



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:36 PM UTC

PDB ID : 1NQF / pdb_00001nqf
Title : OUTER MEMBRANE COBALAMIN TRANSPORTER (BTUB) FROM E. COLI, METHIONINE SUBSTITUTION CONSTRUCT FOR SE-MET SAD PHASING
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Deposited on : 2003-01-21
Resolution : 2.70 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

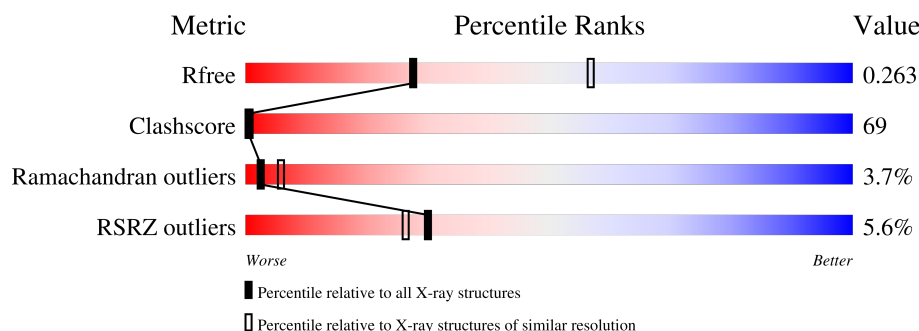
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	594	

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
3	C8E	A	800	-	-	X	-
3	C8E	A	802	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	C8E	A	803	-	-	X	-
3	C8E	A	804	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4490 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 Vitamin B12 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	544	Total	C	N	O	Se	0	0	0
			4294	2700	740	846	8			

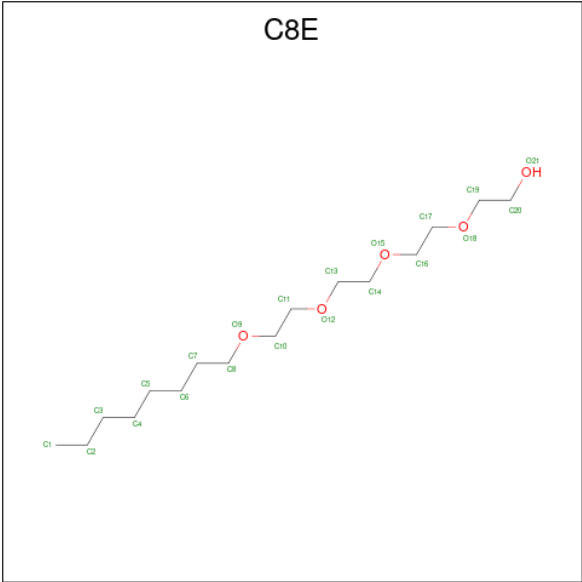
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	293	MSE	MET	engineered mutation	UNP P06129
A	317	MSE	TRP	engineered mutation	UNP P06129
A	319	MSE	LYS	engineered mutation	UNP P06129
A	321	MSE	THR	engineered mutation	UNP P06129
A	516	MSE	TRP	engineered mutation	UNP P06129
A	518	MSE	ILE	engineered mutation	UNP P06129
A	520	MSE	TYR	engineered mutation	UNP P06129
A	541	MSE	MET	engineered mutation	UNP P06129

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

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



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

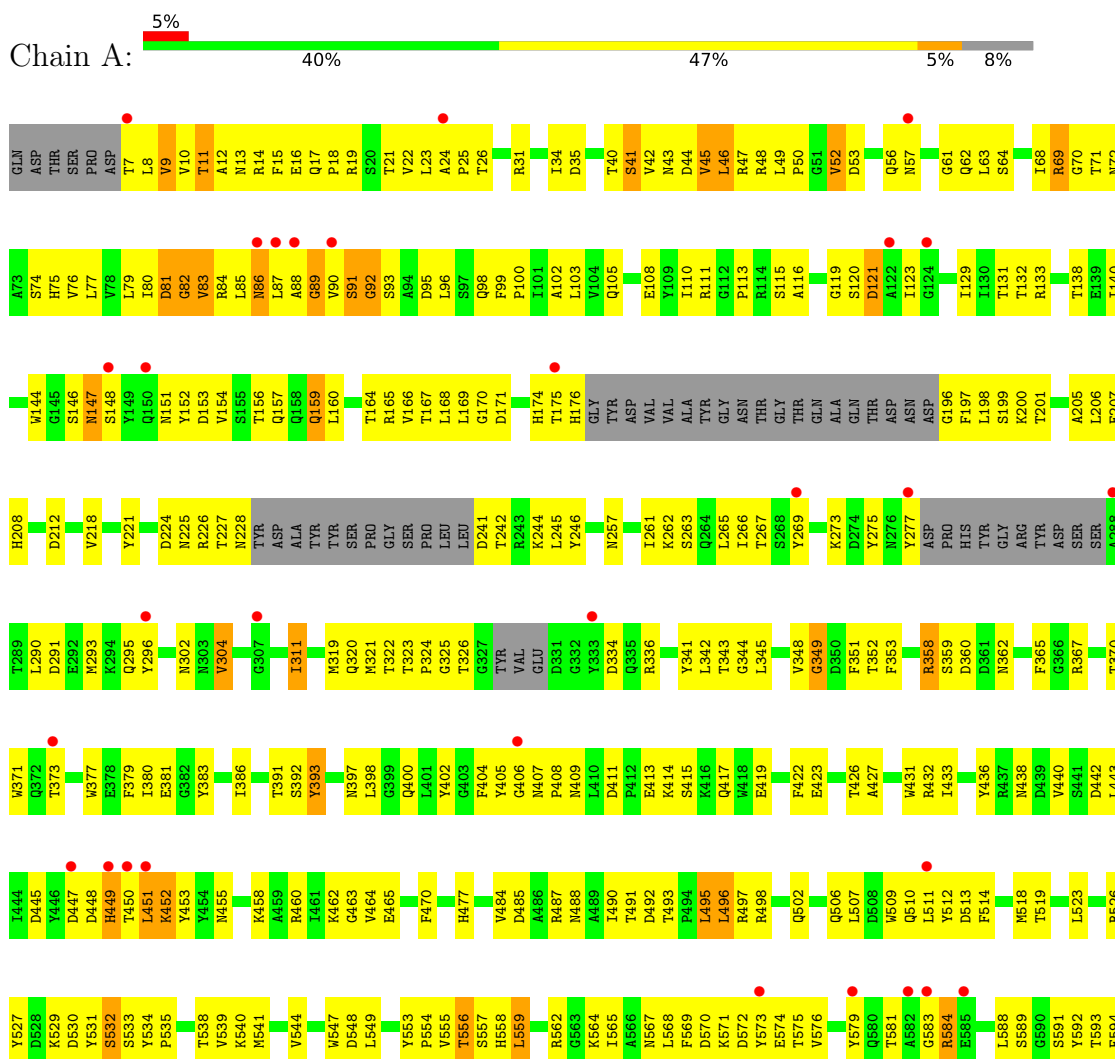
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	69	Total	O	0	0
			69	69		

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: Vitamin B12 receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	81.61Å 81.61Å 226.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.5 (20.00-2.70) 96.1 (20.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.1.24, CNS	Depositor
R, R_{free}	0.244 , 0.288 (Not available) , 0.263	Depositor DCC
R_{free} test set	1222 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	59.8	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 62.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4490	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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: MG, 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	1.08	3/4384 (0.1%)	1.28	18/5940 (0.3%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	548	ASP	CA-C	-5.50	1.46	1.52
1	A	9	VAL	CA-CB	-5.35	1.47	1.54
1	A	544	VAL	N-CA	-5.29	1.39	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	GLY	N-CA-C	12.29	128.24	111.03
1	A	45	VAL	CB-CA-C	-11.74	100.08	113.22
1	A	325	GLY	N-CA-C	-6.80	106.61	115.59
1	A	311	ILE	N-CA-C	-6.45	99.84	108.35
1	A	575	THR	N-CA-C	-6.33	104.60	112.90
1	A	304	VAL	N-CA-C	5.88	118.44	108.86
1	A	45	VAL	CA-C-O	-5.72	117.65	122.63
1	A	212	ASP	N-CA-C	-5.58	107.05	112.97
1	A	159	GLN	N-CA-C	-5.49	101.59	110.32
1	A	69	ARG	NE-CZ-NH1	-5.39	116.11	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	358	ARG	N-CA-C	5.39	117.59	109.23
1	A	52	VAL	N-CA-C	5.33	115.63	108.17
1	A	393	TYR	N-CA-C	5.31	117.33	108.99
1	A	452	LYS	N-CA-C	5.26	117.06	109.07
1	A	485	ASP	CB-CA-C	-5.19	104.16	112.05
1	A	419	GLU	CA-C-N	5.16	125.16	121.65
1	A	419	GLU	C-N-CA	5.16	125.16	121.65
1	A	52	VAL	CB-CA-C	-5.11	103.21	110.83

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	81	ASP	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	4294	0	4071	575	1
2	A	1	0	0	0	0
3	A	126	0	204	68	0
4	A	69	0	0	16	0
All	All	4490	0	4275	604	1

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 69.

All (604) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:THR:HG21	1:A:277:TYR:CZ	1.52	1.45
1:A:89:GLY:HA3	1:A:91:SER:N	1.15	1.43
3:A:802:C8E:H52	3:A:802:C8E:C1	1.49	1.38
1:A:62:GLN:HE21	1:A:62:GLN:N	1.24	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ARG:NH1	1:A:244:LYS:HG3	1.43	1.33
1:A:85:LEU:HD22	1:A:85:LEU:O	1.18	1.33
1:A:86:ASN:O	1:A:87:LEU:HD12	1.31	1.28
1:A:555:VAL:O	1:A:556:THR:HG23	1.18	1.27
1:A:18:PRO:O	1:A:21:THR:CG2	1.85	1.23
1:A:198:LEU:C	1:A:198:LEU:HD12	1.59	1.22
1:A:89:GLY:HA3	1:A:90:VAL:C	1.58	1.22
3:A:802:C8E:H12	3:A:802:C8E:C5	1.70	1.21
1:A:86:ASN:C	1:A:87:LEU:HD12	1.66	1.21
1:A:242:THR:CG2	1:A:277:TYR:CZ	2.23	1.19
1:A:85:LEU:O	1:A:85:LEU:CD2	1.92	1.17
1:A:559:LEU:O	1:A:559:LEU:HD22	1.43	1.17
1:A:91:SER:HB3	4:A:869:HOH:O	1.39	1.16
1:A:62:GLN:HE21	1:A:62:GLN:CA	1.54	1.16
1:A:245:LEU:HD23	1:A:246:TYR:N	1.59	1.15
1:A:120:SER:HB2	1:A:393:TYR:CE1	1.82	1.15
1:A:89:GLY:CA	1:A:91:SER:N	2.08	1.14
1:A:61:GLY:C	1:A:62:GLN:HE21	1.55	1.13
1:A:9:VAL:CG1	1:A:19:ARG:HD3	1.78	1.12
1:A:169:LEU:HD12	1:A:169:LEU:C	1.75	1.12
1:A:174:HIS:CE1	1:A:176:HIS:NE2	2.16	1.12
1:A:342:LEU:HD11	3:A:803:C8E:H51	1.17	1.12
1:A:9:VAL:HG11	1:A:19:ARG:HD3	1.15	1.11
1:A:555:VAL:C	1:A:556:THR:HG23	1.72	1.11
1:A:245:LEU:CD2	1:A:246:TYR:N	2.15	1.10
1:A:160:LEU:HD22	1:A:166:VAL:HG21	1.20	1.09
1:A:62:GLN:N	1:A:62:GLN:NE2	1.98	1.09
1:A:263:SER:HB2	1:A:302:ASN:HD22	1.18	1.06
1:A:358:ARG:O	3:A:800:C8E:C8	2.04	1.05
1:A:103:LEU:N	1:A:103:LEU:HD23	1.71	1.05
1:A:120:SER:O	1:A:121:ASP:HB2	1.27	1.05
1:A:242:THR:HG21	1:A:277:TYR:OH	1.53	1.05
1:A:18:PRO:O	1:A:21:THR:HG22	0.88	1.04
1:A:61:GLY:C	1:A:62:GLN:NE2	2.14	1.04
1:A:88:ALA:O	1:A:92:GLY:HA2	1.56	1.04
1:A:226:ARG:HH22	1:A:244:LYS:HE2	1.21	1.03
3:A:803:C8E:H112	3:A:803:C8E:C16	1.88	1.03
1:A:198:LEU:HD12	1:A:199:SER:N	1.73	1.03
1:A:79:LEU:HB3	1:A:82:GLY:HA3	1.40	1.02
1:A:555:VAL:O	1:A:556:THR:CG2	2.06	1.02
1:A:198:LEU:C	1:A:198:LEU:CD1	2.27	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ARG:HH12	1:A:244:LYS:CG	1.73	1.01
1:A:406:GLY:CA	1:A:452:LYS:HE3	1.89	1.01
1:A:160:LEU:CD2	1:A:166:VAL:HG21	1.91	1.01
1:A:226:ARG:HH12	1:A:244:LYS:HG3	0.95	1.01
1:A:263:SER:HB2	1:A:302:ASN:ND2	1.74	1.01
1:A:174:HIS:C	1:A:174:HIS:CD2	2.38	1.01
1:A:169:LEU:HD12	1:A:169:LEU:O	1.61	1.00
1:A:160:LEU:HD22	1:A:166:VAL:CG2	1.90	1.00
1:A:568:LEU:HB3	1:A:569:PHE:CD1	1.97	0.99
1:A:323:THR:O	1:A:326:THR:HB	1.63	0.99
1:A:555:VAL:C	1:A:556:THR:CG2	2.34	0.99
1:A:362:ASN:HD22	1:A:365:PHE:H	1.12	0.98
1:A:160:LEU:CD2	1:A:166:VAL:CG2	2.42	0.98
1:A:120:SER:CB	1:A:393:TYR:CE1	2.47	0.97
1:A:398:LEU:CD2	1:A:398:LEU:H	1.77	0.97
1:A:496:LEU:O	1:A:497:ARG:HB2	1.60	0.97
1:A:147:ASN:O	1:A:148:SER:OG	1.81	0.96
1:A:539:VAL:HG23	1:A:540:LYS:N	1.77	0.96
1:A:18:PRO:HD2	1:A:21:THR:HG21	1.48	0.95
1:A:362:ASN:ND2	1:A:365:PHE:CD2	2.34	0.95
1:A:559:LEU:HD22	1:A:559:LEU:C	1.90	0.94
1:A:169:LEU:C	1:A:169:LEU:CD1	2.40	0.94
1:A:342:LEU:CD1	3:A:803:C8E:H51	1.98	0.94
1:A:568:LEU:HB3	1:A:569:PHE:HD1	1.32	0.94
1:A:572:ASP:HA	4:A:864:HOH:O	1.67	0.94
1:A:406:GLY:HA3	1:A:452:LYS:CE	1.97	0.94
1:A:539:VAL:CG2	1:A:540:LYS:N	2.31	0.93
1:A:120:SER:O	1:A:121:ASP:CB	2.14	0.93
1:A:103:LEU:N	1:A:103:LEU:CD2	2.30	0.93
1:A:539:VAL:HG23	1:A:540:LYS:H	1.33	0.93
1:A:86:ASN:C	1:A:87:LEU:CD1	2.43	0.92
1:A:245:LEU:HD23	1:A:246:TYR:H	1.27	0.92
1:A:555:VAL:HG12	1:A:556:THR:HG22	1.53	0.91
1:A:64:SER:O	1:A:95:ASP:OD1	1.89	0.91
1:A:85:LEU:O	1:A:87:LEU:N	2.04	0.91
1:A:464:VAL:HG11	3:A:804:C8E:H51	1.53	0.91
1:A:62:GLN:CA	1:A:62:GLN:NE2	2.25	0.90
1:A:198:LEU:CD1	1:A:199:SER:N	2.32	0.89
1:A:518:MSE:HG3	1:A:549:LEU:CD1	2.02	0.89
1:A:323:THR:O	1:A:326:THR:CB	2.19	0.89
3:A:803:C8E:H112	3:A:803:C8E:O15	1.67	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLY:HA3	1:A:91:SER:H	1.37	0.89
1:A:224:ASP:O	1:A:224:ASP:OD1	1.89	0.89
1:A:506:GLN:NE2	1:A:519:THR:HB	1.88	0.89
1:A:85:LEU:HD22	1:A:87:LEU:HD13	1.53	0.89
1:A:447:ASP:HA	4:A:818:HOH:O	1.74	0.88
1:A:13:ASN:HD22	1:A:13:ASN:C	1.80	0.88
1:A:398:LEU:H	1:A:398:LEU:HD23	1.38	0.88
3:A:802:C8E:C1	3:A:802:C8E:C5	2.38	0.88
1:A:555:VAL:HG12	1:A:556:THR:CG2	2.04	0.88
1:A:495:LEU:O	1:A:496:LEU:HB2	1.71	0.88
1:A:174:HIS:CD2	1:A:175:THR:N	2.43	0.87
3:A:802:C8E:C14	3:A:802:C8E:H101	2.04	0.87
1:A:518:MSE:HE1	1:A:547:TRP:CZ3	2.10	0.87
1:A:245:LEU:CD2	1:A:245:LEU:C	2.45	0.86
3:A:803:C8E:H112	3:A:803:C8E:H162	1.57	0.86
1:A:174:HIS:C	1:A:174:HIS:HD2	1.82	0.86
1:A:10:VAL:HG12	1:A:11:THR:N	1.90	0.85
1:A:13:ASN:C	1:A:13:ASN:ND2	2.35	0.84
1:A:174:HIS:HD2	1:A:175:THR:N	1.75	0.84
1:A:426:THR:HG22	1:A:431:TRP:HE1	1.41	0.84
1:A:9:VAL:HG11	1:A:19:ARG:CD	2.05	0.84
1:A:151:ASN:C	1:A:152:TYR:HD2	1.85	0.84
1:A:464:VAL:CG1	3:A:804:C8E:H51	2.08	0.84
1:A:242:THR:CG2	1:A:277:TYR:CE2	2.60	0.83
1:A:98:GLN:HE21	1:A:225:ASN:HD22	1.26	0.83
1:A:426:THR:CG2	1:A:431:TRP:HE1	1.90	0.83
1:A:62:GLN:HE21	1:A:62:GLN:HA	1.42	0.83
1:A:358:ARG:C	3:A:800:C8E:C7	2.51	0.83
1:A:95:ASP:O	1:A:96:LEU:HB2	1.79	0.83
1:A:518:MSE:HG3	1:A:549:LEU:HD12	1.60	0.83
1:A:556:THR:OG1	1:A:557:SER:N	2.08	0.83
1:A:559:LEU:C	1:A:559:LEU:CD2	2.49	0.83
1:A:159:GLN:HA	1:A:160:LEU:HB3	1.60	0.82
1:A:242:THR:HG22	1:A:277:TYR:CE2	2.15	0.82
1:A:174:HIS:CE1	1:A:176:HIS:CE1	2.68	0.82
1:A:89:GLY:CA	1:A:90:VAL:C	2.38	0.82
1:A:342:LEU:HD11	3:A:803:C8E:C5	2.05	0.82
1:A:559:LEU:O	1:A:559:LEU:CD2	2.25	0.82
1:A:174:HIS:CE1	1:A:176:HIS:CD2	2.68	0.82
1:A:511:LEU:N	1:A:511:LEU:CD1	2.43	0.82
1:A:13:ASN:ND2	1:A:15:PHE:H	1.77	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ASN:C	1:A:148:SER:OG	2.23	0.81
1:A:518:MSE:HE1	1:A:547:TRP:HZ3	1.41	0.81
1:A:89:GLY:HA3	1:A:91:SER:CA	2.11	0.81
1:A:406:GLY:CA	1:A:452:LYS:CE	2.58	0.81
1:A:174:HIS:CD2	1:A:175:THR:O	2.33	0.81
1:A:488:ASN:CG	1:A:491:THR:HG22	2.06	0.81
1:A:407:ASN:C	1:A:407:ASN:HD22	1.88	0.80
1:A:509:TRP:NE1	1:A:511:LEU:HD11	1.97	0.80
1:A:10:VAL:O	1:A:12:ALA:N	2.15	0.80
1:A:88:ALA:O	1:A:92:GLY:CA	2.30	0.80
1:A:224:ASP:CG	1:A:226:ARG:HH21	1.90	0.80
1:A:358:ARG:O	3:A:800:C8E:C7	2.29	0.79
1:A:509:TRP:CD1	1:A:511:LEU:HD11	2.17	0.79
1:A:85:LEU:CD2	1:A:85:LEU:C	2.55	0.79
3:A:802:C8E:H101	3:A:802:C8E:H142	1.64	0.79
1:A:153:ASP:OD1	1:A:154:VAL:N	2.16	0.79
1:A:120:SER:CB	1:A:393:TYR:CZ	2.65	0.79
1:A:144:TRP:CD1	1:A:144:TRP:C	2.61	0.79
1:A:244:LYS:NZ	1:A:246:TYR:HB2	1.98	0.79
1:A:362:ASN:ND2	1:A:365:PHE:H	1.79	0.79
3:A:802:C8E:C14	3:A:802:C8E:C10	2.61	0.79
1:A:98:GLN:NE2	1:A:225:ASN:HD22	1.80	0.78
1:A:245:LEU:HD22	1:A:246:TYR:N	1.97	0.78
1:A:406:GLY:HA3	1:A:452:LYS:HE2	1.66	0.78
1:A:406:GLY:HA3	1:A:452:LYS:HE3	1.59	0.78
1:A:62:GLN:NE2	1:A:62:GLN:HA	1.96	0.78
1:A:56:GLN:HG3	1:A:64:SER:HB3	1.65	0.78
1:A:558:HIS:HB2	1:A:593:THR:O	1.84	0.78
1:A:405:TYR:CD2	1:A:451:LEU:HD13	2.19	0.77
1:A:370:THR:H	3:A:800:C8E:H81	1.50	0.77
1:A:555:VAL:HB	1:A:559:LEU:HD13	1.67	0.77
1:A:405:TYR:CD2	1:A:451:LEU:CD1	2.68	0.77
1:A:18:PRO:C	1:A:21:THR:HG22	2.02	0.77
1:A:570:ASP:HB2	1:A:584:ARG:HE	1.50	0.77
1:A:569:PHE:CD1	1:A:569:PHE:N	2.52	0.76
1:A:53:ASP:HB3	1:A:502:GLN:HE22	1.49	0.76
1:A:206:LEU:HB2	1:A:218:VAL:CG2	2.16	0.76
1:A:558:HIS:CB	1:A:593:THR:O	2.34	0.76
1:A:569:PHE:HD1	1:A:569:PHE:N	1.83	0.76
1:A:131:THR:O	1:A:131:THR:OG1	2.02	0.76
3:A:803:C8E:H202	3:A:803:C8E:H32	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:TYR:CE1	1:A:540:LYS:HG3	2.20	0.76
1:A:358:ARG:C	3:A:800:C8E:H72	2.10	0.76
1:A:159:GLN:HA	1:A:160:LEU:CB	2.16	0.75
1:A:160:LEU:HD23	1:A:166:VAL:CG2	2.17	0.75
1:A:26:THR:HG22	1:A:110:ILE:HG23	1.68	0.75
1:A:358:ARG:O	3:A:800:C8E:H82	1.83	0.75
1:A:245:LEU:CD2	1:A:246:TYR:O	2.35	0.74
1:A:571:LYS:HE2	1:A:572:ASP:O	1.87	0.74
1:A:263:SER:CB	1:A:302:ASN:ND2	2.50	0.74
1:A:447:ASP:OD1	4:A:870:HOH:O	2.04	0.74
1:A:342:LEU:HD11	3:A:803:C8E:H21	1.68	0.74
1:A:245:LEU:C	1:A:245:LEU:HD22	2.12	0.74
3:A:804:C8E:C7	3:A:804:C8E:H32	2.17	0.74
1:A:242:THR:HG22	1:A:277:TYR:CZ	2.22	0.74
1:A:405:TYR:HD2	1:A:451:LEU:HD13	1.53	0.73
1:A:445:ASP:OD1	1:A:445:ASP:N	2.21	0.73
1:A:407:ASN:HD22	1:A:408:PRO:N	1.87	0.73
1:A:31:ARG:NH1	1:A:35:ASP:OD1	2.20	0.73
1:A:242:THR:HG21	1:A:277:TYR:HH	1.54	0.73
3:A:802:C8E:H142	3:A:802:C8E:C10	2.19	0.73
1:A:42:VAL:HG11	1:A:96:LEU:HD13	1.71	0.73
1:A:77:LEU:HD13	1:A:121:ASP:HB3	1.70	0.72
1:A:527:TYR:CE1	1:A:540:LYS:CG	2.71	0.72
1:A:174:HIS:NE2	1:A:176:HIS:CD2	2.57	0.72
1:A:13:ASN:HD22	1:A:15:PHE:H	1.36	0.71
1:A:245:LEU:HD21	1:A:246:TYR:O	1.90	0.71
1:A:583:GLY:O	1:A:584:ARG:HB2	1.90	0.71
1:A:400:GLN:O	1:A:406:GLY:O	2.09	0.71
1:A:526:ARG:HD2	4:A:872:HOH:O	1.89	0.71
1:A:407:ASN:HD22	1:A:408:PRO:CD	2.03	0.70
1:A:495:LEU:O	1:A:496:LEU:CB	2.39	0.70
1:A:88:ALA:CB	1:A:293:MSE:HE1	2.21	0.70
1:A:487:ARG:NH1	1:A:492:ASP:O	2.24	0.70
3:A:802:C8E:H52	3:A:802:C8E:H12	0.74	0.70
1:A:407:ASN:C	1:A:407:ASN:ND2	2.48	0.70
1:A:567:ASN:HA	4:A:814:HOH:O	1.91	0.70
3:A:803:C8E:H82	3:A:805:C8E:H11	1.74	0.70
1:A:323:THR:HG23	1:A:324:PRO:HD2	1.73	0.70
3:A:804:C8E:H32	3:A:804:C8E:H71	1.73	0.70
1:A:511:LEU:N	1:A:511:LEU:HD12	2.05	0.70
1:A:120:SER:HB3	1:A:393:TYR:CZ	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:805:C8E:H202	4:A:832:HOH:O	1.92	0.69
1:A:588:LEU:HD13	1:A:589:SER:N	2.07	0.69
1:A:263:SER:CB	1:A:302:ASN:HD22	2.01	0.69
1:A:174:HIS:HD2	1:A:175:THR:CA	2.05	0.69
1:A:407:ASN:ND2	1:A:409:ASN:H	1.91	0.69
1:A:85:LEU:O	1:A:87:LEU:HD13	1.93	0.68
1:A:413:GLU:HG2	1:A:443:LEU:HA	1.74	0.68
1:A:175:THR:O	1:A:176:HIS:CB	2.42	0.68
1:A:197:PHE:CD2	1:A:227:THR:OG1	2.46	0.68
1:A:226:ARG:NH2	1:A:244:LYS:HE2	2.03	0.68
1:A:174:HIS:NE2	1:A:175:THR:O	2.27	0.68
1:A:448:ASP:O	1:A:449:HIS:HB2	1.94	0.68
1:A:53:ASP:HB3	1:A:502:GLN:NE2	2.08	0.68
1:A:83:VAL:HG12	1:A:83:VAL:O	1.94	0.68
1:A:174:HIS:CD2	1:A:175:THR:C	2.72	0.67
1:A:198:LEU:HD12	1:A:199:SER:CA	2.24	0.67
1:A:397:ASN:OD1	1:A:400:GLN:HG3	1.94	0.67
1:A:411:ASP:H	1:A:455:ASN:HD21	1.42	0.67
1:A:405:TYR:HD2	1:A:451:LEU:CD1	2.06	0.67
1:A:564:LYS:HG2	1:A:565:ILE:N	2.09	0.67
1:A:463:GLY:O	3:A:804:C8E:H191	1.95	0.67
1:A:311:ILE:O	1:A:311:ILE:HG22	1.93	0.67
1:A:405:TYR:CE2	1:A:451:LEU:CD1	2.78	0.67
1:A:19:ARG:HB3	1:A:19:ARG:HH11	1.58	0.66
1:A:74:SER:HA	1:A:93:SER:HB2	1.75	0.66
1:A:506:GLN:HE22	1:A:519:THR:CG2	2.07	0.66
1:A:242:THR:CG2	1:A:277:TYR:CE1	2.78	0.66
1:A:568:LEU:HB3	1:A:569:PHE:CE1	2.31	0.66
1:A:531:TYR:O	1:A:533:SER:N	2.29	0.66
1:A:89:GLY:HA2	1:A:92:GLY:CA	2.26	0.66
1:A:527:TYR:CD1	1:A:540:LYS:HG3	2.30	0.65
1:A:44:ASP:OD1	1:A:47:ARG:NH1	2.29	0.65
1:A:43:ASN:N	4:A:866:HOH:O	2.19	0.65
1:A:245:LEU:CD2	1:A:246:TYR:C	2.69	0.65
1:A:534:TYR:HA	1:A:535:PRO:C	2.22	0.65
1:A:175:THR:O	1:A:176:HIS:HB2	1.96	0.65
1:A:518:MSE:CE	1:A:547:TRP:CZ3	2.80	0.65
3:A:803:C8E:H82	3:A:805:C8E:C1	2.26	0.65
1:A:151:ASN:O	1:A:152:TYR:HD2	1.79	0.65
1:A:206:LEU:CB	1:A:218:VAL:CG2	2.75	0.65
1:A:358:ARG:O	3:A:800:C8E:H81	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:HIS:HE1	1:A:176:HIS:CE1	2.14	0.65
1:A:558:HIS:ND1	1:A:558:HIS:N	2.45	0.65
1:A:113:PRO:HD3	1:A:417:GLN:CD	2.21	0.65
1:A:509:TRP:CD1	1:A:511:LEU:CD1	2.79	0.64
1:A:52:VAL:HG12	1:A:52:VAL:O	1.97	0.64
1:A:224:ASP:OD1	1:A:224:ASP:C	2.39	0.64
1:A:245:LEU:HD23	1:A:273:LYS:O	1.98	0.64
3:A:802:C8E:H11	3:A:802:C8E:H172	1.79	0.64
1:A:324:PRO:C	1:A:326:THR:H	2.05	0.64
1:A:102:ALA:C	1:A:103:LEU:HD23	2.22	0.64
1:A:77:LEU:HD21	1:A:79:LEU:HD21	1.79	0.63
1:A:144:TRP:HD1	1:A:144:TRP:O	1.81	0.63
1:A:242:THR:HG21	1:A:277:TYR:CE1	2.26	0.63
1:A:159:GLN:HB3	1:A:164:THR:O	1.97	0.63
1:A:527:TYR:HE1	1:A:540:LYS:CG	2.09	0.63
1:A:82:GLY:HA2	1:A:83:VAL:CB	2.29	0.63
1:A:85:LEU:C	1:A:87:LEU:H	2.06	0.63
1:A:398:LEU:CD2	1:A:398:LEU:N	2.52	0.62
1:A:362:ASN:CG	1:A:365:PHE:CE2	2.77	0.62
1:A:13:ASN:ND2	1:A:15:PHE:N	2.46	0.62
1:A:89:GLY:HA2	1:A:92:GLY:HA2	1.81	0.62
1:A:198:LEU:HD13	1:A:199:SER:N	2.14	0.62
1:A:82:GLY:HA2	1:A:83:VAL:HB	1.80	0.62
1:A:85:LEU:C	1:A:87:LEU:N	2.56	0.62
1:A:506:GLN:HE21	1:A:519:THR:HB	1.64	0.62
1:A:151:ASN:O	1:A:152:TYR:CD2	2.52	0.62
1:A:45:VAL:O	1:A:46:LEU:HG	2.00	0.62
1:A:518:MSE:HG3	1:A:549:LEU:HD13	1.81	0.62
1:A:164:THR:OG1	1:A:208:HIS:HD2	1.83	0.61
1:A:506:GLN:HE22	1:A:519:THR:CB	2.13	0.61
1:A:53:ASP:OD1	1:A:53:ASP:C	2.43	0.61
1:A:82:GLY:HA2	1:A:83:VAL:O	2.00	0.61
1:A:567:ASN:C	4:A:814:HOH:O	2.44	0.61
1:A:495:LEU:O	1:A:496:LEU:CD1	2.48	0.61
1:A:120:SER:HB3	1:A:393:TYR:CE1	2.33	0.60
1:A:68:ILE:O	1:A:71:THR:HG23	2.01	0.60
1:A:334:ASP:OD2	1:A:336:ARG:NH2	2.33	0.60
1:A:398:LEU:H	1:A:398:LEU:HD22	1.66	0.60
1:A:405:TYR:HE2	1:A:451:LEU:HD11	1.66	0.60
1:A:506:GLN:NE2	1:A:519:THR:CB	2.63	0.60
1:A:57:ASN:HB3	1:A:579:TYR:CD2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ARG:O	1:A:34:ILE:N	2.35	0.60
1:A:103:LEU:HD21	1:A:201:THR:HG21	1.83	0.60
1:A:406:GLY:HA2	1:A:452:LYS:HE3	1.80	0.60
3:A:803:C8E:H162	3:A:803:C8E:C11	2.29	0.60
1:A:82:GLY:HA2	1:A:83:VAL:C	2.26	0.59
1:A:436:TYR:C	3:A:804:C8E:H202	2.27	0.59
1:A:198:LEU:HD12	1:A:198:LEU:O	2.00	0.59
1:A:529:LYS:NZ	1:A:538:THR:HG22	2.17	0.59
3:A:805:C8E:O21	3:A:805:C8E:H161	2.03	0.59
1:A:17:GLN:HG3	1:A:21:THR:CG2	2.33	0.58
1:A:47:ARG:HG3	1:A:48:ARG:N	2.18	0.58
1:A:98:GLN:NE2	4:A:823:HOH:O	2.36	0.58
1:A:511:LEU:N	1:A:511:LEU:HD13	2.19	0.58
1:A:588:LEU:HD13	1:A:588:LEU:C	2.26	0.58
1:A:175:THR:O	1:A:176:HIS:CG	2.56	0.58
1:A:224:ASP:OD2	1:A:226:ARG:NH2	2.35	0.58
1:A:13:ASN:O	1:A:14:ARG:HB2	2.03	0.58
1:A:88:ALA:HB3	1:A:293:MSE:HE1	1.86	0.58
1:A:491:THR:HG23	1:A:493:THR:HG23	1.85	0.58
1:A:296:TYR:HE1	1:A:321:MSE:CG	2.17	0.57
1:A:380:ILE:O	1:A:381:GLU:C	2.46	0.57
1:A:553:TYR:CE2	1:A:555:VAL:HG22	2.39	0.57
1:A:153:ASP:OD1	1:A:153:ASP:C	2.45	0.57
1:A:436:TYR:O	3:A:804:C8E:H202	2.04	0.57
1:A:447:ASP:O	1:A:448:ASP:HB2	2.04	0.57
1:A:116:ALA:HA	1:A:370:THR:CG2	2.34	0.57
3:A:804:C8E:H71	3:A:804:C8E:C3	2.35	0.57
1:A:89:GLY:CA	1:A:92:GLY:HA2	2.33	0.57
1:A:342:LEU:C	1:A:342:LEU:HD12	2.29	0.57
1:A:405:TYR:CE2	1:A:451:LEU:HD11	2.40	0.57
1:A:495:LEU:O	1:A:496:LEU:HD13	2.05	0.57
1:A:534:TYR:CG	1:A:535:PRO:HA	2.39	0.57
1:A:438:ASN:C	1:A:438:ASN:OD1	2.47	0.57
1:A:553:TYR:HD2	1:A:555:VAL:CG2	2.18	0.57
1:A:323:THR:HG23	1:A:324:PRO:CD	2.35	0.57
1:A:116:ALA:HA	1:A:370:THR:HG22	1.87	0.57
1:A:553:TYR:HD2	1:A:555:VAL:HG23	1.70	0.56
1:A:518:MSE:CE	1:A:547:TRP:CE3	2.88	0.56
1:A:10:VAL:O	1:A:11:THR:C	2.48	0.56
1:A:87:LEU:CD1	1:A:87:LEU:N	2.65	0.56
1:A:502:GLN:HG2	1:A:523:LEU:HD22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:MSE:HE3	1:A:547:TRP:CE3	2.40	0.56
1:A:592:TYR:CE1	1:A:594:PHE:HB3	2.41	0.56
1:A:52:VAL:HG22	1:A:68:ILE:HD13	1.87	0.56
1:A:160:LEU:CD2	1:A:166:VAL:HG23	2.35	0.56
1:A:113:PRO:HD3	1:A:417:GLN:NE2	2.20	0.56
1:A:567:ASN:ND2	1:A:571:LYS:H	2.03	0.56
1:A:7:THR:O	1:A:7:THR:HG22	2.05	0.56
1:A:120:SER:HB2	1:A:393:TYR:CD1	2.35	0.56
1:A:406:GLY:HA3	1:A:407:ASN:HB2	1.88	0.56
1:A:491:THR:HG23	1:A:493:THR:H	1.71	0.56
1:A:433:ILE:HD12	3:A:802:C8E:H13	1.88	0.56
1:A:531:TYR:O	1:A:532:SER:C	2.48	0.56
1:A:568:LEU:O	1:A:584:ARG:NH2	2.39	0.56
1:A:10:VAL:N	1:A:108:GLU:OE1	2.39	0.55
1:A:86:ASN:O	1:A:87:LEU:CD1	2.27	0.55
1:A:205:ALA:O	1:A:206:LEU:HD12	2.06	0.55
1:A:218:VAL:HG23	1:A:218:VAL:O	2.05	0.55
1:A:13:ASN:HD21	1:A:15:PHE:HB2	1.70	0.55
1:A:323:THR:O	1:A:326:THR:OG1	2.24	0.55
1:A:558:HIS:O	1:A:559:LEU:HB2	2.07	0.55
1:A:197:PHE:HD2	1:A:227:THR:HG1	1.52	0.55
1:A:407:ASN:HB2	1:A:452:LYS:HE2	1.87	0.55
1:A:226:ARG:HH12	1:A:244:LYS:CD	2.19	0.55
1:A:464:VAL:CG2	3:A:804:C8E:C5	2.84	0.55
1:A:18:PRO:CD	1:A:21:THR:HG21	2.30	0.55
1:A:52:VAL:HG22	1:A:68:ILE:CD1	2.36	0.55
1:A:102:ALA:C	1:A:103:LEU:CD2	2.79	0.55
1:A:144:TRP:CD1	1:A:144:TRP:O	2.58	0.55
1:A:506:GLN:HE22	1:A:519:THR:HB	1.65	0.55
1:A:562:ARG:O	1:A:588:LEU:HD22	2.07	0.55
1:A:115:SER:OG	1:A:119:GLY:O	2.25	0.55
1:A:460:ARG:HE	1:A:462:LYS:HE3	1.71	0.55
1:A:226:ARG:NH1	1:A:244:LYS:CG	2.38	0.55
1:A:153:ASP:HB2	1:A:171:ASP:OD1	2.06	0.54
1:A:436:TYR:O	3:A:804:C8E:C20	2.56	0.54
1:A:80:ILE:O	1:A:83:VAL:CG1	2.55	0.54
1:A:407:ASN:HD22	1:A:408:PRO:HD2	1.72	0.54
1:A:477:HIS:CE1	1:A:507:LEU:HD11	2.42	0.54
1:A:529:LYS:HZ3	1:A:538:THR:HG22	1.72	0.54
1:A:534:TYR:CD1	1:A:534:TYR:C	2.85	0.54
1:A:151:ASN:C	1:A:152:TYR:CD2	2.75	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LEU:HD22	1:A:246:TYR:C	2.32	0.54
1:A:165:ARG:HG2	1:A:207:GLU:HB2	1.89	0.54
1:A:206:LEU:HB2	1:A:218:VAL:HG21	1.88	0.54
1:A:226:ARG:CZ	1:A:244:LYS:HG3	2.29	0.54
1:A:75:HIS:O	1:A:123:ILE:O	2.26	0.54
1:A:244:LYS:HZ2	1:A:246:TYR:HB2	1.71	0.54
1:A:579:TYR:CD1	1:A:579:TYR:N	2.76	0.54
1:A:358:ARG:N	3:A:800:C8E:H71	2.23	0.54
1:A:373:THR:HG23	3:A:803:C8E:H102	1.89	0.54
1:A:362:ASN:ND2	1:A:365:PHE:CE2	2.76	0.54
1:A:120:SER:HB3	1:A:393:TYR:OH	2.09	0.53
1:A:25:PRO:C	1:A:26:THR:CG2	2.81	0.53
1:A:40:THR:O	1:A:41:SER:CB	2.55	0.53
1:A:166:VAL:HG13	1:A:206:LEU:CD1	2.38	0.53
1:A:557:SER:HB3	1:A:558:HIS:CE1	2.42	0.53
1:A:527:TYR:HE1	1:A:540:LYS:CD	2.22	0.53
1:A:21:THR:OG1	1:A:345:LEU:HD11	2.08	0.53
1:A:19:ARG:C	1:A:21:THR:H	2.15	0.53
1:A:296:TYR:HE1	1:A:321:MSE:HG3	1.72	0.53
1:A:464:VAL:CG2	3:A:804:C8E:H51	2.39	0.53
1:A:24:ALA:HB2	4:A:856:HOH:O	2.07	0.53
1:A:69:ARG:HD3	1:A:436:TYR:CZ	2.43	0.53
1:A:558:HIS:O	1:A:592:TYR:CD2	2.60	0.53
1:A:18:PRO:HD2	1:A:21:THR:CG2	2.31	0.53
1:A:85:LEU:O	1:A:86:ASN:C	2.48	0.53
1:A:367:ARG:HH21	3:A:800:C8E:H172	1.72	0.53
1:A:553:TYR:CD2	1:A:555:VAL:HG22	2.43	0.53
1:A:19:ARG:C	1:A:21:THR:N	2.67	0.52
1:A:198:LEU:HD11	1:A:200:LYS:HG3	1.90	0.52
1:A:527:TYR:CE1	1:A:540:LYS:HD2	2.44	0.52
1:A:567:ASN:CA	4:A:814:HOH:O	2.53	0.52
1:A:244:LYS:HZ1	1:A:246:TYR:HB2	1.72	0.52
1:A:98:GLN:HE22	1:A:225:ASN:CB	2.23	0.52
1:A:553:TYR:CD2	1:A:555:VAL:CG2	2.93	0.52
1:A:592:TYR:HE1	1:A:594:PHE:CG	2.28	0.52
1:A:88:ALA:HB3	1:A:293:MSE:CE	2.40	0.52
1:A:74:SER:CA	1:A:93:SER:HB2	2.39	0.51
1:A:98:GLN:HE22	1:A:225:ASN:HB3	1.75	0.51
1:A:261:ILE:HG12	1:A:304:VAL:CG1	2.40	0.51
1:A:400:GLN:O	1:A:407:ASN:N	2.43	0.51
1:A:458:LYS:HD2	1:A:490:ILE:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:THR:HG22	1:A:156:THR:OG1	2.09	0.51
1:A:157:GLN:HB2	1:A:167:THR:HG23	1.91	0.51
1:A:174:HIS:HB2	1:A:198:LEU:HA	1.93	0.51
1:A:319:MSE:HG3	1:A:336:ARG:HG2	1.92	0.51
1:A:451:LEU:C	1:A:452:LYS:CG	2.83	0.51
1:A:151:ASN:C	1:A:151:ASN:OD1	2.53	0.51
1:A:45:VAL:O	1:A:46:LEU:CG	2.59	0.51
1:A:206:LEU:HB2	1:A:218:VAL:HG23	1.90	0.51
1:A:49:LEU:HB3	1:A:50:PRO:HD2	1.93	0.51
1:A:140:ILE:HG12	1:A:154:VAL:HG22	1.92	0.51
1:A:464:VAL:HG21	3:A:804:C8E:C5	2.41	0.50
1:A:513:ASP:O	1:A:554:PRO:HD2	2.11	0.50
1:A:527:TYR:HE1	1:A:540:LYS:HD2	1.77	0.50
1:A:81:ASP:OD2	1:A:131:THR:HG23	2.12	0.50
1:A:426:THR:O	1:A:427:ALA:C	2.55	0.50
1:A:488:ASN:CB	1:A:491:THR:HG22	2.42	0.50
1:A:567:ASN:HD21	1:A:571:LYS:H	1.58	0.50
1:A:68:ILE:HG13	1:A:76:VAL:CG2	2.42	0.50
1:A:80:ILE:O	1:A:83:VAL:HG12	2.12	0.50
1:A:85:LEU:CD2	1:A:87:LEU:HD13	2.32	0.50
1:A:226:ARG:NH1	1:A:226:ARG:HG3	2.26	0.50
1:A:555:VAL:O	1:A:556:THR:CB	2.58	0.50
1:A:89:GLY:CA	1:A:91:SER:H	2.05	0.50
1:A:324:PRO:C	1:A:326:THR:N	2.70	0.50
1:A:398:LEU:N	1:A:398:LEU:HD22	2.22	0.49
1:A:451:LEU:O	1:A:452:LYS:HG2	2.11	0.49
1:A:241:ASP:OD2	1:A:241:ASP:N	2.45	0.49
1:A:559:LEU:HA	1:A:591:SER:O	2.12	0.49
1:A:370:THR:H	3:A:800:C8E:C8	2.21	0.49
1:A:7:THR:O	1:A:7:THR:CG2	2.61	0.49
1:A:406:GLY:N	1:A:452:LYS:HE3	2.27	0.49
3:A:805:C8E:H161	3:A:805:C8E:C20	2.32	0.49
1:A:422:PHE:CD2	3:A:801:C8E:H11	2.48	0.49
1:A:506:GLN:HE22	1:A:519:THR:HG22	1.75	0.49
1:A:373:THR:HG21	3:A:803:C8E:H131	1.94	0.49
1:A:400:GLN:O	1:A:406:GLY:C	2.55	0.49
1:A:414:LYS:HE3	1:A:442:ASP:OD1	2.12	0.49
1:A:568:LEU:N	4:A:814:HOH:O	2.46	0.49
1:A:265:LEU:C	1:A:266:ILE:HG13	2.37	0.49
1:A:23:LEU:O	1:A:24:ALA:HB2	2.12	0.49
1:A:510:GLN:C	1:A:511:LEU:HD12	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:GLY:CA	1:A:484:VAL:HG11	2.43	0.48
1:A:371:TRP:H	1:A:391:THR:HG22	1.77	0.48
1:A:46:LEU:O	1:A:52:VAL:HG11	2.14	0.48
1:A:445:ASP:O	1:A:453:TYR:HD1	1.97	0.48
3:A:803:C8E:H202	3:A:803:C8E:C3	2.39	0.48
1:A:275:TYR:CZ	1:A:290:LEU:HD13	2.48	0.48
1:A:464:VAL:HG21	3:A:804:C8E:H51	1.95	0.48
1:A:464:VAL:HG13	3:A:804:C8E:C4	2.43	0.48
1:A:426:THR:CG2	1:A:431:TRP:NE1	2.69	0.48
1:A:573:TYR:CE1	1:A:581:THR:HG21	2.49	0.48
1:A:79:LEU:HA	1:A:84:ARG:HA	1.95	0.48
1:A:89:GLY:HA2	1:A:92:GLY:N	2.29	0.48
3:A:805:C8E:H142	3:A:805:C8E:H172	1.41	0.48
1:A:63:LEU:HD23	1:A:63:LEU:N	2.29	0.47
1:A:495:LEU:HA	1:A:495:LEU:HD23	1.56	0.47
1:A:70:GLY:HA3	1:A:484:VAL:HG11	1.95	0.47
1:A:370:THR:HB	4:A:839:HOH:O	2.13	0.47
1:A:44:ASP:HA	1:A:47:ARG:HD3	1.95	0.47
1:A:512:TYR:CD2	1:A:512:TYR:N	2.82	0.47
1:A:53:ASP:OD1	1:A:53:ASP:O	2.31	0.47
1:A:77:LEU:CD1	1:A:121:ASP:HB3	2.43	0.47
1:A:319:MSE:CG	1:A:336:ARG:HG2	2.44	0.47
1:A:43:ASN:CG	4:A:866:HOH:O	2.56	0.47
1:A:147:ASN:HD22	1:A:147:ASN:HA	1.51	0.47
1:A:221:TYR:CD1	1:A:221:TYR:C	2.92	0.47
1:A:488:ASN:HB3	1:A:491:THR:HG22	1.97	0.47
1:A:269:TYR:HA	1:A:295:GLN:O	2.14	0.47
1:A:85:LEU:C	1:A:85:LEU:HD23	2.38	0.47
1:A:98:GLN:NE2	1:A:225:ASN:CB	2.78	0.47
1:A:72:ASN:OD1	1:A:498:ARG:NH2	2.41	0.47
1:A:275:TYR:CE2	1:A:290:LEU:HD13	2.49	0.47
1:A:322:THR:HG22	1:A:326:THR:HG21	1.97	0.46
1:A:319:MSE:HG2	1:A:336:ARG:HG3	1.97	0.46
1:A:342:LEU:CD1	3:A:803:C8E:H21	2.42	0.46
1:A:13:ASN:ND2	1:A:13:ASN:O	2.49	0.46
1:A:323:THR:HG22	1:A:326:THR:OG1	2.16	0.46
1:A:377:TRP:CD1	1:A:377:TRP:C	2.89	0.46
1:A:49:LEU:HB3	1:A:50:PRO:CD	2.46	0.46
1:A:80:ILE:HD13	1:A:129:ILE:HB	1.96	0.46
1:A:245:LEU:HD22	1:A:246:TYR:CA	2.46	0.46
1:A:523:LEU:HD22	1:A:523:LEU:HA	1.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ARG:C	3:A:800:C8E:H71	2.37	0.46
1:A:383:TYR:OH	1:A:426:THR:HB	2.16	0.46
1:A:17:GLN:HG3	1:A:21:THR:HG21	1.97	0.46
1:A:132:THR:HG22	1:A:133:ARG:N	2.31	0.46
3:A:800:C8E:H141	3:A:800:C8E:H112	1.37	0.46
1:A:88:ALA:O	1:A:92:GLY:C	2.59	0.45
1:A:344:GLY:C	3:A:803:C8E:H191	2.41	0.45
1:A:423:GLU:HB2	1:A:432:ARG:HG3	1.98	0.45
1:A:17:GLN:HE21	1:A:21:THR:HG23	1.81	0.45
1:A:559:LEU:O	1:A:559:LEU:CG	2.63	0.45
1:A:541:MSE:CE	1:A:574:GLU:HB2	2.46	0.45
1:A:379:PHE:O	1:A:380:ILE:HG13	2.15	0.45
1:A:17:GLN:HE21	1:A:22:VAL:HG22	1.82	0.45
1:A:323:THR:CG2	1:A:324:PRO:N	2.78	0.45
1:A:451:LEU:C	1:A:452:LYS:HG2	2.41	0.45
1:A:245:LEU:CD2	1:A:246:TYR:CA	2.94	0.45
1:A:511:LEU:HB3	1:A:512:TYR:CD2	2.51	0.45
3:A:802:C8E:H101	3:A:802:C8E:H141	1.95	0.45
1:A:8:LEU:HD23	1:A:16:GLU:OE2	2.16	0.45
1:A:146:SER:O	1:A:147:ASN:HB2	2.17	0.45
1:A:359:SER:HB2	3:A:800:C8E:H72	1.98	0.45
1:A:82:GLY:CA	1:A:83:VAL:HB	2.47	0.45
1:A:558:HIS:HB3	1:A:593:THR:O	2.16	0.45
1:A:576:VAL:O	1:A:579:TYR:HD1	2.01	0.44
3:A:802:C8E:H142	3:A:802:C8E:H102	1.96	0.44
1:A:358:ARG:CA	3:A:800:C8E:H71	2.48	0.44
1:A:527:TYR:CE1	1:A:540:LYS:CD	3.01	0.44
1:A:353:PHE:HB3	3:A:803:C8E:H171	1.99	0.44
1:A:470:PHE:CE1	1:A:477:HIS:CG	3.05	0.44
1:A:496:LEU:HD21	1:A:529:LYS:HG3	1.98	0.44
1:A:25:PRO:C	1:A:26:THR:HG23	2.43	0.44
1:A:422:PHE:CG	3:A:801:C8E:H11	2.53	0.44
1:A:448:ASP:O	1:A:449:HIS:CB	2.62	0.44
1:A:529:LYS:NZ	1:A:538:THR:CG2	2.80	0.44
1:A:159:GLN:H	1:A:159:GLN:HG2	1.62	0.44
1:A:10:VAL:HG13	1:A:14:ARG:C	2.42	0.44
1:A:164:THR:OG1	1:A:208:HIS:CD2	2.67	0.44
1:A:197:PHE:HD2	1:A:227:THR:OG1	1.93	0.44
1:A:379:PHE:C	1:A:380:ILE:HG13	2.43	0.44
1:A:159:GLN:CA	1:A:160:LEU:CB	2.88	0.43
1:A:588:LEU:HD22	1:A:588:LEU:HA	1.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:MSE:HG2	1:A:336:ARG:CG	2.48	0.43
1:A:323:THR:HG23	1:A:324:PRO:N	2.32	0.43
1:A:573:TYR:CD1	1:A:573:TYR:C	2.95	0.43
1:A:349:GLY:O	1:A:351:PHE:N	2.51	0.43
1:A:584:ARG:HD3	1:A:584:ARG:HA	1.21	0.43
1:A:349:GLY:O	1:A:351:PHE:HD1	2.01	0.43
1:A:341:TYR:CD1	1:A:341:TYR:C	2.96	0.43
1:A:99:PHE:HA	1:A:100:PRO:HD3	1.72	0.43
1:A:174:HIS:CD2	1:A:174:HIS:O	2.68	0.43
1:A:291:ASP:HA	1:A:326:THR:HG23	2.00	0.43
1:A:406:GLY:HA3	1:A:407:ASN:CB	2.49	0.43
1:A:169:LEU:CD1	1:A:170:GLY:N	2.81	0.43
1:A:360:ASP:O	1:A:367:ARG:HA	2.19	0.43
1:A:541:MSE:HE2	1:A:574:GLU:O	2.18	0.43
1:A:103:LEU:HD23	1:A:103:LEU:H	1.71	0.42
1:A:88:ALA:HB2	1:A:320:GLN:OE1	2.19	0.42
1:A:105:GLN:OE1	1:A:133:ARG:HD2	2.19	0.42
1:A:460:ARG:NE	1:A:462:LYS:HE3	2.34	0.42
1:A:120:SER:CA	1:A:393:TYR:CZ	3.02	0.42
1:A:261:ILE:HG12	1:A:304:VAL:HG12	2.01	0.42
1:A:402:TYR:HE2	1:A:408:PRO:HB3	1.85	0.42
1:A:9:VAL:HG13	1:A:19:ARG:HD3	1.84	0.42
1:A:111:ARG:NH2	1:A:465:GLU:OE2	2.44	0.42
1:A:152:TYR:CD2	1:A:152:TYR:N	2.87	0.42
1:A:342:LEU:HD12	1:A:343:THR:N	2.34	0.42
1:A:592:TYR:CE1	1:A:594:PHE:CD1	3.08	0.42
1:A:116:ALA:CA	1:A:370:THR:CG2	2.98	0.42
1:A:167:THR:C	1:A:168:LEU:HG	2.44	0.42
1:A:451:LEU:HA	1:A:451:LEU:HD22	1.74	0.42
1:A:512:TYR:C	1:A:514:PHE:H	2.28	0.42
3:A:803:C8E:H71	3:A:803:C8E:H41	1.78	0.42
1:A:89:GLY:HA3	1:A:91:SER:C	2.44	0.42
1:A:13:ASN:HD22	1:A:14:ARG:N	2.16	0.42
1:A:196:GLY:HA3	1:A:228:ASN:HB2	2.02	0.42
1:A:531:TYR:C	1:A:533:SER:N	2.78	0.42
1:A:265:LEU:C	1:A:265:LEU:HD13	2.45	0.41
1:A:322:THR:HG22	1:A:326:THR:CG2	2.50	0.41
1:A:541:MSE:HE3	1:A:574:GLU:HB2	2.03	0.41
1:A:164:THR:HA	1:A:207:GLU:O	2.20	0.41
1:A:512:TYR:C	1:A:514:PHE:N	2.78	0.41
1:A:166:VAL:HG13	1:A:206:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:ASP:CG	1:A:584:ARG:HG2	2.45	0.41
1:A:311:ILE:HD11	3:A:803:C8E:C1	2.50	0.41
1:A:404:PHE:O	1:A:404:PHE:HD2	2.04	0.41
1:A:415:SER:HB2	1:A:440:VAL:HG22	2.01	0.41
1:A:17:GLN:HA	1:A:18:PRO:HD3	1.85	0.41
1:A:23:LEU:HD22	1:A:386:ILE:HD13	2.03	0.41
1:A:98:GLN:NE2	1:A:225:ASN:ND2	2.59	0.41
1:A:267:THR:HG22	1:A:267:THR:O	2.21	0.41
1:A:68:ILE:O	1:A:69:ARG:C	2.61	0.41
1:A:407:ASN:ND2	1:A:408:PRO:HD2	2.35	0.41
1:A:452:LYS:HE2	1:A:452:LYS:HB3	1.76	0.41
1:A:23:LEU:HD11	1:A:352:THR:HG22	2.01	0.41
1:A:49:LEU:CB	1:A:50:PRO:CD	2.98	0.41
1:A:98:GLN:HE21	1:A:98:GLN:HB3	1.72	0.41
1:A:123:ILE:HG12	1:A:392:SER:HB2	2.03	0.41
1:A:257:ASN:OD1	1:A:262:LYS:HE2	2.21	0.41
1:A:445:ASP:O	1:A:453:TYR:CD1	2.74	0.41
1:A:488:ASN:OD1	1:A:488:ASN:C	2.63	0.40
1:A:359:SER:N	3:A:800:C8E:H72	2.36	0.40
1:A:530:ASP:OD1	1:A:530:ASP:C	2.59	0.40
1:A:160:LEU:HD23	1:A:166:VAL:HG23	1.99	0.40
3:A:805:C8E:C20	4:A:832:HOH:O	2.61	0.40
1:A:88:ALA:C	1:A:92:GLY:HA2	2.39	0.40
1:A:344:GLY:O	3:A:803:C8E:H191	2.22	0.40
1:A:348:VAL:O	1:A:349:GLY:O	2.40	0.40
1:A:445:ASP:O	1:A:453:TYR:HA	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ARG:NH1	1:A:427:ALA:O[6_655]	1.77	0.43

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	534/594 (90%)	468 (88%)	46 (9%)	20 (4%)	2 6

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	THR
1	A	41	SER
1	A	86	ASN
1	A	147	ASN
1	A	449	HIS
1	A	450	THR
1	A	496	LEU
1	A	559	LEU
1	A	584	ARG
1	A	46	LEU
1	A	121	ASP
1	A	349	GLY
1	A	451	LEU
1	A	495	LEU
1	A	532	SER
1	A	556	THR
1	A	83	VAL
1	A	89	GLY
1	A	91	SER
1	A	92	GLY

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	C8E	A	804	-	20,20,20	0.35	0	19,19,19	0.51	0
3	C8E	A	800	-	20,20,20	0.39	0	19,19,19	0.76	1 (5%)
3	C8E	A	801	-	20,20,20	0.34	0	19,19,19	0.60	0
3	C8E	A	805	-	20,20,20	0.41	0	19,19,19	0.31	0
3	C8E	A	803	-	20,20,20	0.43	0	19,19,19	0.67	0
3	C8E	A	802	-	20,20,20	0.36	0	19,19,19	0.77	1 (5%)

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
3	C8E	A	804	-	-	12/18/18/18	-
3	C8E	A	800	-	-	10/18/18/18	-
3	C8E	A	801	-	-	12/18/18/18	-
3	C8E	A	805	-	-	16/18/18/18	-
3	C8E	A	803	-	-	11/18/18/18	-
3	C8E	A	802	-	-	10/18/18/18	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	C8E	C10-O9-C8	-2.15	103.87	113.26
3	A	800	C8E	C6-C7-C8	-2.09	104.37	113.47

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	804	C8E	C11-C10-O9-C8
3	A	805	C8E	C17-C16-O15-C14
3	A	805	C8E	C16-C17-O18-C19
3	A	800	C8E	C14-C13-O12-C11
3	A	803	C8E	C14-C13-O12-C11
3	A	805	C8E	C11-C10-O9-C8
3	A	802	C8E	C10-C11-O12-C13
3	A	803	C8E	C7-C8-O9-C10
3	A	804	C8E	O9-C10-C11-O12
3	A	800	C8E	O9-C10-C11-O12
3	A	803	C8E	O15-C16-C17-O18
3	A	805	C8E	O9-C10-C11-O12
3	A	800	C8E	O12-C13-C14-O15
3	A	804	C8E	O15-C16-C17-O18
3	A	803	C8E	C2-C3-C4-C5
3	A	805	C8E	O15-C16-C17-O18
3	A	800	C8E	C6-C7-C8-O9
3	A	801	C8E	O9-C10-C11-O12
3	A	801	C8E	O12-C13-C14-O15
3	A	802	C8E	O12-C13-C14-O15
3	A	805	C8E	O18-C19-C20-O21
3	A	800	C8E	O15-C16-C17-O18
3	A	801	C8E	O18-C19-C20-O21
3	A	801	C8E	C6-C7-C8-O9
3	A	805	C8E	C2-C3-C4-C5
3	A	803	C8E	C5-C6-C7-C8
3	A	801	C8E	C4-C5-C6-C7
3	A	802	C8E	O18-C19-C20-O21
3	A	805	C8E	C6-C7-C8-O9
3	A	802	C8E	C6-C7-C8-O9
3	A	804	C8E	O12-C13-C14-O15
3	A	805	C8E	C5-C6-C7-C8
3	A	804	C8E	C3-C4-C5-C6
3	A	805	C8E	C3-C4-C5-C6
3	A	805	C8E	C1-C2-C3-C4
3	A	804	C8E	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
3	A	801	C8E	C5-C6-C7-C8
3	A	801	C8E	O15-C16-C17-O18
3	A	801	C8E	C16-C17-O18-C19
3	A	803	C8E	C10-C11-O12-C13
3	A	805	C8E	C10-C11-O12-C13
3	A	805	C8E	C14-C13-O12-C11
3	A	800	C8E	C10-C11-O12-C13
3	A	803	C8E	C13-C14-O15-C16
3	A	801	C8E	C13-C14-O15-C16
3	A	800	C8E	C13-C14-O15-C16
3	A	802	C8E	O9-C10-C11-O12
3	A	802	C8E	C2-C3-C4-C5
3	A	800	C8E	C17-C16-O15-C14
3	A	804	C8E	C14-C13-O12-C11
3	A	803	C8E	C11-C10-O9-C8
3	A	800	C8E	C7-C8-O9-C10
3	A	803	C8E	C4-C5-C6-C7
3	A	805	C8E	C4-C5-C6-C7
3	A	804	C8E	C17-C16-O15-C14
3	A	801	C8E	C20-C19-O18-C17
3	A	801	C8E	C1-C2-C3-C4
3	A	803	C8E	C16-C17-O18-C19
3	A	800	C8E	C16-C17-O18-C19
3	A	802	C8E	C17-C16-O15-C14
3	A	804	C8E	C10-C11-O12-C13
3	A	803	C8E	C1-C2-C3-C4
3	A	802	C8E	O15-C16-C17-O18
3	A	805	C8E	C7-C8-O9-C10
3	A	802	C8E	C16-C17-O18-C19
3	A	804	C8E	C20-C19-O18-C17
3	A	801	C8E	C3-C4-C5-C6
3	A	804	C8E	C2-C3-C4-C5
3	A	802	C8E	C3-C4-C5-C6
3	A	804	C8E	C7-C8-O9-C10
3	A	805	C8E	C20-C19-O18-C17

There are no ring outliers.

6 monomers are involved in 68 short contacts:

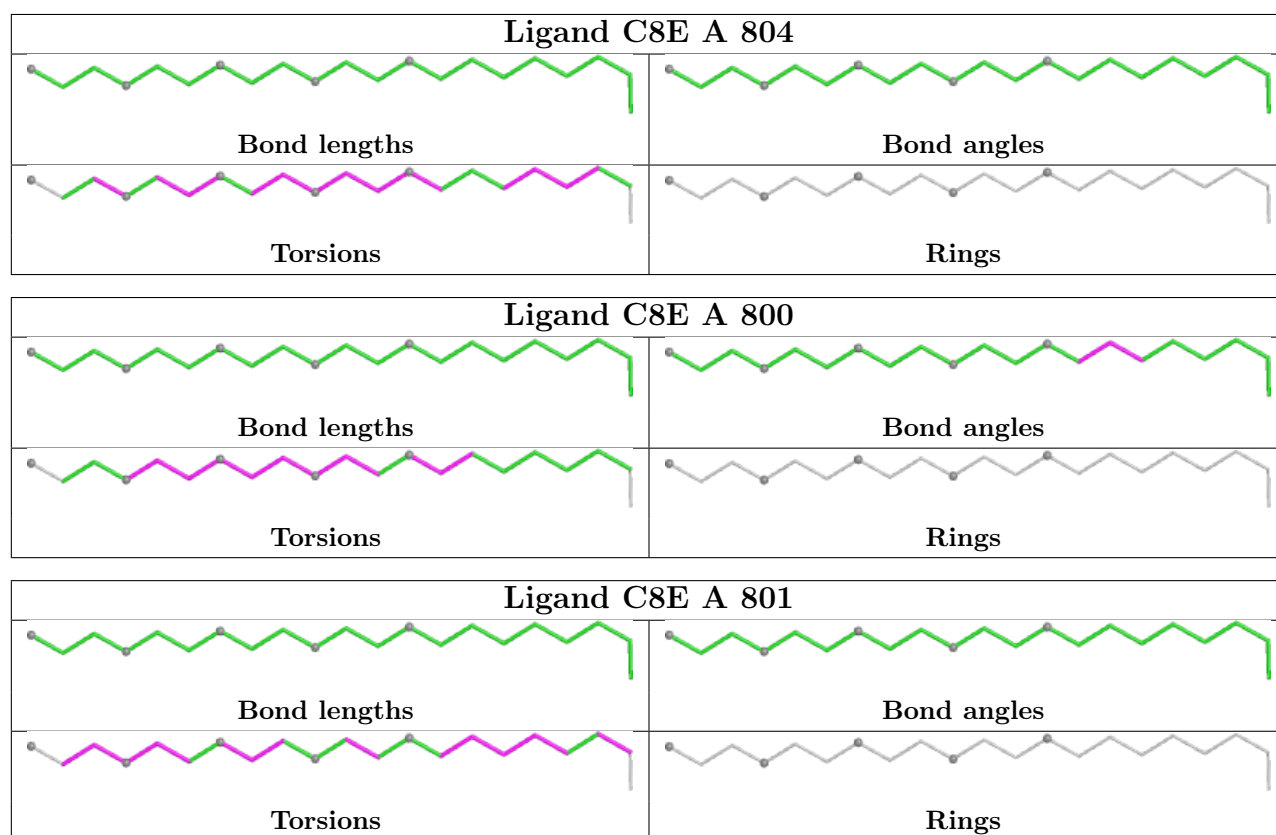
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	804	C8E	14	0
3	A	800	C8E	15	0

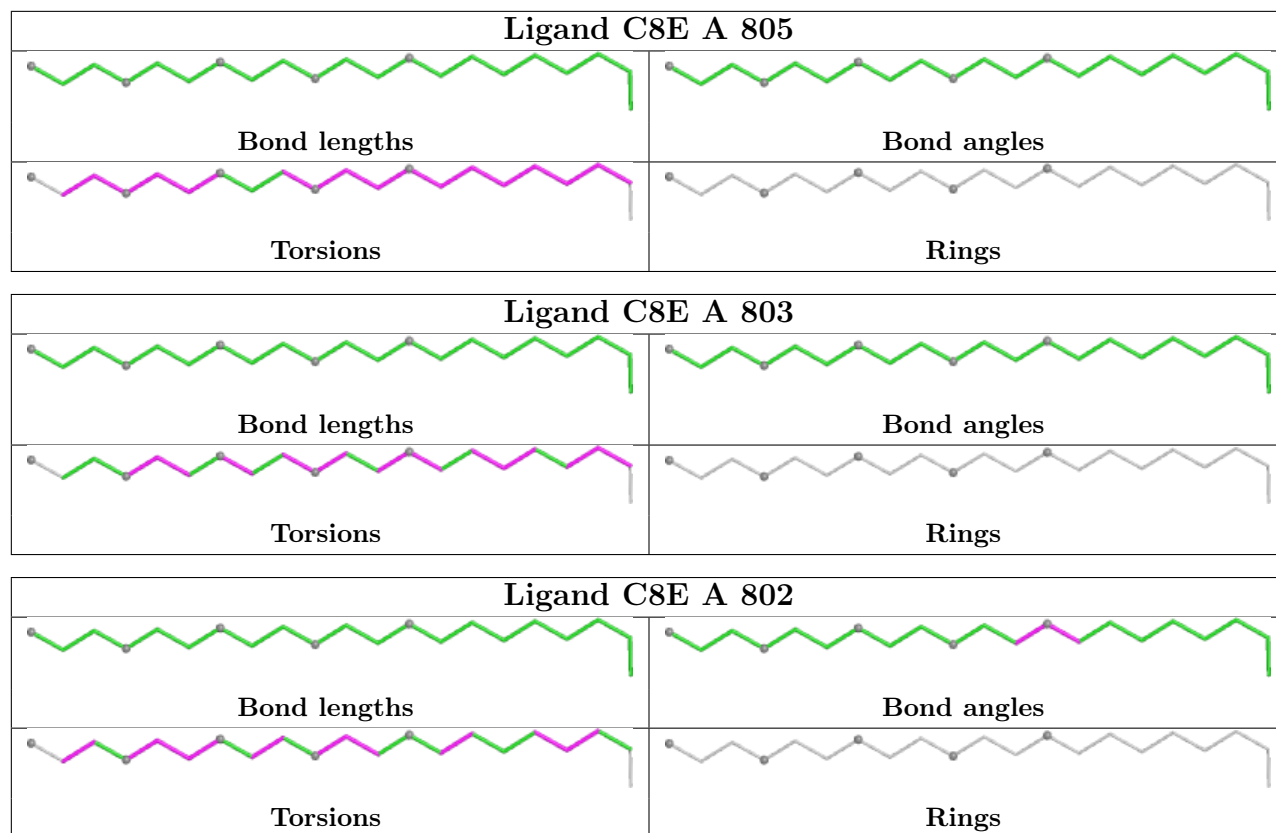
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	C8E	2	0
3	A	805	C8E	7	0
3	A	803	C8E	20	0
3	A	802	C8E	12	0

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	536/594 (90%)	0.37	30 (5%) 30 26	18, 36, 65, 102	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	90	VAL	4.7
1	A	175	THR	4.6
1	A	579	TYR	4.4
1	A	573	TYR	3.6
1	A	450	THR	3.5
1	A	447	ASP	3.5
1	A	582	ALA	3.5
1	A	88	ALA	3.5
1	A	406	GLY	3.4
1	A	583	GLY	3.0
1	A	296	TYR	2.9
1	A	86	ASN	2.9
1	A	7	THR	2.8
1	A	148	SER	2.7
1	A	585	GLU	2.6
1	A	288	ALA	2.6
1	A	511	LEU	2.6
1	A	277	TYR	2.6
1	A	57	ASN	2.6
1	A	451	LEU	2.4
1	A	87	LEU	2.4
1	A	124	GLY	2.4
1	A	373	THR	2.3
1	A	307	GLY	2.1
1	A	122	ALA	2.1
1	A	150	GLN	2.1
1	A	449	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	269	TYR	2.1
1	A	24	ALA	2.0
1	A	333	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

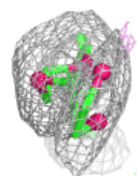
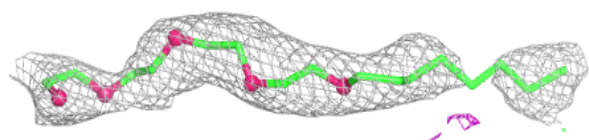
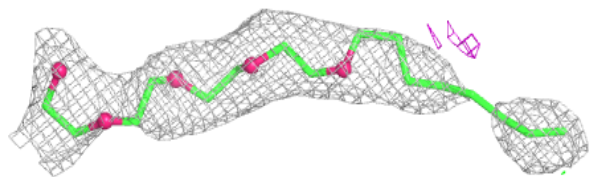
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	C8E	A	801	21/21	0.82	0.19	39,66,118,123	0
2	MG	A	806	1/1	0.84	0.24	73,73,73,73	0
3	C8E	A	803	21/21	0.84	0.17	57,79,114,123	0
3	C8E	A	805	21/21	0.85	0.20	41,85,184,197	0
3	C8E	A	800	21/21	0.87	0.16	29,62,92,116	0
3	C8E	A	804	21/21	0.88	0.16	32,55,95,98	0
3	C8E	A	802	21/21	0.88	0.17	47,57,93,103	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.

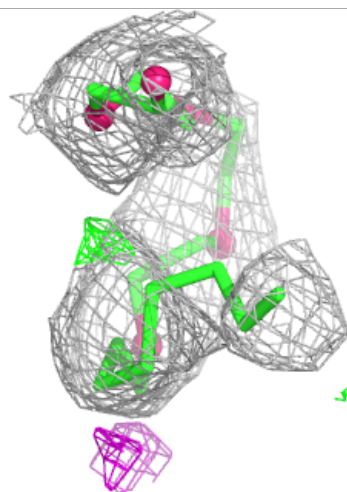
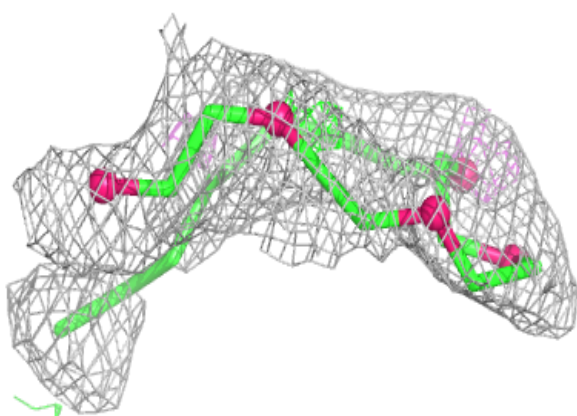
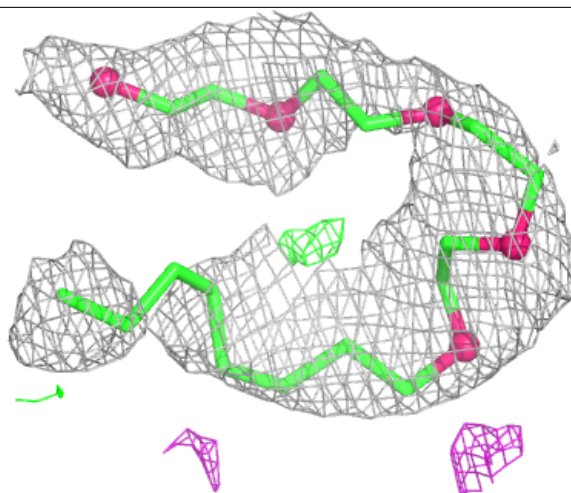
Electron density around C8E A 801:

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



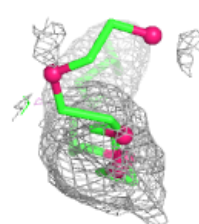
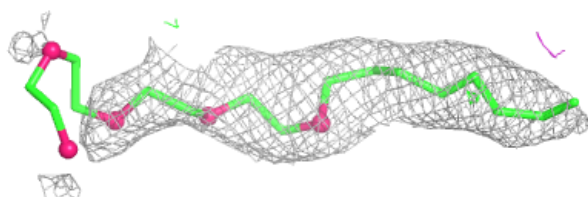
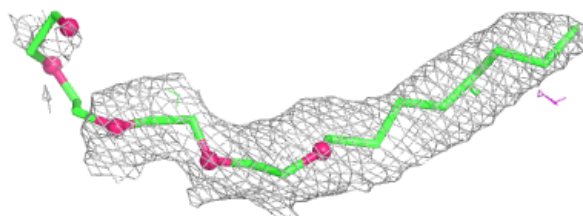
Electron density around C8E A 803:

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

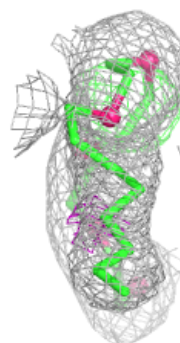
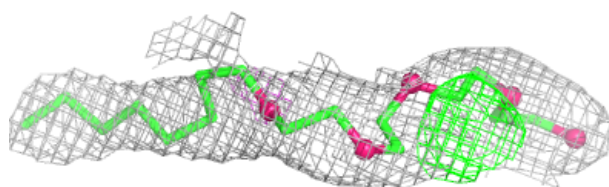
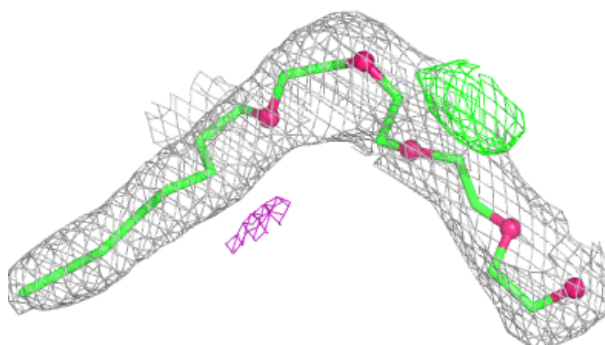


Electron density around C8E A 805:

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

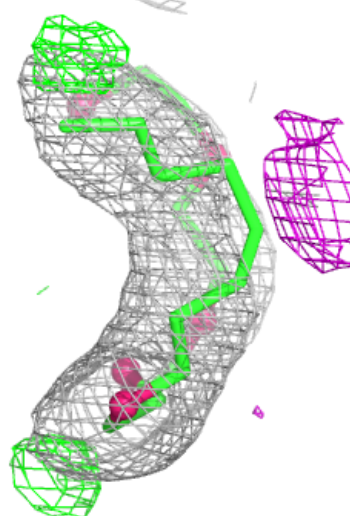
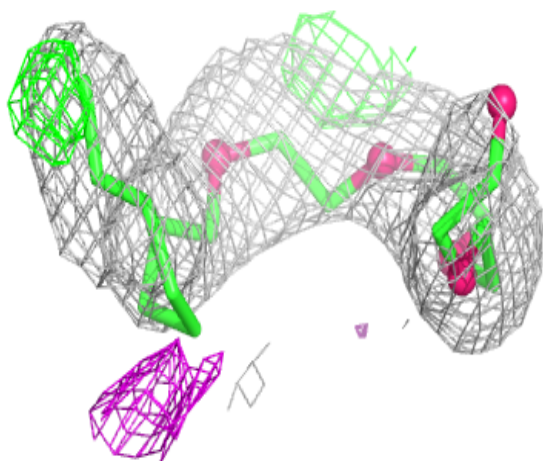
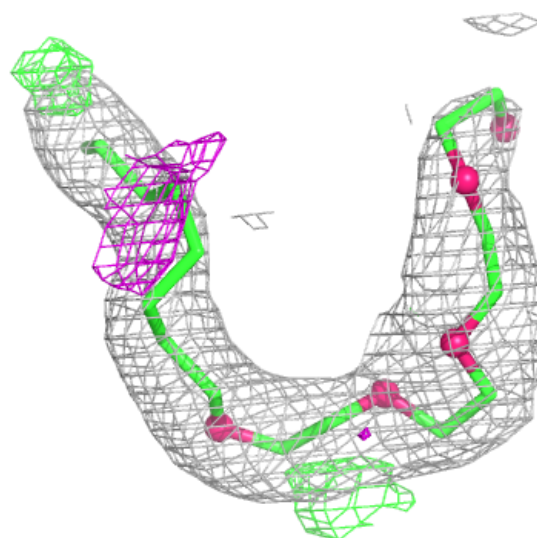
**Electron density around C8E A 800:**

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



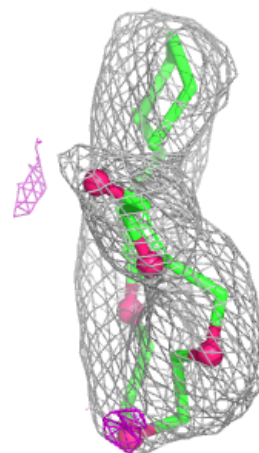
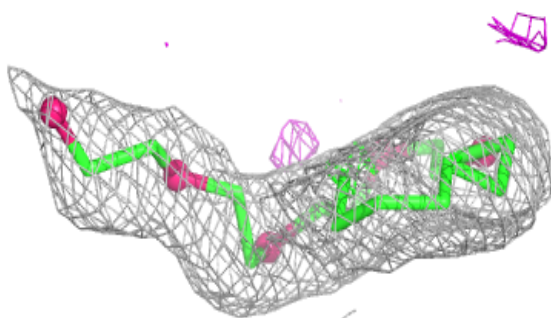
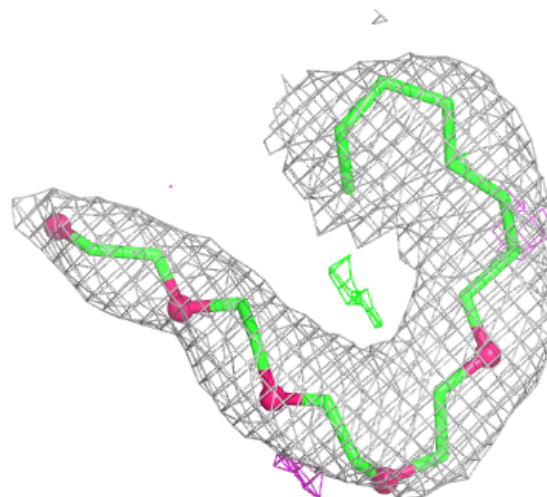
Electron density around C8E A 804:

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



Electron density around C8E A 802:

$2mF_o-DF_c$ (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.