



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:22 AM UTC

PDB ID : 6FE7 / pdb_00006fe7
Title : Crystal structure of human phosphodiesterase 4D2 catalytic domain with inhibitor NPD-356
Authors : Singh, A.K.; Brown, D.G.
Deposited on : 2017-12-29
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

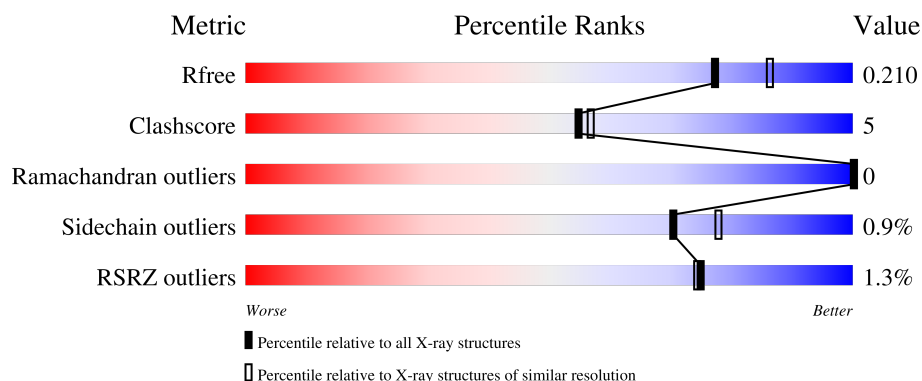
1 Overall quality at a glance

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	83% 7% 9%
1	B	364	83% 6% 11%
1	C	364	80% 8% 11%
1	D	364	82% 7% 11%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	D	522	-	X	-	-
8	PG4	C	521	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11789 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	0	0
			2669	1690	455	510	14			
1	B	323	Total	C	N	O	S	0	1	0
			2619	1657	447	501	14			
1	C	324	Total	C	N	O	S	0	0	0
			2622	1659	448	501	14			
1	D	324	Total	C	N	O	S	0	0	0
			2622	1659	448	501	14			

There are 16 discrepancies between the modelled and reference sequences:

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

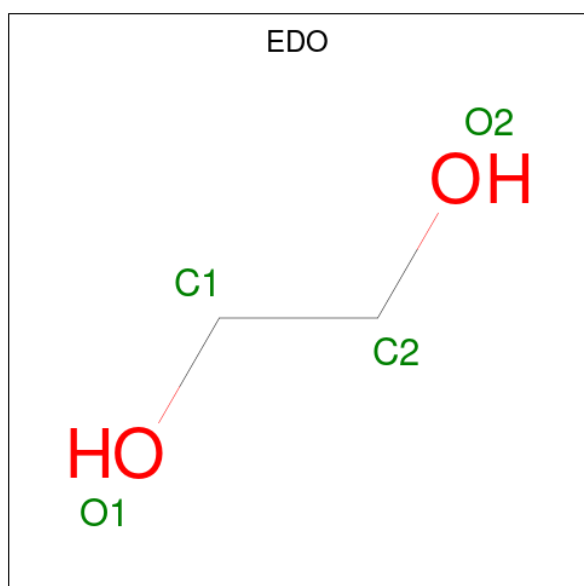
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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

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

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



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

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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	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		

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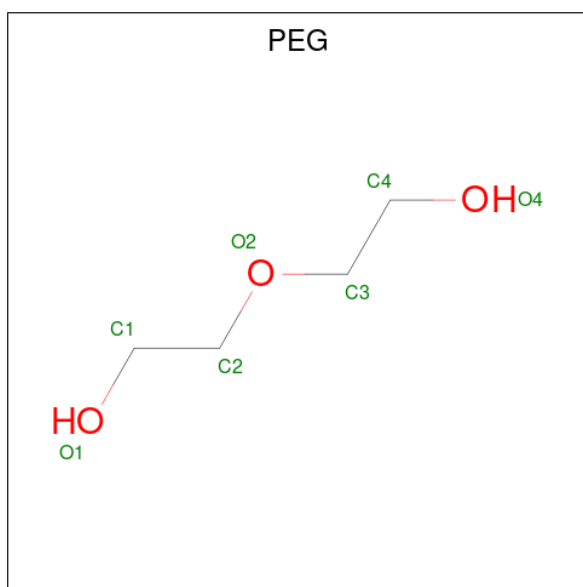
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total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

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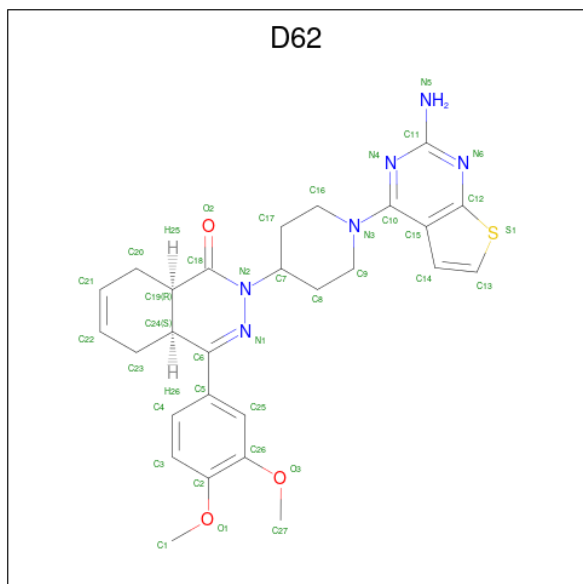
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0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

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



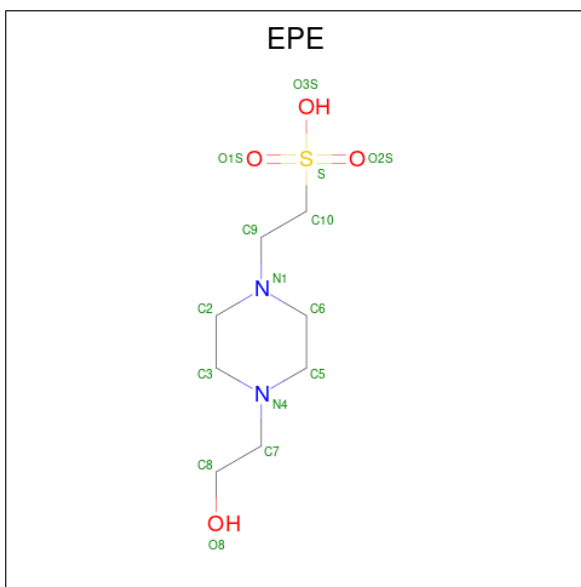
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total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

- Molecule 6 is (4a*S*,8a*R*)-2-(1-{2-aminothieno[2,3-*d*]pyrimidin-4-yl}piperidin-4-yl)-4-(3,4-dimethoxyphenyl)-1,2,4a,5,8,8a-hexahydrophthalazin-1-one (CCD ID: D62) (formula: $C_{27}H_{30}N_6O_3S$).



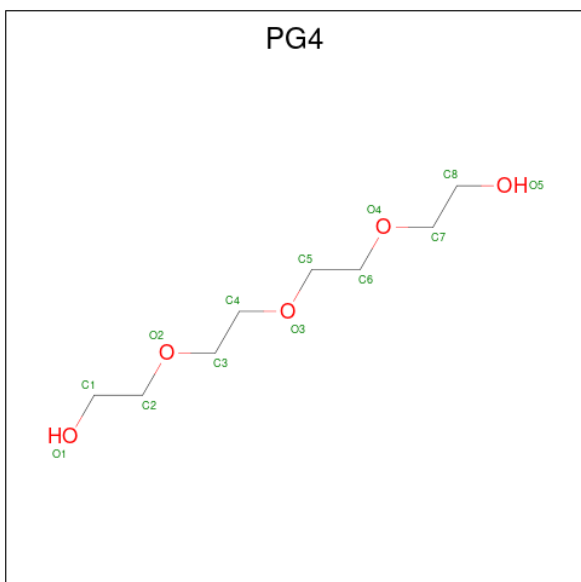
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			37	27	6	3	1		
6	B	1	Total	C	N	O	S	0	0
			37	27	6	3	1		
6	C	1	Total	C	N	O	S	0	0
			37	27	6	3	1		
6	D	1	Total	C	N	O	S	0	0
			37	27	6	3	1		

- 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 TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



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

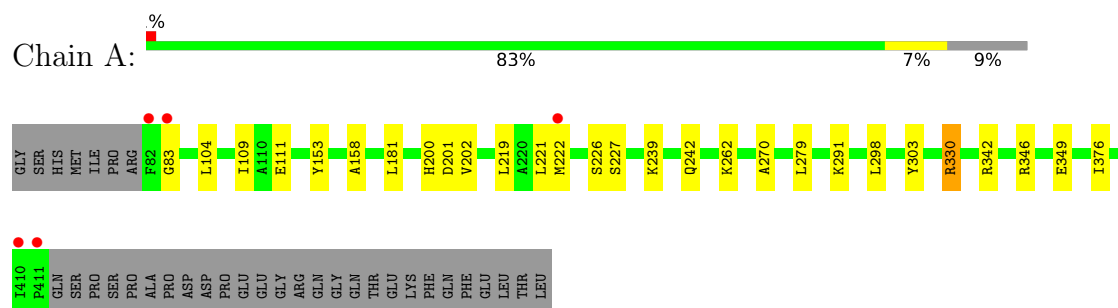
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	172	Total	O	0	0
			172	172		
9	B	182	Total	O	0	0
			182	182		
9	C	119	Total	O	0	0
			119	119		
9	D	197	Total	O	0	0
			197	197		

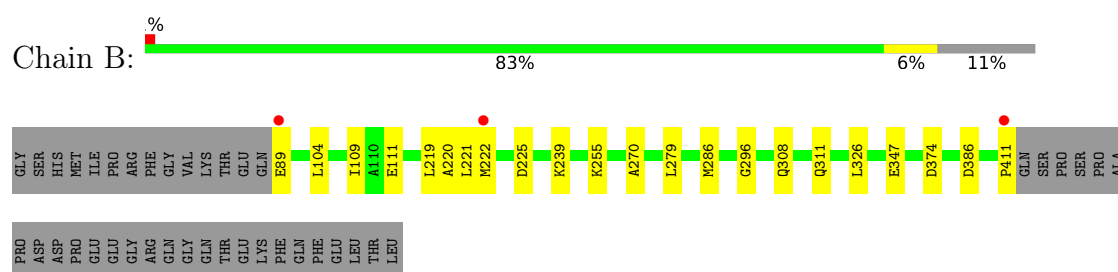
3 Residue-property plots [i](#)

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.

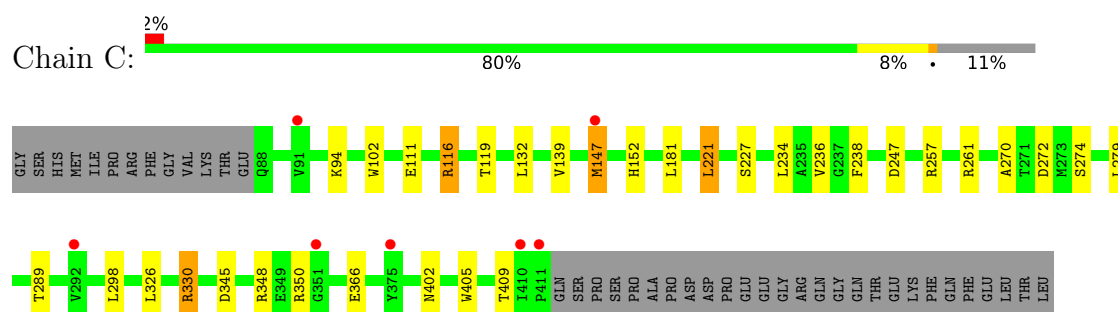
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



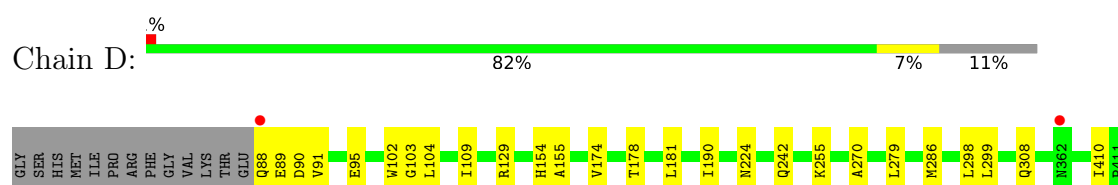
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



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



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



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

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.22Å 111.03Å 160.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.30 – 2.00 54.30 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (54.30-2.00) 100.0 (54.30-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.170 , 0.200 0.182 , 0.210	Depositor DCC
R_{free} test set	6067 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11789	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 2.99% 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: D62, EDO, EPE, ZN, MG, PG4, PEG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.27	3/2724 (0.1%)	1.02	5/3700 (0.1%)
1	B	1.20	5/2673 (0.2%)	0.98	1/3632 (0.0%)
1	C	1.17	0/2676	0.98	2/3636 (0.1%)
1	D	1.19	4/2676 (0.1%)	0.99	2/3636 (0.1%)
All	All	1.21	12/10749 (0.1%)	0.99	10/14604 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	410	ILE	CA-C	7.50	1.60	1.52
1	B	219	LEU	C-O	-6.51	1.16	1.24
1	D	154	HIS	C-O	-6.37	1.16	1.24
1	A	219	LEU	C-O	-5.69	1.17	1.24
1	D	95	GLU	C-O	-5.66	1.17	1.24
1	B	296	GLY	C-O	-5.60	1.16	1.24
1	B	221	LEU	C-O	-5.59	1.17	1.24
1	D	103	GLY	N-CA	5.44	1.52	1.45
1	A	303	TYR	C-O	-5.39	1.17	1.24
1	B	347	GLU	C-O	-5.30	1.18	1.24
1	B	220	ALA	C-O	-5.25	1.18	1.24
1	A	202	VAL	C-O	-5.14	1.18	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	HIS	N-CA-C	8.66	122.84	111.75
1	A	158	ALA	N-CA-C	6.74	118.70	111.36
1	D	102	TRP	CA-C-N	-5.80	112.74	122.25
1	D	102	TRP	C-N-CA	-5.80	112.74	122.25
1	C	102	TRP	CA-C-N	-5.51	113.21	122.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	102	TRP	C-N-CA	-5.51	113.21	122.25
1	B	326	LEU	N-CA-C	5.30	120.11	111.37
1	A	349	GLU	CB-CA-C	-5.07	102.06	110.68
1	A	83	GLY	N-CA-C	5.03	120.67	114.69
1	A	330	ARG	NE-CZ-NH1	-5.01	116.49	121.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2669	0	2625	21	0
1	B	2619	0	2574	17	0
1	C	2622	0	2578	45	0
1	D	2622	0	2578	18	0
2	A	1	0	0	1	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	60	0	90	4	0
4	B	60	0	90	1	0
4	C	56	0	84	3	0
4	D	56	0	84	4	0
5	A	42	0	60	5	0
5	B	7	0	10	2	0
5	C	14	0	20	3	0
5	D	35	0	50	2	0
6	A	37	0	0	2	0
6	B	37	0	0	0	0
6	C	37	0	0	0	0
6	D	37	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	15	0	18	1	0
7	B	30	0	36	4	0
7	C	15	0	18	5	0
7	D	15	0	17	2	0
8	C	26	0	36	14	0
9	A	172	0	0	2	0
9	B	182	0	0	3	0
9	C	119	0	0	3	0
9	D	197	0	0	0	0
All	All	11789	0	10968	107	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 5.

All (107) 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:222:MET:HE1	1:B:222:MET:HE3	1.33	1.02
1:C:116:ARG:HE	1:C:147:MET:HE1	1.31	0.96
1:C:111:GLU:OE2	7:C:514:EPE:H32	1.65	0.95
1:C:116:ARG:NE	1:C:147:MET:HE1	1.85	0.92
1:B:111:GLU:OE1	7:B:521:EPE:H72	1.74	0.87
1:B:386:ASP:OD2	4:B:504:EDO:H22	1.75	0.87
1:C:116:ARG:HE	1:C:147:MET:CE	1.90	0.84
1:A:342:ARG:NH2	1:A:346:ARG:HH21	1.76	0.83
1:A:222:MET:HE1	1:B:222:MET:CE	2.08	0.82
1:C:330:ARG:HH11	1:C:330:ARG:HG2	1.46	0.81
1:D:286:MET:HE3	1:D:308:GLN:OE1	1.80	0.81
1:B:111:GLU:OE2	7:B:521:EPE:H52	1.82	0.80
8:C:521:PG4:H51	1:D:224:ASN:OD1	1.82	0.79
1:C:116:ARG:NE	1:C:147:MET:CE	2.47	0.77
1:D:129:ARG:HB3	4:D:521:EDO:H22	1.67	0.77
1:A:342:ARG:NH2	1:A:346:ARG:NH2	2.33	0.76
1:C:119:THR:OG1	1:C:147:MET:HE3	1.87	0.75
1:C:132:LEU:HD22	1:C:139:VAL:HG22	1.67	0.75
8:C:521:PG4:H31	8:C:521:PG4:H61	1.71	0.72
1:D:286:MET:CE	1:D:308:GLN:OE1	2.38	0.72
1:D:88:GLN:HG3	1:D:90:ASP:H	1.56	0.70
1:C:330:ARG:HG2	1:C:330:ARG:NH1	2.04	0.69
1:A:201:ASP:OD2	2:A:501:ZN:ZN	1.42	0.68
1:B:286:MET:HE3	1:B:308:GLN:OE1	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:ASP:OD1	1:C:348:ARG:NH2	2.27	0.67
1:A:242:GLN:OE1	1:D:242:GLN:OE1	2.11	0.67
1:C:261:ARG:HE	8:C:521:PG4:C8	2.07	0.66
1:C:330:ARG:HH11	1:C:330:ARG:CG	2.08	0.66
1:C:261:ARG:NE	8:C:521:PG4:H82	2.10	0.65
1:A:376:ILE:HD12	6:A:520:D62:C14	2.28	0.63
1:C:181:LEU:HD21	1:C:298:LEU:HD12	1.79	0.63
1:C:366:GLU:HG2	1:C:409:THR:OG1	1.99	0.63
1:C:132:LEU:CD2	1:C:139:VAL:HG22	2.28	0.63
5:A:518:PEG:H21	1:C:236:VAL:HG22	1.81	0.62
1:C:261:ARG:HE	8:C:521:PG4:H82	1.65	0.62
1:C:111:GLU:OE2	7:C:514:EPE:H71	2.00	0.61
8:C:502:PG4:H41	9:C:698:HOH:O	2.00	0.61
1:A:104:LEU:HD11	1:A:109:ILE:HD11	1.82	0.61
1:D:181:LEU:HD21	1:D:298:LEU:HD12	1.83	0.60
1:C:234:LEU:HB3	8:C:521:PG4:H52	1.82	0.60
7:D:523:EPE:O8	7:D:523:EPE:H51	2.03	0.58
9:A:603:HOH:O	1:C:350:ARG:NH2	2.37	0.58
1:D:88:GLN:HB3	1:D:91:VAL:HG23	1.86	0.57
4:A:525:EDO:H22	9:C:654:HOH:O	2.04	0.57
1:A:227:SER:HA	5:A:516:PEG:H31	1.86	0.56
1:C:152:HIS:HE1	8:C:502:PG4:H52	1.71	0.56
1:D:190:ILE:HD13	4:D:521:EDO:H21	1.87	0.56
1:B:286:MET:CE	1:B:308:GLN:OE1	2.54	0.56
1:B:111:GLU:CD	7:B:521:EPE:H52	2.30	0.56
7:C:514:EPE:H92	9:C:705:HOH:O	2.06	0.56
1:A:291:LYS:H	4:A:508:EDO:H11	1.70	0.55
1:C:326:LEU:HB2	4:C:515:EDO:H21	1.89	0.55
1:C:402:ASN:OD1	4:C:515:EDO:H12	2.08	0.54
1:A:181:LEU:HD21	1:A:298:LEU:HD12	1.89	0.54
1:D:174:VAL:HG12	5:D:519:PEG:H12	1.88	0.54
1:D:178:THR:OG1	5:D:519:PEG:H42	2.07	0.54
8:C:521:PG4:H61	8:C:521:PG4:C3	2.37	0.53
1:B:374:ASP:HA	5:B:508:PEG:H42	1.90	0.53
1:C:147:MET:HE2	1:C:147:MET:HA	1.89	0.53
1:A:376:ILE:HD12	6:A:520:D62:C13	2.38	0.53
1:C:111:GLU:OE2	7:C:514:EPE:C3	2.49	0.53
1:A:181:LEU:CD2	1:A:298:LEU:HD12	2.39	0.52
1:A:270:ALA:HB1	1:A:279:LEU:HD11	1.91	0.52
1:C:261:ARG:HB2	4:C:509:EDO:H12	1.91	0.52
1:D:104:LEU:HD11	1:D:109:ILE:CD1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:PHE:CD2	8:C:521:PG4:H72	2.46	0.51
1:C:227:SER:H	5:C:519:PEG:H32	1.76	0.51
1:A:104:LEU:HD11	1:A:109:ILE:CD1	2.41	0.50
1:B:270:ALA:HB1	1:B:279:LEU:HD11	1.93	0.50
1:A:153:TYR:O	4:A:525:EDO:H11	2.12	0.50
1:A:262:LYS:HG3	5:A:517:PEG:H32	1.93	0.49
1:C:119:THR:CB	1:C:147:MET:HE3	2.41	0.49
5:A:517:PEG:H41	1:B:225:ASP:CB	2.42	0.49
1:B:255:LYS:HD3	9:B:693:HOH:O	2.12	0.49
1:C:405:TRP:O	1:C:409:THR:HG23	2.11	0.48
1:C:152:HIS:CE1	8:C:502:PG4:H52	2.49	0.48
1:C:261:ARG:NE	8:C:521:PG4:C8	2.73	0.48
1:B:239:LYS:NZ	9:B:604:HOH:O	2.37	0.48
1:D:270:ALA:HB1	1:D:279:LEU:HD11	1.95	0.47
1:B:374:ASP:HA	5:B:508:PEG:C4	2.44	0.47
1:C:270:ALA:HB1	1:C:279:LEU:HD11	1.96	0.47
1:C:350:ARG:HH11	1:C:350:ARG:HD3	1.56	0.47
1:C:181:LEU:CD2	1:C:298:LEU:HD12	2.43	0.46
8:C:521:PG4:C3	8:C:521:PG4:C6	2.92	0.46
1:C:272:ASP:OD2	5:C:519:PEG:H31	2.16	0.46
1:C:119:THR:OG1	1:C:147:MET:CE	2.62	0.45
1:D:299:LEU:C	1:D:299:LEU:HD13	2.42	0.45
1:B:111:GLU:OE1	7:B:521:EPE:C7	2.54	0.45
1:A:342:ARG:CZ	1:A:346:ARG:NH2	2.79	0.45
1:D:181:LEU:CD2	1:D:298:LEU:HD12	2.46	0.45
1:C:152:HIS:HE1	8:C:502:PG4:C5	2.30	0.45
1:D:104:LEU:HD11	1:D:109:ILE:HD11	1.99	0.45
1:A:226:SER:HA	5:A:516:PEG:O1	2.17	0.44
1:C:289:THR:O	1:C:289:THR:HG22	2.17	0.44
1:D:129:ARG:CB	4:D:521:EDO:H22	2.43	0.44
1:B:311:GLN:OE1	9:B:601:HOH:O	2.21	0.43
1:A:239:LYS:HE3	1:A:242:GLN:OE1	2.18	0.43
4:A:521:EDO:O2	9:A:601:HOH:O	2.21	0.43
1:B:104:LEU:HD11	1:B:109:ILE:CD1	2.48	0.43
1:C:111:GLU:CD	7:C:514:EPE:H71	2.44	0.43
1:A:111:GLU:OE1	7:A:524:EPE:H52	2.20	0.41
1:C:274:SER:OG	5:C:519:PEG:H42	2.20	0.41
1:D:155:ALA:HA	4:D:513:EDO:H11	2.02	0.41
7:D:523:EPE:H102	7:D:523:EPE:H22	1.67	0.41
1:C:116:ARG:HA	1:C:116:ARG:HD2	1.87	0.41
1:C:221:LEU:HD13	1:C:221:LEU:C	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:ASP:OD2	1:C:257:ARG:NH1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	328/364 (90%)	321 (98%)	7 (2%)	0	100	100
1	B	322/364 (88%)	317 (98%)	5 (2%)	0	100	100
1	C	322/364 (88%)	318 (99%)	4 (1%)	0	100	100
1	D	322/364 (88%)	316 (98%)	6 (2%)	0	100	100
All	All	1294/1456 (89%)	1272 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	301/331 (91%)	299 (99%)	2 (1%)	76	82
1	B	296/331 (89%)	294 (99%)	2 (1%)	76	82
1	C	296/331 (89%)	291 (98%)	5 (2%)	53	60
1	D	296/331 (89%)	294 (99%)	2 (1%)	76	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1189/1324 (90%)	1178 (99%)	11 (1%)	70	78

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	LEU
1	A	330	ARG
1	B	89	GLU
1	B	411	PRO
1	C	94	LYS
1	C	116	ARG
1	C	147	MET
1	C	221	LEU
1	C	330	ARG
1	D	89	GLU
1	D	255	LYS

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	224	ASN
1	A	250	GLN
1	A	258	GLN
1	A	389	HIS
1	B	210	GLN
1	B	250	GLN
1	B	321	ASN
1	C	152	HIS
1	C	210	GLN
1	D	105	HIS
1	D	250	GLN
1	D	321	ASN

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 91 ligands modelled in this entry, 8 are monoatomic - leaving 83 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EDO	D	501	-	3,3,3	0.75	0	2,2,2	0.34	0
4	EDO	D	511	-	3,3,3	0.47	0	2,2,2	0.86	0
4	EDO	C	508	-	3,3,3	0.44	0	2,2,2	0.65	0
4	EDO	A	506	-	3,3,3	0.70	0	2,2,2	1.04	0
5	PEG	D	510	-	6,6,6	0.34	0	5,5,5	0.88	0
4	EDO	C	504	-	3,3,3	0.40	0	2,2,2	0.20	0
4	EDO	B	514	-	3,3,3	0.76	0	2,2,2	0.29	0
4	EDO	B	517	-	3,3,3	0.19	0	2,2,2	1.36	0
4	EDO	D	504	-	3,3,3	0.76	0	2,2,2	0.21	0
4	EDO	C	511	-	3,3,3	0.59	0	2,2,2	0.61	0
4	EDO	D	505	-	3,3,3	0.46	0	2,2,2	0.48	0
4	EDO	A	514	-	3,3,3	0.52	0	2,2,2	0.75	0
4	EDO	B	503	-	3,3,3	0.40	0	2,2,2	1.19	0
4	EDO	B	513	-	3,3,3	0.55	0	2,2,2	0.66	0
4	EDO	C	510	-	3,3,3	0.17	0	2,2,2	0.93	0
5	PEG	C	519	-	6,6,6	0.91	0	5,5,5	1.20	0
4	EDO	C	512	-	3,3,3	0.94	0	2,2,2	0.61	0
4	EDO	A	503	-	3,3,3	0.34	0	2,2,2	0.74	0
5	PEG	A	510	-	6,6,6	0.51	0	5,5,5	0.74	0
4	EDO	D	521	-	3,3,3	0.59	0	2,2,2	0.88	0
5	PEG	D	509	-	6,6,6	0.99	0	5,5,5	1.62	1 (20%)
4	EDO	D	512	-	3,3,3	0.45	0	2,2,2	0.16	0
4	EDO	D	520	-	3,3,3	0.30	0	2,2,2	0.91	0
4	EDO	C	517	-	3,3,3	0.30	0	2,2,2	0.71	0
4	EDO	B	515	-	3,3,3	0.35	0	2,2,2	0.54	0
4	EDO	B	505	-	3,3,3	0.42	0	2,2,2	0.55	0
8	PG4	C	502	-	12,12,12	1.04	0	11,11,11	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	521	-	3,3,3	0.50	0	2,2,2	0.77	0
6	D62	C	520	-	41,42,42	0.68	1 (2%)	50,61,61	2.07	8 (16%)
4	EDO	A	512	-	3,3,3	0.29	0	2,2,2	1.22	0
4	EDO	B	507	-	3,3,3	0.29	0	2,2,2	1.53	0
6	D62	A	520	-	41,42,42	0.76	1 (2%)	50,61,61	1.60	7 (14%)
4	EDO	A	505	-	3,3,3	0.49	0	2,2,2	0.29	0
5	PEG	A	519	-	6,6,6	0.44	0	5,5,5	0.44	0
4	EDO	C	518	-	3,3,3	0.28	0	2,2,2	0.71	0
4	EDO	C	501	-	3,3,3	0.55	0	2,2,2	0.23	0
4	EDO	A	509	-	3,3,3	0.52	0	2,2,2	0.39	0
4	EDO	C	516	-	3,3,3	1.02	0	2,2,2	0.88	0
7	EPE	B	521	-	15,15,15	2.08	1 (6%)	19,20,20	1.00	0
5	PEG	A	517	-	6,6,6	0.54	0	5,5,5	0.52	0
5	PEG	A	518	-	6,6,6	0.62	0	5,5,5	0.67	0
5	PEG	D	518	-	6,6,6	1.09	0	5,5,5	1.29	0
4	EDO	A	523	-	3,3,3	0.48	0	2,2,2	0.77	0
5	PEG	C	513	-	6,6,6	0.52	0	5,5,5	0.92	0
4	EDO	C	515	-	3,3,3	0.79	0	2,2,2	0.26	0
7	EPE	A	524	-	15,15,15	2.43	1 (6%)	19,20,20	2.33	7 (36%)
5	PEG	D	508	-	6,6,6	0.49	0	5,5,5	1.20	0
4	EDO	A	525	-	3,3,3	0.75	0	2,2,2	0.07	0
4	EDO	C	507	-	3,3,3	0.41	0	2,2,2	0.34	0
4	EDO	B	510	-	3,3,3	0.46	0	2,2,2	0.88	0
5	PEG	D	519	-	6,6,6	0.49	0	5,5,5	1.27	0
4	EDO	D	513	-	3,3,3	0.79	0	2,2,2	1.07	0
4	EDO	A	515	-	3,3,3	1.16	0	2,2,2	0.41	0
4	EDO	D	515	-	3,3,3	0.43	0	2,2,2	1.30	0
4	EDO	B	511	-	3,3,3	0.69	0	2,2,2	1.18	0
4	EDO	B	520	-	3,3,3	0.41	0	2,2,2	0.66	0
4	EDO	A	507	-	3,3,3	0.26	0	2,2,2	1.48	0
4	EDO	D	507	-	3,3,3	0.45	0	2,2,2	0.42	0
4	EDO	D	514	-	3,3,3	0.97	0	2,2,2	0.56	0
7	EPE	B	509	-	15,15,15	1.36	1 (6%)	19,20,20	2.22	7 (36%)
4	EDO	D	506	-	3,3,3	0.32	0	2,2,2	1.15	0
5	PEG	B	508	-	6,6,6	0.77	0	5,5,5	1.38	1 (20%)
4	EDO	B	504	-	3,3,3	0.24	0	2,2,2	0.65	0
4	EDO	C	509	-	3,3,3	0.29	0	2,2,2	0.44	0
8	PG4	C	521	-	12,12,12	1.27	2 (16%)	11,11,11	1.57	2 (18%)
4	EDO	D	522	-	3,3,3	2.60	2 (66%)	2,2,2	2.17	1 (50%)
4	EDO	A	508	-	3,3,3	0.42	0	2,2,2	0.36	0
4	EDO	D	516	-	3,3,3	0.50	0	2,2,2	1.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	D62	B	516	-	41,42,42	0.66	0	50,61,61	1.57	6 (12%)
7	EPE	C	514	-	15,15,15	2.08	1 (6%)	19,20,20	0.98	0
4	EDO	A	504	-	3,3,3	0.39	0	2,2,2	0.93	0
5	PEG	A	511	-	6,6,6	0.41	0	5,5,5	0.59	0
4	EDO	B	519	-	3,3,3	0.28	0	2,2,2	1.11	0
4	EDO	A	522	-	3,3,3	0.56	0	2,2,2	0.47	0
4	EDO	C	503	-	3,3,3	0.41	0	2,2,2	0.50	0
6	D62	D	517	-	41,42,42	0.75	0	50,61,61	2.25	7 (14%)
5	PEG	A	516	-	6,6,6	0.72	0	5,5,5	1.13	0
7	EPE	D	523	-	15,15,15	3.04	3 (20%)	19,20,20	1.69	5 (26%)
4	EDO	B	518	-	3,3,3	0.80	0	2,2,2	0.27	0
4	EDO	B	506	-	3,3,3	0.34	0	2,2,2	1.45	1 (50%)
4	EDO	B	512	-	3,3,3	0.09	0	2,2,2	1.11	0
4	EDO	A	513	-	3,3,3	0.27	0	2,2,2	1.46	1 (50%)
4	EDO	C	522	-	3,3,3	0.42	0	2,2,2	0.50	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	501	-	-	1/1/1/1	-
4	EDO	D	511	-	-	1/1/1/1	-
4	EDO	C	508	-	-	1/1/1/1	-
4	EDO	A	506	-	-	0/1/1/1	-
5	PEG	D	510	-	-	0/4/4/4	-
4	EDO	C	504	-	-	1/1/1/1	-
4	EDO	B	514	-	-	0/1/1/1	-
4	EDO	B	517	-	-	0/1/1/1	-
4	EDO	D	504	-	-	0/1/1/1	-
4	EDO	C	511	-	-	0/1/1/1	-
4	EDO	D	505	-	-	0/1/1/1	-
4	EDO	A	514	-	-	1/1/1/1	-
4	EDO	B	503	-	-	0/1/1/1	-
4	EDO	B	513	-	-	0/1/1/1	-
4	EDO	C	510	-	-	1/1/1/1	-
5	PEG	C	519	-	-	2/4/4/4	-
4	EDO	C	512	-	-	1/1/1/1	-
4	EDO	A	503	-	-	0/1/1/1	-
5	PEG	A	510	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	521	-	-	1/1/1/1	-
5	PEG	D	509	-	-	3/4/4/4	-
4	EDO	D	512	-	-	1/1/1/1	-
4	EDO	D	520	-	-	1/1/1/1	-
4	EDO	C	517	-	-	1/1/1/1	-
4	EDO	B	515	-	-	1/1/1/1	-
4	EDO	B	505	-	-	1/1/1/1	-
8	PG4	C	502	-	-	5/10/10/10	-
4	EDO	A	521	-	-	1/1/1/1	-
6	D62	C	520	-	-	2/16/53/53	0/6/6/6
4	EDO	A	512	-	-	0/1/1/1	-
4	EDO	B	507	-	-	1/1/1/1	-
6	D62	A	520	-	-	1/16/53/53	0/6/6/6
4	EDO	A	505	-	-	0/1/1/1	-
5	PEG	A	519	-	-	2/4/4/4	-
4	EDO	C	518	-	-	1/1/1/1	-
4	EDO	C	501	-	-	1/1/1/1	-
4	EDO	A	509	-	-	1/1/1/1	-
4	EDO	C	516	-	-	0/1/1/1	-
7	EPE	B	521	-	-	2/9/19/19	0/1/1/1
5	PEG	A	517	-	-	3/4/4/4	-
5	PEG	A	518	-	-	2/4/4/4	-
5	PEG	D	518	-	-	1/4/4/4	-
4	EDO	A	523	-	-	1/1/1/1	-
5	PEG	C	513	-	-	3/4/4/4	-
4	EDO	C	515	-	-	0/1/1/1	-
7	EPE	A	524	-	-	3/9/19/19	0/1/1/1
5	PEG	D	508	-	-	3/4/4/4	-
4	EDO	A	525	-	-	0/1/1/1	-
4	EDO	C	507	-	-	1/1/1/1	-
4	EDO	B	510	-	-	0/1/1/1	-
5	PEG	D	519	-	-	3/4/4/4	-
4	EDO	D	513	-	-	0/1/1/1	-
4	EDO	A	515	-	-	0/1/1/1	-
4	EDO	D	515	-	-	1/1/1/1	-
4	EDO	B	511	-	-	1/1/1/1	-
4	EDO	B	520	-	-	1/1/1/1	-
4	EDO	A	507	-	-	1/1/1/1	-
4	EDO	D	507	-	-	1/1/1/1	-
4	EDO	D	514	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EPE	B	509	-	-	2/9/19/19	0/1/1/1
4	EDO	D	506	-	-	0/1/1/1	-
5	PEG	B	508	-	-	1/4/4/4	-
4	EDO	B	504	-	-	1/1/1/1	-
4	EDO	C	509	-	-	0/1/1/1	-
8	PG4	C	521	-	-	7/10/10/10	-
4	EDO	D	522	-	-	0/1/1/1	-
4	EDO	A	508	-	-	1/1/1/1	-
4	EDO	D	516	-	-	0/1/1/1	-
6	D62	B	516	-	-	2/16/53/53	0/6/6/6
7	EPE	C	514	-	-	6/9/19/19	0/1/1/1
4	EDO	A	504	-	-	1/1/1/1	-
5	PEG	A	511	-	-	4/4/4/4	-
4	EDO	B	519	-	-	1/1/1/1	-
4	EDO	A	522	-	-	1/1/1/1	-
4	EDO	C	503	-	-	1/1/1/1	-
6	D62	D	517	-	-	2/16/53/53	0/6/6/6
5	PEG	A	516	-	-	3/4/4/4	-
7	EPE	D	523	-	-	4/9/19/19	0/1/1/1
4	EDO	B	518	-	-	1/1/1/1	-
4	EDO	B	506	-	-	0/1/1/1	-
4	EDO	B	512	-	-	1/1/1/1	-
4	EDO	A	513	-	-	0/1/1/1	-
4	EDO	C	522	-	-	0/1/1/1	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	523	EPE	C10-S	-11.03	1.62	1.77
7	A	524	EPE	C10-S	-8.90	1.65	1.77
7	C	514	EPE	C10-S	-7.82	1.66	1.77
7	B	521	EPE	C10-S	-7.82	1.66	1.77
7	B	509	EPE	C10-S	-4.30	1.71	1.77
4	D	522	EDO	O1-C1	3.29	1.58	1.42
6	A	520	D62	C15-C12	-2.68	1.38	1.41
4	D	522	EDO	O2-C2	2.52	1.54	1.42
6	C	520	D62	C15-C12	-2.36	1.38	1.41
8	C	521	PG4	C6-C5	2.34	1.60	1.49
7	D	523	EPE	O2S-S	-2.32	1.38	1.45
7	D	523	EPE	O1S-S	-2.19	1.38	1.45
8	C	521	PG4	O2-C3	2.14	1.51	1.42

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	517	D62	C12-S1-C13	-11.26	87.28	90.62
6	C	520	D62	C12-S1-C13	-10.65	87.46	90.62
6	B	516	D62	C12-S1-C13	-6.69	88.63	90.62
7	A	524	EPE	O3S-S-C10	5.95	117.65	106.00
6	D	517	D62	C15-C12-N6	-5.79	122.65	126.55
6	A	520	D62	C12-S1-C13	-5.72	88.92	90.62
6	C	520	D62	C15-C12-N6	-5.39	122.92	126.55
7	A	524	EPE	O2S-S-C10	-5.38	98.60	106.73
6	A	520	D62	C15-C12-N6	-5.07	123.13	126.55
6	B	516	D62	C15-C12-N6	-4.73	123.36	126.55
7	B	509	EPE	C5-N4-C3	4.43	118.38	108.84
6	D	517	D62	C8-C7-N2	-4.34	106.15	110.89
7	B	509	EPE	O2S-S-C10	4.05	112.85	106.73
7	B	509	EPE	O1S-S-C10	4.03	112.81	106.73
6	C	520	D62	C8-C7-N2	-3.63	106.93	110.89
7	A	524	EPE	O3S-S-O2S	-3.51	102.62	111.40
7	D	523	EPE	O2S-S-O1S	-3.46	102.57	113.82
6	D	517	D62	C4-C5-C6	3.27	124.66	120.74
8	C	521	PG4	C3-O2-C2	3.21	127.32	113.26
6	D	517	D62	C12-C15-C14	-3.11	108.99	111.76
6	D	517	D62	C25-C5-C6	-2.96	116.57	120.24
7	B	509	EPE	C2-C3-N4	2.94	116.58	110.65
7	D	523	EPE	C3-C2-N1	-2.92	104.75	110.65
6	A	520	D62	C8-C7-N2	-2.92	107.71	110.89
5	D	509	PEG	C3-O2-C2	2.89	125.90	113.26
8	C	521	PG4	O2-C2-C1	2.85	122.68	110.11
7	D	523	EPE	C5-C6-N1	-2.82	104.96	110.65
6	A	520	D62	C25-C5-C6	-2.73	116.85	120.24
6	B	516	D62	C8-C7-N2	-2.61	108.04	110.89
7	A	524	EPE	O1S-S-C10	2.58	110.63	106.73
7	B	509	EPE	C5-C6-N1	-2.57	105.47	110.65
7	D	523	EPE	O2S-S-C10	2.56	110.60	106.73
6	B	516	D62	O2-C18-N2	-2.56	118.58	121.63
6	D	517	D62	C15-C12-S1	2.53	113.42	111.38
6	B	516	D62	C11-N4-C10	2.47	120.14	113.51
4	D	522	EDO	O1-C1-C2	2.45	131.02	112.39
6	A	520	D62	C11-N4-C10	2.41	119.97	113.51
6	C	520	D62	S1-C12-N6	2.35	125.24	122.51
6	A	520	D62	C12-C15-C14	-2.30	109.71	111.76
6	C	520	D62	C25-C5-C6	-2.29	117.39	120.24
7	A	524	EPE	C5-N4-C3	2.26	113.72	108.84
6	C	520	D62	C12-C15-C14	-2.24	109.76	111.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	523	EPE	O1S-S-C10	2.21	110.07	106.73
7	B	509	EPE	O3S-S-O2S	-2.20	105.88	111.40
6	C	520	D62	C11-N4-C10	2.20	119.42	113.51
6	B	516	D62	O2-C18-C19	2.18	127.01	121.95
7	A	524	EPE	C3-C2-N1	-2.13	106.34	110.65
7	B	509	EPE	O2S-S-O1S	-2.09	107.04	113.82
5	B	508	PEG	O4-C4-C3	2.08	124.04	111.82
6	A	520	D62	C4-C5-C6	2.07	123.22	120.74
4	A	513	EDO	O1-C1-C2	-2.07	96.65	112.39
6	C	520	D62	C27-O3-C26	2.06	120.53	117.51
4	B	506	EDO	O2-C2-C1	-2.04	96.87	112.39
7	A	524	EPE	C7-N4-C3	2.02	116.62	111.24

There are no chirality outliers.

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	524	EPE	C8-C7-N4-C3
7	B	509	EPE	C10-C9-N1-C6
7	C	514	EPE	C10-C9-N1-C6
7	C	514	EPE	C9-C10-S-O2S
7	D	523	EPE	C10-C9-N1-C2
7	D	523	EPE	C8-C7-N4-C5
7	D	523	EPE	C9-C10-S-O1S
6	C	520	D62	N4-C10-N3-C9
8	C	521	PG4	O2-C3-C4-O3
5	C	519	PEG	C4-C3-O2-C2
8	C	521	PG4	O3-C5-C6-O4
5	D	519	PEG	C1-C2-O2-C3
6	C	520	D62	C15-C10-N3-C9
8	C	521	PG4	C1-C2-O2-C3
6	D	517	D62	N4-C10-N3-C9
5	C	513	PEG	O1-C1-C2-O2
5	D	518	PEG	O1-C1-C2-O2
8	C	521	PG4	O1-C1-C2-O2
4	D	507	EDO	O1-C1-C2-O2
7	C	514	EPE	C9-C10-S-O3S
5	A	510	PEG	O2-C3-C4-O4
5	C	519	PEG	O2-C3-C4-O4
5	D	508	PEG	O2-C3-C4-O4
8	C	502	PG4	O1-C1-C2-O2
5	A	511	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
5	A	516	PEG	O1-C1-C2-O2
5	A	517	PEG	O2-C3-C4-O4
5	B	508	PEG	O1-C1-C2-O2
5	D	509	PEG	O1-C1-C2-O2
5	A	516	PEG	O2-C3-C4-O4
4	A	514	EDO	O1-C1-C2-O2
4	B	515	EDO	O1-C1-C2-O2
4	C	512	EDO	O1-C1-C2-O2
4	D	520	EDO	O1-C1-C2-O2
6	D	517	D62	C15-C10-N3-C9
6	B	516	D62	N4-C10-N3-C9
7	A	524	EPE	S-C10-C9-N1
5	A	511	PEG	O1-C1-C2-O2
4	A	522	EDO	O1-C1-C2-O2
4	B	512	EDO	O1-C1-C2-O2
4	C	510	EDO	O1-C1-C2-O2
4	C	517	EDO	O1-C1-C2-O2
4	D	515	EDO	O1-C1-C2-O2
8	C	502	PG4	O3-C5-C6-O4
7	B	509	EPE	C10-C9-N1-C2
5	D	519	PEG	O2-C3-C4-O4
8	C	521	PG4	C6-C5-O3-C4
8	C	521	PG4	O4-C7-C8-O5
4	A	508	EDO	O1-C1-C2-O2
4	A	523	EDO	O1-C1-C2-O2
4	B	507	EDO	O1-C1-C2-O2
5	A	511	PEG	C4-C3-O2-C2
7	C	514	EPE	C9-C10-S-O1S
6	B	516	D62	C15-C10-N3-C9
5	D	509	PEG	C4-C3-O2-C2
5	A	510	PEG	C1-C2-O2-C3
5	A	518	PEG	O2-C3-C4-O4
5	C	513	PEG	O2-C3-C4-O4
5	D	519	PEG	O1-C1-C2-O2
7	B	521	EPE	S-C10-C9-N1
7	C	514	EPE	S-C10-C9-N1
4	A	509	EDO	O1-C1-C2-O2
4	B	519	EDO	O1-C1-C2-O2
5	A	518	PEG	C4-C3-O2-C2
5	A	517	PEG	C4-C3-O2-C2
5	A	517	PEG	C1-C2-O2-C3
8	C	521	PG4	C5-C6-O4-C7

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Mol	Chain	Res	Type	Atoms
5	D	508	PEG	O1-C1-C2-O2
5	A	510	PEG	C4-C3-O2-C2
5	D	508	PEG	C1-C2-O2-C3
7	B	521	EPE	N4-C7-C8-O8
5	D	509	PEG	O2-C3-C4-O4
4	A	521	EDO	O1-C1-C2-O2
4	B	511	EDO	O1-C1-C2-O2
4	B	518	EDO	O1-C1-C2-O2
4	B	520	EDO	O1-C1-C2-O2
4	C	508	EDO	O1-C1-C2-O2
8	C	502	PG4	C5-C6-O4-C7
8	C	502	PG4	C1-C2-O2-C3
4	C	518	EDO	O1-C1-C2-O2
4	A	504	EDO	O1-C1-C2-O2
4	B	504	EDO	O1-C1-C2-O2
4	C	501	EDO	O1-C1-C2-O2
4	C	507	EDO	O1-C1-C2-O2
4	D	511	EDO	O1-C1-C2-O2
4	D	512	EDO	O1-C1-C2-O2
4	D	521	EDO	O1-C1-C2-O2
7	A	524	EPE	C9-C10-S-O2S
5	A	511	PEG	C1-C2-O2-C3
5	A	516	PEG	C4-C3-O2-C2
7	C	514	EPE	N4-C7-C8-O8
4	A	507	EDO	O1-C1-C2-O2
4	C	503	EDO	O1-C1-C2-O2
4	C	504	EDO	O1-C1-C2-O2
6	A	520	D62	N4-C10-N3-C9
5	A	519	PEG	O1-C1-C2-O2
4	B	505	EDO	O1-C1-C2-O2
4	D	501	EDO	O1-C1-C2-O2
7	D	523	EPE	C9-C10-S-O3S
5	C	513	PEG	C1-C2-O2-C3
8	C	502	PG4	O2-C3-C4-O3
5	A	519	PEG	O2-C3-C4-O4

There are no ring outliers.

21 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	519	PEG	3	0
4	D	521	EDO	3	0

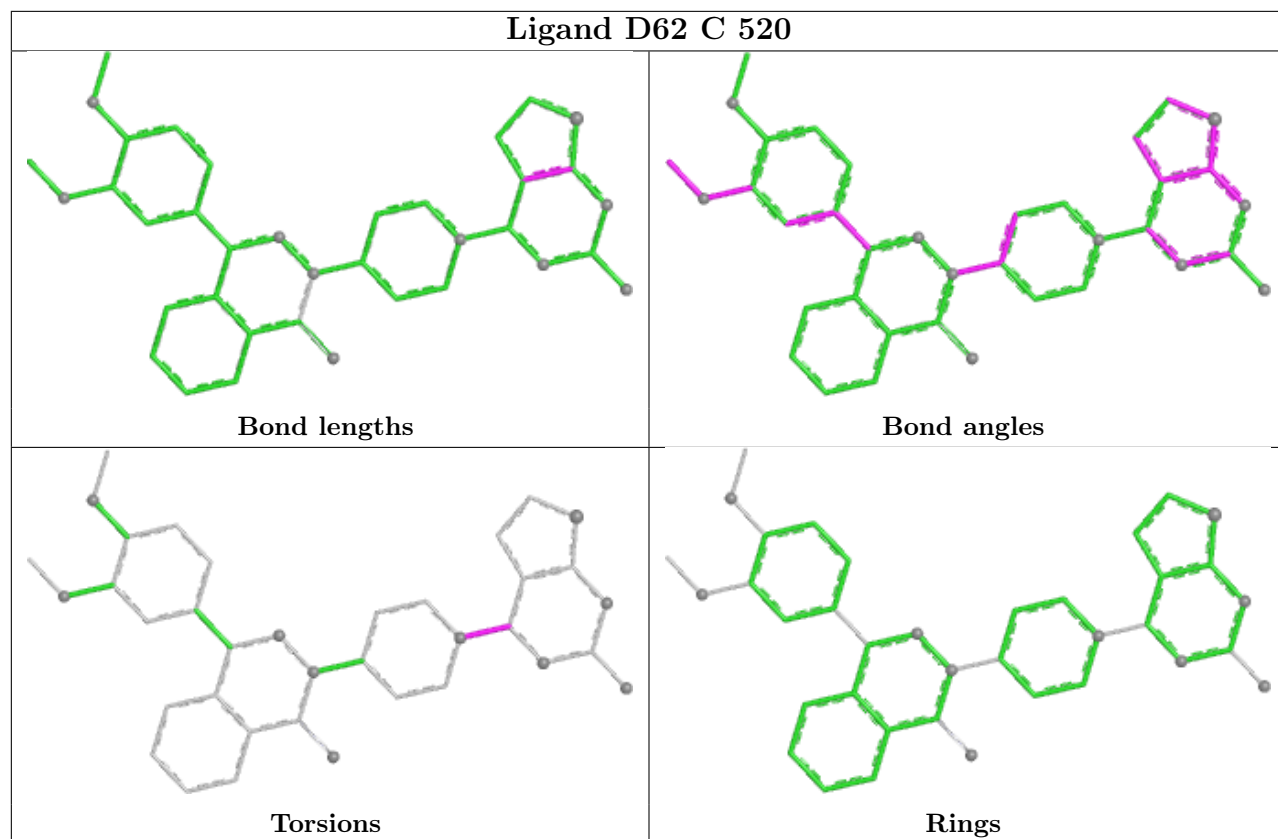
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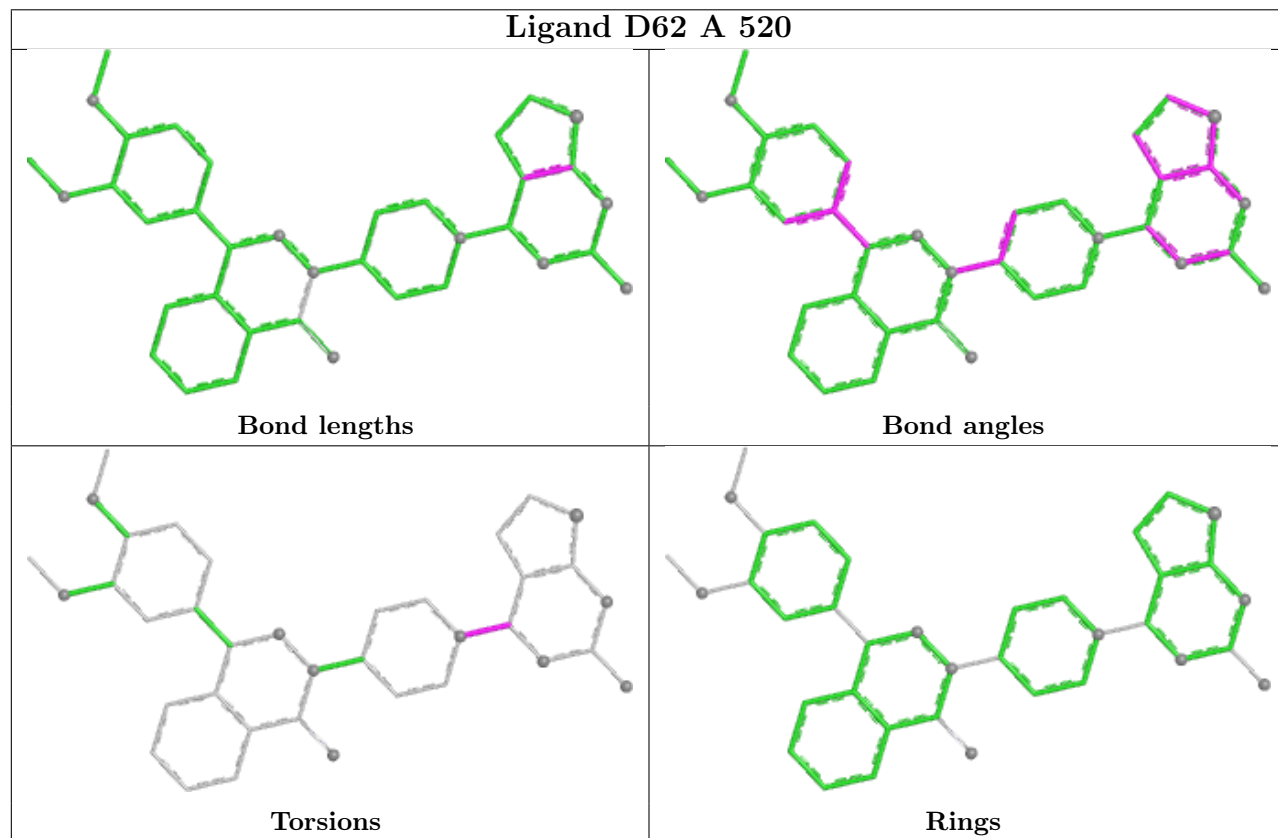
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	502	PG4	4	0
4	A	521	EDO	1	0
6	A	520	D62	2	0
7	B	521	EPE	4	0
5	A	517	PEG	2	0
5	A	518	PEG	1	0
4	C	515	EDO	2	0
7	A	524	EPE	1	0
4	A	525	EDO	2	0
5	D	519	PEG	2	0
4	D	513	EDO	1	0
5	B	508	PEG	2	0
4	B	504	EDO	1	0
4	C	509	EDO	1	0
8	C	521	PG4	10	0
4	A	508	EDO	1	0
7	C	514	EPE	5	0
5	A	516	PEG	2	0
7	D	523	EPE	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.

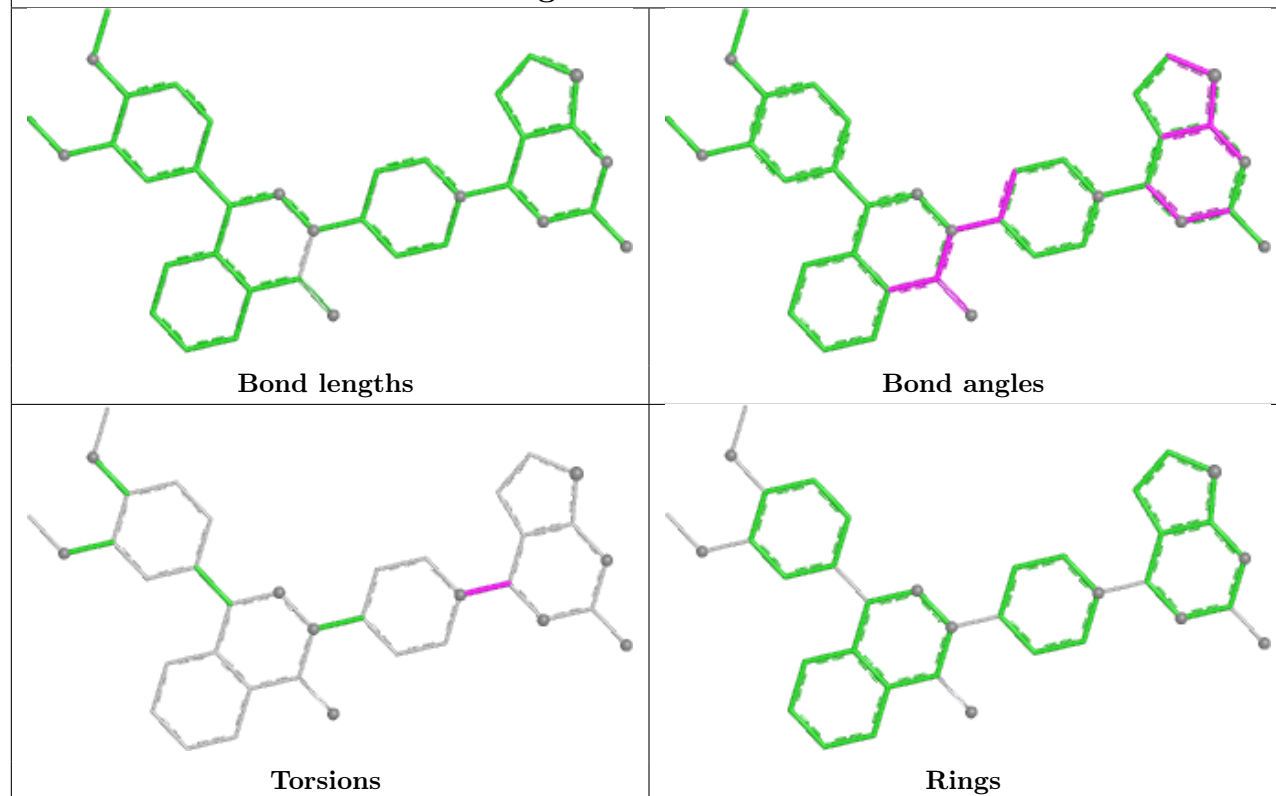
Ligand D62 C 520



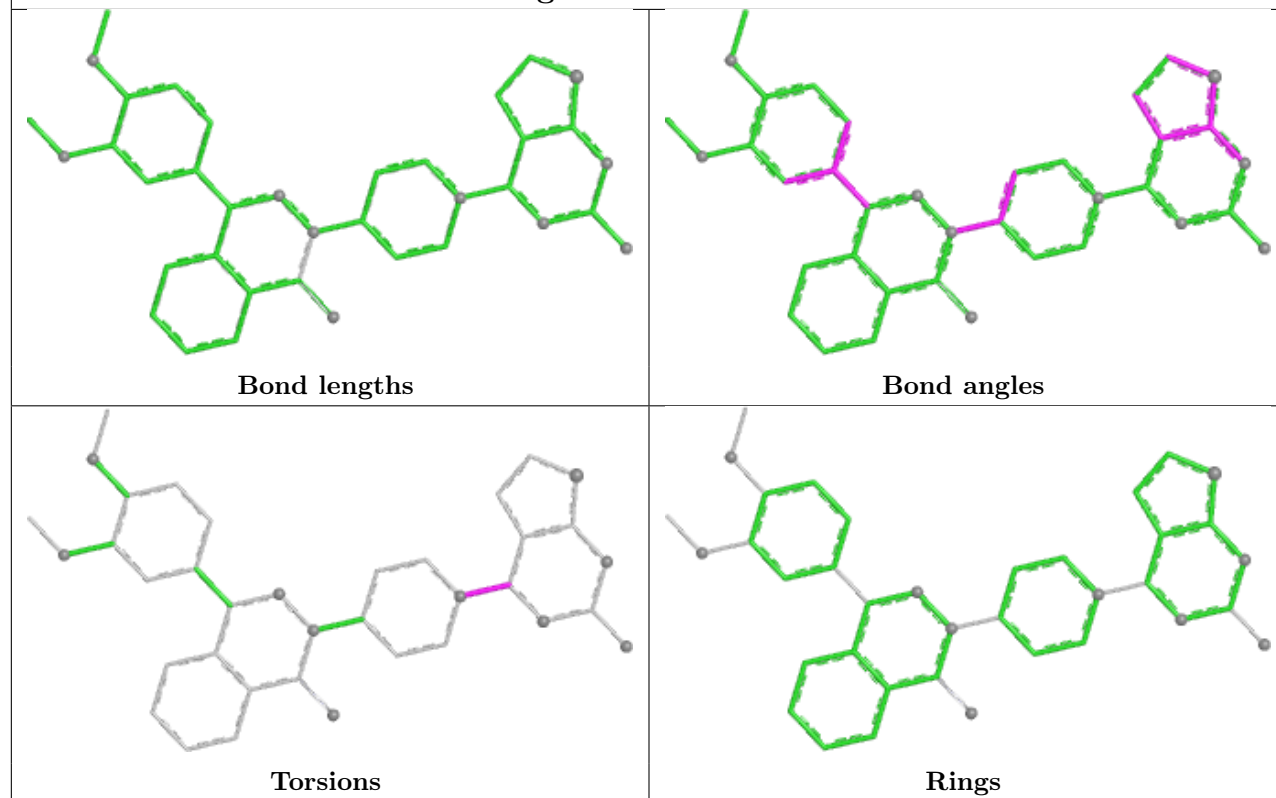
Ligand D62 A 520



Ligand D62 B 516



Ligand D62 D 517



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.02	5 (1%) 72 71	24, 37, 67, 98	0
1	B	323/364 (88%)	0.15	3 (0%) 81 80	18, 40, 60, 91	1 (0%)
1	C	324/364 (89%)	0.14	7 (2%) 62 61	25, 40, 73, 92	0
1	D	324/364 (89%)	-0.30	2 (0%) 85 85	23, 31, 54, 83	0
All	All	1301/1456 (89%)	0.00	17 (1%) 75 74	18, 37, 65, 98	1 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	82	PHE	4.2
1	C	411	PRO	3.6
1	A	411	PRO	2.9
1	A	222	MET	2.8
1	A	410	ILE	2.8
1	B	89	GLU	2.6
1	A	83	GLY	2.5
1	C	147	MET	2.4
1	C	292	VAL	2.4
1	D	362	ASN	2.3
1	C	91	VAL	2.2
1	B	222	MET	2.2
1	B	411	PRO	2.1
1	C	375	TYR	2.1
1	C	351	GLY	2.1
1	C	410	ILE	2.0
1	D	88	GLN	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	A	525	4/4	0.74	0.22	58,64,64,70	0
4	EDO	C	512	4/4	0.74	0.30	63,68,70,75	0
4	EDO	B	512	4/4	0.80	0.16	60,62,67,80	0
5	PEG	A	519	7/7	0.80	0.17	58,64,71,73	0
4	EDO	C	503	4/4	0.81	0.25	73,78,78,84	0
4	EDO	B	511	4/4	0.81	0.22	52,58,58,62	0
4	EDO	B	510	4/4	0.81	0.19	54,57,62,62	0
5	PEG	C	513	7/7	0.81	0.18	53,58,64,68	0
4	EDO	C	510	4/4	0.82	0.18	59,67,72,72	0
4	EDO	B	517	4/4	0.82	0.26	66,69,75,79	0
5	PEG	D	509	7/7	0.82	0.20	44,55,69,75	0
8	PG4	C	521	13/13	0.82	0.17	38,46,59,65	0
4	EDO	D	522	4/4	0.83	0.18	39,40,45,48	0
4	EDO	D	520	4/4	0.84	0.18	64,65,68,74	0
4	EDO	B	504	4/4	0.84	0.19	70,75,77,82	0
4	EDO	B	514	4/4	0.84	0.15	57,62,69,69	0
4	EDO	C	518	4/4	0.85	0.15	64,64,67,77	0
5	PEG	A	516	7/7	0.85	0.19	39,59,73,75	0
4	EDO	A	504	4/4	0.85	0.15	53,65,67,78	0
4	EDO	D	506	4/4	0.86	0.20	51,52,53,61	0
4	EDO	D	513	4/4	0.86	0.17	43,45,47,55	0
4	EDO	D	515	4/4	0.86	0.17	53,65,68,76	0
5	PEG	C	519	7/7	0.86	0.18	43,57,66,75	0
4	EDO	C	516	4/4	0.86	0.15	43,47,50,52	0
4	EDO	B	515	4/4	0.86	0.17	50,54,61,65	0
4	EDO	C	517	4/4	0.87	0.14	66,67,71,76	0
5	PEG	B	508	7/7	0.87	0.15	49,67,72,80	0
5	PEG	D	518	7/7	0.87	0.16	50,56,60,68	0
4	EDO	A	508	4/4	0.87	0.19	60,69,69,80	0
4	EDO	A	509	4/4	0.88	0.16	66,67,72,76	0
5	PEG	A	511	7/7	0.88	0.18	44,68,77,80	0
4	EDO	A	521	4/4	0.89	0.17	54,65,68,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	C	508	4/4	0.89	0.15	57,58,63,66	0
4	EDO	B	518	4/4	0.89	0.18	48,54,57,67	0
5	PEG	A	510	7/7	0.89	0.16	55,71,76,78	0
4	EDO	C	501	4/4	0.89	0.15	48,48,60,66	0
4	EDO	C	515	4/4	0.89	0.15	58,66,70,70	0
8	PG4	C	502	13/13	0.89	0.17	46,73,84,85	0
5	PEG	A	518	7/7	0.89	0.15	59,63,70,71	0
4	EDO	B	513	4/4	0.90	0.14	47,55,62,63	0
4	EDO	C	511	4/4	0.90	0.16	52,56,60,61	0
4	EDO	B	520	4/4	0.90	0.14	50,52,59,65	0
5	PEG	D	510	7/7	0.90	0.16	56,69,80,92	0
4	EDO	A	522	4/4	0.90	0.14	49,56,64,69	0
7	EPE	B	521	15/15	0.90	0.14	52,77,92,93	0
4	EDO	A	515	4/4	0.90	0.14	36,48,53,53	0
4	EDO	A	512	4/4	0.90	0.14	44,47,48,49	0
4	EDO	C	522	4/4	0.91	0.13	49,49,58,68	0
5	PEG	D	508	7/7	0.91	0.15	43,60,69,72	0
4	EDO	A	506	4/4	0.91	0.13	39,43,46,50	0
4	EDO	C	507	4/4	0.91	0.13	52,52,63,63	0
4	EDO	B	505	4/4	0.91	0.12	54,58,63,63	0
7	EPE	A	524	15/15	0.91	0.14	44,77,92,96	0
4	EDO	D	516	4/4	0.91	0.10	37,39,45,47	0
4	EDO	A	523	4/4	0.91	0.12	51,56,56,58	0
4	EDO	A	513	4/4	0.91	0.16	45,51,53,64	0
5	PEG	D	519	7/7	0.92	0.12	37,42,49,51	0
4	EDO	B	506	4/4	0.92	0.13	54,57,60,62	0
4	EDO	D	501	4/4	0.92	0.13	51,53,53,54	0
4	EDO	A	514	4/4	0.92	0.13	49,50,55,57	0
4	EDO	A	507	4/4	0.92	0.13	50,61,65,67	0
4	EDO	C	504	4/4	0.93	0.11	51,56,56,60	0
6	D62	A	520	37/37	0.93	0.11	32,40,96,104	0
4	EDO	D	521	4/4	0.93	0.12	34,42,48,51	0
7	EPE	B	509	15/15	0.93	0.12	53,62,70,73	0
4	EDO	B	503	4/4	0.93	0.10	37,41,41,43	0
4	EDO	B	507	4/4	0.93	0.14	52,55,61,62	0
4	EDO	B	519	4/4	0.93	0.17	63,63,68,70	0
4	EDO	D	514	4/4	0.94	0.10	30,41,43,47	0
4	EDO	D	511	4/4	0.94	0.11	42,43,43,61	0
7	EPE	D	523	15/15	0.94	0.13	36,72,91,103	0
6	D62	C	520	37/37	0.94	0.10	33,39,100,107	0
4	EDO	C	509	4/4	0.94	0.13	54,55,59,59	0
5	PEG	A	517	7/7	0.95	0.10	31,43,48,53	0

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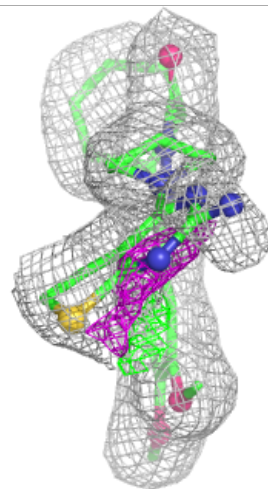
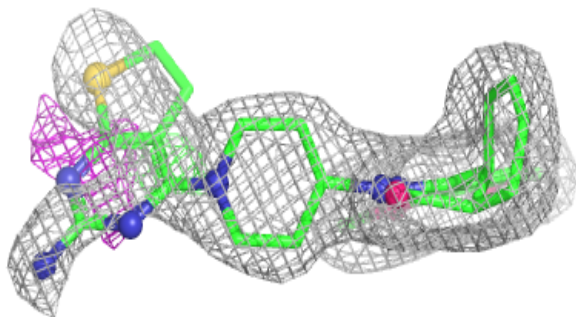
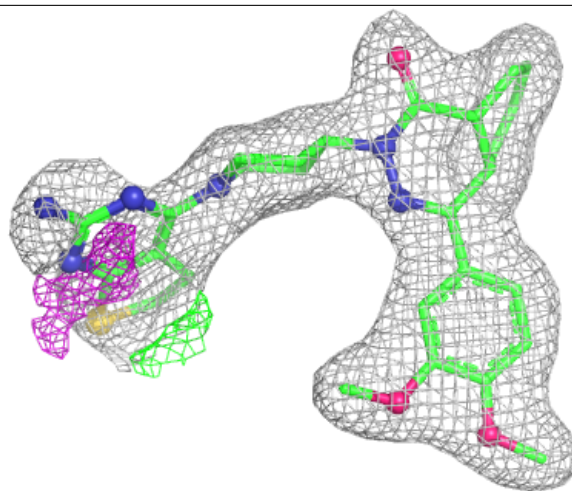
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	EPE	C	514	15/15	0.95	0.11	40,46,80,101	0
6	D62	D	517	37/37	0.95	0.09	26,32,74,89	0
4	EDO	A	503	4/4	0.95	0.09	51,53,54,56	0
4	EDO	D	505	4/4	0.95	0.09	41,43,43,48	0
6	D62	B	516	37/37	0.96	0.07	27,33,74,78	0
4	EDO	A	505	4/4	0.96	0.08	42,49,54,65	0
4	EDO	D	512	4/4	0.96	0.07	38,41,43,46	0
4	EDO	D	504	4/4	0.96	0.07	31,32,32,33	0
4	EDO	D	507	4/4	0.96	0.10	38,50,52,55	0
3	MG	C	506	1/1	0.99	0.04	21,21,21,21	0
2	ZN	A	501	1/1	0.99	0.04	33,33,33,33	0
3	MG	B	502	1/1	0.99	0.04	22,22,22,22	0
2	ZN	C	505	1/1	1.00	0.01	33,33,33,33	0
3	MG	D	503	1/1	1.00	0.02	18,18,18,18	0
2	ZN	D	502	1/1	1.00	0.01	30,30,30,30	0
3	MG	A	502	1/1	1.00	0.01	19,19,19,19	0
2	ZN	B	501	1/1	1.00	0.02	33,33,33,33	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.

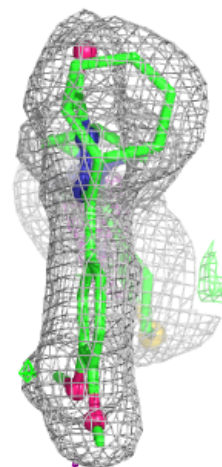
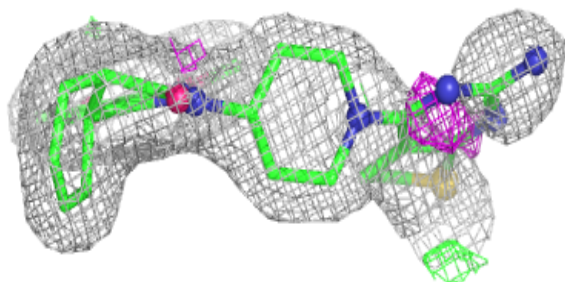
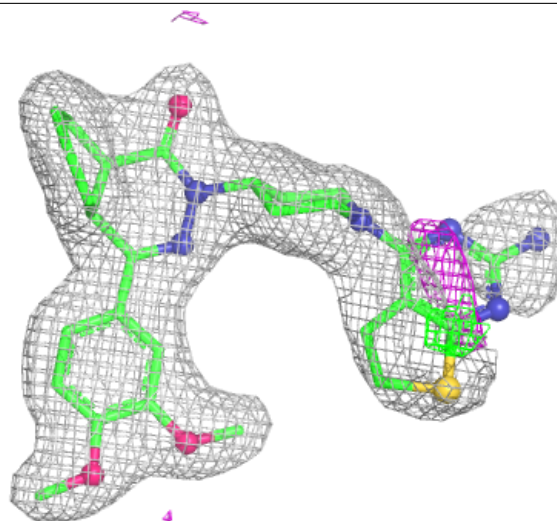
Electron density around D62 A 520:

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



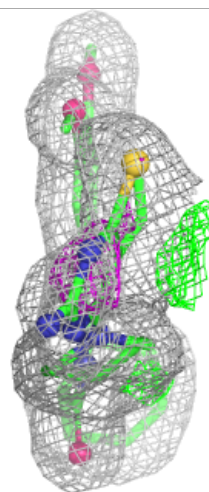
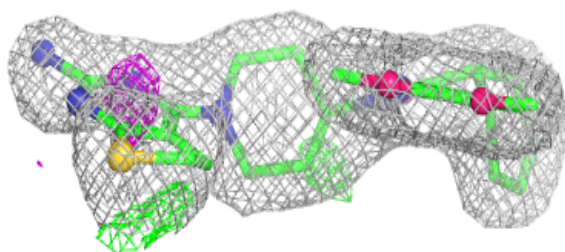
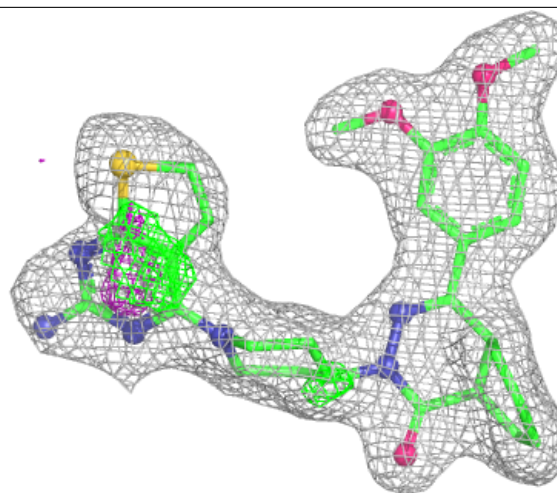
Electron density around D62 C 520:

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



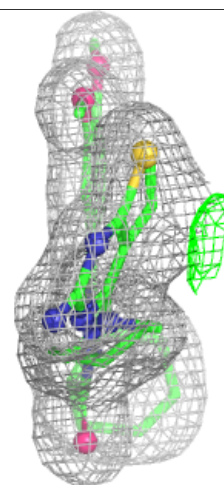
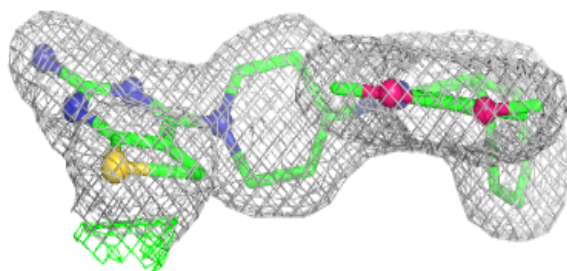
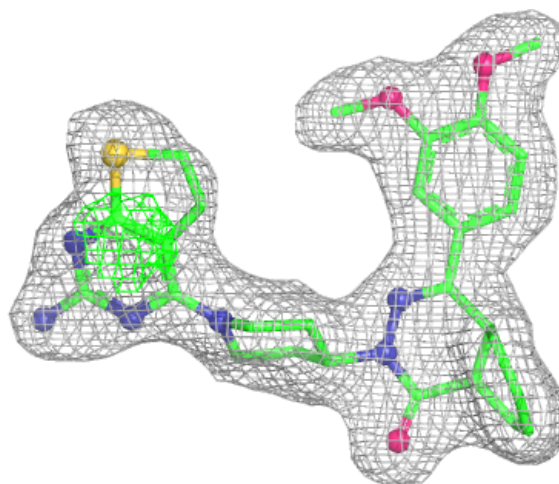
Electron density around D62 D 517:

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



Electron density around D62 B 516:

$2mF_o-DF_c$ (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.