



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:57 PM EDT

PDB ID : 7ABJ / pdb_00007abj
Title : Crystal structure of human phosphodiesterase 4D2 catalytic domain with inhibitor NPD-1361
Authors : Singh, A.K.; Blaazer, A.R.; Zara, L.; de Esch, I.J.P.; Leurs, R.; Brown, D.G.
Deposited on : 2020-09-07
Resolution : 2.11 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

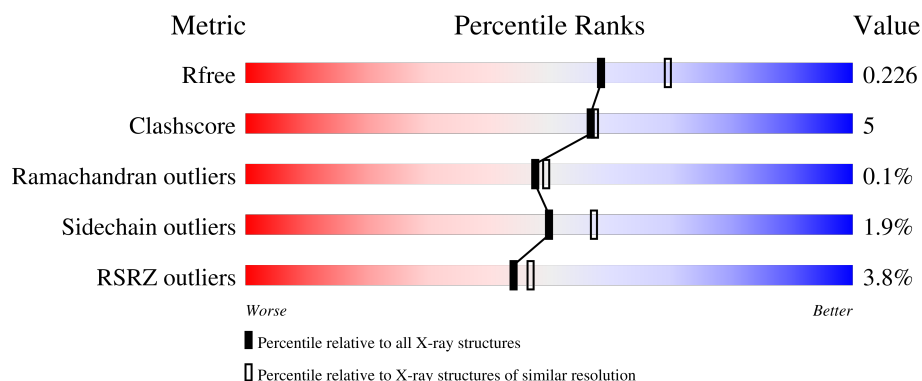
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	364	5% 81% 9% 10%
1	B	364	4% 82% 6% 11%
1	C	364	4% 80% 8% 11%
1	D	364	% 82% 7% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	B	508	-	-	X	-
8	PEG	D	514	-	-	X	-
8	PEG	D	515	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11436 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2658	1681	454	509	14			
1	B	324	Total	C	N	O	S	0	0	0
			2622	1659	448	501	14			
1	C	324	Total	C	N	O	S	0	0	0
			2622	1659	448	501	14			
1	D	324	Total	C	N	O	S	0	0	0
			2622	1659	448	501	14			

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

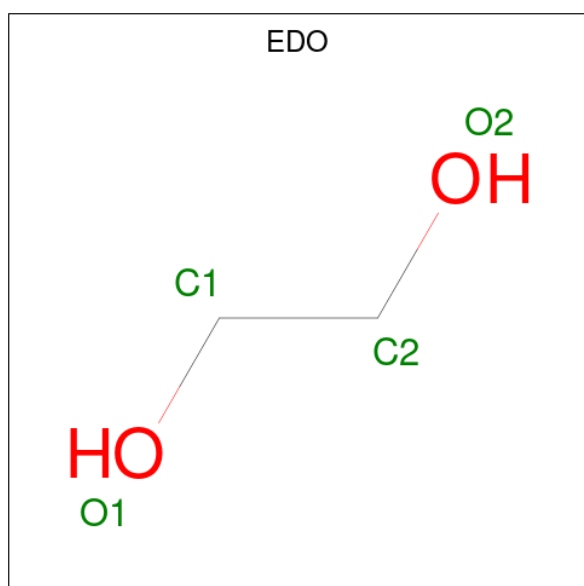
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

Continued on next page...

Continued from previous page...

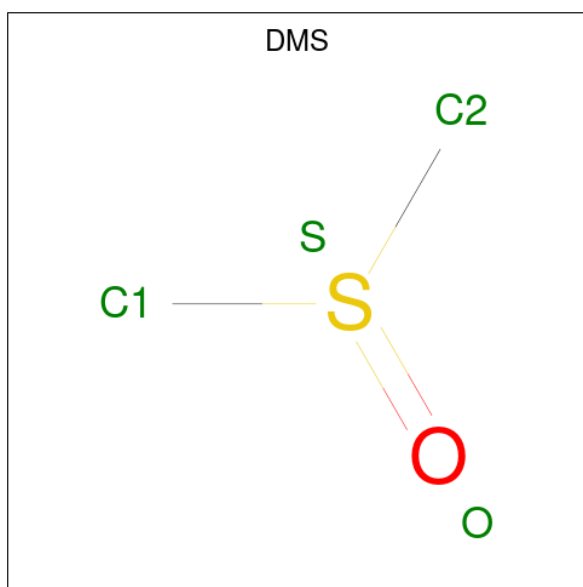
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0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

Continued on next page...

Continued from previous page...

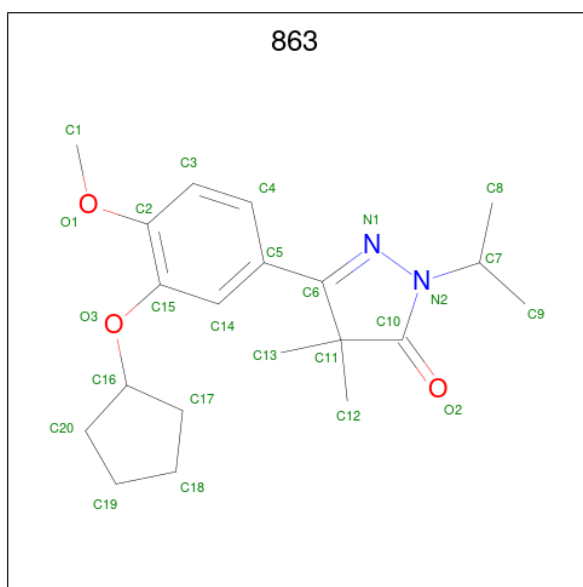
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0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

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



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

- Molecule 6 is 5-(3-(cyclopentyloxy)-4-methoxyphenyl)-2-isopropyl-4,4-dimethyl-2,4-dihydro-3H-pyrazol-3-one (CCD ID: 863) (formula: $C_{20}H_{28}N_2O_3$) (labeled as "Ligand of Interest" by depositor).



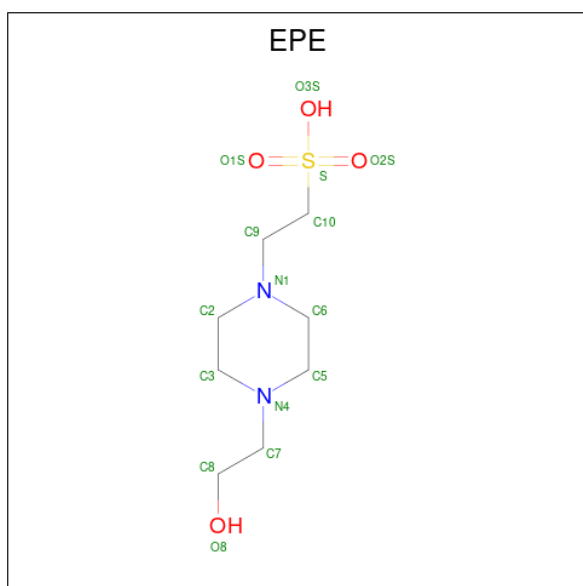
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			25	20	2	3		

Continued on next page...

Continued from previous page...

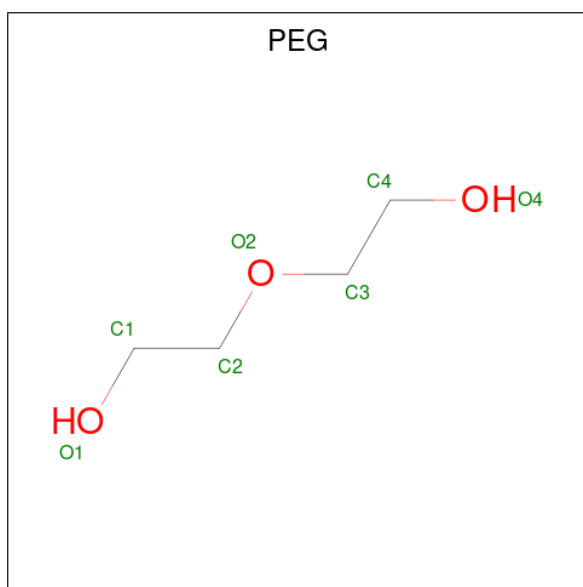
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			25	20	2	3		
6	C	1	Total	C	N	O	0	0
			25	20	2	3		
6	D	1	Total	C	N	O	0	0
			25	20	2	3		

- Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



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

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

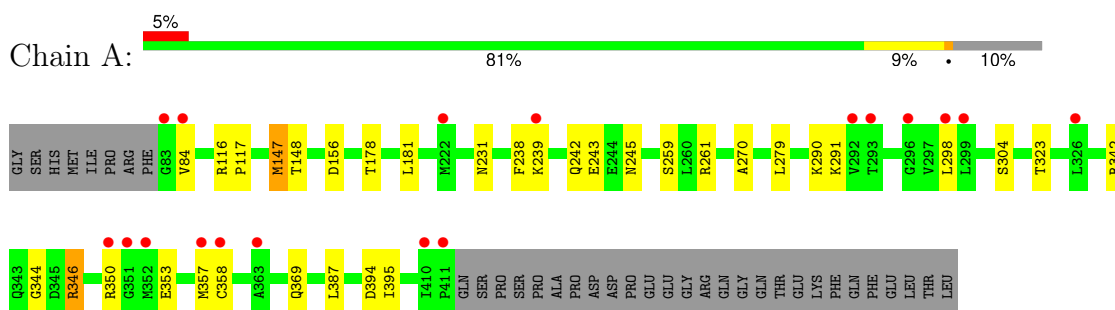
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	138	Total O 138 138	0	0
9	B	128	Total O 128 128	0	0
9	C	92	Total O 92 92	0	0
9	D	176	Total O 176 176	0	0

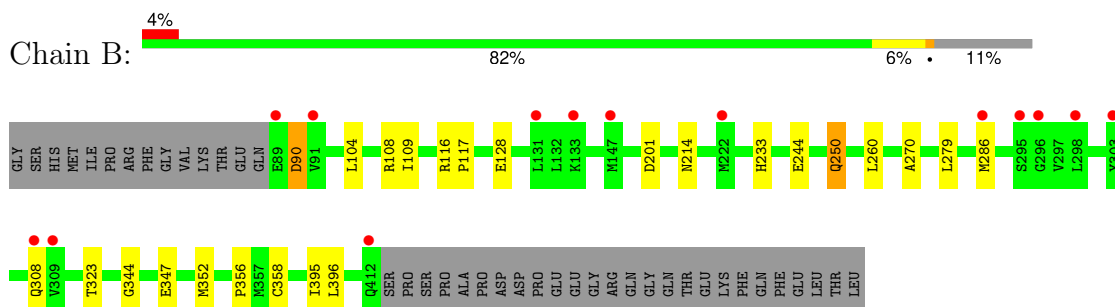
3 Residue-property plots [i](#)

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.

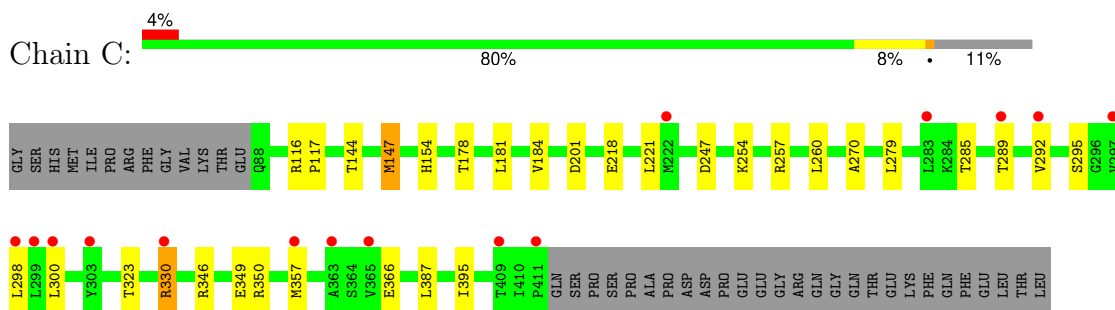
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



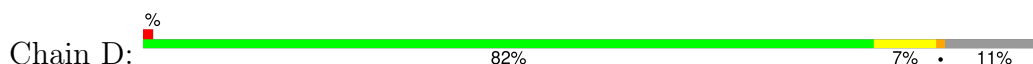
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

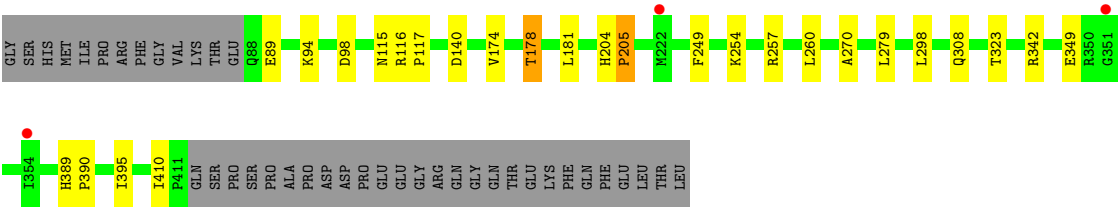


- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.00Å 111.04Å 160.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.41 – 2.11 84.41 – 2.11	Depositor EDS
% Data completeness (in resolution range)	99.8 (84.41-2.11) 99.8 (84.41-2.11)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.181 , 0.218 0.190 , 0.226	Depositor DCC
R_{free} test set	5224 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11436	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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: EPE, 863, ZN, EDO, DMS, MG, 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	1.07	0/2712	1.32	0/3684
1	B	1.04	1/2676 (0.0%)	1.32	2/3636 (0.1%)
1	C	1.04	0/2676	1.31	2/3636 (0.1%)
1	D	1.13	2/2676 (0.1%)	1.33	4/3636 (0.1%)
All	All	1.07	3/10740 (0.0%)	1.32	8/14592 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	205	PRO	N-CA	16.81	1.69	1.47
1	D	204	HIS	C-N	8.66	1.44	1.33
1	B	233	HIS	CE1-NE2	6.23	1.38	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	204	HIS	CA-C-N	17.17	137.08	119.56
1	D	204	HIS	C-N-CA	17.17	137.08	119.56
1	B	250	GLN	CB-CA-C	-7.20	98.80	110.74
1	D	205	PRO	CA-N-CD	-6.53	102.86	112.00
1	B	201	ASP	CA-CB-CG	5.19	117.79	112.60
1	C	349	GLU	CB-CA-C	-5.16	101.92	110.68
1	D	349	GLU	CB-CA-C	-5.16	101.92	110.68
1	C	201	ASP	CA-CB-CG	5.13	117.73	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2658	0	2616	31	0
1	B	2622	0	2578	19	0
1	C	2622	0	2578	25	1
1	D	2622	0	2578	27	1
2	A	1	0	0	0	0
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	52	0	78	11	0
4	B	24	0	36	7	0
4	C	32	0	48	3	0
4	D	44	0	66	7	0
5	A	4	0	6	3	0
5	B	4	0	6	1	0
6	A	25	0	0	2	0
6	B	25	0	0	0	0
6	C	25	0	0	0	0
6	D	25	0	0	0	0
7	A	15	0	18	0	0
7	B	30	0	36	0	0
7	C	15	0	17	0	0
7	D	15	0	17	0	0
8	B	7	0	10	0	0
8	C	7	0	10	0	0
8	D	21	0	30	9	0
9	A	138	0	0	0	0
9	B	128	0	0	0	0
9	C	92	0	0	0	0
9	D	176	0	0	1	0
All	All	11436	0	10728	99	1

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 5.

All (99) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:PRO:CA	1:D:205:PRO:N	1.69	1.37
1:A:346:ARG:O	1:A:350:ARG:HG2	1.68	0.93
1:A:357:MET:SD	6:A:516:863:C18	2.64	0.86
1:B:352:MET:HE2	4:B:508:EDO:C2	2.06	0.85
1:D:257:ARG:HH21	8:D:514:PEG:H21	1.39	0.85
1:B:352:MET:HE2	4:B:508:EDO:H22	1.57	0.85
1:A:156:ASP:OD1	4:C:501:EDO:O1	1.96	0.82
1:B:214:ASN:HD22	4:B:508:EDO:H21	1.45	0.82
1:A:231:ASN:HD21	4:A:506:EDO:H12	1.44	0.80
1:D:257:ARG:HH21	8:D:514:PEG:C2	1.94	0.79
1:A:242:GLN:HB2	4:A:510:EDO:H21	1.65	0.79
1:C:154:HIS:CG	4:C:501:EDO:H21	2.22	0.74
1:C:116:ARG:NE	1:C:147:MET:CE	2.54	0.70
1:D:257:ARG:NH2	8:D:514:PEG:H21	2.10	0.67
1:B:286:MET:HE3	1:B:308:GLN:NE2	2.08	0.67
1:D:254:LYS:H	8:D:514:PEG:H42	1.59	0.67
1:A:231:ASN:HD21	4:A:506:EDO:C1	2.09	0.66
1:A:261:ARG:HB2	5:A:514:DMS:H21	1.78	0.65
1:D:115:ASN:HD21	4:D:508:EDO:C1	2.10	0.65
1:A:259:SER:OG	4:A:513:EDO:H12	1.98	0.63
1:C:116:ARG:NE	1:C:147:MET:HE3	2.13	0.63
1:A:245:ASN:H	4:A:512:EDO:H11	1.62	0.63
1:D:115:ASN:HD21	4:D:508:EDO:H11	1.64	0.62
1:A:369:GLN:NE2	6:A:516:863:C20	2.62	0.62
1:D:178:THR:OG1	8:D:515:PEG:C4	2.49	0.61
1:D:181:LEU:HD21	1:D:298:LEU:HD12	1.85	0.58
1:A:238:PHE:CE1	5:A:514:DMS:H11	2.38	0.58
1:B:286:MET:HE3	1:B:308:GLN:HE22	1.68	0.57
1:D:140:ASP:OD2	4:D:510:EDO:H22	2.04	0.57
1:C:116:ARG:HD2	1:C:147:MET:HE3	1.87	0.56
1:A:323:THR:HB	1:A:395:ILE:HG23	1.88	0.56
1:C:116:ARG:CD	1:C:147:MET:HE3	2.37	0.54
1:A:148:THR:HG23	4:A:511:EDO:H12	1.90	0.53
1:B:244:GLU:OE2	1:C:254:LYS:HE2	2.10	0.52
1:A:116:ARG:NE	1:A:147:MET:HE2	2.25	0.51
1:C:260:LEU:C	1:C:260:LEU:HD13	2.35	0.51
1:A:259:SER:CB	4:A:513:EDO:H12	2.40	0.51
1:D:115:ASN:ND2	4:D:508:EDO:H11	2.25	0.51
1:B:214:ASN:ND2	4:B:508:EDO:H21	2.20	0.50
1:C:298:LEU:HD11	1:C:387:LEU:HG	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:THR:O	1:C:289:THR:HG22	2.11	0.50
1:A:353:GLU:OE2	1:A:353:GLU:N	2.45	0.50
1:A:243:GLU:OE1	4:A:511:EDO:H12	2.12	0.49
1:B:214:ASN:HD22	4:B:508:EDO:C2	2.19	0.49
1:D:205:PRO:N	1:D:205:PRO:C	2.63	0.49
1:D:178:THR:OG1	8:D:515:PEG:H41	2.13	0.49
1:A:238:PHE:CD1	5:A:514:DMS:H11	2.48	0.49
1:A:350:ARG:HD2	1:C:144:THR:HG23	1.94	0.49
1:B:323:THR:HB	1:B:395:ILE:HG23	1.95	0.49
1:B:286:MET:CE	1:B:308:GLN:NE2	2.76	0.48
1:D:181:LEU:CD2	1:D:298:LEU:HD12	2.42	0.48
1:C:116:ARG:NE	1:C:147:MET:HE2	2.28	0.48
1:A:342:ARG:HG3	1:A:346:ARG:NH1	2.28	0.48
1:D:178:THR:OG1	8:D:515:PEG:H42	2.13	0.48
1:B:286:MET:CE	1:B:308:GLN:HE22	2.27	0.47
1:C:154:HIS:CD2	4:C:501:EDO:H21	2.47	0.47
1:C:181:LEU:HD21	1:C:298:LEU:HD12	1.97	0.47
1:C:116:ARG:HD2	1:C:147:MET:CE	2.46	0.46
1:A:298:LEU:HD11	1:A:387:LEU:HG	1.98	0.45
1:D:323:THR:HB	1:D:395:ILE:HG23	1.98	0.45
1:D:257:ARG:HH21	8:D:514:PEG:H22	1.78	0.45
1:C:178:THR:HG22	1:C:181:LEU:HD12	1.98	0.45
1:A:270:ALA:HB1	1:A:279:LEU:HD11	1.99	0.45
1:B:270:ALA:HB1	1:B:279:LEU:HD11	1.99	0.45
1:A:342:ARG:CG	1:A:346:ARG:NH1	2.81	0.44
1:A:116:ARG:N	1:A:117:PRO:CD	2.81	0.44
1:A:148:THR:HG23	4:A:511:EDO:C1	2.46	0.44
1:D:98:ASP:OD2	4:D:509:EDO:O2	2.35	0.44
1:C:116:ARG:N	1:C:117:PRO:CD	2.81	0.44
1:B:347:GLU:OE2	4:B:508:EDO:H12	2.17	0.44
1:D:140:ASP:OD2	4:D:510:EDO:C2	2.66	0.44
1:B:356:PRO:O	5:B:510:DMS:H22	2.18	0.43
1:C:270:ALA:HB1	1:C:279:LEU:HD11	2.00	0.43
1:C:323:THR:HB	1:C:395:ILE:HG23	2.00	0.43
1:C:184:VAL:HG11	1:C:300:LEU:HD12	2.01	0.43
1:A:231:ASN:ND2	4:A:506:EDO:H12	2.23	0.43
1:C:116:ARG:CD	1:C:147:MET:CE	2.96	0.43
1:D:249:PHE:CD2	4:D:506:EDO:H11	2.54	0.43
1:B:116:ARG:N	1:B:117:PRO:CD	2.82	0.42
1:C:247:ASP:OD2	1:C:257:ARG:NH2	2.52	0.42
1:D:116:ARG:N	1:D:117:PRO:CD	2.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:ARG:HG2	1:D:342:ARG:HH21	1.84	0.42
1:D:174:VAL:HG12	8:D:515:PEG:H12	2.00	0.42
1:A:242:GLN:CB	4:A:510:EDO:H21	2.42	0.42
1:C:181:LEU:CD2	1:C:298:LEU:HD12	2.50	0.42
1:A:323:THR:HB	1:A:395:ILE:CG2	2.49	0.42
1:D:308:GLN:HG3	9:D:757:HOH:O	2.19	0.42
1:A:239:LYS:HE3	1:C:218:GLU:OE1	2.19	0.42
1:A:178:THR:HG22	1:A:181:LEU:HD12	2.01	0.41
1:A:344:GLY:HA3	1:A:358:CYS:O	2.20	0.41
1:B:286:MET:HE3	1:B:286:MET:HB2	1.98	0.41
1:D:342:ARG:HG2	1:D:342:ARG:NH2	2.36	0.41
1:B:352:MET:HE2	4:B:508:EDO:C1	2.51	0.41
1:D:389:HIS:HA	1:D:390:PRO:HA	1.81	0.41
1:B:104:LEU:HD11	1:B:109:ILE:HD11	2.03	0.41
1:D:270:ALA:HB1	1:D:279:LEU:HD11	2.03	0.41
1:C:366:GLU:H	1:C:366:GLU:CD	2.29	0.40
1:B:344:GLY:HA3	1:B:358:CYS:O	2.20	0.40
1:C:346:ARG:O	1:C:350:ARG:HD2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:ARG:NH2	1:D:410:ILE:O[2_575]	1.66	0.54

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	327/364 (90%)	321 (98%)	6 (2%)	0	100	100
1	B	322/364 (88%)	317 (98%)	4 (1%)	1 (0%)	36	36

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	322/364 (88%)	316 (98%)	6 (2%)	0	100	100
1	D	322/364 (88%)	319 (99%)	3 (1%)	0	100	100
All	All	1293/1456 (89%)	1273 (98%)	19 (2%)	1 (0%)	48	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	90	ASP

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	300/331 (91%)	293 (98%)	7 (2%)	44	50
1	B	296/331 (89%)	290 (98%)	6 (2%)	48	55
1	C	296/331 (89%)	290 (98%)	6 (2%)	48	55
1	D	296/331 (89%)	292 (99%)	4 (1%)	59	67
All	All	1188/1324 (90%)	1165 (98%)	23 (2%)	50	57

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	VAL
1	A	147	MET
1	A	290	LYS
1	A	291	LYS
1	A	304	SER
1	A	346	ARG
1	A	394	ASP
1	B	90	ASP
1	B	108	ARG
1	B	128	GLU
1	B	250	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	260	LEU
1	B	396	LEU
1	C	147	MET
1	C	221	LEU
1	C	292	VAL
1	C	295	SER
1	C	330	ARG
1	C	357	MET
1	D	89	GLU
1	D	94	LYS
1	D	178	THR
1	D	260	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	ASN
1	A	331	GLN
1	A	369	GLN
1	B	224	ASN
1	B	242	GLN
1	B	258	GLN
1	B	321	ASN
1	C	210	GLN
1	C	250	GLN
1	C	321	ASN
1	C	331	GLN
1	D	210	GLN
1	D	308	GLN
1	D	312	ASN
1	D	369	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 62 ligands modelled in this entry, 8 are monoatomic - leaving 54 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	D	507	-	3,3,3	0.36	0	2,2,2	0.28	0
4	EDO	D	512	-	3,3,3	0.12	0	2,2,2	0.83	0
4	EDO	A	504	-	3,3,3	0.06	0	2,2,2	0.24	0
8	PEG	D	513	-	6,6,6	0.36	0	5,5,5	0.26	0
4	EDO	C	513	-	3,3,3	0.12	0	2,2,2	0.18	0
8	PEG	D	514	-	6,6,6	0.14	0	5,5,5	0.16	0
4	EDO	C	508	-	3,3,3	0.42	0	2,2,2	0.27	0
6	863	B	512	-	26,27,27	0.46	0	32,40,40	0.80	0
4	EDO	A	506	-	3,3,3	0.39	0	2,2,2	0.22	0
4	EDO	C	506	-	3,3,3	0.12	0	2,2,2	0.31	0
8	PEG	D	515	-	6,6,6	0.46	0	5,5,5	0.72	0
4	EDO	C	511	-	3,3,3	0.51	0	2,2,2	0.53	0
6	863	D	517	-	26,27,27	0.51	0	32,40,40	0.84	1 (3%)
7	EPE	B	513	-	15,15,15	1.99	1 (6%)	19,20,20	1.59	2 (10%)
4	EDO	C	505	-	3,3,3	0.11	0	2,2,2	0.06	0
4	EDO	D	505	-	3,3,3	0.12	0	2,2,2	0.24	0
6	863	C	512	-	26,27,27	0.50	0	32,40,40	1.17	3 (9%)
4	EDO	D	509	-	3,3,3	0.26	0	2,2,2	0.39	0
4	EDO	D	506	-	3,3,3	0.27	0	2,2,2	0.48	0
4	EDO	D	508	-	3,3,3	0.21	0	2,2,2	0.70	0
4	EDO	B	507	-	3,3,3	0.37	0	2,2,2	0.55	0
4	EDO	C	501	-	3,3,3	0.30	0	2,2,2	0.11	0
4	EDO	D	504	-	3,3,3	0.21	0	2,2,2	0.37	0
4	EDO	A	515	-	3,3,3	0.25	0	2,2,2	0.86	0
4	EDO	C	507	-	3,3,3	0.17	0	2,2,2	0.30	0
7	EPE	D	518	-	15,15,15	3.14	2 (13%)	19,20,20	1.89	5 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	506	-	3,3,3	0.07	0	2,2,2	0.20	0
4	EDO	B	505	-	3,3,3	0.01	0	2,2,2	0.32	0
4	EDO	A	509	-	3,3,3	0.34	0	2,2,2	0.20	0
4	EDO	B	503	-	3,3,3	0.04	0	2,2,2	0.07	0
4	EDO	B	508	-	3,3,3	0.38	0	2,2,2	0.69	0
4	EDO	C	509	-	3,3,3	0.33	0	2,2,2	0.47	0
5	DMS	B	510	-	3,3,3	0.25	0	3,3,3	0.15	0
4	EDO	D	516	-	3,3,3	0.49	0	2,2,2	0.39	0
4	EDO	A	507	-	3,3,3	0.25	0	2,2,2	0.23	0
4	EDO	A	511	-	3,3,3	0.42	0	2,2,2	0.36	0
7	EPE	B	511	-	15,15,15	1.66	1 (6%)	19,20,20	1.81	3 (15%)
4	EDO	A	508	-	3,3,3	0.13	0	2,2,2	0.40	0
4	EDO	A	510	-	3,3,3	0.24	0	2,2,2	0.80	0
4	EDO	A	503	-	3,3,3	0.05	0	2,2,2	0.14	0
4	EDO	D	510	-	3,3,3	0.16	0	2,2,2	0.19	0
5	DMS	A	514	-	3,3,3	0.26	0	3,3,3	0.47	0
7	EPE	A	518	-	15,15,15	2.02	1 (6%)	19,20,20	1.44	3 (15%)
4	EDO	D	503	-	3,3,3	0.49	0	2,2,2	0.51	0
4	EDO	D	511	-	3,3,3	0.51	0	2,2,2	0.47	0
4	EDO	B	504	-	3,3,3	0.22	0	2,2,2	0.23	0
4	EDO	A	512	-	3,3,3	0.14	0	2,2,2	0.52	0
4	EDO	A	513	-	3,3,3	0.54	0	2,2,2	0.49	0
4	EDO	A	517	-	3,3,3	0.24	0	2,2,2	0.26	0
4	EDO	A	505	-	3,3,3	0.48	0	2,2,2	0.10	0
6	863	A	516	-	26,27,27	0.41	0	32,40,40	0.89	2 (6%)
7	EPE	C	510	-	15,15,15	2.12	1 (6%)	19,20,20	1.66	4 (21%)
8	PEG	C	502	-	6,6,6	0.15	0	5,5,5	0.11	0
8	PEG	B	509	-	6,6,6	0.56	0	5,5,5	0.38	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	D	507	-	-	1/1/1/1	-
4	EDO	D	512	-	-	1/1/1/1	-
4	EDO	A	504	-	-	1/1/1/1	-
8	PEG	D	513	-	-	2/4/4/4	-
4	EDO	C	513	-	-	1/1/1/1	-
8	PEG	D	514	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	508	-	-	0/1/1/1	-
6	863	B	512	-	-	0/14/41/41	0/3/3/3
4	EDO	A	506	-	-	1/1/1/1	-
4	EDO	C	506	-	-	1/1/1/1	-
8	PEG	D	515	-	-	2/4/4/4	-
4	EDO	C	511	-	-	0/1/1/1	-
6	863	D	517	-	-	0/14/41/41	0/3/3/3
7	EPE	B	513	-	-	4/9/19/19	0/1/1/1
4	EDO	C	505	-	-	1/1/1/1	-
4	EDO	D	505	-	-	0/1/1/1	-
6	863	C	512	-	-	3/14/41/41	0/3/3/3
4	EDO	D	509	-	-	1/1/1/1	-
4	EDO	D	506	-	-	0/1/1/1	-
4	EDO	D	508	-	-	1/1/1/1	-
4	EDO	B	507	-	-	1/1/1/1	-
4	EDO	C	501	-	-	1/1/1/1	-
4	EDO	D	504	-	-	0/1/1/1	-
4	EDO	A	515	-	-	1/1/1/1	-
4	EDO	C	507	-	-	0/1/1/1	-
7	EPE	D	518	-	-	5/9/19/19	0/1/1/1
4	EDO	B	506	-	-	1/1/1/1	-
4	EDO	B	505	-	-	1/1/1/1	-
4	EDO	A	509	-	-	1/1/1/1	-
4	EDO	B	503	-	-	1/1/1/1	-
4	EDO	B	508	-	-	1/1/1/1	-
4	EDO	C	509	-	-	0/1/1/1	-
4	EDO	D	516	-	-	0/1/1/1	-
4	EDO	A	507	-	-	1/1/1/1	-
4	EDO	A	511	-	-	1/1/1/1	-
7	EPE	B	511	-	-	5/9/19/19	0/1/1/1
4	EDO	A	508	-	-	1/1/1/1	-
4	EDO	A	510	-	-	1/1/1/1	-
4	EDO	A	503	-	-	1/1/1/1	-
4	EDO	D	510	-	-	1/1/1/1	-
7	EPE	A	518	-	-	5/9/19/19	0/1/1/1
4	EDO	D	503	-	-	0/1/1/1	-
4	EDO	D	511	-	-	1/1/1/1	-
4	EDO	B	504	-	-	1/1/1/1	-
4	EDO	A	512	-	-	1/1/1/1	-
4	EDO	A	513	-	-	0/1/1/1	-
4	EDO	A	517	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	505	-	-	0/1/1/1	-
6	863	A	516	-	-	3/14/41/41	0/3/3/3
7	EPE	C	510	-	-	2/9/19/19	0/1/1/1
8	PEG	C	502	-	-	3/4/4/4	-
8	PEG	B	509	-	-	2/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	518	EPE	C10-S	-11.59	1.61	1.77
7	C	510	EPE	C10-S	-7.78	1.66	1.77
7	A	518	EPE	C10-S	-7.36	1.67	1.77
7	B	513	EPE	C10-S	-7.32	1.67	1.77
7	B	511	EPE	C10-S	-5.70	1.69	1.77
7	D	518	EPE	O2S-S	-2.18	1.39	1.45

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	513	EPE	O3S-S-C10	5.49	116.75	106.00
7	B	511	EPE	O1S-S-C10	5.06	114.38	106.73
7	C	510	EPE	O3S-S-C10	4.63	115.06	106.00
7	D	518	EPE	O1S-S-C10	4.12	112.95	106.73
7	D	518	EPE	O2S-S-O1S	-3.66	101.91	113.82
7	B	511	EPE	O3S-S-C10	3.55	112.95	106.00
7	A	518	EPE	O2S-S-C10	3.37	111.82	106.73
7	D	518	EPE	C9-N1-C2	-3.23	102.63	111.24
7	A	518	EPE	O3S-S-O1S	-2.96	104.00	111.40
7	C	510	EPE	O3S-S-O1S	-2.90	104.14	111.40
6	C	512	863	O3-C15-C14	-2.87	117.44	123.87
7	B	513	EPE	O3S-S-O2S	-2.86	104.25	111.40
7	D	518	EPE	O2S-S-C10	2.82	110.99	106.73
6	C	512	863	O2-C10-C11	-2.79	124.24	126.93
7	B	511	EPE	O3S-S-O1S	-2.78	104.45	111.40
6	C	512	863	O2-C10-N2	2.53	129.13	127.01
7	A	518	EPE	O3S-S-C10	2.51	110.92	106.00
7	C	510	EPE	O2S-S-C10	2.46	110.44	106.73
7	D	518	EPE	C6-N1-C2	2.40	114.02	108.84
6	A	516	863	O3-C15-C14	-2.32	118.68	123.87
6	A	516	863	C15-O3-C16	-2.25	112.91	120.14
7	C	510	EPE	O3S-S-O2S	-2.05	106.26	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	517	863	O3-C15-C14	-2.01	119.37	123.87

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	512	863	C17-C16-O3-C15
6	C	512	863	C20-C16-O3-C15
7	A	518	EPE	C9-C10-S-O2S
7	B	511	EPE	C8-C7-N4-C3
7	B	513	EPE	C9-C10-S-O1S
7	D	518	EPE	S-C10-C9-N1
8	D	515	PEG	C4-C3-O2-C2
8	D	515	PEG	O1-C1-C2-O2
7	D	518	EPE	N4-C7-C8-O8
7	A	518	EPE	C9-C10-S-O3S
7	D	518	EPE	C9-C10-S-O3S
8	C	502	PEG	O1-C1-C2-O2
7	A	518	EPE	C8-C7-N4-C5
7	B	513	EPE	C8-C7-N4-C5
4	A	504	EDO	O1-C1-C2-O2
4	C	501	EDO	O1-C1-C2-O2
8	B	509	PEG	O2-C3-C4-O4
4	A	512	EDO	O1-C1-C2-O2
4	A	515	EDO	O1-C1-C2-O2
4	A	517	EDO	O1-C1-C2-O2
4	B	505	EDO	O1-C1-C2-O2
4	C	506	EDO	O1-C1-C2-O2
4	D	511	EDO	O1-C1-C2-O2
8	C	502	PEG	O2-C3-C4-O4
4	B	504	EDO	O1-C1-C2-O2
4	D	512	EDO	O1-C1-C2-O2
7	A	518	EPE	C9-C10-S-O1S
7	B	513	EPE	C9-C10-S-O2S
7	D	518	EPE	C9-C10-S-O1S
7	D	518	EPE	C9-C10-S-O2S
6	A	516	863	C20-C16-O3-C15
7	A	518	EPE	S-C10-C9-N1
8	D	514	PEG	C4-C3-O2-C2
8	B	509	PEG	O1-C1-C2-O2
8	D	514	PEG	O1-C1-C2-O2
4	A	508	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	B	513	EPE	N4-C7-C8-O8
8	D	513	PEG	C1-C2-O2-C3
7	B	511	EPE	C10-C9-N1-C2
7	B	511	EPE	C10-C9-N1-C6
6	A	516	863	C17-C16-O3-C15
8	C	502	PEG	C1-C2-O2-C3
8	D	513	PEG	C4-C3-O2-C2
4	B	506	EDO	O1-C1-C2-O2
4	C	505	EDO	O1-C1-C2-O2
6	A	516	863	C2-C15-O3-C16
7	B	511	EPE	N4-C7-C8-O8
4	A	507	EDO	O1-C1-C2-O2
4	A	509	EDO	O1-C1-C2-O2
4	B	503	EDO	O1-C1-C2-O2
4	B	507	EDO	O1-C1-C2-O2
4	D	507	EDO	O1-C1-C2-O2
7	C	510	EPE	C8-C7-N4-C3
4	A	503	EDO	O1-C1-C2-O2
4	C	513	EDO	O1-C1-C2-O2
4	D	508	EDO	O1-C1-C2-O2
4	D	510	EDO	O1-C1-C2-O2
7	B	511	EPE	C9-C10-S-O2S
7	C	510	EPE	C8-C7-N4-C5
4	A	510	EDO	O1-C1-C2-O2
4	A	511	EDO	O1-C1-C2-O2
4	A	506	EDO	O1-C1-C2-O2
4	B	508	EDO	O1-C1-C2-O2
4	D	509	EDO	O1-C1-C2-O2
6	C	512	863	C2-C15-O3-C16

There are no ring outliers.

16 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	514	PEG	5	0
4	A	506	EDO	3	0
8	D	515	PEG	4	0
4	D	509	EDO	1	0
4	D	506	EDO	1	0
4	D	508	EDO	3	0
4	C	501	EDO	3	0
4	B	508	EDO	7	0

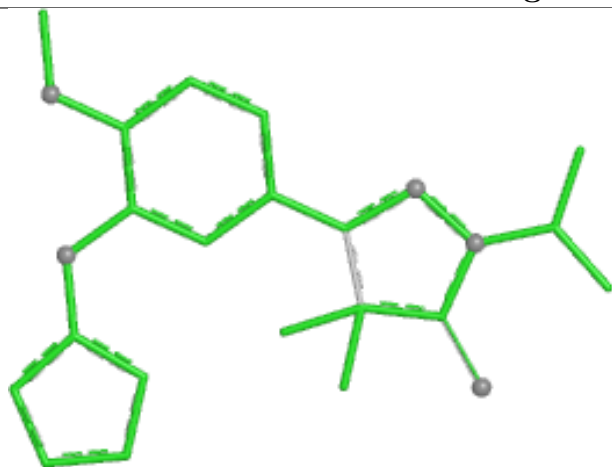
Continued on next page...

Continued from previous page...

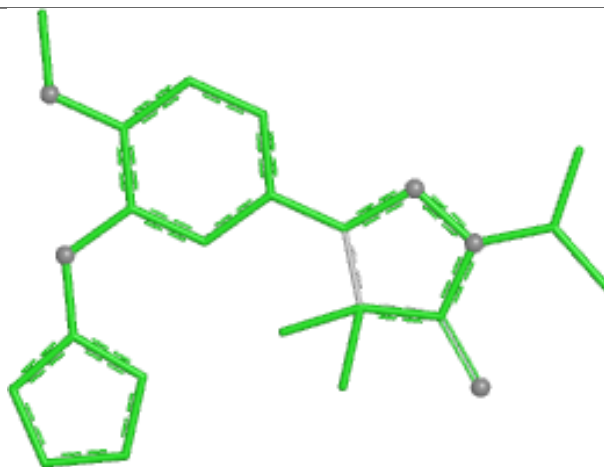
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	510	DMS	1	0
4	A	511	EDO	3	0
4	A	510	EDO	2	0
4	D	510	EDO	2	0
5	A	514	DMS	3	0
4	A	512	EDO	1	0
4	A	513	EDO	2	0
6	A	516	863	2	0

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.

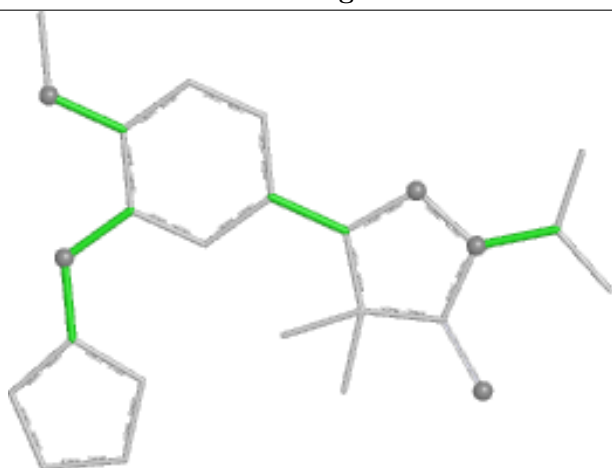
Ligand 863 B 512



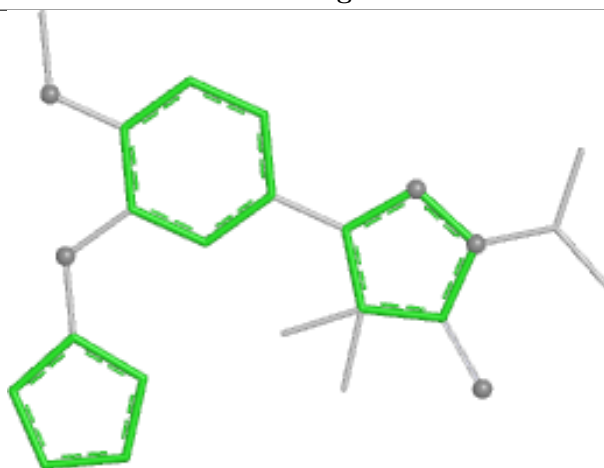
Bond lengths



Bond angles

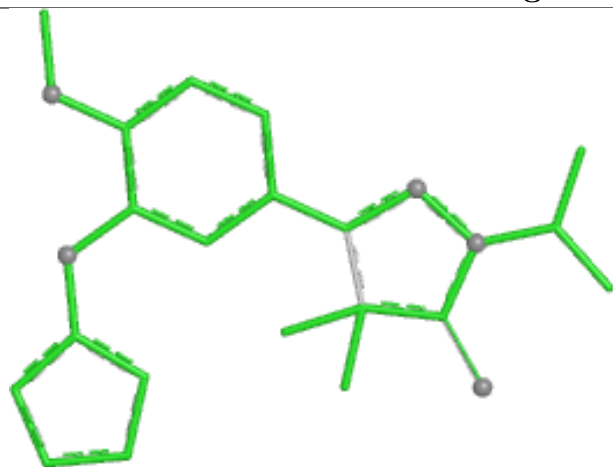


Torsions

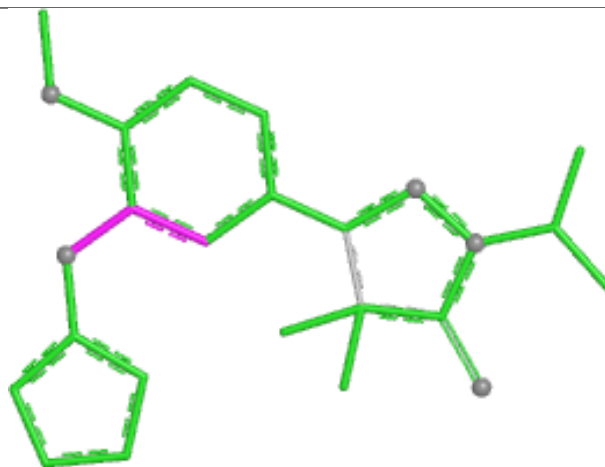


Rings

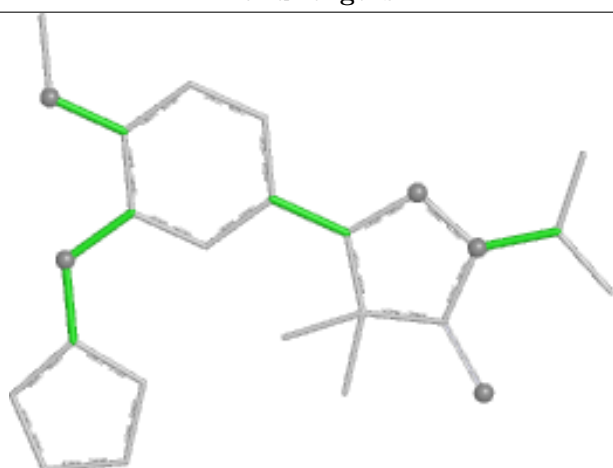
Ligand 863 D 517



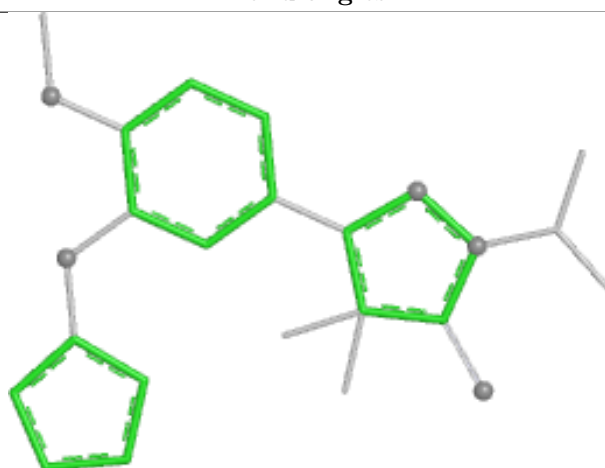
Bond lengths



Bond angles

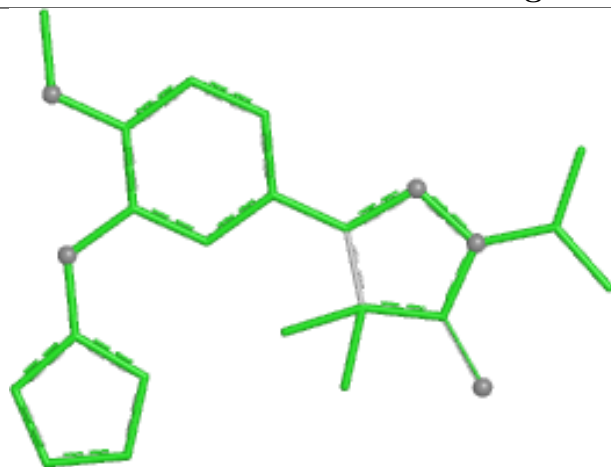


Torsions

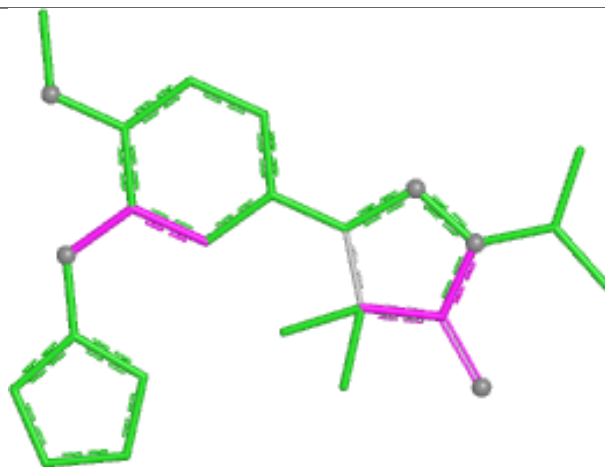


Rings

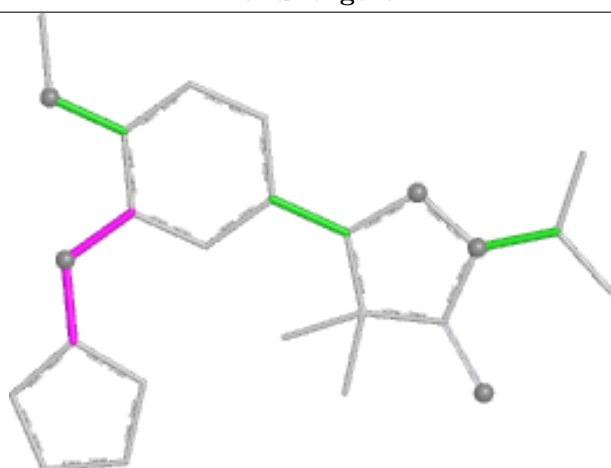
Ligand 863 C 512



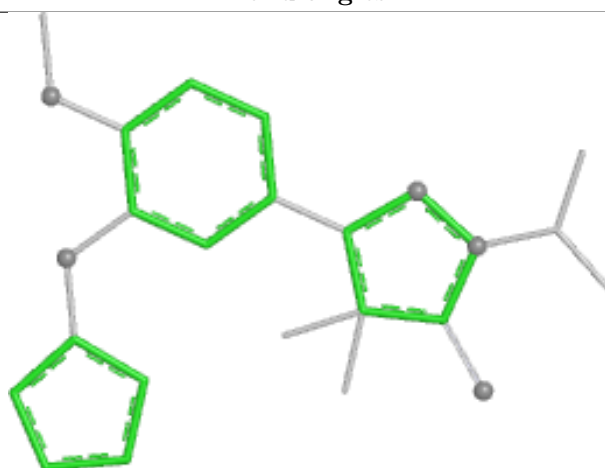
Bond lengths



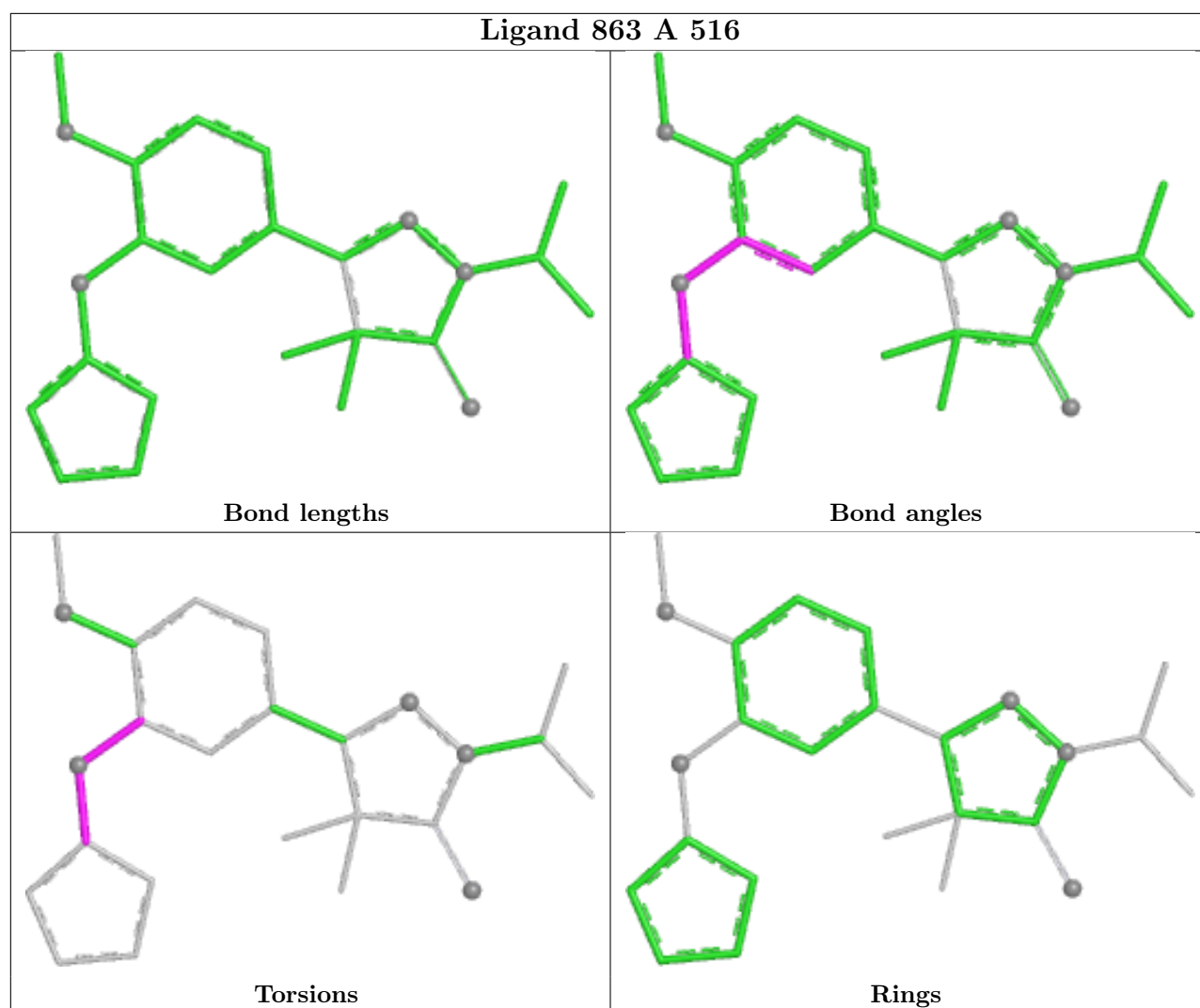
Bond angles



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	329/364 (90%)	0.36	18 (5%) 30 33	28, 47, 85, 124	0
1	B	324/364 (89%)	0.66	14 (4%) 40 42	30, 54, 76, 104	0
1	C	324/364 (89%)	0.52	15 (4%) 37 40	30, 50, 86, 116	0
1	D	324/364 (89%)	0.03	3 (0%) 81 83	27, 40, 69, 90	0
All	All	1301/1456 (89%)	0.39	50 (3%) 44 47	27, 48, 80, 124	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	293	THR	3.9
1	C	299	LEU	3.6
1	A	83	GLY	3.5
1	A	411	PRO	3.4
1	A	222	MET	3.3
1	A	299	LEU	3.3
1	B	91	VAL	3.2
1	D	351	GLY	3.2
1	A	84	VAL	3.1
1	B	89	GLU	2.9
1	C	292	VAL	2.9
1	B	147	MET	2.9
1	C	357	MET	2.9
1	C	411	PRO	2.9
1	D	354	ILE	2.8
1	A	292	VAL	2.7
1	A	351	GLY	2.7
1	A	298	LEU	2.7
1	B	286	MET	2.6
1	C	297	VAL	2.6
1	B	295	SER	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	308	GLN	2.5
1	B	133	LYS	2.5
1	C	363	ALA	2.5
1	C	283	LEU	2.5
1	C	298	LEU	2.5
1	C	303	TYR	2.4
1	A	352	MET	2.3
1	D	222	MET	2.3
1	A	296	GLY	2.3
1	B	298	LEU	2.3
1	B	222	MET	2.3
1	C	365	VAL	2.3
1	A	350	ARG	2.3
1	C	289	THR	2.2
1	A	326	LEU	2.2
1	B	131	LEU	2.2
1	B	296	GLY	2.2
1	B	303	TYR	2.2
1	B	412	GLN	2.1
1	C	300	LEU	2.1
1	A	363	ALA	2.1
1	A	239	LYS	2.1
1	A	410	ILE	2.1
1	C	330	ARG	2.1
1	B	309	VAL	2.1
1	C	222	MET	2.0
1	C	409	THR	2.0
1	A	357	MET	2.0
1	A	358	CYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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	C	501	4/4	0.69	0.21	71,79,81,84	0
8	PEG	B	509	7/7	0.76	0.26	71,77,82,86	0
8	PEG	D	514	7/7	0.76	0.17	65,70,75,80	0
4	EDO	A	506	4/4	0.81	0.18	66,72,72,76	0
4	EDO	A	512	4/4	0.83	0.22	57,60,67,70	0
4	EDO	D	512	4/4	0.83	0.21	71,77,85,86	0
4	EDO	A	513	4/4	0.84	0.25	69,72,75,77	0
4	EDO	C	508	4/4	0.85	0.19	62,63,66,74	0
8	PEG	D	513	7/7	0.85	0.20	71,74,81,84	0
4	EDO	B	504	4/4	0.85	0.18	60,77,77,78	0
4	EDO	C	509	4/4	0.86	0.22	61,65,72,72	0
4	EDO	D	508	4/4	0.86	0.19	59,60,62,65	0
4	EDO	A	510	4/4	0.86	0.32	45,60,60,71	0
4	EDO	A	507	4/4	0.87	0.17	66,73,74,76	0
4	EDO	C	513	4/4	0.87	0.15	76,78,81,82	0
4	EDO	D	506	4/4	0.87	0.22	53,56,56,72	0
4	EDO	B	506	4/4	0.87	0.14	66,67,68,70	0
4	EDO	D	510	4/4	0.87	0.15	74,74,78,79	0
4	EDO	B	507	4/4	0.87	0.15	65,70,72,76	0
5	DMS	B	510	4/4	0.87	0.24	68,86,92,102	0
7	EPE	B	511	15/15	0.87	0.16	85,91,95,102	0
4	EDO	A	508	4/4	0.87	0.18	68,71,76,79	0
4	EDO	C	506	4/4	0.87	0.17	66,71,72,75	0
4	EDO	A	509	4/4	0.87	0.18	61,66,69,76	0
4	EDO	B	503	4/4	0.88	0.19	65,68,70,78	0
4	EDO	A	517	4/4	0.88	0.18	57,57,59,66	0
4	EDO	D	511	4/4	0.88	0.17	47,51,51,60	0
7	EPE	D	518	15/15	0.89	0.18	49,75,90,91	0
6	863	B	512	25/25	0.89	0.15	55,59,81,82	0
8	PEG	C	502	7/7	0.89	0.21	83,86,95,101	0
4	EDO	B	505	4/4	0.89	0.16	63,70,72,85	0
7	EPE	B	513	15/15	0.89	0.16	55,108,124,126	0
4	EDO	D	505	4/4	0.90	0.16	66,70,72,73	0
4	EDO	C	507	4/4	0.90	0.15	69,70,74,74	0
4	EDO	B	508	4/4	0.90	0.25	45,55,57,57	0
4	EDO	A	504	4/4	0.90	0.14	58,65,65,72	0
4	EDO	A	511	4/4	0.90	0.18	56,63,66,66	0

Continued on next page...

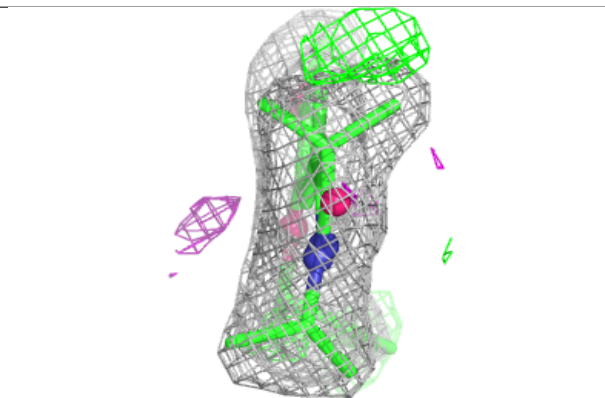
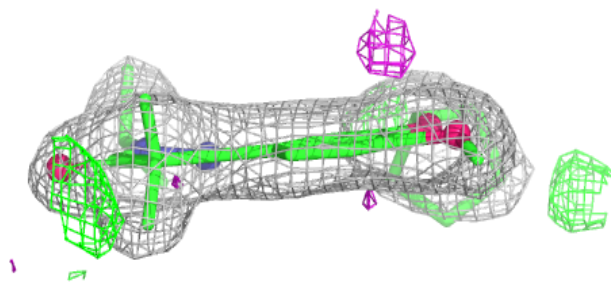
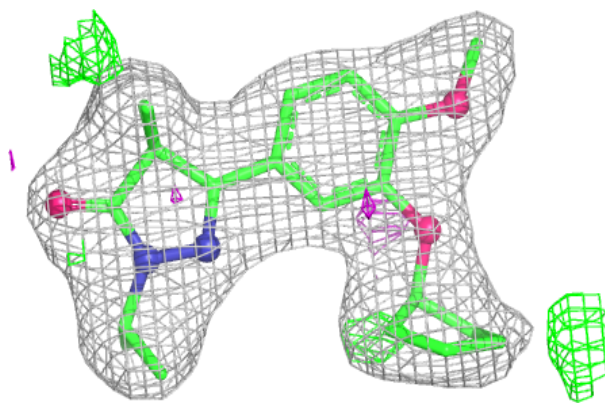
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	D	516	4/4	0.91	0.16	49,56,62,64	0
6	863	C	512	25/25	0.91	0.15	53,64,72,74	0
7	EPE	A	518	15/15	0.91	0.14	62,91,105,108	0
4	EDO	C	511	4/4	0.91	0.16	46,62,64,74	0
6	863	A	516	25/25	0.91	0.17	61,80,105,105	0
8	PEG	D	515	7/7	0.91	0.14	49,50,53,53	0
4	EDO	A	503	4/4	0.92	0.12	64,69,70,72	0
4	EDO	A	505	4/4	0.92	0.14	46,67,67,69	0
4	EDO	D	503	4/4	0.93	0.11	41,45,45,46	0
4	EDO	C	505	4/4	0.93	0.14	67,68,69,76	0
6	863	D	517	25/25	0.93	0.13	49,59,74,79	0
4	EDO	D	509	4/4	0.93	0.15	71,72,73,74	0
4	EDO	D	504	4/4	0.94	0.11	63,63,64,68	0
5	DMS	A	514	4/4	0.94	0.14	51,63,71,72	0
4	EDO	A	515	4/4	0.95	0.09	41,45,48,51	0
4	EDO	D	507	4/4	0.96	0.08	45,50,51,52	0
7	EPE	C	510	15/15	0.96	0.09	52,60,79,90	0
3	MG	D	502	1/1	0.98	0.06	26,26,26,26	0
3	MG	C	504	1/1	0.99	0.03	27,27,27,27	0
2	ZN	C	503	1/1	1.00	0.01	41,41,41,41	0
2	ZN	D	501	1/1	1.00	0.01	36,36,36,36	0
3	MG	A	502	1/1	1.00	0.01	29,29,29,29	0
3	MG	B	502	1/1	1.00	0.03	31,31,31,31	0
2	ZN	A	501	1/1	1.00	0.02	40,40,40,40	0
2	ZN	B	501	1/1	1.00	0.04	44,44,44,44	0

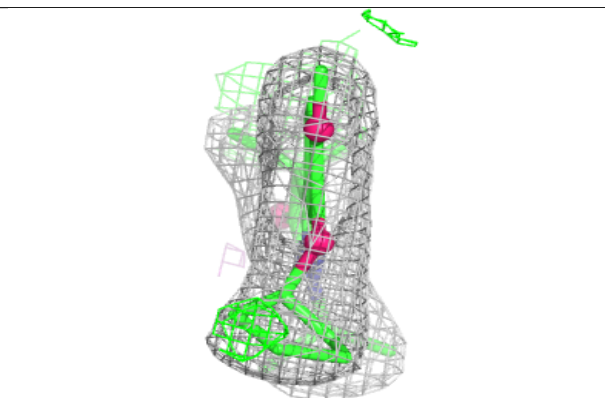
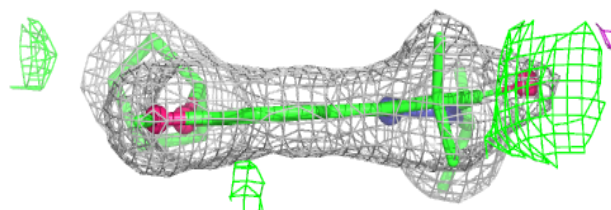
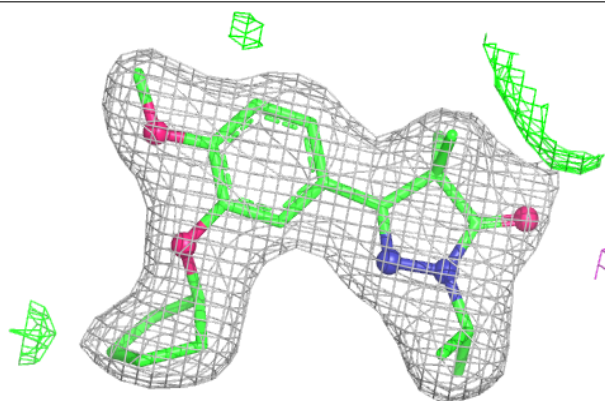
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 863 B 512:

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

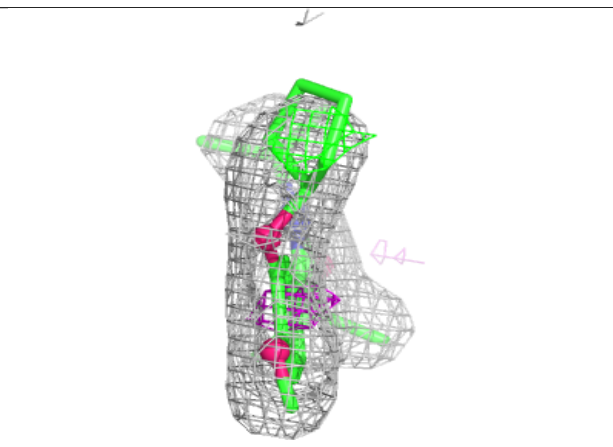
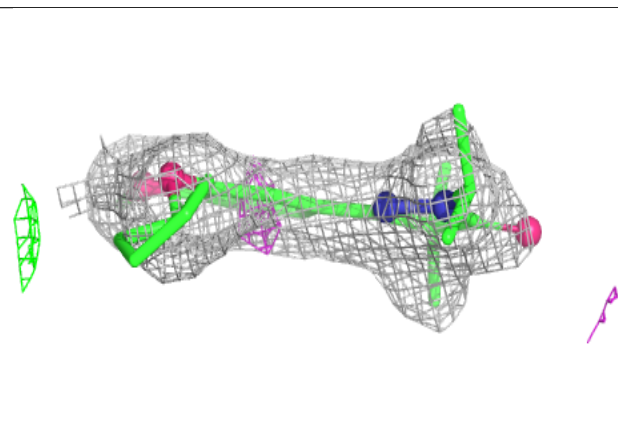
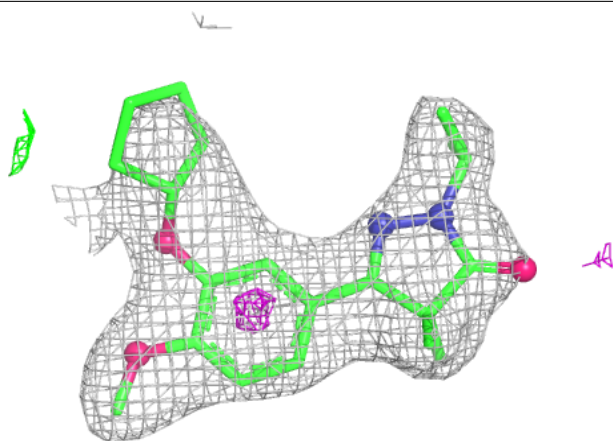
**Electron density around 863 C 512:**

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

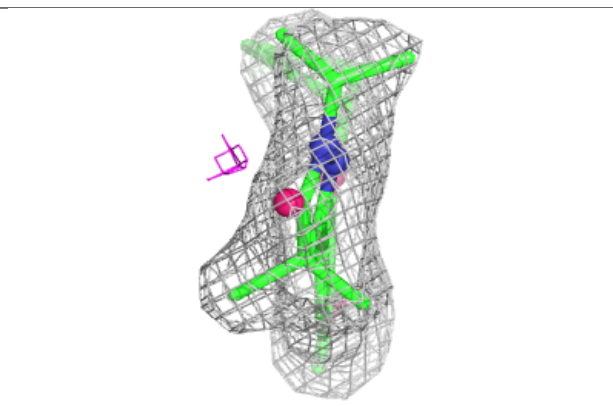
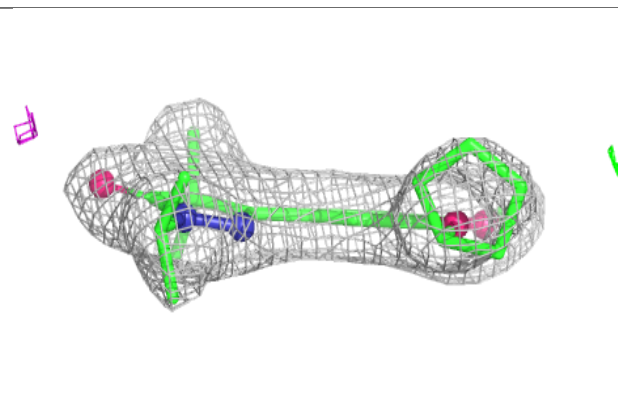
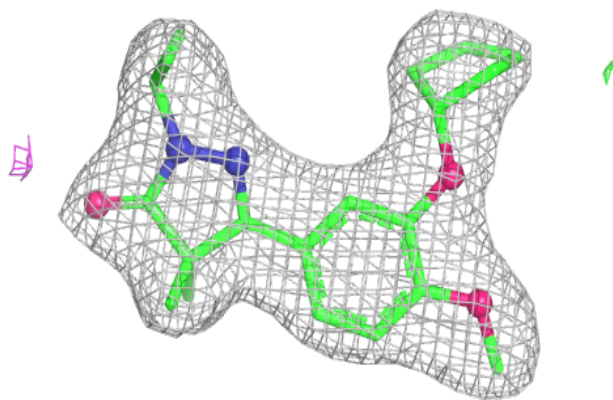


Electron density around 863 A 516:

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

**Electron density around 863 D 517:**

$2mF_o-DF_c$ (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.