



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:33 PM UTC

PDB ID : 5EGF / pdb_00005egf
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

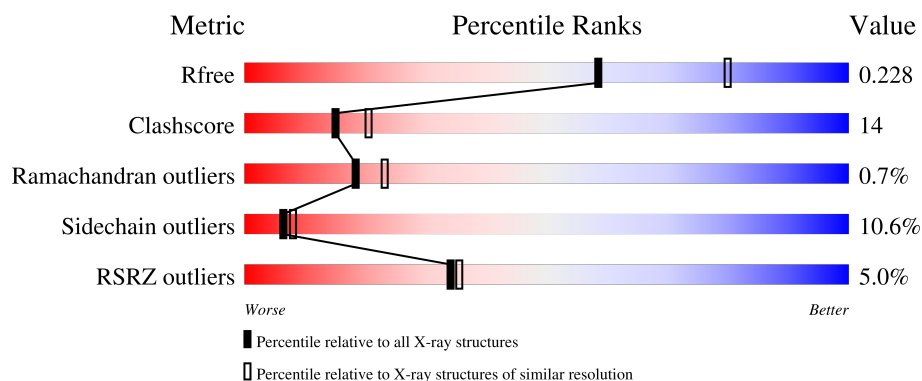
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 ≥ 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	5% 63% 24% • 9%
1	B	486	3% 66% 22% • 9%
1	C	486	6% 62% 26% • 9%
1	D	486	5% 61% 26% • 9%

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	-
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:

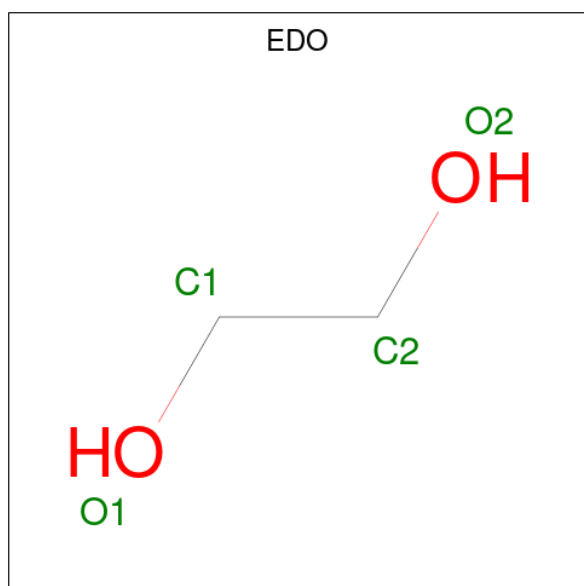
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	HIS	-	expression tag	UNP F1CWE4
A	3	HIS	-	expression tag	UNP F1CWE4
A	4	HIS	-	expression tag	UNP F1CWE4
A	5	HIS	-	expression tag	UNP F1CWE4
A	6	HIS	-	expression tag	UNP F1CWE4
A	7	HIS	-	expression tag	UNP F1CWE4
A	35	ALA	LYS	engineered mutation	UNP 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 (CCD ID: EDO) (formula: C₂H₆O₂).



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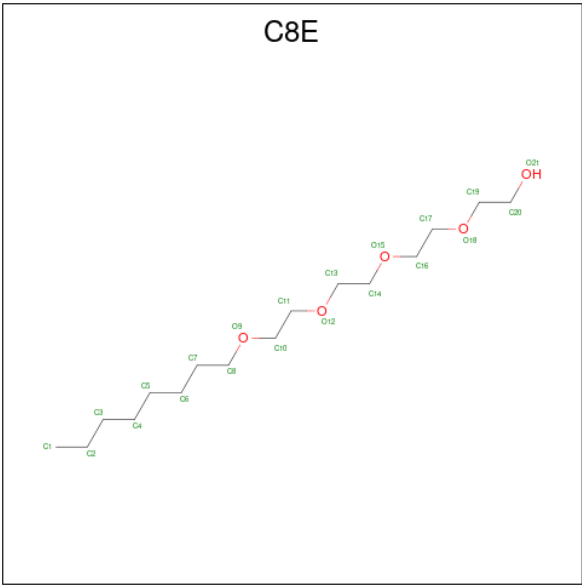
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0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

- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (CCD ID: C8E) (formula: C₁₆H₃₄O₅).



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

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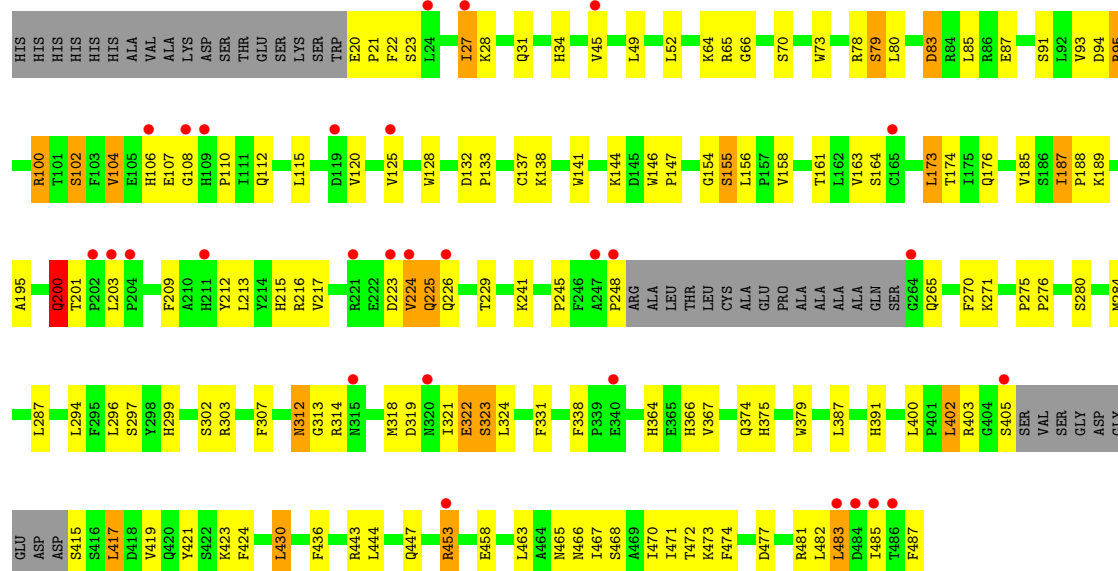
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			21	16	5		

- Molecule 4 is water.

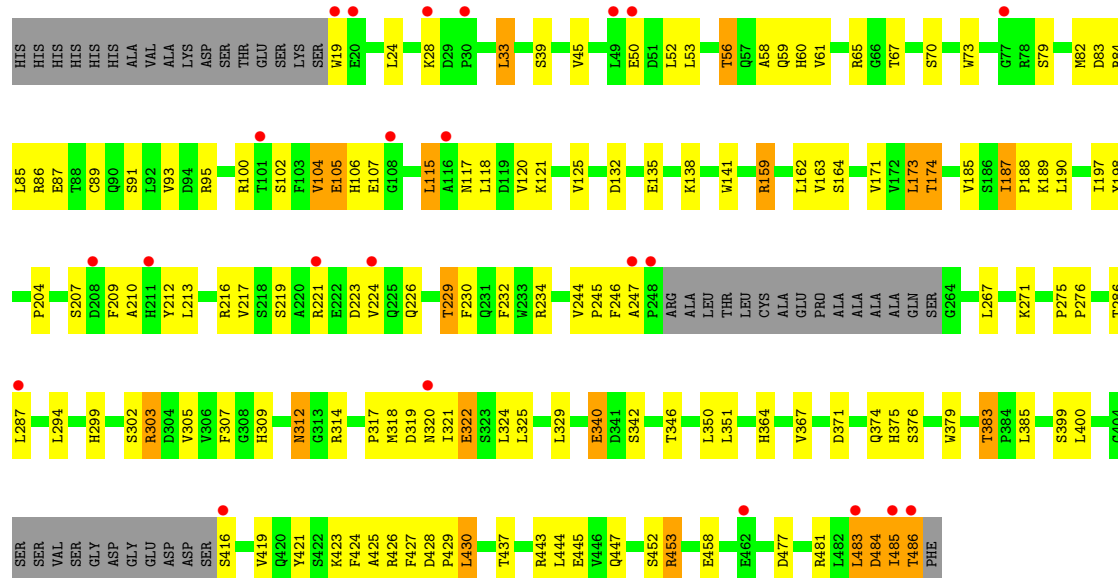
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	115	Total	O	0	0
			115	115		
4	B	179	Total	O	0	0
			179	179		
4	C	134	Total	O	0	0
			134	134		
4	D	98	Total	O	0	0
			98	98		



- 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, α , β , γ	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) 85.0 (29.75-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.94 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.7_650	Depositor
R, R_{free}	0.225 , 0.266 0.227 , 0.228	Depositor DCC
R_{free} test set	1880 reflections (1.55%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14879	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.54	0/3626	0.90	2/4946 (0.0%)
1	B	0.61	1/3623 (0.0%)	0.94	8/4941 (0.2%)
1	C	0.54	1/3645 (0.0%)	0.89	2/4970 (0.0%)
1	D	0.51	0/3626	0.89	6/4946 (0.1%)
All	All	0.56	2/14520 (0.0%)	0.91	18/19803 (0.1%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	187	ILE	CA-CB	5.30	1.57	1.53
1	C	187	ILE	CA-CB	5.13	1.57	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	485	ILE	N-CA-C	9.61	120.08	111.81
1	D	477	ASP	CA-C-N	6.99	126.69	119.56
1	D	477	ASP	C-N-CA	6.99	126.69	119.56
1	B	247	ALA	N-CA-C	6.75	124.74	109.81
1	B	109	HIS	CA-C-N	6.47	126.23	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	HIS	C-N-CA	6.47	126.23	119.76
1	D	33	LEU	N-CA-C	-6.03	104.79	111.36
1	B	187	ILE	N-CA-CB	6.00	114.28	110.50
1	D	303	ARG	N-CA-C	-5.98	105.95	113.72
1	B	275	PRO	CA-C-N	5.82	126.11	119.83
1	B	275	PRO	C-N-CA	5.82	126.11	119.83
1	D	305	VAL	N-CA-C	5.66	116.09	108.17
1	A	282	ILE	N-CA-C	5.32	115.43	107.51
1	C	477	ASP	CA-C-N	5.25	125.33	119.87
1	C	477	ASP	C-N-CA	5.25	125.33	119.87
1	D	187	ILE	N-CA-CB	5.10	113.72	110.50
1	B	485	ILE	N-CA-C	5.06	119.86	109.34
1	B	209	PHE	N-CA-C	-5.03	105.98	111.82

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 [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	3529	0	3454	93	0
1	B	3527	0	3452	80	0
1	C	3544	0	3466	104	0
1	D	3529	0	3454	100	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	392	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 14.

All (392) 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
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: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:D:223:ASP:HB3	1:D:226:GLN:CD	2.13	0.72
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:312:ASN:HD22	1:C:312:ASN:C	2.00	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: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
1:C:20:GLU:N	1:C:23:SER:HG	1.92	0.67
2:C:501:EDO:H21	3:C:509:C8E:C8	2.20	0.67
1:D:322:GLU:CD	1:D:322:GLU:H	2.03	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:A:289:LYS:HZ1	1:A:309:HIS:HD2	1.42	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:D:379:TRP:H	1:D:379:TRP:CD1	2.12	0.66
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: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:B:79:SER:HG	1:B:415:SER:N	1.96	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:A:244:VAL:O	1:D:299:HIS:CD2	2.50	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:C:473:LYS:HZ3	1:C:485:ILE:H	1.49	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CD1	1:D:379:TRP:N	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:B:48:THR:HG23	1:B:116:ALA:C	2.31	0.55
1:C:52:LEU:C	1:C:52:LEU:HD23	2.31	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:B:52:LEU:C	1:B:52:LEU:HD23	2.31	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
1:C:70:SER:HB2	1:C:141:TRP:CZ3	2.42	0.53
1:C:224:VAL:C	1:C:226:GLN:H	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:289:LYS:HZ3	1:A:309:HIS:HD2	1.55	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:D:232:PHE:CD1	1:D:232:PHE:C	2.86	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: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
1:C:225:GLN:H	1:C:225:GLN:CD	2.19	0.50
1:C:241:LYS:NZ	4:C:606:HOH:O	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:O	1:D:485:ILE:HG13	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: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:C:287:LEU:HD22	1:C:471:ILE:HG23	1.96	0.48
1:A:199:ASN:O	1:A:200:GLN:HB2	2.14	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:A:339:PRO:O	1:A:340:GLU:C	2.57	0.47
1:B:112:GLN:HE22	1:B:213:LEU:HD11	1.80	0.47
1:D:190:LEU:HD23	1:D:190:LEU:C	2.39	0.47
1:A:133:PRO:HB2	1:A:172:VAL:HG23	1.96	0.47
1:A:341:ASP:C	1:A:343:THR:H	2.23	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:THR:HA	1:A:364:HIS:ND1	2.30	0.46
1:B:190:LEU:C	1:B:190:LEU:HD23	2.41	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:109:HIS:N	1:B:109:HIS:HD1	2.14	0.46
1:B:307:PHE:CB	2:B:508:EDO:H12	2.45	0.46
1:A:473:LYS:HZ1	1:A:485:ILE:HG13	1.80	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: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: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:23:SER:C	1:B:25:SER:H	2.26	0.44
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
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:C:322:GLU:CD	1:C:322:GLU:H	2.26	0.44
1:A:82:MSE:HE3	1:A:82:MSE:HB3	1.90	0.44
1:A:144:LYS:HZ1	1:B:131:GLU:HG3	1.82	0.44
1:A:396:LEU:HD13	1:A:440:HIS:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:VAL:HB	1:B:163:VAL:HG13	2.00	0.44
1:C:312:ASN:C	1:C:312:ASN:ND2	2.71	0.44
1:C:200:GLN:HE21	1:C:200:GLN:HB3	1.66	0.43
1:D:52:LEU:HD23	1:D:52:LEU:C	2.43	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:52:LEU:C	1:A:52:LEU:HD23	2.42	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:A:278:LEU:O	1:A:279:PRO:C	2.61	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:A:289:LYS:HZ1	1:A:309:HIS:CD2	2.28	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:232:PHE:CD1	1:A:232:PHE:C	2.96	0.43
1:A:318:MSE:HB3	1:A:321:ILE:HB	1.99	0.43
3:A:508:C8E:H31	3:D:511:C8E:H13	2.01	0.42
1:C:106:HIS:O	1:C:107:GLU:HB2	2.18	0.42
1:C:287:LEU:HD23	1:C:287:LEU:C	2.44	0.42
1:C:296:LEU:HD11	1:C:387:LEU:HD23	2.01	0.42
1:C:34:HIS:CD2	1:C:34:HIS:C	2.97	0.42
1:B:450:ALA:O	2:B:506:EDO:H22	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:314:ARG:NH1	1:B:328:THR:HG1	2.18	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:B:104:VAL:HG13	1:B:105:GLU:N	2.34	0.42
1:C:224:VAL:C	1:C:226:GLN:N	2.77	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:167:GLY:C	1:A:168:ASN:HD22	2.28	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:D:350:LEU:O	1:D:351:LEU:C	2.62	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%)	18	23
1	B	438/486 (90%)	413 (94%)	21 (5%)	4 (1%)	14	17
1	C	440/486 (90%)	415 (94%)	22 (5%)	3 (1%)	18	23
1	D	437/486 (90%)	412 (94%)	22 (5%)	3 (1%)	18	23
All	All	1752/1944 (90%)	1650 (94%)	89 (5%)	13 (1%)	18	23

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%)	353 (89%)	44 (11%)	6	7
1	B	398/424 (94%)	361 (91%)	37 (9%)	8	11
1	C	400/424 (94%)	357 (89%)	43 (11%)	6	7
1	D	397/424 (94%)	353 (89%)	44 (11%)	6	7
All	All	1592/1696 (94%)	1424 (89%)	168 (11%)	6	8

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLU
1	A	25	SER
1	A	28	LYS
1	A	45	VAL
1	A	46	THR
1	A	53	LEU
1	A	60	HIS
1	A	79	SER
1	A	95	ARG
1	A	102	SER
1	A	104	VAL
1	A	105	GLU
1	A	111	ILE
1	A	115	LEU
1	A	117	ASN
1	A	162	LEU
1	A	173	LEU
1	A	185	VAL
1	A	216	ARG
1	A	219	SER
1	A	224	VAL
1	A	225	GLN
1	A	265	GLN
1	A	274	VAL
1	A	286	THR
1	A	287	LEU
1	A	302	SER
1	A	309	HIS
1	A	312	ASN
1	A	322	GLU
1	A	342	SER
1	A	343	THR
1	A	344	ASP

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Mol	Chain	Res	Type
1	A	374	GLN
1	A	377	THR
1	A	399	SER
1	A	430	LEU
1	A	435	ILE
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	20	GLU
1	B	31	GLN
1	B	40	LYS
1	B	45	VAL
1	B	48	THR
1	B	67	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	111	ILE
1	B	115	LEU
1	B	117	ASN
1	B	118	LEU
1	B	121	LYS
1	B	164	SER
1	B	173	LEU
1	B	185	VAL
1	B	218	SER
1	B	221	ARG
1	B	224	VAL
1	B	241	LYS
1	B	249	ARG
1	B	287	LEU
1	B	388	ILE
1	B	397	SER
1	B	415	SER
1	B	418	ASP

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Mol	Chain	Res	Type
1	B	430	LEU
1	B	458	GLU
1	B	473	LYS
1	B	482	LEU
1	B	485	ILE
1	B	486	THR
1	C	27	ILE
1	C	45	VAL
1	C	64	LYS
1	C	78	ARG
1	C	79	SER
1	C	83	ASP
1	C	85	LEU
1	C	95	ARG
1	C	100	ARG
1	C	102	SER
1	C	104	VAL
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	217	VAL
1	C	224	VAL
1	C	225	GLN
1	C	265	GLN
1	C	280	SER
1	C	312	ASN
1	C	319	ASP
1	C	322	GLU
1	C	323	SER
1	C	324	LEU
1	C	374	GLN
1	C	402	LEU
1	C	415	SER
1	C	417	LEU
1	C	423	LYS
1	C	430	LEU
1	C	443	ARG

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Mol	Chain	Res	Type
1	C	444	LEU
1	C	453	ARG
1	C	468	SER
1	C	472	THR
1	C	482	LEU
1	C	483	LEU
1	C	487	PHE
1	D	19	TRP
1	D	28	LYS
1	D	45	VAL
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	189	LYS
1	D	207	SER
1	D	219	SER
1	D	221	ARG
1	D	229	THR
1	D	271	LYS
1	D	286	THR
1	D	302	SER
1	D	309	HIS
1	D	312	ASN
1	D	322	GLU
1	D	340	GLU
1	D	342	SER
1	D	367	VAL
1	D	374	GLN
1	D	383	THR
1	D	399	SER
1	D	416	SER

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Mol	Chain	Res	Type
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 (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	HIS
1	A	168	ASN
1	A	235	HIS
1	A	299	HIS
1	A	309	HIS
1	A	312	ASN
1	A	352	HIS
1	A	374	GLN
1	A	375	HIS
1	A	390	GLN
1	A	457	GLN
1	B	31	GLN
1	B	69	HIS
1	B	81	ASN
1	B	112	GLN
1	B	176	GLN
1	B	235	HIS
1	B	374	GLN
1	B	390	GLN
1	C	31	GLN
1	C	117	ASN
1	C	168	ASN
1	C	170	HIS
1	C	299	HIS
1	C	312	ASN
1	C	352	HIS
1	C	391	HIS
1	C	447	GLN
1	D	31	GLN

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Mol	Chain	Res	Type
1	D	109	HIS
1	D	231	GLN
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 oligosaccharides 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	B	503	-	3,3,3	0.62	0	2,2,2	0.15	0
2	EDO	B	504	-	3,3,3	0.69	0	2,2,2	0.12	0
2	EDO	B	507	-	3,3,3	0.50	0	2,2,2	0.24	0
2	EDO	A	507	-	3,3,3	0.46	0	2,2,2	0.32	0
2	EDO	B	505	-	3,3,3	0.45	0	2,2,2	0.37	0
3	C8E	C	509	-	20,20,20	0.40	0	19,19,19	0.76	0
3	C8E	B	512	-	20,20,20	0.34	0	19,19,19	0.63	0
2	EDO	D	502	-	3,3,3	0.47	0	2,2,2	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	D	508	-	3,3,3	0.49	0	2,2,2	0.37	0
2	EDO	C	502	-	3,3,3	0.46	0	2,2,2	0.29	0
2	EDO	D	504	-	3,3,3	0.52	0	2,2,2	0.19	0
2	EDO	B	508	-	3,3,3	0.66	0	2,2,2	0.09	0
2	EDO	B	511	-	3,3,3	0.47	0	2,2,2	0.41	0
2	EDO	D	507	-	3,3,3	0.48	0	2,2,2	0.18	0
2	EDO	D	505	-	3,3,3	0.50	0	2,2,2	0.28	0
3	C8E	D	511	-	20,20,20	0.46	0	19,19,19	0.40	0
2	EDO	D	503	-	3,3,3	0.53	0	2,2,2	0.19	0
2	EDO	B	502	-	3,3,3	0.38	0	2,2,2	0.39	0
2	EDO	C	506	-	3,3,3	0.43	0	2,2,2	0.31	0
2	EDO	A	503	-	3,3,3	0.54	0	2,2,2	0.15	0
2	EDO	D	510	-	3,3,3	0.50	0	2,2,2	0.60	0
2	EDO	A	506	-	3,3,3	0.45	0	2,2,2	0.37	0
2	EDO	C	504	-	3,3,3	0.59	0	2,2,2	0.21	0
2	EDO	A	502	-	3,3,3	0.51	0	2,2,2	0.23	0
2	EDO	B	509	-	3,3,3	0.50	0	2,2,2	0.30	0
2	EDO	C	501	-	3,3,3	0.44	0	2,2,2	0.30	0
2	EDO	C	507	-	3,3,3	0.50	0	2,2,2	0.24	0
2	EDO	C	505	-	3,3,3	0.44	0	2,2,2	0.38	0
2	EDO	B	506	-	3,3,3	0.35	0	2,2,2	0.38	0
2	EDO	D	509	-	3,3,3	0.46	0	2,2,2	0.33	0
2	EDO	D	506	-	3,3,3	0.45	0	2,2,2	0.31	0
2	EDO	C	508	-	3,3,3	0.47	0	2,2,2	0.37	0
2	EDO	C	503	-	3,3,3	0.46	0	2,2,2	0.27	0
2	EDO	B	501	-	3,3,3	0.51	0	2,2,2	0.31	0
2	EDO	A	504	-	3,3,3	0.43	0	2,2,2	0.44	0
3	C8E	A	508	-	20,20,20	0.44	0	19,19,19	0.38	0
2	EDO	A	505	-	3,3,3	0.59	0	2,2,2	0.17	0
2	EDO	A	501	-	3,3,3	0.53	0	2,2,2	0.24	0
2	EDO	D	501	-	3,3,3	0.47	0	2,2,2	0.37	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	B	503	-	-	0/1/1/1	-
2	EDO	B	504	-	-	0/1/1/1	-
2	EDO	B	507	-	-	1/1/1/1	-
2	EDO	A	507	-	-	1/1/1/1	-
2	EDO	B	505	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	C8E	C	509	-	-	12/18/18/18	-
3	C8E	B	512	-	-	10/18/18/18	-
2	EDO	D	502	-	-	1/1/1/1	-
2	EDO	D	508	-	-	0/1/1/1	-
2	EDO	C	502	-	-	0/1/1/1	-
2	EDO	D	504	-	-	1/1/1/1	-
2	EDO	B	508	-	-	1/1/1/1	-
2	EDO	B	511	-	-	1/1/1/1	-
2	EDO	D	507	-	-	0/1/1/1	-
2	EDO	D	505	-	-	1/1/1/1	-
3	C8E	D	511	-	-	13/18/18/18	-
2	EDO	D	503	-	-	0/1/1/1	-
2	EDO	B	502	-	-	0/1/1/1	-
2	EDO	C	506	-	-	1/1/1/1	-
2	EDO	A	503	-	-	1/1/1/1	-
2	EDO	D	510	-	-	1/1/1/1	-
2	EDO	A	506	-	-	0/1/1/1	-
2	EDO	C	504	-	-	1/1/1/1	-
2	EDO	A	502	-	-	0/1/1/1	-
2	EDO	B	509	-	-	1/1/1/1	-
2	EDO	C	501	-	-	0/1/1/1	-
2	EDO	C	507	-	-	0/1/1/1	-
2	EDO	C	505	-	-	0/1/1/1	-
2	EDO	B	506	-	-	0/1/1/1	-
2	EDO	D	509	-	-	1/1/1/1	-
2	EDO	D	506	-	-	1/1/1/1	-
2	EDO	C	508	-	-	1/1/1/1	-
2	EDO	C	503	-	-	0/1/1/1	-
2	EDO	B	501	-	-	0/1/1/1	-
2	EDO	A	504	-	-	0/1/1/1	-
3	C8E	A	508	-	-	9/18/18/18	-
2	EDO	A	505	-	-	1/1/1/1	-
2	EDO	A	501	-	-	0/1/1/1	-
2	EDO	D	501	-	-	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	D	511	C8E	O12-C13-C14-O15
3	A	508	C8E	C6-C7-C8-O9
3	C	509	C8E	O18-C19-C20-O21
3	D	511	C8E	O18-C19-C20-O21
3	D	511	C8E	C6-C7-C8-O9
3	C	509	C8E	O15-C16-C17-O18
3	C	509	C8E	C6-C7-C8-O9
3	A	508	C8E	O9-C10-C11-O12
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	A	508	C8E	C5-C6-C7-C8
3	C	509	C8E	C2-C3-C4-C5
3	D	511	C8E	C3-C4-C5-C6
3	D	511	C8E	O15-C16-C17-O18
3	B	512	C8E	C6-C7-C8-O9
3	D	511	C8E	C16-C17-O18-C19
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	A	508	C8E	C2-C3-C4-C5
3	C	509	C8E	C1-C2-C3-C4
3	B	512	C8E	O12-C13-C14-O15
3	D	511	C8E	C1-C2-C3-C4
3	B	512	C8E	C16-C17-O18-C19
2	A	507	EDO	O1-C1-C2-O2
2	D	505	EDO	O1-C1-C2-O2
3	C	509	C8E	C11-C10-O9-C8
3	D	511	C8E	O9-C10-C11-O12
3	C	509	C8E	C20-C19-O18-C17
3	B	512	C8E	C17-C16-O15-C14
2	B	507	EDO	O1-C1-C2-O2
2	D	506	EDO	O1-C1-C2-O2
3	B	512	C8E	C20-C19-O18-C17
3	D	511	C8E	C14-C13-O12-C11
3	D	511	C8E	C10-C11-O12-C13
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	C	509	C8E	C13-C14-O15-C16

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

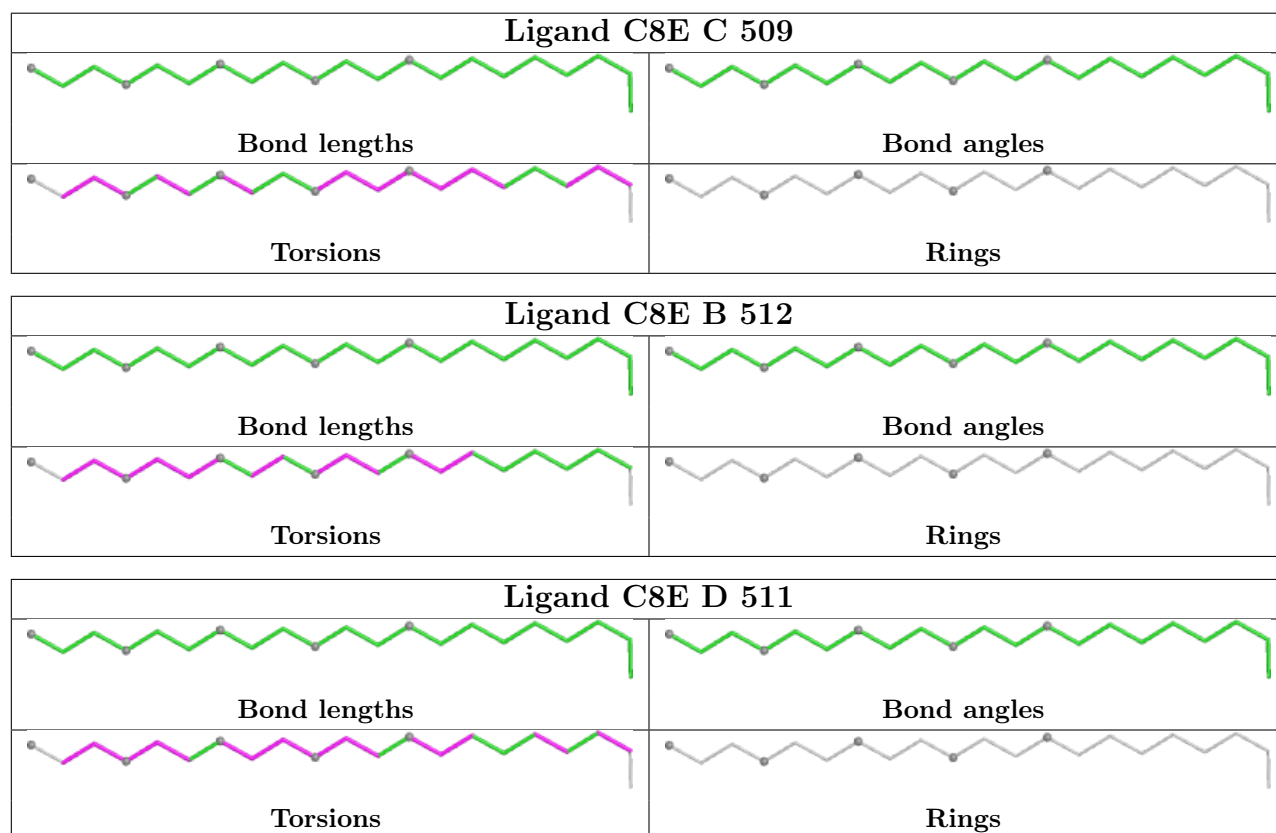
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	504	EDO	1	0
2	B	505	EDO	3	0
3	C	509	C8E	12	0
3	B	512	C8E	16	0
2	D	502	EDO	1	0
2	D	508	EDO	1	0
2	C	502	EDO	1	0
2	D	504	EDO	1	0
2	B	508	EDO	4	0
2	D	507	EDO	1	0
3	D	511	C8E	9	0
2	D	503	EDO	3	0
2	B	502	EDO	6	0
2	C	506	EDO	1	0
2	A	503	EDO	3	0
2	D	510	EDO	1	0
2	A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

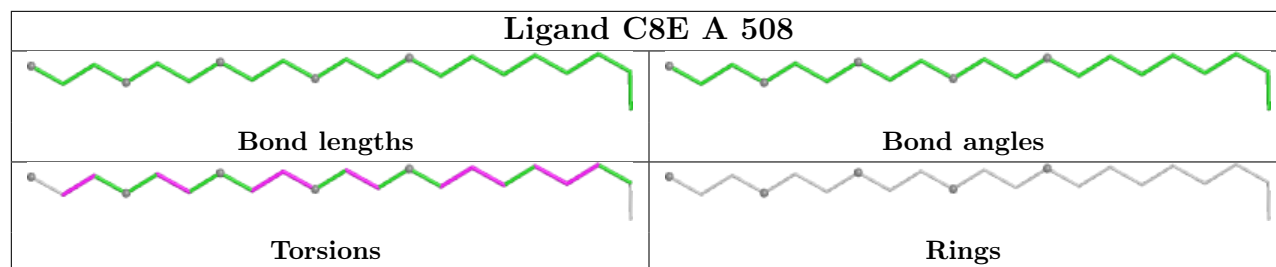
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	EDO	9	0
2	C	505	EDO	1	0
2	B	506	EDO	6	0
2	D	506	EDO	1	0
2	A	504	EDO	4	0
3	A	508	C8E	9	0
2	A	505	EDO	1	0

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	436/486 (89%)	0.49	23 (5%) 32 34	31, 53, 85, 153	1 (0%)
1	B	437/486 (89%)	0.27	13 (2%) 52 54	25, 44, 79, 139	1 (0%)
1	C	438/486 (90%)	0.46	29 (6%) 24 26	27, 50, 92, 144	2 (0%)
1	D	436/486 (89%)	0.62	23 (5%) 32 34	34, 56, 91, 133	1 (0%)
All	All	1747/1944 (89%)	0.46	88 (5%) 34 35	25, 51, 88, 153	5 (0%)

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	485	ILE	5.9
1	A	485	ILE	5.4
1	D	19	TRP	4.9
1	B	485	ILE	4.9
1	B	250	ALA	4.8
1	B	416	SER	4.6
1	D	247	ALA	4.2
1	C	109	HIS	4.1
1	C	485	ILE	4.0
1	D	483	LEU	3.9
1	D	486	THR	3.9
1	B	263	SER	3.5
1	C	108	GLY	3.4
1	A	483	LEU	3.3
1	A	19	TRP	3.1
1	C	221	ARG	3.0
1	D	248	PRO	3.0
1	C	486	THR	2.9
1	C	247	ALA	2.9
1	D	101	THR	2.9
1	D	30	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	125	VAL	2.8
1	C	202	PRO	2.8
1	B	247	ALA	2.8
1	D	28	LYS	2.8
1	D	208	ASP	2.8
1	A	272	GLY	2.8
1	A	341	ASP	2.7
1	C	484	ASP	2.7
1	B	248	PRO	2.7
1	C	211	HIS	2.7
1	D	462	GLU	2.6
1	A	486	THR	2.6
1	C	483	LEU	2.6
1	C	264	GLY	2.6
1	C	405	SER	2.6
1	C	315	ASN	2.6
1	B	483	LEU	2.5
1	C	223	ASP	2.5
1	C	106	HIS	2.5
1	D	287	LEU	2.5
1	B	402	LEU	2.4
1	D	20	GLU	2.4
1	B	415	SER	2.4
1	A	52	LEU	2.4
1	D	49	LEU	2.4
1	D	116	ALA	2.4
1	C	165	CYS	2.4
1	D	211[A]	HIS	2.4
1	C	224	VAL	2.4
1	C	204	PRO	2.3
1	D	221	ARG	2.3
1	D	108	GLY	2.3
1	A	230	PHE	2.3
1	A	274	VAL	2.3
1	B	205	PRO	2.3
1	C	340	GLU	2.3
1	D	224	VAL	2.3
1	A	313	GLY	2.3
1	A	404	GLY	2.3
1	A	25	SER	2.3
1	B	109	HIS	2.3
1	A	484	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	27	ILE	2.2
1	C	248	PRO	2.2
1	D	77	GLY	2.2
1	A	462	GLU	2.2
1	C	45	VAL	2.2
1	C	226	GLN	2.2
1	C	453	ARG	2.2
1	C	320	ASN	2.1
1	A	116	ALA	2.1
1	C	24	LEU	2.1
1	C	119	ASP	2.1
1	A	226	GLN	2.1
1	A	247	ALA	2.1
1	B	212	TYR	2.1
1	D	320	ASN	2.1
1	B	31	GLN	2.1
1	C	203	LEU	2.1
1	A	208	ASP	2.1
1	A	339	PRO	2.1
1	A	343	THR	2.0
1	A	476	THR	2.0
1	D	50	GLU	2.0
1	A	378	ASN	2.0
1	A	323	SER	2.0
1	D	416	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

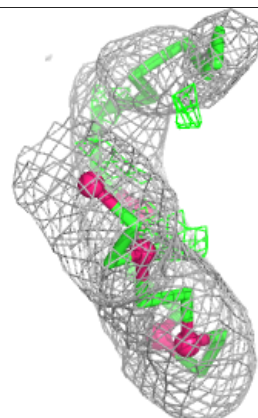
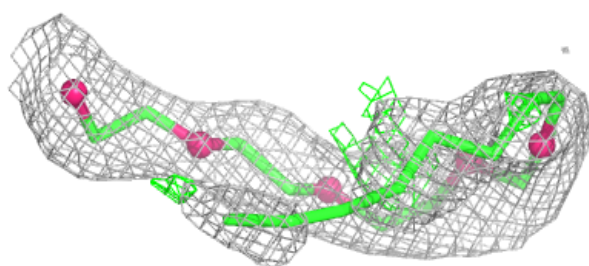
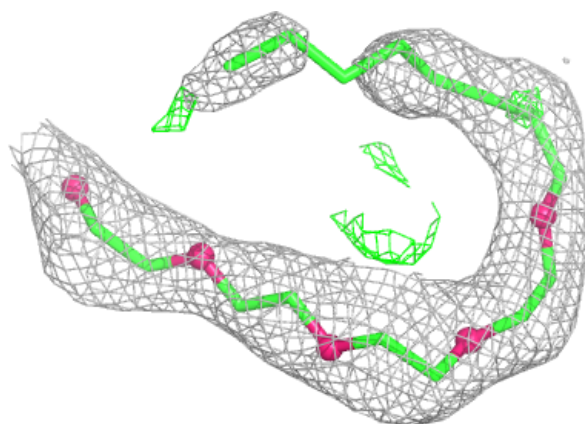
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	D	509	4/4	0.60	0.17	85,85,85,85	0
2	EDO	D	501	4/4	0.66	0.18	78,78,78,78	0
2	EDO	A	507	4/4	0.69	0.23	84,84,84,84	0
2	EDO	D	506	4/4	0.73	0.16	83,83,83,83	0
2	EDO	C	508	4/4	0.75	0.26	82,82,82,82	0
2	EDO	D	505	4/4	0.76	0.27	91,91,91,91	0
2	EDO	A	503	4/4	0.77	0.18	65,65,65,65	0
2	EDO	A	505	4/4	0.79	0.16	64,64,64,64	0
2	EDO	B	508	4/4	0.80	0.21	58,58,58,58	0
2	EDO	B	509	4/4	0.83	0.17	62,62,62,62	0
2	EDO	C	504	4/4	0.84	0.21	51,51,51,51	0
2	EDO	D	504	4/4	0.85	0.18	68,68,68,68	0
2	EDO	B	503	4/4	0.85	0.16	56,56,56,56	0
2	EDO	A	504	4/4	0.86	0.23	54,54,54,54	0
2	EDO	B	507	4/4	0.87	0.15	67,67,67,67	0
2	EDO	A	506	4/4	0.87	0.11	72,72,72,72	0
2	EDO	D	510	4/4	0.87	0.10	57,57,57,57	0
3	C8E	A	508	21/21	0.88	0.17	66,66,66,66	0
3	C8E	D	511	21/21	0.89	0.14	65,65,65,65	0
2	EDO	B	511	4/4	0.90	0.14	71,71,71,71	0
2	EDO	B	501	4/4	0.90	0.12	62,62,62,62	0
2	EDO	D	502	4/4	0.90	0.13	71,71,71,71	0
2	EDO	D	508	4/4	0.90	0.12	67,67,67,67	0
2	EDO	A	502	4/4	0.91	0.12	74,74,74,74	0
2	EDO	C	501	4/4	0.91	0.23	53,53,53,53	0
2	EDO	A	501	4/4	0.91	0.11	45,45,45,45	0
2	EDO	C	505	4/4	0.91	0.19	60,60,60,60	0
2	EDO	B	504	4/4	0.91	0.12	38,38,38,38	0
2	EDO	B	502	4/4	0.92	0.17	48,48,48,48	0
2	EDO	D	503	4/4	0.93	0.08	49,49,49,49	0
2	EDO	C	506	4/4	0.93	0.12	63,63,63,63	0
2	EDO	B	506	4/4	0.93	0.19	42,42,42,42	0
2	EDO	D	507	4/4	0.94	0.09	44,44,44,44	0
2	EDO	C	507	4/4	0.94	0.09	38,38,38,38	0
3	C8E	B	512	21/21	0.94	0.10	42,42,42,42	0
3	C8E	C	509	21/21	0.94	0.09	42,42,42,42	0
2	EDO	B	505	4/4	0.94	0.07	45,45,45,45	0
2	EDO	C	502	4/4	0.95	0.11	59,59,59,59	0
2	EDO	C	503	4/4	0.96	0.18	57,57,57,57	0

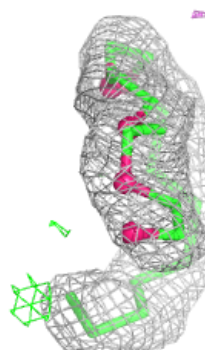
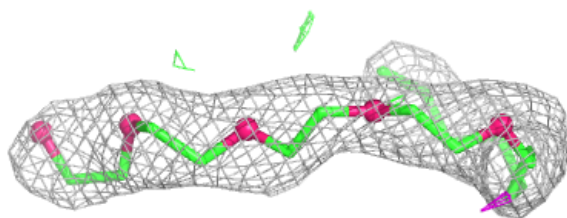
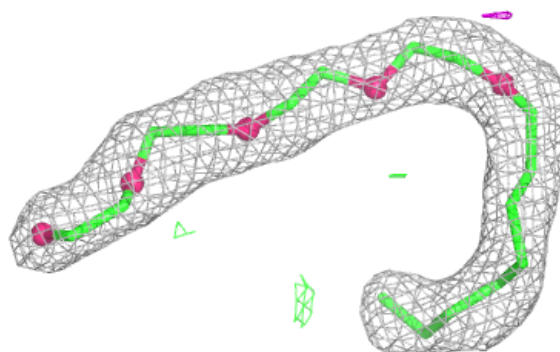
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around C8E A 508:

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

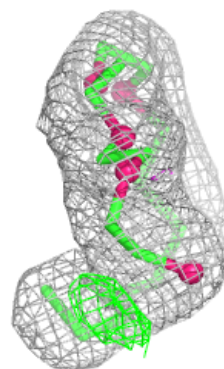
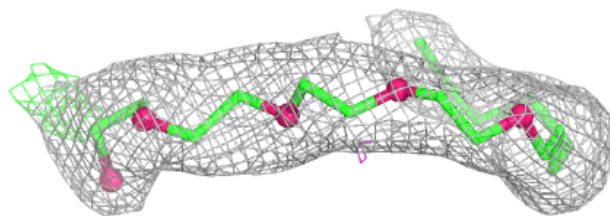
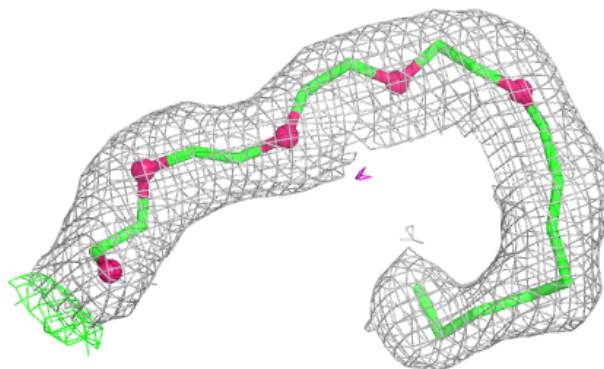
**Electron density around C8E D 511:**

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

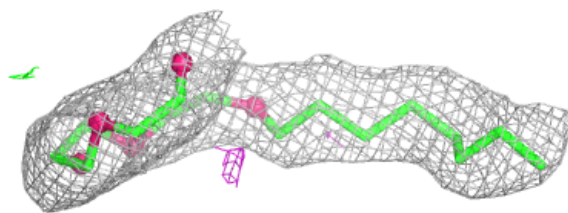
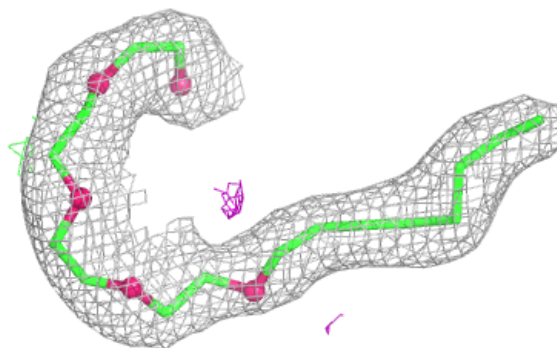


Electron density around C8E B 512:

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

**Electron density around C8E C 509:**

$2mF_o-DF_c$ (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.