,63	0
2	EDO	A	6	4/4	0.94	0.16	27,30,31,34	0
2	EDO	A	5	4/4	0.94	0.20	44,47,48,54	0
2	EDO	A	11	4/4	0.94	0.16	25,27,31,33	0
2	EDO	A	1	4/4	0.94	0.19	40,44,47,49	0
6	PO4	B	4	5/5	0.95	0.14	36,41,43,45	2
2	EDO	A	8	4/4	0.95	0.13	27,35,41,43	0
2	EDO	C	440	4/4	0.95	0.22	43,45,46,46	0
2	EDO	A	13	4/4	0.95	0.18	27,33,33,38	0
2	EDO	A	440	4/4	0.96	0.15	32,35,37,45	0
2	EDO	D	7	4/4	0.97	0.32	36,37,37,41	0
2	EDO	D	4	4/4	0.97	0.17	27,33,36,44	0
3	ZN	C	4	1/1	0.98	0.07	65,65,65,65	0
6	PO4	C	6	5/5	0.98	0.07	43,45,48,51	0
3	ZN	D	6	1/1	0.99	0.08	59,59,59,59	0
3	ZN	B	3	1/1	0.99	0.10	39,39,39,39	0
3	ZN	B	2	1/1	0.99	0.03	64,64,64,64	0
3	ZN	A	4	1/1	0.99	0.04	58,58,58,58	0
3	ZN	D	440	1/1	0.99	0.11	29,29,29,29	0
3	ZN	C	5	1/1	0.99	0.10	38,38,38,38	0
3	ZN	A	3	1/1	1.00	0.10	34,34,34,34	0

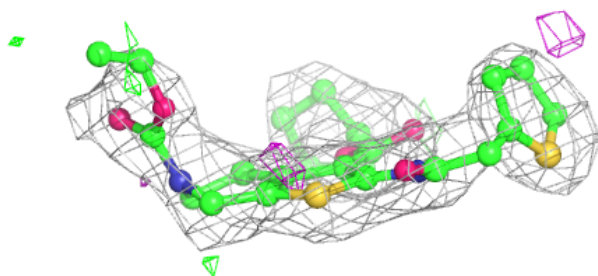
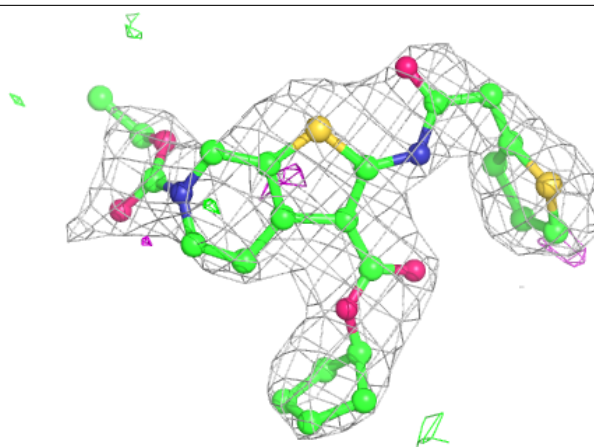
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

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

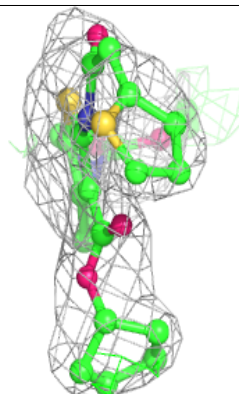
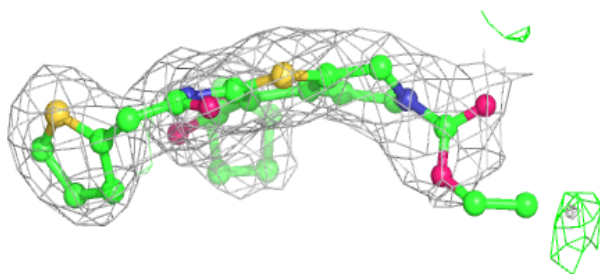
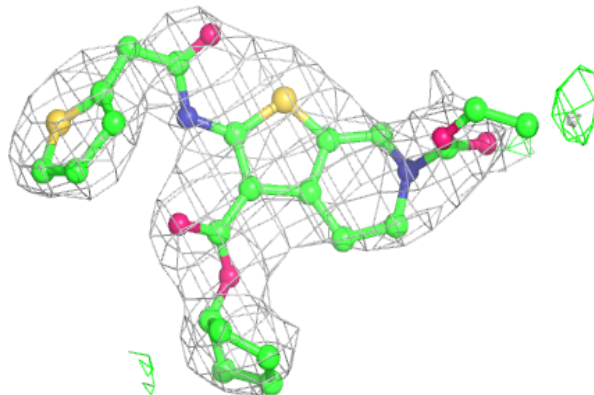


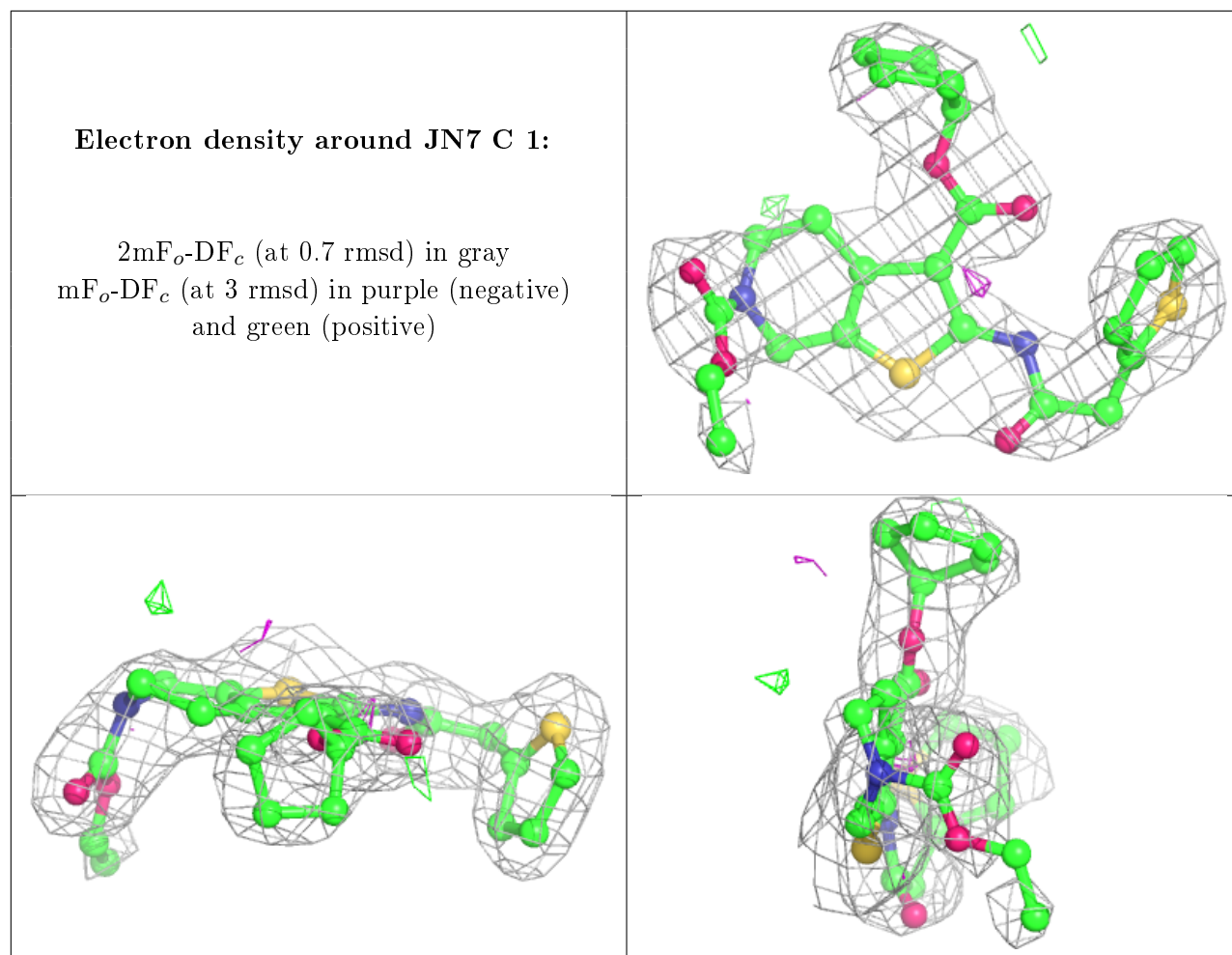
Electron density around JN7 B 1:

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

**Electron density around JN7 D 1:**

$2mF_o-DF_c$ (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.