



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:27 AM UTC

PDB ID : 7AAG / pdb_00007aag
Title : Crystal structure of human phosphodiesterase 4D2 catalytic domain with inhibitor NPD-617
Authors : Singh, A.K.; Blaazer, A.R.; Zara, L.; de Esch, I.J.P.; Leurs, R.; Brown, D.G.
Deposited on : 2020-09-04
Resolution : 1.79 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

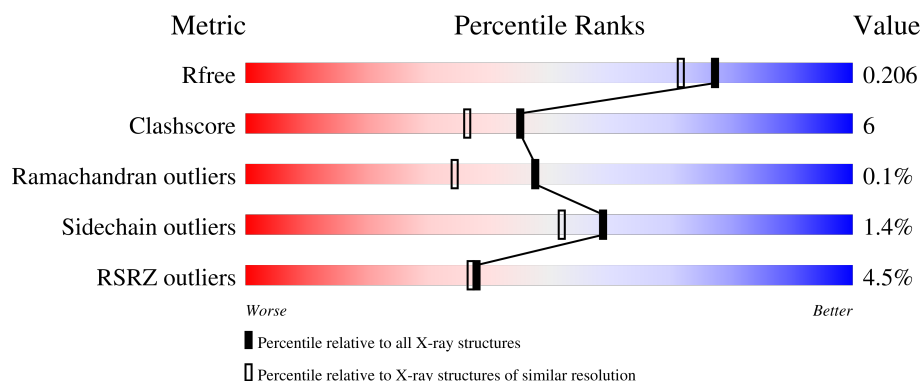
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

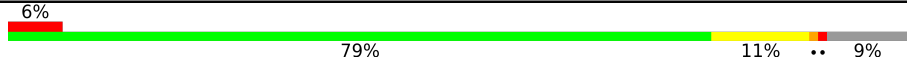
The reported resolution of this entry is 1.79 Å.

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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	
1	B	364	
1	C	364	
1	D	364	

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
5	EDO	B	512	-	-	X	-
6	PEG	D	501	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 11980 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	330	Total	C	N	O	S	0	1	0
			2675	1694	456	511	14			
1	B	324	Total	C	N	O	S	0	2	0
			2633	1665	450	504	14			
1	C	322	Total	C	N	O	S	0	2	0
			2624	1658	448	503	15			
1	D	324	Total	C	N	O	S	0	1	0
			2628	1663	448	503	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

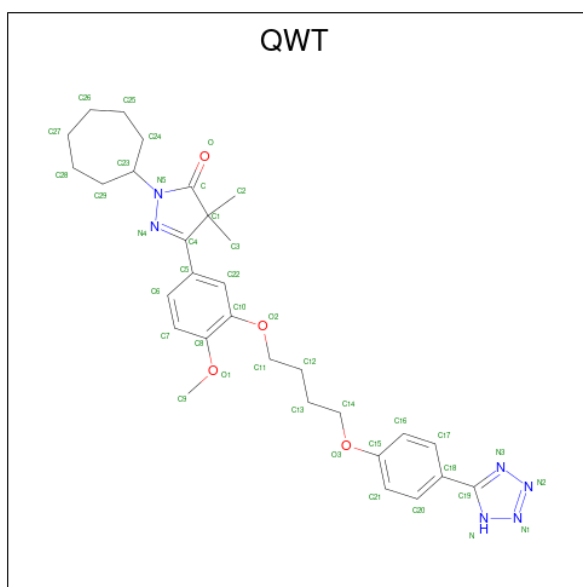
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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	2	Total	Mg	0	0
			2	2		
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-cycloheptyl-3-(4-methoxy-3-{4-[4-(1H-1,2,3,4-tetrazol-5-yl)phenoxy]butoxy}phenyl)-4,4-dimethyl-4,5-dihydro-1H-pyrazol-5-one (CCD ID: QWT) (formula: C₃₀H₃₈N₆O₄) (labeled as "Ligand of Interest" by depositor).



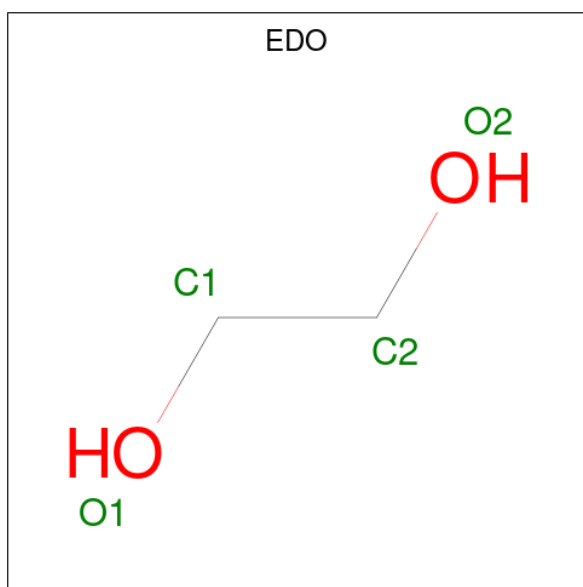
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			40	30	6	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			40	30	6	4		
4	C	1	Total	C	N	O	0	0
			40	30	6	4		
4	D	1	Total	C	N	O	0	0
			40	30	6	4		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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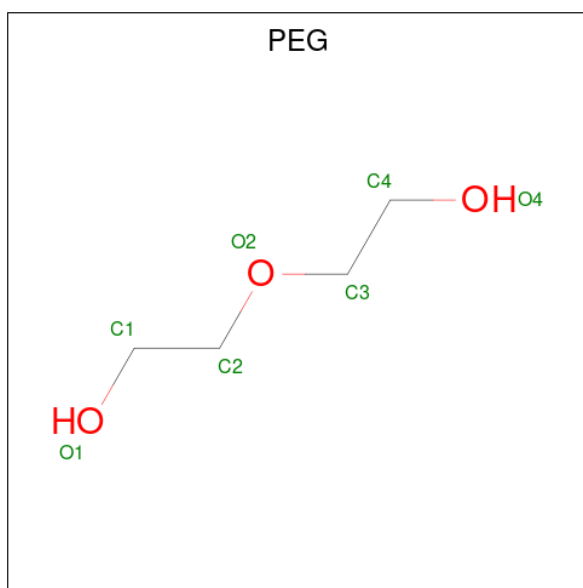
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0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

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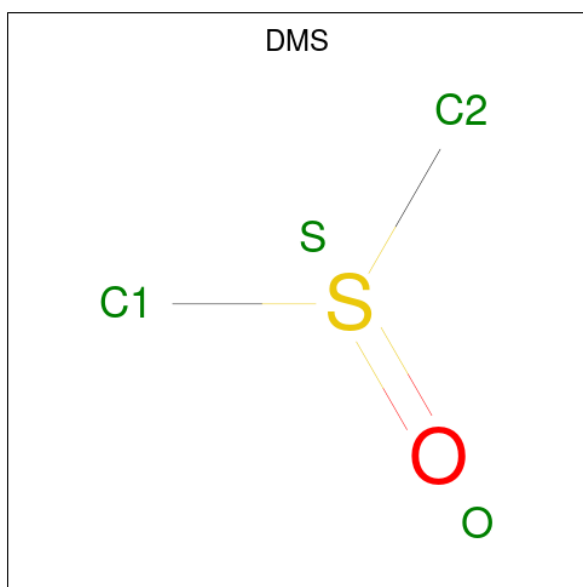
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



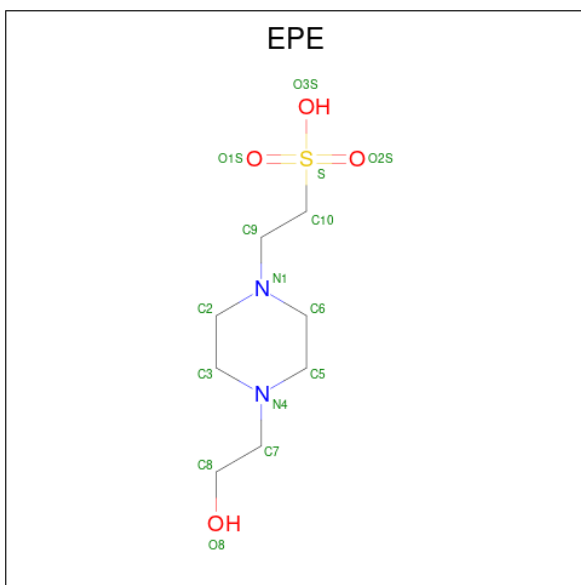
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	C	1	Total	C	O	0	0
			7	4	3		
6	D	1	Total	C	O	0	0
			7	4	3		
6	D	1	Total	C	O	0	0
			7	4	3		
6	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



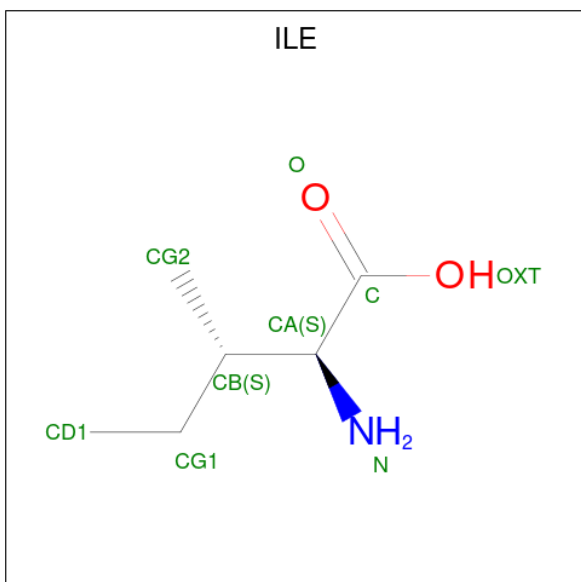
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	S	0	0
			4	2	1	1		
7	A	1	Total	C	O	S	0	0
			4	2	1	1		
7	A	1	Total	C	O	S	0	0
			4	2	1	1		
7	A	1	Total	C	O	S	0	0
			4	2	1	1		
7	B	1	Total	C	O	S	0	0
			4	2	1	1		
7	B	1	Total	C	O	S	0	0
			4	2	1	1		
7	B	1	Total	C	O	S	0	0
			4	2	1	1		
7	C	1	Total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

- Molecule 8 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



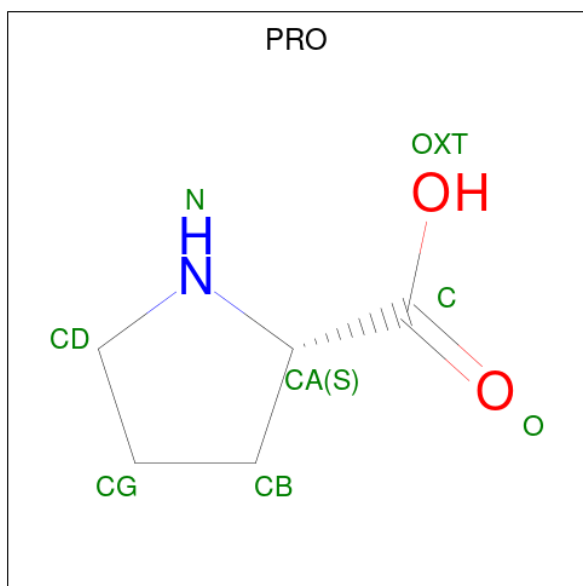
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
8	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
8	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
8	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
8	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 9 is ISOLEUCINE (CCD ID: ILE) (formula: $C_6H_{13}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	C	N	O	0	0
			8	6	1	1		

- Molecule 10 is PROLINE (CCD ID: PRO) (formula: $C_5H_9NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	C	1	Total	C	N	O	0	0
			7	5	1	1		

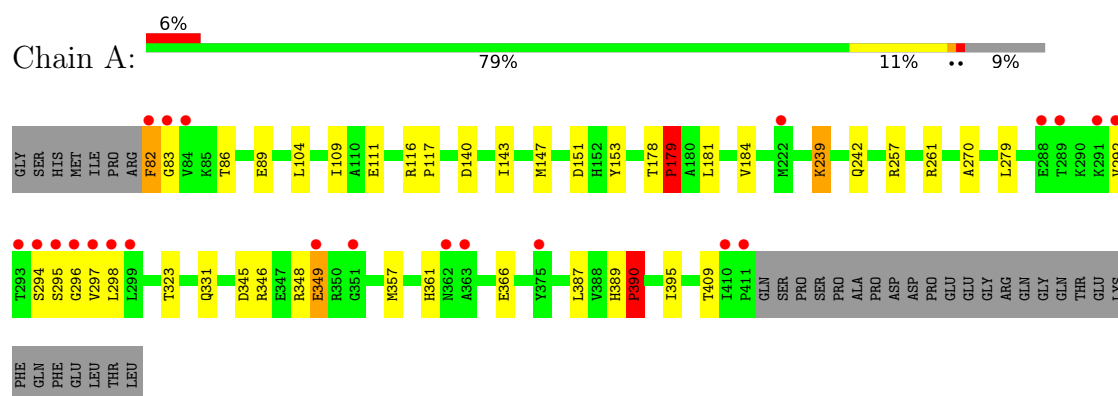
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	217	Total	O	0	0
			217	217		
11	B	235	Total	O	0	0
			235	235		
11	C	181	Total	O	0	0
			181	181		
11	D	245	Total	O	0	0
			245	245		

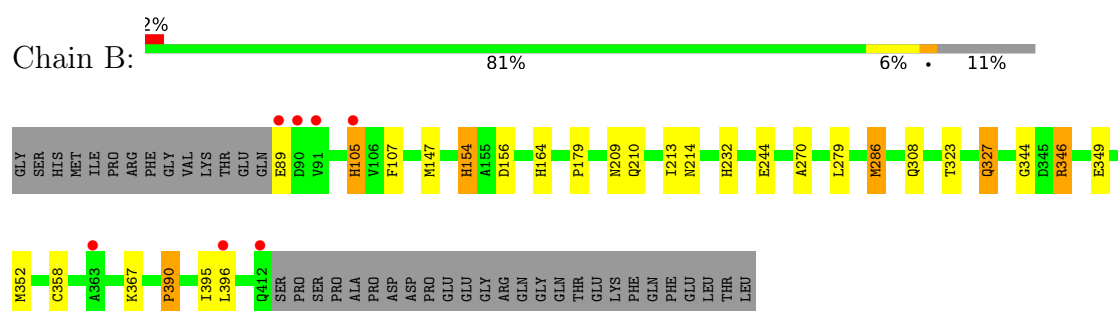
3 Residue-property plots

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.

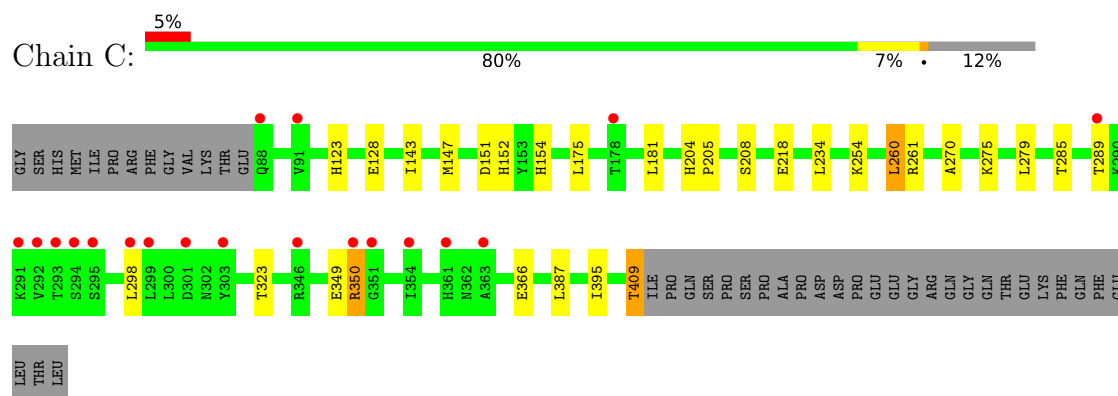
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



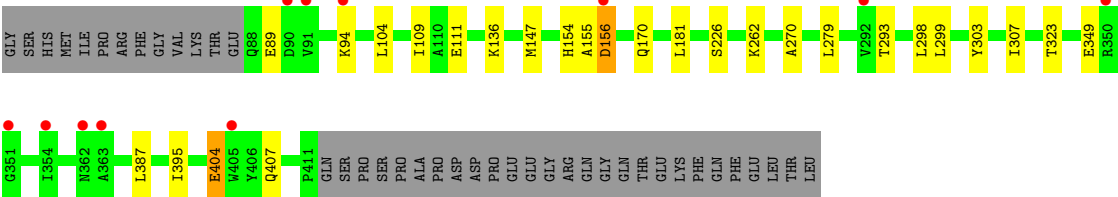
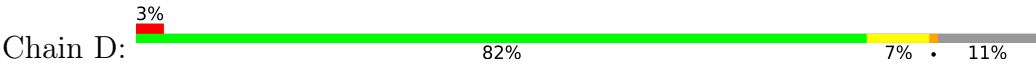
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



- 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	98.44Å 110.82Å 161.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.94 – 1.79 66.94 – 1.79	Depositor EDS
% Data completeness (in resolution range)	100.0 (66.94-1.79) 100.0 (66.94-1.79)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.167 , 0.197 0.180 , 0.206	Depositor DCC
R_{free} test set	8357 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.2	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	11980	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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, QWT, DMS, EPE, PEG, EDO, ZN

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	7/2733 (0.3%)	1.33	11/3712 (0.3%)
1	B	1.13	5/2690 (0.2%)	1.24	1/3655 (0.0%)
1	C	1.15	4/2677 (0.1%)	1.28	7/3635 (0.2%)
1	D	1.14	5/2685 (0.2%)	1.24	5/3648 (0.1%)
All	All	1.16	21/10785 (0.2%)	1.28	24/14650 (0.2%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	PRO	N-CA	15.98	1.67	1.47
1	C	205	PRO	N-CA	15.07	1.67	1.47
1	A	390	PRO	N-CA	13.29	1.69	1.47
1	D	156	ASP	CG-OD1	-7.72	1.10	1.25
1	C	204	HIS	C-N	7.71	1.42	1.34
1	B	232	HIS	CE1-NE2	7.45	1.40	1.32
1	D	404[A]	GLU	C-O	7.05	1.32	1.24
1	D	404[B]	GLU	C-O	7.05	1.32	1.24
1	B	179	PRO	C-O	-6.98	1.15	1.24
1	B	105	HIS	CE1-NE2	-6.01	1.26	1.32
1	A	117	PRO	C-O	-5.96	1.16	1.24
1	B	164	HIS	CE1-NE2	5.93	1.38	1.32
1	A	179	PRO	C-O	-5.84	1.16	1.24
1	B	154	HIS	CE1-NE2	5.50	1.38	1.32
1	A	242[A]	GLN	C-O	5.49	1.31	1.24
1	A	242[B]	GLN	C-O	5.49	1.31	1.24
1	C	154	HIS	CE1-NE2	5.29	1.37	1.32
1	D	156	ASP	N-CA	5.28	1.52	1.46
1	A	389	HIS	C-N	5.27	1.44	1.34
1	C	205	PRO	C-O	-5.06	1.17	1.24
1	D	293	THR	C-O	5.04	1.30	1.23

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	204	HIS	CA-C-N	14.98	135.45	119.87
1	C	204	HIS	C-N-CA	14.98	135.45	119.87
1	A	178	THR	CA-C-N	12.13	135.00	119.84
1	A	178	THR	C-N-CA	12.13	135.00	119.84
1	D	404[A]	GLU	CA-C-O	9.09	130.37	120.10
1	D	404[B]	GLU	CA-C-O	9.09	130.37	120.10
1	A	242[A]	GLN	CA-C-O	8.72	130.54	119.12
1	A	242[B]	GLN	CA-C-O	8.72	130.54	119.12
1	C	205	PRO	N-CA-C	-7.00	105.42	114.03
1	C	205	PRO	CB-CA-C	6.77	121.66	111.44
1	A	242[A]	GLN	N-CA-C	6.69	121.30	113.20
1	A	242[B]	GLN	N-CA-C	6.69	121.30	113.20
1	A	390	PRO	CA-N-CD	-6.36	102.60	111.50
1	D	404[A]	GLU	N-CA-C	6.25	118.89	111.71
1	D	404[B]	GLU	N-CA-C	6.25	118.89	111.71
1	A	179	PRO	CA-N-CD	-5.76	103.93	112.00
1	A	83	GLY	O-C-N	5.63	127.32	121.97
1	C	205	PRO	CA-N-CD	-5.43	104.40	112.00
1	A	82	PHE	CA-CB-CG	5.30	119.10	113.80
1	D	155	ALA	O-C-N	-5.29	115.34	122.43
1	C	349	GLU	CB-CG-CD	5.28	121.57	112.60
1	A	349	GLU	CB-CA-C	5.27	121.33	110.31
1	C	154	HIS	CA-CB-CG	-5.07	108.73	113.80
1	B	390	PRO	N-CA-CB	-5.01	97.09	102.60

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	2675	0	2633	36	0
1	B	2633	0	2588	38	0
1	C	2624	0	2573	31	0
1	D	2628	0	2584	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	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	0	2	0
4	B	40	0	0	0	0
4	C	40	0	0	0	0
4	D	40	0	0	0	0
5	A	60	0	90	4	0
5	B	40	0	60	11	0
5	C	40	0	59	7	0
5	D	60	0	89	1	0
6	A	7	0	10	0	0
6	C	7	0	10	0	0
6	D	21	0	30	17	0
7	A	20	0	30	5	0
7	B	12	0	18	3	0
7	C	8	0	12	2	0
7	D	8	0	12	3	0
8	A	15	0	17	5	0
8	B	30	0	36	3	0
8	C	15	0	17	0	0
8	D	15	0	17	1	0
9	C	8	0	10	0	0
10	C	7	0	7	0	0
11	A	217	0	0	1	0
11	B	235	0	0	1	0
11	C	181	0	0	1	0
11	D	245	0	0	3	0
All	All	11980	0	10902	129	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (129) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:PRO:N	1:A:179:PRO:CA	1.67	1.41
1:A:390:PRO:N	1:A:390:PRO:CA	1.69	1.37
1:D:154:HIS:ND1	6:D:501:PEG:H21	1.53	1.24
1:D:154:HIS:ND1	6:D:501:PEG:H31	1.62	1.13
1:C:366:GLU:HG2	1:C:409:THR:CG2	1.79	1.13
1:A:153:TYR:O	5:A:520:EDO:H11	1.46	1.11
1:A:151:ASP:O	5:A:520:EDO:H21	1.51	1.10
1:A:331:GLN:OE1	8:A:519:EPE:H81	1.58	1.02
1:D:154:HIS:ND1	6:D:501:PEG:C2	2.25	0.99
1:B:105:HIS:HB2	8:B:516:EPE:O3S	1.66	0.95
1:D:154:HIS:ND1	6:D:501:PEG:C3	2.30	0.94
1:C:366:GLU:HG2	1:C:409:THR:HG22	1.46	0.94
1:D:262:LYS:HD3	7:D:519:DMS:H21	1.54	0.88
1:D:154:HIS:CG	6:D:501:PEG:H21	2.10	0.86
1:B:210:GLN:OE1	7:B:514:DMS:H21	1.76	0.85
5:A:520:EDO:H12	5:A:521:EDO:O1	1.77	0.84
1:B:352:MET:HE2	5:B:512:EDO:C2	2.10	0.81
1:C:123:HIS:ND1	1:C:143:ILE:HD11	1.96	0.81
1:B:352:MET:HE2	5:B:512:EDO:C1	2.12	0.80
1:A:296:GLY:O	7:A:515:DMS:H13	1.82	0.79
1:D:156:ASP:N	1:D:156:ASP:OD1	2.11	0.78
1:A:239:LYS:HD2	1:C:218:GLU:OE1	1.87	0.74
1:D:303:TYR:CE1	7:D:519:DMS:H23	2.23	0.73
1:B:286:MET:HE3	1:B:308:GLN:NE2	2.04	0.72
1:B:154:HIS:HB3	6:D:501:PEG:H42	1.73	0.71
1:B:105:HIS:HB2	8:B:516:EPE:S	2.31	0.70
1:B:154:HIS:ND1	6:D:501:PEG:O2	2.24	0.69
1:A:179:PRO:N	1:A:179:PRO:C	2.51	0.67
1:A:357:MET:SD	4:A:503:QWT:C14	2.83	0.67
1:B:156:ASP:OD1	6:D:501:PEG:H41	1.96	0.65
1:C:234:LEU:HB3	6:D:518:PEG:H22	1.78	0.65
1:A:257:ARG:HB3	7:A:513:DMS:H21	1.78	0.64
1:C:366:GLU:HG2	1:C:409:THR:HG21	1.76	0.64
1:A:346:ARG:HD3	1:C:151:ASP:OD2	1.99	0.63
1:D:154:HIS:CG	6:D:501:PEG:H31	2.33	0.62
1:A:292:VAL:HG11	7:A:515:DMS:H11	1.81	0.62
1:B:154:HIS:CG	6:D:501:PEG:H42	2.36	0.61
1:B:105:HIS:HE1	1:B:107:PHE:HB2	1.67	0.60
1:D:154:HIS:ND1	6:D:501:PEG:O2	2.33	0.60
1:A:361:HIS:HE1	11:A:778:HOH:O	1.84	0.59
1:C:181:LEU:HD21	1:C:298:LEU:HD12	1.84	0.59
1:A:143:ILE:O	1:A:147:MET:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:511:EDO:H22	11:B:705:HOH:O	2.03	0.58
1:C:260:LEU:C	1:C:260:LEU:HD13	2.28	0.58
1:A:86:THR:OG1	1:A:89:GLU:HG3	2.04	0.57
5:C:507:EDO:O2	5:C:515:EDO:C1	2.52	0.57
1:B:214:ASN:HD22	5:B:512:EDO:H21	1.70	0.57
1:D:226:SER:HB2	11:D:673:HOH:O	2.04	0.56
1:B:105:HIS:CD2	1:B:327:GLN:OE1	2.58	0.56
5:C:507:EDO:O2	5:C:515:EDO:H11	2.06	0.55
1:B:352:MET:HE2	5:B:512:EDO:H11	1.89	0.55
1:B:154:HIS:CB	6:D:501:PEG:H42	2.37	0.55
1:C:254:LYS:NZ	11:C:601:HOH:O	2.40	0.54
1:B:105:HIS:CE1	1:B:107:PHE:HB2	2.43	0.54
1:A:111:GLU:OE2	8:A:519:EPE:H31	2.07	0.54
1:A:357:MET:SD	4:A:503:QWT:C13	2.96	0.54
1:C:123:HIS:CE1	1:C:143:ILE:HD11	2.44	0.53
1:C:234:LEU:CB	6:D:518:PEG:H22	2.39	0.53
1:B:352:MET:CE	5:B:512:EDO:H11	2.39	0.52
1:C:128:GLU:HG3	5:C:516:EDO:H12	1.91	0.52
8:A:519:EPE:N4	8:A:519:EPE:H92	2.23	0.52
8:A:519:EPE:N4	8:A:519:EPE:C9	2.72	0.52
1:A:181:LEU:HD21	1:A:298:LEU:HD12	1.91	0.52
1:A:270:ALA:HB1	1:A:279:LEU:HD11	1.91	0.52
1:B:270:ALA:HB1	1:B:279:LEU:HD11	1.92	0.51
1:C:261:ARG:HB2	5:C:508:EDO:H12	1.93	0.51
1:C:298:LEU:HD11	1:C:387:LEU:HG	1.92	0.51
1:B:352:MET:HB3	5:B:512:EDO:H22	1.92	0.50
1:C:366:GLU:CG	1:C:409:THR:HG22	2.30	0.50
1:B:323:THR:HB	1:B:395:ILE:HG23	1.94	0.50
1:A:349:GLU:HG3	1:C:147[B]:MET:CE	2.41	0.49
1:B:209:ASN:HB3	7:B:514:DMS:H13	1.94	0.49
1:C:175:LEU:HD23	5:C:510:EDO:H21	1.94	0.49
1:B:352:MET:HE2	5:B:512:EDO:H22	1.94	0.49
1:B:286:MET:CE	1:B:308:GLN:NE2	2.75	0.48
1:D:407:GLN:CD	5:D:524:EDO:H11	2.37	0.48
1:B:346:ARG:HD2	11:D:603:HOH:O	2.12	0.48
1:D:299:LEU:C	1:D:299:LEU:HD13	2.39	0.48
1:C:350:ARG:HA	7:C:501:DMS:H21	1.96	0.48
1:D:136:LYS:HE2	7:D:520:DMS:H11	1.95	0.48
1:B:286:MET:HE3	1:B:308:GLN:HE22	1.78	0.47
1:C:270:ALA:HB1	1:C:279:LEU:HD11	1.97	0.47
1:C:285:THR:O	1:C:289:THR:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ASN:HD22	5:B:512:EDO:C2	2.27	0.47
1:D:111:GLU:OE2	8:D:522:EPE:H32	2.15	0.47
1:B:213:ILE:HD12	7:B:514:DMS:H11	1.97	0.47
1:D:181:LEU:HD21	1:D:298:LEU:HD12	1.95	0.47
1:B:105:HIS:HB2	8:B:516:EPE:HOS3	1.73	0.47
1:D:270:ALA:HB1	1:D:279:LEU:HD11	1.96	0.46
1:A:140:ASP:HB2	7:C:501:DMS:H12	1.98	0.46
1:D:404[A]:GLU:HG2	11:D:622:HOH:O	2.16	0.46
1:A:349:GLU:HG3	1:C:147[B]:MET:HE1	1.98	0.45
1:A:184:VAL:CG2	1:A:297:VAL:HG13	2.46	0.45
5:A:510:EDO:H11	1:C:152:HIS:CD2	2.52	0.45
1:B:156:ASP:OD1	6:D:501:PEG:C4	2.64	0.45
1:A:111:GLU:OE1	8:A:519:EPE:H21	2.17	0.45
1:A:298:LEU:HD11	1:A:387:LEU:HG	1.97	0.44
1:A:323:THR:HB	1:A:395:ILE:HG23	1.99	0.44
1:B:244:GLU:OE1	1:C:254:LYS:HE2	2.17	0.44
1:B:352:MET:CE	5:B:512:EDO:C1	2.87	0.44
1:D:154:HIS:HB3	6:D:501:PEG:H32	1.99	0.44
1:B:147:MET:SD	1:D:349:GLU:HB3	2.57	0.44
1:D:298:LEU:HD11	1:D:387:LEU:HG	1.99	0.44
1:A:181:LEU:CD2	1:A:298:LEU:HD12	2.48	0.44
1:A:261:ARG:HD2	7:A:513:DMS:H13	2.00	0.44
1:A:345:ASP:OD1	1:A:348:ARG:NH2	2.50	0.44
1:A:257:ARG:CB	7:A:513:DMS:H21	2.48	0.43
1:B:349:GLU:HG3	1:D:147:MET:SD	2.59	0.43
1:C:181:LEU:CD2	1:C:298:LEU:HD12	2.48	0.43
1:D:104:LEU:HD11	1:D:109:ILE:HD11	2.00	0.43
1:D:104:LEU:HD22	1:D:170:GLN:HG3	2.01	0.43
1:D:323:THR:HB	1:D:395:ILE:HG23	2.01	0.43
1:B:286:MET:HE3	1:B:308:GLN:HE21	1.78	0.42
1:B:286:MET:HE3	1:B:286:MET:HB2	1.95	0.42
1:D:307:ILE:HD12	1:D:307:ILE:HA	1.91	0.42
1:A:104:LEU:HD11	1:A:109:ILE:CD1	2.50	0.42
1:A:366:GLU:HG2	1:A:409:THR:OG1	2.19	0.42
1:A:116:ARG:HH11	1:A:116:ARG:HD3	1.67	0.42
1:A:143:ILE:O	1:A:147:MET:CG	2.68	0.42
1:A:349:GLU:HG3	1:C:147[B]:MET:SD	2.60	0.41
1:C:208:SER:HB3	5:C:515:EDO:H12	2.01	0.41
1:D:104:LEU:HD11	1:D:109:ILE:CD1	2.50	0.41
1:C:261:ARG:HB2	5:C:508:EDO:C1	2.51	0.41
1:A:239:LYS:HD2	1:C:218:GLU:CD	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:MET:HE2	5:B:512:EDO:H21	1.97	0.41
1:C:323:THR:HB	1:C:395:ILE:HG23	2.02	0.41
1:B:154:HIS:ND1	6:D:501:PEG:H42	2.35	0.41
1:B:344:GLY:HA3	1:B:358:CYS:O	2.21	0.40
1:C:275:LYS:HA	1:C:275:LYS:HD3	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	329/364 (90%)	324 (98%)	4 (1%)	1 (0%)	36	25
1	B	324/364 (89%)	321 (99%)	3 (1%)	0	100	100
1	C	322/364 (88%)	320 (99%)	2 (1%)	0	100	100
1	D	323/364 (89%)	318 (98%)	5 (2%)	0	100	100
All	All	1298/1456 (89%)	1283 (99%)	14 (1%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	295	SER

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	302/331 (91%)	297 (98%)	5 (2%)	53	45
1	B	298/331 (90%)	291 (98%)	7 (2%)	44	33
1	C	296/331 (89%)	293 (99%)	3 (1%)	68	64
1	D	297/331 (90%)	295 (99%)	2 (1%)	76	73
All	All	1193/1324 (90%)	1176 (99%)	17 (1%)	59	52

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	PHE
1	A	179	PRO
1	A	239	LYS
1	A	294	SER
1	A	390	PRO
1	B	89	GLU
1	B	286	MET
1	B	327	GLN
1	B	346	ARG
1	B	367	LYS
1	B	390	PRO
1	B	396	LEU
1	C	260	LEU
1	C	350	ARG
1	C	409	THR
1	D	89	GLU
1	D	94	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	A	224	ASN
1	A	250	GLN
1	B	105	HIS
1	B	321	ASN
1	B	389	HIS
1	C	210	GLN
1	C	250	GLN
1	C	308	GLN
1	D	105	HIS

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Mol	Chain	Res	Type
1	D	210	GLN
1	D	258	GLN
1	D	321	ASN
1	D	407	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 87 ligands modelled in this entry, 9 are monoatomic - leaving 78 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	$\# Z > 2$
5	EDO	C	517	-	3,3,3	0.59	0	2,2,2	0.73	0
6	PEG	D	518	-	6,6,6	0.75	0	5,5,5	0.53	0
5	EDO	B	512	-	3,3,3	0.61	0	2,2,2	0.75	0
7	DMS	A	517	-	3,3,3	0.39	0	3,3,3	0.02	0
5	EDO	D	509	-	3,3,3	0.21	0	2,2,2	0.44	0
5	EDO	B	507	-	3,3,3	0.19	0	2,2,2	0.15	0
5	EDO	C	518	-	3,3,3	0.12	0	2,2,2	0.18	0
5	EDO	A	518	-	3,3,3	0.68	0	2,2,2	0.43	0
5	EDO	C	507	-	3,3,3	0.51	0	2,2,2	0.20	0
7	DMS	C	501	-	3,3,3	0.22	0	3,3,3	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	A	504	-	3,3,3	0.24	0	2,2,2	0.23	0
5	EDO	A	505	-	3,3,3	0.19	0	2,2,2	0.39	0
6	PEG	C	512	-	6,6,6	0.23	0	5,5,5	0.28	0
7	DMS	A	513	-	3,3,3	0.46	0	3,3,3	0.49	0
7	DMS	B	513	-	3,3,3	0.59	0	3,3,3	0.14	0
5	EDO	D	512	-	3,3,3	0.36	0	2,2,2	0.25	0
5	EDO	D	507	-	3,3,3	0.30	0	2,2,2	0.54	0
5	EDO	A	522	-	3,3,3	0.30	0	2,2,2	0.31	0
5	EDO	B	509	-	3,3,3	0.29	0	2,2,2	0.34	0
9	ILE	C	502	-	6,7,8	0.62	0	4,8,10	1.31	1 (25%)
6	PEG	A	512	-	6,6,6	0.21	0	5,5,5	0.07	0
6	PEG	D	501	-	6,6,6	0.84	0	5,5,5	1.28	1 (20%)
5	EDO	C	511	-	3,3,3	0.20	0	2,2,2	0.27	0
5	EDO	C	515	-	3,3,3	0.65	0	2,2,2	0.14	0
5	EDO	D	511	-	3,3,3	0.46	0	2,2,2	0.52	0
5	EDO	B	517	-	3,3,3	0.05	0	2,2,2	0.01	0
7	DMS	B	514	-	3,3,3	0.24	0	3,3,3	0.45	0
7	DMS	D	519	-	3,3,3	0.34	0	3,3,3	0.39	0
5	EDO	C	510	-	3,3,3	0.17	0	2,2,2	0.44	0
7	DMS	B	518	-	3,3,3	0.26	0	3,3,3	0.14	0
5	EDO	B	508	-	3,3,3	0.19	0	2,2,2	0.38	0
5	EDO	C	509	-	3,3,3	0.68	0	2,2,2	0.54	0
8	EPE	C	514	-	15,15,15	2.50	1 (6%)	19,20,20	1.50	3 (15%)
5	EDO	D	510	-	3,3,3	0.25	0	2,2,2	0.49	0
5	EDO	C	508	-	3,3,3	0.42	0	2,2,2	0.10	0
5	EDO	A	506	-	3,3,3	0.23	0	2,2,2	0.11	0
5	EDO	B	510	-	3,3,3	0.26	0	2,2,2	0.34	0
5	EDO	D	508	-	3,3,3	0.36	0	2,2,2	0.49	0
5	EDO	B	501	-	3,3,3	0.31	0	2,2,2	0.23	0
4	QWT	C	506	-	43,44,44	0.97	1 (2%)	53,61,61	1.59	8 (15%)
7	DMS	A	515	-	3,3,3	0.30	0	3,3,3	0.25	0
5	EDO	B	506	-	3,3,3	0.23	0	2,2,2	0.28	0
7	DMS	D	520	-	3,3,3	0.24	0	3,3,3	0.12	0
5	EDO	A	511	-	3,3,3	0.18	0	2,2,2	0.28	0
4	QWT	D	505	-	43,44,44	0.90	2 (4%)	53,61,61	2.07	8 (15%)
5	EDO	A	524	-	3,3,3	0.11	0	2,2,2	0.23	0
5	EDO	D	521	-	3,3,3	1.54	1 (33%)	2,2,2	0.95	0
5	EDO	A	523	-	3,3,3	0.23	0	2,2,2	0.23	0
5	EDO	D	523	-	3,3,3	0.20	0	2,2,2	0.12	0
4	QWT	B	504	-	43,44,44	1.13	3 (6%)	53,61,61	1.71	8 (15%)
8	EPE	B	515	-	15,15,15	1.66	1 (6%)	19,20,20	2.09	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	EPE	A	519	-	15,15,15	2.45	2 (13%)	19,20,20	2.08	7 (36%)
8	EPE	D	522	-	15,15,15	2.02	1 (6%)	19,20,20	1.61	3 (15%)
5	EDO	A	520	-	3,3,3	0.26	0	2,2,2	0.53	0
6	PEG	D	517	-	6,6,6	0.14	0	5,5,5	0.10	0
5	EDO	B	505	-	3,3,3	0.24	0	2,2,2	0.64	0
5	EDO	C	516	-	3,3,3	0.32	0	2,2,2	0.11	0
5	EDO	A	507	-	3,3,3	0.41	0	2,2,2	0.36	0
5	EDO	D	524	-	3,3,3	0.15	0	2,2,2	0.18	0
10	PRO	C	503	-	6,7,8	0.53	0	7,8,10	1.76	3 (42%)
5	EDO	C	519	-	3,3,3	0.08	0	2,2,2	0.06	0
7	DMS	A	514	-	3,3,3	0.36	0	3,3,3	0.20	0
5	EDO	D	502	-	3,3,3	0.09	0	2,2,2	0.16	0
5	EDO	D	514	-	3,3,3	0.16	0	2,2,2	0.31	0
5	EDO	A	509	-	3,3,3	0.11	0	2,2,2	0.11	0
4	QWT	A	503	-	43,44,44	1.01	4 (9%)	53,61,61	1.61	7 (13%)
5	EDO	D	516	-	3,3,3	0.64	0	2,2,2	0.60	0
5	EDO	A	521	-	3,3,3	0.33	0	2,2,2	0.56	0
5	EDO	B	511	-	3,3,3	0.43	0	2,2,2	0.29	0
5	EDO	A	510	-	3,3,3	0.15	0	2,2,2	0.03	0
7	DMS	A	516	-	3,3,3	0.40	0	3,3,3	0.36	0
5	EDO	D	513	-	3,3,3	0.14	0	2,2,2	0.32	0
5	EDO	D	515	-	3,3,3	0.35	0	2,2,2	0.16	0
5	EDO	A	526	-	3,3,3	0.26	0	2,2,2	0.28	0
7	DMS	C	513	-	3,3,3	0.30	0	3,3,3	0.21	0
5	EDO	A	508	-	3,3,3	0.32	0	2,2,2	0.40	0
5	EDO	D	506	-	3,3,3	0.36	0	2,2,2	0.56	0
8	EPE	B	516	-	15,15,15	1.76	2 (13%)	19,20,20	1.57	2 (10%)

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
5	EDO	B	506	-	-	0/1/1/1	-
5	EDO	C	517	-	-	1/1/1/1	-
5	EDO	D	524	-	-	0/1/1/1	-
5	EDO	D	507	-	-	0/1/1/1	-
10	PRO	C	503	-	-	0/0/9/11	0/1/1/1
5	EDO	A	522	-	-	0/1/1/1	-
6	PEG	D	518	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	C	519	-	-	1/1/1/1	-
5	EDO	A	511	-	-	0/1/1/1	-
5	EDO	B	509	-	-	1/1/1/1	-
9	ILE	C	502	-	-	0/7/8/10	-
5	EDO	B	512	-	-	1/1/1/1	-
5	EDO	D	502	-	-	1/1/1/1	-
5	EDO	D	514	-	-	0/1/1/1	-
6	PEG	A	512	-	-	3/4/4/4	-
6	PEG	D	501	-	-	1/4/4/4	-
5	EDO	C	511	-	-	1/1/1/1	-
8	EPE	B	516	-	-	3/9/19/19	0/1/1/1
5	EDO	C	515	-	-	1/1/1/1	-
5	EDO	A	509	-	-	1/1/1/1	-
5	EDO	D	511	-	-	1/1/1/1	-
4	QWT	D	505	-	-	3/21/52/52	0/5/5/5
5	EDO	B	517	-	-	0/1/1/1	-
5	EDO	D	509	-	-	1/1/1/1	-
5	EDO	A	524	-	-	1/1/1/1	-
5	EDO	B	507	-	-	0/1/1/1	-
5	EDO	C	510	-	-	1/1/1/1	-
5	EDO	C	518	-	-	1/1/1/1	-
5	EDO	B	508	-	-	0/1/1/1	-
5	EDO	A	518	-	-	1/1/1/1	-
4	QWT	A	503	-	-	5/21/52/52	0/5/5/5
5	EDO	A	523	-	-	1/1/1/1	-
5	EDO	D	516	-	-	1/1/1/1	-
5	EDO	C	509	-	-	0/1/1/1	-
5	EDO	D	521	-	-	0/1/1/1	-
5	EDO	D	523	-	-	1/1/1/1	-
4	QWT	B	504	-	-	3/21/52/52	0/5/5/5
5	EDO	A	521	-	-	0/1/1/1	-
5	EDO	B	511	-	-	0/1/1/1	-
8	EPE	C	514	-	-	1/9/19/19	0/1/1/1
5	EDO	A	510	-	-	1/1/1/1	-
5	EDO	C	507	-	-	0/1/1/1	-
5	EDO	D	510	-	-	1/1/1/1	-
5	EDO	A	504	-	-	0/1/1/1	-
5	EDO	A	505	-	-	0/1/1/1	-
5	EDO	C	508	-	-	1/1/1/1	-
6	PEG	C	512	-	-	4/4/4/4	-
5	EDO	D	513	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	D	515	-	-	1/1/1/1	-
8	EPE	B	515	-	-	5/9/19/19	0/1/1/1
5	EDO	A	526	-	-	1/1/1/1	-
5	EDO	A	506	-	-	1/1/1/1	-
5	EDO	B	510	-	-	0/1/1/1	-
8	EPE	A	519	-	-	3/9/19/19	0/1/1/1
5	EDO	A	508	-	-	0/1/1/1	-
5	EDO	A	520	-	-	0/1/1/1	-
5	EDO	D	506	-	-	0/1/1/1	-
8	EPE	D	522	-	-	5/9/19/19	0/1/1/1
6	PEG	D	517	-	-	2/4/4/4	-
5	EDO	B	505	-	-	0/1/1/1	-
5	EDO	B	501	-	-	0/1/1/1	-
5	EDO	D	508	-	-	1/1/1/1	-
4	QWT	C	506	-	-	3/21/52/52	0/5/5/5
5	EDO	D	512	-	-	1/1/1/1	-
5	EDO	C	516	-	-	1/1/1/1	-
5	EDO	A	507	-	-	1/1/1/1	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	514	EPE	C10-S	-9.30	1.64	1.77
8	A	519	EPE	C10-S	-8.81	1.65	1.77
8	D	522	EPE	C10-S	-6.67	1.68	1.77
8	B	516	EPE	C10-S	-5.77	1.69	1.77
8	B	515	EPE	C10-S	-5.52	1.69	1.77
4	C	506	QWT	C1-C	4.91	1.57	1.52
4	B	504	QWT	C-N5	-4.20	1.32	1.35
4	B	504	QWT	C29-C23	-3.75	1.43	1.53
4	A	503	QWT	C24-C23	-3.53	1.44	1.53
4	D	505	QWT	C-N5	-3.47	1.33	1.35
4	D	505	QWT	C1-C	2.63	1.55	1.52
4	A	503	QWT	C-N5	-2.60	1.33	1.35
4	A	503	QWT	C4-N4	-2.51	1.25	1.29
5	D	521	EDO	O1-C1	2.33	1.53	1.42
8	B	516	EPE	O2S-S	2.32	1.51	1.45
4	A	503	QWT	N5-N4	-2.15	1.34	1.38
8	A	519	EPE	O1S-S	-2.06	1.39	1.45
4	B	504	QWT	N5-N4	-2.04	1.34	1.38

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	505	QWT	O-C-C1	8.99	135.60	126.93
8	B	515	EPE	O1S-S-C10	7.60	118.21	106.73
4	D	505	QWT	O-C-N5	-6.71	121.37	127.01
4	A	503	QWT	O-C-C1	6.58	133.27	126.93
4	B	504	QWT	O-C-C1	6.42	133.12	126.93
4	C	506	QWT	O-C-C1	5.43	132.17	126.93
4	B	504	QWT	C23-N5-C	-5.24	122.00	131.27
4	D	505	QWT	C23-N5-C	-4.88	122.63	131.27
4	C	506	QWT	O-C-N5	-4.81	122.96	127.01
4	A	503	QWT	C-N5-N4	4.73	116.42	113.43
4	A	503	QWT	C23-N5-C	-4.55	123.22	131.27
4	D	505	QWT	C-N5-N4	4.39	116.20	113.43
4	B	504	QWT	C-N5-N4	4.26	116.12	113.43
4	C	506	QWT	C23-N5-C	-4.14	123.95	131.27
8	B	516	EPE	O3S-S-O1S	-4.12	101.09	111.40
8	A	519	EPE	O1S-S-C10	3.98	112.75	106.73
8	A	519	EPE	O3S-S-O2S	-3.81	101.86	111.40
4	B	504	QWT	O-C-N5	-3.79	123.82	127.01
8	D	522	EPE	O2S-S-C10	3.73	112.36	106.73
4	D	505	QWT	N3-N2-N1	-3.67	106.12	110.50
8	A	519	EPE	O2S-S-C10	-3.64	101.23	106.73
4	C	506	QWT	N3-N2-N1	-3.63	106.16	110.50
8	A	519	EPE	C8-C7-N4	-3.61	100.77	113.44
4	A	503	QWT	N3-N2-N1	-3.59	106.21	110.50
4	B	504	QWT	N3-N2-N1	-3.58	106.23	110.50
8	C	514	EPE	O2S-S-C10	3.29	111.70	106.73
8	C	514	EPE	O3S-S-O2S	-3.17	103.47	111.40
8	B	516	EPE	O3S-S-C10	3.08	112.03	106.00
8	D	522	EPE	C7-N4-C3	2.99	119.21	111.24
10	C	503	PRO	O-C-CA	-2.97	117.14	124.77
4	B	504	QWT	N-N1-N2	2.96	110.89	106.68
4	D	505	QWT	N-N1-N2	2.94	110.87	106.68
4	A	503	QWT	N-N1-N2	2.92	110.84	106.68
4	C	506	QWT	N-N1-N2	2.89	110.79	106.68
8	B	515	EPE	O2S-S-O1S	-2.74	104.90	113.82
4	D	505	QWT	C19-N3-N2	2.71	108.98	106.10
4	C	506	QWT	C5-C4-N4	-2.70	115.67	119.72
4	C	506	QWT	C19-N3-N2	2.68	108.95	106.10
4	A	503	QWT	C19-N3-N2	2.67	108.94	106.10
8	D	522	EPE	C6-C5-N4	-2.67	105.27	110.65
4	B	504	QWT	C19-N3-N2	2.66	108.93	106.10
9	C	502	ILE	O-C-CA	-2.52	118.28	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	506	QWT	C24-C23-N5	-2.48	100.77	112.14
10	C	503	PRO	CB-CA-C	-2.45	109.29	112.66
8	A	519	EPE	O3S-S-C10	2.35	110.61	106.00
4	D	505	QWT	C29-C23-N5	-2.24	101.84	112.14
8	C	514	EPE	O1S-S-C10	2.21	110.07	106.73
4	B	504	QWT	C25-C24-C23	2.19	122.44	115.78
10	C	503	PRO	CD-N-CA	2.16	112.69	107.21
8	A	519	EPE	C2-C3-N4	-2.12	106.38	110.65
8	A	519	EPE	C9-N1-C6	-2.08	105.70	111.24
4	A	503	QWT	O-C-N5	-2.08	125.26	127.01
6	D	501	PEG	C3-O2-C2	2.05	122.22	113.26

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	515	EPE	C8-C7-N4-C3
8	B	516	EPE	C9-C10-S-O1S
8	B	516	EPE	C9-C10-S-O3S
8	C	514	EPE	N4-C7-C8-O8
8	A	519	EPE	N4-C7-C8-O8
6	D	501	PEG	O2-C3-C4-O4
6	D	518	PEG	O1-C1-C2-O2
8	B	515	EPE	C9-C10-S-O3S
8	D	522	EPE	C9-C10-S-O3S
6	D	517	PEG	O1-C1-C2-O2
6	D	518	PEG	O2-C3-C4-O4
6	C	512	PEG	O1-C1-C2-O2
5	A	507	EDO	O1-C1-C2-O2
5	C	510	EDO	O1-C1-C2-O2
5	C	511	EDO	O1-C1-C2-O2
5	D	510	EDO	O1-C1-C2-O2
8	A	519	EPE	C8-C7-N4-C3
4	D	505	QWT	C12-C11-O2-C10
4	B	504	QWT	C12-C11-O2-C10
8	D	522	EPE	S-C10-C9-N1
4	A	503	QWT	C12-C13-C14-O3
6	A	512	PEG	O1-C1-C2-O2
8	A	519	EPE	C8-C7-N4-C5
4	C	506	QWT	C12-C11-O2-C10
4	A	503	QWT	O2-C11-C12-C13
4	A	503	QWT	C12-C11-O2-C10

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Mol	Chain	Res	Type	Atoms
5	A	524	EDO	O1-C1-C2-O2
5	A	526	EDO	O1-C1-C2-O2
5	B	509	EDO	O1-C1-C2-O2
5	B	512	EDO	O1-C1-C2-O2
5	D	511	EDO	O1-C1-C2-O2
8	B	515	EPE	C8-C7-N4-C5
4	C	506	QWT	C8-C10-O2-C11
4	A	503	QWT	C8-C10-O2-C11
5	C	516	EDO	O1-C1-C2-O2
5	D	512	EDO	O1-C1-C2-O2
4	D	505	QWT	C8-C10-O2-C11
8	B	515	EPE	C9-C10-S-O1S
8	B	515	EPE	C9-C10-S-O2S
8	B	516	EPE	C9-C10-S-O2S
8	D	522	EPE	C9-C10-S-O1S
8	D	522	EPE	C9-C10-S-O2S
6	C	512	PEG	C1-C2-O2-C3
6	C	512	PEG	C4-C3-O2-C2
8	D	522	EPE	C8-C7-N4-C3
4	C	506	QWT	C22-C10-O2-C11
5	A	506	EDO	O1-C1-C2-O2
4	B	504	QWT	C8-C10-O2-C11
6	A	512	PEG	C4-C3-O2-C2
5	C	517	EDO	O1-C1-C2-O2
5	C	519	EDO	O1-C1-C2-O2
6	A	512	PEG	O2-C3-C4-O4
6	C	512	PEG	O2-C3-C4-O4
5	D	523	EDO	O1-C1-C2-O2
4	D	505	QWT	C22-C10-O2-C11
4	A	503	QWT	C22-C10-O2-C11
6	D	517	PEG	O2-C3-C4-O4
5	A	523	EDO	O1-C1-C2-O2
5	A	509	EDO	O1-C1-C2-O2
5	C	508	EDO	O1-C1-C2-O2
5	C	518	EDO	O1-C1-C2-O2
5	D	508	EDO	O1-C1-C2-O2
5	D	509	EDO	O1-C1-C2-O2
5	D	515	EDO	O1-C1-C2-O2
5	D	516	EDO	O1-C1-C2-O2
6	D	518	PEG	C4-C3-O2-C2
5	A	510	EDO	O1-C1-C2-O2
5	A	518	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	C	515	EDO	O1-C1-C2-O2
5	D	502	EDO	O1-C1-C2-O2
4	B	504	QWT	C22-C10-O2-C11
6	D	518	PEG	C1-C2-O2-C3

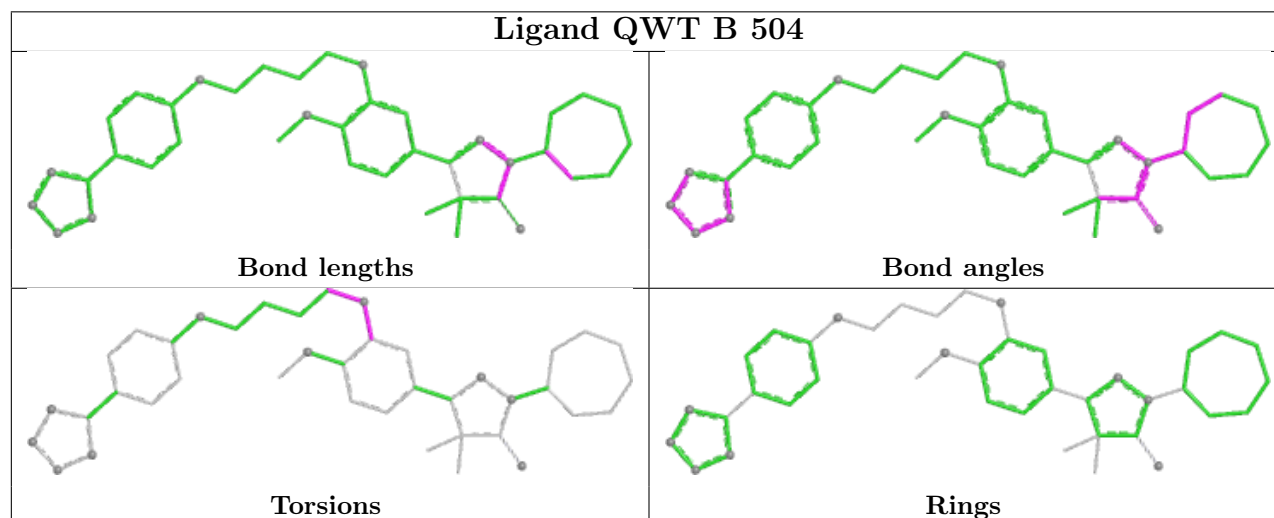
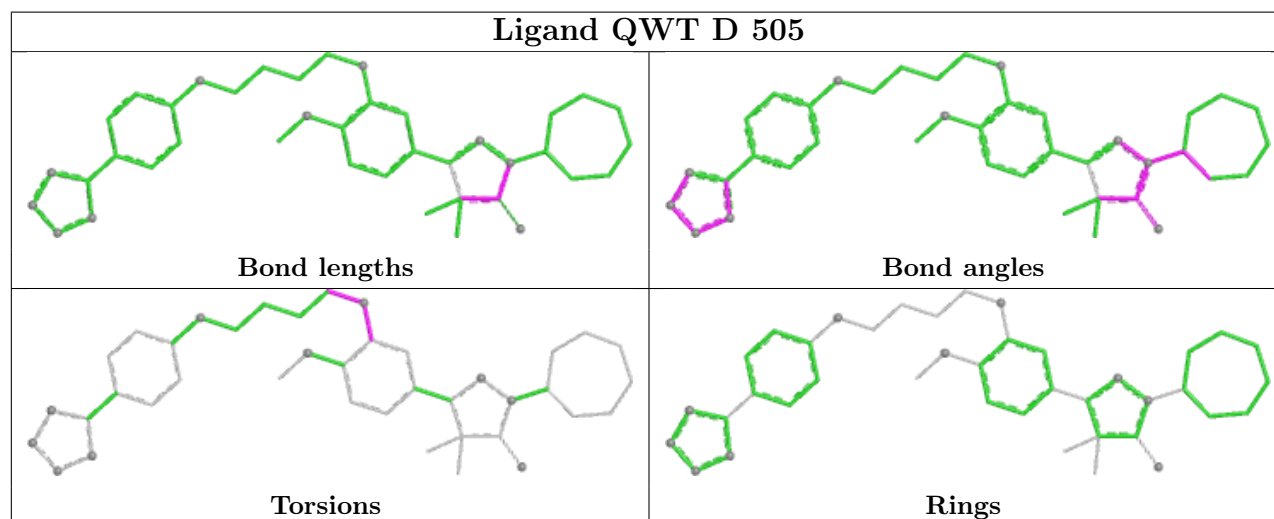
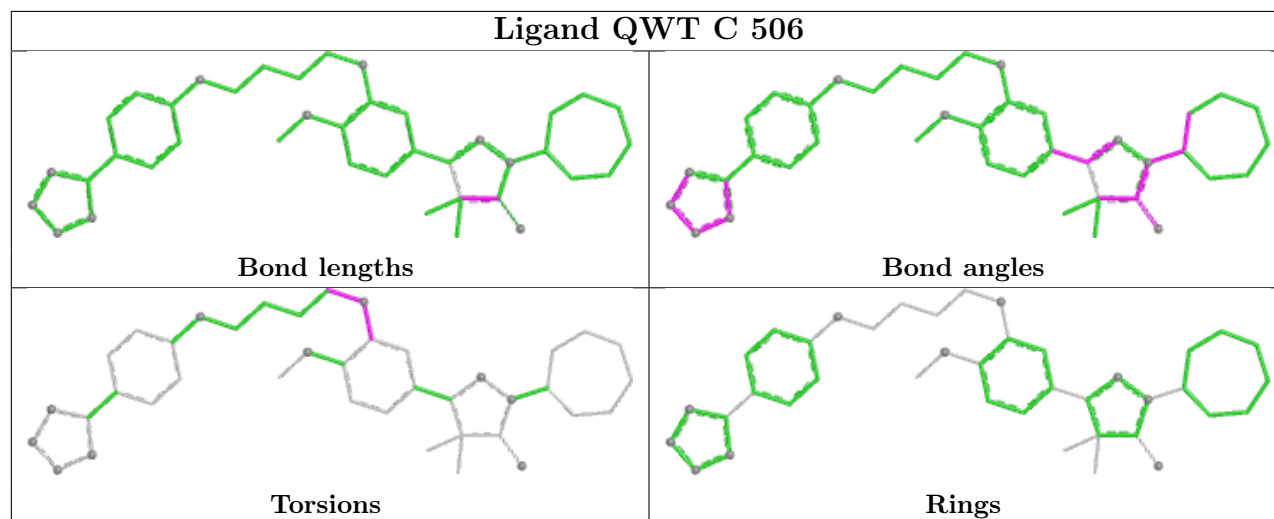
There are no ring outliers.

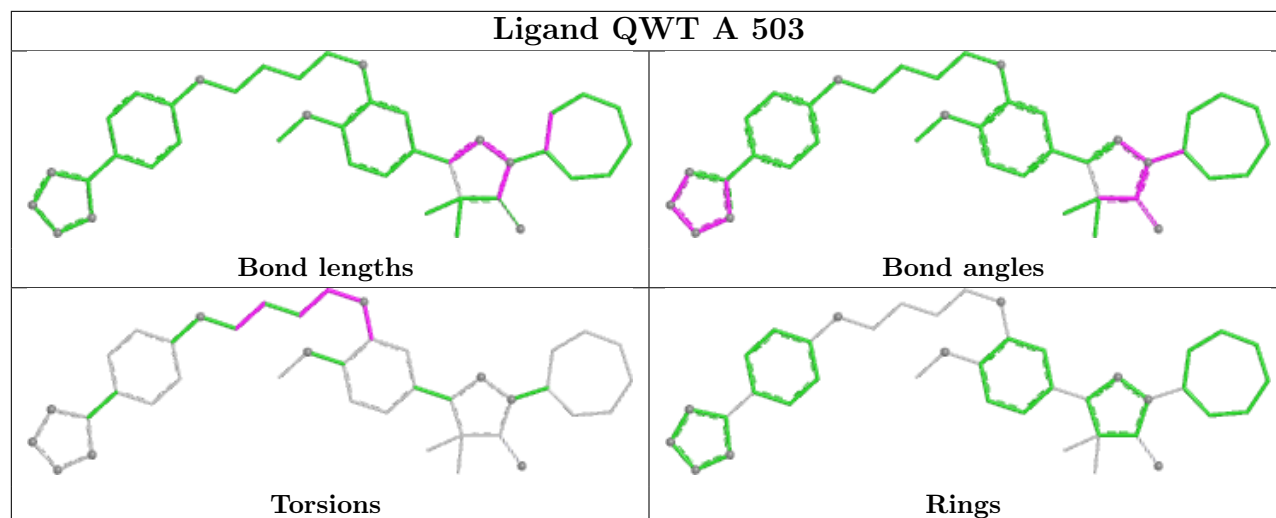
23 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	518	PEG	2	0
5	B	512	EDO	10	0
5	C	507	EDO	2	0
7	C	501	DMS	2	0
7	A	513	DMS	3	0
6	D	501	PEG	15	0
5	C	515	EDO	3	0
7	B	514	DMS	3	0
7	D	519	DMS	2	0
5	C	510	EDO	1	0
5	C	508	EDO	2	0
7	A	515	DMS	2	0
7	D	520	DMS	1	0
8	A	519	EPE	5	0
8	D	522	EPE	1	0
5	A	520	EDO	3	0
5	C	516	EDO	1	0
5	D	524	EDO	1	0
4	A	503	QWT	2	0
5	A	521	EDO	1	0
5	B	511	EDO	1	0
5	A	510	EDO	1	0
8	B	516	EPE	3	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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	330/364 (90%)	0.28	22 (6%) 24 22	15, 28, 57, 103	1 (0%)
1	B	324/364 (89%)	0.31	7 (2%) 62 62	15, 29, 47, 79	2 (0%)
1	C	322/364 (88%)	0.39	19 (5%) 28 27	14, 30, 60, 93	2 (0%)
1	D	324/364 (89%)	-0.01	11 (3%) 48 48	16, 24, 45, 76	1 (0%)
All	All	1300/1456 (89%)	0.24	59 (4%) 38 37	14, 28, 54, 103	6 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	82	PHE	9.9
1	A	293	THR	5.4
1	A	411	PRO	4.6
1	A	296	GLY	4.5
1	A	295	SER	4.0
1	C	292	VAL	3.9
1	C	298	LEU	3.7
1	A	363	ALA	3.6
1	A	83	GLY	3.6
1	A	294	SER	3.6
1	A	297	VAL	3.5
1	B	412	GLN	3.4
1	A	292	VAL	3.3
1	C	351	GLY	3.2
1	A	299	LEU	3.1
1	C	289	THR	3.1
1	C	299	LEU	3.0
1	D	362	ASN	3.0
1	A	222	MET	2.9
1	D	90	ASP	2.9
1	B	89	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	295	SER	2.9
1	D	91	VAL	2.8
1	A	298	LEU	2.8
1	B	91	VAL	2.8
1	D	354	ILE	2.7
1	D	363	ALA	2.7
1	D	351	GLY	2.7
1	A	291	LYS	2.7
1	D	350	ARG	2.6
1	B	90	ASP	2.6
1	C	363	ALA	2.6
1	A	84	VAL	2.6
1	A	351	GLY	2.5
1	C	354	ILE	2.5
1	A	375	TYR	2.5
1	A	410	ILE	2.5
1	D	94	LYS	2.4
1	C	303	TYR	2.4
1	C	294	SER	2.4
1	D	405	TRP	2.4
1	C	301	ASP	2.4
1	C	291	LYS	2.4
1	B	363	ALA	2.3
1	C	293	THR	2.3
1	D	292	VAL	2.3
1	A	288	GLU	2.3
1	C	91	VAL	2.3
1	C	361	HIS	2.2
1	A	349	GLU	2.2
1	B	396	LEU	2.2
1	D	156	ASP	2.2
1	C	350	ARG	2.2
1	C	346	ARG	2.1
1	C	178	THR	2.1
1	C	88	GLN	2.1
1	A	289	THR	2.1
1	B	105	HIS	2.1
1	A	362	ASN	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 [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
5	EDO	A	511	4/4	0.67	0.23	53,65,68,70	0
8	EPE	B	516	15/15	0.70	0.25	73,95,110,115	0
5	EDO	D	523	4/4	0.73	0.25	65,65,66,66	0
6	PEG	C	512	7/7	0.74	0.26	55,62,68,71	0
5	EDO	C	518	4/4	0.76	0.22	58,58,59,59	0
10	PRO	C	503	7/8	0.77	0.19	79,80,81,82	0
7	DMS	D	519	4/4	0.78	0.24	56,70,78,82	0
6	PEG	A	512	7/7	0.80	0.22	59,76,89,89	0
6	PEG	D	517	7/7	0.80	0.20	55,67,71,75	0
7	DMS	A	515	4/4	0.80	0.23	83,85,85,93	0
7	DMS	A	517	4/4	0.81	0.24	70,72,76,77	0
5	EDO	D	510	4/4	0.81	0.20	39,43,50,60	0
7	DMS	D	520	4/4	0.81	0.24	73,79,79,83	0
7	DMS	A	514	4/4	0.81	0.28	59,66,81,83	0
5	EDO	D	524	4/4	0.81	0.17	66,68,72,73	0
5	EDO	C	519	4/4	0.82	0.21	66,66,68,72	0
7	DMS	A	516	4/4	0.82	0.21	38,48,69,71	0
5	EDO	A	526	4/4	0.82	0.21	44,57,58,59	0
7	DMS	B	518	4/4	0.82	0.27	83,85,86,91	0
7	DMS	C	513	4/4	0.83	0.25	76,80,84,85	0
5	EDO	D	521	4/4	0.84	0.17	31,32,34,39	0
6	PEG	D	518	7/7	0.84	0.19	36,42,56,56	0
5	EDO	B	501	4/4	0.85	0.15	49,51,55,56	0
7	DMS	B	513	4/4	0.85	0.23	53,66,68,69	0
5	EDO	B	506	4/4	0.85	0.17	46,47,52,54	0
5	EDO	B	507	4/4	0.85	0.14	38,45,47,55	0
7	DMS	A	513	4/4	0.85	0.23	34,49,64,74	0
5	EDO	B	509	4/4	0.85	0.15	40,43,53,58	0
5	EDO	B	511	4/4	0.85	0.18	50,54,55,57	0
5	EDO	A	520	4/4	0.85	0.16	43,46,52,53	0
5	EDO	A	522	4/4	0.86	0.17	31,38,43,44	0
5	EDO	D	512	4/4	0.86	0.17	44,50,56,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	C	507	4/4	0.86	0.13	41,44,45,46	0
5	EDO	C	511	4/4	0.86	0.16	56,58,59,59	0
5	EDO	C	517	4/4	0.86	0.17	30,49,55,55	0
8	EPE	A	519	15/15	0.86	0.22	31,82,104,104	0
5	EDO	B	508	4/4	0.86	0.15	45,47,50,51	0
5	EDO	A	521	4/4	0.86	0.20	50,52,57,57	0
5	EDO	A	509	4/4	0.87	0.14	48,50,51,52	0
5	EDO	D	502	4/4	0.87	0.17	49,49,51,58	0
5	EDO	D	513	4/4	0.87	0.20	58,58,60,65	0
5	EDO	D	516	4/4	0.87	0.13	30,35,42,44	0
8	EPE	B	515	15/15	0.88	0.17	42,63,69,72	0
5	EDO	C	516	4/4	0.88	0.16	59,63,65,69	0
7	DMS	C	501	4/4	0.88	0.18	64,68,72,77	0
5	EDO	D	508	4/4	0.89	0.16	35,38,42,50	0
5	EDO	A	524	4/4	0.89	0.14	44,48,52,55	0
5	EDO	A	505	4/4	0.89	0.16	43,47,48,55	0
5	EDO	A	506	4/4	0.89	0.14	32,36,46,49	0
5	EDO	D	514	4/4	0.89	0.15	43,54,60,62	0
5	EDO	A	507	4/4	0.89	0.14	32,43,46,46	0
8	EPE	D	522	15/15	0.89	0.20	28,81,103,107	0
4	QWT	A	503	40/40	0.89	0.13	26,40,75,78	0
5	EDO	B	512	4/4	0.90	0.14	41,45,48,52	0
7	DMS	B	514	4/4	0.90	0.23	79,80,81,81	0
5	EDO	B	517	4/4	0.90	0.17	54,62,66,67	0
9	ILE	C	502	8/9	0.90	0.15	54,62,66,74	0
5	EDO	A	510	4/4	0.90	0.14	40,47,50,54	0
5	EDO	B	505	4/4	0.91	0.11	32,33,35,37	0
5	EDO	D	515	4/4	0.91	0.14	55,56,57,65	0
5	EDO	C	508	4/4	0.91	0.14	51,53,54,54	0
5	EDO	A	523	4/4	0.91	0.14	42,45,50,53	0
5	EDO	C	510	4/4	0.92	0.11	41,43,45,50	0
5	EDO	A	504	4/4	0.92	0.13	44,46,46,48	0
5	EDO	C	509	4/4	0.92	0.12	34,39,39,42	0
4	QWT	D	505	40/40	0.93	0.10	23,33,72,81	0
5	EDO	D	511	4/4	0.93	0.10	33,33,38,38	0
5	EDO	D	507	4/4	0.93	0.10	37,40,43,46	0
4	QWT	B	504	40/40	0.93	0.10	22,32,65,71	0
5	EDO	C	515	4/4	0.94	0.10	41,44,49,50	0
8	EPE	C	514	15/15	0.94	0.13	30,47,70,75	0
5	EDO	A	518	4/4	0.94	0.10	28,34,36,37	0
5	EDO	A	508	4/4	0.94	0.12	30,44,51,63	0
4	QWT	C	506	40/40	0.94	0.10	27,36,77,85	0

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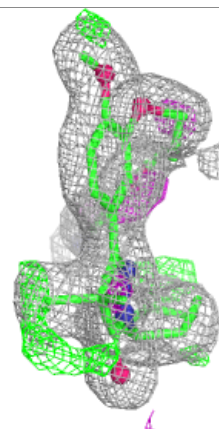
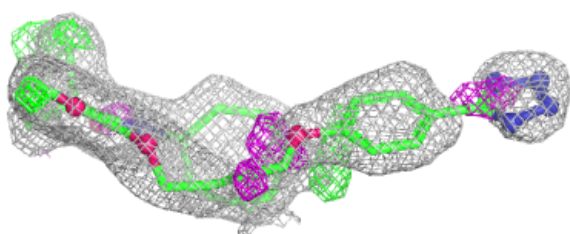
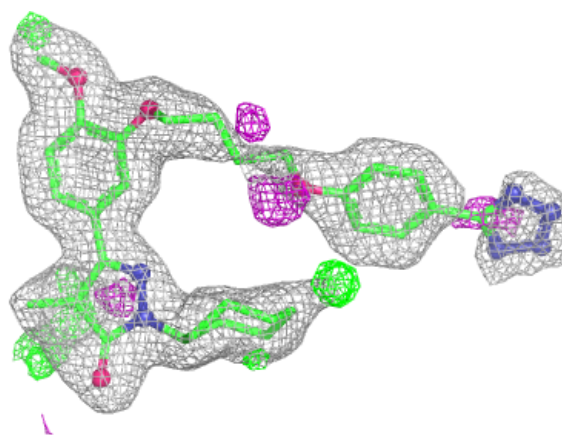
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	D	506	4/4	0.95	0.08	29,29,30,33	0
5	EDO	D	509	4/4	0.95	0.08	31,33,35,38	0
6	PEG	D	501	7/7	0.95	0.15	8,25,44,48	0
5	EDO	B	510	4/4	0.96	0.08	40,42,43,46	0
3	MG	C	505	1/1	0.99	0.05	14,14,14,14	0
3	MG	D	504	1/1	0.99	0.05	11,11,11,11	0
3	MG	A	502	1/1	0.99	0.05	13,13,13,13	0
3	MG	B	503	1/1	0.99	0.05	13,13,13,13	0
2	ZN	C	504	1/1	1.00	0.02	25,25,25,25	0
2	ZN	D	503	1/1	1.00	0.02	22,22,22,22	0
2	ZN	A	501	1/1	1.00	0.02	22,22,22,22	0
3	MG	A	525	1/1	1.00	0.10	8,8,8,8	0
2	ZN	B	502	1/1	1.00	0.02	23,23,23,23	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.

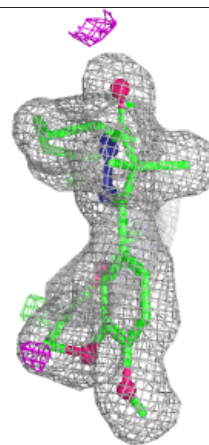
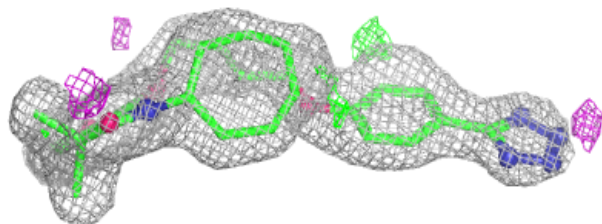
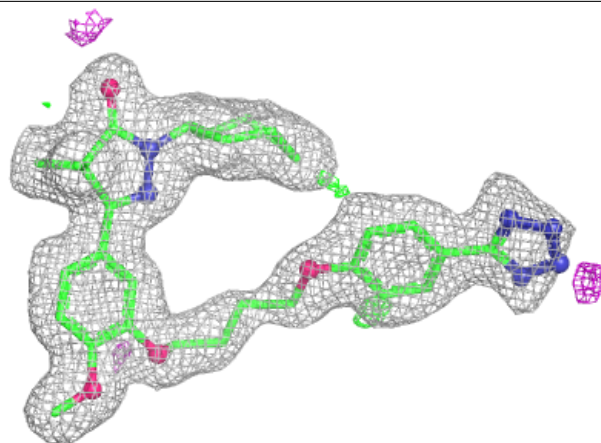
Electron density around QWT A 503:

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



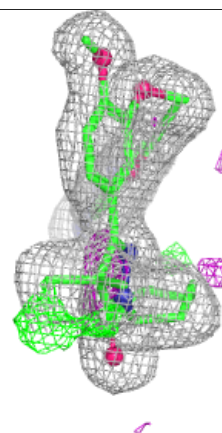
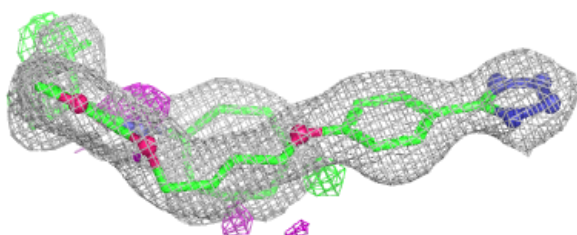
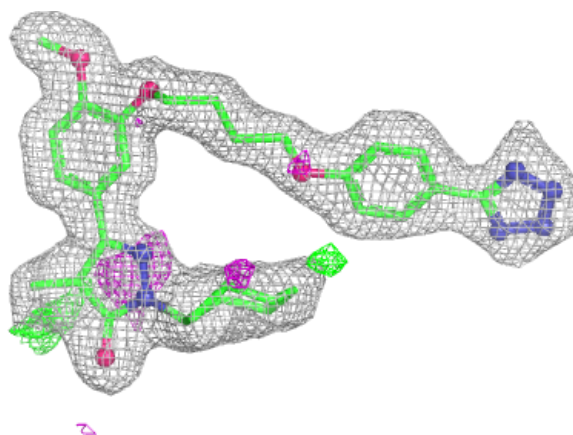
Electron density around QWT D 505:

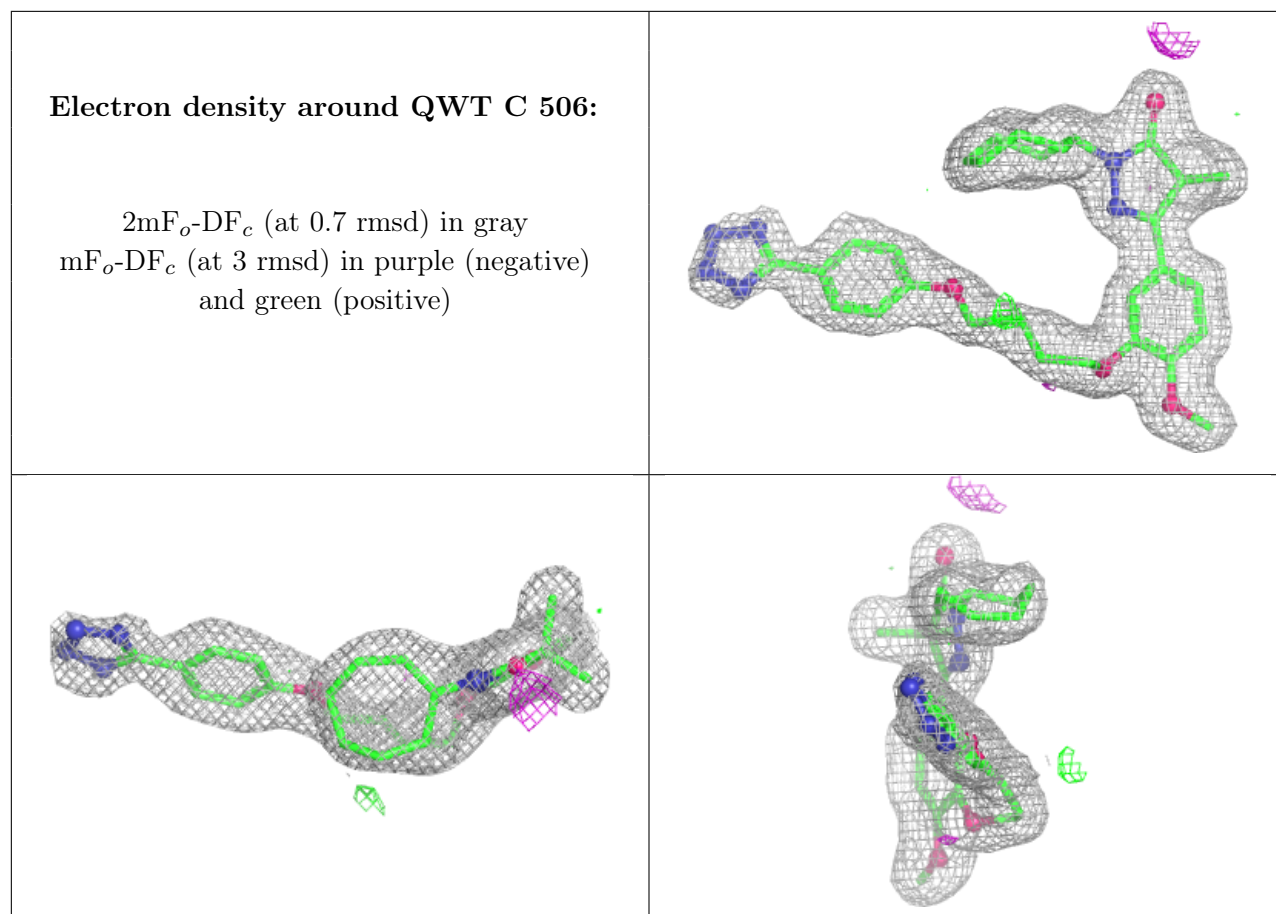
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around QWT B 504:

$2mF_o-DF_c$ (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.