



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:13 PM UTC

PDB ID : 6FET / pdb_00006fet
Title : Crystal structure of human phosphodiesterase 4D2 catalytic domain with inhibitor NPD-1439
Authors : Singh, A.K.; Brown, D.G.
Deposited on : 2018-01-03
Resolution : 1.88 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

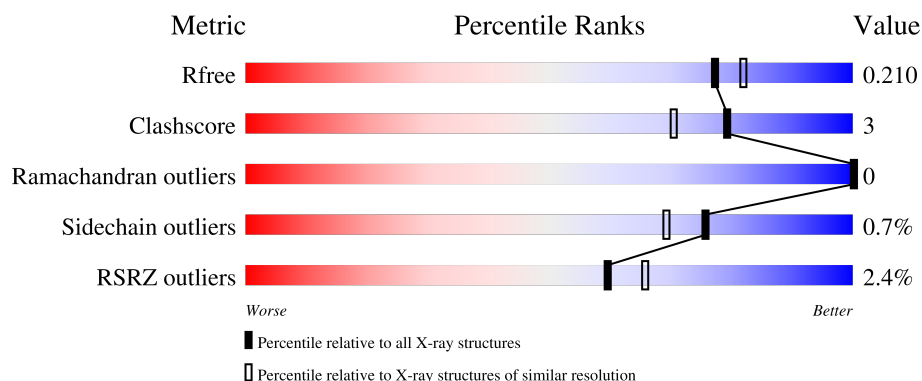
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	3% 84% 6% 10%
1	B	364	% 85% % 11%
1	C	364	4% 82% 6% 11%
1	D	364	% 80% 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
9	PG4	D	502	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 11731 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	323	Total	C	N	O	S	0	0	0
			2613	1654	446	499	14			
1	C	324	Total	C	N	O	S	0	1	0
			2630	1663	450	503	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

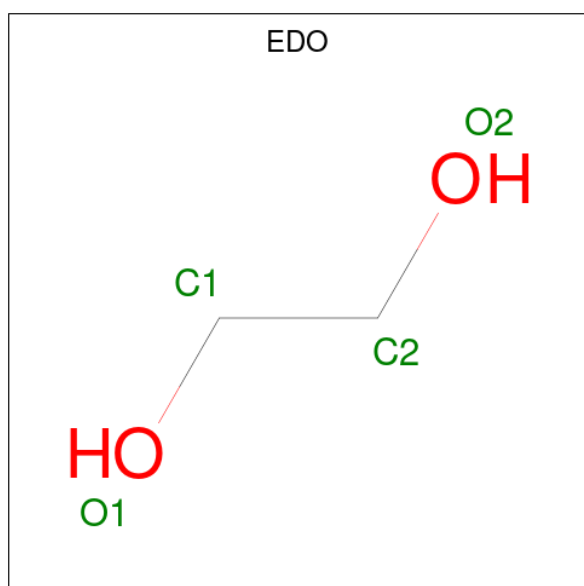
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

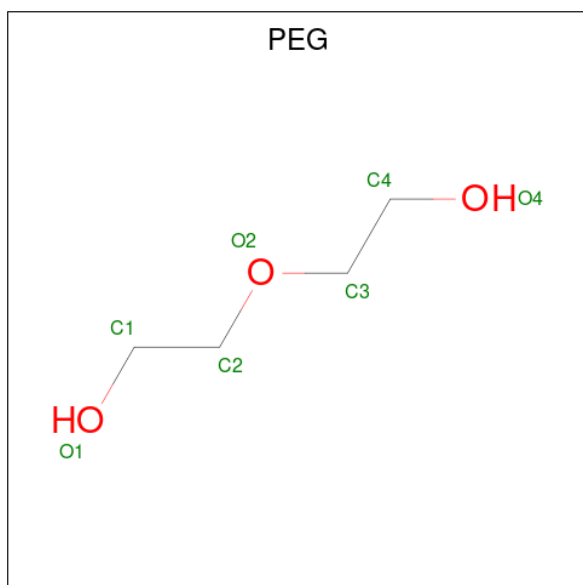
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0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

Continued on next page...

Continued from previous page...

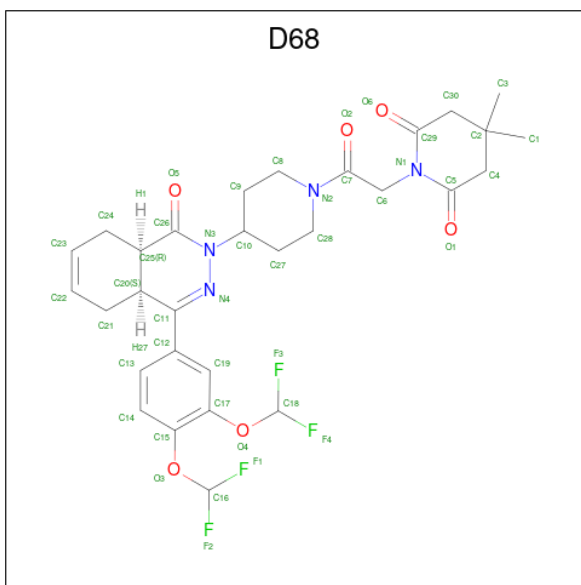
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



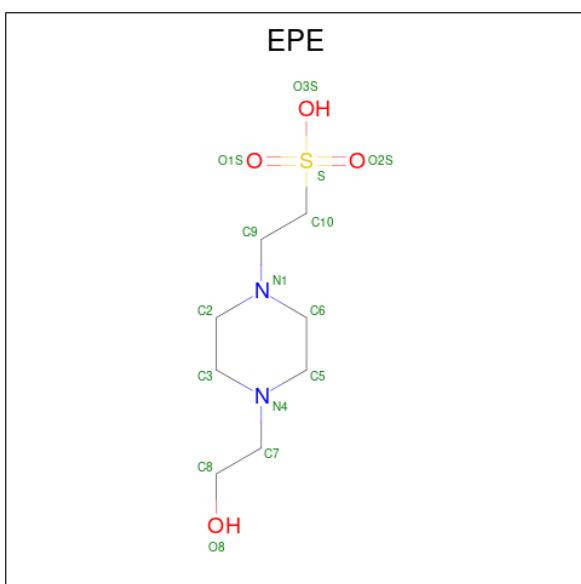
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is 1-(2-{4-[(4aS,8aR)-4-[3,4-bis(difluoromethoxy)phenyl]-1-oxo-1,2,4a,5,8,8a-hexahydrophthalazin-2-yl]piperidin-1-yl}-2-oxoethyl)-4,4-dimethylpiperidine-2,6-dione (CCD ID: D68) (formula: C₃₀H₃₄F₄N₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 44	C 30	F 4	N 4	O 6	0	0
6	B	1	Total 44	C 30	F 4	N 4	O 6	0	0
6	C	1	Total 44	C 30	F 4	N 4	O 6	0	0
6	D	1	Total 44	C 30	F 4	N 4	O 6	0	0

- Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).

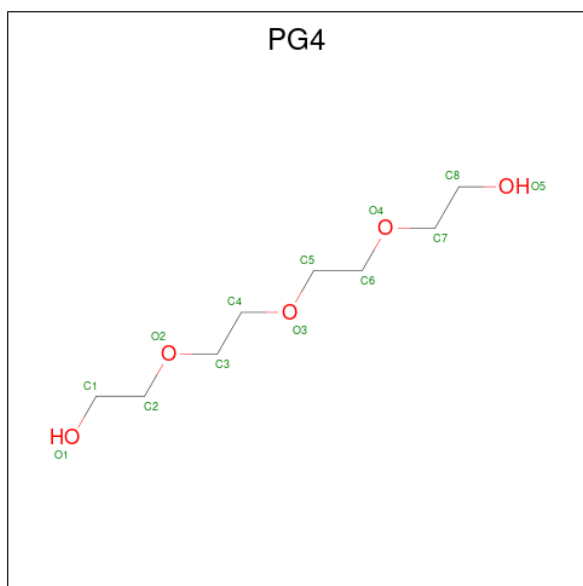


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
7	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
7	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
7	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
7	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 8 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Ni	0	0
			1	1		
8	D	1	Total	Ni	0	0
			1	1		

- Molecule 9 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			13	8	5		
9	D	1	Total	C	O	0	0
			13	8	5		

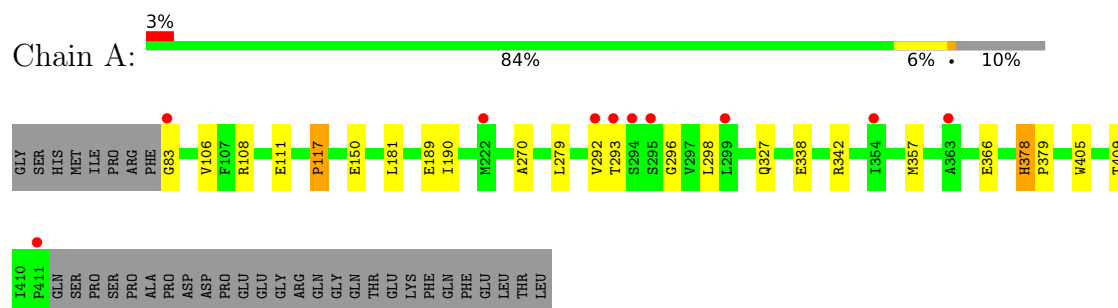
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	163	Total 163	O 163	0	0
10	B	169	Total 169	O 169	0	0
10	C	118	Total 118	O 118	0	0
10	D	175	Total 175	O 175	0	0

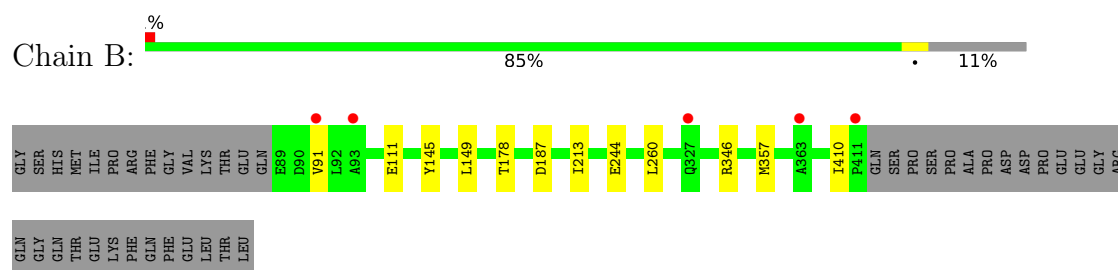
3 Residue-property plots [i](#)

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.

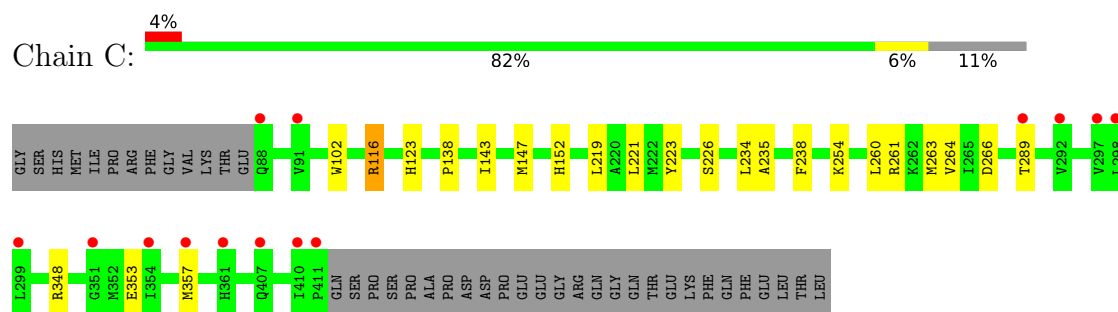
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



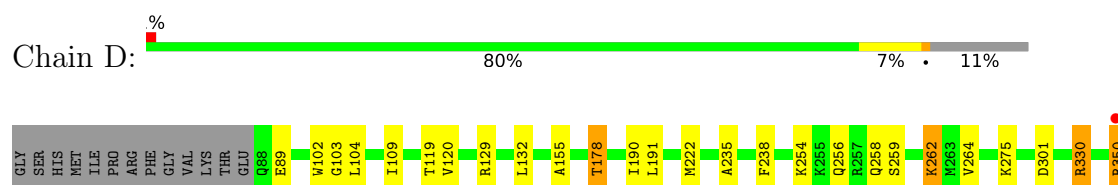
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

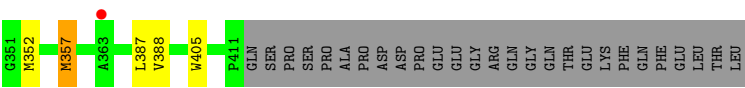


- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



- 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	97.19Å 110.71Å 161.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.35 – 1.88 55.35 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.9 (55.35-1.88) 99.9 (55.35-1.88)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.171 , 0.199 0.184 , 0.210	Depositor DCC
R_{free} test set	7234 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11731	wwPDB-VP
Average B, all atoms (Å ²)	41.0	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: ZN, NI, PG4, EDO, MG, EPE, PEG, D68

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	1.20	4/2712 (0.1%)	0.99	1/3684 (0.0%)
1	B	1.19	5/2667 (0.2%)	0.97	1/3624 (0.0%)
1	C	1.24	7/2684 (0.3%)	1.01	4/3647 (0.1%)
1	D	1.38	14/2676 (0.5%)	1.01	5/3636 (0.1%)
All	All	1.25	30/10739 (0.3%)	1.00	11/14591 (0.1%)

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	348	ARG	N-CA	6.79	1.54	1.46
1	B	187	ASP	CA-C	6.35	1.61	1.52
1	B	213	ILE	C-O	-6.03	1.17	1.24
1	D	132	LEU	C-O	-5.95	1.17	1.24
1	A	378	HIS	C-O	-5.84	1.19	1.24
1	D	103	GLY	N-CA	5.81	1.53	1.45
1	D	178	THR	CA-C	5.67	1.58	1.53
1	D	235	ALA	C-O	-5.61	1.17	1.24
1	D	264	VAL	C-O	-5.57	1.17	1.24
1	C	235	ALA	C-O	-5.51	1.17	1.24
1	C	266	ASP	C-O	-5.49	1.17	1.24
1	B	145	TYR	C-O	-5.37	1.17	1.24
1	C	263	MET	C-O	-5.33	1.17	1.24
1	D	259	SER	C-O	-5.31	1.18	1.24
1	C	260	LEU	C-O	-5.30	1.18	1.24
1	D	119	THR	C-O	-5.29	1.18	1.24
1	D	120	VAL	C-O	-5.29	1.17	1.24
1	D	238	PHE	C-O	-5.27	1.17	1.24
1	D	388	VAL	C-O	-5.27	1.17	1.24
1	D	191	LEU	C-O	-5.23	1.18	1.24
1	D	387	LEU	C-O	-5.18	1.18	1.24
1	C	264	VAL	C-O	-5.13	1.18	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	149	LEU	C-O	-5.12	1.18	1.24
1	D	256	GLN	C-O	-5.09	1.18	1.24
1	D	262	LYS	C-O	-5.09	1.18	1.24
1	B	260	LEU	C-O	-5.08	1.18	1.24
1	A	117	PRO	C-O	-5.07	1.18	1.24
1	A	83	GLY	N-CA	5.04	1.53	1.45
1	A	106	VAL	C-O	-5.04	1.18	1.24
1	C	219	LEU	C-O	-5.04	1.18	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	301	ASP	N-CA-C	7.16	120.88	112.72
1	D	102	TRP	CA-C-N	-6.53	111.55	122.25
1	D	102	TRP	C-N-CA	-6.53	111.55	122.25
1	D	357	MET	N-CA-C	6.37	120.83	113.38
1	C	116	ARG	NE-CZ-NH2	6.19	124.77	119.20
1	D	330	ARG	NE-CZ-NH1	-5.80	115.70	121.50
1	A	357	MET	N-CA-C	5.77	119.91	112.86
1	C	102	TRP	CA-C-N	-5.49	113.25	122.25
1	C	102	TRP	C-N-CA	-5.49	113.25	122.25
1	C	353	GLU	CA-C-O	-5.36	115.72	121.56
1	B	410	ILE	CB-CA-C	-5.31	106.00	110.94

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	17	0
1	B	2613	0	2570	6	0
1	C	2630	0	2583	14	0
1	D	2622	0	2578	15	0
2	A	1	0	0	0	0
2	B	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	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	76	0	114	2	0
4	B	64	0	96	2	0
4	C	48	0	72	4	0
4	D	80	0	120	7	0
5	A	7	0	10	0	0
5	B	7	0	10	0	0
5	C	7	0	10	2	0
5	D	7	0	10	2	0
6	A	44	0	0	0	0
6	B	44	0	0	1	0
6	C	44	0	0	1	0
6	D	44	0	0	0	0
7	A	15	0	17	4	0
7	B	30	0	36	2	0
7	C	15	0	17	1	0
7	D	15	0	17	0	0
8	A	1	0	0	0	0
8	D	1	0	0	0	0
9	C	13	0	18	0	0
9	D	13	0	18	10	0
10	A	163	0	0	0	0
10	B	169	0	0	0	0
10	C	118	0	0	0	0
10	D	175	0	0	2	0
All	All	11731	0	10912	60	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 3.

All (60) 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)
9:D:502:PG4:H42	9:D:502:PG4:H11	1.45	0.99
9:D:502:PG4:H11	9:D:502:PG4:C4	2.07	0.83
1:D:222:MET:HA	9:D:502:PG4:H31	1.70	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ILE:HD11	4:A:524:EDO:H22	1.72	0.70
1:D:350:ARG:HD3	1:D:352:MET:HE2	1.74	0.69
1:A:111:GLU:OE1	7:A:518:EPE:H52	1.92	0.69
1:C:152:HIS:HE1	5:C:511:PEG:H22	1.58	0.68
1:C:261:ARG:HB2	4:C:508:EDO:H12	1.77	0.66
1:A:338:GLU:O	1:A:342:ARG:HG3	1.98	0.64
1:C:116:ARG:HD2	1:C:147:MET:HE1	1.79	0.64
1:D:129:ARG:HB3	4:D:514:EDO:H22	1.80	0.62
4:B:508:EDO:H11	4:D:511:EDO:H21	1.83	0.59
1:B:111:GLU:OE1	7:B:513:EPE:H32	2.04	0.57
1:A:181:LEU:CD2	1:A:298:LEU:HD12	2.36	0.56
1:A:111:GLU:OE2	7:A:518:EPE:H72	2.05	0.55
1:C:138:PRO:HG2	4:C:509:EDO:H22	1.89	0.54
1:C:152:HIS:CE1	5:C:511:PEG:H22	2.43	0.53
1:C:357:MET:HE1	6:C:515:D68:F3	2.00	0.52
9:D:502:PG4:C4	9:D:502:PG4:C1	2.84	0.51
9:D:502:PG4:O4	9:D:502:PG4:H41	2.10	0.51
1:D:275:LYS:NZ	10:D:603:HOH:O	2.42	0.51
1:B:346:ARG:HH22	4:B:508:EDO:H12	1.78	0.49
1:A:117:PRO:HD2	1:A:150:GLU:OE2	2.12	0.49
1:A:189:GLU:HG3	4:A:521:EDO:H22	1.95	0.48
1:B:244:GLU:OE2	1:C:254:LYS:NZ	2.46	0.48
1:A:378:HIS:HB3	1:A:379:PRO:HD3	1.96	0.48
1:A:181:LEU:HD23	1:A:298:LEU:HD12	1.95	0.47
1:C:238:PHE:CD2	9:D:502:PG4:H82	2.48	0.47
1:C:234:LEU:HB3	9:D:502:PG4:H62	1.95	0.47
1:A:111:GLU:CD	7:A:518:EPE:H52	2.39	0.47
1:D:262:LYS:HD3	4:D:507:EDO:C2	2.45	0.46
1:C:261:ARG:HB2	4:C:508:EDO:C1	2.44	0.45
1:A:111:GLU:OE2	7:A:518:EPE:H32	2.17	0.45
1:C:289:THR:O	1:C:289:THR:HG22	2.16	0.45
1:D:254:LYS:O	1:D:258:GLN:HG3	2.16	0.45
1:A:366:GLU:HG2	1:A:409:THR:OG1	2.16	0.45
1:D:104:LEU:HD11	1:D:109:ILE:CD1	2.47	0.45
1:A:181:LEU:HD21	1:A:298:LEU:HD12	1.99	0.44
1:D:155:ALA:HA	4:D:513:EDO:H11	2.00	0.44
1:B:357:MET:HE2	6:B:514:D68:C6	2.47	0.44
7:C:512:EPE:H51	7:C:512:EPE:H81	1.77	0.43
1:D:190:ILE:HD13	4:D:514:EDO:H21	1.98	0.43
9:D:502:PG4:O1	9:D:502:PG4:H71	2.18	0.43
1:A:270:ALA:HB1	1:A:279:LEU:HD11	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:TRP:O	1:A:409:THR:HG23	2.19	0.42
1:C:223:TYR:OH	9:D:502:PG4:H32	2.19	0.42
1:A:292:VAL:C	1:A:293:THR:HG23	2.44	0.42
1:C:123:HIS:ND1	1:C:143:ILE:HD11	2.35	0.42
4:D:510:EDO:C2	10:D:717:HOH:O	2.68	0.42
1:C:152:HIS:NE2	4:C:501:EDO:H12	2.34	0.41
1:D:178:THR:HA	5:D:519:PEG:H11	2.03	0.41
1:D:190:ILE:HD11	4:D:515:EDO:H12	2.03	0.41
1:D:104:LEU:HD11	1:D:109:ILE:HD11	2.02	0.40
1:D:222:MET:HA	9:D:502:PG4:C3	2.46	0.40
1:B:111:GLU:OE1	7:B:513:EPE:H81	2.21	0.40
1:A:292:VAL:CG1	1:A:296:GLY:HA2	2.50	0.40
1:D:330:ARG:HD2	1:D:405:TRP:CZ3	2.57	0.40
1:B:357:MET:HE3	1:B:357:MET:HB2	1.72	0.40
1:D:357:MET:HE3	1:D:357:MET:HB2	1.71	0.40
5:D:519:PEG:H12	5:D:519:PEG:H31	1.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	321/364 (88%)	318 (99%)	3 (1%)	0	100	100
1	C	323/364 (89%)	317 (98%)	6 (2%)	0	100	100
1	D	322/364 (88%)	316 (98%)	6 (2%)	0	100	100
All	All	1293/1456 (89%)	1272 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

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%)	298 (99%)	2 (1%)	76	69
1	B	295/331 (89%)	293 (99%)	2 (1%)	76	69
1	C	297/331 (90%)	295 (99%)	2 (1%)	76	69
1	D	296/331 (89%)	294 (99%)	2 (1%)	76	69
All	All	1188/1324 (90%)	1180 (99%)	8 (1%)	76	69

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ARG
1	A	327	GLN
1	B	91	VAL
1	B	178	THR
1	C	221	LEU
1	C	226	SER
1	D	89	GLU
1	D	350	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	152	HIS
1	A	224	ASN
1	A	250	GLN
1	A	258	GLN
1	A	308	GLN
1	A	369	GLN
1	B	210	GLN
1	B	312	ASN
1	B	321	ASN
1	C	210	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	250	GLN
1	D	127	GLN
1	D	210	GLN
1	D	250	GLN
1	D	308	GLN
1	D	321	ASN
1	D	369	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 92 ligands modelled in this entry, 10 are monoatomic - leaving 82 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	508	-	3,3,3	0.20	0	2,2,2	0.61	0
4	EDO	B	503	-	3,3,3	0.48	0	2,2,2	0.73	0
4	EDO	B	506	-	3,3,3	0.40	0	2,2,2	1.04	0
4	EDO	A	514	-	3,3,3	0.38	0	2,2,2	1.49	0
4	EDO	D	513	-	3,3,3	0.18	0	2,2,2	0.75	0
4	EDO	A	503	-	3,3,3	0.51	0	2,2,2	0.59	0
4	EDO	B	515	-	3,3,3	0.26	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	D	526	-	3,3,3	0.74	0	2,2,2	0.21	0
4	EDO	D	511	-	3,3,3	0.41	0	2,2,2	0.86	0
4	EDO	D	523	-	3,3,3	0.25	0	2,2,2	0.67	0
4	EDO	B	518	-	3,3,3	0.45	0	2,2,2	0.62	0
4	EDO	C	502	-	3,3,3	0.41	0	2,2,2	1.03	0
9	PG4	D	502	-	12,12,12	0.51	0	11,11,11	1.14	2 (18%)
4	EDO	D	501	-	3,3,3	0.31	0	2,2,2	1.53	0
4	EDO	C	506	-	3,3,3	0.15	0	2,2,2	0.39	0
7	EPE	D	521	-	15,15,15	2.97	2 (13%)	19,20,20	1.85	4 (21%)
4	EDO	A	521	-	3,3,3	0.26	0	2,2,2	0.65	0
4	EDO	C	509	-	3,3,3	0.15	0	2,2,2	1.10	0
4	EDO	D	507	-	3,3,3	0.29	0	2,2,2	0.85	0
4	EDO	C	507	-	3,3,3	0.28	0	2,2,2	1.19	0
4	EDO	D	512	-	3,3,3	0.30	0	2,2,2	0.14	0
4	EDO	A	509	-	3,3,3	0.25	0	2,2,2	1.76	0
4	EDO	A	515	-	3,3,3	0.32	0	2,2,2	1.28	0
5	PEG	A	510	-	6,6,6	0.42	0	5,5,5	1.00	0
7	EPE	B	513	-	15,15,15	2.12	1 (6%)	19,20,20	2.46	7 (36%)
6	D68	D	520	-	47,48,48	0.71	2 (4%)	63,71,71	1.31	5 (7%)
9	PG4	C	514	-	12,12,12	0.68	0	11,11,11	0.94	0
4	EDO	D	506	-	3,3,3	0.60	0	2,2,2	0.40	0
4	EDO	D	517	-	3,3,3	0.14	0	2,2,2	1.32	0
4	EDO	A	524	-	3,3,3	0.25	0	2,2,2	0.17	0
4	EDO	D	516	-	3,3,3	0.52	0	2,2,2	1.36	0
4	EDO	D	525	-	3,3,3	0.60	0	2,2,2	0.40	0
5	PEG	C	511	-	6,6,6	0.30	0	5,5,5	0.88	0
4	EDO	D	515	-	3,3,3	0.39	0	2,2,2	0.30	0
4	EDO	C	510	-	3,3,3	0.65	0	2,2,2	0.68	0
4	EDO	B	508	-	3,3,3	0.35	0	2,2,2	0.59	0
4	EDO	B	522	-	3,3,3	0.26	0	2,2,2	0.41	0
4	EDO	C	517	-	3,3,3	0.27	0	2,2,2	0.59	0
5	PEG	D	519	-	6,6,6	0.55	0	5,5,5	0.79	0
4	EDO	C	501	-	3,3,3	0.27	0	2,2,2	0.70	0
7	EPE	C	512	-	15,15,15	2.64	1 (6%)	19,20,20	1.91	6 (31%)
4	EDO	A	513	-	3,3,3	0.15	0	2,2,2	0.43	0
4	EDO	C	516	-	3,3,3	0.45	0	2,2,2	0.53	0
4	EDO	A	504	-	3,3,3	0.95	0	2,2,2	0.24	0
7	EPE	B	507	-	15,15,15	1.29	1 (6%)	19,20,20	1.89	5 (26%)
4	EDO	C	513	-	3,3,3	0.75	0	2,2,2	0.66	0
4	EDO	B	511	-	3,3,3	0.52	0	2,2,2	0.29	0
4	EDO	A	523	-	3,3,3	0.51	0	2,2,2	0.53	0
4	EDO	B	504	-	3,3,3	0.63	0	2,2,2	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	D	522	-	3,3,3	0.52	0	2,2,2	0.50	0
4	EDO	B	510	-	3,3,3	0.49	0	2,2,2	1.20	0
4	EDO	B	521	-	3,3,3	1.07	0	2,2,2	0.73	0
6	D68	B	514	-	47,48,48	0.51	0	63,71,71	1.34	4 (6%)
4	EDO	D	510	-	3,3,3	0.33	0	2,2,2	0.51	0
4	EDO	A	519	-	3,3,3	0.37	0	2,2,2	0.80	0
4	EDO	A	511	-	3,3,3	0.61	0	2,2,2	0.44	0
4	EDO	A	512	-	3,3,3	0.39	0	2,2,2	0.28	0
4	EDO	C	518	-	3,3,3	0.25	0	2,2,2	0.54	0
4	EDO	B	517	-	3,3,3	0.33	0	2,2,2	0.54	0
4	EDO	A	522	-	3,3,3	0.39	0	2,2,2	1.32	0
4	EDO	B	519	-	3,3,3	0.73	0	2,2,2	0.11	0
4	EDO	D	503	-	3,3,3	0.33	0	2,2,2	0.62	0
4	EDO	D	508	-	3,3,3	0.28	0	2,2,2	1.25	0
4	EDO	D	518	-	3,3,3	0.28	0	2,2,2	0.14	0
4	EDO	A	506	-	3,3,3	0.26	0	2,2,2	1.39	0
4	EDO	B	505	-	3,3,3	0.44	0	2,2,2	0.57	0
4	EDO	A	508	-	3,3,3	0.64	0	2,2,2	0.83	0
4	EDO	A	516	-	3,3,3	0.26	0	2,2,2	0.92	0
4	EDO	D	524	-	3,3,3	1.39	0	2,2,2	0.83	0
4	EDO	D	509	-	3,3,3	0.61	0	2,2,2	0.97	0
4	EDO	B	516	-	3,3,3	0.23	0	2,2,2	1.25	0
4	EDO	A	507	-	3,3,3	0.17	0	2,2,2	0.64	0
4	EDO	C	503	-	3,3,3	0.30	0	2,2,2	0.40	0
4	EDO	B	520	-	3,3,3	0.76	0	2,2,2	0.51	0
7	EPE	A	518	-	15,15,15	2.74	2 (13%)	19,20,20	1.59	3 (15%)
4	EDO	A	505	-	3,3,3	0.58	0	2,2,2	0.60	0
6	D68	C	515	-	47,48,48	0.66	1 (2%)	63,71,71	0.84	2 (3%)
4	EDO	A	520	-	3,3,3	0.52	0	2,2,2	0.41	0
4	EDO	B	509	-	3,3,3	0.22	0	2,2,2	0.68	0
5	PEG	B	512	-	6,6,6	0.92	0	5,5,5	1.64	2 (40%)
6	D68	A	517	-	47,48,48	0.61	0	63,71,71	1.11	4 (6%)
4	EDO	D	514	-	3,3,3	0.39	0	2,2,2	0.74	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	508	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	503	-	-	0/1/1/1	-
4	EDO	B	506	-	-	1/1/1/1	-
4	EDO	A	514	-	-	0/1/1/1	-
4	EDO	D	513	-	-	0/1/1/1	-
4	EDO	A	503	-	-	0/1/1/1	-
4	EDO	B	515	-	-	1/1/1/1	-
4	EDO	D	526	-	-	1/1/1/1	-
4	EDO	D	511	-	-	0/1/1/1	-
4	EDO	D	523	-	-	0/1/1/1	-
4	EDO	B	518	-	-	1/1/1/1	-
4	EDO	C	502	-	-	1/1/1/1	-
9	PG4	D	502	-	-	9/10/10/10	-
4	EDO	D	501	-	-	1/1/1/1	-
4	EDO	C	506	-	-	1/1/1/1	-
7	EPE	D	521	-	-	2/9/19/19	0/1/1/1
4	EDO	A	521	-	-	0/1/1/1	-
4	EDO	C	509	-	-	0/1/1/1	-
4	EDO	D	507	-	-	0/1/1/1	-
4	EDO	C	507	-	-	1/1/1/1	-
4	EDO	D	512	-	-	1/1/1/1	-
4	EDO	A	509	-	-	1/1/1/1	-
4	EDO	A	515	-	-	0/1/1/1	-
5	PEG	A	510	-	-	4/4/4/4	-
7	EPE	B	513	-	-	4/9/19/19	0/1/1/1
6	D68	D	520	-	-	2/24/79/79	0/5/5/5
9	PG4	C	514	-	-	4/10/10/10	-
4	EDO	D	506	-	-	0/1/1/1	-
4	EDO	D	517	-	-	0/1/1/1	-
4	EDO	A	524	-	-	1/1/1/1	-
4	EDO	D	516	-	-	1/1/1/1	-
4	EDO	D	525	-	-	1/1/1/1	-
5	PEG	C	511	-	-	3/4/4/4	-
4	EDO	D	515	-	-	1/1/1/1	-
4	EDO	C	510	-	-	0/1/1/1	-
4	EDO	B	508	-	-	0/1/1/1	-
4	EDO	B	522	-	-	1/1/1/1	-
4	EDO	C	517	-	-	1/1/1/1	-
5	PEG	D	519	-	-	2/4/4/4	-
4	EDO	C	501	-	-	1/1/1/1	-
7	EPE	C	512	-	-	6/9/19/19	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	513	-	-	0/1/1/1	-
4	EDO	C	516	-	-	0/1/1/1	-
4	EDO	A	504	-	-	0/1/1/1	-
7	EPE	B	507	-	-	3/9/19/19	0/1/1/1
4	EDO	C	513	-	-	0/1/1/1	-
4	EDO	B	511	-	-	1/1/1/1	-
4	EDO	A	523	-	-	1/1/1/1	-
4	EDO	B	504	-	-	0/1/1/1	-
4	EDO	D	522	-	-	1/1/1/1	-
4	EDO	B	510	-	-	1/1/1/1	-
4	EDO	B	521	-	-	0/1/1/1	-
6	D68	B	514	-	-	2/24/79/79	0/5/5/5
4	EDO	D	510	-	-	1/1/1/1	-
4	EDO	A	519	-	-	0/1/1/1	-
4	EDO	A	511	-	-	1/1/1/1	-
4	EDO	A	512	-	-	0/1/1/1	-
4	EDO	C	518	-	-	1/1/1/1	-
4	EDO	B	517	-	-	1/1/1/1	-
4	EDO	A	522	-	-	1/1/1/1	-
4	EDO	B	519	-	-	0/1/1/1	-
4	EDO	D	503	-	-	1/1/1/1	-
4	EDO	D	508	-	-	0/1/1/1	-
4	EDO	D	518	-	-	0/1/1/1	-
4	EDO	A	506	-	-	1/1/1/1	-
4	EDO	B	505	-	-	0/1/1/1	-
4	EDO	A	508	-	-	0/1/1/1	-
4	EDO	A	516	-	-	1/1/1/1	-
4	EDO	D	524	-	-	1/1/1/1	-
4	EDO	D	509	-	-	0/1/1/1	-
4	EDO	B	516	-	-	0/1/1/1	-
4	EDO	A	507	-	-	1/1/1/1	-
4	EDO	C	503	-	-	1/1/1/1	-
4	EDO	B	520	-	-	0/1/1/1	-
7	EPE	A	518	-	-	5/9/19/19	0/1/1/1
4	EDO	A	505	-	-	0/1/1/1	-
6	D68	C	515	-	-	2/24/79/79	0/5/5/5
4	EDO	A	520	-	-	1/1/1/1	-
4	EDO	B	509	-	-	0/1/1/1	-
5	PEG	B	512	-	-	2/4/4/4	-
6	D68	A	517	-	-	2/24/79/79	0/5/5/5
4	EDO	D	514	-	-	1/1/1/1	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	521	EPE	C10-S	-10.61	1.62	1.77
7	A	518	EPE	C10-S	-10.03	1.63	1.77
7	C	512	EPE	C10-S	-9.68	1.64	1.77
7	B	513	EPE	C10-S	-7.65	1.66	1.77
7	B	507	EPE	C10-S	-3.95	1.72	1.77
7	D	521	EPE	O1S-S	-3.36	1.35	1.45
6	D	520	D68	C6-N1	2.74	1.50	1.46
6	D	520	D68	C21-C20	-2.62	1.49	1.53
7	A	518	EPE	O3S-S	-2.20	1.38	1.47
6	C	515	D68	N3-N4	-2.08	1.33	1.37

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	513	EPE	O2S-S-C10	6.35	116.33	106.73
7	A	518	EPE	O2S-S-C10	5.36	114.83	106.73
7	D	521	EPE	O1S-S-C10	4.97	114.24	106.73
7	C	512	EPE	O3S-S-C10	4.79	115.38	106.00
6	B	514	D68	C13-C12-C11	4.71	126.38	120.74
6	B	514	D68	C19-C12-C11	-4.55	114.59	120.24
6	B	514	D68	C17-O4-C18	4.48	134.70	118.50
6	D	520	D68	C13-C12-C11	4.42	126.03	120.74
7	D	521	EPE	O2S-S-O1S	-4.41	99.49	113.82
7	B	513	EPE	O2S-S-O1S	-4.32	99.77	113.82
6	D	520	D68	C19-C12-C11	-4.22	114.99	120.24
6	D	520	D68	C17-O4-C18	4.05	133.13	118.50
7	B	507	EPE	O1S-S-C10	4.00	112.77	106.73
7	B	513	EPE	O3S-S-O1S	3.89	121.12	111.40
6	A	517	D68	C17-O4-C18	3.87	132.47	118.50
7	C	512	EPE	O2S-S-C10	3.86	112.56	106.73
7	B	507	EPE	O2S-S-C10	3.75	112.40	106.73
7	B	507	EPE	C2-C3-N4	3.21	117.13	110.65
7	B	513	EPE	O3S-S-O2S	-3.20	103.38	111.40
6	B	514	D68	O5-C26-N3	-2.77	118.33	121.63
6	C	515	D68	C17-O4-C18	2.74	128.38	118.50
6	A	517	D68	C19-C12-C11	-2.69	116.90	120.24
7	C	512	EPE	C9-N1-C2	-2.64	104.21	111.24
7	B	513	EPE	C2-C3-N4	2.60	115.90	110.65
5	B	512	PEG	C3-O2-C2	2.56	124.45	113.26
7	B	507	EPE	O2S-S-O1S	-2.55	105.52	113.82
6	A	517	D68	C27-C10-N3	2.53	113.66	110.89
6	A	517	D68	C13-C12-C11	2.49	123.72	120.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	512	PEG	O2-C3-C4	2.49	121.07	110.11
7	A	518	EPE	O3S-S-O2S	-2.44	105.29	111.40
7	C	512	EPE	O2S-S-O1S	-2.42	105.94	113.82
7	B	513	EPE	C7-N4-C3	2.32	117.42	111.24
7	C	512	EPE	C3-C2-N1	2.30	115.30	110.65
7	B	513	EPE	C5-N4-C3	2.28	113.75	108.84
7	D	521	EPE	O2S-S-C10	2.23	110.10	106.73
6	D	520	D68	C6-N1-C29	2.22	119.48	117.80
6	D	520	D68	O4-C17-C19	2.15	128.69	123.87
7	D	521	EPE	O3S-S-C10	2.14	110.19	106.00
7	B	507	EPE	C6-C5-N4	2.12	114.93	110.65
7	A	518	EPE	C7-N4-C3	-2.10	105.65	111.24
9	D	502	PG4	O2-C2-C1	2.06	119.18	110.11
7	C	512	EPE	C10-C9-N1	2.03	120.05	112.36
9	D	502	PG4	C3-O2-C2	2.03	122.15	113.26
6	C	515	D68	C29-N1-C5	2.01	125.01	123.98

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	518	EPE	C9-C10-S-O1S
7	A	518	EPE	C9-C10-S-O3S
7	B	507	EPE	C9-C10-S-O2S
7	B	507	EPE	C9-C10-S-O3S
7	B	513	EPE	C8-C7-N4-C3
7	B	513	EPE	C9-C10-S-O2S
7	C	512	EPE	C10-C9-N1-C6
7	C	512	EPE	C8-C7-N4-C5
7	C	512	EPE	C9-C10-S-O2S
7	D	521	EPE	C8-C7-N4-C3
5	B	512	PEG	C4-C3-O2-C2
9	D	502	PG4	C1-C2-O2-C3
9	D	502	PG4	C4-C3-O2-C2
5	D	519	PEG	C1-C2-O2-C3
5	A	510	PEG	O1-C1-C2-O2
5	D	519	PEG	O2-C3-C4-O4
4	B	510	EDO	O1-C1-C2-O2
4	C	507	EDO	O1-C1-C2-O2
4	D	503	EDO	O1-C1-C2-O2
4	D	526	EDO	O1-C1-C2-O2
6	A	517	D68	F3-C18-O4-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	B	514	D68	F3-C18-O4-C17
6	C	515	D68	F4-C18-O4-C17
6	D	520	D68	F3-C18-O4-C17
5	B	512	PEG	O2-C3-C4-O4
5	C	511	PEG	O2-C3-C4-O4
7	B	513	EPE	S-C10-C9-N1
7	C	512	EPE	S-C10-C9-N1
4	A	511	EDO	O1-C1-C2-O2
4	C	502	EDO	O1-C1-C2-O2
4	C	503	EDO	O1-C1-C2-O2
4	D	512	EDO	O1-C1-C2-O2
4	D	515	EDO	O1-C1-C2-O2
4	D	524	EDO	O1-C1-C2-O2
9	D	502	PG4	C6-C5-O3-C4
7	B	513	EPE	C9-C10-S-O3S
9	C	514	PG4	O2-C3-C4-O3
4	C	501	EDO	O1-C1-C2-O2
6	A	517	D68	F4-C18-O4-C17
6	B	514	D68	F4-C18-O4-C17
6	D	520	D68	F4-C18-O4-C17
7	C	512	EPE	C9-C10-S-O3S
7	A	518	EPE	C9-C10-S-O2S
7	B	507	EPE	C9-C10-S-O1S
7	C	512	EPE	C9-C10-S-O1S
9	C	514	PG4	C5-C6-O4-C7
5	C	511	PEG	C4-C3-O2-C2
7	A	518	EPE	S-C10-C9-N1
5	A	510	PEG	C1-C2-O2-C3
4	A	509	EDO	O1-C1-C2-O2
4	D	514	EDO	O1-C1-C2-O2
9	D	502	PG4	O2-C3-C4-O3
7	A	518	EPE	C8-C7-N4-C5
5	C	511	PEG	C1-C2-O2-C3
9	D	502	PG4	O1-C1-C2-O2
9	C	514	PG4	C6-C5-O3-C4
5	A	510	PEG	O2-C3-C4-O4
9	D	502	PG4	C3-C4-O3-C5
9	D	502	PG4	O4-C7-C8-O5
6	C	515	D68	F3-C18-O4-C17
4	A	520	EDO	O1-C1-C2-O2
4	D	516	EDO	O1-C1-C2-O2
9	D	502	PG4	C8-C7-O4-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	511	EDO	O1-C1-C2-O2
4	B	522	EDO	O1-C1-C2-O2
4	D	501	EDO	O1-C1-C2-O2
4	D	510	EDO	O1-C1-C2-O2
4	D	522	EDO	O1-C1-C2-O2
4	D	525	EDO	O1-C1-C2-O2
5	A	510	PEG	C4-C3-O2-C2
9	D	502	PG4	C5-C6-O4-C7
4	A	507	EDO	O1-C1-C2-O2
4	A	522	EDO	O1-C1-C2-O2
4	B	518	EDO	O1-C1-C2-O2
4	C	506	EDO	O1-C1-C2-O2
4	C	517	EDO	O1-C1-C2-O2
7	D	521	EPE	C9-C10-S-O1S
4	A	524	EDO	O1-C1-C2-O2
4	B	515	EDO	O1-C1-C2-O2
4	C	518	EDO	O1-C1-C2-O2
4	A	506	EDO	O1-C1-C2-O2
4	A	516	EDO	O1-C1-C2-O2
4	A	523	EDO	O1-C1-C2-O2
4	B	506	EDO	O1-C1-C2-O2
9	C	514	PG4	O1-C1-C2-O2
4	B	517	EDO	O1-C1-C2-O2

There are no ring outliers.

20 monomers are involved in 37 short contacts:

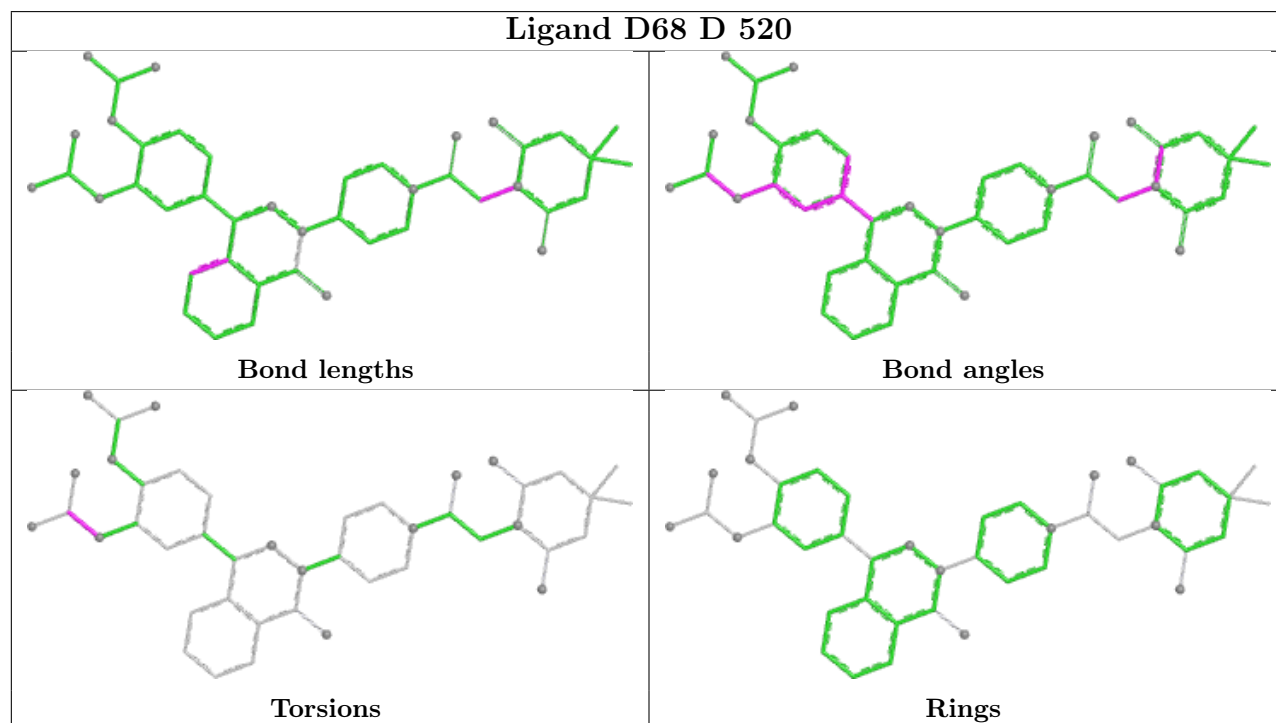
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	508	EDO	2	0
4	D	513	EDO	1	0
4	D	511	EDO	1	0
9	D	502	PG4	10	0
4	A	521	EDO	1	0
4	C	509	EDO	1	0
4	D	507	EDO	1	0
7	B	513	EPE	2	0
4	A	524	EDO	1	0
5	C	511	PEG	2	0
4	D	515	EDO	1	0
4	B	508	EDO	2	0
5	D	519	PEG	2	0
4	C	501	EDO	1	0

Continued on next page...

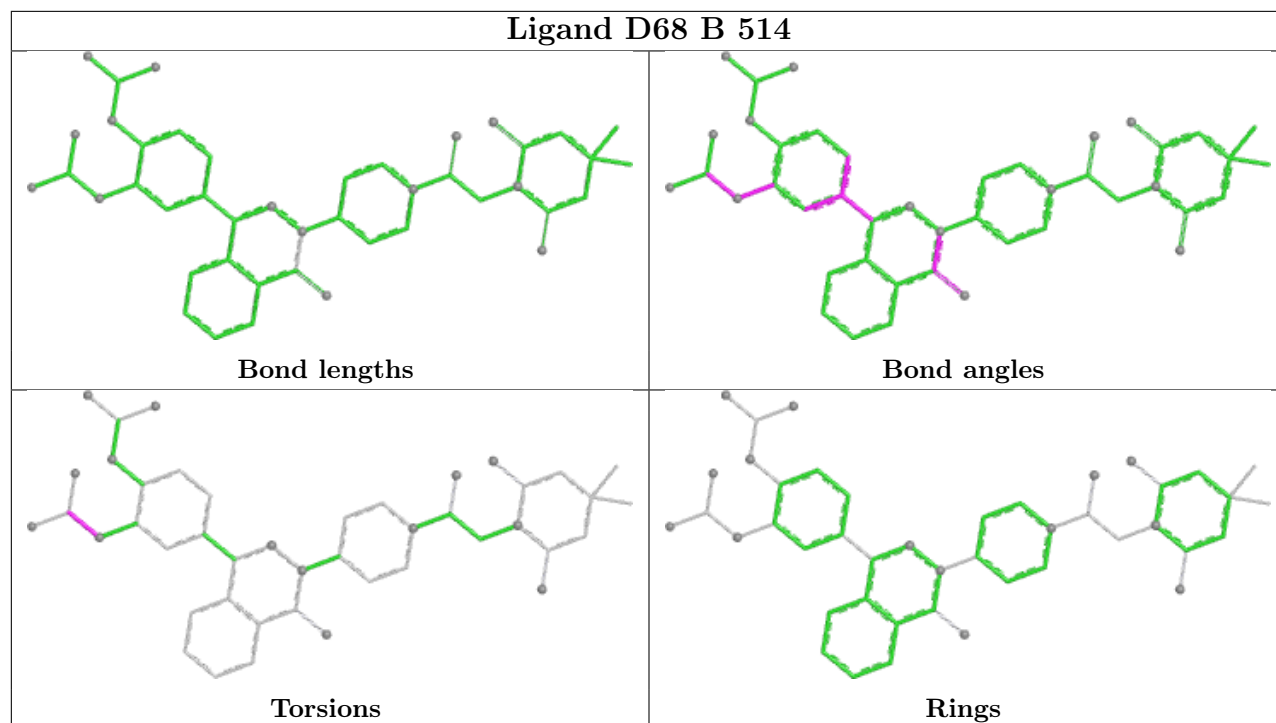
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	512	EPE	1	0
6	B	514	D68	1	0
4	D	510	EDO	1	0
7	A	518	EPE	4	0
6	C	515	D68	1	0
4	D	514	EDO	2	0

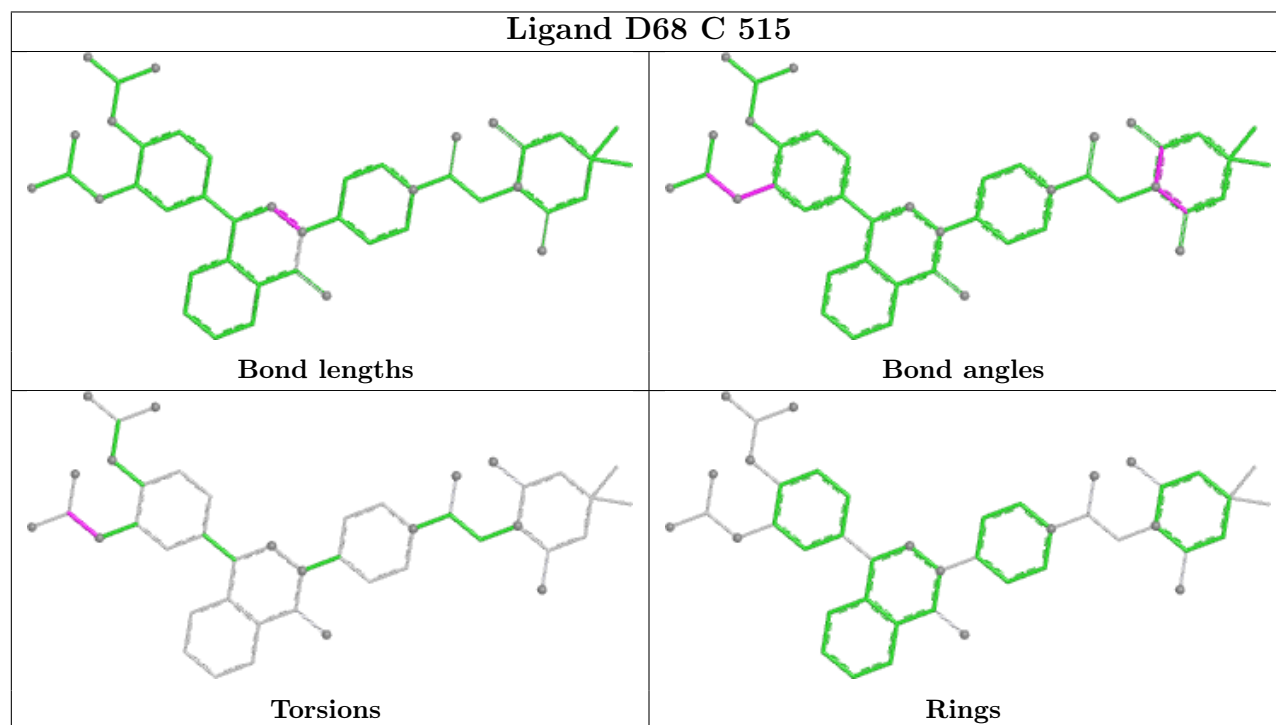
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

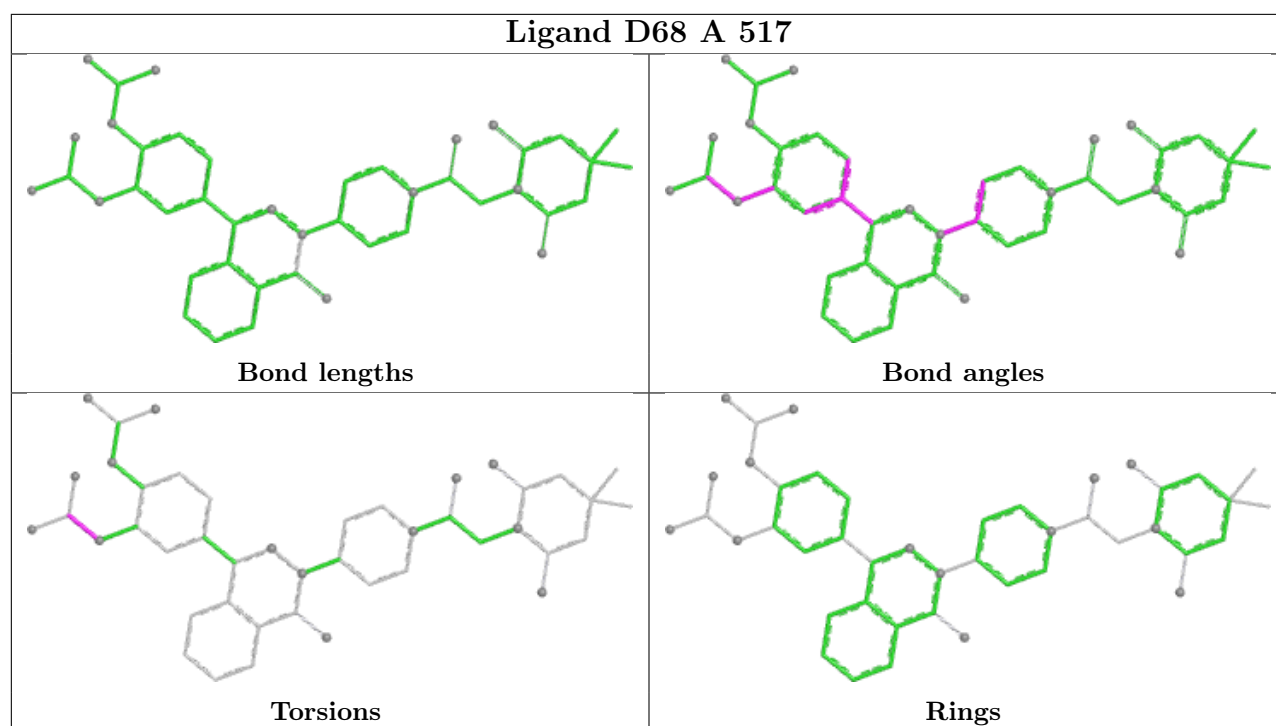


Ligand D68 B 514



Ligand D68 C 515





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%)	0.22	10 (3%) 52 57	24, 38, 70, 106	0
1	B	323/364 (88%)	0.24	5 (1%) 72 77	24, 39, 58, 86	0
1	C	324/364 (89%)	0.36	14 (4%) 40 43	15, 40, 72, 94	1 (0%)
1	D	324/364 (89%)	-0.11	2 (0%) 85 89	22, 32, 54, 78	0
All	All	1300/1456 (89%)	0.18	31 (2%) 59 66	15, 37, 66, 106	1 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	411	PRO	4.1
1	A	354	ILE	3.7
1	A	83	GLY	3.6
1	A	293	THR	3.6
1	A	294	SER	3.5
1	A	411	PRO	3.4
1	C	354	ILE	3.3
1	B	91	VAL	3.3
1	C	292	VAL	2.9
1	A	295	SER	2.8
1	C	289	THR	2.6
1	C	410	ILE	2.5
1	C	91	VAL	2.5
1	D	363	ALA	2.5
1	A	299	LEU	2.4
1	C	357	MET	2.4
1	C	299	LEU	2.4
1	A	292	VAL	2.4
1	B	327	GLN	2.2
1	C	298	LEU	2.2
1	B	411	PRO	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	350	ARG	2.2
1	B	93	ALA	2.2
1	A	222	MET	2.1
1	C	361	HIS	2.1
1	A	363	ALA	2.1
1	C	88	GLN	2.1
1	C	297	VAL	2.1
1	C	407	GLN	2.1
1	C	351	GLY	2.0
1	B	363	ALA	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	EDO	D	525	4/4	0.78	0.18	68,70,73,75	0
9	PG4	D	502	13/13	0.80	0.19	39,50,65,66	0
4	EDO	D	524	4/4	0.82	0.20	42,48,54,55	0
4	EDO	C	513	4/4	0.83	0.18	58,66,71,77	0
4	EDO	B	517	4/4	0.84	0.16	75,81,87,89	0
4	EDO	D	513	4/4	0.84	0.20	43,43,50,59	0
5	PEG	C	511	7/7	0.84	0.20	55,67,77,83	0
4	EDO	D	523	4/4	0.84	0.17	58,59,59,63	0
4	EDO	B	519	4/4	0.85	0.20	68,75,85,86	0
4	EDO	C	502	4/4	0.85	0.14	49,51,52,63	0
4	EDO	C	509	4/4	0.85	0.18	62,62,65,83	0
5	PEG	A	510	7/7	0.85	0.19	62,72,75,81	0
4	EDO	B	508	4/4	0.85	0.16	47,55,57,62	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	A	520	4/4	0.85	0.16	59,60,67,75	0
4	EDO	C	501	4/4	0.86	0.17	49,55,59,69	0
4	EDO	C	518	4/4	0.86	0.17	57,59,66,72	0
4	EDO	B	518	4/4	0.86	0.15	70,71,71,73	0
4	EDO	D	522	4/4	0.86	0.19	63,66,69,71	0
4	EDO	A	522	4/4	0.86	0.14	56,60,60,62	0
4	EDO	A	524	4/4	0.87	0.16	39,59,61,67	0
4	EDO	D	509	4/4	0.87	0.18	47,48,54,65	0
4	EDO	A	515	4/4	0.88	0.17	38,53,57,66	0
4	EDO	A	506	4/4	0.88	0.17	68,68,70,71	0
4	EDO	B	509	4/4	0.88	0.16	45,54,60,66	0
4	EDO	A	507	4/4	0.88	0.18	42,59,62,68	0
4	EDO	A	523	4/4	0.88	0.16	64,73,74,76	0
4	EDO	D	518	4/4	0.89	0.15	44,49,53,59	0
4	EDO	D	526	4/4	0.89	0.14	55,58,59,65	0
4	EDO	C	506	4/4	0.89	0.16	52,54,65,75	0
5	PEG	B	512	7/7	0.89	0.15	56,60,62,64	0
4	EDO	B	516	4/4	0.89	0.21	56,61,63,83	0
9	PG4	C	514	13/13	0.89	0.14	61,64,76,88	0
4	EDO	A	512	4/4	0.89	0.15	41,47,50,59	0
4	EDO	A	503	4/4	0.90	0.15	65,69,70,71	0
4	EDO	B	504	4/4	0.90	0.14	53,64,65,65	0
4	EDO	C	516	4/4	0.90	0.15	53,54,55,65	0
4	EDO	A	521	4/4	0.90	0.16	40,53,59,66	0
4	EDO	A	509	4/4	0.90	0.14	50,59,59,62	0
4	EDO	B	515	4/4	0.90	0.16	66,68,72,72	0
4	EDO	D	514	4/4	0.90	0.13	29,37,48,50	0
4	EDO	D	516	4/4	0.90	0.12	34,37,41,50	0
5	PEG	D	519	7/7	0.90	0.13	37,41,51,59	0
4	EDO	D	517	4/4	0.90	0.17	50,57,62,67	0
4	EDO	A	519	4/4	0.90	0.16	62,66,69,70	0
4	EDO	B	506	4/4	0.91	0.14	56,56,57,63	0
4	EDO	C	508	4/4	0.91	0.15	59,60,64,65	0
4	EDO	B	521	4/4	0.91	0.14	39,46,53,53	0
4	EDO	C	510	4/4	0.91	0.15	52,56,57,59	0
7	EPE	A	518	15/15	0.91	0.14	44,81,90,92	0
4	EDO	B	511	4/4	0.91	0.14	52,59,68,75	0
4	EDO	A	504	4/4	0.91	0.12	37,43,43,43	0
4	EDO	B	510	4/4	0.92	0.12	43,53,58,59	0
4	EDO	D	503	4/4	0.92	0.14	54,60,61,62	0
4	EDO	D	507	4/4	0.92	0.12	53,56,66,82	0
4	EDO	A	514	4/4	0.92	0.14	48,48,51,57	0

Continued on next page...

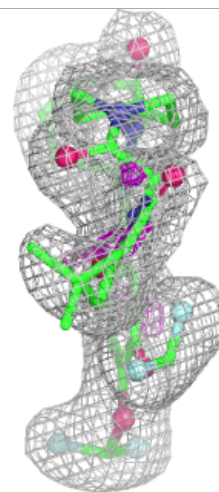
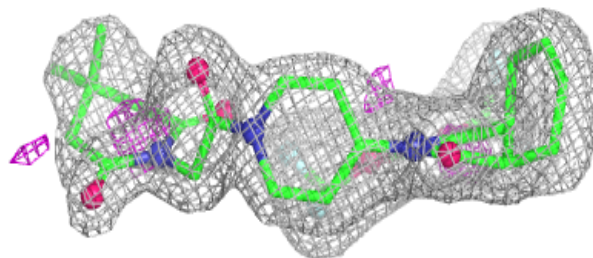
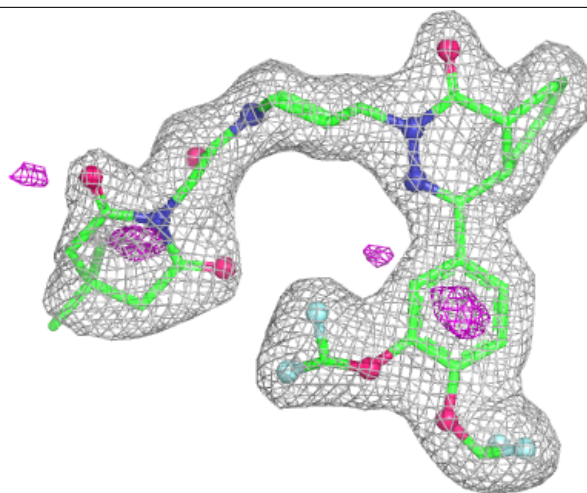
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	C	507	4/4	0.92	0.15	58,62,63,74	0
7	EPE	B	513	15/15	0.92	0.14	47,76,94,100	0
4	EDO	A	511	4/4	0.92	0.13	43,48,53,59	0
4	EDO	C	517	4/4	0.92	0.13	44,50,58,69	0
4	EDO	B	520	4/4	0.93	0.12	38,56,59,61	0
4	EDO	D	501	4/4	0.93	0.14	54,58,60,63	0
4	EDO	A	508	4/4	0.93	0.11	37,39,40,46	0
4	EDO	B	505	4/4	0.93	0.12	60,62,66,67	0
4	EDO	D	508	4/4	0.93	0.13	51,53,59,64	0
4	EDO	A	516	4/4	0.93	0.13	50,53,55,59	0
4	EDO	A	505	4/4	0.94	0.11	54,59,60,66	0
7	EPE	B	507	15/15	0.94	0.11	50,56,63,66	0
4	EDO	D	511	4/4	0.94	0.13	42,43,47,60	0
7	EPE	D	521	15/15	0.94	0.13	38,67,82,84	0
6	D68	A	517	44/44	0.94	0.10	35,42,73,80	0
6	D68	C	515	44/44	0.94	0.10	33,40,70,81	0
4	EDO	B	503	4/4	0.95	0.10	44,46,49,49	0
4	EDO	C	503	4/4	0.95	0.11	56,57,66,66	0
4	EDO	B	522	4/4	0.95	0.09	47,50,50,55	0
4	EDO	D	515	4/4	0.95	0.09	29,44,45,47	0
4	EDO	A	513	4/4	0.95	0.08	38,42,42,47	0
4	EDO	D	510	4/4	0.95	0.13	39,44,53,61	0
7	EPE	C	512	15/15	0.96	0.09	42,51,65,78	0
6	D68	B	514	44/44	0.96	0.08	30,36,60,70	0
4	EDO	D	512	4/4	0.96	0.09	46,48,48,49	0
6	D68	D	520	44/44	0.96	0.08	29,35,61,67	0
4	EDO	D	506	4/4	0.97	0.07	33,34,37,39	0
3	MG	C	505	1/1	0.98	0.03	23,23,23,23	0
8	NI	A	525	1/1	0.99	0.06	41,41,41,41	0
8	NI	D	527	1/1	0.99	0.02	29,29,29,29	1
3	MG	B	502	1/1	0.99	0.04	22,22,22,22	0
3	MG	D	505	1/1	0.99	0.04	20,20,20,20	0
2	ZN	C	504	1/1	1.00	0.02	34,34,34,34	0
2	ZN	D	504	1/1	1.00	0.01	29,29,29,29	0
3	MG	A	502	1/1	1.00	0.03	23,23,23,23	0
2	ZN	A	501	1/1	1.00	0.02	33,33,33,33	0
2	ZN	B	501	1/1	1.00	0.03	32,32,32,32	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.

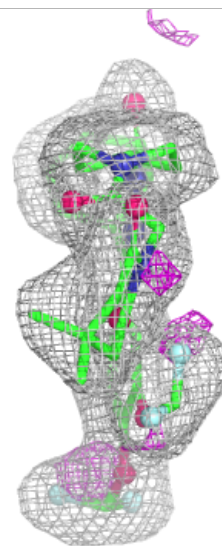
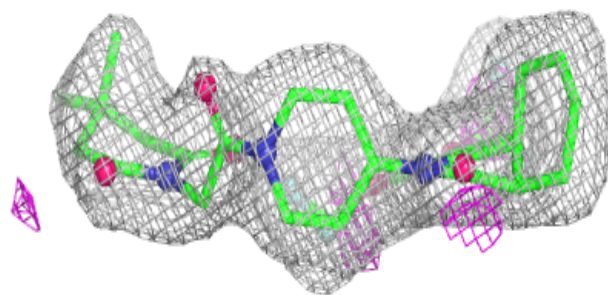
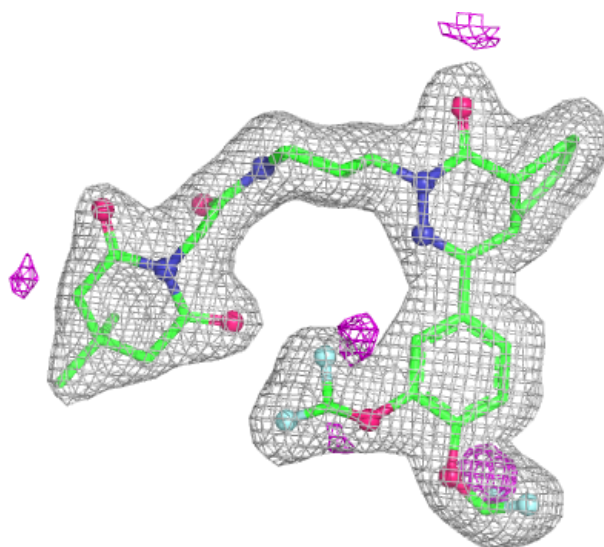
Electron density around D68 A 517:

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



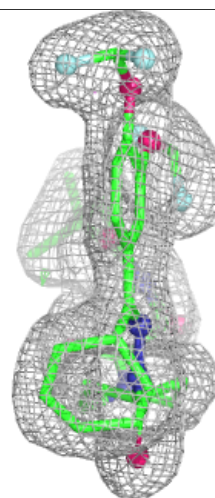
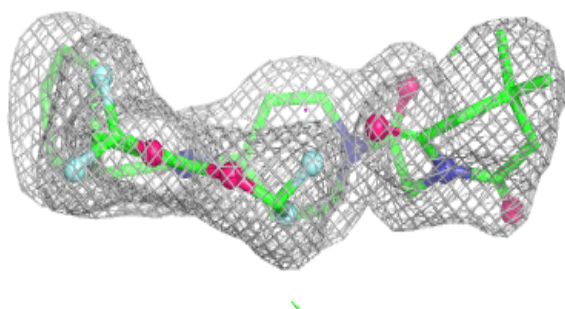
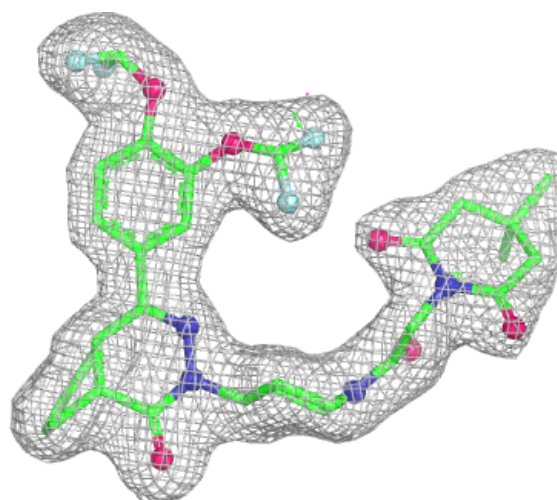
Electron density around D68 C 515:

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



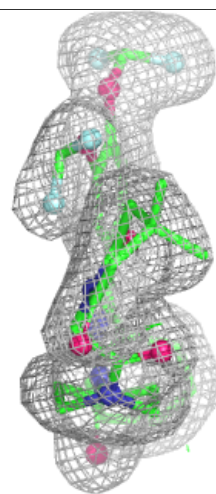
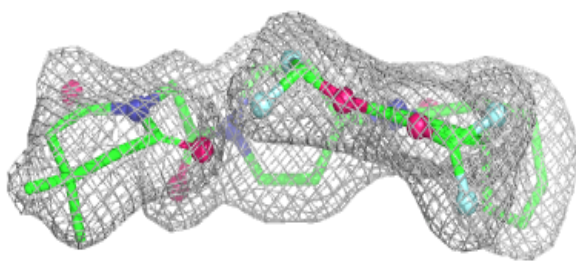
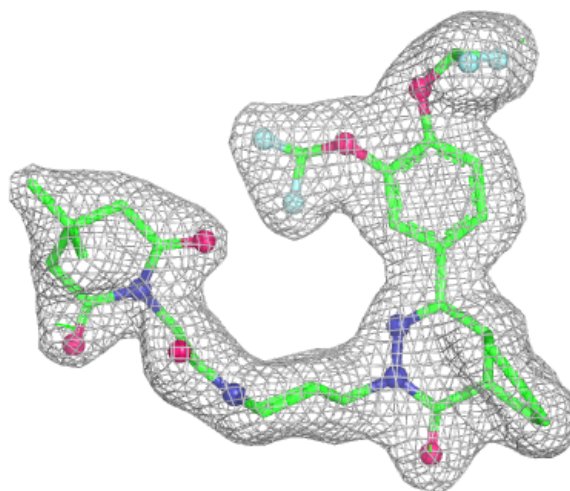
Electron density around D68 B 514:

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



Electron density around D68 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.