Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 11:39 AM EDT

PDB ID	:	6IBF
Title	:	Crystal structure of human phosphodiesterase 4D2 catalytic domain with inhibitor NPD-417
Authors	:	Singh, A.K.; Brown, D.G.
Deposited on	:	2018-11-29
Resolution	:	2.31 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:

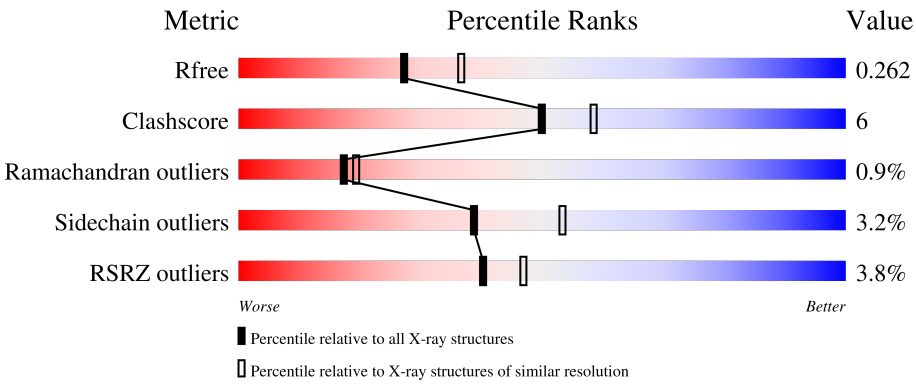
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.31 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	364	6%, 76%, 11%, •, 10%
1	B	364	%, 76%, 12%, •, 11%
1	C	364	5%, 74%, 13%, •, 11%
1	D	364	%, 78%, 11%, 11%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 11476 atoms, of which 6 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	329	2667	1686	456	511	14	0	1	0
1	B	324	2622	1659	448	501	14	0	0	0
1	C	323	2613	1654	446	499	14	0	0	0
1	D	324	2622	1659	448	501	14	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	75	GLY	-	expression tag	UNP Q08499
A	76	SER	-	expression tag	UNP Q08499
A	77	HIS	-	expression tag	UNP Q08499
A	78	MET	-	expression tag	UNP Q08499
B	75	GLY	-	expression tag	UNP Q08499
B	76	SER	-	expression tag	UNP Q08499
B	77	HIS	-	expression tag	UNP Q08499
B	78	MET	-	expression tag	UNP Q08499
C	75	GLY	-	expression tag	UNP Q08499
C	76	SER	-	expression tag	UNP Q08499
C	77	HIS	-	expression tag	UNP Q08499
C	78	MET	-	expression tag	UNP Q08499
D	75	GLY	-	expression tag	UNP Q08499
D	76	SER	-	expression tag	UNP Q08499
D	77	HIS	-	expression tag	UNP Q08499
D	78	MET	-	expression tag	UNP Q08499

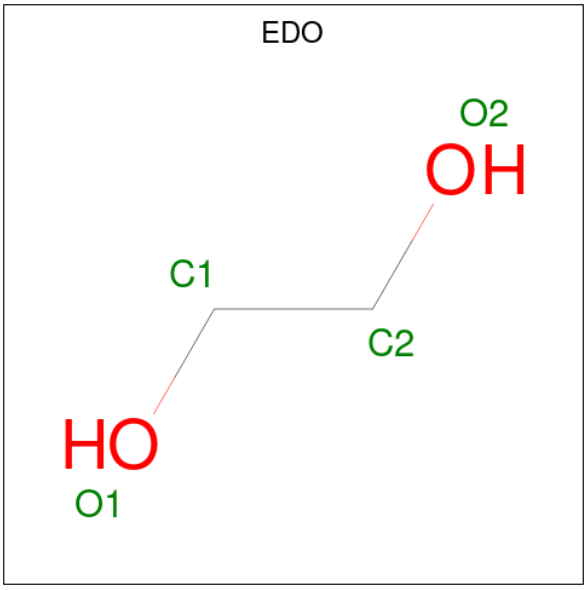
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

Continued on next page...

Continued from previous page...

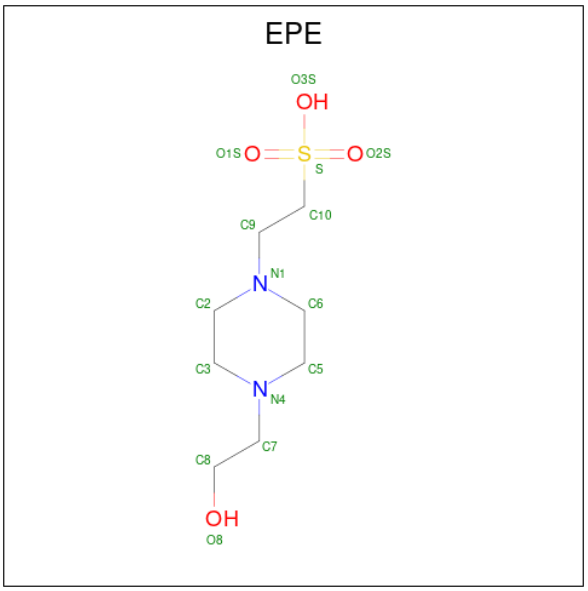
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0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

Continued on next page...

Continued from previous page...

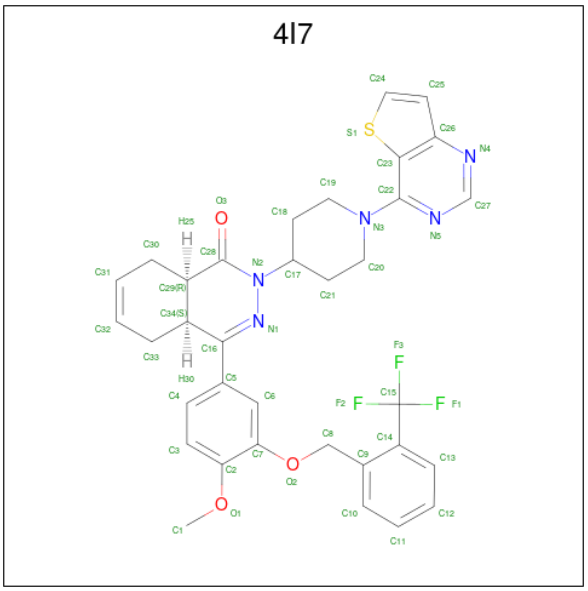
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C H O 10 2 6 2	0	0

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



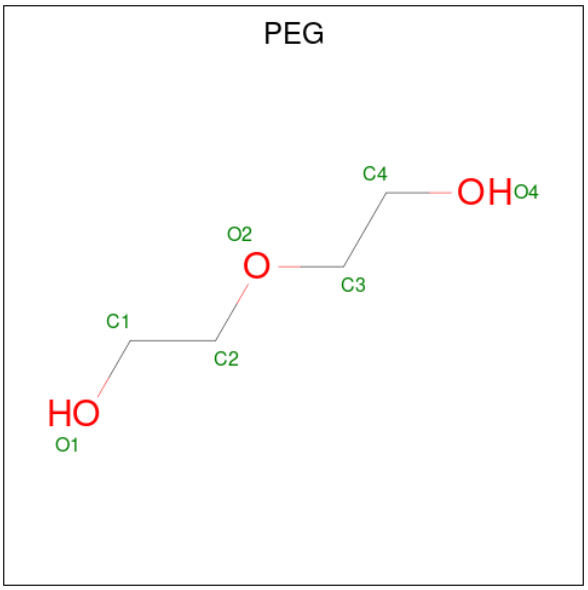
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	A	1	15	8	2	4	1	0	0
			Total	C	N	O	S		
5	B	1	15	8	2	4	1	0	0
			Total	C	N	O	S		
5	C	1	15	8	2	4	1	0	0
			Total	C	N	O	S		
5	D	1	15	8	2	4	1	0	0

- Molecule 6 is (4 {a} {S},8 {a} {R})-4-[4-methoxy-3-[[2-(trifluoromethyl)phenyl]methoxy]phenyl]-2-(1-thieno[3,2-d]pyrimidin-4-ylpiperidin-4-yl)-4 {a},5,8,8 {a}-tetrahydrophthalazin-1-one (three-letter code: 4I7) (formula: $C_{34}H_{32}F_3N_5O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	S		
6	A	1	46	34	3	5	3	1	0	0
			Total	C	F	N	O	S		
6	B	1	46	34	3	5	3	1	0	0
			Total	C	F	N	O	S		
6	C	1	46	34	3	5	3	1	0	0
			Total	C	F	N	O	S		
6	D	1	46	34	3	5	3	1	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 8 is water.

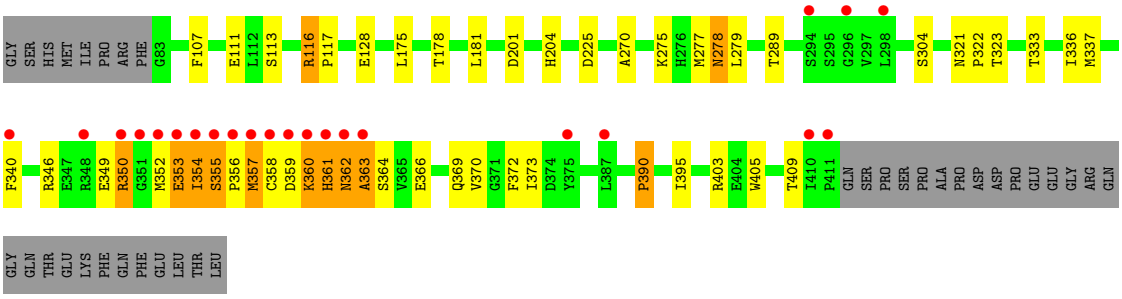
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	131	131	131	0	0
			Total	O		
8	B	118	118	118	0	0
			Total	O		
8	C	102	102	102	0	0
			Total	O		
8	D	177	177	177	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

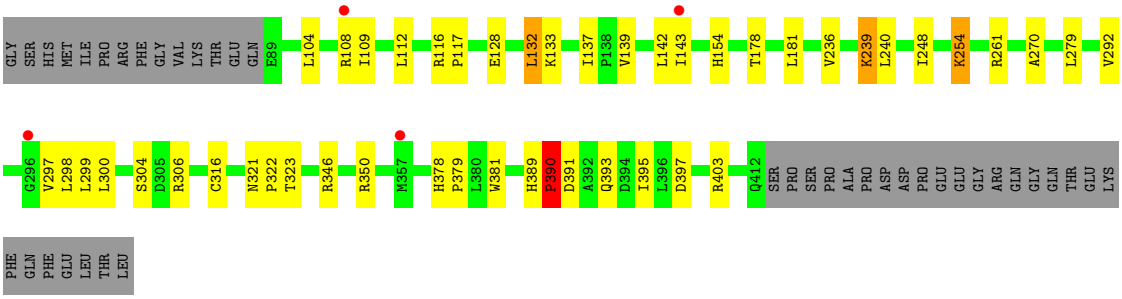
• Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain A:



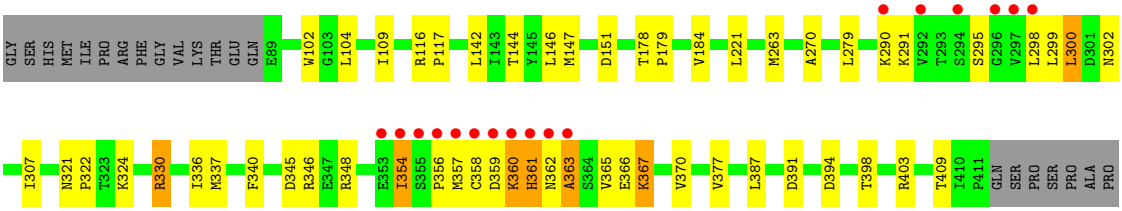
• Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain B:



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

Chain C:



ASP ASP PRO GLU GLU GLY ARG GLN GLY GLN THR GLU LYS PHE GLN PHE GLU LEU THR LEU

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

Chain D:

GLY SER HIS MET ILE PRO ARG PHE GLY VAL LYS THR GLU Q88 E89 L104 R108 I109 A110 E111 V168 V174 T178 P179 A192 A196 H200 Q210 N214 E218 E243 C246 F249 L260 A270 K275 L279 M286 S295

L298 Y303 S304 Q308 N321 P322 P325 L326 Q327 L328 D345 R348 I354 S355 P356 M357 N362 K367 H389 P390 E404 P411 GLN SER PRO SER PRO ALA PRO ASP ASP PRO GLU GLU GLY ARG GLN GLY GLN THR GLU LYS PHE GLN PHE GLU LEU THR

LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	98.48Å 110.51Å 160.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.11 – 2.31 80.15 – 2.31	Depositor EDS
% Data completeness (in resolution range)	97.4 (80.11-2.31) 97.4 (80.15-2.31)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.203 , 0.262 0.210 , 0.262	Depositor DCC
R_{free} test set	3778 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	33.6	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11476	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, EPE, 4I7, PEG, EDO, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.71	0/2721	0.80	1/3696 (0.0%)
1	B	0.70	0/2676	0.81	1/3636 (0.0%)
1	C	0.72	0/2667	0.79	0/3624
1	D	0.76	0/2676	0.79	0/3636
All	All	0.72	0/10740	0.80	2/14592 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	390	PRO	N-CA-CB	-6.12	95.87	102.60
1	A	390	PRO	N-CA-CB	-5.93	96.08	102.60

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	2667	0	2623	41	0
1	B	2622	0	2578	24	0
1	C	2613	0	2570	43	0
1	D	2622	0	2578	22	0
2	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	36	0	54	1	0
4	B	36	0	54	0	0
4	C	20	0	30	0	0
4	D	60	6	90	3	0
5	A	15	0	18	0	0
5	B	15	0	18	0	0
5	C	15	0	18	0	0
5	D	15	0	18	1	0
6	A	46	0	0	1	0
6	B	46	0	0	0	0
6	C	46	0	0	0	0
6	D	46	0	0	0	0
7	D	14	0	20	3	0
8	A	131	0	0	1	0
8	B	118	0	0	1	0
8	C	102	0	0	2	0
8	D	177	0	0	4	0
All	All	11470	6	10669	125	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 6.

All (125) 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:A:355:SER:HB2	1:A:356:PRO:HD2	1.28	1.13
1:A:355:SER:HB2	1:A:356:PRO:CD	1.92	0.98
1:A:353:GLU:O	1:A:354:ILE:O	1.97	0.83
1:C:360:LYS:O	1:C:362:ASN:N	2.15	0.79
1:C:184:VAL:CG1	1:C:300:LEU:HD12	2.16	0.75
1:A:360:LYS:C	1:A:362:ASN:H	1.89	0.74
1:A:360:LYS:O	1:A:362:ASN:N	2.16	0.74
1:C:354:ILE:HD12	1:C:354:ILE:H	1.52	0.74
1:A:356:PRO:O	1:A:358:CYS:N	2.21	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:PHE:HB3	1:C:358:CYS:SG	2.30	0.71
1:A:346:ARG:HD3	1:C:151:ASP:OD2	1.94	0.66
1:A:275:LYS:HE2	8:A:649:HOH:O	1.96	0.66
1:A:270:ALA:HB1	1:A:279:LEU:HD11	1.77	0.65
1:C:359:ASP:O	1:C:362:ASN:O	2.15	0.64
1:B:139:VAL:O	1:B:143:ILE:HG22	1.98	0.63
1:B:378:HIS:HB3	1:B:379:PRO:HD3	1.81	0.62
1:C:330:ARG:HG2	1:C:330:ARG:NH1	2.15	0.60
1:C:104:LEU:HD11	1:C:109:ILE:HD11	1.83	0.60
1:D:275:LYS:HE2	8:D:643:HOH:O	2.01	0.60
1:A:361:HIS:O	1:A:362:ASN:HB2	2.01	0.59
1:D:243:GLU:HB2	1:D:246:CYS:SG	2.43	0.59
1:C:345:ASP:OD1	1:C:348:ARG:NH2	2.37	0.58
1:D:174:VAL:HG12	7:D:511:PEG:H41	1.85	0.58
1:B:254:LYS:HZ2	1:B:254:LYS:HB3	1.70	0.57
1:D:111:GLU:OE2	5:D:516:EPE:H32	2.03	0.57
1:D:178:THR:OG1	7:D:511:PEG:H11	2.04	0.57
1:D:321:ASN:HB2	1:D:322:PRO:HD3	1.86	0.56
1:D:104:LEU:HD11	1:D:109:ILE:CD1	2.37	0.55
1:D:325:PRO:HD2	1:D:328:LEU:HD12	1.89	0.55
1:C:184:VAL:HG11	1:C:300:LEU:HD12	1.87	0.55
1:C:354:ILE:HG21	1:C:359:ASP:OD2	2.06	0.54
1:A:107:PHE:O	1:A:111:GLU:HG3	2.08	0.54
1:B:270:ALA:HB1	1:B:279:LEU:HD11	1.89	0.54
1:A:178:THR:HG22	1:A:181:LEU:HD12	1.90	0.53
1:C:362:ASN:O	1:C:363:ALA:CB	2.56	0.53
1:C:290:LYS:HG3	1:C:298:LEU:HD21	1.91	0.53
1:C:298:LEU:HD11	1:C:387:LEU:CD1	2.40	0.52
1:C:184:VAL:HG11	1:C:300:LEU:CD1	2.40	0.52
1:B:132:LEU:HA	1:B:137:ILE:HB	1.92	0.52
1:C:102:TRP:CE2	1:C:324:LYS:HE2	2.45	0.52
1:D:192:ALA:HB2	1:D:260:LEU:HD12	1.90	0.51
1:C:330:ARG:NH1	1:C:330:ARG:CG	2.73	0.51
1:D:179:PRO:HG2	7:D:512:PEG:H21	1.93	0.51
1:C:330:ARG:CG	1:C:330:ARG:HH11	2.23	0.51
1:A:116:ARG:N	1:A:117:PRO:CD	2.74	0.51
1:B:393:GLN:NE2	1:B:397:ASP:OD1	2.44	0.50
1:D:270:ALA:HB1	1:D:279:LEU:HD11	1.94	0.50
1:A:360:LYS:C	1:A:362:ASN:N	2.59	0.50
1:C:354:ILE:HD12	1:C:354:ILE:N	2.24	0.50
1:B:350:ARG:NH1	8:D:601:HOH:O	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:303:TYR:CD1	4:D:509:EDO:H22	2.46	0.50
1:D:286:MET:SD	1:D:308:GLN:NE2	2.85	0.50
1:A:333:THR:O	1:A:337:MET:HG2	2.10	0.49
1:A:225:ASP:OD1	1:B:261:ARG:NH2	2.41	0.49
1:A:359:ASP:OD2	1:A:361:HIS:ND1	2.46	0.49
1:A:340:PHE:HB3	1:A:358:CYS:SG	2.53	0.49
1:A:372:PHE:HB2	6:A:513:4I7:F2	2.03	0.49
1:B:236:VAL:O	1:B:240:LEU:HG	2.13	0.48
1:A:337:MET:HE3	1:A:337:MET:HA	1.95	0.48
1:C:142:LEU:O	1:C:146:LEU:HG	2.14	0.48
1:B:108:ARG:NH1	1:B:112:LEU:HD21	2.29	0.47
1:A:349:GLU:HG3	1:C:147:MET:HG2	1.96	0.47
1:D:218:GLU:OE2	4:D:521:EDO:H12	2.14	0.47
1:A:175:LEU:HD23	4:A:506:EDO:H21	1.96	0.47
1:A:333:THR:HA	1:A:336:ILE:HG22	1.95	0.47
1:A:350:ARG:CG	1:C:144:THR:HG23	2.45	0.46
1:A:353:GLU:C	1:A:354:ILE:O	2.53	0.46
1:B:323:THR:HB	1:B:395:ILE:HG23	1.96	0.46
1:A:353:GLU:O	1:A:354:ILE:C	2.53	0.46
1:A:359:ASP:O	1:A:363:ALA:HB3	2.17	0.45
1:B:292:VAL:HG12	1:B:298:LEU:HA	1.98	0.45
1:C:356:PRO:O	1:C:357:MET:HB2	2.16	0.45
1:A:354:ILE:C	1:A:354:ILE:HD12	2.36	0.45
1:B:104:LEU:HD11	1:B:109:ILE:HD11	1.99	0.45
1:A:350:ARG:HG3	1:C:144:THR:HG23	1.98	0.45
1:D:196:ALA:O	1:D:200:HIS:HB3	2.16	0.45
1:C:340:PHE:HB3	1:C:358:CYS:CB	2.46	0.44
1:B:142:LEU:HA	1:B:248:ILE:CG2	2.48	0.44
1:C:104:LEU:HD11	1:C:109:ILE:CD1	2.46	0.44
1:C:366:GLU:O	1:C:370:VAL:HG23	2.18	0.44
1:A:366:GLU:O	1:A:370:VAL:HG23	2.17	0.44
1:A:369:GLN:O	1:A:373:ILE:HG13	2.18	0.44
1:C:179:PRO:HD2	1:C:391:ASP:CG	2.37	0.44
1:C:337:MET:HG2	1:C:365:VAL:HG22	2.00	0.44
1:C:366:GLU:HG2	1:C:409:THR:CG2	2.47	0.44
1:D:303:TYR:CE1	4:D:509:EDO:H22	2.53	0.44
1:B:116:ARG:N	1:B:117:PRO:CD	2.81	0.44
1:B:346:ARG:O	1:B:350:ARG:HG3	2.17	0.44
1:B:297:VAL:HA	8:B:602:HOH:O	2.18	0.43
1:C:263:MET:HG2	1:C:307:ILE:HD13	1.99	0.43
1:A:178:THR:CG2	1:A:181:LEU:HD12	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:THR:HG22	1:A:289:THR:O	2.18	0.43
1:A:323:THR:HB	1:A:395:ILE:HG23	1.99	0.43
1:A:405:TRP:O	1:A:409:THR:HG23	2.18	0.43
1:C:321:ASN:HB2	1:C:322:PRO:HD3	2.00	0.43
1:B:154:HIS:HA	8:D:602:HOH:O	2.18	0.43
1:C:360:LYS:O	1:C:361:HIS:C	2.57	0.43
1:D:168:VAL:HG21	1:D:200:HIS:CE1	2.53	0.43
1:C:116:ARG:N	1:C:117:PRO:CD	2.82	0.43
1:C:367:LYS:HE2	1:C:367:LYS:HB2	1.77	0.43
1:D:249:PHE:CZ	1:D:260:LEU:HD21	2.53	0.42
1:C:337:MET:CE	8:C:631:HOH:O	2.67	0.42
1:D:345:ASP:OD1	1:D:348:ARG:NH2	2.52	0.42
1:B:178:THR:HG22	1:B:181:LEU:HD12	2.02	0.42
1:C:322:PRO:HG2	1:C:377:VAL:HG21	2.00	0.42
1:C:346:ARG:HD2	8:C:666:HOH:O	2.19	0.42
1:D:389:HIS:HA	1:D:390:PRO:HA	1.82	0.42
1:A:352:MET:O	1:A:353:GLU:CB	2.67	0.42
1:C:359:ASP:O	1:C:360:LYS:C	2.58	0.42
1:C:336:ILE:HG23	1:C:337:MET:HE2	2.02	0.41
1:A:321:ASN:HB2	1:A:322:PRO:HD3	2.01	0.41
1:A:201:ASP:O	1:A:204:HIS:HB2	2.20	0.41
1:A:277:MET:O	1:A:278:ASN:CB	2.68	0.41
1:B:321:ASN:HB2	1:B:322:PRO:HD3	2.03	0.41
1:C:270:ALA:HB1	1:C:279:LEU:HD11	2.02	0.41
1:A:362:ASN:O	1:A:363:ALA:O	2.37	0.41
1:B:239:LYS:HD3	1:B:239:LYS:HA	1.72	0.41
1:B:389:HIS:HA	1:B:390:PRO:HA	1.71	0.41
1:B:316:CYS:HB3	1:B:381:TRP:CZ2	2.56	0.41
1:D:243:GLU:OE1	8:D:601:HOH:O	2.21	0.41
1:C:394:ASP:O	1:C:398:THR:OG1	2.31	0.41
1:B:300:LEU:HB2	1:B:306:ARG:HG2	2.02	0.40
1:A:113:SER:O	1:A:116:ARG:HB2	2.22	0.40
1:C:298:LEU:HD11	1:C:387:LEU:HG	2.03	0.40
1:D:210:GLN:NE2	1:D:214:ASN:OD1	2.51	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	328/364 (90%)	304 (93%)	16 (5%)	8 (2%)	6 4
1	B	322/364 (88%)	311 (97%)	11 (3%)	0	100 100
1	C	321/364 (88%)	302 (94%)	15 (5%)	4 (1%)	13 13
1	D	322/364 (88%)	313 (97%)	9 (3%)	0	100 100
All	All	1293/1456 (89%)	1230 (95%)	51 (4%)	12 (1%)	17 19

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	ASN
1	A	354	ILE
1	A	357	MET
1	A	361	HIS
1	A	362	ASN
1	A	363	ALA
1	C	361	HIS
1	C	363	ALA
1	C	360	LYS
1	A	353	GLU
1	A	355	SER
1	C	302	ASN

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	301/331 (91%)	292 (97%)	9 (3%)	41	56
1	B	296/331 (89%)	286 (97%)	10 (3%)	37	51
1	C	295/331 (89%)	285 (97%)	10 (3%)	37	51
1	D	296/331 (89%)	287 (97%)	9 (3%)	41	56
All	All	1188/1324 (90%)	1150 (97%)	38 (3%)	39	53

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	ARG
1	A	128	GLU
1	A	304	SER
1	A	350	ARG
1	A	357	MET
1	A	360	LYS
1	A	364	SER
1	A	390	PRO
1	A	403	ARG
1	B	128	GLU
1	B	132	LEU
1	B	133	LYS
1	B	239	LYS
1	B	254	LYS
1	B	299	LEU
1	B	304	SER
1	B	390	PRO
1	B	391	ASP
1	B	403	ARG
1	C	178	THR
1	C	221	LEU
1	C	291	LYS
1	C	295	SER
1	C	299	LEU
1	C	300	LEU
1	C	330	ARG
1	C	354	ILE
1	C	367	LYS
1	C	403	ARG
1	D	89	GLU
1	D	108	ARG
1	D	295	SER
1	D	298	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	304	SER
1	D	327	GLN
1	D	357	MET
1	D	367	LYS
1	D	404	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 56 ligands modelled in this entry, 8 are monoatomic - leaving 48 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	EDO	C	503	-	3,3,3	0.16	0	2,2,2	0.27	0
4	EDO	D	518	-	3,3,3	0.07	0	2,2,2	0.05	0
4	EDO	B	512	-	3,3,3	0.38	0	2,2,2	0.34	0
4	EDO	D	514	-	3,3,3	0.44	0	2,2,2	0.55	0
4	EDO	B	511	-	3,3,3	0.57	0	2,2,2	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	EPE	A	510	-	15,15,15	1.94	1 (6%)	19,20,20	5.43	6 (31%)
4	EDO	D	504	-	3,3,3	0.27	0	2,2,2	0.31	0
4	EDO	D	507	-	3,3,3	0.07	0	2,2,2	0.18	0
4	EDO	B	506	-	3,3,3	0.28	0	2,2,2	0.50	0
4	EDO	D	513	-	3,3,3	0.25	0	2,2,2	0.29	0
4	EDO	A	504	-	3,3,3	0.22	0	2,2,2	0.14	0
4	EDO	A	511	-	3,3,3	0.14	0	2,2,2	0.09	0
4	EDO	C	504	-	3,3,3	0.22	0	2,2,2	0.36	0
5	EPE	C	505	-	15,15,15	2.11	1 (6%)	19,20,20	1.39	2 (10%)
4	EDO	A	509	-	3,3,3	0.19	0	2,2,2	0.03	0
4	EDO	D	510	-	3,3,3	0.34	0	2,2,2	0.23	0
4	EDO	D	521	-	3,3,3	0.34	0	2,2,2	0.21	0
4	EDO	A	507	-	3,3,3	0.05	0	2,2,2	0.18	0
6	4I7	A	513	-	50,52,52	0.63	1 (2%)	58,76,76	1.34	9 (15%)
4	EDO	A	512	-	3,3,3	0.19	0	2,2,2	0.39	0
4	EDO	B	504	-	3,3,3	0.13	0	2,2,2	0.12	0
4	EDO	B	505	-	3,3,3	0.02	0	2,2,2	0.07	0
4	EDO	A	506	-	3,3,3	0.04	0	2,2,2	0.15	0
4	EDO	A	508	-	3,3,3	0.18	0	2,2,2	0.22	0
4	EDO	C	506	-	3,3,3	0.22	0	2,2,2	0.06	0
4	EDO	D	509	-	3,3,3	0.19	0	2,2,2	0.08	0
4	EDO	D	517	-	3,3,3	0.08	0	2,2,2	0.09	0
6	4I7	B	513	-	50,52,52	0.65	1 (2%)	58,76,76	1.48	9 (15%)
4	EDO	D	519	-	3,3,3	0.31	0	2,2,2	0.32	0
4	EDO	B	507	-	3,3,3	0.25	0	2,2,2	0.47	0
5	EPE	B	510	-	15,15,15	1.88	1 (6%)	19,20,20	1.70	4 (21%)
4	EDO	B	503	-	3,3,3	0.04	0	2,2,2	0.06	0
4	EDO	C	507	-	3,3,3	0.23	0	2,2,2	0.23	0
6	4I7	C	508	-	50,52,52	0.62	1 (2%)	58,76,76	1.48	8 (13%)
4	EDO	D	503	-	3,3,3	0.15	0	2,2,2	0.09	0
4	EDO	D	505	-	3,3,3	0.20	0	2,2,2	0.28	0
5	EPE	D	516	-	15,15,15	1.75	1 (6%)	19,20,20	4.77	5 (26%)
7	PEG	D	511	-	6,6,6	0.44	0	5,5,5	0.46	0
4	EDO	B	508	-	3,3,3	0.16	0	2,2,2	0.09	0
6	4I7	D	520	-	50,52,52	0.65	0	58,76,76	1.04	6 (10%)
4	EDO	D	506	-	3,3,3	0.12	0	2,2,2	0.21	0
4	EDO	D	508	-	3,3,3	0.15	0	2,2,2	0.42	0
4	EDO	B	509	-	3,3,3	0.11	0	2,2,2	0.18	0
4	EDO	C	509	-	3,3,3	0.20	0	2,2,2	0.34	0
4	EDO	A	503	-	3,3,3	0.07	0	2,2,2	0.03	0
7	PEG	D	512	-	6,6,6	0.47	0	5,5,5	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	EDO	A	505	-	3,3,3	0.17	0	2,2,2	0.19	0
4	EDO	D	515	-	3,3,3	0.12	0	2,2,2	0.04	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	EDO	C	503	-	-	1/1/1/1	-
4	EDO	D	518	-	-	1/1/1/1	-
4	EDO	B	512	-	-	0/1/1/1	-
4	EDO	D	514	-	-	0/1/1/1	-
4	EDO	B	511	-	-	0/1/1/1	-
5	EPE	A	510	-	-	3/9/19/19	0/1/1/1
4	EDO	D	504	-	-	1/1/1/1	-
4	EDO	D	507	-	-	1/1/1/1	-
4	EDO	B	506	-	-	1/1/1/1	-
4	EDO	D	513	-	-	1/1/1/1	-
4	EDO	A	504	-	-	0/1/1/1	-
4	EDO	A	511	-	-	1/1/1/1	-
4	EDO	C	504	-	-	0/1/1/1	-
5	EPE	C	505	-	-	2/9/19/19	0/1/1/1
4	EDO	A	509	-	-	0/1/1/1	-
4	EDO	D	510	-	-	1/1/1/1	-
4	EDO	D	521	-	-	1/1/1/1	-
4	EDO	A	507	-	-	1/1/1/1	-
6	4I7	A	513	-	-	5/25/62/62	0/7/7/7
4	EDO	A	512	-	-	1/1/1/1	-
4	EDO	B	504	-	-	0/1/1/1	-
4	EDO	B	505	-	-	1/1/1/1	-
4	EDO	A	506	-	-	1/1/1/1	-
4	EDO	A	508	-	-	1/1/1/1	-
4	EDO	C	506	-	-	1/1/1/1	-
4	EDO	D	509	-	-	0/1/1/1	-
4	EDO	D	517	-	-	1/1/1/1	-
6	4I7	B	513	-	-	2/25/62/62	0/7/7/7
4	EDO	D	519	-	-	1/1/1/1	-
4	EDO	B	507	-	-	1/1/1/1	-
5	EPE	B	510	-	-	7/9/19/19	0/1/1/1
4	EDO	B	503	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	507	-	-	1/1/1/1	-
6	4I7	C	508	-	-	5/25/62/62	0/7/7/7
4	EDO	D	503	-	-	1/1/1/1	-
4	EDO	D	505	-	-	1/1/1/1	-
5	EPE	D	516	-	-	4/9/19/19	0/1/1/1
7	PEG	D	511	-	-	3/4/4/4	-
4	EDO	B	508	-	-	0/1/1/1	-
6	4I7	D	520	-	-	4/25/62/62	0/7/7/7
4	EDO	D	506	-	-	1/1/1/1	-
4	EDO	D	508	-	-	1/1/1/1	-
4	EDO	B	509	-	-	1/1/1/1	-
4	EDO	C	509	-	-	0/1/1/1	-
4	EDO	A	503	-	-	0/1/1/1	-
7	PEG	D	512	-	-	1/4/4/4	-
4	EDO	A	505	-	-	0/1/1/1	-
4	EDO	D	515	-	-	1/1/1/1	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	505	EPE	C10-S	-7.84	1.66	1.77
5	A	510	EPE	C10-S	-6.91	1.67	1.77
5	B	510	EPE	C10-S	-6.77	1.68	1.77
5	D	516	EPE	C10-S	-6.39	1.68	1.77
6	A	513	4I7	C17-N2	2.29	1.50	1.47
6	C	508	4I7	C22-N5	2.18	1.35	1.32
6	B	513	4I7	C17-N2	2.10	1.49	1.47

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	510	EPE	O2S-S-C10	-15.83	82.80	106.73
5	A	510	EPE	O1S-S-C10	-15.20	83.76	106.73
5	D	516	EPE	O2S-S-C10	-14.79	84.37	106.73
5	D	516	EPE	O3S-S-C10	-10.43	85.60	106.00
5	D	516	EPE	O1S-S-C10	-7.40	95.54	106.73
5	A	510	EPE	O3S-S-C10	-6.86	92.59	106.00
6	B	513	4I7	C18-C17-N2	5.05	116.42	110.89
6	C	508	4I7	C18-C17-N2	4.74	116.08	110.89
5	C	505	EPE	O3S-S-C10	4.41	114.64	106.00
6	C	508	4I7	C6-C5-C16	-4.38	114.80	120.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	513	4I7	C23-C22-N3	4.37	128.94	120.52
5	D	516	EPE	O3S-S-O2S	4.24	122.01	111.40
5	D	516	EPE	O3S-S-O1S	4.17	121.84	111.40
6	C	508	4I7	C4-C5-C16	4.09	125.63	120.74
5	B	510	EPE	O3S-S-C10	4.01	113.86	106.00
6	C	508	4I7	C23-C22-N3	3.87	127.97	120.52
6	B	513	4I7	C27-N5-C22	3.87	120.63	116.84
6	C	508	4I7	C27-N5-C22	3.54	120.31	116.84
6	A	513	4I7	C21-C17-N2	3.48	114.70	110.89
6	A	513	4I7	C23-C22-N3	3.42	127.11	120.52
6	A	513	4I7	C6-C5-C16	-3.37	116.06	120.24
6	B	513	4I7	C6-C5-C16	-3.36	116.06	120.24
6	D	520	4I7	C18-C17-N2	3.35	114.56	110.89
6	A	513	4I7	C4-C5-C16	3.33	124.73	120.74
6	B	513	4I7	C4-C5-C16	3.31	124.71	120.74
6	A	513	4I7	C27-N5-C22	3.21	119.98	116.84
6	A	513	4I7	C18-C17-N2	3.01	114.18	110.89
5	A	510	EPE	O2S-S-O1S	2.80	122.94	113.82
5	A	510	EPE	O3S-S-O1S	2.76	118.32	111.40
6	D	520	4I7	C27-N5-C22	2.75	119.54	116.84
6	B	513	4I7	C19-N3-C22	2.73	125.89	116.86
5	C	505	EPE	O3S-S-O1S	-2.65	104.77	111.40
6	D	520	4I7	C15-C14-C9	2.64	123.59	121.06
5	B	510	EPE	C6-N1-C2	2.58	114.39	108.84
6	A	513	4I7	C19-N3-C22	2.54	125.25	116.86
6	C	508	4I7	C19-N3-C22	2.52	125.19	116.86
6	D	520	4I7	C23-C22-N3	2.50	125.34	120.52
6	D	520	4I7	C19-N3-C22	2.48	125.07	116.86
5	B	510	EPE	C2-C3-N4	-2.45	105.71	110.65
6	D	520	4I7	C28-N2-N1	-2.45	122.13	125.13
5	A	510	EPE	O3S-S-O2S	2.43	117.47	111.40
6	A	513	4I7	C15-C14-C9	2.36	123.33	121.06
6	B	513	4I7	C25-C26-C23	2.32	112.32	110.62
6	B	513	4I7	C28-N2-N1	-2.27	122.35	125.13
5	B	510	EPE	C5-C6-N1	2.26	115.22	110.65
6	A	513	4I7	C25-C26-C23	2.21	112.23	110.62
6	C	508	4I7	C15-C14-C9	2.17	123.14	121.06
6	C	508	4I7	C20-N3-C19	2.14	116.38	111.57
6	B	513	4I7	C15-C14-C9	2.07	123.05	121.06

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	513	4I7	C23-C22-N3-C19
6	A	513	4I7	C21-C17-N2-N1
6	C	508	4I7	C23-C22-N3-C19
6	C	508	4I7	N5-C22-N3-C19
6	C	508	4I7	C21-C17-N2-N1
6	A	513	4I7	C21-C17-N2-C28
7	D	511	PEG	C4-C3-O2-C2
5	B	510	EPE	C9-C10-S-O3S
5	D	516	EPE	C9-C10-S-O3S
6	A	513	4I7	N5-C22-N3-C19
4	D	505	EDO	O1-C1-C2-O2
4	D	507	EDO	O1-C1-C2-O2
4	D	515	EDO	O1-C1-C2-O2
7	D	511	PEG	O2-C3-C4-O4
5	A	510	EPE	S-C10-C9-N1
5	B	510	EPE	S-C10-C9-N1
4	A	506	EDO	O1-C1-C2-O2
4	A	511	EDO	O1-C1-C2-O2
4	B	503	EDO	O1-C1-C2-O2
4	B	506	EDO	O1-C1-C2-O2
4	D	506	EDO	O1-C1-C2-O2
4	D	508	EDO	O1-C1-C2-O2
6	C	508	4I7	C21-C17-N2-C28
5	B	510	EPE	C10-C9-N1-C6
5	C	505	EPE	C10-C9-N1-C2
5	D	516	EPE	C8-C7-N4-C3
5	B	510	EPE	N4-C7-C8-O8
6	D	520	4I7	C9-C8-O2-C7
5	B	510	EPE	C9-C10-S-O1S
5	B	510	EPE	C9-C10-S-O2S
5	D	516	EPE	C9-C10-S-O1S
5	D	516	EPE	C9-C10-S-O2S
6	C	508	4I7	C9-C8-O2-C7
6	B	513	4I7	C9-C8-O2-C7
7	D	512	PEG	C1-C2-O2-C3
5	A	510	EPE	C10-C9-N1-C2
5	A	510	EPE	C10-C9-N1-C6
5	B	510	EPE	C10-C9-N1-C2
5	C	505	EPE	C10-C9-N1-C6
4	A	512	EDO	O1-C1-C2-O2
4	B	507	EDO	O1-C1-C2-O2
4	B	509	EDO	O1-C1-C2-O2
4	D	510	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	513	4I7	C9-C8-O2-C7
4	B	505	EDO	O1-C1-C2-O2
4	A	508	EDO	O1-C1-C2-O2
4	C	507	EDO	O1-C1-C2-O2
4	D	504	EDO	O1-C1-C2-O2
4	D	513	EDO	O1-C1-C2-O2
4	D	518	EDO	O1-C1-C2-O2
7	D	511	PEG	O1-C1-C2-O2
4	C	503	EDO	O1-C1-C2-O2
4	C	506	EDO	O1-C1-C2-O2
4	D	503	EDO	O1-C1-C2-O2
4	D	517	EDO	O1-C1-C2-O2
4	D	519	EDO	O1-C1-C2-O2
6	D	520	4I7	N5-C22-N3-C20
4	D	521	EDO	O1-C1-C2-O2
6	D	520	4I7	C18-C17-N2-C28
6	B	513	4I7	C23-C22-N3-C19
6	D	520	4I7	C23-C22-N3-C20
4	A	507	EDO	O1-C1-C2-O2

There are no ring outliers.

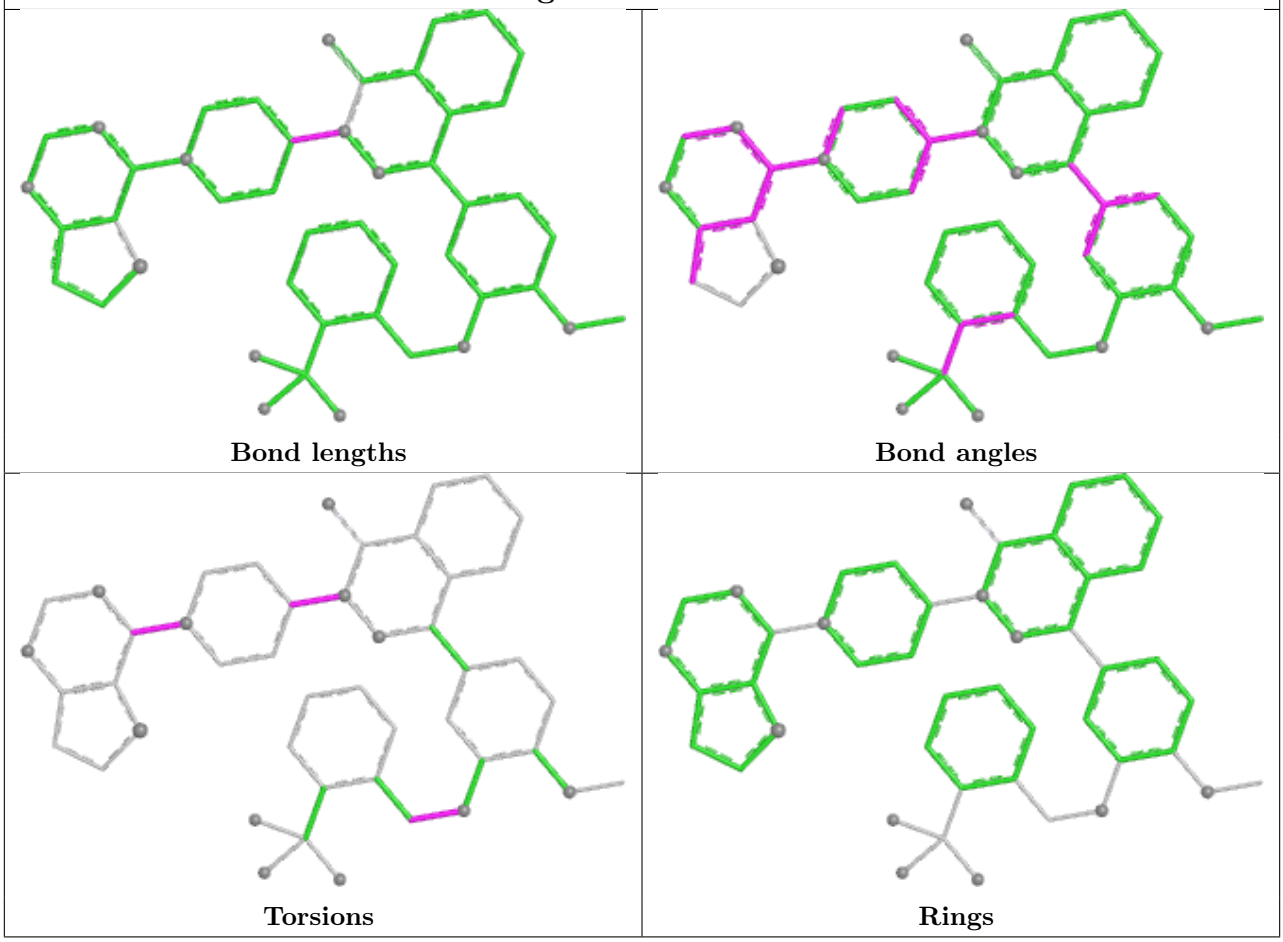
7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	521	EDO	1	0
6	A	513	4I7	1	0
4	A	506	EDO	1	0
4	D	509	EDO	2	0
5	D	516	EPE	1	0
7	D	511	PEG	2	0
7	D	512	PEG	1	0

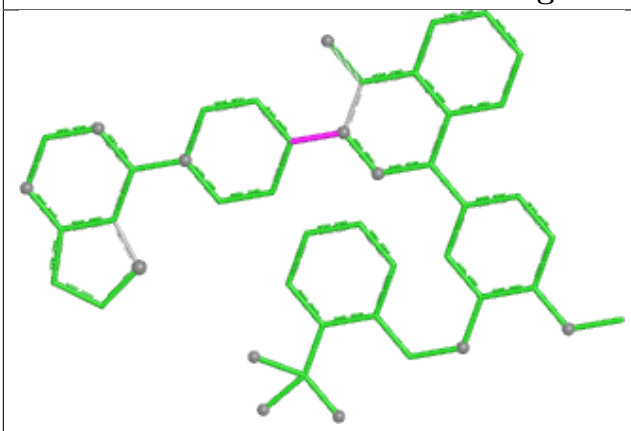
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

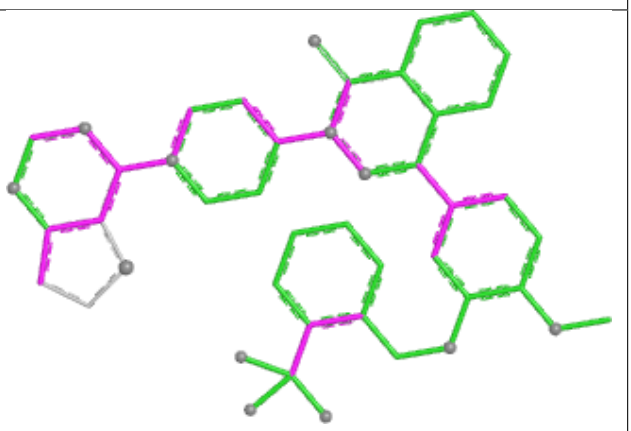
Ligand 4I7 A 513



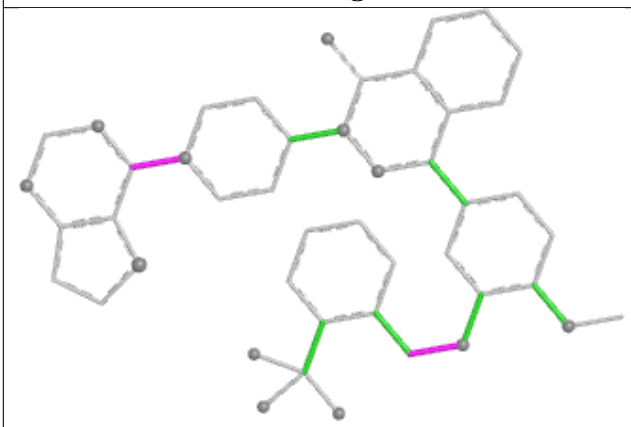
Ligand 4I7 B 513



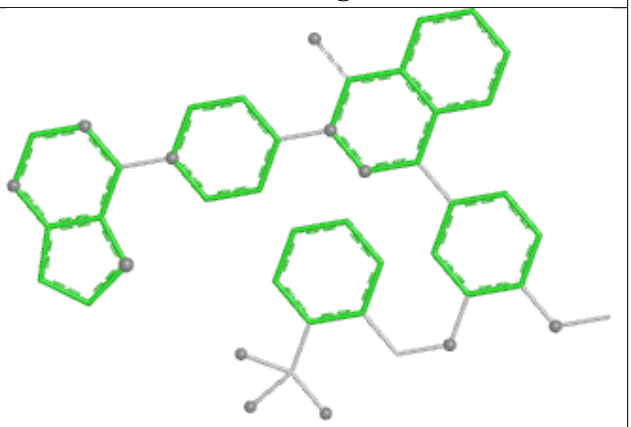
Bond lengths



Bond angles

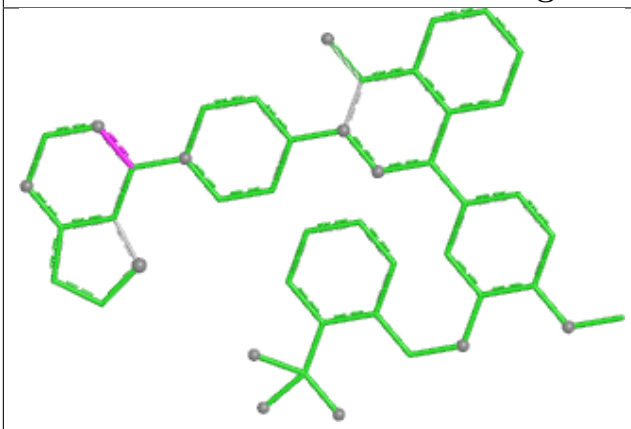


Torsions

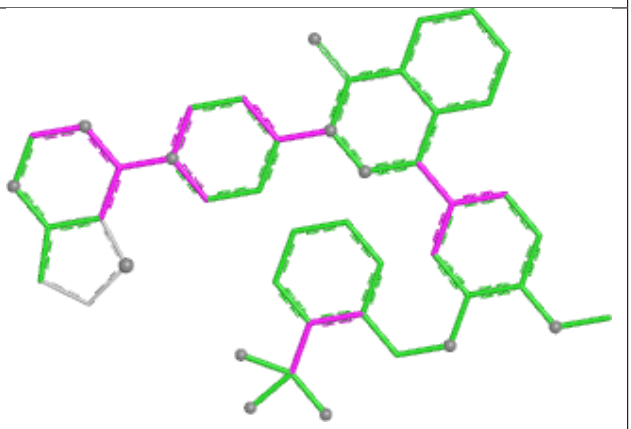


Rings

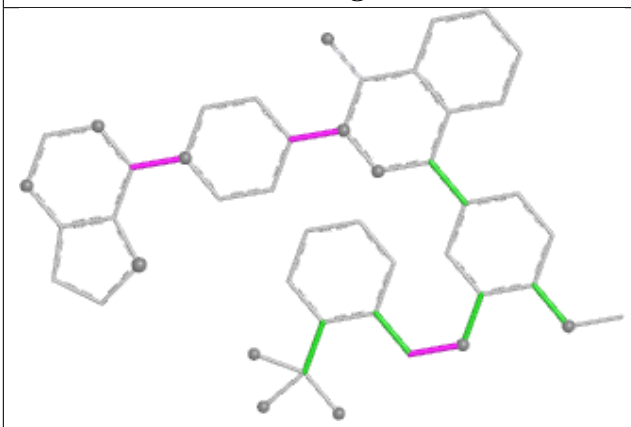
Ligand 4I7 C 508



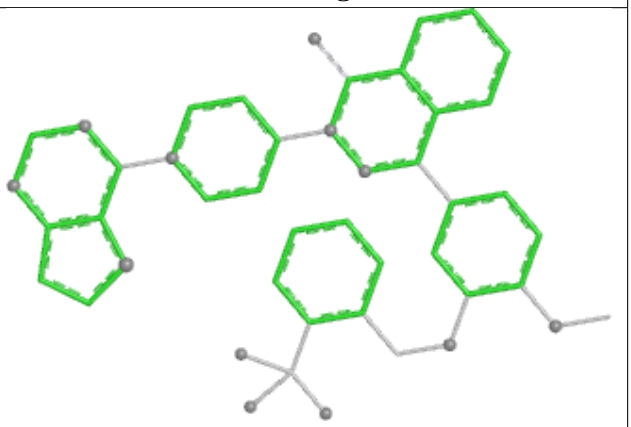
Bond lengths



Bond angles

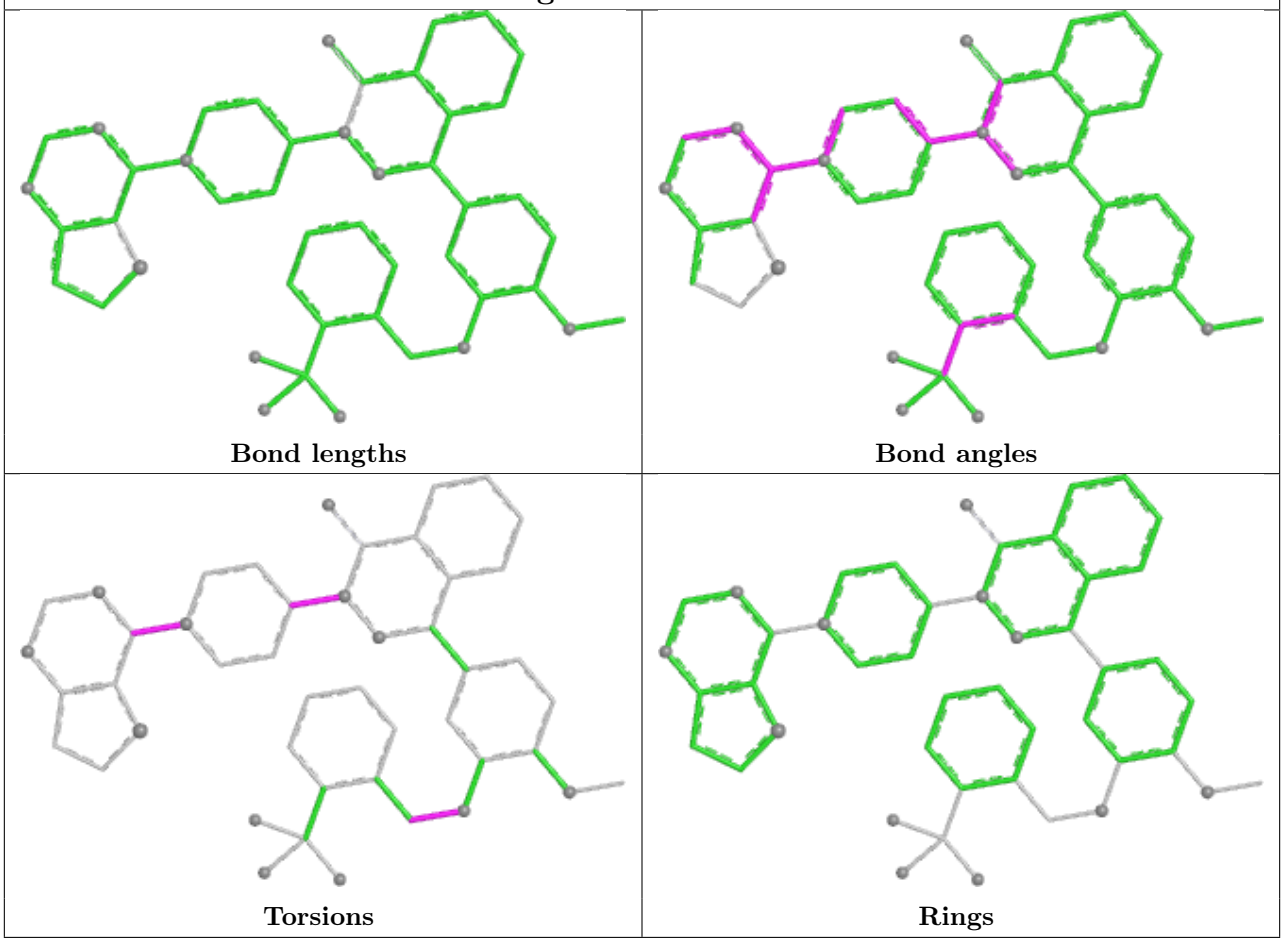


Torsions



Rings

Ligand 4I7 D 520



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	329/364 (90%)	0.14	23 (6%)	16	22	23, 42, 83, 126	13 (3%)
1	B	324/364 (89%)	-0.08	4 (1%)	79	83	24, 45, 68, 107	0
1	C	323/364 (88%)	0.21	17 (5%)	26	33	24, 45, 82, 114	11 (3%)
1	D	324/364 (89%)	-0.17	5 (1%)	73	79	21, 32, 68, 112	0
All	All	1300/1456 (89%)	0.03	49 (3%)	40	47	21, 41, 78, 126	24 (1%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	358	CYS	11.4
1	C	356	PRO	10.5
1	C	360	LYS	9.4
1	C	357	MET	9.0
1	A	363	ALA	7.8
1	C	354	ILE	7.6
1	A	362	ASN	6.3
1	A	358	CYS	5.5
1	A	361	HIS	5.3
1	C	359	ASP	5.2
1	A	354	ILE	5.2
1	A	356	PRO	5.0
1	C	361	HIS	4.8
1	A	357	MET	4.6
1	A	360	LYS	4.2
1	A	352	MET	3.8
1	C	298	LEU	3.7
1	C	355	SER	3.7
1	A	294	SER	3.7
1	B	143	ILE	3.5
1	A	410	ILE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	296	GLY	3.2
1	A	355	SER	3.1
1	C	362	ASN	3.0
1	D	356	PRO	3.0
1	A	350	ARG	2.9
1	D	362	ASN	2.8
1	D	357	MET	2.8
1	A	375	TYR	2.8
1	A	359	ASP	2.6
1	C	292	VAL	2.6
1	A	411	PRO	2.6
1	A	348	ARG	2.6
1	A	353	GLU	2.6
1	B	357	MET	2.5
1	C	353	GLU	2.5
1	A	340	PHE	2.4
1	D	354	ILE	2.4
1	C	297	VAL	2.3
1	A	298	LEU	2.2
1	D	89	GLU	2.2
1	C	296	GLY	2.2
1	B	296	GLY	2.2
1	C	363	ALA	2.1
1	A	351	GLY	2.1
1	B	108	ARG	2.1
1	A	387	LEU	2.1
1	C	290	LYS	2.1
1	C	294	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	B	506	4/4	0.63	0.26	60,74,79,85	0
4	EDO	B	509	4/4	0.68	0.32	80,82,85,88	0
4	EDO	C	504	4/4	0.75	0.18	80,81,82,84	0
4	EDO	A	512	4/4	0.77	0.25	60,64,64,66	0
4	EDO	C	509	4/4	0.78	0.19	65,68,71,74	0
4	EDO	A	511	4/4	0.82	0.21	66,69,72,73	0
7	PEG	D	512	7/7	0.82	0.18	41,45,59,59	0
4	EDO	D	506	4/4	0.85	0.21	72,75,76,78	0
4	EDO	D	513	4/4	0.85	0.14	54,55,57,57	0
4	EDO	B	512	4/4	0.85	0.17	54,58,60,62	0
4	EDO	B	508	4/4	0.86	0.16	59,61,61,61	0
4	EDO	C	506	4/4	0.86	0.25	49,53,57,60	0
4	EDO	C	503	4/4	0.87	0.13	61,63,64,64	0
4	EDO	B	504	4/4	0.87	0.51	67,68,70,71	0
4	EDO	D	519	4/4	0.87	0.29	48,49,52,53	0
4	EDO	D	521	4/4	0.87	0.51	20,20,20,20	0
6	4I7	A	513	46/46	0.87	0.23	48,73,126,132	0
4	EDO	D	503	4/4	0.87	0.19	67,69,73,74	0
4	EDO	A	507	4/4	0.88	0.17	55,60,66,70	0
6	4I7	D	520	46/46	0.88	0.21	38,61,116,122	0
4	EDO	B	511	4/4	0.88	0.26	49,51,55,58	0
4	EDO	D	517	4/4	0.89	0.12	67,68,71,74	0
4	EDO	D	518	4/4	0.89	0.18	59,63,65,66	0
4	EDO	D	505	4/4	0.89	0.18	51,51,53,55	0
4	EDO	C	507	4/4	0.89	0.20	42,46,47,50	0
4	EDO	D	507	4/4	0.89	0.17	48,54,57,65	0
6	4I7	B	513	46/46	0.89	0.20	39,66,114,127	0
4	EDO	D	509	4/4	0.89	0.19	55,58,59,69	0
4	EDO	D	504	4/4	0.89	0.16	36,39,41,41	0
4	EDO	A	508	4/4	0.90	0.13	58,63,64,66	0
7	PEG	D	511	7/7	0.90	0.17	40,44,52,53	0
5	EPE	A	510	15/15	0.90	0.21	71,93,109,110	0
4	EDO	B	503	4/4	0.91	0.18	68,70,71,74	0
4	EDO	D	514	4/4	0.91	0.17	54,59,60,62	0
4	EDO	A	509	4/4	0.91	0.17	43,46,48,48	0
6	4I7	C	508	46/46	0.92	0.16	41,54,98,106	0
5	EPE	B	510	15/15	0.92	0.17	65,96,103,104	0
4	EDO	B	505	4/4	0.92	0.31	63,64,64,65	0
4	EDO	A	506	4/4	0.92	0.14	49,53,56,63	0
4	EDO	D	510	4/4	0.93	0.18	43,43,44,46	0
4	EDO	D	515	4/4	0.93	0.19	54,54,55,60	0

Continued on next page...

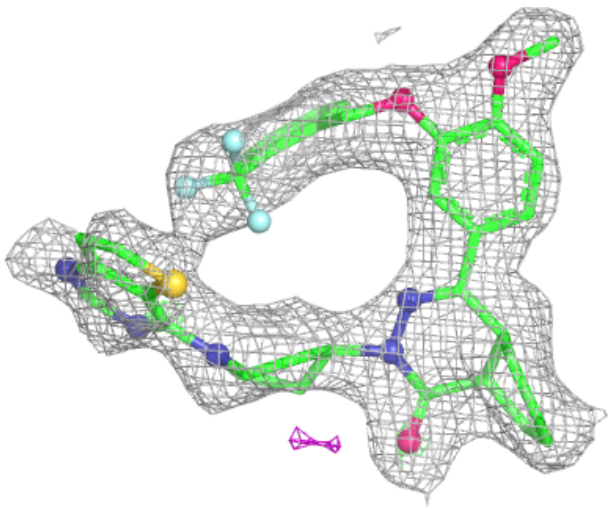
Continued from previous page...

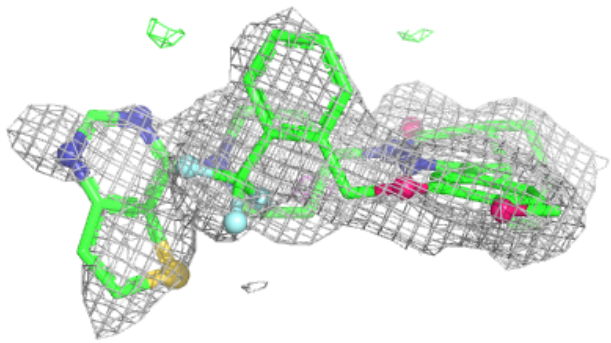
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	A	503	4/4	0.94	0.15	64,67,68,72	0
4	EDO	D	508	4/4	0.95	0.20	54,57,57,58	0
4	EDO	A	505	4/4	0.95	0.12	39,43,44,45	0
4	EDO	B	507	4/4	0.96	0.21	56,56,56,61	0
5	EPE	D	516	15/15	0.96	0.18	44,83,105,109	0
4	EDO	A	504	4/4	0.97	0.17	32,39,42,48	0
5	EPE	C	505	15/15	0.98	0.15	52,69,80,82	0
3	MG	D	502	1/1	0.98	0.13	16,16,16,16	0
3	MG	C	502	1/1	0.99	0.13	18,18,18,18	0
2	ZN	A	501	1/1	0.99	0.14	37,37,37,37	0
2	ZN	B	501	1/1	0.99	0.09	39,39,39,39	0
3	MG	A	502	1/1	0.99	0.14	23,23,23,23	0
3	MG	B	502	1/1	0.99	0.13	21,21,21,21	0
2	ZN	C	501	1/1	1.00	0.12	36,36,36,36	0
2	ZN	D	501	1/1	1.00	0.12	30,30,30,30	0

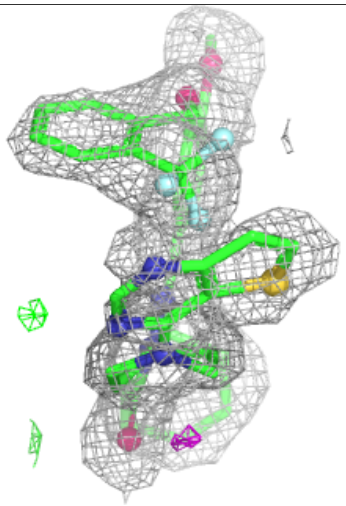
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 4I7 A 513:

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

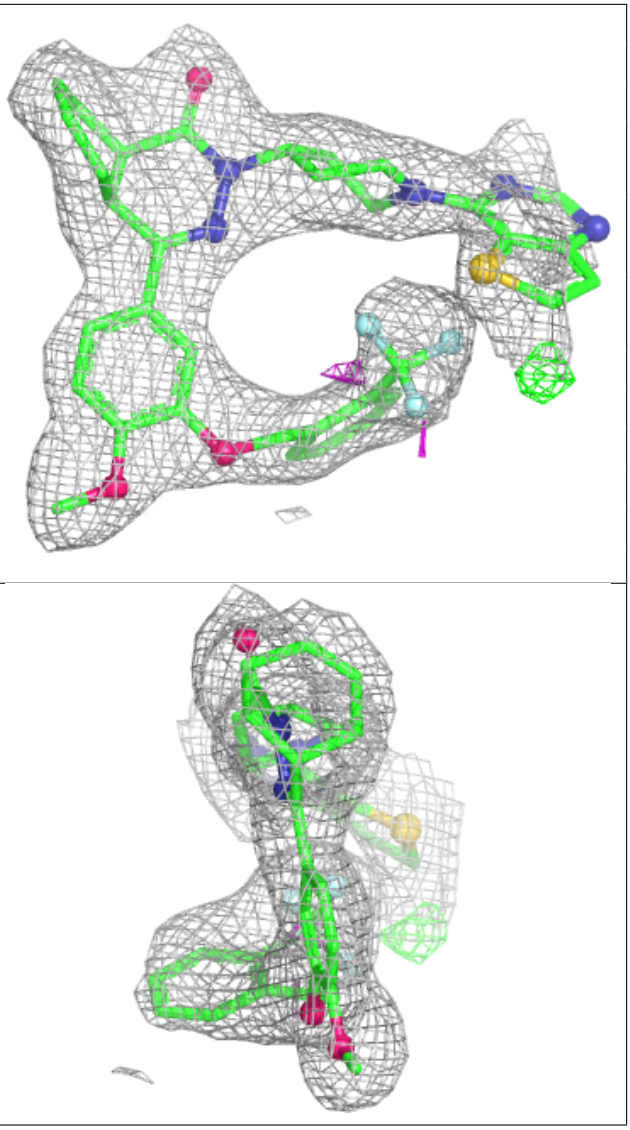






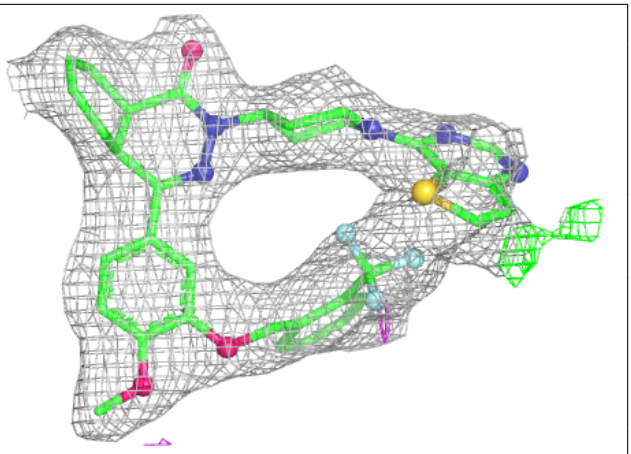
Electron density around 4I7 D 520:

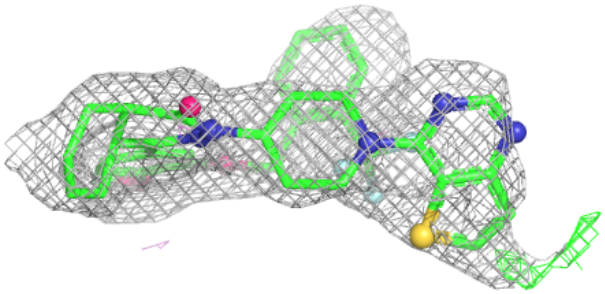
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

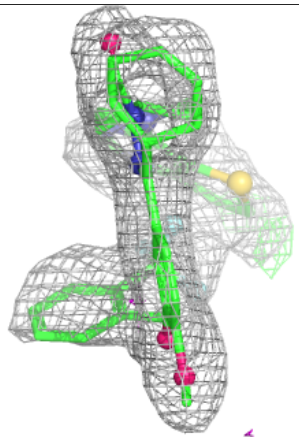


Electron density around 4I7 B 513:

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

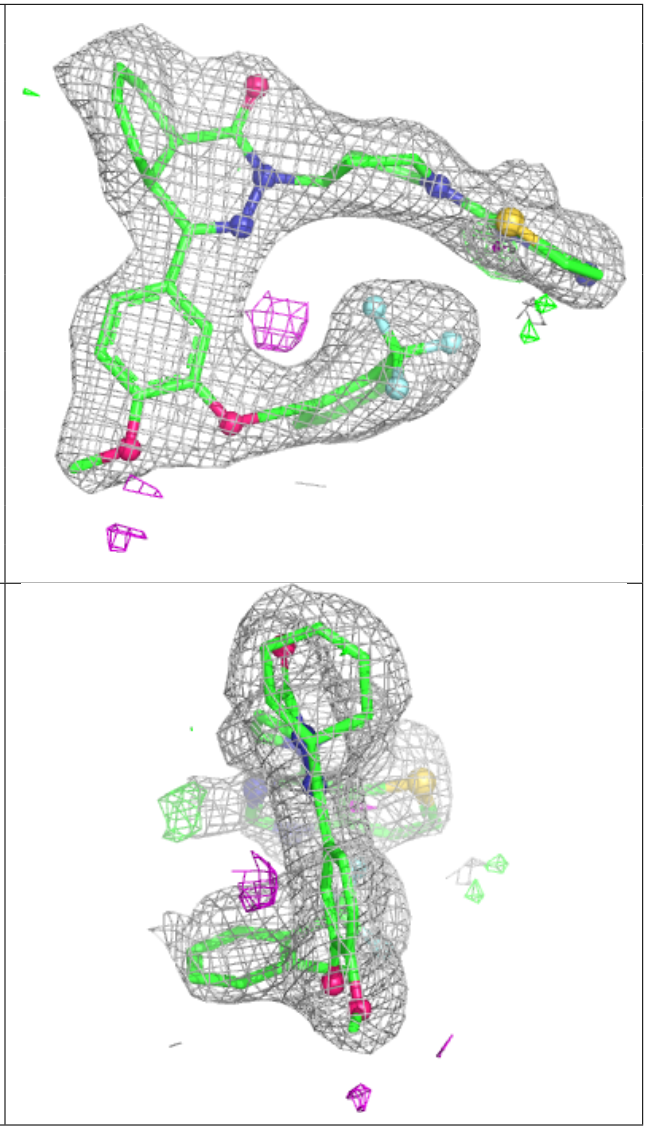






Electron density around 4I7 C 508:

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



6.5 Other polymers (i)

There are no such residues in this entry.