



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 10:13 PM UTC

PDB ID : 6IAG / pdb_00006iag
Title : Crystal structure of human phosphodiesterase 4D2 catalytic domain with inhibitor NPD-637
Authors : Singh, A.K.; Brown, D.G.
Deposited on : 2018-11-26
Resolution : 2.00 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

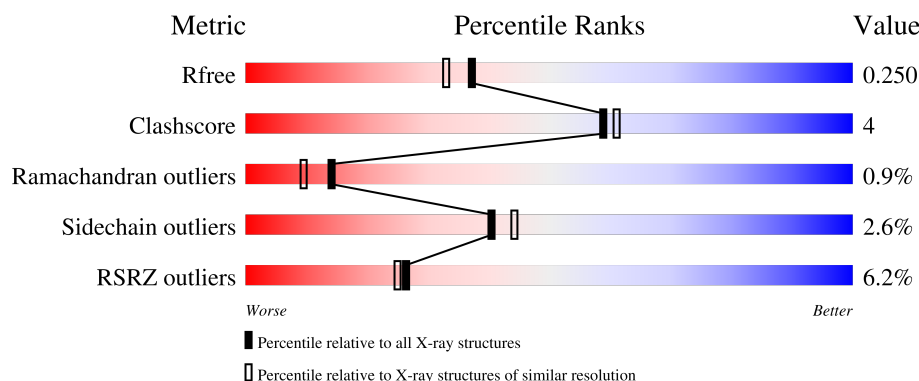
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	 10% 81% 9% • 10%
1	B	364	 3% 79% 9% • 11%
1	C	364	 7% 77% 11% • 11%
1	D	364	 2% 77% 11% • 11%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11530 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	323	Total	C	N	O	S	0	0	0
			2613	1654	446	499	14			
1	D	324	Total	C	N	O	S	0	1	0
			2628	1663	449	502	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

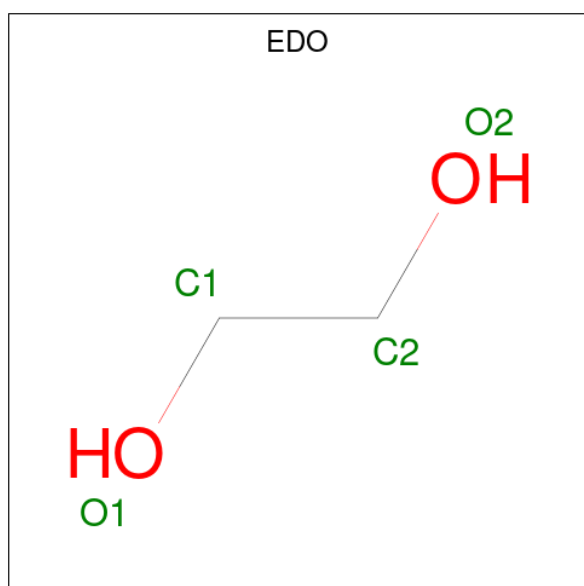
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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		

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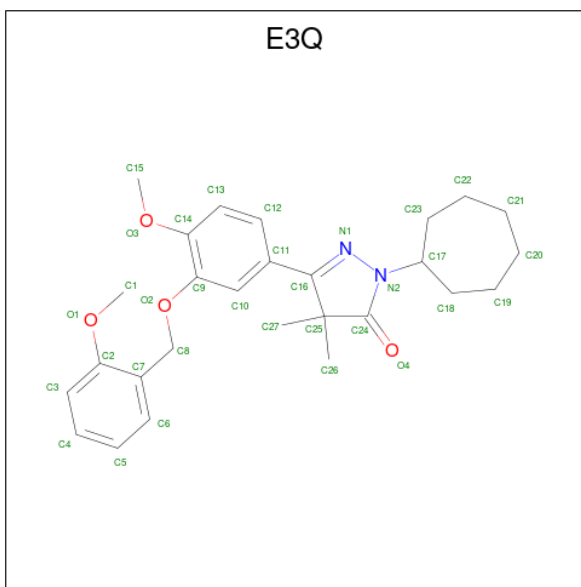
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0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

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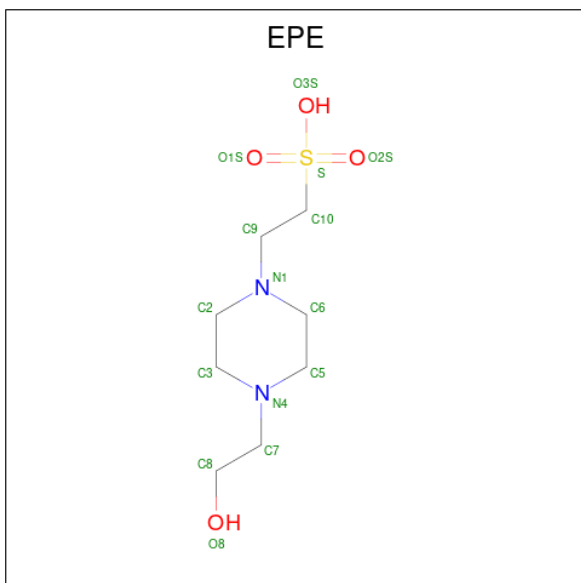
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total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

- Molecule 5 is 1-cycloheptyl-3-{4-methoxy-3-[(2-methoxyphenyl)methoxy]phenyl}-4,4-dimethyl-4,5-dihydro-1H-pyrazol-5-one (CCD ID: E3Q) (formula: C₂₇H₃₄N₂O₄) (labeled as "Ligand of Interest" by depositor).



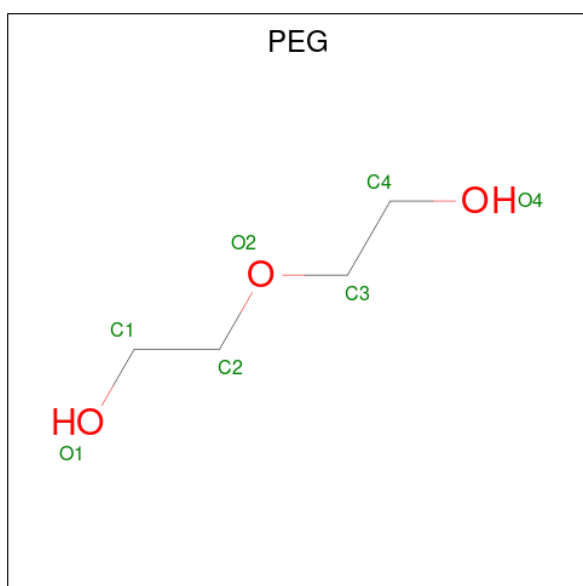
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			33	27	2	4		
5	B	1	Total	C	N	O	0	0
			33	27	2	4		
5	C	1	Total	C	N	O	0	0
			33	27	2	4		
5	D	1	Total	C	N	O	0	0
			33	27	2	4		

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



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

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

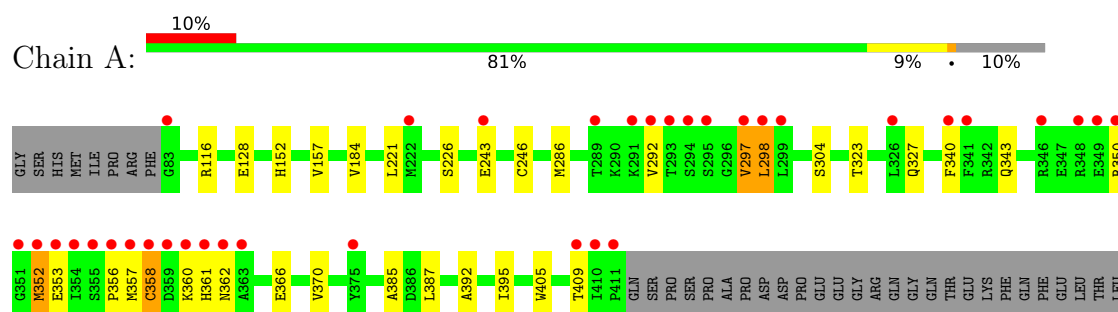
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	165	Total	O	0	0
			165	165		
8	B	161	Total	O	0	0
			161	161		
8	C	129	Total	O	0	0
			129	129		
8	D	200	Total	O	0	0
			200	200		

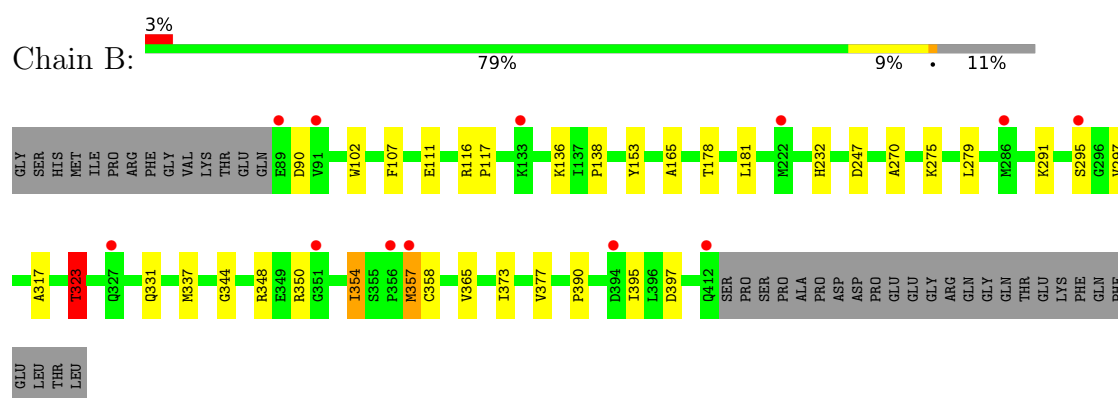
3 Residue-property plots [i](#)

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.

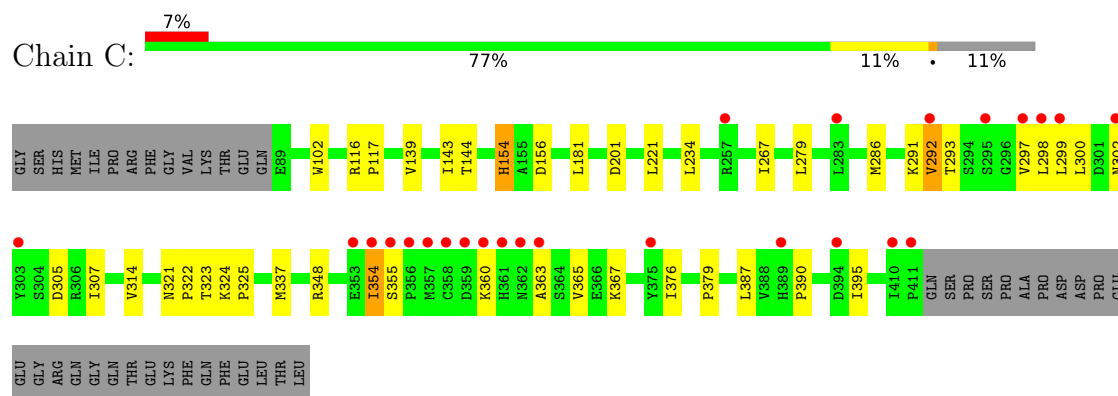
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



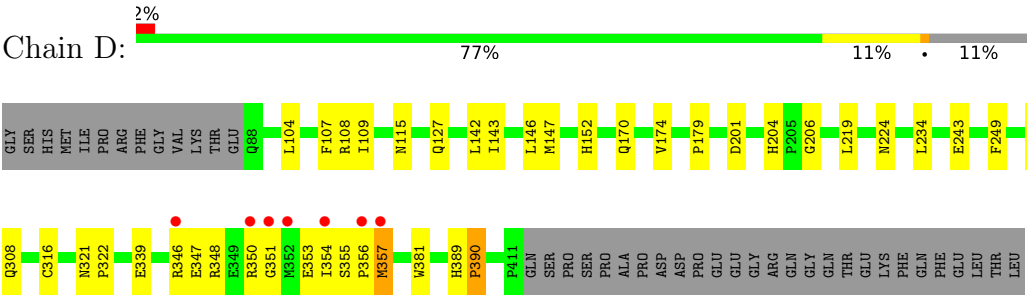
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



- 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	99.11Å 110.31Å 160.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.50 – 2.00 84.50 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (84.50-2.00) 98.2 (84.50-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.200 , 0.246 0.210 , 0.250	Depositor DCC
R_{free} test set	6003 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.6	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	0.95	EDS
Total number of atoms	11530	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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: MG, EDO, PEG, ZN, E3Q, EPE

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	1.15	2/2712 (0.1%)	1.42	5/3684 (0.1%)
1	B	1.11	2/2676 (0.1%)	1.46	3/3636 (0.1%)
1	C	1.10	0/2667	1.43	3/3624 (0.1%)
1	D	1.11	1/2685 (0.0%)	1.36	2/3648 (0.1%)
All	All	1.12	5/10740 (0.0%)	1.42	13/14592 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	116	ARG	C-N	10.92	1.50	1.33
1	D	234	LEU	C-O	5.97	1.30	1.24
1	A	152	HIS	C-O	-5.71	1.16	1.24
1	B	232	HIS	CE1-NE2	5.31	1.37	1.32
1	B	317	ALA	C-O	5.01	1.29	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	ARG	O-C-N	-7.15	113.10	121.32
1	A	116	ARG	CA-C-N	6.88	127.17	119.32
1	A	116	ARG	C-N-CA	6.88	127.17	119.32
1	B	323	THR	N-CA-C	-6.41	105.38	113.72
1	B	323	THR	N-CA-CB	-5.66	102.33	110.65
1	A	343	GLN	N-CA-C	-5.42	105.45	111.36
1	B	397	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	116	ARG	CB-CG-CD	-5.20	99.35	111.30
1	C	201	ASP	CA-CB-CG	5.16	117.76	112.60
1	D	127	GLN	CA-C-N	5.15	127.44	120.38
1	D	127	GLN	C-N-CA	5.15	127.44	120.38
1	C	154	HIS	CA-C-N	5.08	127.59	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	154	HIS	C-N-CA	5.08	127.59	120.28

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	12	0
1	B	2622	0	2578	26	0
1	C	2613	0	2570	23	0
1	D	2628	0	2586	32	0
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	40	0	60	1	0
4	B	24	0	36	3	0
4	C	20	0	30	0	0
4	D	56	0	84	9	0
5	A	33	0	0	2	0
5	B	33	0	0	1	0
5	C	33	0	0	0	0
5	D	33	0	0	1	0
6	B	30	0	34	4	0
6	C	15	0	18	0	0
6	D	15	0	18	2	0
7	D	14	0	20	3	0
8	A	165	0	0	0	0
8	B	161	0	0	3	0
8	C	129	0	0	0	0
8	D	200	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11530	0	10650	94	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 4.

All (94) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:ILE:HG12	8:B:602:HOH:O	1.66	0.94
1:B:107:PHE:HB2	6:B:508:EPE:H101	1.64	0.77
1:D:286:MET:HE3	1:D:308[A]:GLN:OE1	1.86	0.75
1:D:346:ARG:NH2	8:D:601:HOH:O	2.21	0.74
1:D:115:ASN:HD21	4:D:505:EDO:H12	1.53	0.73
1:D:115:ASN:HD21	4:D:505:EDO:C1	2.02	0.72
1:D:143:ILE:HG22	1:D:147:MET:HE2	1.70	0.72
1:D:174:VAL:HG12	7:D:511:PEG:H41	1.71	0.72
1:D:286:MET:CE	1:D:308[A]:GLN:OE1	2.41	0.68
1:B:102:TRP:HE1	1:B:323:THR:HG23	1.59	0.68
1:C:348:ARG:HH11	1:C:354:ILE:HD11	1.59	0.66
1:C:348:ARG:NH1	1:C:354:ILE:HD11	2.12	0.64
1:A:243:GLU:HB2	1:A:246:CYS:SG	2.41	0.61
1:D:107:PHE:HB2	6:D:516:EPE:H91	1.83	0.60
1:D:115:ASN:ND2	4:D:505:EDO:H12	2.16	0.59
1:C:234:LEU:HB2	4:D:515:EDO:H11	1.85	0.59
1:A:298:LEU:HD21	1:A:387:LEU:HD11	1.85	0.58
1:B:348:ARG:NH2	8:B:602:HOH:O	2.36	0.57
1:B:354:ILE:N	1:B:354:ILE:HD12	2.20	0.56
1:B:337:MET:HE2	1:B:365:VAL:HG22	1.90	0.54
1:A:350:ARG:HG2	1:C:144:THR:HG23	1.90	0.53
1:C:139:VAL:O	1:C:143:ILE:HG12	2.08	0.53
1:B:116:ARG:N	1:B:117:PRO:CD	2.73	0.52
1:B:323:THR:HG23	1:B:395:ILE:HG23	1.92	0.52
1:A:323:THR:HB	1:A:395:ILE:HG23	1.92	0.52
1:D:179:PRO:HG2	7:D:512:PEG:H21	1.90	0.52
1:C:234:LEU:CB	4:D:515:EDO:H11	2.39	0.52
1:C:321:ASN:HB2	1:C:322:PRO:HD3	1.92	0.52
1:B:136:LYS:O	1:B:138:PRO:HD3	2.10	0.51
1:D:224:ASN:OD1	4:D:515:EDO:H12	2.10	0.51
1:B:102:TRP:HE1	1:B:323:THR:CG2	2.22	0.50
7:D:512:PEG:H21	7:D:512:PEG:O4	2.11	0.50
1:A:366:GLU:O	1:A:370:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:MET:HA	8:B:637:HOH:O	2.12	0.50
1:D:346:ARG:HG3	8:D:775:HOH:O	2.11	0.49
4:B:510:EDO:H21	1:D:243:GLU:OE1	2.13	0.49
1:A:405:TRP:O	1:A:409:THR:HG23	2.13	0.48
1:B:331:GLN:HE22	6:B:508:EPE:H102	1.79	0.48
1:D:142:LEU:O	1:D:146:LEU:HG	2.14	0.47
1:A:340:PHE:HD2	5:A:513:E3Q:C5	2.27	0.47
1:B:337:MET:HE1	1:B:357:MET:HG3	1.95	0.47
1:D:321:ASN:HB2	1:D:322:PRO:HD3	1.95	0.47
1:B:247:ASP:OD1	1:B:247:ASP:C	2.58	0.47
1:D:357:MET:HB2	5:D:517:E3Q:C4	2.45	0.47
1:B:357:MET:HB3	5:B:509:E3Q:C4	2.45	0.46
1:B:270:ALA:HB1	1:B:279:LEU:HD11	1.97	0.46
1:C:116:ARG:N	1:C:117:PRO:CD	2.79	0.46
1:D:303:TYR:CE1	4:D:509:EDO:H12	2.51	0.46
1:C:298:LEU:HD11	1:C:387:LEU:HG	1.97	0.46
1:D:355:SER:HB3	4:D:503:EDO:H21	1.97	0.46
4:B:510:EDO:H22	1:D:152:HIS:HE1	1.81	0.45
1:A:184:VAL:CG2	1:A:297:VAL:HG13	2.47	0.45
1:A:286:MET:HG3	4:A:512:EDO:O2	2.16	0.45
1:C:181:LEU:HD21	1:C:298:LEU:HD12	1.98	0.45
1:C:292:VAL:HG23	1:C:293:THR:N	2.32	0.45
1:A:340:PHE:HB3	1:A:358:CYS:SG	2.57	0.45
1:B:178:THR:CG2	1:B:181:LEU:HD12	2.46	0.45
1:C:286:MET:HE1	1:C:305:ASP:OD1	2.17	0.45
1:D:348:ARG:HD3	1:D:354:ILE:HD11	1.99	0.45
1:C:286:MET:CE	1:C:305:ASP:OD1	2.65	0.45
1:D:350:ARG:NH1	8:D:611:HOH:O	2.50	0.45
1:D:104:LEU:HD11	1:D:109:ILE:CD1	2.47	0.44
1:D:304:SER:O	1:D:308[B]:GLN:HG3	2.18	0.44
1:D:347:GLU:OE1	1:D:354:ILE:HA	2.18	0.44
1:C:267:ILE:HG21	1:C:314:VAL:HG21	1.99	0.44
1:A:340:PHE:CD2	5:A:513:E3Q:C5	3.01	0.43
1:B:178:THR:HG22	1:B:181:LEU:HD12	2.00	0.43
1:C:154:HIS:HB3	1:C:156:ASP:OD1	2.18	0.43
1:D:201:ASP:O	1:D:204:HIS:HB2	2.19	0.43
1:B:153:TYR:CZ	1:B:165:ALA:HB2	2.54	0.43
1:D:108:ARG:H	6:D:516:EPE:HOS3	1.66	0.42
6:B:508:EPE:H32	6:B:508:EPE:H81	1.79	0.42
1:C:307:ILE:HD12	1:C:307:ILE:HA	1.93	0.42
1:C:337:MET:HG3	1:C:365:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:GLY:HA3	1:B:358:CYS:O	2.19	0.42
1:C:221:LEU:HD23	1:C:221:LEU:C	2.44	0.42
1:B:350:ARG:NH2	4:B:510:EDO:O2	2.53	0.42
1:C:324:LYS:O	1:C:325:PRO:C	2.63	0.42
1:C:279:LEU:HD23	1:C:279:LEU:HA	1.87	0.41
1:C:376:ILE:C	1:C:379:PRO:HD2	2.45	0.41
1:A:385:ALA:HA	1:A:392:ALA:HB3	2.03	0.41
1:B:337:MET:HE1	1:B:357:MET:CG	2.51	0.41
1:B:373:ILE:HA	1:B:377:VAL:HB	2.03	0.41
1:C:323:THR:HB	1:C:395:ILE:HG23	2.02	0.41
1:D:249:PHE:CD2	4:D:518:EDO:H11	2.55	0.41
1:D:389:HIS:HA	1:D:390:PRO:HA	1.92	0.41
1:D:206:GLY:HA2	1:D:339:GLU:OE2	2.21	0.41
1:B:295:SER:OG	1:B:297:VAL:HG23	2.21	0.41
1:D:316:CYS:HB3	1:D:381:TRP:CZ2	2.55	0.41
1:B:111:GLU:CD	6:B:508:EPE:H61	2.45	0.40
1:B:350:ARG:HH11	1:B:350:ARG:HD3	1.74	0.40
1:C:102:TRP:CE2	1:C:324:LYS:HE2	2.57	0.40
1:D:219:LEU:HD23	1:D:219:LEU:HA	1.93	0.40
1:D:104:LEU:HD22	1:D:170:GLN:HG3	2.02	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%)	310 (95%)	12 (4%)	5 (2%)	8	4
1	B	322/364 (88%)	317 (98%)	5 (2%)	0	100	100
1	C	321/364 (88%)	307 (96%)	11 (3%)	3 (1%)	14	9
1	D	323/364 (89%)	315 (98%)	5 (2%)	3 (1%)	14	9
All	All	1293/1456 (89%)	1249 (97%)	33 (3%)	11 (1%)	14	9

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	352	MET
1	A	362	ASN
1	C	302	ASN
1	C	360	LYS
1	A	353	GLU
1	C	363	ALA
1	D	353	GLU
1	A	361	HIS
1	A	356	PRO
1	D	351	GLY
1	D	356	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	300/331 (91%)	287 (96%)	13 (4%)	26	25
1	B	296/331 (89%)	289 (98%)	7 (2%)	43	47
1	C	295/331 (89%)	286 (97%)	9 (3%)	35	37
1	D	297/331 (90%)	295 (99%)	2 (1%)	76	82
All	All	1188/1324 (90%)	1157 (97%)	31 (3%)	40	44

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	GLU
1	A	157	VAL
1	A	221	LEU
1	A	226	SER
1	A	292	VAL
1	A	297	VAL
1	A	298	LEU
1	A	304	SER
1	A	327	GLN

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Mol	Chain	Res	Type
1	A	352	MET
1	A	357	MET
1	A	358	CYS
1	A	360	LYS
1	B	90	ASP
1	B	275	LYS
1	B	291	LYS
1	B	323	THR
1	B	354	ILE
1	B	357	MET
1	B	390	PRO
1	C	291	LYS
1	C	292	VAL
1	C	297	VAL
1	C	299	LEU
1	C	300	LEU
1	C	354	ILE
1	C	355	SER
1	C	367	LYS
1	C	390	PRO
1	D	357	MET
1	D	390	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	250	GLN
1	A	321	ASN
1	B	210	GLN
1	B	242	GLN
1	B	331	GLN
1	C	210	GLN
1	C	250	GLN
1	D	210	GLN
1	D	258	GLN
1	D	321	ASN
1	D	389	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 53 ligands modelled in this entry, 8 are monoatomic - leaving 45 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	A	505	-	3,3,3	0.19	0	2,2,2	0.09	0
4	EDO	A	503	-	3,3,3	0.02	0	2,2,2	0.06	0
4	EDO	D	510	-	3,3,3	0.38	0	2,2,2	0.04	0
4	EDO	A	504	-	3,3,3	0.72	0	2,2,2	0.48	0
4	EDO	C	503	-	3,3,3	0.13	0	2,2,2	0.26	0
4	EDO	D	508	-	3,3,3	0.23	0	2,2,2	0.42	0
5	E3Q	C	507	-	35,36,36	0.73	2 (5%)	43,51,51	1.45	6 (13%)
4	EDO	C	504	-	3,3,3	0.16	0	2,2,2	0.18	0
4	EDO	A	506	-	3,3,3	0.20	0	2,2,2	0.41	0
5	E3Q	A	513	-	35,36,36	0.78	1 (2%)	43,51,51	1.64	6 (13%)
6	EPE	B	511	-	15,15,15	1.85	1 (6%)	19,20,20	1.34	3 (15%)
4	EDO	A	511	-	3,3,3	0.11	0	2,2,2	0.13	0
7	PEG	D	512	-	6,6,6	0.38	0	5,5,5	0.50	0
4	EDO	D	505	-	3,3,3	0.10	0	2,2,2	0.40	0
4	EDO	D	514	-	3,3,3	0.19	0	2,2,2	0.26	0
4	EDO	D	518	-	3,3,3	0.30	0	2,2,2	0.52	0
4	EDO	A	508	-	3,3,3	0.09	0	2,2,2	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	506	-	3,3,3	0.25	0	2,2,2	0.53	0
4	EDO	B	507	-	3,3,3	0.13	0	2,2,2	0.03	0
4	EDO	D	504	-	3,3,3	0.05	0	2,2,2	0.08	0
4	EDO	D	513	-	3,3,3	0.12	0	2,2,2	0.23	0
5	E3Q	B	509	-	35,36,36	0.88	2 (5%)	43,51,51	1.45	5 (11%)
4	EDO	A	507	-	3,3,3	0.15	0	2,2,2	0.29	0
4	EDO	B	503	-	3,3,3	0.11	0	2,2,2	0.26	0
5	E3Q	D	517	-	35,36,36	0.85	2 (5%)	43,51,51	1.41	4 (9%)
4	EDO	D	520	-	3,3,3	0.12	0	2,2,2	0.21	0
7	PEG	D	511	-	6,6,6	0.28	0	5,5,5	0.37	0
4	EDO	C	508	-	3,3,3	0.23	0	2,2,2	0.19	0
4	EDO	A	509	-	3,3,3	0.55	0	2,2,2	0.36	0
4	EDO	A	512	-	3,3,3	0.06	0	2,2,2	0.18	0
4	EDO	B	505	-	3,3,3	0.16	0	2,2,2	0.31	0
4	EDO	D	506	-	3,3,3	0.11	0	2,2,2	0.11	0
4	EDO	D	519	-	3,3,3	0.31	0	2,2,2	0.29	0
4	EDO	C	509	-	3,3,3	0.09	0	2,2,2	0.14	0
4	EDO	D	503	-	3,3,3	0.24	0	2,2,2	0.18	0
4	EDO	B	504	-	3,3,3	0.19	0	2,2,2	0.13	0
6	EPE	C	505	-	15,15,15	2.43	1 (6%)	19,20,20	1.41	4 (21%)
4	EDO	B	510	-	3,3,3	0.21	0	2,2,2	0.19	0
4	EDO	D	509	-	3,3,3	0.13	0	2,2,2	0.18	0
4	EDO	D	515	-	3,3,3	0.38	0	2,2,2	0.24	0
4	EDO	A	510	-	3,3,3	0.25	0	2,2,2	0.38	0
6	EPE	D	516	-	15,15,15	1.99	1 (6%)	19,20,20	5.04	5 (26%)
6	EPE	B	508	-	15,15,15	2.87	2 (13%)	19,20,20	1.49	3 (15%)
4	EDO	C	506	-	3,3,3	0.16	0	2,2,2	0.14	0
4	EDO	D	507	-	3,3,3	1.07	0	2,2,2	0.80	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	A	505	-	-	1/1/1/1	-
4	EDO	A	503	-	-	1/1/1/1	-
4	EDO	D	510	-	-	1/1/1/1	-
4	EDO	A	504	-	-	1/1/1/1	-
4	EDO	C	503	-	-	1/1/1/1	-
4	EDO	D	508	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	E3Q	C	507	-	-	6/15/46/46	0/4/4/4
4	EDO	C	504	-	-	1/1/1/1	-
4	EDO	A	506	-	-	1/1/1/1	-
5	E3Q	A	513	-	-	1/15/46/46	0/4/4/4
6	EPE	B	511	-	-	4/9/19/19	0/1/1/1
4	EDO	A	511	-	-	0/1/1/1	-
7	PEG	D	512	-	-	1/4/4/4	-
4	EDO	D	505	-	-	1/1/1/1	-
4	EDO	D	514	-	-	1/1/1/1	-
4	EDO	D	518	-	-	0/1/1/1	-
4	EDO	A	508	-	-	1/1/1/1	-
4	EDO	B	506	-	-	1/1/1/1	-
4	EDO	B	507	-	-	1/1/1/1	-
4	EDO	D	504	-	-	1/1/1/1	-
4	EDO	D	513	-	-	0/1/1/1	-
5	E3Q	B	509	-	-	3/15/46/46	0/4/4/4
4	EDO	A	507	-	-	1/1/1/1	-
4	EDO	B	503	-	-	1/1/1/1	-
5	E3Q	D	517	-	-	2/15/46/46	0/4/4/4
4	EDO	D	520	-	-	1/1/1/1	-
7	PEG	D	511	-	-	3/4/4/4	-
4	EDO	C	508	-	-	1/1/1/1	-
4	EDO	A	509	-	-	0/1/1/1	-
4	EDO	A	512	-	-	1/1/1/1	-
4	EDO	B	505	-	-	0/1/1/1	-
4	EDO	D	506	-	-	0/1/1/1	-
4	EDO	D	519	-	-	1/1/1/1	-
4	EDO	C	509	-	-	1/1/1/1	-
4	EDO	D	503	-	-	1/1/1/1	-
4	EDO	B	504	-	-	1/1/1/1	-
6	EPE	C	505	-	-	5/9/19/19	0/1/1/1
4	EDO	B	510	-	-	1/1/1/1	-
4	EDO	D	509	-	-	0/1/1/1	-
4	EDO	D	515	-	-	1/1/1/1	-
4	EDO	A	510	-	-	0/1/1/1	-
6	EPE	D	516	-	-	1/9/19/19	0/1/1/1
6	EPE	B	508	-	-	6/9/19/19	0/1/1/1
4	EDO	C	506	-	-	1/1/1/1	-
4	EDO	D	507	-	-	1/1/1/1	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	508	EPE	C10-S	-10.67	1.62	1.77
6	C	505	EPE	C10-S	-8.93	1.65	1.77
6	D	516	EPE	C10-S	-7.34	1.67	1.77
6	B	511	EPE	C10-S	-6.96	1.67	1.77
5	D	517	E3Q	C24-N2	3.26	1.38	1.35
5	B	509	E3Q	C24-N2	3.07	1.38	1.35
5	B	509	E3Q	C17-N2	2.69	1.50	1.47
5	C	507	E3Q	C24-N2	2.62	1.37	1.35
5	A	513	E3Q	C24-N2	2.62	1.37	1.35
6	B	508	EPE	O2S-S	-2.33	1.38	1.45
5	D	517	E3Q	C17-N2	2.26	1.50	1.47
5	C	507	E3Q	C17-N2	2.08	1.49	1.47

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	516	EPE	O2S-S-C10	-14.08	85.45	106.73
6	D	516	EPE	O1S-S-C10	-12.81	87.38	106.73
6	D	516	EPE	O3S-S-C10	-9.50	87.43	106.00
5	A	513	E3Q	C16-N1-N2	-6.75	100.15	108.30
5	D	517	E3Q	C16-N1-N2	-6.38	100.60	108.30
5	B	509	E3Q	C16-N1-N2	-6.24	100.78	108.30
5	C	507	E3Q	C16-N1-N2	-6.20	100.83	108.30
5	C	507	E3Q	C11-C16-N1	-4.28	113.30	119.72
5	D	517	E3Q	C11-C16-N1	-4.18	113.44	119.72
5	B	509	E3Q	C11-C16-N1	-4.09	113.59	119.72
5	A	513	E3Q	C11-C16-N1	-3.76	114.08	119.72
5	A	513	E3Q	O2-C9-C14	3.59	123.17	115.75
6	B	511	EPE	O1S-S-C10	3.55	112.09	106.73
6	D	516	EPE	O3S-S-O1S	3.50	120.17	111.40
6	B	508	EPE	O1S-S-C10	3.32	111.75	106.73
6	D	516	EPE	O3S-S-O2S	3.22	119.45	111.40
5	A	513	E3Q	O2-C9-C10	-3.20	116.58	123.49
6	B	508	EPE	O2S-S-O1S	-3.02	103.99	113.82
5	A	513	E3Q	O1-C2-C7	2.69	119.97	115.96
6	B	508	EPE	O3S-S-C10	2.61	111.12	106.00
5	A	513	E3Q	O1-C2-C3	-2.61	119.91	124.30
5	C	507	E3Q	O1-C2-C7	2.47	119.63	115.96
6	C	505	EPE	O3S-S-O1S	-2.44	105.30	111.40
5	B	509	E3Q	O4-C24-N2	-2.43	124.96	127.01
5	C	507	E3Q	O4-C24-N2	-2.42	124.98	127.01
5	C	507	E3Q	O1-C2-C3	-2.40	120.25	124.30
5	C	507	E3Q	C17-N2-C24	-2.38	127.06	131.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	505	EPE	O1S-S-C10	2.29	110.18	106.73
6	B	511	EPE	O3S-S-C10	2.28	110.47	106.00
5	B	509	E3Q	C17-N2-C24	-2.23	127.32	131.27
6	C	505	EPE	O2S-S-C10	2.22	110.09	106.73
5	D	517	E3Q	O4-C24-C25	-2.21	124.80	126.93
5	D	517	E3Q	C17-N2-C24	-2.14	127.49	131.27
5	B	509	E3Q	O1-C2-C7	2.04	119.00	115.96
6	B	511	EPE	O3S-S-O1S	-2.03	106.31	111.40
6	C	505	EPE	C3-C2-N1	2.03	114.75	110.65

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	508	EPE	C8-C7-N4-C3
6	B	511	EPE	C10-C9-N1-C6
6	B	511	EPE	C9-C10-S-O2S
6	B	511	EPE	C9-C10-S-O3S
6	C	505	EPE	C10-C9-N1-C2
6	C	505	EPE	C10-C9-N1-C6
6	C	505	EPE	C9-C10-S-O1S
5	C	507	E3Q	C3-C2-O1-C1
6	C	505	EPE	C9-C10-S-O3S
5	C	507	E3Q	C7-C2-O1-C1
6	D	516	EPE	N4-C7-C8-O8
7	D	511	PEG	O2-C3-C4-O4
4	A	507	EDO	O1-C1-C2-O2
4	A	508	EDO	O1-C1-C2-O2
4	C	503	EDO	O1-C1-C2-O2
4	D	507	EDO	O1-C1-C2-O2
4	D	519	EDO	O1-C1-C2-O2
5	A	513	E3Q	C7-C8-O2-C9
5	C	507	E3Q	C7-C8-O2-C9
5	B	509	E3Q	C7-C8-O2-C9
6	B	508	EPE	C9-C10-S-O3S
5	D	517	E3Q	C7-C8-O2-C9
7	D	511	PEG	O1-C1-C2-O2
6	B	508	EPE	N4-C7-C8-O8
4	B	510	EDO	O1-C1-C2-O2
4	C	504	EDO	O1-C1-C2-O2
4	D	505	EDO	O1-C1-C2-O2
4	D	510	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	D	515	EDO	O1-C1-C2-O2
4	A	504	EDO	O1-C1-C2-O2
7	D	511	PEG	C4-C3-O2-C2
6	B	508	EPE	C9-C10-S-O1S
6	B	508	EPE	C9-C10-S-O2S
6	B	511	EPE	C9-C10-S-O1S
6	C	505	EPE	C9-C10-S-O2S
6	B	508	EPE	S-C10-C9-N1
7	D	512	PEG	C1-C2-O2-C3
4	A	503	EDO	O1-C1-C2-O2
4	B	504	EDO	O1-C1-C2-O2
5	C	507	E3Q	C14-C9-O2-C8
5	B	509	E3Q	C14-C9-O2-C8
4	A	506	EDO	O1-C1-C2-O2
4	D	514	EDO	O1-C1-C2-O2
5	C	507	E3Q	C18-C17-N2-C24
4	A	505	EDO	O1-C1-C2-O2
4	B	503	EDO	O1-C1-C2-O2
4	B	506	EDO	O1-C1-C2-O2
5	D	517	E3Q	C14-C9-O2-C8
4	B	507	EDO	O1-C1-C2-O2
4	C	506	EDO	O1-C1-C2-O2
4	C	508	EDO	O1-C1-C2-O2
4	D	520	EDO	O1-C1-C2-O2
5	B	509	E3Q	C10-C9-O2-C8
4	A	512	EDO	O1-C1-C2-O2
4	D	503	EDO	O1-C1-C2-O2
4	D	504	EDO	O1-C1-C2-O2
4	C	509	EDO	O1-C1-C2-O2
4	D	508	EDO	O1-C1-C2-O2
5	C	507	E3Q	C10-C9-O2-C8

There are no ring outliers.

14 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	513	E3Q	2	0
7	D	512	PEG	2	0
4	D	505	EDO	3	0
4	D	518	EDO	1	0
5	B	509	E3Q	1	0
5	D	517	E3Q	1	0

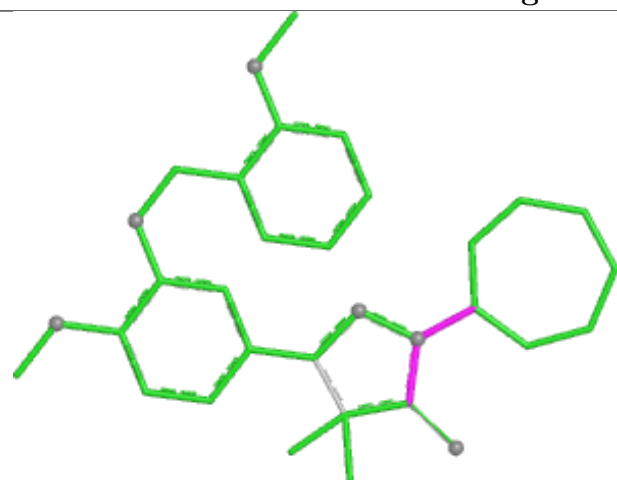
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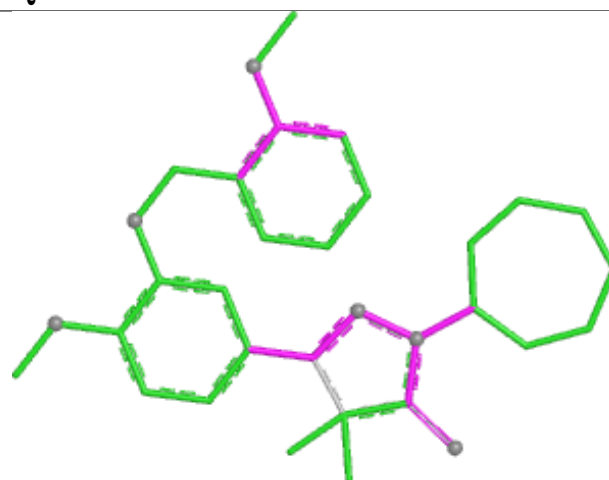
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	511	PEG	1	0
4	A	512	EDO	1	0
4	D	503	EDO	1	0
4	B	510	EDO	3	0
4	D	509	EDO	1	0
4	D	515	EDO	3	0
6	D	516	EPE	2	0
6	B	508	EPE	4	0

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.

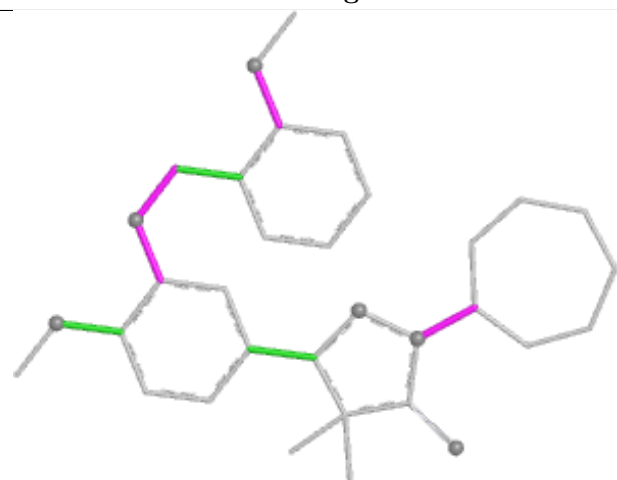
Ligand E3Q C 507



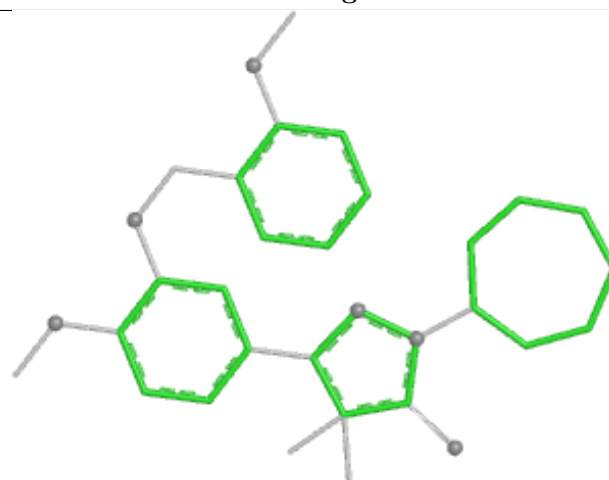
Bond lengths



Bond angles

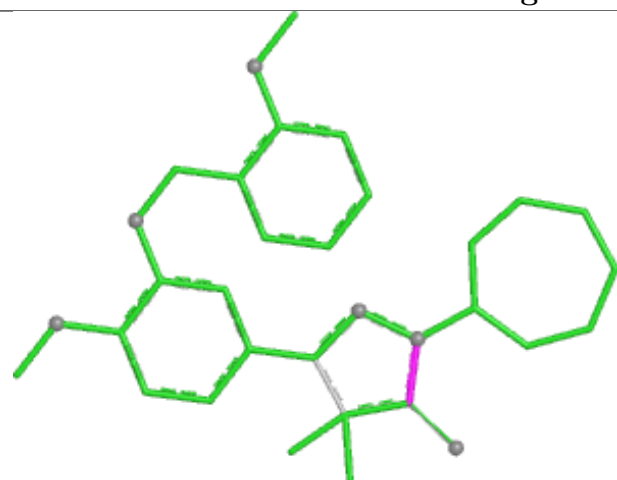


Torsions

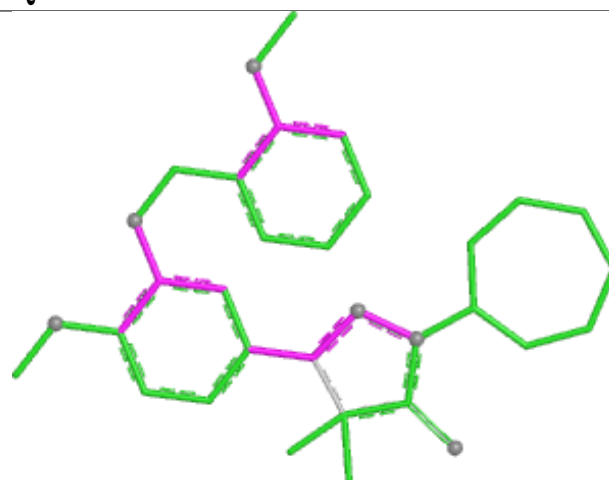


Rings

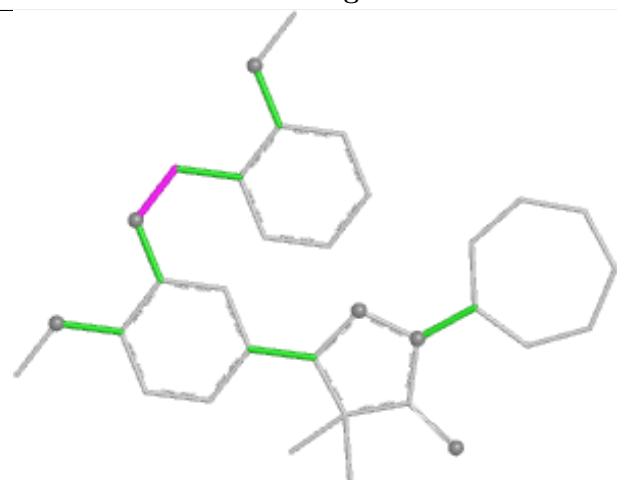
Ligand E3Q A 513



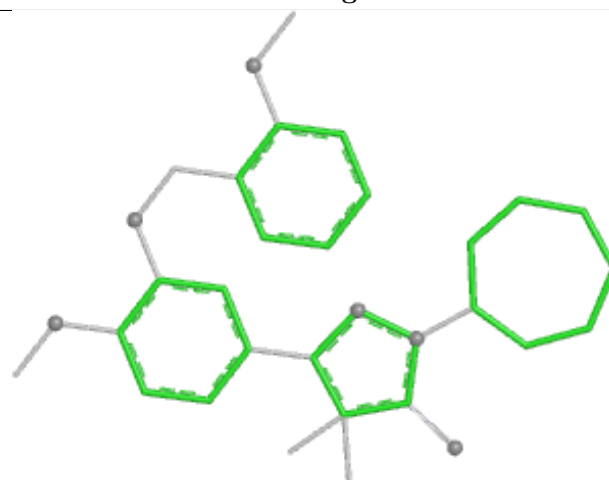
Bond lengths



Bond angles

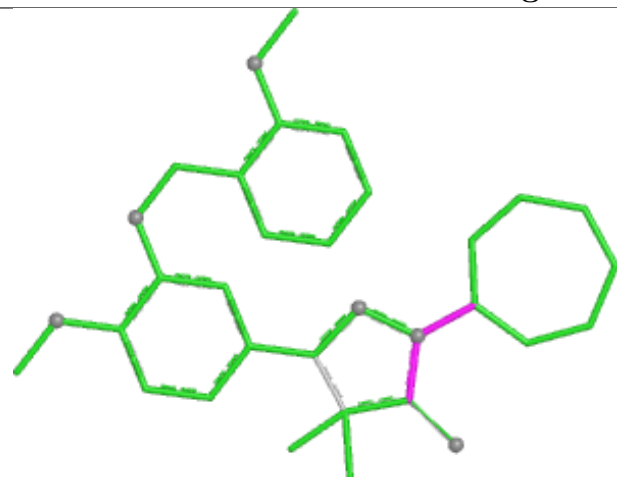


Torsions

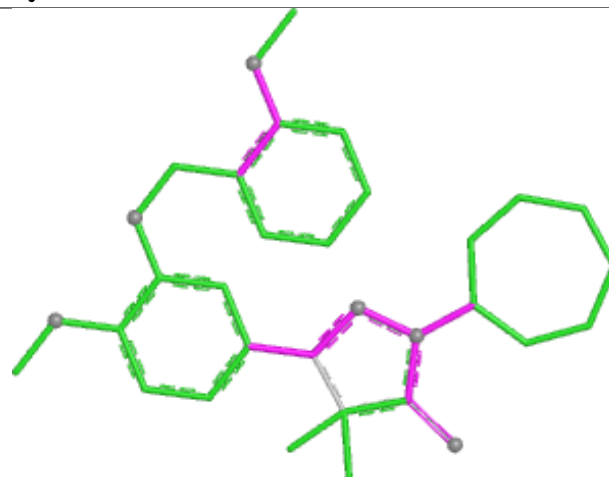


Rings

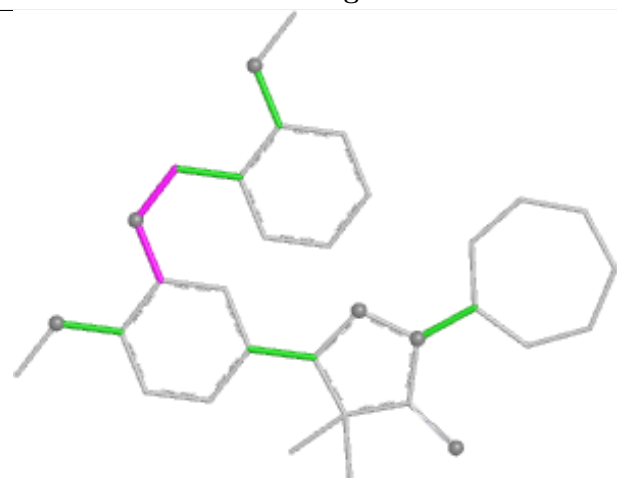
Ligand E3Q B 509



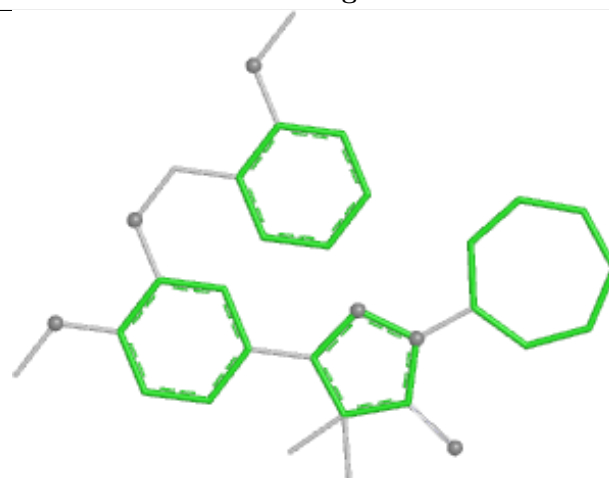
Bond lengths



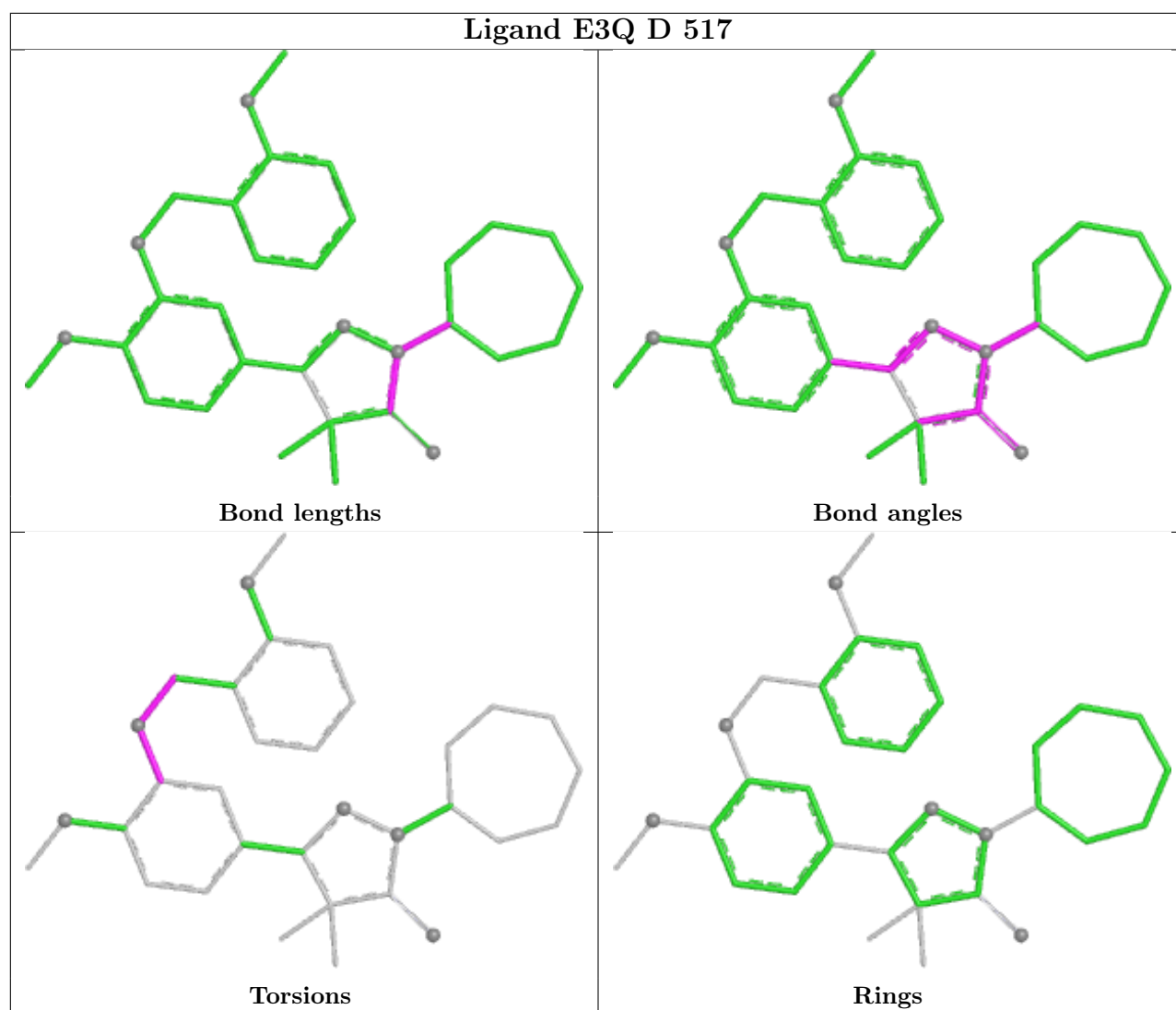
Bond angles



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%)	0.77	36 (10%) 10 9	19, 33, 68, 104	13 (3%)
1	B	324/364 (89%)	0.45	12 (3%) 45 44	21, 37, 57, 88	0
1	C	323/364 (88%)	0.91	25 (7%) 19 18	12, 35, 70, 93	11 (3%)
1	D	324/364 (89%)	0.06	7 (2%) 62 61	16, 28, 58, 98	1 (0%)
All	All	1300/1456 (89%)	0.55	80 (6%) 26 25	12, 34, 63, 104	25 (1%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	360	LYS	28.3
1	A	354	ILE	17.4
1	C	358	CYS	13.6
1	A	357	MET	13.1
1	A	356	PRO	12.8
1	C	357	MET	12.7
1	C	363	ALA	12.6
1	A	358	CYS	12.5
1	A	360	LYS	12.4
1	C	354	ILE	11.9
1	C	359	ASP	11.6
1	C	356	PRO	11.3
1	A	352	MET	11.1
1	A	359	ASP	10.4
1	A	363	ALA	10.0
1	C	361	HIS	9.8
1	A	351	GLY	9.4
1	C	355	SER	9.1
1	A	355	SER	9.0
1	A	361	HIS	8.4
1	C	362	ASN	7.4

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Mol	Chain	Res	Type	RSRZ
1	C	353	GLU	7.0
1	A	353	GLU	6.7
1	A	350	ARG	5.5
1	A	362	ASN	5.5
1	D	357	MET	4.6
1	B	357	MET	4.3
1	A	340	PHE	4.2
1	C	411	PRO	3.8
1	A	299	LEU	3.8
1	A	411	PRO	3.7
1	D	354	ILE	3.6
1	A	83	GLY	3.6
1	A	349	GLU	3.4
1	B	412	GLN	3.3
1	C	257	ARG	3.3
1	A	298	LEU	3.2
1	C	299	LEU	3.2
1	A	292	VAL	3.1
1	D	351	GLY	3.1
1	C	375	TYR	3.0
1	C	297	VAL	3.0
1	C	303	TYR	3.0
1	A	293	THR	2.9
1	C	298	LEU	2.9
1	A	346	ARG	2.8
1	A	341	PHE	2.7
1	A	375	TYR	2.7
1	A	222	MET	2.7
1	D	356	PRO	2.7
1	B	222	MET	2.6
1	C	292	VAL	2.6
1	A	410	ILE	2.6
1	A	289	THR	2.6
1	A	294	SER	2.6
1	B	327	GLN	2.4
1	A	295	SER	2.4
1	C	283	LEU	2.4
1	A	243	GLU	2.4
1	A	409	THR	2.4
1	A	348	ARG	2.3
1	C	394	ASP	2.3
1	A	326	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	295	SER	2.2
1	A	297	VAL	2.2
1	D	350	ARG	2.2
1	B	394	ASP	2.2
1	A	291	LYS	2.2
1	C	410	ILE	2.2
1	C	302	ASN	2.2
1	B	91	VAL	2.1
1	B	351	GLY	2.1
1	D	352	MET	2.1
1	C	389	HIS	2.1
1	B	286	MET	2.1
1	B	356	PRO	2.1
1	B	295	SER	2.1
1	D	346	ARG	2.0
1	B	133	LYS	2.0
1	B	89	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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(Å ²)	Q<0.9
5	E3Q	A	513	33/33	0.73	0.27	64,92,101,103	0
4	EDO	C	504	4/4	0.79	0.20	56,56,57,61	0
4	EDO	C	508	4/4	0.79	0.19	53,53,53,62	0
4	EDO	A	512	4/4	0.79	0.24	62,74,80,87	0
5	E3Q	B	509	33/33	0.79	0.23	39,59,81,89	0
5	E3Q	D	517	33/33	0.80	0.21	48,59,85,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	E3Q	C	507	33/33	0.82	0.21	52,64,83,85	0
4	EDO	B	507	4/4	0.82	0.15	55,56,57,58	0
4	EDO	B	505	4/4	0.83	0.19	50,52,54,61	0
4	EDO	B	504	4/4	0.83	0.20	53,54,54,61	0
4	EDO	D	508	4/4	0.83	0.20	61,64,65,67	0
4	EDO	D	509	4/4	0.83	0.20	44,51,57,67	0
6	EPE	B	511	15/15	0.83	0.19	62,72,78,78	0
4	EDO	D	520	4/4	0.84	0.18	61,61,62,65	0
4	EDO	D	513	4/4	0.84	0.20	55,56,60,61	0
4	EDO	D	507	4/4	0.85	0.17	34,42,45,46	0
4	EDO	A	504	4/4	0.85	0.20	32,44,46,47	0
4	EDO	C	506	4/4	0.85	0.17	50,52,55,56	0
4	EDO	A	506	4/4	0.85	0.19	45,49,50,62	0
4	EDO	D	506	4/4	0.85	0.27	74,77,78,80	0
4	EDO	A	510	4/4	0.86	0.18	32,40,40,50	0
4	EDO	D	519	4/4	0.86	0.17	48,51,54,63	0
7	PEG	D	512	7/7	0.86	0.14	32,35,42,47	0
4	EDO	D	510	4/4	0.87	0.16	38,44,44,47	0
4	EDO	A	503	4/4	0.87	0.19	50,55,60,72	0
4	EDO	D	514	4/4	0.87	0.17	50,56,60,63	0
4	EDO	D	515	4/4	0.87	0.15	41,44,44,46	0
4	EDO	C	509	4/4	0.88	0.15	53,55,55,59	0
4	EDO	B	510	4/4	0.88	0.17	40,42,46,56	0
4	EDO	B	506	4/4	0.88	0.22	58,59,60,61	0
6	EPE	D	516	15/15	0.88	0.19	37,69,85,88	0
4	EDO	D	518	4/4	0.88	0.19	41,46,50,54	0
4	EDO	D	505	4/4	0.90	0.15	44,46,48,49	0
4	EDO	A	511	4/4	0.90	0.15	53,54,54,55	0
6	EPE	B	508	15/15	0.90	0.15	45,79,87,89	0
4	EDO	A	507	4/4	0.91	0.12	57,57,57,58	0
7	PEG	D	511	7/7	0.91	0.14	39,40,44,46	0
4	EDO	A	509	4/4	0.91	0.12	35,35,38,41	0
4	EDO	D	503	4/4	0.92	0.13	52,52,58,61	0
4	EDO	A	508	4/4	0.92	0.14	58,63,63,70	0
4	EDO	C	503	4/4	0.93	0.10	45,45,46,46	0
4	EDO	B	503	4/4	0.93	0.14	48,53,55,57	0
4	EDO	A	505	4/4	0.93	0.09	34,34,34,35	0
4	EDO	D	504	4/4	0.94	0.08	34,36,38,41	0
6	EPE	C	505	15/15	0.95	0.11	37,50,67,74	0
2	ZN	C	501	1/1	0.99	0.03	31,31,31,31	0
3	MG	A	502	1/1	0.99	0.04	19,19,19,19	0
3	MG	C	502	1/1	0.99	0.03	17,17,17,17	0

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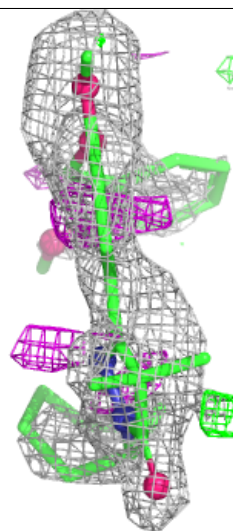
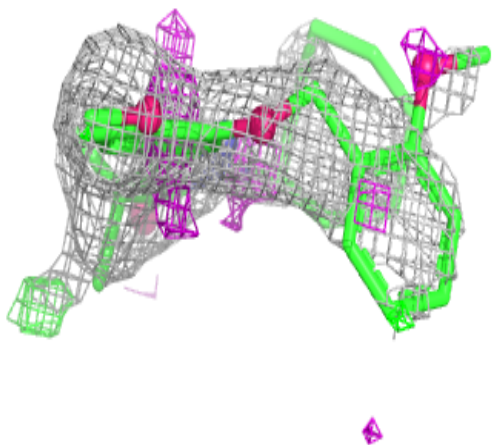
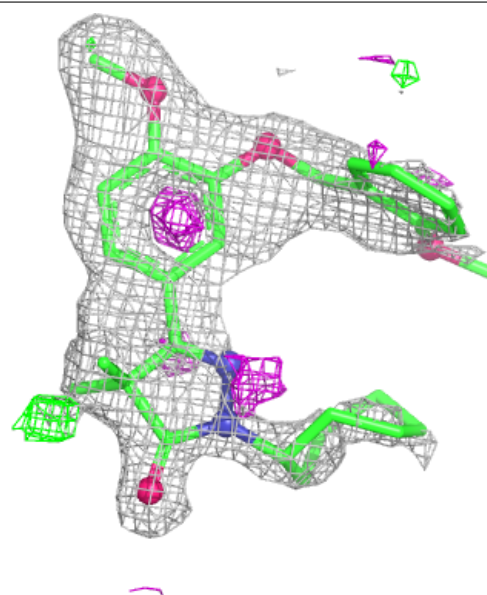
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	B	501	1/1	0.99	0.04	31,31,31,31	0
3	MG	B	502	1/1	1.00	0.02	17,17,17,17	0
2	ZN	D	501	1/1	1.00	0.02	26,26,26,26	0
3	MG	D	502	1/1	1.00	0.03	15,15,15,15	0
2	ZN	A	501	1/1	1.00	0.02	29,29,29,29	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.

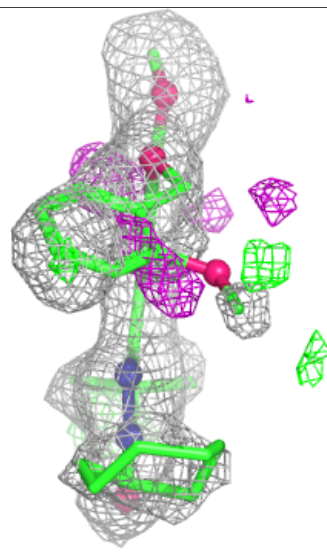
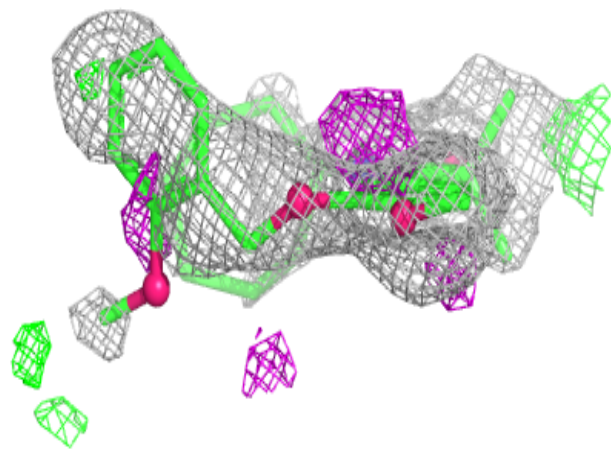
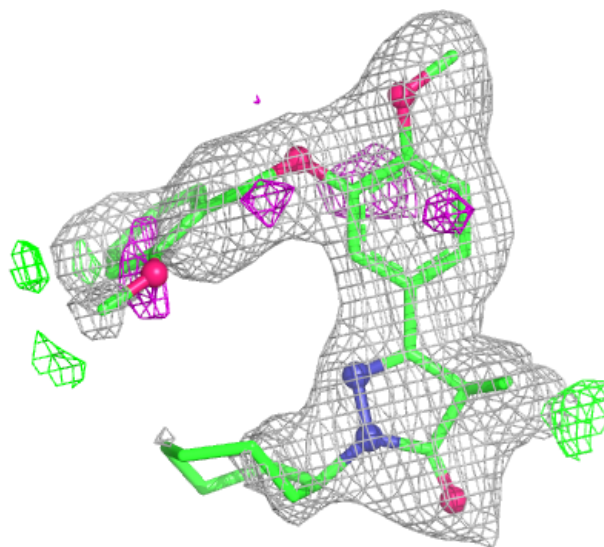
Electron density around E3Q A 513:

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



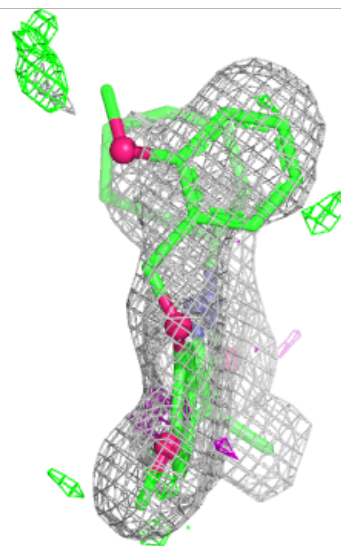
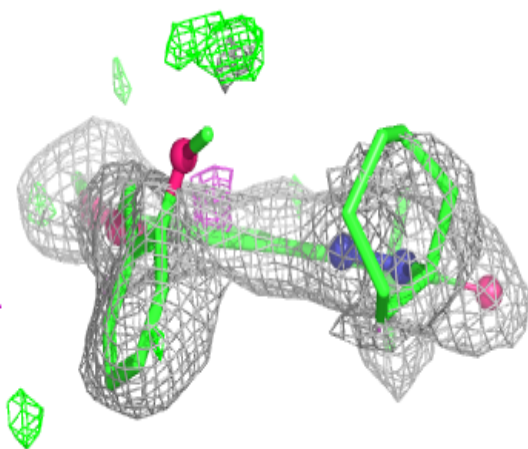
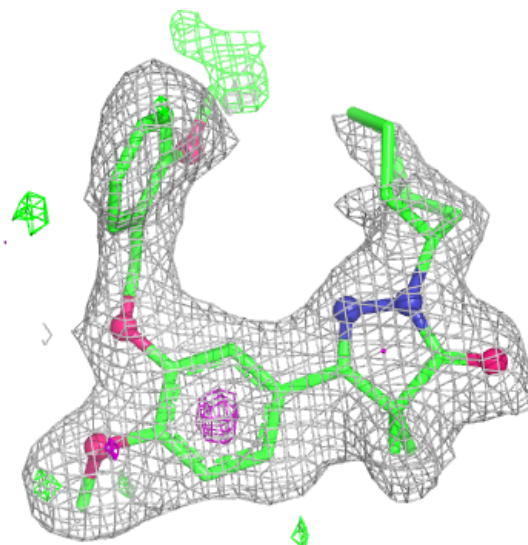
Electron density around E3Q B 509:

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



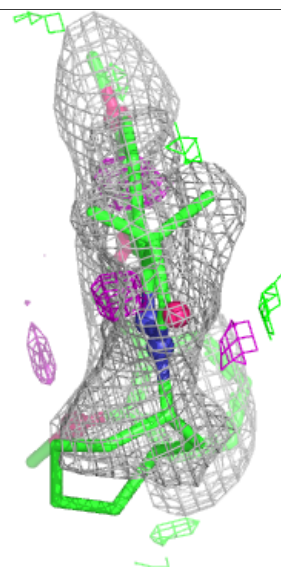
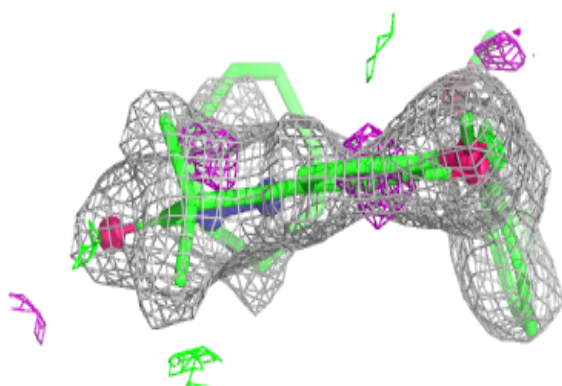
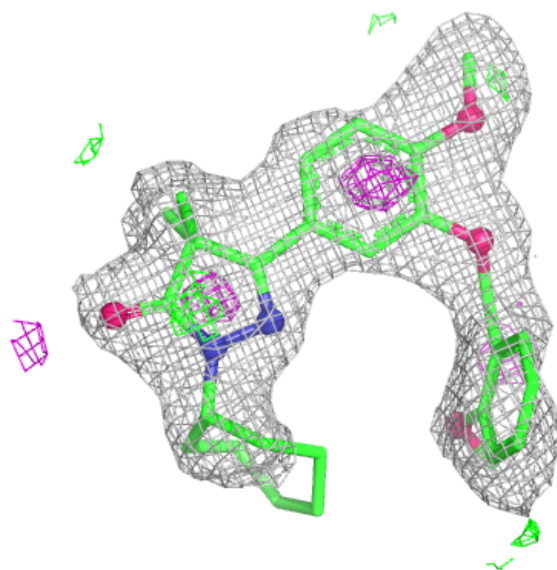
Electron density around E3Q D 517:

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



Electron density around E3Q C 507:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.