Full wwPDB X-ray Structure Validation Report ⓘ

Nov 30, 2020 – 10:15 AM JST

PDB ID	:	6LGO
Title	:	Crystal structure of cystathionine gamma synthase from Xanthomonas oryzae pv. oryzae in complex with homolanthionine
Authors	:	Ngo, H.P.T.; Nguyen, T.D.Q.; Kang, L.W.
Deposited on	:	2019-12-05
Resolution	:	2.39 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 following versions of software and data (see references ⓘ) were used in the production of this report:

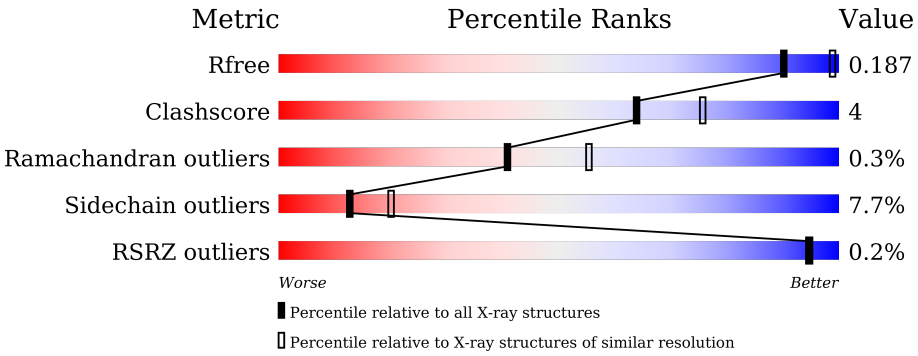
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 2.39 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on 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 <=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	408	81% 12% • 5%
1	B	408	81% 10% •• 5%
1	C	408	80% 11% • 5%
1	D	408	81% 11% • 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11993 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.

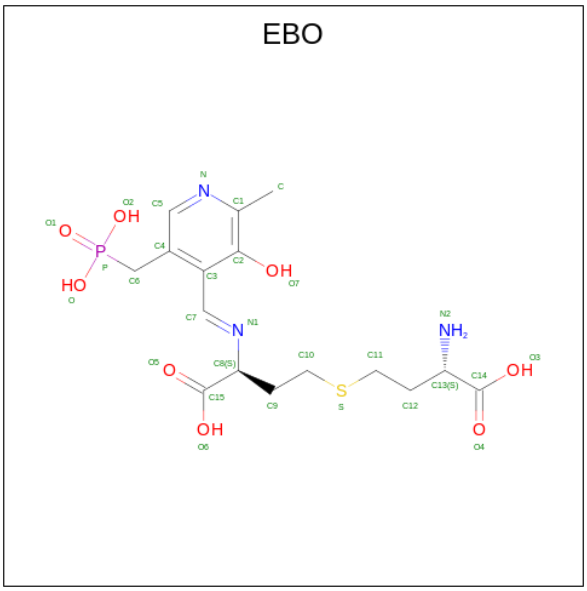
- Molecule 1 is a protein called Cystathionine gamma-synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			2870	1814	506	543	7			
1	B	387	Total	C	N	O	S	0	0	0
			2870	1814	506	543	7			
1	C	387	Total	C	N	O	S	0	0	0
			2870	1814	506	543	7			
1	D	387	Total	C	N	O	S	0	0	0
			2870	1814	506	543	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q5H1U9
A	-1	SER	-	expression tag	UNP Q5H1U9
A	0	HIS	-	expression tag	UNP Q5H1U9
A	134	VAL	ASP	engineered mutation	UNP Q5H1U9
B	-2	GLY	-	expression tag	UNP Q5H1U9
B	-1	SER	-	expression tag	UNP Q5H1U9
B	0	HIS	-	expression tag	UNP Q5H1U9
B	134	VAL	ASP	engineered mutation	UNP Q5H1U9
C	-2	GLY	-	expression tag	UNP Q5H1U9
C	-1	SER	-	expression tag	UNP Q5H1U9
C	0	HIS	-	expression tag	UNP Q5H1U9
C	134	VAL	ASP	engineered mutation	UNP Q5H1U9
D	-2	GLY	-	expression tag	UNP Q5H1U9
D	-1	SER	-	expression tag	UNP Q5H1U9
D	0	HIS	-	expression tag	UNP Q5H1U9
D	134	VAL	ASP	engineered mutation	UNP Q5H1U9

- Molecule 2 is (2 {S})-2-azanyl-4-[(3 {S})-3-[({E})-[2-methyl-3-oxidanyl-5-(phosphonomethyl)pyridin-4-yl]methylideneamino]-4-oxidanyl-4-oxidanylidene-butyl]sulfanyl-butanoic acid (three-letter code: EBO) (formula: $C_{16}H_{24}N_3O_8PS$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			29	16	3	8	1	1		
2	B	1	Total	C	N	O	P	S	0	0
			29	16	3	8	1	1		
2	C	1	Total	C	N	O	P	S	0	0
			29	16	3	8	1	1		
2	D	1	Total	C	N	O	P	S	0	0
			29	16	3	8	1	1		

- Molecule 3 is water.

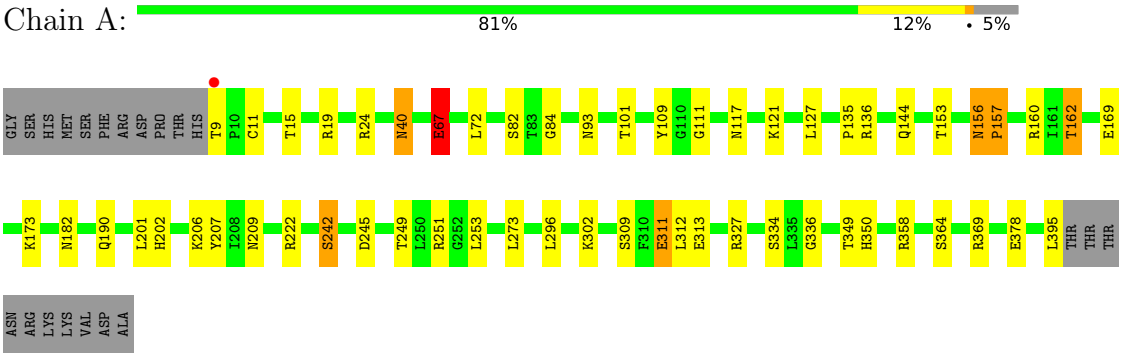
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	95	Total	O	0	0
			95	95		
3	B	98	Total	O	0	0
			98	98		
3	C	105	Total	O	0	0
			105	105		
3	D	99	Total	O	0	0
			99	99		

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.

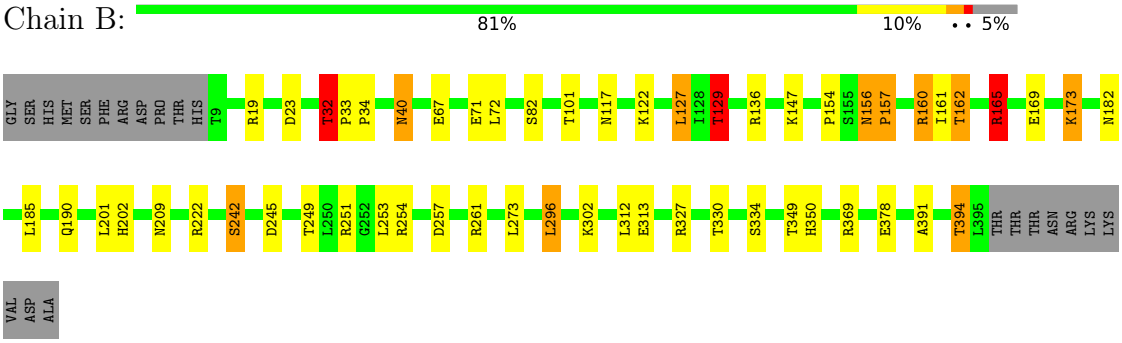
• Molecule 1: Cystathionine gamma-synthase

Chain A:



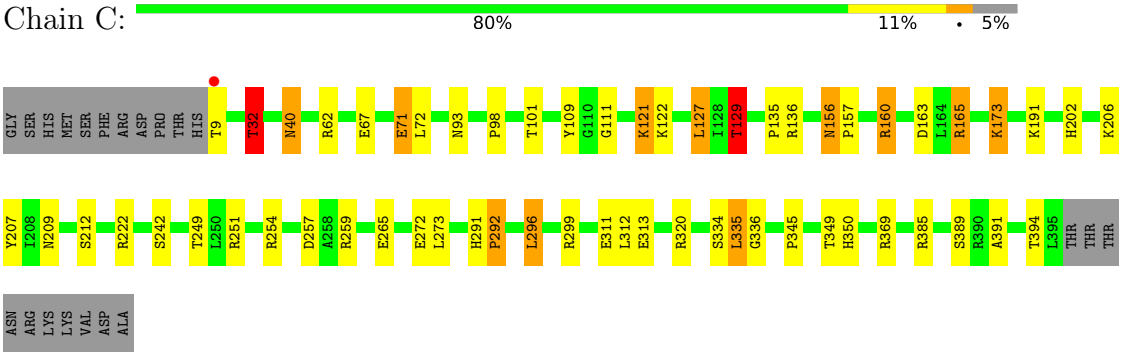
• Molecule 1: Cystathionine gamma-synthase

Chain B:



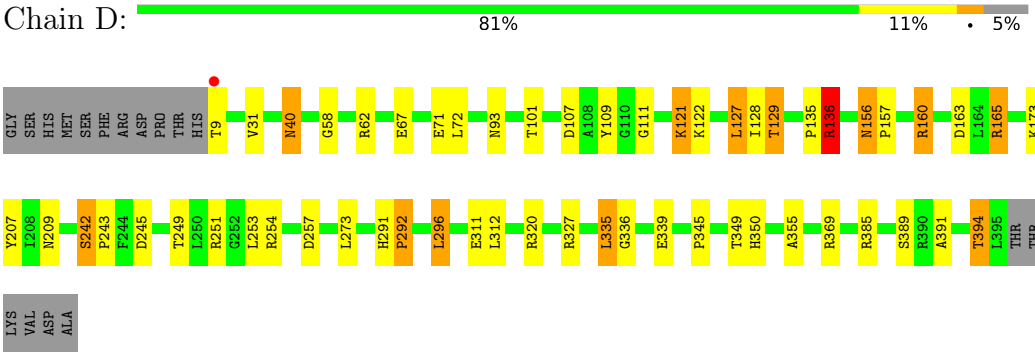
• Molecule 1: Cystathionine gamma-synthase

Chain C:



• Molecule 1: Cystathionine gamma-synthase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	161.22Å 161.22Å 244.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.07 – 2.39 47.07 – 2.39	Depositor EDS
% Data completeness (in resolution range)	96.2 (47.07-2.39) 96.2 (47.07-2.39)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.42 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.154 , 0.181 0.162 , 0.187	Depositor DCC
R_{free} test set	5900 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	29.8	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 7.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.486 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11993	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 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EBO

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	1.02	4/2924 (0.1%)	1.18	11/3980 (0.3%)
1	B	1.05	6/2924 (0.2%)	1.22	18/3980 (0.5%)
1	C	1.09	5/2924 (0.2%)	1.26	17/3980 (0.4%)
1	D	1.10	7/2924 (0.2%)	1.25	17/3980 (0.4%)
All	All	1.07	22/11696 (0.2%)	1.23	63/15920 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	3
1	D	0	3
All	All	0	10

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	67	GLU	CD-OE2	9.27	1.35	1.25
1	A	67	GLU	CD-OE2	8.63	1.35	1.25
1	C	389	SER	CB-OG	-7.06	1.33	1.42
1	D	389	SER	CB-OG	-7.04	1.33	1.42
1	C	257	ASP	CG-OD2	6.86	1.41	1.25
1	A	378	GLU	CD-OE1	6.60	1.32	1.25
1	D	67	GLU	CD-OE2	6.24	1.32	1.25
1	A	169	GLU	CD-OE1	6.16	1.32	1.25
1	D	339	GLU	CD-OE1	6.10	1.32	1.25
1	C	67	GLU	CD-OE2	5.93	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	378	GLU	CD-OE1	5.89	1.32	1.25
1	B	169	GLU	CD-OE1	5.75	1.31	1.25
1	D	67	GLU	CD-OE1	5.71	1.31	1.25
1	C	265	GLU	CD-OE2	-5.71	1.19	1.25
1	D	245	ASP	CG-OD2	5.69	1.38	1.25
1	D	58	GLY	C-O	5.63	1.32	1.23
1	D	257	ASP	CG-OD2	5.43	1.37	1.25
1	A	84	GLY	C-O	5.41	1.32	1.23
1	B	257	ASP	CG-OD1	5.29	1.37	1.25
1	B	23	ASP	CG-OD1	5.22	1.37	1.25
1	C	71	GLU	CD-OE1	5.21	1.31	1.25
1	B	330	THR	C-O	5.07	1.32	1.23

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	160	ARG	NE-CZ-NH1	17.14	128.87	120.30
1	D	160	ARG	NE-CZ-NH2	-15.59	112.51	120.30
1	C	160	ARG	NE-CZ-NH2	-14.45	113.08	120.30
1	C	160	ARG	NE-CZ-NH1	14.13	127.36	120.30
1	B	160	ARG	NE-CZ-NH2	-12.83	113.89	120.30
1	A	160	ARG	NE-CZ-NH2	-11.89	114.35	120.30
1	D	385	ARG	NE-CZ-NH1	10.97	125.78	120.30
1	C	385	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	B	160	ARG	NE-CZ-NH1	9.47	125.04	120.30
1	D	385	ARG	NE-CZ-NH2	-9.16	115.72	120.30
1	C	385	ARG	NE-CZ-NH2	-8.87	115.87	120.30
1	D	160	ARG	CD-NE-CZ	8.41	135.37	123.60
1	B	222	ARG	NE-CZ-NH2	8.31	124.45	120.30
1	B	32	THR	N-CA-CB	-7.94	95.22	110.30
1	A	160	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	B	160	ARG	CG-CD-NE	-7.91	95.19	111.80
1	B	129	THR	CA-CB-OG1	-7.89	92.43	109.00
1	A	160	ARG	CB-CA-C	7.83	126.06	110.40
1	B	165	ARG	CG-CD-NE	-7.66	95.72	111.80
1	A	358	ARG	NE-CZ-NH2	-7.65	116.48	120.30
1	D	160	ARG	CG-CD-NE	-7.49	96.06	111.80
1	B	261	ARG	NE-CZ-NH2	-7.45	116.57	120.30
1	C	160	ARG	CG-CD-NE	-7.35	96.37	111.80
1	A	222	ARG	NE-CZ-NH2	7.17	123.88	120.30
1	A	19	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	D	136	ARG	NE-CZ-NH1	7.14	123.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	129	THR	CB-CA-C	7.11	130.79	111.60
1	A	358	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	D	62	ARG	NE-CZ-NH1	7.05	123.82	120.30
1	C	62	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	C	160	ARG	CD-NE-CZ	6.83	133.17	123.60
1	A	117	ASN	CB-CA-C	6.54	123.48	110.40
1	D	62	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	222	ARG	NE-CZ-NH1	-6.37	117.12	120.30
1	C	257	ASP	CB-CG-OD1	-6.32	112.61	118.30
1	C	254	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	C	32	THR	N-CA-CB	-6.25	98.43	110.30
1	A	19	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	B	19	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	B	254	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	B	222	ARG	NE-CZ-NH1	-6.03	117.29	120.30
1	B	129	THR	CA-CB-CG2	5.98	120.77	112.40
1	C	129	THR	CA-CB-CG2	5.96	120.74	112.40
1	B	173	LYS	CB-CA-C	5.86	122.12	110.40
1	C	292	PRO	C-N-CA	-5.81	110.09	122.30
1	B	67	GLU	CB-CA-C	5.81	122.01	110.40
1	C	129	THR	CB-CA-C	5.78	127.21	111.60
1	C	259	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	160	ARG	CD-NE-CZ	5.65	131.51	123.60
1	D	320	ARG	NE-CZ-NH2	5.65	123.12	120.30
1	C	165	ARG	CB-CA-C	-5.65	99.11	110.40
1	D	165	ARG	CG-CD-NE	-5.51	100.22	111.80
1	B	32	THR	CB-CA-C	5.51	126.47	111.60
1	D	292	PRO	C-N-CA	-5.45	110.85	122.30
1	C	222	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	C	320	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	D	254	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	B	117	ASN	CB-CA-C	5.23	120.86	110.40
1	A	160	ARG	CB-CG-CD	5.23	125.20	111.60
1	D	107	ASP	CB-CG-OD1	5.13	122.92	118.30
1	D	257	ASP	CB-CG-OD1	-5.12	113.70	118.30
1	D	355	ALA	CB-CA-C	5.12	117.77	110.10
1	D	245	ASP	CB-CG-OD1	-5.01	113.79	118.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	HIS	Peptide
1	A	309	SER	Mainchain
1	B	160	ARG	Sidechain
1	B	202	HIS	Peptide
1	C	160	ARG	Sidechain
1	C	202	HIS	Peptide
1	C	9	THR	Peptide
1	D	160	ARG	Sidechain
1	D	202	HIS	Peptide
1	D	9	THR	Peptide

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	2870	0	2873	28	0
1	B	2870	0	2873	29	0
1	C	2870	0	2873	27	0
1	D	2870	0	2873	31	0
2	A	29	0	0	0	0
2	B	29	0	0	0	0
2	C	29	0	0	0	0
2	D	29	0	0	1	0
3	A	95	0	0	3	0
3	B	98	0	0	5	0
3	C	105	0	0	1	0
3	D	99	0	0	0	0
All	All	11993	0	11492	98	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (98) 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:C:32:THR:HG23	3:C:660:HOH:O	1.73	0.88
1:C:93:ASN:O	1:D:122:LYS:NZ	2.06	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:LYS:NZ	1:D:93:ASN:O	2.13	0.81
1:B:391:ALA:O	1:B:394:THR:HB	1.82	0.79
1:B:32:THR:HG23	3:B:684:HOH:O	1.80	0.79
1:B:251:ARG:HH22	1:C:209:ASN:HD21	1.31	0.79
1:D:391:ALA:O	1:D:394:THR:HB	1.87	0.74
1:A:251:ARG:HH22	1:D:209:ASN:HD21	1.37	0.73
1:D:209:ASN:HD22	1:D:249:THR:HA	1.54	0.72
1:C:391:ALA:O	1:C:394:THR:HB	1.91	0.71
1:A:40:ASN:HD22	1:A:40:ASN:H	1.41	0.68
1:C:209:ASN:HD22	1:C:249:THR:HA	1.58	0.68
1:A:156:ASN:HD21	1:A:369:ARG:HH11	1.43	0.67
1:B:349:THR:OG1	1:B:350:HIS:HD2	1.79	0.66
1:B:209:ASN:HD22	1:B:249:THR:HA	1.60	0.66
1:B:251:ARG:NH2	1:C:209:ASN:HD21	1.93	0.66
1:B:40:ASN:H	1:B:40:ASN:HD22	1.46	0.63
1:A:251:ARG:NH2	1:D:209:ASN:HD21	1.95	0.63
1:D:349:THR:OG1	1:D:350:HIS:HD2	1.80	0.63
1:A:209:ASN:HD22	1:A:249:THR:HA	1.64	0.61
1:C:40:ASN:HD22	1:C:40:ASN:H	1.48	0.61
1:A:349:THR:OG1	1:A:350:HIS:HD2	1.84	0.61
1:D:136:ARG:HH11	1:D:136:ARG:CG	2.14	0.61
1:B:165:ARG:NH1	3:B:601:HOH:O	2.27	0.60
1:A:209:ASN:HD21	1:D:251:ARG:HH22	1.50	0.59
1:D:156:ASN:HD21	1:D:369:ARG:HH11	1.50	0.59
1:D:40:ASN:H	1:D:40:ASN:HD22	1.51	0.59
1:C:156:ASN:HD21	1:C:369:ARG:HH11	1.53	0.57
1:C:291:HIS:CD2	1:C:292:PRO:O	2.58	0.56
1:B:182:ASN:HD21	1:B:190:GLN:HB3	1.69	0.56
1:A:162:THR:CG2	3:A:654:HOH:O	2.54	0.56
1:A:24:ARG:NH1	1:A:67:GLU:OE2	2.40	0.55
1:C:349:THR:OG1	1:C:350:HIS:HD2	1.89	0.55
1:C:127:LEU:HD13	1:C:129:THR:HG22	1.89	0.54
1:C:163:ASP:HB2	1:C:296:LEU:HD11	1.89	0.54
1:A:162:THR:HG21	3:A:675:HOH:O	2.06	0.54
1:C:173:LYS:HE3	1:C:173:LYS:HA	1.90	0.54
1:B:162:THR:CG2	3:B:656:HOH:O	2.56	0.53
1:D:40:ASN:N	1:D:40:ASN:HD22	2.05	0.53
1:B:201:LEU:HD12	1:B:201:LEU:C	2.29	0.53
1:B:162:THR:HG21	3:B:681:HOH:O	2.08	0.52
1:C:40:ASN:N	1:C:40:ASN:HD22	2.07	0.52
1:A:201:LEU:C	1:A:201:LEU:HD12	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:ASP:HB2	1:D:296:LEU:HD11	1.93	0.51
1:D:109:TYR:CE2	1:D:111:GLY:HA3	2.46	0.51
1:A:162:THR:HG22	3:A:654:HOH:O	2.09	0.50
1:A:182:ASN:HD21	1:A:190:GLN:HB3	1.76	0.50
1:B:209:ASN:HD21	1:C:251:ARG:HH22	1.60	0.50
1:D:127:LEU:HD13	1:D:129:THR:HG22	1.94	0.49
1:C:109:TYR:CE2	1:C:111:GLY:HA3	2.47	0.49
1:B:156:ASN:HD21	1:B:369:ARG:HH11	1.60	0.49
1:A:93:ASN:O	1:B:122:LYS:NZ	2.45	0.49
1:D:206:LYS:HD2	1:D:335:LEU:HG	1.95	0.48
1:B:40:ASN:N	1:B:40:ASN:HD22	2.09	0.47
1:A:251:ARG:HH22	1:D:209:ASN:ND2	2.09	0.47
1:D:156:ASN:HA	1:D:157:PRO:HA	1.75	0.47
1:D:291:HIS:CD2	1:D:292:PRO:O	2.67	0.47
1:A:40:ASN:N	1:A:40:ASN:HD22	2.05	0.47
1:A:245:ASP:OD2	1:B:242:SER:HB2	2.15	0.47
1:B:162:THR:HG22	3:B:656:HOH:O	2.13	0.47
1:A:242:SER:HB2	1:B:245:ASP:OD2	2.15	0.46
1:B:127:LEU:HD13	1:B:129:THR:HG22	1.96	0.46
1:A:109:TYR:CE2	1:A:111:GLY:HA3	2.51	0.46
1:A:82:SER:HB3	1:B:82:SER:HB3	1.97	0.46
1:B:32:THR:HG21	1:C:212:SER:O	2.14	0.46
1:D:136:ARG:HH11	1:D:136:ARG:HG2	1.80	0.46
1:A:153:THR:HB	1:A:162:THR:HG23	1.98	0.45
1:A:209:ASN:HD21	1:D:251:ARG:NH2	2.12	0.45
1:A:156:ASN:ND2	1:A:369:ARG:HH11	2.12	0.45
1:A:11:CYS:HB2	1:A:15:THR:HB	1.98	0.45
1:B:156:ASN:HA	1:B:157:PRO:HA	1.77	0.45
1:C:206:LYS:HD2	1:C:335:LEU:HG	1.98	0.45
1:D:136:ARG:NH1	1:D:136:ARG:CG	2.78	0.45
2:D:501:EBO:N1	2:D:501:EBO:O7	2.47	0.44
1:D:207:TYR:CE1	1:D:336:GLY:HA2	2.53	0.44
1:B:40:ASN:ND2	1:D:31:VAL:HB	2.32	0.44
1:B:161:ILE:HG22	1:B:296:LEU:HD13	2.00	0.43
1:C:156:ASN:HD22	1:C:157:PRO:CA	2.31	0.43
1:C:98:PRO:HD2	1:D:122:LYS:O	2.18	0.43
1:C:157:PRO:HD3	1:C:350:HIS:CE1	2.54	0.42
1:D:156:ASN:HD22	1:D:157:PRO:CA	2.32	0.42
1:B:209:ASN:HD21	1:C:251:ARG:NH2	2.18	0.42
1:C:345:PRO:HA	1:C:349:THR:OG1	2.20	0.42
1:A:207:TYR:CE1	1:A:336:GLY:HA2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:PRO:HD3	1:B:185:LEU:CD1	2.49	0.42
1:C:207:TYR:CE1	1:C:336:GLY:HA2	2.54	0.42
1:A:311:GLU:OE1	1:A:364:SER:OG	2.30	0.41
1:D:156:ASN:ND2	1:D:369:ARG:HH11	2.16	0.41
1:D:345:PRO:HA	1:D:349:THR:OG1	2.20	0.41
1:A:156:ASN:HA	1:A:157:PRO:HA	1.84	0.41
1:A:40:ASN:N	1:A:40:ASN:ND2	2.69	0.41
1:C:121:LYS:HE2	1:C:121:LYS:HB3	1.55	0.41
1:C:156:ASN:HA	1:C:157:PRO:HA	1.85	0.41
1:B:33:PRO:HA	1:B:34:PRO:HD3	1.83	0.41
1:D:101:THR:HG21	1:D:128:ILE:HD12	2.02	0.41
1:D:242:SER:HA	1:D:243:PRO:HD3	1.81	0.41
1:B:154:PRO:HD3	1:B:185:LEU:HD12	2.02	0.40
1:D:121:LYS:HB3	1:D:121:LYS:HE2	1.69	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	385/408 (94%)	376 (98%)	7 (2%)	2 (0%)	29	41
1	B	385/408 (94%)	375 (97%)	9 (2%)	1 (0%)	41	55
1	C	385/408 (94%)	378 (98%)	6 (2%)	1 (0%)	41	55
1	D	385/408 (94%)	378 (98%)	7 (2%)	0	100	100
All	All	1540/1632 (94%)	1507 (98%)	29 (2%)	4 (0%)	41	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	334	SER

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Mol	Chain	Res	Type
1	B	334	SER
1	A	206	LYS
1	C	334	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	291/310 (94%)	267 (92%)	24 (8%)	11	17
1	B	291/310 (94%)	268 (92%)	23 (8%)	12	19
1	C	291/310 (94%)	268 (92%)	23 (8%)	12	19
1	D	291/310 (94%)	271 (93%)	20 (7%)	15	25
All	All	1164/1240 (94%)	1074 (92%)	90 (8%)	13	20

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	40	ASN
1	A	67	GLU
1	A	72	LEU
1	A	101	THR
1	A	121	LYS
1	A	127	LEU
1	A	135	PRO
1	A	136	ARG
1	A	144	GLN
1	A	156	ASN
1	A	157	PRO
1	A	162	THR
1	A	173	LYS
1	A	242	SER
1	A	253	LEU
1	A	273	LEU
1	A	296	LEU

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Mol	Chain	Res	Type
1	A	302	LYS
1	A	311	GLU
1	A	312	LEU
1	A	313	GLU
1	A	327	ARG
1	A	395	LEU
1	B	32	THR
1	B	40	ASN
1	B	71	GLU
1	B	72	LEU
1	B	101	THR
1	B	127	LEU
1	B	129	THR
1	B	136	ARG
1	B	147	LYS
1	B	156	ASN
1	B	157	PRO
1	B	162	THR
1	B	165	ARG
1	B	173	LYS
1	B	242	SER
1	B	253	LEU
1	B	273	LEU
1	B	296	LEU
1	B	302	LYS
1	B	312	LEU
1	B	313	GLU
1	B	327	ARG
1	B	394	THR
1	C	32	THR
1	C	40	ASN
1	C	71	GLU
1	C	72	LEU
1	C	101	THR
1	C	121	LYS
1	C	127	LEU
1	C	129	THR
1	C	135	PRO
1	C	136	ARG
1	C	156	ASN
1	C	165	ARG
1	C	173	LYS

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Mol	Chain	Res	Type
1	C	191	LYS
1	C	242	SER
1	C	272	GLU
1	C	273	LEU
1	C	296	LEU
1	C	299	ARG
1	C	311	GLU
1	C	312	LEU
1	C	313	GLU
1	C	335	LEU
1	D	40	ASN
1	D	71	GLU
1	D	72	LEU
1	D	121	LYS
1	D	127	LEU
1	D	129	THR
1	D	135	PRO
1	D	136	ARG
1	D	156	ASN
1	D	165	ARG
1	D	173	LYS
1	D	242	SER
1	D	253	LEU
1	D	273	LEU
1	D	296	LEU
1	D	311	GLU
1	D	312	LEU
1	D	327	ARG
1	D	335	LEU
1	D	394	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	48	ASN
1	A	97	GLN
1	A	156	ASN
1	A	182	ASN
1	A	190	GLN
1	A	209	ASN
1	A	350	HIS

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Mol	Chain	Res	Type
1	B	40	ASN
1	B	48	ASN
1	B	97	GLN
1	B	156	ASN
1	B	182	ASN
1	B	190	GLN
1	B	209	ASN
1	B	350	HIS
1	C	40	ASN
1	C	48	ASN
1	C	97	GLN
1	C	117	ASN
1	C	156	ASN
1	C	182	ASN
1	C	190	GLN
1	C	209	ASN
1	C	291	HIS
1	C	350	HIS
1	D	40	ASN
1	D	97	GLN
1	D	156	ASN
1	D	182	ASN
1	D	209	ASN
1	D	291	HIS
1	D	301	GLN
1	D	350	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	EBO	C	501	-	22,29,29	3.05	10 (45%)	27,40,40	5.31	16 (59%)
2	EBO	D	501	-	22,29,29	2.60	9 (40%)	27,40,40	5.88	18 (66%)
2	EBO	A	501	-	22,29,29	3.18	11 (50%)	27,40,40	5.43	17 (62%)
2	EBO	B	501	-	22,29,29	3.72	11 (50%)	27,40,40	5.42	15 (55%)

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
2	EBO	C	501	-	-	10/18/26/26	0/1/1/1
2	EBO	D	501	-	-	10/18/26/26	0/1/1/1
2	EBO	A	501	-	-	6/18/26/26	0/1/1/1
2	EBO	B	501	-	-	8/18/26/26	0/1/1/1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	EBO	C2-C1	8.96	1.49	1.40
2	B	501	EBO	C3-C4	7.92	1.51	1.42
2	C	501	EBO	C3-C4	7.82	1.51	1.42
2	D	501	EBO	C3-C4	6.87	1.50	1.42
2	A	501	EBO	P-C6	6.34	1.89	1.79
2	A	501	EBO	C3-C4	6.27	1.49	1.42
2	B	501	EBO	C9-C8	5.75	1.60	1.53
2	A	501	EBO	C2-C1	5.70	1.46	1.40
2	C	501	EBO	P-C6	5.52	1.88	1.79
2	B	501	EBO	P-C6	5.30	1.88	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	EBO	C2-C1	5.25	1.46	1.40
2	B	501	EBO	C5-C4	5.13	1.48	1.37
2	A	501	EBO	C5-C4	4.87	1.47	1.37
2	A	501	EBO	C9-C8	4.78	1.59	1.53
2	A	501	EBO	P-O1	4.19	1.59	1.50
2	B	501	EBO	P-O1	4.14	1.58	1.50
2	D	501	EBO	P-O1	4.11	1.58	1.50
2	C	501	EBO	C10-S	-4.08	1.66	1.81
2	D	501	EBO	P-C6	3.97	1.86	1.79
2	C	501	EBO	C9-C8	3.74	1.58	1.53
2	D	501	EBO	C9-C8	-3.70	1.48	1.53
2	D	501	EBO	C11-S	-3.54	1.68	1.81
2	C	501	EBO	C5-C4	3.46	1.44	1.37
2	B	501	EBO	C10-S	-3.42	1.68	1.81
2	D	501	EBO	C5-C4	3.39	1.44	1.37
2	C	501	EBO	C3-C2	3.38	1.45	1.40
2	C	501	EBO	C8-N1	-3.36	1.43	1.46
2	A	501	EBO	C8-N1	3.07	1.50	1.46
2	B	501	EBO	C3-C2	3.04	1.45	1.40
2	D	501	EBO	C3-C2	2.85	1.45	1.40
2	A	501	EBO	C6-C4	2.85	1.55	1.51
2	B	501	EBO	C8-N1	2.80	1.49	1.46
2	A	501	EBO	C10-S	-2.74	1.71	1.81
2	B	501	EBO	P-O	-2.74	1.48	1.54
2	D	501	EBO	C2-C1	2.53	1.43	1.40
2	B	501	EBO	C11-S	-2.53	1.72	1.81
2	A	501	EBO	P-O2	-2.42	1.49	1.54
2	C	501	EBO	C11-S	-2.27	1.73	1.81
2	A	501	EBO	C11-S	-2.27	1.73	1.81
2	D	501	EBO	C-C1	2.07	1.53	1.50
2	C	501	EBO	C-C1	2.00	1.53	1.50

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	EBO	P-C6-C4	15.85	141.02	113.85
2	C	501	EBO	P-C6-C4	15.71	140.78	113.85
2	A	501	EBO	P-C6-C4	15.61	140.60	113.85
2	B	501	EBO	P-C6-C4	14.73	139.10	113.85
2	D	501	EBO	C6-C4-C3	13.72	136.08	122.04
2	C	501	EBO	C6-C4-C3	13.35	135.69	122.04
2	A	501	EBO	O2-P-C6	12.41	135.87	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	EBO	O2-P-C6	12.32	135.66	106.92
2	B	501	EBO	O-P-C6	12.08	135.10	106.92
2	B	501	EBO	C6-C4-C3	10.92	133.21	122.04
2	C	501	EBO	O1-P-C6	10.15	134.12	111.13
2	A	501	EBO	C6-C4-C3	9.64	131.90	122.04
2	D	501	EBO	O-P-O1	-7.45	92.68	112.39
2	D	501	EBO	O2-P-O1	-7.07	93.70	112.39
2	D	501	EBO	C2-C3-C4	7.05	123.67	118.26
2	A	501	EBO	C-C1-C2	-6.96	112.29	120.89
2	B	501	EBO	O-P-O1	-6.55	95.06	112.39
2	A	501	EBO	O2-P-O1	-6.17	96.07	112.39
2	A	501	EBO	C8-N1-C7	6.04	125.59	117.40
2	C	501	EBO	C2-C3-C4	5.95	122.82	118.26
2	B	501	EBO	O2-P-O1	-5.91	96.75	112.39
2	C	501	EBO	O-P-O1	-5.91	96.75	112.39
2	B	501	EBO	C5-C4-C3	-5.70	107.65	118.15
2	B	501	EBO	C8-N1-C7	5.66	125.07	117.40
2	A	501	EBO	C5-C4-C3	-5.49	108.05	118.15
2	C	501	EBO	C5-C4-C3	-5.49	108.05	118.15
2	D	501	EBO	C5-C4-C3	-5.45	108.11	118.15
2	A	501	EBO	O-P-O1	-5.38	98.16	112.39
2	A	501	EBO	C4-C5-N	5.29	132.63	123.82
2	B	501	EBO	C-C1-C2	-5.22	114.44	120.89
2	B	501	EBO	O1-P-C6	-5.12	99.54	111.13
2	A	501	EBO	C9-C10-S	-4.98	102.15	113.31
2	B	501	EBO	C4-C5-N	4.97	132.10	123.82
2	B	501	EBO	C9-C10-S	-4.80	102.55	113.31
2	D	501	EBO	O-P-C6	4.56	117.56	106.92
2	D	501	EBO	C-C1-N	4.48	126.42	117.67
2	D	501	EBO	C6-C4-C5	-4.43	114.31	119.28
2	D	501	EBO	C9-C10-S	-4.41	103.42	113.31
2	B	501	EBO	O2-P-C6	4.38	117.13	106.92
2	C	501	EBO	C10-C9-C8	-4.14	102.96	113.97
2	C	501	EBO	C4-C5-N	3.95	130.39	123.82
2	C	501	EBO	C-C1-C2	-3.92	116.05	120.89
2	D	501	EBO	C-C1-C2	-3.89	116.09	120.89
2	A	501	EBO	O1-P-C6	-3.88	102.35	111.13
2	B	501	EBO	C2-C3-C4	3.80	121.18	118.26
2	C	501	EBO	C-C1-N	3.69	124.87	117.67
2	A	501	EBO	C-C1-N	3.65	124.80	117.67
2	C	501	EBO	C6-C4-C5	-3.64	115.19	119.28
2	B	501	EBO	C-C1-N	3.56	124.62	117.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	EBO	C2-C3-C7	-3.47	113.94	120.41
2	C	501	EBO	O-P-O2	-3.45	98.00	108.08
2	A	501	EBO	C2-C3-C4	3.38	120.86	118.26
2	C	501	EBO	O2-P-O1	-3.27	103.75	112.39
2	C	501	EBO	O2-P-C6	2.97	113.84	106.92
2	C	501	EBO	C2-C3-C7	-2.90	115.01	120.41
2	D	501	EBO	O1-P-C6	-2.88	104.62	111.13
2	D	501	EBO	C12-C11-S	-2.87	106.87	113.31
2	A	501	EBO	O-P-C6	2.83	113.52	106.92
2	B	501	EBO	C12-C11-S	-2.76	107.11	113.31
2	D	501	EBO	C4-C5-N	2.69	128.30	123.82
2	D	501	EBO	C2-C1-N	-2.54	117.48	120.77
2	D	501	EBO	O-P-O2	-2.38	101.13	108.08
2	A	501	EBO	C12-C11-S	-2.21	108.34	113.31
2	A	501	EBO	C5-N-C1	-2.20	115.08	119.17
2	A	501	EBO	C11-S-C10	-2.04	95.68	101.87
2	C	501	EBO	C12-C11-S	-2.02	108.79	113.31

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	EBO	C15-C8-N1-C7
2	C	501	EBO	C9-C8-N1-C7
2	C	501	EBO	S-C11-C12-C13
2	C	501	EBO	C3-C4-C6-P
2	C	501	EBO	C5-C4-C6-P
2	C	501	EBO	C4-C6-P-O1
2	D	501	EBO	C15-C8-N1-C7
2	D	501	EBO	C9-C8-N1-C7
2	D	501	EBO	S-C10-C9-C8
2	D	501	EBO	C11-C12-C13-C14
2	D	501	EBO	C11-C12-C13-N2
2	D	501	EBO	C3-C4-C6-P
2	D	501	EBO	C5-C4-C6-P
2	A	501	EBO	C15-C8-C9-C10
2	A	501	EBO	N1-C8-C9-C10
2	A	501	EBO	C15-C8-N1-C7
2	A	501	EBO	C9-C8-N1-C7
2	A	501	EBO	C3-C4-C6-P
2	A	501	EBO	C5-C4-C6-P
2	B	501	EBO	C15-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
2	B	501	EBO	N1-C8-C9-C10
2	B	501	EBO	C15-C8-N1-C7
2	B	501	EBO	C9-C8-N1-C7
2	B	501	EBO	C3-C4-C6-P
2	B	501	EBO	C5-C4-C6-P
2	B	501	EBO	C4-C6-P-O
2	D	501	EBO	C4-C6-P-O2
2	C	501	EBO	C15-C8-C9-C10
2	C	501	EBO	N1-C8-C9-C10
2	C	501	EBO	C4-C6-P-O
2	D	501	EBO	C4-C6-P-O1
2	C	501	EBO	C9-C10-S-C11
2	D	501	EBO	C9-C10-S-C11
2	B	501	EBO	C9-C10-S-C11

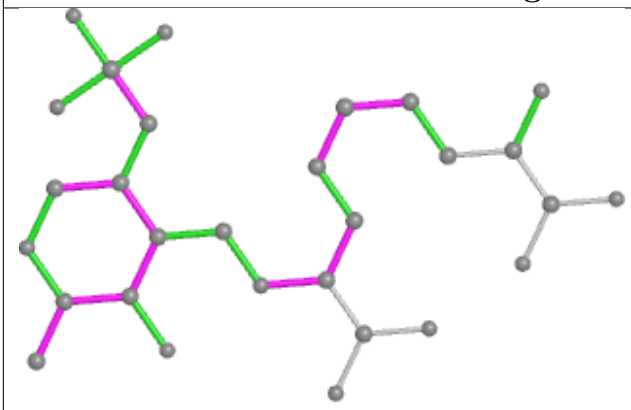
There are no ring outliers.

1 monomer is involved in 1 short contact:

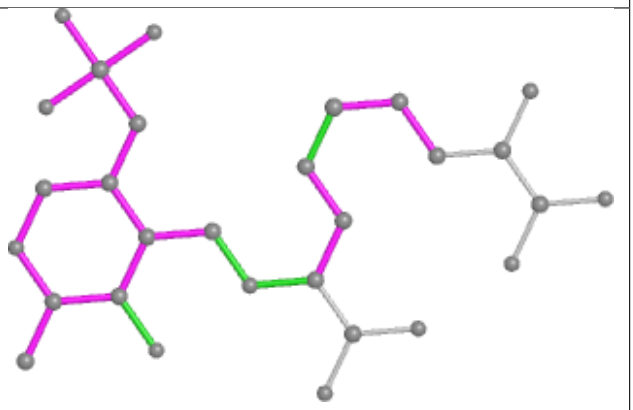
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	EBO	1	0

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 then 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.

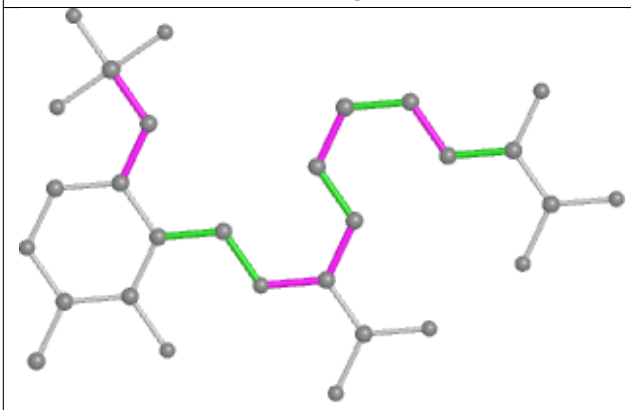
Ligand EBO C 501



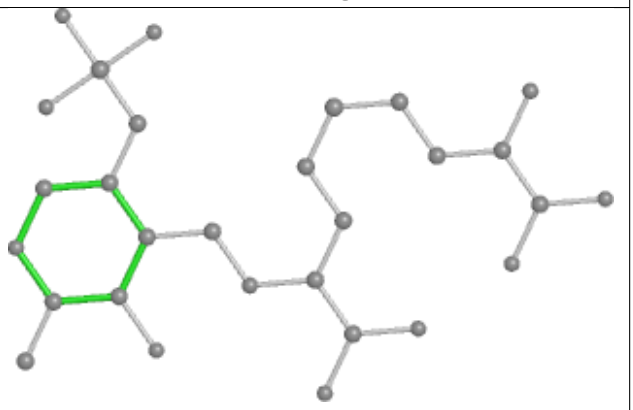
Bond lengths



Bond angles

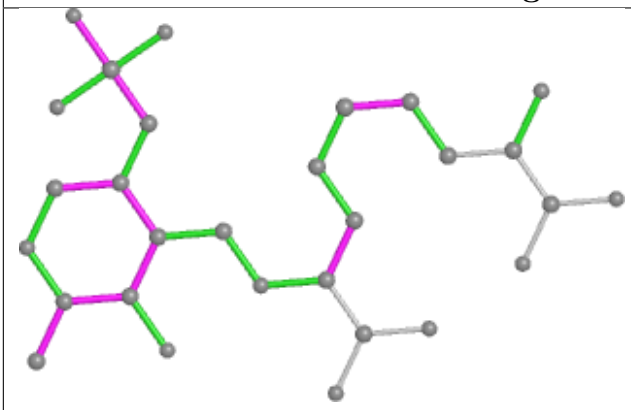


Torsions

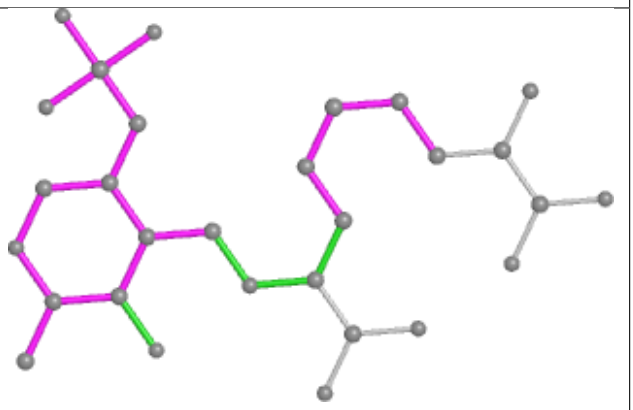


Rings

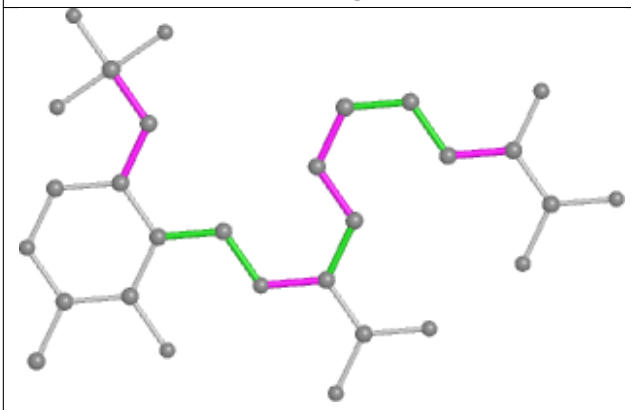
Ligand EBO D 501



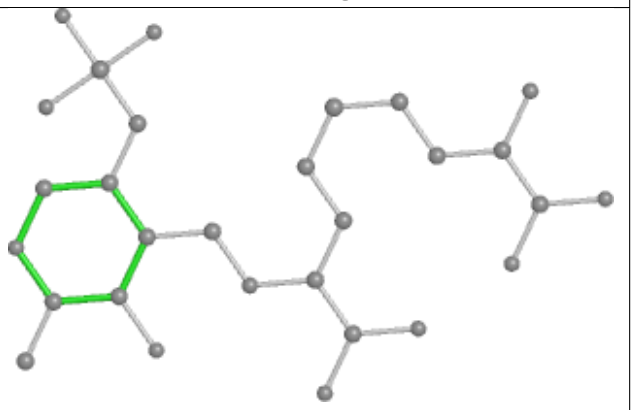
Bond lengths



Bond angles

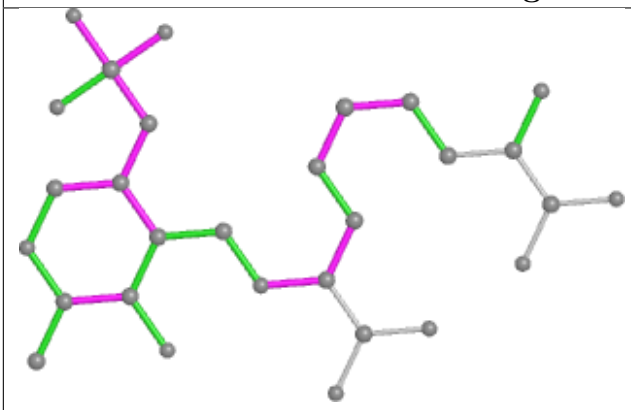


Torsions

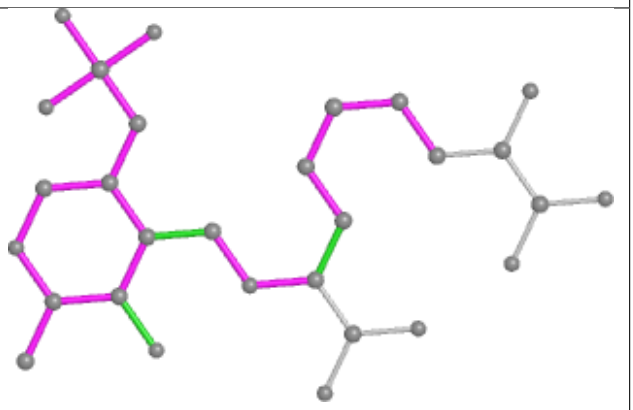


Rings

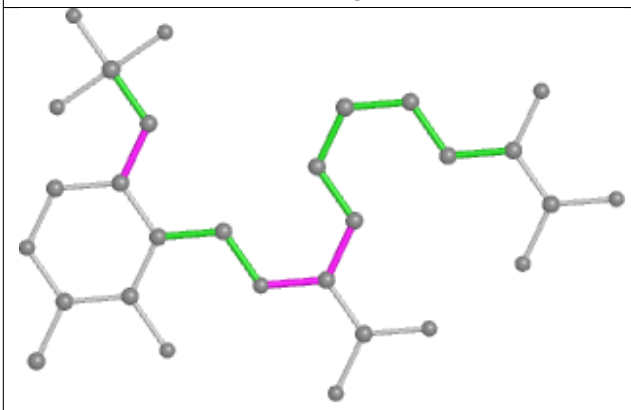
Ligand EBO A 501



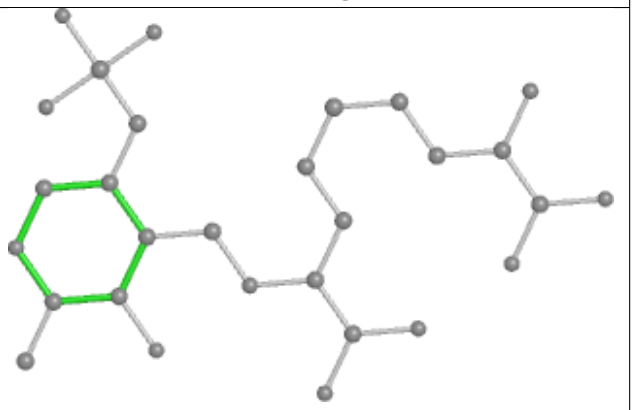
Bond lengths



Bond angles

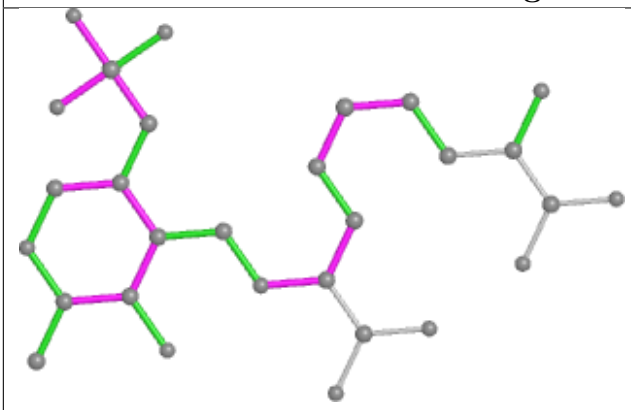


Torsions

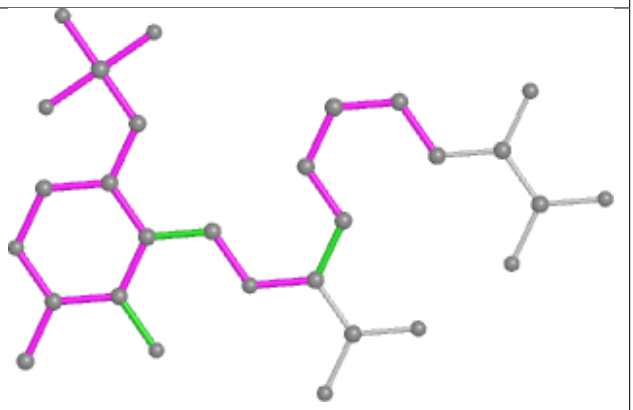


Rings

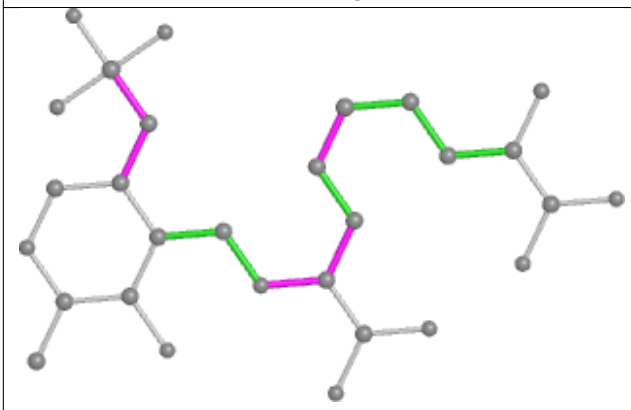
Ligand EBO B 501



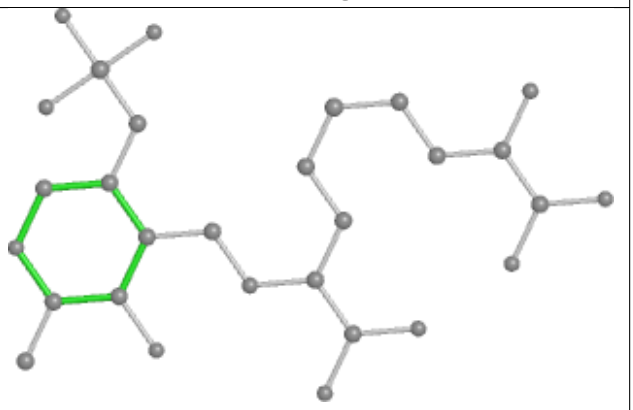
Bond lengths



Bond angles



Torsions



Rings

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	387/408 (94%)	-0.42	1 (0%) 94 93	20, 29, 49, 83	0
1	B	387/408 (94%)	-0.42	0 100 100	20, 29, 51, 84	0
1	C	387/408 (94%)	-0.42	1 (0%) 94 93	19, 30, 52, 100	0
1	D	387/408 (94%)	-0.43	1 (0%) 94 93	20, 30, 52, 98	0
All	All	1548/1632 (94%)	-0.42	3 (0%) 95 94	19, 29, 52, 100	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	9	THR	4.0
1	C	9	THR	3.6
1	A	9	THR	2.1

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

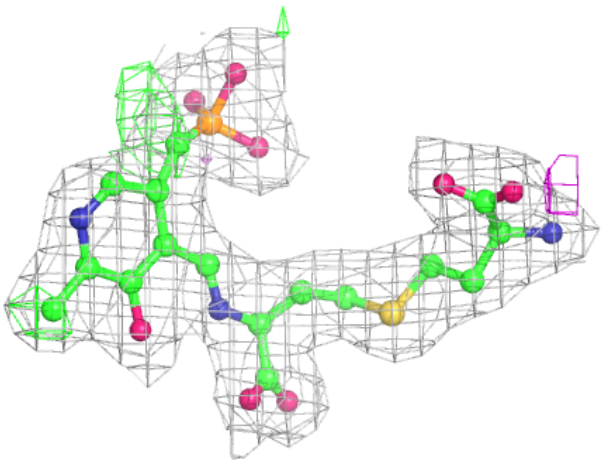
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

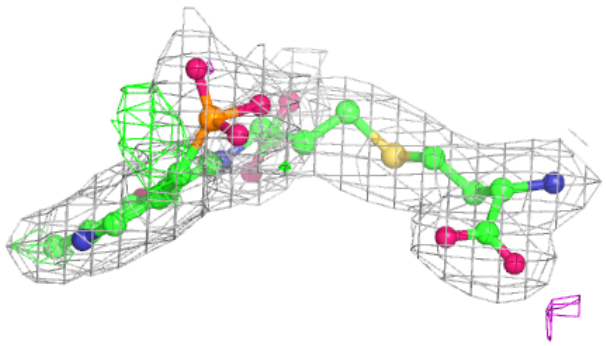
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EBO	D	501	29/29	0.97	0.10	17,26,33,42	0
2	EBO	A	501	29/29	0.97	0.12	18,26,35,41	0
2	EBO	B	501	29/29	0.97	0.12	19,26,34,41	0
2	EBO	C	501	29/29	0.98	0.12	19,24,39,44	0

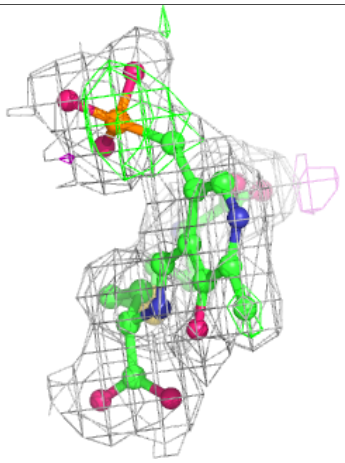
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EBO D 501:

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

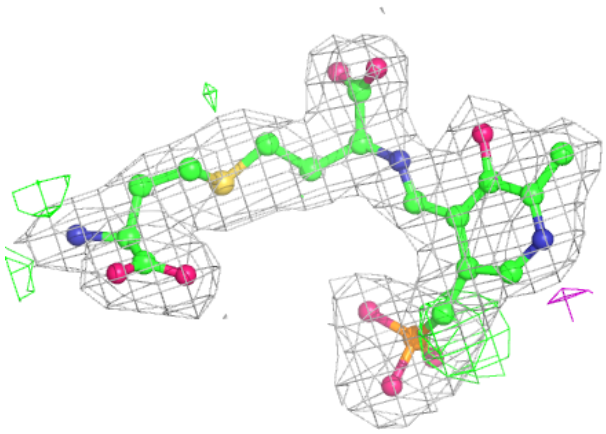


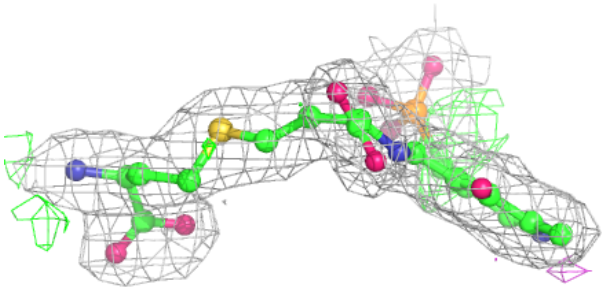


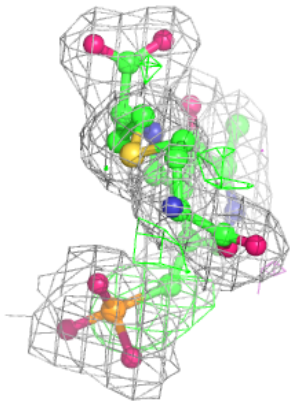


Electron density around EBO A 501:

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

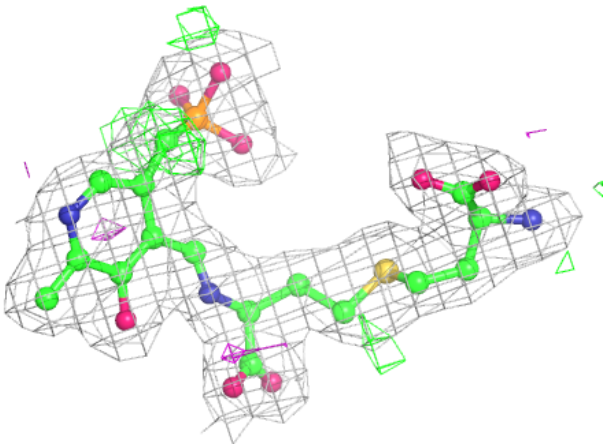


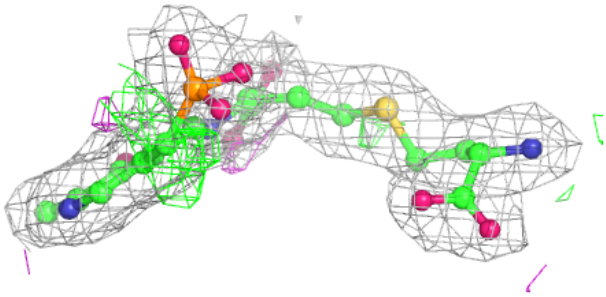




Electron density around EBO B 501:

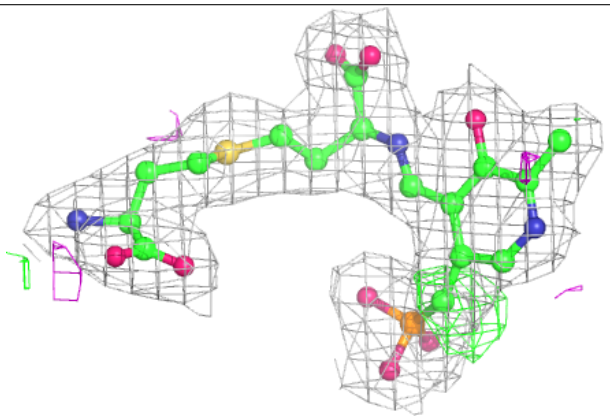
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

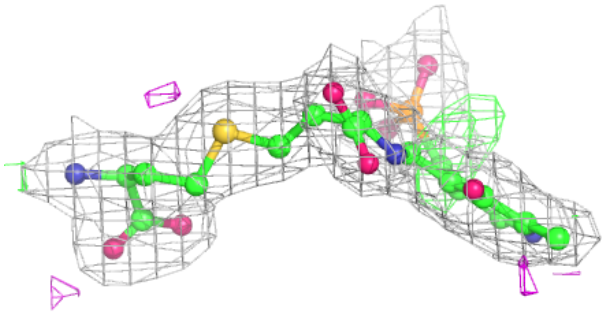


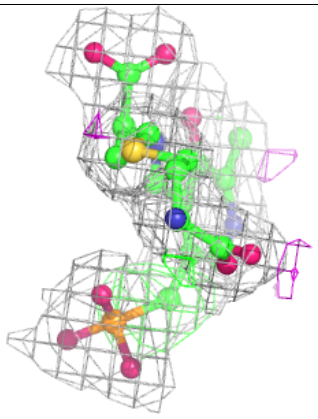


Electron density around EBO C 501:

$2mF_o$-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.