



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 03:47 PM EDT

PDB ID : 5EGF  
Title : The crystal structure of SeMet-CT  
Authors : Zhang, J.R.; Tang, Y.; Zhou, J.H.  
Deposited on : 2015-10-27  
Resolution : 2.29 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](mailto: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>.

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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	:	2.37.1
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)	:	2.37.1

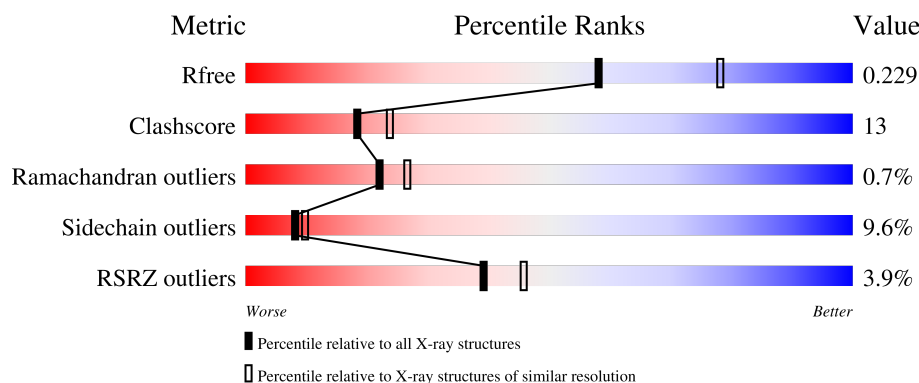
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.29 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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  $\geq 3$ , 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	486	<div> <div>3%</div> <div> <div></div> <div>65%</div> <div>23%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	486	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>21%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	486	<div> <div>4%</div> <div> <div></div> <div>62%</div> <div>25%</div> <div>•</div> <div>9%</div> </div> </div>
1	D	486	<div> <div>4%</div> <div> <div></div> <div>63%</div> <div>25%</div> <div>•</div> <div>9%</div> </div> </div>

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
2	EDO	A	504	-	-	X	-
2	EDO	B	502	-	-	X	-
2	EDO	B	506	-	-	X	-
2	EDO	B	508	-	-	X	-
2	EDO	C	501	-	-	X	-
2	EDO	C	504	-	-	X	-
2	EDO	C	508	-	-	-	X
2	EDO	D	505	-	-	-	X
3	C8E	A	508	-	-	X	-
3	C8E	B	512	-	-	X	-
3	C8E	C	509	-	-	X	-
3	C8E	D	511	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14879 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 TqaA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	Se	0	1	0
			3529	2257	609	650	7	6			
1	B	443	Total	C	N	O	S	Se	0	1	0
			3527	2252	609	653	7	6			
1	C	444	Total	C	N	O	S	Se	0	2	0
			3544	2265	612	654	7	6			
1	D	442	Total	C	N	O	S	Se	0	1	0
			3529	2257	609	650	7	6			

There are 32 discrepancies between the modelled and reference sequences:

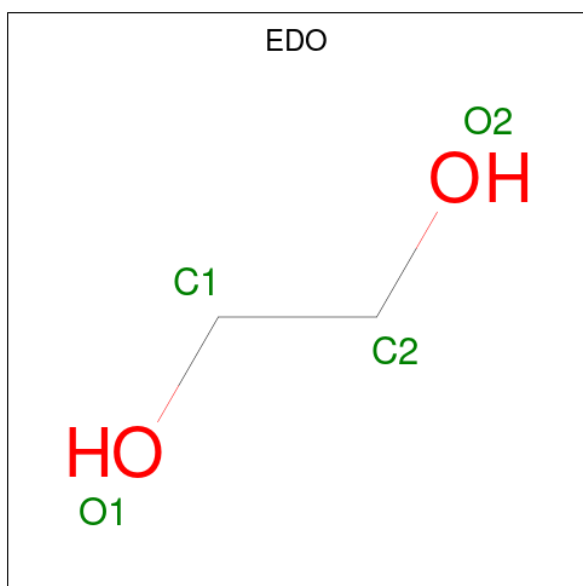
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	HIS	-	expression tag	UNP F1CWE4
A	3	HIS	-	expression tag	UNP F1CWE4
A	4	HIS	-	expression tag	UNP F1CWE4
A	5	HIS	-	expression tag	UNP F1CWE4
A	6	HIS	-	expression tag	UNP F1CWE4
A	7	HIS	-	expression tag	UNP F1CWE4
A	35	ALA	LYS	engineered mutation	UNP F1CWE4
A	36	ALA	GLU	engineered mutation	UNP F1CWE4
B	2	HIS	-	expression tag	UNP F1CWE4
B	3	HIS	-	expression tag	UNP F1CWE4
B	4	HIS	-	expression tag	UNP F1CWE4
B	5	HIS	-	expression tag	UNP F1CWE4
B	6	HIS	-	expression tag	UNP F1CWE4
B	7	HIS	-	expression tag	UNP F1CWE4
B	35	ALA	LYS	engineered mutation	UNP F1CWE4
B	36	ALA	GLU	engineered mutation	UNP F1CWE4
C	2	HIS	-	expression tag	UNP F1CWE4
C	3	HIS	-	expression tag	UNP F1CWE4
C	4	HIS	-	expression tag	UNP F1CWE4
C	5	HIS	-	expression tag	UNP F1CWE4
C	6	HIS	-	expression tag	UNP F1CWE4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	7	HIS	-	expression tag	UNP F1CWE4
C	35	ALA	LYS	engineered mutation	UNP F1CWE4
C	36	ALA	GLU	engineered mutation	UNP F1CWE4
D	2	HIS	-	expression tag	UNP F1CWE4
D	3	HIS	-	expression tag	UNP F1CWE4
D	4	HIS	-	expression tag	UNP F1CWE4
D	5	HIS	-	expression tag	UNP F1CWE4
D	6	HIS	-	expression tag	UNP F1CWE4
D	7	HIS	-	expression tag	UNP F1CWE4
D	35	ALA	LYS	engineered mutation	UNP F1CWE4
D	36	ALA	GLU	engineered mutation	UNP F1CWE4

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

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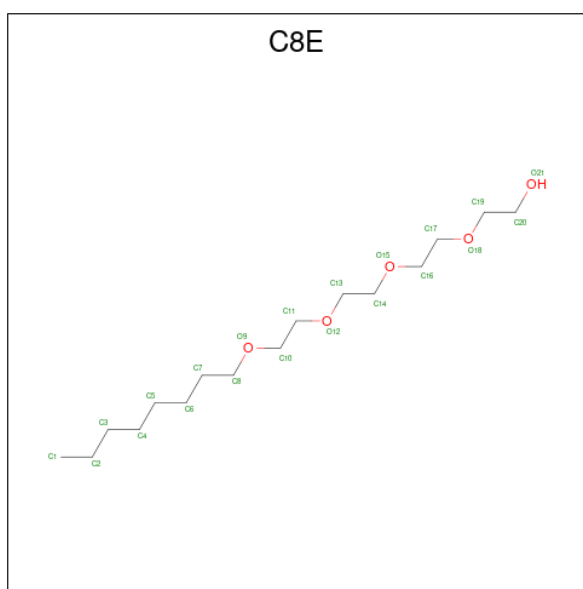
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0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

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

- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula:  $C_{16}H_{34}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	16	5		
3	B	1	Total	C	O	0	0
			21	16	5		
3	C	1	Total	C	O	0	0
			21	16	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			21	16	5		

- Molecule 4 is water.

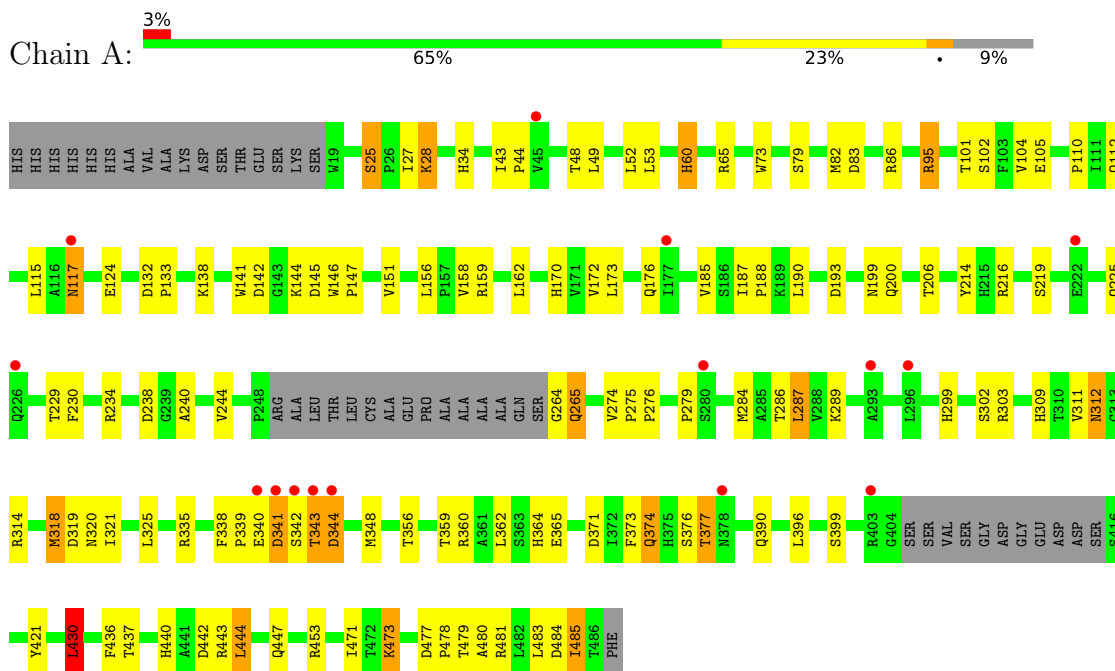
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	115	Total	O	0	0
			115	115		
4	B	179	Total	O	0	0
			179	179		
4	C	134	Total	O	0	0
			134	134		
4	D	98	Total	O	0	0
			98	98		



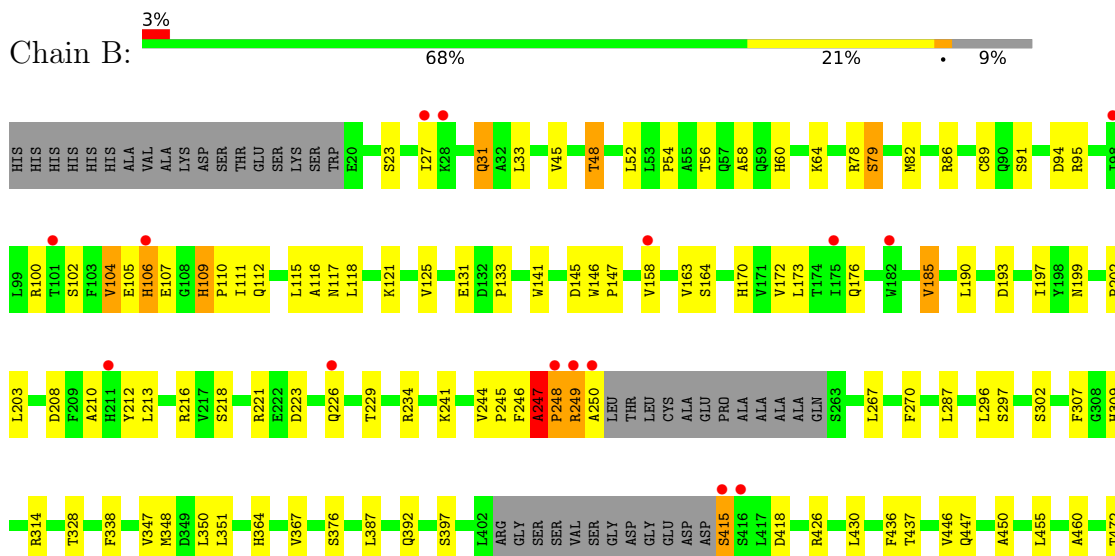
### 3 Residue-property plots

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: TqaA

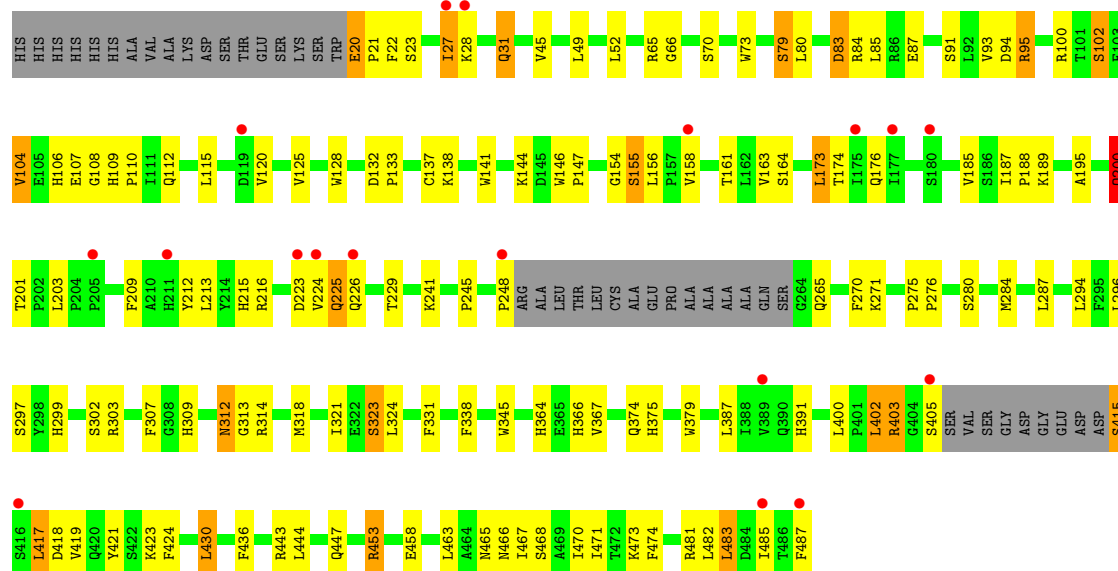


- Molecule 1: TqaA

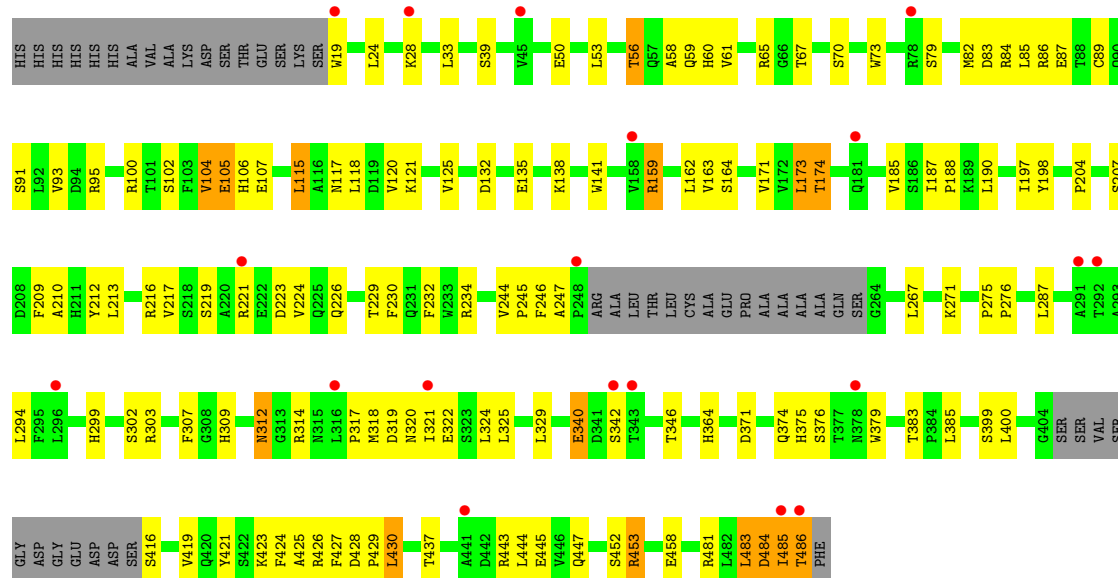




• Molecule 1: TqaA



• Molecule 1: TqaA



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	216.60Å 100.28Å 128.23Å 90.00° 100.18° 90.00°	Depositor
Resolution (Å)	29.75 – 2.29 29.75 – 2.29	Depositor EDS
% Data completeness (in resolution range)	85.4 (29.75-2.29) 85.1 (29.75-2.29)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.94 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.7_650	Depositor
R, $R_{free}$	0.225 , 0.266 0.226 , 0.229	Depositor DCC
$R_{free}$ test set	1880 reflections (1.66%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.5	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 40.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14879	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, C8E

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	0.45	0/3626	0.61	0/4946
1	B	0.50	0/3623	0.63	1/4941 (0.0%)
1	C	0.44	0/3645	0.58	0/4970
1	D	0.41	0/3626	0.57	0/4946
All	All	0.45	0/14520	0.60	1/19803 (0.0%)

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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	247	ALA	N-CA-C	5.09	124.74	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	484	ASP	Peptide
1	B	247	ALA	Peptide

## 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	3529	0	3454	89	0
1	B	3527	0	3452	78	0
1	C	3544	0	3466	100	0
1	D	3529	0	3454	96	0
2	A	28	0	42	9	0
2	B	40	0	60	20	0
2	C	32	0	48	16	0
2	D	40	0	60	9	0
3	A	21	0	34	9	0
3	B	21	0	34	16	0
3	C	21	0	34	12	0
3	D	21	0	34	9	0
4	A	115	0	0	2	0
4	B	179	0	0	6	0
4	C	134	0	0	9	0
4	D	98	0	0	5	0
All	All	14879	0	14172	378	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 13.

All (378) 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)
2:B:502:EDO:H11	3:B:512:C8E:H13	1.34	1.08
2:C:501:EDO:H21	3:C:509:C8E:H81	1.36	1.02
2:B:502:EDO:H22	3:B:512:C8E:H32	1.44	0.99
1:B:95:ARG:HH21	1:B:203:LEU:HB3	1.25	0.98
1:D:56:THR:HG22	1:D:59:GLN:H	1.30	0.97
1:B:267:LEU:HB2	2:B:506:EDO:H11	1.50	0.93
3:A:508:C8E:H21	1:D:246:PHE:H	1.36	0.90
1:B:472:THR:O	1:B:476:THR:HG23	1.74	0.87
3:A:508:C8E:H12	3:D:511:C8E:H142	1.57	0.84
1:D:485:ILE:HD12	1:D:486:THR:HG22	1.59	0.84
2:B:502:EDO:C1	3:B:512:C8E:H13	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:VAL:O	1:D:299:HIS:HD2	1.63	0.81
1:C:303:ARG:H	2:C:505:EDO:H11	1.45	0.80
1:D:483:LEU:HD12	1:D:484:ASP:HB2	1.64	0.80
1:A:289:LYS:NZ	1:A:309:HIS:HD2	1.79	0.80
1:B:267:LEU:CB	2:B:506:EDO:H11	2.12	0.79
1:A:151:VAL:H	2:A:504:EDO:H21	1.47	0.78
1:C:20:GLU:N	1:C:23:SER:HG	1.82	0.77
1:B:95:ARG:NH2	1:B:203:LEU:HB3	2.00	0.75
1:C:307:PHE:HA	2:C:502:EDO:H12	1.68	0.75
1:B:202:PRO:HD2	4:B:756:HOH:O	1.86	0.74
1:C:366[B]:HIS:HD2	4:C:609:HOH:O	1.69	0.73
1:B:314:ARG:NH1	1:B:328:THR:OG1	2.23	0.72
1:B:460:ALA:CB	2:B:506:EDO:H12	2.20	0.72
1:C:312:ASN:HD22	1:C:313:GLY:N	1.87	0.72
1:A:141:TRP:HA	1:A:145:ASP:HB2	1.72	0.71
1:B:23:SER:O	4:B:601:HOH:O	2.07	0.71
1:C:229:THR:HG21	1:C:367:VAL:HG11	1.72	0.71
1:C:187:ILE:HG22	1:C:188:PRO:HD3	1.72	0.71
1:D:73:TRP:CZ3	1:D:421:TYR:HB2	2.25	0.71
1:A:25:SER:HB3	1:A:52:LEU:HD22	1.73	0.71
2:B:502:EDO:C2	3:B:512:C8E:H32	2.19	0.71
1:D:53:LEU:HD22	1:D:213:LEU:HD12	1.73	0.70
1:A:151:VAL:N	2:A:504:EDO:H21	2.07	0.70
1:D:187:ILE:CG2	1:D:188:PRO:HD3	2.22	0.69
1:D:187:ILE:HG22	1:D:188:PRO:HD3	1.73	0.69
1:B:33:LEU:HD22	1:B:106:HIS:HD2	1.55	0.69
1:B:387:LEU:HB3	2:B:508:EDO:H11	1.73	0.68
1:A:318:MSE:HE3	1:A:321:ILE:HD13	1.75	0.68
1:D:223:ASP:HB3	1:D:226:GLN:CD	2.13	0.68
1:A:299:HIS:HB3	3:D:511:C8E:H161	1.76	0.68
1:D:445:GLU:HG2	1:D:447:GLN:HE21	1.59	0.67
2:C:501:EDO:H21	3:C:509:C8E:C8	2.20	0.67
2:B:502:EDO:H22	3:B:512:C8E:C3	2.21	0.67
1:D:385:LEU:H	2:D:508:EDO:H21	1.60	0.67
1:A:287:LEU:HD13	1:A:471:ILE:HG23	1.76	0.66
1:D:312:ASN:HD22	1:D:314:ARG:H	1.43	0.66
1:B:56:THR:HB	2:B:505:EDO:H22	1.76	0.66
1:B:307:PHE:HA	2:B:508:EDO:H12	1.77	0.66
2:C:501:EDO:O2	3:C:509:C8E:H102	1.96	0.66
1:D:174:THR:HG21	4:D:635:HOH:O	1.95	0.66
1:C:312:ASN:HD22	1:C:312:ASN:C	2.00	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:508:C8E:H191	1:D:299:HIS:HB3	1.78	0.65
1:C:212:TYR:CE2	1:C:216:ARG:HD2	2.31	0.65
1:A:289:LYS:HZ3	1:A:309:HIS:HD2	1.43	0.65
1:A:436:PHE:HB2	1:A:447:GLN:HB2	1.79	0.64
1:D:209:PHE:O	1:D:212:TYR:HB3	1.97	0.64
1:C:147:PRO:HG3	2:C:506:EDO:H22	1.78	0.64
1:A:319:ASP:O	1:A:320:ASN:HB2	1.98	0.64
1:A:190:LEU:HD12	1:A:325:LEU:HD21	1.81	0.63
1:A:312:ASN:HD22	1:A:314:ARG:H	1.46	0.63
1:B:141:TRP:HA	1:B:145:ASP:HB2	1.80	0.63
1:D:33:LEU:HD13	1:D:106:HIS:CD2	2.34	0.63
1:A:28:LYS:HD3	1:A:28:LYS:N	2.14	0.63
1:A:73:TRP:CZ3	1:A:421:TYR:HB2	2.34	0.62
1:B:60:HIS:CE1	1:B:64:LYS:HE2	2.34	0.62
1:D:322:GLU:CD	1:D:322:GLU:H	2.03	0.62
1:A:244:VAL:O	1:D:299:HIS:CD2	2.50	0.62
3:A:508:C8E:H21	1:D:246:PHE:N	2.11	0.62
1:B:426:ARG:HA	2:B:504:EDO:H21	1.81	0.62
1:B:212:TYR:CE2	1:B:216:ARG:HD2	2.35	0.61
1:B:244:VAL:O	1:C:299:HIS:HD2	1.83	0.61
1:C:65:ARG:NH2	1:C:430:LEU:HD22	2.15	0.61
1:D:121:LYS:HB3	4:D:636:HOH:O	1.99	0.61
1:C:146:TRP:CG	1:C:147:PRO:HD3	2.36	0.61
1:B:248:PRO:HG3	4:B:699:HOH:O	2.01	0.60
1:A:187:ILE:HG22	1:A:188:PRO:HD3	1.82	0.60
3:B:512:C8E:H162	3:C:509:C8E:H101	1.84	0.60
1:D:314:ARG:NH2	1:D:324:LEU:O	2.35	0.60
1:C:331:PHE:HB2	2:C:504:EDO:C2	2.31	0.60
1:B:79:SER:HG	1:B:415:SER:N	1.98	0.60
1:B:297:SER:HB2	1:B:302:SER:O	2.01	0.59
1:A:156:LEU:O	2:A:503:EDO:H22	2.01	0.59
2:C:501:EDO:H11	3:C:509:C8E:H191	1.83	0.59
3:B:512:C8E:H171	1:C:299:HIS:HB3	1.84	0.59
1:D:294:LEU:HD21	1:D:485:ILE:HG21	1.84	0.59
1:B:229:THR:HA	1:B:364:HIS:ND1	2.18	0.59
1:C:215[B]:HIS:CG	1:C:318:MSE:HE2	2.38	0.59
1:C:215[A]:HIS:CG	1:C:318:MSE:HE2	2.38	0.59
1:A:146:TRP:CD2	1:A:147:PRO:HD3	2.38	0.59
3:A:508:C8E:H11	3:D:511:C8E:H62	1.85	0.58
1:C:93:VAL:HG13	1:C:100:ARG:HG2	1.84	0.58
1:A:264:GLY:HA2	1:A:453:ARG:HD2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:GLY:HA2	4:C:640:HOH:O	2.02	0.58
1:A:477:ASP:OD1	1:A:479:THR:HB	2.02	0.58
1:D:95:ARG:NH2	1:D:204:PRO:O	2.35	0.58
1:B:485:ILE:HG23	1:B:486:THR:H	1.68	0.58
1:A:187:ILE:CG2	1:A:188:PRO:HD3	2.33	0.58
1:B:267:LEU:HB2	2:B:506:EDO:C1	2.32	0.57
1:C:473:LYS:HZ3	1:C:485:ILE:H	1.49	0.57
1:B:348:MSE:CE	1:B:478:PRO:HB2	2.34	0.57
1:D:485:ILE:HD12	1:D:486:THR:CG2	2.33	0.57
2:C:501:EDO:H11	3:C:509:C8E:H171	1.85	0.57
1:C:466:ASN:O	1:C:470:ILE:HG13	2.04	0.57
1:A:234:ARG:N	1:A:376:SER:HB3	2.20	0.57
1:C:83:ASP:O	1:C:87:GLU:HG3	2.04	0.57
1:C:270:PHE:CD2	1:C:447:GLN:HG2	2.40	0.57
1:A:158:VAL:HA	1:A:176:GLN:O	2.04	0.57
2:C:501:EDO:C2	3:C:509:C8E:H81	2.23	0.57
1:D:83:ASP:O	1:D:87:GLU:HG3	2.05	0.57
3:B:512:C8E:H11	2:C:501:EDO:O1	2.05	0.56
1:D:275:PRO:HD3	1:D:443:ARG:HA	1.87	0.56
1:D:379:TRP:N	1:D:379:TRP:CD1	2.71	0.56
3:B:512:C8E:H71	3:C:509:C8E:H22	1.87	0.56
1:C:303:ARG:HG2	1:C:338:PHE:HB2	1.87	0.56
1:C:473:LYS:NZ	1:C:485:ILE:H	2.02	0.56
1:D:303:ARG:HG3	4:D:685:HOH:O	2.05	0.56
1:B:86:ARG:O	1:B:89:CYS:HB2	2.06	0.56
1:C:297:SER:HB2	1:C:302:SER:O	2.04	0.56
1:B:270:PHE:CD2	1:B:447:GLN:HG2	2.41	0.56
1:B:250:ALA:O	1:C:458:GLU:HG3	2.05	0.55
1:A:34:HIS:HB2	1:A:49:LEU:HD22	1.87	0.55
1:A:65:ARG:CZ	1:A:430:LEU:HD22	2.36	0.55
1:C:155:SER:HB3	4:C:608:HOH:O	2.06	0.55
1:A:28:LYS:N	1:A:28:LYS:CD	2.69	0.55
1:C:331:PHE:HB2	2:C:504:EDO:H21	1.88	0.55
1:C:400:LEU:HB3	1:C:419:VAL:HG11	1.88	0.55
1:D:245:PRO:HA	3:D:511:C8E:H142	1.89	0.55
1:C:91:SER:O	1:C:94:ASP:HB2	2.07	0.55
1:A:146:TRP:CG	1:A:147:PRO:HD3	2.42	0.54
1:D:307:PHE:HA	2:D:502:EDO:H21	1.89	0.54
1:C:65:ARG:CZ	1:C:430:LEU:HD22	2.37	0.54
1:B:296:LEU:HD11	1:B:387:LEU:HD23	1.90	0.53
1:D:138:LYS:HD3	1:D:424:PHE:CE1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:SER:HB2	1:C:141:TRP:CZ3	2.42	0.53
1:A:276:PRO:HD2	1:A:284:MSE:HE1	1.91	0.53
1:D:383:THR:HA	2:D:506:EDO:H11	1.90	0.53
1:A:340:GLU:O	1:A:341:ASP:HB3	2.08	0.53
3:B:512:C8E:H141	3:C:509:C8E:H71	1.90	0.53
1:C:112:GLN:HE22	1:C:213:LEU:HD11	1.73	0.53
1:C:21:PRO:HB2	1:C:22:PHE:HD1	1.74	0.53
1:D:65:ARG:CZ	1:D:430:LEU:HD22	2.39	0.53
3:A:508:C8E:H13	3:D:511:C8E:C1	2.40	0.52
1:A:240:ALA:HB2	1:A:335:ARG:CZ	2.39	0.52
1:C:436:PHE:HB2	1:C:447:GLN:HB2	1.91	0.52
1:A:151:VAL:H	2:A:504:EDO:C2	2.18	0.52
1:A:299:HIS:HD2	1:D:244:VAL:O	1.92	0.52
1:B:246:PHE:O	1:B:247:ALA:HB3	2.10	0.52
1:C:331:PHE:HD2	2:C:504:EDO:H22	1.73	0.52
1:C:187:ILE:CG2	1:C:188:PRO:HD3	2.39	0.52
1:D:224:VAL:HG11	1:D:375:HIS:CG	2.44	0.52
1:B:158:VAL:HA	1:B:176:GLN:O	2.10	0.52
1:C:195:ALA:HB2	1:C:400:LEU:HD12	1.91	0.52
1:D:93:VAL:HG12	1:D:100:ARG:HG3	1.91	0.52
1:D:190:LEU:HD12	1:D:325:LEU:HD21	1.92	0.52
1:A:340:GLU:O	1:A:341:ASP:CB	2.59	0.51
1:B:82:MSE:HB3	1:B:86:ARG:HH12	1.74	0.51
1:C:73:TRP:CZ3	1:C:421:TYR:HB2	2.46	0.51
1:C:284:MSE:CG	1:C:391:HIS:CE1	2.93	0.51
1:D:70:SER:HB3	1:D:424:PHE:HB2	1.92	0.51
1:A:60:HIS:NE2	1:A:110:PRO:HB3	2.26	0.51
1:B:247:ALA:HB3	1:B:248:PRO:HA	1.91	0.51
1:B:82:MSE:HB3	1:B:86:ARG:NH1	2.26	0.51
1:D:93:VAL:HG12	1:D:100:ARG:CG	2.40	0.51
1:C:52:LEU:C	1:C:52:LEU:HD23	2.31	0.51
1:C:271:LYS:HD3	1:C:465:ASN:OD1	2.11	0.51
1:A:311:VAL:HG21	1:A:365:GLU:HB2	1.92	0.51
1:B:27:ILE:HD11	1:B:52:LEU:HD11	1.93	0.51
1:B:146:TRP:CG	1:B:147:PRO:HD3	2.45	0.51
1:C:245:PRO:HB3	2:C:501:EDO:H12	1.93	0.51
1:A:28:LYS:HE3	1:A:28:LYS:H	1.74	0.50
1:A:284:MSE:H	2:A:506:EDO:H21	1.76	0.50
1:B:52:LEU:C	1:B:52:LEU:HD23	2.31	0.50
1:D:229:THR:HA	1:D:364:HIS:ND1	2.26	0.50
1:A:138:LYS:HE2	1:A:142:ASP:OD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:THR:HG23	1:B:116:ALA:C	2.31	0.50
1:B:234:ARG:N	1:B:376:SER:HB3	2.27	0.50
1:B:203:LEU:N	4:B:607:HOH:O	2.41	0.50
1:A:27:ILE:HA	1:A:28:LYS:HD3	1.94	0.49
1:A:373:PHE:HA	1:A:377:THR:OG1	2.12	0.49
1:C:323:SER:HB2	4:C:638:HOH:O	2.12	0.49
1:C:93:VAL:CG1	1:C:100:ARG:HG2	2.42	0.49
1:D:329:LEU:HD21	2:D:510:EDO:H21	1.94	0.49
1:C:102:SER:HB2	1:C:154:GLY:O	2.13	0.49
1:D:427:PHE:HB2	2:D:504:EDO:H11	1.95	0.49
1:A:48:THR:HG23	1:A:117:ASN:HB2	1.95	0.49
1:D:138:LYS:HD3	1:D:424:PHE:CZ	2.47	0.49
1:C:132:ASP:OD1	1:C:133:PRO:HD2	2.13	0.49
1:C:331:PHE:CD2	2:C:504:EDO:H22	2.47	0.49
1:D:453:ARG:O	1:D:453:ARG:HD3	2.12	0.49
1:C:224:VAL:C	1:C:226:GLN:H	2.16	0.49
1:A:214:TYR:CE1	4:A:601:HOH:O	2.55	0.49
1:A:230:PHE:CZ	1:A:371:ASP:HB3	2.47	0.49
1:C:284:MSE:HG3	1:C:391:HIS:CE1	2.48	0.49
1:D:485:ILE:HG13	1:D:485:ILE:O	2.09	0.49
1:D:312:ASN:ND2	1:D:314:ARG:H	2.11	0.48
1:A:377:THR:HG22	4:A:615:HOH:O	2.13	0.48
1:A:275:PRO:HD3	1:A:443:ARG:HA	1.96	0.48
1:C:20:GLU:N	1:C:23:SER:H	2.10	0.48
1:A:289:LYS:HZ3	1:A:309:HIS:CD2	2.28	0.48
1:D:340:GLU:H	1:D:340:GLU:HG3	1.36	0.48
1:A:144:LYS:NZ	1:B:131:GLU:HG3	2.29	0.48
1:A:199:ASN:O	1:A:200:GLN:HB2	2.14	0.48
1:A:289:LYS:HZ1	1:A:309:HIS:HD2	1.55	0.48
1:C:287:LEU:HD22	1:C:471:ILE:HG23	1.96	0.48
1:C:80:LEU:HB3	4:C:667:HOH:O	2.13	0.48
1:C:312:ASN:ND2	1:C:314:ARG:H	2.11	0.48
1:A:289:LYS:HE2	1:A:309:HIS:HB2	1.96	0.48
1:B:54:PRO:HA	1:B:111:ILE:HG22	1.95	0.48
1:C:366[B]:HIS:CD2	4:C:609:HOH:O	2.55	0.47
1:D:141:TRP:HE1	2:D:503:EDO:C2	2.27	0.47
1:B:112:GLN:HE22	1:B:213:LEU:HD11	1.80	0.47
1:A:133:PRO:HB2	1:A:172:VAL:HG23	1.96	0.47
1:C:138:LYS:HD3	1:C:424:PHE:CE1	2.50	0.47
1:C:209:PHE:O	1:C:212:TYR:HB3	2.14	0.47
1:C:31:GLN:HE22	1:C:49:LEU:HB3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:THR:HB	1:D:59:GLN:OE1	2.14	0.47
1:D:84:ARG:HG2	1:D:198:TYR:CD1	2.50	0.47
1:D:89:CYS:O	1:D:93:VAL:HG23	2.15	0.47
1:A:348:MSE:HE2	1:A:478:PRO:HB3	1.96	0.47
1:A:264:GLY:HA3	1:A:453:ARG:NH1	2.30	0.47
3:B:512:C8E:H12	3:C:509:C8E:H31	1.96	0.46
1:D:56:THR:HG22	1:D:59:GLN:N	2.14	0.46
1:D:212:TYR:CE2	1:D:216:ARG:HD2	2.51	0.46
1:C:173:LEU:HD22	1:C:174:THR:N	2.31	0.46
1:C:402:LEU:HD12	1:C:402:LEU:HA	1.74	0.46
1:D:125:VAL:HB	1:D:163:VAL:HG13	1.98	0.46
1:A:82:MSE:O	1:A:86:ARG:HG3	2.15	0.46
1:A:229:THR:HA	1:A:364:HIS:ND1	2.30	0.46
1:D:232:PHE:CD1	1:D:232:PHE:C	2.86	0.46
1:D:346:THR:HA	1:D:481:ARG:HA	1.98	0.46
1:B:199:ASN:HB3	4:B:616:HOH:O	2.15	0.46
1:D:229:THR:HG23	1:D:364:HIS:HB3	1.97	0.46
3:A:508:C8E:H13	3:D:511:C8E:H12	1.98	0.46
1:B:185:VAL:HG12	4:B:722:HOH:O	2.15	0.46
3:B:512:C8E:H41	3:C:509:C8E:H22	1.97	0.46
1:D:425:ALA:H	2:D:503:EDO:H21	1.81	0.46
1:A:312:ASN:ND2	1:A:314:ARG:H	2.11	0.46
1:B:307:PHE:CB	2:B:508:EDO:H12	2.45	0.46
1:D:24:LEU:HD11	1:D:217:VAL:HG21	1.96	0.46
1:B:58:ALA:HB2	2:B:505:EDO:H11	1.98	0.45
1:C:223:ASP:HB3	1:C:226:GLN:OE1	2.17	0.45
1:C:225:GLN:CD	1:C:225:GLN:H	2.19	0.45
1:B:229:THR:HG21	1:B:367:VAL:HG11	1.98	0.45
1:D:56:THR:HG23	4:D:657:HOH:O	2.17	0.45
1:D:425:ALA:N	2:D:503:EDO:H21	2.32	0.45
1:A:477:ASP:OD2	1:A:480:ALA:HB2	2.17	0.45
1:D:318:MSE:HE3	1:D:321:ILE:HD13	1.98	0.45
1:B:193:ASP:O	1:B:197:ILE:HG13	2.16	0.45
1:B:347:VAL:O	1:B:351:LEU:HG	2.17	0.45
1:D:164:SER:OG	1:D:171:VAL:HG22	2.17	0.45
1:A:43:ILE:HB	1:A:44:PRO:HD2	1.99	0.45
1:C:79:SER:HG	1:C:415:SER:N	2.15	0.45
1:D:82:MSE:O	1:D:86:ARG:HG3	2.17	0.45
1:B:307:PHE:CA	2:B:508:EDO:H12	2.47	0.45
1:B:48:THR:HG23	1:B:116:ALA:HB3	1.98	0.44
1:B:91:SER:HB3	1:B:197:ILE:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:TRP:CZ2	1:D:159:ARG:HB3	2.52	0.44
1:C:287:LEU:HD23	1:C:287:LEU:O	2.17	0.44
1:A:374:GLN:HE21	1:A:374:GLN:HB2	1.56	0.44
1:C:379:TRP:CD1	1:C:379:TRP:N	2.85	0.44
1:D:267:LEU:HG	1:D:452:SER:HB3	2.00	0.44
1:A:124:GLU:O	1:B:125:VAL:HA	2.17	0.44
1:B:223:ASP:OD2	1:B:226:GLN:HG3	2.17	0.44
1:A:82:MSE:HE3	1:A:82:MSE:HB3	1.90	0.44
1:A:396:LEU:HD13	1:A:440:HIS:CE1	2.53	0.44
1:A:473:LYS:HZ1	1:A:485:ILE:HG13	1.82	0.44
1:B:125:VAL:HB	1:B:163:VAL:HG13	2.00	0.44
1:C:200:GLN:HE21	1:C:200:GLN:HB3	1.66	0.43
1:D:223:ASP:HB3	1:D:226:GLN:OE1	2.18	0.43
1:C:229:THR:HG21	1:C:367:VAL:CG1	2.46	0.43
1:D:234:ARG:N	1:D:376:SER:HB3	2.34	0.43
1:D:287:LEU:HD23	1:D:287:LEU:O	2.18	0.43
1:A:132:ASP:OD1	1:A:133:PRO:HD2	2.18	0.43
1:B:392:GLN:OE1	1:B:392:GLN:HA	2.17	0.43
1:C:158:VAL:HA	1:C:176:GLN:O	2.18	0.43
1:D:162:LEU:HD12	1:D:162:LEU:HA	1.84	0.43
1:A:344:ASP:HA	1:A:481:ARG:HD2	1.99	0.43
1:C:125:VAL:HB	1:C:163:VAL:HG13	2.00	0.43
1:D:428:ASP:HA	1:D:429:PRO:HD2	1.90	0.43
1:B:208:ASP:HB3	1:B:210:ALA:H	1.83	0.43
2:B:502:EDO:H12	3:B:512:C8E:O15	2.19	0.43
1:D:426:ARG:HA	2:D:507:EDO:H21	2.00	0.43
1:A:158:VAL:O	1:A:158:VAL:HG12	2.18	0.43
1:C:248:PRO:HB2	1:C:453:ARG:HD3	2.00	0.43
1:C:481:ARG:NH2	1:C:483:LEU:HD23	2.33	0.43
1:A:390:GLN:HE21	1:A:390:GLN:HB2	1.73	0.43
1:C:28:LYS:HB3	1:C:28:LYS:HE2	1.73	0.43
1:B:455:LEU:HD13	3:B:512:C8E:H42	2.00	0.43
1:C:21:PRO:O	1:C:22:PHE:HB2	2.18	0.43
1:C:294:LEU:HD22	1:C:474:PHE:CZ	2.54	0.43
1:D:173:LEU:HD22	1:D:174:THR:H	1.83	0.43
1:A:159:ARG:CZ	2:A:503:EDO:H21	2.48	0.43
1:A:356:THR:O	1:A:360:ARG:HG3	2.19	0.43
1:C:318:MSE:HG2	1:C:321:ILE:HB	2.00	0.43
1:A:318:MSE:HB3	1:A:321:ILE:HB	1.99	0.43
1:A:339:PRO:O	1:A:340:GLU:C	2.57	0.42
3:A:508:C8E:H31	3:D:511:C8E:H13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:HIS:O	1:C:107:GLU:HB2	2.18	0.42
1:C:296:LEU:HD11	1:C:387:LEU:HD23	2.01	0.42
1:D:190:LEU:HD23	1:D:190:LEU:C	2.39	0.42
1:A:341:ASP:C	1:A:343:THR:H	2.23	0.42
1:B:450:ALA:O	2:B:506:EDO:H22	2.18	0.42
1:D:93:VAL:HG21	1:D:120:VAL:HG21	2.01	0.42
1:D:210:ALA:O	1:D:213:LEU:N	2.51	0.42
1:B:348:MSE:HE1	1:B:478:PRO:HB2	2.00	0.42
1:C:31:GLN:NE2	1:C:49:LEU:HB3	2.34	0.42
1:C:137:CYS:SG	1:C:163:VAL:HG21	2.60	0.42
1:C:275:PRO:HA	1:C:276:PRO:HD3	1.82	0.42
1:D:321:ILE:HG23	1:D:322:GLU:N	2.33	0.42
1:A:485:ILE:HD12	1:A:485:ILE:HA	1.79	0.42
1:A:206:THR:HG23	2:A:505:EDO:H11	2.02	0.42
1:B:338:PHE:CE2	1:B:350:LEU:HD13	2.53	0.42
1:B:104:VAL:HG13	1:B:105:GLU:N	2.34	0.42
1:D:104:VAL:HG13	1:D:105:GLU:N	2.35	0.42
1:A:303:ARG:HB2	1:A:338:PHE:HB2	2.02	0.42
1:C:241:LYS:NZ	4:C:606:HOH:O	2.44	0.42
2:C:501:EDO:C1	3:C:509:C8E:H171	2.48	0.42
1:D:58:ALA:O	1:D:61:VAL:HB	2.20	0.42
1:D:118:LEU:HD12	1:D:118:LEU:HA	1.87	0.42
1:D:319:ASP:O	1:D:320:ASN:HB2	2.20	0.42
1:A:151:VAL:HB	2:A:504:EDO:H22	2.01	0.42
1:A:264:GLY:CA	1:A:453:ARG:HD2	2.50	0.42
1:B:436:PHE:HB2	1:B:447:GLN:HB2	2.02	0.42
1:C:95:ARG:NH1	1:C:203:LEU:HD13	2.35	0.42
1:C:107:GLU:HG3	4:C:645:HOH:O	2.19	0.42
1:D:132:ASP:OD2	1:D:135:GLU:HG3	2.20	0.42
1:A:95:ARG:HD3	1:A:193:ASP:OD2	2.20	0.41
1:D:173:LEU:HD22	1:D:174:THR:N	2.35	0.41
1:D:234:ARG:HE	1:D:376:SER:HA	1.84	0.41
1:A:144:LYS:HZ1	1:B:131:GLU:HG3	1.85	0.41
1:B:91:SER:O	1:B:94:ASP:HB2	2.20	0.41
1:D:230:PHE:CZ	1:D:371:ASP:HB3	2.55	0.41
1:A:159:ARG:NH2	2:A:503:EDO:H21	2.36	0.41
1:A:473:LYS:N	1:A:473:LYS:HD3	2.36	0.41
1:B:245:PRO:HG3	3:B:512:C8E:H82	2.02	0.41
1:C:284:MSE:HG2	1:C:391:HIS:CE1	2.55	0.41
1:D:275:PRO:HA	1:D:276:PRO:HD3	1.87	0.41
1:D:400:LEU:HB3	1:D:419:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:HIS:CD2	1:D:244:VAL:O	2.72	0.41
1:B:244:VAL:O	1:C:299:HIS:CD2	2.70	0.41
1:B:437:THR:HG22	1:B:446:VAL:HG22	2.02	0.41
1:C:417:LEU:HA	1:C:417:LEU:HD12	1.82	0.41
1:B:267:LEU:HB3	2:B:506:EDO:H11	1.96	0.41
1:C:402:LEU:O	1:C:403:ARG:HB3	2.20	0.41
1:B:31:GLN:HE21	1:B:31:GLN:HB3	1.72	0.41
1:B:146:TRP:CD2	1:B:147:PRO:HD3	2.56	0.41
1:C:187:ILE:N	1:C:188:PRO:CD	2.83	0.41
1:B:60:HIS:CE1	1:B:110:PRO:HG3	2.55	0.41
1:B:109:HIS:ND1	1:B:109:HIS:N	2.68	0.41
1:C:156:LEU:O	4:C:601:HOH:O	2.22	0.41
1:C:161:THR:HB	1:C:174:THR:OG1	2.21	0.41
1:D:39:SER:HA	4:D:642:HOH:O	2.20	0.41
1:D:91:SER:HB2	1:D:197:ILE:HG21	2.02	0.41
1:D:100:ARG:HD2	1:D:115:LEU:O	2.20	0.41
1:A:101:THR:CG2	1:A:112:GLN:HB2	2.51	0.41
1:B:190:LEU:C	1:B:190:LEU:HD23	2.41	0.41
1:C:229:THR:HA	1:C:364:HIS:ND1	2.36	0.41
1:D:85:LEU:HD23	1:D:85:LEU:HA	1.95	0.41
1:B:133:PRO:HB2	1:B:172:VAL:HG23	2.03	0.40
1:C:287:LEU:CD2	1:C:471:ILE:HG23	2.50	0.40
1:A:359:THR:HA	1:A:362:LEU:HG	2.03	0.40
1:C:93:VAL:HG21	1:C:120:VAL:HG21	2.03	0.40
1:C:104:VAL:O	1:C:110:PRO:HA	2.21	0.40
1:C:463:LEU:O	1:C:467:ILE:HG12	2.21	0.40
1:A:348:MSE:HE2	1:A:348:MSE:HB2	2.00	0.40
1:B:31:GLN:H	1:B:31:GLN:HG2	1.64	0.40
1:C:27:ILE:HD11	1:C:52:LEU:HD11	2.03	0.40
1:C:79:SER:HB2	1:C:405:SER:N	2.37	0.40
1:D:141:TRP:CE2	1:D:424:PHE:HB3	2.56	0.40
1:A:265:GLN:O	1:A:265:GLN:HG2	2.21	0.40
1:A:444:LEU:HD23	1:A:444:LEU:HA	1.75	0.40
1:B:56:THR:CB	2:B:505:EDO:H22	2.49	0.40
1:C:224:VAL:HG11	1:C:375:HIS:CG	2.56	0.40
1:D:245:PRO:HB3	3:D:511:C8E:H62	2.03	0.40
3:A:508:C8E:C1	3:D:511:C8E:H32	2.52	0.40
3:B:512:C8E:H71	3:B:512:C8E:H41	1.97	0.40
1:D:106:HIS:CE1	1:D:107:GLU:HG3	2.57	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	437/486 (90%)	410 (94%)	24 (6%)	3 (1%)	22	26
1	B	438/486 (90%)	413 (94%)	21 (5%)	4 (1%)	17	20
1	C	440/486 (90%)	415 (94%)	22 (5%)	3 (1%)	22	26
1	D	437/486 (90%)	412 (94%)	22 (5%)	3 (1%)	22	26
All	All	1752/1944 (90%)	1650 (94%)	89 (5%)	13 (1%)	22	26

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	341	ASP
1	B	247	ALA
1	B	249	ARG
1	D	247	ALA
1	B	485	ILE
1	C	108	GLY
1	C	144	LYS
1	C	200	GLN
1	A	279	PRO
1	D	484	ASP
1	A	430	LEU
1	B	248	PRO
1	D	317	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	397/424 (94%)	357 (90%)	40 (10%)	7	9
1	B	398/424 (94%)	366 (92%)	32 (8%)	12	15
1	C	400/424 (94%)	357 (89%)	43 (11%)	6	7
1	D	397/424 (94%)	360 (91%)	37 (9%)	9	10
All	All	1592/1696 (94%)	1440 (90%)	152 (10%)	8	10

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	28	LYS
1	A	53	LEU
1	A	60	HIS
1	A	79	SER
1	A	83	ASP
1	A	95	ARG
1	A	102	SER
1	A	104	VAL
1	A	105	GLU
1	A	115	LEU
1	A	117	ASN
1	A	162	LEU
1	A	170	HIS
1	A	173	LEU
1	A	185	VAL
1	A	216	ARG
1	A	219	SER
1	A	225	GLN
1	A	238	ASP
1	A	265	GLN
1	A	274	VAL
1	A	286	THR
1	A	287	LEU
1	A	302	SER
1	A	312	ASN
1	A	318	MSE
1	A	342	SER
1	A	343	THR
1	A	344	ASP
1	A	374	GLN
1	A	377	THR
1	A	399	SER

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Mol	Chain	Res	Type
1	A	430	LEU
1	A	437	THR
1	A	442	ASP
1	A	444	LEU
1	A	473	LYS
1	A	483	LEU
1	A	485	ILE
1	B	31	GLN
1	B	45	VAL
1	B	48	THR
1	B	78	ARG
1	B	79	SER
1	B	100	ARG
1	B	102	SER
1	B	104	VAL
1	B	106	HIS
1	B	107	GLU
1	B	109	HIS
1	B	115	LEU
1	B	117	ASN
1	B	118	LEU
1	B	121	LYS
1	B	164	SER
1	B	170	HIS
1	B	173	LEU
1	B	185	VAL
1	B	218	SER
1	B	221	ARG
1	B	241	LYS
1	B	249	ARG
1	B	287	LEU
1	B	309	HIS
1	B	397	SER
1	B	415	SER
1	B	418	ASP
1	B	430	LEU
1	B	473	LYS
1	B	482	LEU
1	B	485	ILE
1	C	20	GLU
1	C	27	ILE
1	C	31	GLN

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Mol	Chain	Res	Type
1	C	45	VAL
1	C	79	SER
1	C	83	ASP
1	C	84	ARG
1	C	85	LEU
1	C	95	ARG
1	C	102	SER
1	C	104	VAL
1	C	109	HIS
1	C	115	LEU
1	C	155	SER
1	C	164	SER
1	C	173	LEU
1	C	185	VAL
1	C	189	LYS
1	C	200	GLN
1	C	201	THR
1	C	225	GLN
1	C	265	GLN
1	C	280	SER
1	C	309	HIS
1	C	312	ASN
1	C	323	SER
1	C	324	LEU
1	C	345	TRP
1	C	374	GLN
1	C	402	LEU
1	C	403	ARG
1	C	415	SER
1	C	417	LEU
1	C	418	ASP
1	C	423	LYS
1	C	430	LEU
1	C	443	ARG
1	C	444	LEU
1	C	453	ARG
1	C	468	SER
1	C	482	LEU
1	C	483	LEU
1	C	487	PHE
1	D	19	TRP
1	D	28	LYS

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Mol	Chain	Res	Type
1	D	50	GLU
1	D	56	THR
1	D	60	HIS
1	D	67	THR
1	D	79	SER
1	D	102	SER
1	D	104	VAL
1	D	105	GLU
1	D	115	LEU
1	D	117	ASN
1	D	159	ARG
1	D	173	LEU
1	D	174	THR
1	D	185	VAL
1	D	207	SER
1	D	219	SER
1	D	221	ARG
1	D	271	LYS
1	D	302	SER
1	D	309	HIS
1	D	312	ASN
1	D	340	GLU
1	D	342	SER
1	D	374	GLN
1	D	399	SER
1	D	416	SER
1	D	423	LYS
1	D	430	LEU
1	D	437	THR
1	D	444	LEU
1	D	453	ARG
1	D	458	GLU
1	D	483	LEU
1	D	485	ILE
1	D	486	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	ASN
1	A	299	HIS
1	A	309	HIS

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Mol	Chain	Res	Type
1	A	312	ASN
1	A	352	HIS
1	A	374	GLN
1	A	375	HIS
1	A	390	GLN
1	B	31	GLN
1	B	106	HIS
1	B	374	GLN
1	B	390	GLN
1	C	31	GLN
1	C	168	ASN
1	C	170	HIS
1	C	299	HIS
1	C	312	ASN
1	C	390	GLN
1	C	447	GLN
1	D	31	GLN
1	D	106	HIS
1	D	299	HIS
1	D	312	ASN
1	D	390	GLN
1	D	447	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

39 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	EDO	A	506	-	3,3,3	0.48	0	2,2,2	0.33	0
2	EDO	D	509	-	3,3,3	0.50	0	2,2,2	0.29	0
2	EDO	D	501	-	3,3,3	0.50	0	2,2,2	0.32	0
2	EDO	D	502	-	3,3,3	0.50	0	2,2,2	0.27	0
3	C8E	A	508	-	20,20,20	0.43	0	19,19,19	0.39	0
2	EDO	B	505	-	3,3,3	0.48	0	2,2,2	0.33	0
2	EDO	B	507	-	3,3,3	0.54	0	2,2,2	0.19	0
3	C8E	C	509	-	20,20,20	0.40	0	19,19,19	0.76	0
2	EDO	D	506	-	3,3,3	0.48	0	2,2,2	0.26	0
2	EDO	A	505	-	3,3,3	0.63	0	2,2,2	0.15	0
2	EDO	B	508	-	3,3,3	0.69	0	2,2,2	0.10	0
2	EDO	D	504	-	3,3,3	0.55	0	2,2,2	0.14	0
2	EDO	B	502	-	3,3,3	0.41	0	2,2,2	0.34	0
2	EDO	A	507	-	3,3,3	0.50	0	2,2,2	0.27	0
2	EDO	C	507	-	3,3,3	0.53	0	2,2,2	0.20	0
2	EDO	A	502	-	3,3,3	0.54	0	2,2,2	0.18	0
2	EDO	A	501	-	3,3,3	0.56	0	2,2,2	0.21	0
2	EDO	B	509	-	3,3,3	0.54	0	2,2,2	0.25	0
3	C8E	D	511	-	20,20,20	0.46	0	19,19,19	0.41	0
2	EDO	C	504	-	3,3,3	0.63	0	2,2,2	0.20	0
2	EDO	B	511	-	3,3,3	0.51	0	2,2,2	0.37	0
2	EDO	B	501	-	3,3,3	0.54	0	2,2,2	0.28	0
2	EDO	D	510	-	3,3,3	0.54	0	2,2,2	0.57	0
2	EDO	C	505	-	3,3,3	0.48	0	2,2,2	0.34	0
2	EDO	B	506	-	3,3,3	0.38	0	2,2,2	0.34	0
2	EDO	D	503	-	3,3,3	0.57	0	2,2,2	0.14	0
2	EDO	C	508	-	3,3,3	0.50	0	2,2,2	0.32	0
2	EDO	D	507	-	3,3,3	0.51	0	2,2,2	0.16	0
2	EDO	A	504	-	3,3,3	0.46	0	2,2,2	0.40	0
2	EDO	C	502	-	3,3,3	0.50	0	2,2,2	0.24	0
2	EDO	B	504	-	3,3,3	0.72	0	2,2,2	0.16	0
2	EDO	D	508	-	3,3,3	0.52	0	2,2,2	0.33	0
2	EDO	C	501	-	3,3,3	0.47	0	2,2,2	0.26	0
2	EDO	D	505	-	3,3,3	0.53	0	2,2,2	0.22	0
2	EDO	C	503	-	3,3,3	0.49	0	2,2,2	0.22	0
2	EDO	A	503	-	3,3,3	0.57	0	2,2,2	0.11	0
2	EDO	B	503	-	3,3,3	0.64	0	2,2,2	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	C8E	B	512	-	20,20,20	0.34	0	19,19,19	0.64	0
2	EDO	C	506	-	3,3,3	0.46	0	2,2,2	0.26	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
2	EDO	A	506	-	-	0/1/1/1	-
2	EDO	D	509	-	-	1/1/1/1	-
2	EDO	D	501	-	-	1/1/1/1	-
2	EDO	D	502	-	-	1/1/1/1	-
3	C8E	A	508	-	-	9/18/18/18	-
2	EDO	B	505	-	-	1/1/1/1	-
2	EDO	B	507	-	-	1/1/1/1	-
3	C8E	C	509	-	-	12/18/18/18	-
2	EDO	D	506	-	-	1/1/1/1	-
2	EDO	A	505	-	-	1/1/1/1	-
2	EDO	B	508	-	-	1/1/1/1	-
2	EDO	D	504	-	-	1/1/1/1	-
2	EDO	B	502	-	-	0/1/1/1	-
2	EDO	A	507	-	-	1/1/1/1	-
2	EDO	C	507	-	-	0/1/1/1	-
2	EDO	A	502	-	-	0/1/1/1	-
2	EDO	A	501	-	-	0/1/1/1	-
2	EDO	B	509	-	-	1/1/1/1	-
3	C8E	D	511	-	-	13/18/18/18	-
2	EDO	C	504	-	-	1/1/1/1	-
2	EDO	B	511	-	-	1/1/1/1	-
2	EDO	B	501	-	-	0/1/1/1	-
2	EDO	D	510	-	-	1/1/1/1	-
2	EDO	C	505	-	-	0/1/1/1	-
2	EDO	B	506	-	-	0/1/1/1	-
2	EDO	D	503	-	-	0/1/1/1	-
2	EDO	C	508	-	-	1/1/1/1	-
2	EDO	D	507	-	-	0/1/1/1	-
2	EDO	A	504	-	-	0/1/1/1	-
2	EDO	C	502	-	-	0/1/1/1	-
2	EDO	B	504	-	-	0/1/1/1	-
2	EDO	D	508	-	-	0/1/1/1	-
2	EDO	C	501	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	D	505	-	-	1/1/1/1	-
2	EDO	C	503	-	-	0/1/1/1	-
2	EDO	A	503	-	-	1/1/1/1	-
2	EDO	B	503	-	-	0/1/1/1	-
3	C8E	B	512	-	-	10/18/18/18	-
2	EDO	C	506	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	509	C8E	O9-C10-C11-O12
3	A	508	C8E	C6-C7-C8-O9
3	D	511	C8E	O12-C13-C14-O15
3	D	511	C8E	C6-C7-C8-O9
3	C	509	C8E	O18-C19-C20-O21
3	D	511	C8E	O18-C19-C20-O21
3	C	509	C8E	O15-C16-C17-O18
3	A	508	C8E	O9-C10-C11-O12
3	C	509	C8E	C6-C7-C8-O9
3	A	508	C8E	O18-C19-C20-O21
3	A	508	C8E	C3-C4-C5-C6
3	B	512	C8E	O9-C10-C11-O12
3	C	509	C8E	C2-C3-C4-C5
3	D	511	C8E	C3-C4-C5-C6
3	A	508	C8E	C5-C6-C7-C8
2	B	508	EDO	O1-C1-C2-O2
2	C	508	EDO	O1-C1-C2-O2
2	D	501	EDO	O1-C1-C2-O2
2	D	502	EDO	O1-C1-C2-O2
2	D	504	EDO	O1-C1-C2-O2
3	D	511	C8E	O15-C16-C17-O18
3	D	511	C8E	C16-C17-O18-C19
3	A	508	C8E	C2-C3-C4-C5
3	B	512	C8E	C6-C7-C8-O9
3	C	509	C8E	C1-C2-C3-C4
2	D	505	EDO	O1-C1-C2-O2
3	B	512	C8E	C16-C17-O18-C19
3	B	512	C8E	O12-C13-C14-O15

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Mol	Chain	Res	Type	Atoms
3	D	511	C8E	C1-C2-C3-C4
2	A	505	EDO	O1-C1-C2-O2
2	A	507	EDO	O1-C1-C2-O2
2	B	507	EDO	O1-C1-C2-O2
2	D	506	EDO	O1-C1-C2-O2
3	D	511	C8E	O9-C10-C11-O12
3	C	509	C8E	C11-C10-O9-C8
3	B	512	C8E	C17-C16-O15-C14
3	C	509	C8E	C20-C19-O18-C17
3	B	512	C8E	C20-C19-O18-C17
2	A	503	EDO	O1-C1-C2-O2
2	D	509	EDO	O1-C1-C2-O2
3	D	511	C8E	C7-C8-O9-C10
3	D	511	C8E	C14-C13-O12-C11
3	D	511	C8E	C10-C11-O12-C13
3	C	509	C8E	C7-C8-O9-C10
3	C	509	C8E	C13-C14-O15-C16
3	D	511	C8E	C20-C19-O18-C17
3	B	512	C8E	C7-C8-O9-C10
3	B	512	C8E	C10-C11-O12-C13
3	C	509	C8E	C10-C11-O12-C13
2	B	511	EDO	O1-C1-C2-O2
3	A	508	C8E	O12-C13-C14-O15
3	A	508	C8E	C14-C13-O12-C11
3	D	511	C8E	C13-C14-O15-C16
2	B	505	EDO	O1-C1-C2-O2
2	B	509	EDO	O1-C1-C2-O2
2	C	504	EDO	O1-C1-C2-O2
2	C	506	EDO	O1-C1-C2-O2
2	D	510	EDO	O1-C1-C2-O2
3	A	508	C8E	O15-C16-C17-O18
3	B	512	C8E	O15-C16-C17-O18
3	B	512	C8E	O18-C19-C20-O21
3	C	509	C8E	C5-C6-C7-C8

There are no ring outliers.

25 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	506	EDO	1	0
2	D	502	EDO	1	0
3	A	508	C8E	9	0

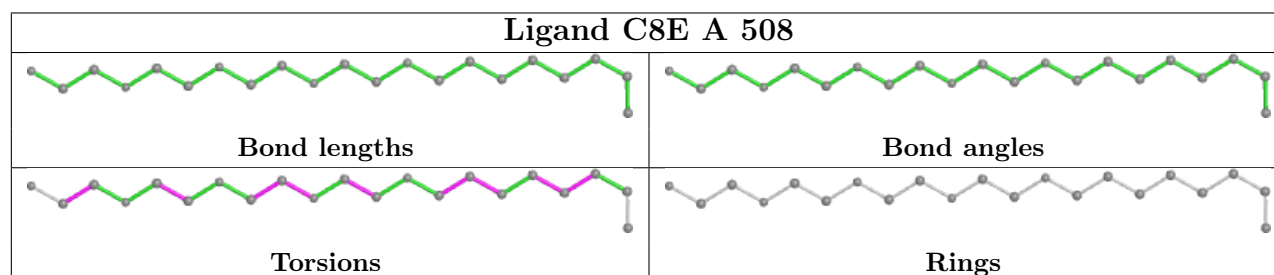
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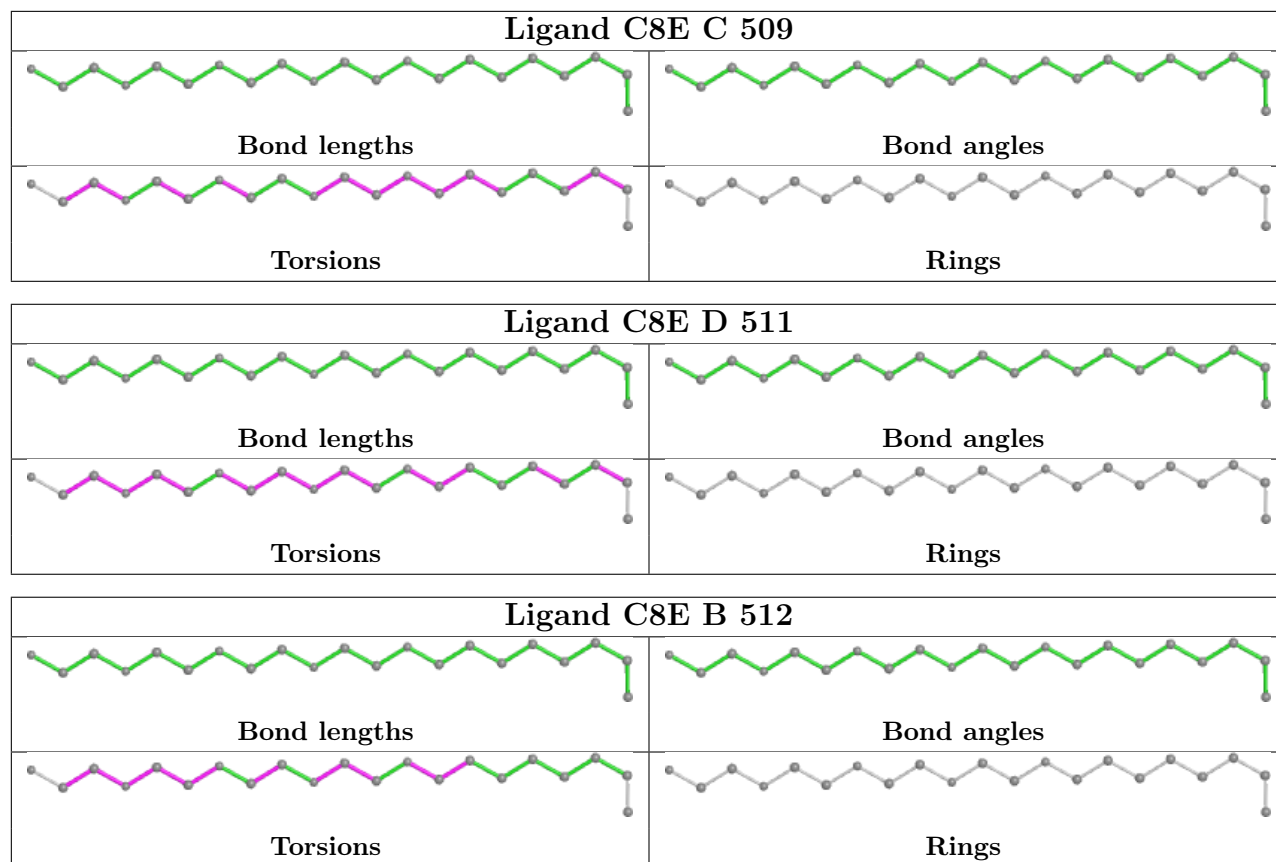


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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	505	EDO	3	0
3	C	509	C8E	12	0
2	D	506	EDO	1	0
2	A	505	EDO	1	0
2	B	508	EDO	4	0
2	D	504	EDO	1	0
2	B	502	EDO	6	0
3	D	511	C8E	9	0
2	C	504	EDO	4	0
2	D	510	EDO	1	0
2	C	505	EDO	1	0
2	B	506	EDO	6	0
2	D	503	EDO	3	0
2	D	507	EDO	1	0
2	A	504	EDO	4	0
2	C	502	EDO	1	0
2	B	504	EDO	1	0
2	D	508	EDO	1	0
2	C	501	EDO	9	0
2	A	503	EDO	3	0
3	B	512	C8E	16	0
2	C	506	EDO	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 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 ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	436/486 (89%)	0.12	15 (3%) 45 52	31, 53, 85, 153	0
1	B	437/486 (89%)	0.06	17 (3%) 39 46	25, 44, 79, 139	0
1	C	438/486 (90%)	0.15	18 (4%) 37 44	27, 50, 92, 144	0
1	D	436/486 (89%)	0.17	19 (4%) 34 41	34, 56, 91, 133	0
All	All	1747/1944 (89%)	0.12	69 (3%) 39 46	25, 51, 88, 153	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	342	SER	5.0
1	C	485	ILE	4.5
1	D	486	THR	3.8
1	D	485	ILE	3.8
1	C	28	LYS	3.7
1	B	485	ILE	3.7
1	D	342	SER	3.6
1	D	343	THR	3.5
1	B	248	PRO	3.4
1	C	158	VAL	3.3
1	B	416	SER	3.2
1	D	321	ILE	3.1
1	A	341	ASP	3.1
1	A	344	ASP	3.1
1	D	28	LYS	3.0
1	D	248	PRO	3.0
1	D	291	ALA	2.9
1	D	316	LEU	2.9
1	B	415	SER	2.8
1	A	378	ASN	2.8
1	A	343	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	19	TRP	2.7
1	C	27	ILE	2.7
1	C	177	ILE	2.7
1	C	416	SER	2.6
1	A	403	ARG	2.6
1	C	180	SER	2.6
1	A	226	GLN	2.6
1	A	117	ASN	2.6
1	D	78	ARG	2.6
1	B	486	THR	2.5
1	C	223	ASP	2.5
1	C	405	SER	2.5
1	D	292	THR	2.5
1	A	280	SER	2.5
1	B	28	LYS	2.5
1	B	101	THR	2.4
1	D	441	ALA	2.3
1	C	389	VAL	2.3
1	C	487	PHE	2.3
1	A	222	GLU	2.3
1	D	181	GLN	2.3
1	B	27	ILE	2.3
1	A	340	GLU	2.2
1	C	224	VAL	2.2
1	B	175	ILE	2.2
1	C	119	ASP	2.2
1	D	158	VAL	2.2
1	B	226	GLN	2.2
1	B	211	HIS	2.2
1	A	45	VAL	2.1
1	A	177	ILE	2.1
1	C	248	PRO	2.1
1	C	211	HIS	2.1
1	B	158	VAL	2.1
1	D	45	VAL	2.1
1	B	249	ARG	2.1
1	B	250	ALA	2.1
1	B	98	ILE	2.1
1	C	175	ILE	2.1
1	C	205	PRO	2.1
1	D	378	ASN	2.1
1	B	182	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	226	GLN	2.0
1	A	296	LEU	2.0
1	A	293	ALA	2.0
1	B	106	HIS	2.0
1	D	221	ARG	2.0
1	D	296	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	EDO	D	505	4/4	0.56	0.40	91,91,91,91	0
2	EDO	D	504	4/4	0.62	0.30	68,68,68,68	0
2	EDO	D	509	4/4	0.64	0.25	85,85,85,85	0
2	EDO	C	508	4/4	0.66	0.45	82,82,82,82	0
2	EDO	D	506	4/4	0.68	0.38	83,83,83,83	0
2	EDO	A	503	4/4	0.70	0.34	65,65,65,65	0
2	EDO	B	503	4/4	0.72	0.33	56,56,56,56	0
2	EDO	A	505	4/4	0.72	0.23	64,64,64,64	0
2	EDO	A	504	4/4	0.77	0.34	54,54,54,54	0
2	EDO	A	502	4/4	0.77	0.22	74,74,74,74	0
2	EDO	B	507	4/4	0.78	0.31	67,67,67,67	0
2	EDO	B	508	4/4	0.81	0.38	58,58,58,58	0
2	EDO	B	509	4/4	0.82	0.22	62,62,62,62	0
2	EDO	D	501	4/4	0.82	0.19	78,78,78,78	0
2	EDO	A	506	4/4	0.83	0.27	72,72,72,72	0
2	EDO	A	507	4/4	0.83	0.21	84,84,84,84	0
2	EDO	D	510	4/4	0.84	0.22	57,57,57,57	0

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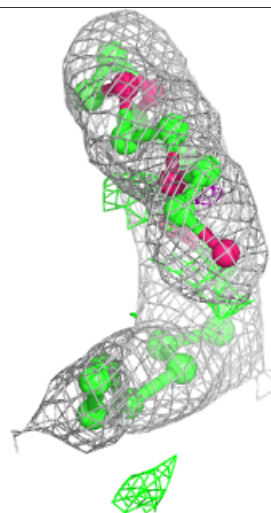
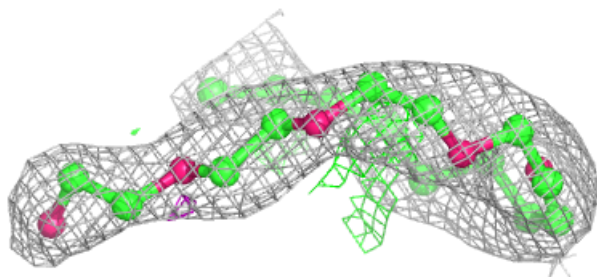
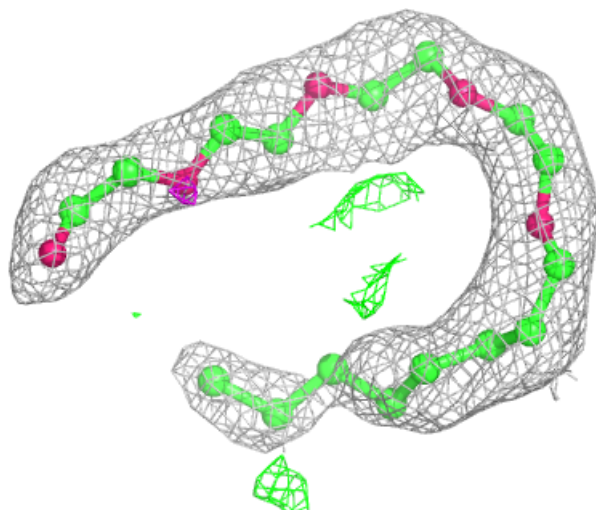
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EDO	D	502	4/4	0.85	0.30	71,71,71,71	0
2	EDO	C	504	4/4	0.85	0.26	51,51,51,51	0
2	EDO	C	506	4/4	0.86	0.45	63,63,63,63	0
3	C8E	A	508	21/21	0.86	0.27	66,66,66,66	0
2	EDO	C	505	4/4	0.87	0.22	60,60,60,60	0
2	EDO	B	501	4/4	0.88	0.24	62,62,62,62	0
2	EDO	B	511	4/4	0.89	0.23	71,71,71,71	0
2	EDO	C	501	4/4	0.92	0.24	53,53,53,53	0
3	C8E	D	511	21/21	0.93	0.20	65,65,65,65	0
2	EDO	D	507	4/4	0.94	0.11	44,44,44,44	0
2	EDO	D	508	4/4	0.94	0.16	67,67,67,67	0
2	EDO	D	503	4/4	0.94	0.14	49,49,49,49	0
2	EDO	B	506	4/4	0.94	0.26	42,42,42,42	0
2	EDO	B	502	4/4	0.94	0.20	48,48,48,48	0
3	C8E	B	512	21/21	0.94	0.22	42,42,42,42	0
2	EDO	C	502	4/4	0.94	0.24	59,59,59,59	0
3	C8E	C	509	21/21	0.95	0.17	42,42,42,42	0
2	EDO	B	504	4/4	0.95	0.09	38,38,38,38	0
2	EDO	C	503	4/4	0.96	0.15	57,57,57,57	0
2	EDO	B	505	4/4	0.96	0.26	45,45,45,45	0
2	EDO	C	507	4/4	0.96	0.11	38,38,38,38	0
2	EDO	A	501	4/4	0.97	0.08	45,45,45,45	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.

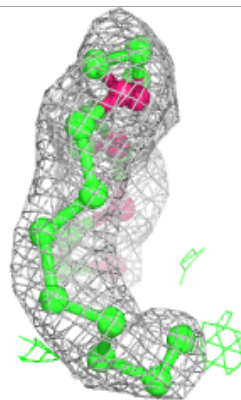
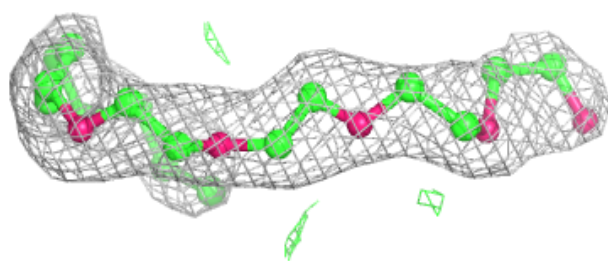
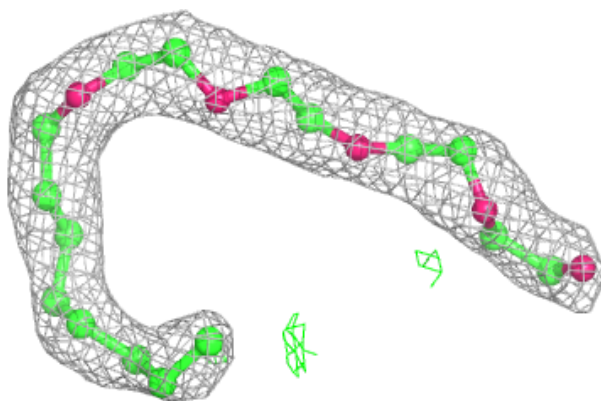
**Electron density around C8E A 508:**

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

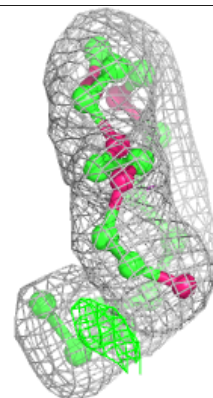
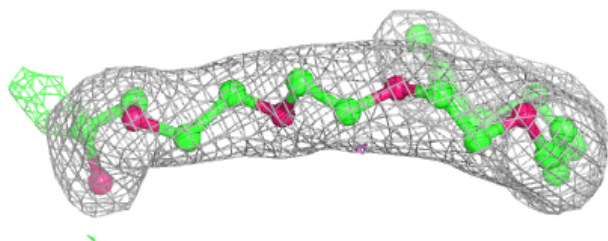
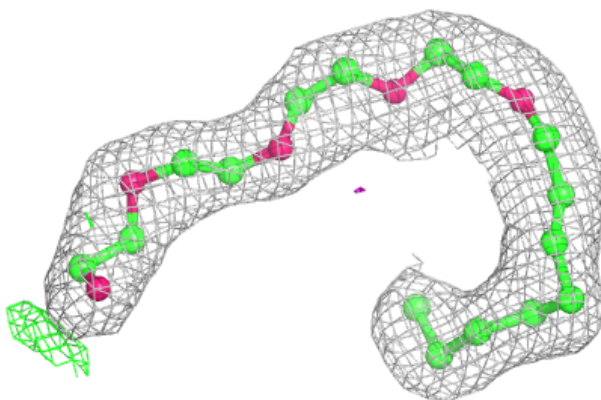


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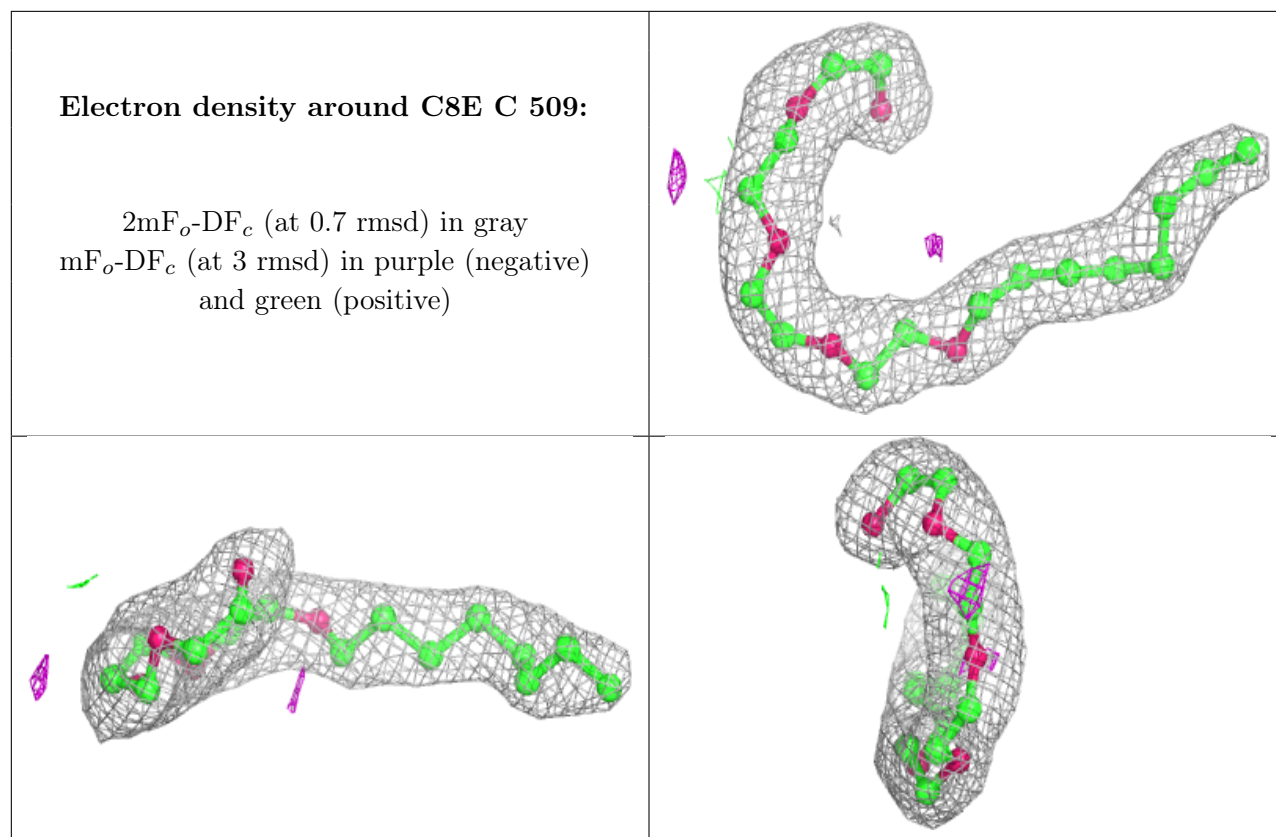
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around C8E B 512:**

$2mF_o-DF_c$  (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.