



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:36 PM UTC

PDB ID : 5IXM / pdb_00005ixm
Title : The LPS Transporter LptDE from Yersinia pestis, core complex
Authors : Botos, I.; Mayclin, S.J.; McCarthy, J.G.; Buchanan, S.K.
Deposited on : 2016-03-23
Resolution : 2.75 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:

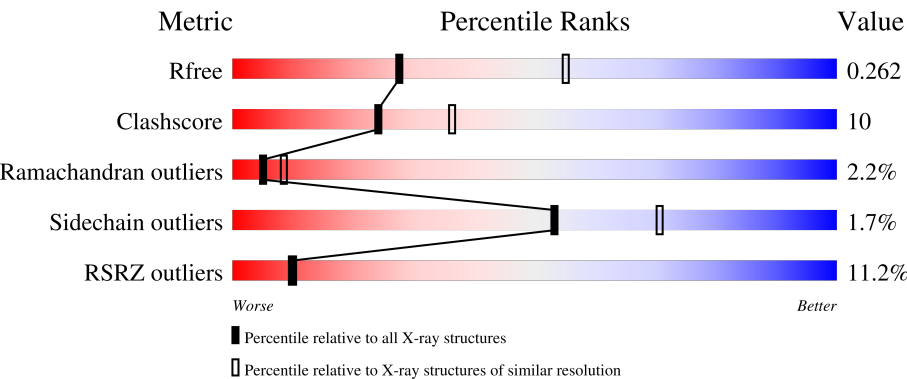
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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.



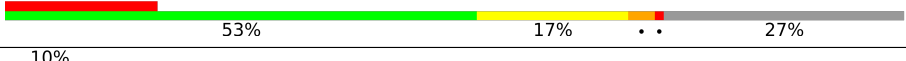
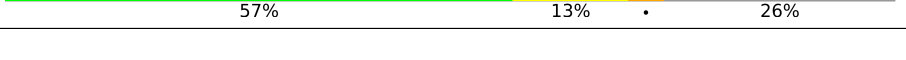
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	577	
1	C	577	
1	E	577	
1	G	577	
2	B	198	

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Mol	Chain	Length	Quality of chain
2	D	198	 14% 57% 15% •• 26%
2	F	198	 17% 53% 17% •• 27%
2	H	198	 10% 57% 13% • 26%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22831 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 LPS-assembly protein LptD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	543	Total	C	N	O	S	0	0	0
			4349	2765	742	829	13			
1	C	541	Total	C	N	O	S	0	0	0
			4346	2762	742	829	13			
1	E	538	Total	C	N	O	S	0	0	0
			4304	2737	736	818	13			
1	G	539	Total	C	N	O	S	0	0	0
			4329	2753	740	824	12			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP Q8ZIK3
A	-19	SER	-	expression tag	UNP Q8ZIK3
A	-18	ASN	-	expression tag	UNP Q8ZIK3
A	-17	HIS	-	expression tag	UNP Q8ZIK3
A	-16	HIS	-	expression tag	UNP Q8ZIK3
A	-15	HIS	-	expression tag	UNP Q8ZIK3
A	-14	HIS	-	expression tag	UNP Q8ZIK3
A	-13	HIS	-	expression tag	UNP Q8ZIK3
A	-12	HIS	-	expression tag	UNP Q8ZIK3
A	-11	HIS	-	expression tag	UNP Q8ZIK3
A	-10	HIS	-	expression tag	UNP Q8ZIK3
A	-9	HIS	-	expression tag	UNP Q8ZIK3
A	-8	HIS	-	expression tag	UNP Q8ZIK3
A	-7	GLU	-	expression tag	UNP Q8ZIK3
A	-6	ASN	-	expression tag	UNP Q8ZIK3
A	-5	LEU	-	expression tag	UNP Q8ZIK3
A	-4	TYR	-	expression tag	UNP Q8ZIK3
A	-3	PHE	-	expression tag	UNP Q8ZIK3
A	-2	GLN	-	expression tag	UNP Q8ZIK3
A	-1	SER	-	expression tag	UNP Q8ZIK3
A	0	MET	-	expression tag	UNP Q8ZIK3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	MET	-	initiating methionine	UNP Q8ZIK3
C	-19	SER	-	expression tag	UNP Q8ZIK3
C	-18	ASN	-	expression tag	UNP Q8ZIK3
C	-17	HIS	-	expression tag	UNP Q8ZIK3
C	-16	HIS	-	expression tag	UNP Q8ZIK3
C	-15	HIS	-	expression tag	UNP Q8ZIK3
C	-14	HIS	-	expression tag	UNP Q8ZIK3
C	-13	HIS	-	expression tag	UNP Q8ZIK3
C	-12	HIS	-	expression tag	UNP Q8ZIK3
C	-11	HIS	-	expression tag	UNP Q8ZIK3
C	-10	HIS	-	expression tag	UNP Q8ZIK3
C	-9	HIS	-	expression tag	UNP Q8ZIK3
C	-8	HIS	-	expression tag	UNP Q8ZIK3
C	-7	GLU	-	expression tag	UNP Q8ZIK3
C	-6	ASN	-	expression tag	UNP Q8ZIK3
C	-5	LEU	-	expression tag	UNP Q8ZIK3
C	-4	TYR	-	expression tag	UNP Q8ZIK3
C	-3	PHE	-	expression tag	UNP Q8ZIK3
C	-2	GLN	-	expression tag	UNP Q8ZIK3
C	-1	SER	-	expression tag	UNP Q8ZIK3
C	0	MET	-	expression tag	UNP Q8ZIK3
E	-20	MET	-	initiating methionine	UNP Q8ZIK3
E	-19	SER	-	expression tag	UNP Q8ZIK3
E	-18	ASN	-	expression tag	UNP Q8ZIK3
E	-17	HIS	-	expression tag	UNP Q8ZIK3
E	-16	HIS	-	expression tag	UNP Q8ZIK3
E	-15	HIS	-	expression tag	UNP Q8ZIK3
E	-14	HIS	-	expression tag	UNP Q8ZIK3
E	-13	HIS	-	expression tag	UNP Q8ZIK3
E	-12	HIS	-	expression tag	UNP Q8ZIK3
E	-11	HIS	-	expression tag	UNP Q8ZIK3
E	-10	HIS	-	expression tag	UNP Q8ZIK3
E	-9	HIS	-	expression tag	UNP Q8ZIK3
E	-8	HIS	-	expression tag	UNP Q8ZIK3
E	-7	GLU	-	expression tag	UNP Q8ZIK3
E	-6	ASN	-	expression tag	UNP Q8ZIK3
E	-5	LEU	-	expression tag	UNP Q8ZIK3
E	-4	TYR	-	expression tag	UNP Q8ZIK3
E	-3	PHE	-	expression tag	UNP Q8ZIK3
E	-2	GLN	-	expression tag	UNP Q8ZIK3
E	-1	SER	-	expression tag	UNP Q8ZIK3
E	0	MET	-	expression tag	UNP Q8ZIK3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-20	MET	-	initiating methionine	UNP Q8ZIK3
G	-19	SER	-	expression tag	UNP Q8ZIK3
G	-18	ASN	-	expression tag	UNP Q8ZIK3
G	-17	HIS	-	expression tag	UNP Q8ZIK3
G	-16	HIS	-	expression tag	UNP Q8ZIK3
G	-15	HIS	-	expression tag	UNP Q8ZIK3
G	-14	HIS	-	expression tag	UNP Q8ZIK3
G	-13	HIS	-	expression tag	UNP Q8ZIK3
G	-12	HIS	-	expression tag	UNP Q8ZIK3
G	-11	HIS	-	expression tag	UNP Q8ZIK3
G	-10	HIS	-	expression tag	UNP Q8ZIK3
G	-9	HIS	-	expression tag	UNP Q8ZIK3
G	-8	HIS	-	expression tag	UNP Q8ZIK3
G	-7	GLU	-	expression tag	UNP Q8ZIK3
G	-6	ASN	-	expression tag	UNP Q8ZIK3
G	-5	LEU	-	expression tag	UNP Q8ZIK3
G	-4	TYR	-	expression tag	UNP Q8ZIK3
G	-3	PHE	-	expression tag	UNP Q8ZIK3
G	-2	GLN	-	expression tag	UNP Q8ZIK3
G	-1	SER	-	expression tag	UNP Q8ZIK3
G	0	MET	-	expression tag	UNP Q8ZIK3

- Molecule 2 is a protein called LPS-assembly lipoprotein LptE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	141	Total	C	N	O	S	0	0	0
			1107	694	200	212	1			
2	D	146	Total	C	N	O	S	0	0	0
			1133	710	205	217	1			
2	F	145	Total	C	N	O	S	0	0	0
			1128	709	207	211	1			
2	H	147	Total	C	N	O	S	0	0	0
			1154	722	210	220	2			

There are 44 discrepancies between the modelled and reference sequences:

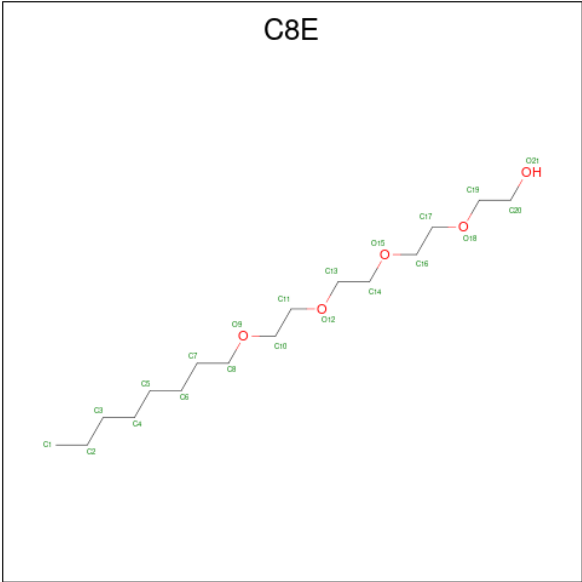
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	ALA	-	expression tag	UNP Q7CJV2
B	-3	PRO	-	expression tag	UNP Q7CJV2
B	-2	ASN	-	expression tag	UNP Q7CJV2
B	-1	THR	-	expression tag	UNP Q7CJV2
B	0	SER	-	expression tag	UNP Q7CJV2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	188	HIS	-	expression tag	UNP Q7CJV2
B	189	HIS	-	expression tag	UNP Q7CJV2
B	190	HIS	-	expression tag	UNP Q7CJV2
B	191	HIS	-	expression tag	UNP Q7CJV2
B	192	HIS	-	expression tag	UNP Q7CJV2
B	193	HIS	-	expression tag	UNP Q7CJV2
D	-4	ALA	-	expression tag	UNP Q7CJV2
D	-3	PRO	-	expression tag	UNP Q7CJV2
D	-2	ASN	-	expression tag	UNP Q7CJV2
D	-1	THR	-	expression tag	UNP Q7CJV2
D	0	SER	-	expression tag	UNP Q7CJV2
D	188	HIS	-	expression tag	UNP Q7CJV2
D	189	HIS	-	expression tag	UNP Q7CJV2
D	190	HIS	-	expression tag	UNP Q7CJV2
D	191	HIS	-	expression tag	UNP Q7CJV2
D	192	HIS	-	expression tag	UNP Q7CJV2
D	193	HIS	-	expression tag	UNP Q7CJV2
F	-4	ALA	-	expression tag	UNP Q7CJV2
F	-3	PRO	-	expression tag	UNP Q7CJV2
F	-2	ASN	-	expression tag	UNP Q7CJV2
F	-1	THR	-	expression tag	UNP Q7CJV2
F	0	SER	-	expression tag	UNP Q7CJV2
F	188	HIS	-	expression tag	UNP Q7CJV2
F	189	HIS	-	expression tag	UNP Q7CJV2
F	190	HIS	-	expression tag	UNP Q7CJV2
F	191	HIS	-	expression tag	UNP Q7CJV2
F	192	HIS	-	expression tag	UNP Q7CJV2
F	193	HIS	-	expression tag	UNP Q7CJV2
H	-4	ALA	-	expression tag	UNP Q7CJV2
H	-3	PRO	-	expression tag	UNP Q7CJV2
H	-2	ASN	-	expression tag	UNP Q7CJV2
H	-1	THR	-	expression tag	UNP Q7CJV2
H	0	SER	-	expression tag	UNP Q7CJV2
H	188	HIS	-	expression tag	UNP Q7CJV2
H	189	HIS	-	expression tag	UNP Q7CJV2
H	190	HIS	-	expression tag	UNP Q7CJV2
H	191	HIS	-	expression tag	UNP Q7CJV2
H	192	HIS	-	expression tag	UNP Q7CJV2
H	193	HIS	-	expression tag	UNP Q7CJV2

- 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	C	1	Total	C	O	0	0
			21	16	5		
3	C	1	Total	C	O	0	0
			21	16	5		
3	C	1	Total	C	O	0	0
			21	16	5		
3	C	1	Total	C	O	0	0
			21	16	5		
3	C	1	Total	C	O	0	0
			21	16	5		
3	C	1	Total	C	O	0	0
			21	16	5		
3	C	1	Total	C	O	0	0
			21	16	5		
3	C	1	Total	C	O	0	0
			21	16	5		

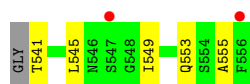
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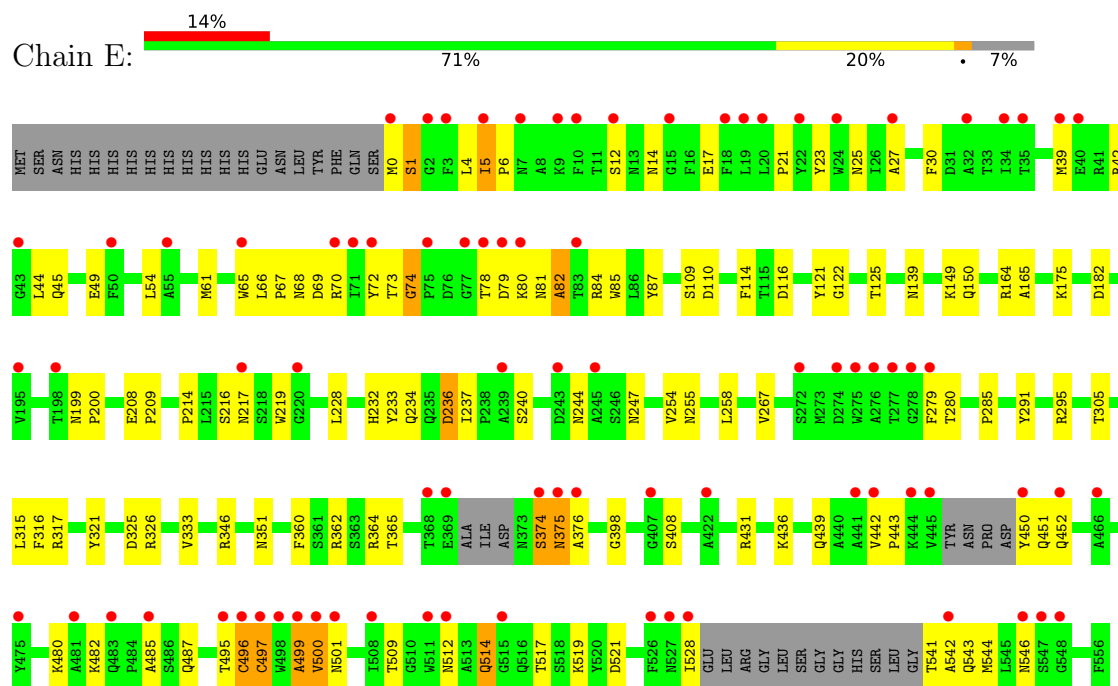
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C O 21 16 5	0	0
3	E	1	Total C O 21 16 5	0	0
3	E	1	Total C O 21 16 5	0	0
3	E	1	Total C O 21 16 5	0	0
3	G	1	Total C O 21 16 5	0	0
3	G	1	Total C O 21 16 5	0	0
3	G	1	Total C O 21 16 5	0	0

- Molecule 4 is water.

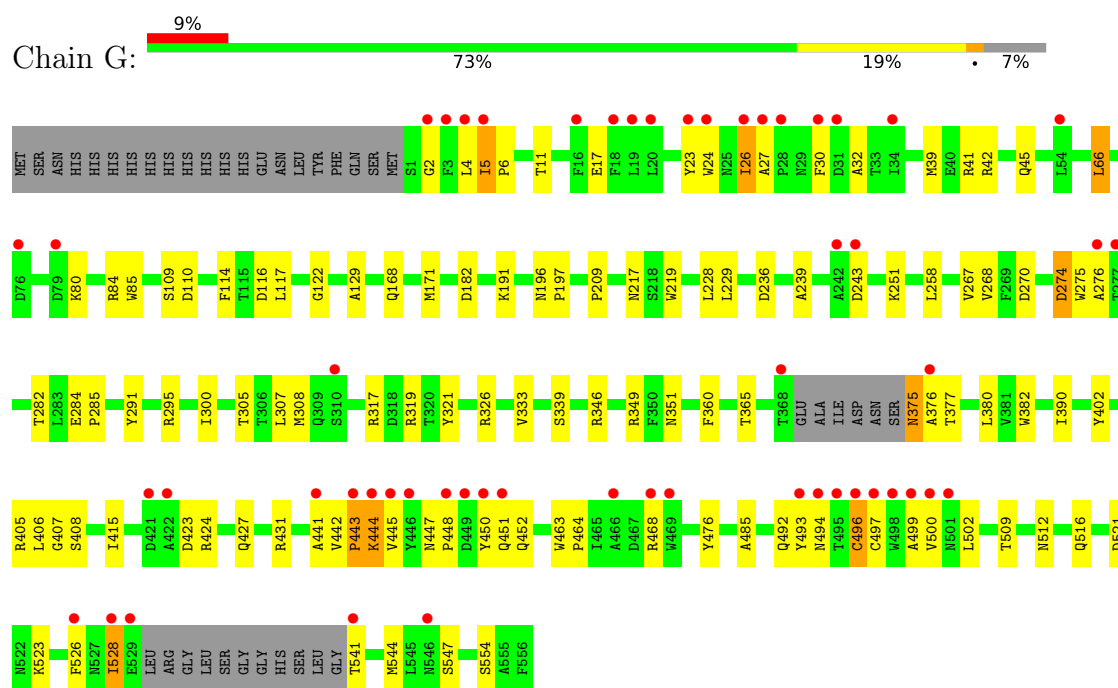
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	148	Total O 148 148	0	0
4	B	38	Total O 38 38	0	0
4	C	125	Total O 125 125	0	0
4	D	27	Total O 27 27	0	0
4	E	75	Total O 75 75	0	0
4	F	16	Total O 16 16	0	0
4	G	92	Total O 92 92	0	0
4	H	19	Total O 19 19	0	0



- Molecule 1: LPS-assembly protein LptD

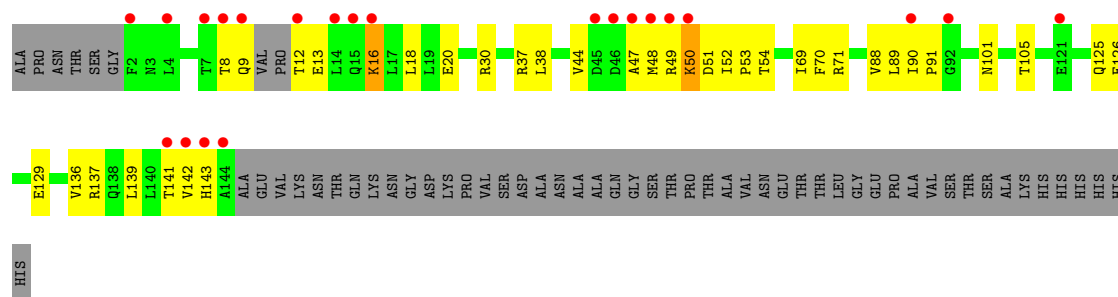


- Molecule 1: LPS-assembly protein LptD

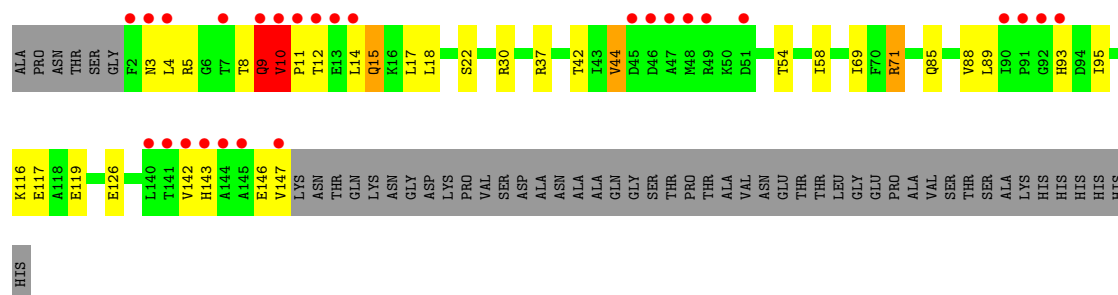


- Molecule 2: LPS-assembly lipoprotein LptE

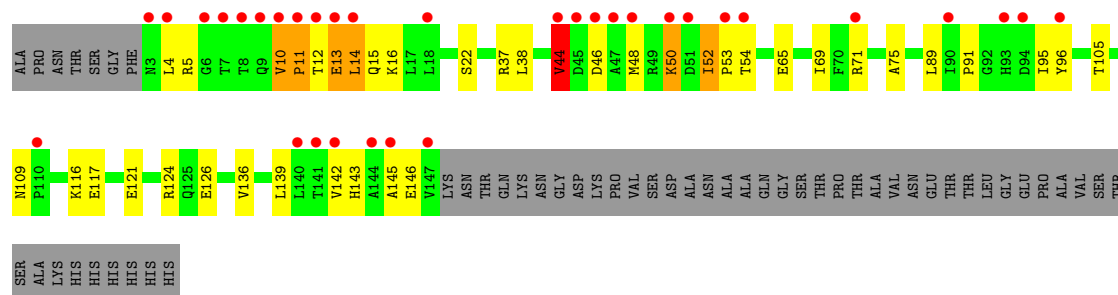




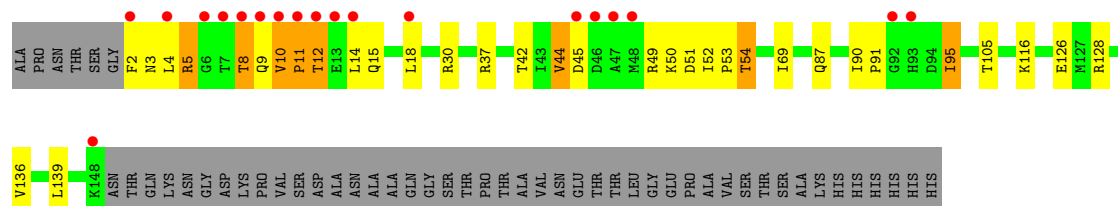
• Molecule 2: LPS-assembly lipoprotein LptE



• Molecule 2: LPS-assembly lipoprotein LptE



• Molecule 2: LPS-assembly lipoprotein LptE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.89Å 176.35Å 143.85Å 90.00° 96.11° 90.00°	Depositor
Resolution (Å)	40.13 – 2.75 40.13 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.3 (40.13-2.75) 94.2 (40.13-2.75)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.212 , 0.261 0.218 , 0.262	Depositor DCC
R_{free} test set	5392 reflections (3.47%)	wwPDB-VP
Wilson B-factor (Å ²)	33.9	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22831	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.07 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.5355e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 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	0.33	0/4471	0.78	5/6091 (0.1%)
1	C	0.33	0/4468	0.77	6/6087 (0.1%)
1	E	0.35	0/4423	0.82	7/6024 (0.1%)
1	G	0.34	0/4451	0.78	8/6065 (0.1%)
2	B	0.36	0/1121	0.86	1/1523 (0.1%)
2	D	0.37	0/1148	0.90	4/1564 (0.3%)
2	F	0.40	1/1143 (0.1%)	0.87	3/1555 (0.2%)
2	H	0.34	0/1169	0.87	3/1589 (0.2%)
All	All	0.34	1/22394 (0.0%)	0.81	37/30498 (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	C	0	1
1	E	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	44	VAL	CA-CB	5.37	1.61	1.54

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	446	TYR	N-CA-C	9.05	124.43	113.12
1	C	447	ASN	N-CA-C	8.46	128.52	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	10	VAL	N-CA-CB	7.42	121.61	111.21
1	A	447	ASN	CA-C-N	-7.00	111.09	119.84
1	A	447	ASN	C-N-CA	-7.00	111.09	119.84
2	F	14	LEU	N-CA-C	6.56	121.14	113.20
2	D	9	GLN	CA-C-N	6.38	133.94	122.13
2	D	9	GLN	C-N-CA	6.38	133.94	122.13
1	E	68	ASN	N-CA-C	5.96	119.04	107.71
1	E	500	VAL	N-CA-C	5.93	121.67	109.34
2	D	15	GLN	N-CA-C	-5.90	106.62	113.88
1	E	499	ALA	N-CA-C	5.81	118.24	109.23
2	F	52	ILE	CA-C-N	5.78	125.73	119.78
2	F	52	ILE	C-N-CA	5.78	125.73	119.78
1	G	442	VAL	CA-C-N	5.71	126.98	119.84
1	G	442	VAL	C-N-CA	5.71	126.98	119.84
1	A	408	SER	CB-CA-C	-5.59	109.63	117.23
2	B	13	GLU	N-CA-C	-5.56	102.25	110.48
1	C	408	SER	CB-CA-C	-5.54	109.70	117.23
1	G	408	SER	CB-CA-C	-5.52	109.73	117.23
1	E	408	SER	CB-CA-C	-5.51	109.74	117.23
1	C	501	ASN	N-CA-C	5.51	117.88	108.90
1	C	73	THR	CB-CA-C	-5.38	109.92	117.23
1	G	444	LYS	N-CA-C	5.35	122.19	110.80
1	A	423	ASP	N-CA-C	-5.32	108.56	114.62
2	H	45	ASP	N-CA-C	5.29	120.01	113.50
1	G	496	CYS	CB-CA-C	-5.26	110.53	116.63
2	H	10	VAL	CA-C-N	-5.24	113.29	119.84
2	H	10	VAL	C-N-CA	-5.24	113.29	119.84
1	E	237	ILE	N-CA-C	5.24	113.70	107.73
1	C	423	ASP	N-CA-C	-5.15	108.75	114.62
1	G	66	LEU	CA-C-N	5.10	126.22	119.84
1	G	66	LEU	C-N-CA	5.10	126.22	119.84
1	E	237	ILE	CA-C-N	5.09	125.37	119.92
1	E	237	ILE	C-N-CA	5.09	125.37	119.92
1	G	376	ALA	N-CA-C	5.08	116.24	108.42
1	A	499	ALA	N-CA-C	5.03	117.03	109.23

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	78	THR	Peptide
1	E	374	SER	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4349	0	4105	83	1
1	C	4346	0	4108	81	1
1	E	4304	0	4065	94	0
1	G	4329	0	4092	84	0
2	B	1107	0	1111	29	0
2	D	1133	0	1139	33	0
2	F	1128	0	1149	30	0
2	H	1154	0	1172	29	0
3	A	105	0	170	13	0
3	C	189	0	306	13	0
3	E	84	0	136	2	0
3	G	63	0	102	5	0
4	A	148	0	0	19	1
4	B	38	0	0	9	0
4	C	125	0	0	17	1
4	D	27	0	0	4	0
4	E	75	0	0	28	2
4	F	16	0	0	5	0
4	G	92	0	0	20	2
4	H	19	0	0	5	0
All	All	22831	0	21655	439	4

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 10.

All (439) 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:298:ASP:OD1	4:A:701:HOH:O	1.82	0.95
2:F:13:GLU:HG3	2:F:14:LEU:HG	1.51	0.93
2:B:12:THR:N	4:B:202:HOH:O	2.01	0.93
1:A:168:GLN:NE2	4:A:704:HOH:O	2.00	0.92
1:G:443:PRO:O	1:G:445:VAL:N	2.04	0.91
1:G:291:TYR:OH	4:G:701:HOH:O	1.90	0.88
1:E:482:LYS:HE3	2:H:8:THR:HG21	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ARG:HH22	3:A:602:C8E:H42	1.41	0.85
1:A:429:ASN:OD1	4:A:702:HOH:O	1.94	0.85
1:G:168:GLN:NE2	4:G:706:HOH:O	2.09	0.85
1:A:54:LEU:O	4:A:703:HOH:O	1.94	0.84
1:G:502:LEU:HD13	1:G:526:PHE:HE1	1.42	0.84
1:E:39:MET:SD	4:E:768:HOH:O	2.33	0.84
1:G:447:ASN:HB3	1:G:450:TYR:HB3	1.61	0.83
1:G:349:ARG:NH1	4:G:708:HOH:O	2.12	0.82
1:C:497:CYS:SG	1:C:498:TRP:N	2.53	0.81
2:D:30:ARG:NH1	4:D:202:HOH:O	2.12	0.81
1:E:546:ASN:OD1	4:E:702:HOH:O	1.97	0.81
1:G:407:GLY:O	4:G:703:HOH:O	1.99	0.81
1:A:84:ARG:NH2	1:A:116:ASP:OD2	2.13	0.81
1:E:23:TYR:O	4:E:703:HOH:O	1.98	0.80
1:C:466:ALA:HB3	1:C:469:TRP:HB2	1.62	0.79
2:B:20:GLU:OE1	4:B:201:HOH:O	2.01	0.79
1:C:25:ASN:OD1	4:C:701:HOH:O	2.01	0.78
1:C:47:GLN:OE1	4:C:702:HOH:O	2.01	0.78
1:C:441:ALA:O	4:C:703:HOH:O	2.02	0.78
1:E:541:THR:O	1:E:543:GLN:N	2.17	0.78
1:A:176:ASN:OD1	4:A:705:HOH:O	2.01	0.77
1:E:72:TYR:O	1:E:74:GLY:N	2.18	0.77
1:G:4:LEU:HD11	1:G:23:TYR:HB3	1.66	0.77
1:E:79:ASP:OD2	1:E:82:ALA:HB2	1.84	0.76
1:E:139:ASN:O	4:E:704:HOH:O	2.03	0.76
2:D:22:SER:O	4:D:201:HOH:O	2.05	0.75
1:E:214:PRO:O	4:E:705:HOH:O	2.04	0.75
1:E:4:LEU:HD11	1:E:23:TYR:HB2	1.69	0.74
1:G:300:ILE:O	4:G:705:HOH:O	2.05	0.74
2:B:91:PRO:O	4:B:203:HOH:O	2.05	0.74
1:C:64:ASP:OD1	4:C:704:HOH:O	2.07	0.73
1:A:4:LEU:HB2	1:A:21:PRO:HG2	1.69	0.72
1:E:255:ASN:OD1	4:E:707:HOH:O	2.08	0.72
1:E:316:PHE:O	4:E:706:HOH:O	2.07	0.72
1:C:225:GLU:OE2	4:C:706:HOH:O	2.09	0.71
1:A:547:SER:O	4:A:706:HOH:O	2.09	0.71
1:G:24:TRP:HB3	1:G:32:ALA:HB3	1.72	0.71
1:G:502:LEU:HD13	1:G:526:PHE:CE1	2.25	0.71
1:E:315:LEU:O	4:E:709:HOH:O	2.09	0.70
1:G:468:ARG:HD2	1:G:493:TYR:HE1	1.57	0.70
2:F:14:LEU:HD12	2:F:53:PRO:HG2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:LYS:NZ	2:B:52:ILE:HD12	2.07	0.70
2:F:116:LYS:NZ	4:F:203:HOH:O	2.25	0.69
1:A:521:ASP:OD2	4:A:707:HOH:O	2.09	0.69
1:E:279:PHE:O	4:E:708:HOH:O	2.09	0.69
1:A:158:GLY:O	4:A:708:HOH:O	2.11	0.69
1:E:69:ASP:N	1:E:81:ASN:O	2.24	0.69
1:E:70:ARG:N	4:E:701:HOH:O	1.86	0.69
1:E:501:ASN:HD22	1:E:528:ILE:HA	1.58	0.68
2:F:89:LEU:HG	2:F:95:ILE:HD12	1.74	0.68
1:G:415:ILE:HD11	1:G:427:GLN:HE21	1.57	0.68
2:H:87:GLN:HB3	2:H:95:ILE:HD11	1.75	0.67
1:G:84:ARG:NH2	1:G:116:ASP:OD2	2.26	0.67
1:C:84:ARG:NH2	1:C:116:ASP:OD2	2.24	0.67
2:B:125:GLN:OE1	4:B:204:HOH:O	2.12	0.66
1:E:79:ASP:CG	1:E:82:ALA:HB2	2.20	0.66
1:A:483:GLN:OE1	4:A:710:HOH:O	2.14	0.66
2:B:16:LYS:HZ1	2:B:52:ILE:HD12	1.59	0.66
1:G:117:LEU:O	4:G:710:HOH:O	2.13	0.66
1:G:182:ASP:OD2	2:H:37:ARG:NH1	2.28	0.66
1:G:390:ILE:O	4:G:709:HOH:O	2.13	0.66
1:A:512:ASN:OD1	4:A:709:HOH:O	2.13	0.66
3:A:601:C8E:H141	1:C:384:GLY:HA3	1.76	0.66
1:E:480:LYS:O	4:E:711:HOH:O	2.13	0.65
1:E:234:GLN:OE1	4:E:710:HOH:O	2.13	0.65
1:C:11:THR:HG22	1:C:523:LYS:HG2	1.78	0.65
1:C:143:ASN:OD1	4:C:707:HOH:O	2.15	0.65
1:C:449:ASP:O	1:C:451:GLN:N	2.30	0.64
2:B:47:ALA:O	2:B:49:ARG:N	2.31	0.64
1:G:217:ASN:HB2	3:G:602:C8E:H171	1.80	0.64
1:E:495:THR:O	1:E:497:CYS:N	2.30	0.64
1:G:450:TYR:HD2	1:G:451:GLN:HG3	1.62	0.63
1:C:260:GLN:NE2	4:C:717:HOH:O	2.31	0.63
2:H:2:PHE:O	4:H:201:HOH:O	2.15	0.63
2:B:8:THR:HG22	2:B:9:GLN:H	1.65	0.62
2:D:126:GLU:OE1	4:D:203:HOH:O	2.16	0.62
1:G:26:ILE:HG22	4:G:712:HOH:O	1.98	0.62
1:A:249:LYS:NZ	4:A:713:HOH:O	2.20	0.62
2:B:88:VAL:HG11	2:B:142:VAL:HG11	1.82	0.62
1:A:259:PRO:HG3	3:C:602:C8E:H141	1.82	0.61
2:B:30:ARG:NH1	4:B:207:HOH:O	2.22	0.61
1:E:528:ILE:O	4:E:712:HOH:O	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:ASP:O	4:C:708:HOH:O	2.16	0.61
1:G:448:PRO:O	1:G:452:GLN:HG3	2.00	0.61
2:D:10:VAL:O	2:D:12:THR:N	2.31	0.60
1:A:51:ARG:NH1	4:A:723:HOH:O	2.31	0.60
2:D:89:LEU:HG	2:D:95:ILE:HD12	1.81	0.60
1:G:468:ARG:HD2	1:G:493:TYR:CE1	2.34	0.60
1:E:244:ASN:HB3	1:E:247:ASN:HB2	1.82	0.60
1:A:1:SER:OG	1:A:24:TRP:O	2.11	0.60
1:C:272:SER:O	2:D:3:ASN:ND2	2.30	0.60
2:D:9:GLN:O	2:D:10:VAL:HG23	2.02	0.60
1:E:450:TYR:OH	2:F:71:ARG:NH1	2.34	0.60
3:A:603:C8E:H192	1:C:428:LEU:HD21	1.83	0.60
1:C:349:ARG:HH22	3:C:602:C8E:H191	1.67	0.59
1:C:496:CYS:O	1:C:497:CYS:HB3	2.01	0.59
2:D:10:VAL:C	2:D:12:THR:H	2.10	0.59
1:G:4:LEU:HD11	1:G:23:TYR:CB	2.32	0.59
2:F:117:GLU:OE1	4:F:201:HOH:O	2.17	0.59
1:A:446:TYR:OH	1:A:449:ASP:OD2	2.17	0.59
1:C:375:ASN:OD1	1:C:376:ALA:N	2.28	0.59
1:C:446:TYR:CD2	1:C:447:ASN:HB2	2.38	0.59
2:B:50:LYS:O	2:B:52:ILE:HG12	2.03	0.59
1:E:45:GLN:HG3	1:E:66:LEU:HB2	1.84	0.59
2:H:30:ARG:NH1	4:H:204:HOH:O	2.35	0.59
1:C:481:ALA:HB2	2:D:71:ARG:HH11	1.68	0.59
1:E:232:HIS:ND1	4:E:707:HOH:O	2.09	0.59
1:A:319:ARG:NH1	4:A:727:HOH:O	2.37	0.58
1:E:66:LEU:HD23	1:E:84:ARG:HG3	1.86	0.58
1:A:452:GLN:HG3	1:A:453:GLY:H	1.68	0.58
1:E:4:LEU:HB2	1:E:21:PRO:HG2	1.86	0.58
1:A:216:SER:OG	2:B:38:LEU:O	2.12	0.57
1:A:307:LEU:HD23	1:A:441:ALA:HA	1.84	0.57
1:A:495:THR:O	1:A:497:CYS:N	2.37	0.57
2:B:101:ASN:ND2	4:B:210:HOH:O	2.37	0.57
2:H:15:GLN:O	2:H:42:THR:N	2.36	0.57
1:A:466:ALA:HB3	1:A:469:TRP:HB2	1.87	0.56
1:C:285:PRO:HB2	3:C:601:C8E:H42	1.87	0.56
1:G:450:TYR:CD2	1:G:451:GLN:HG3	2.40	0.56
2:F:121:GLU:OE2	2:F:124:ARG:NH2	2.38	0.56
1:C:389:ARG:NH1	4:C:729:HOH:O	2.38	0.56
1:E:512:ASN:HB2	1:E:519:LYS:HE3	1.88	0.56
1:C:20:LEU:O	1:C:36:PRO:HD2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:44:VAL:HG23	2:F:46:ASP:H	1.71	0.56
1:E:487:GLN:OE1	4:E:713:HOH:O	2.18	0.56
1:A:213:LEU:HD22	3:A:601:C8E:H61	1.87	0.55
1:C:73:THR:HB	1:C:78:THR:HB	1.89	0.55
2:B:129:GLU:OE2	4:B:205:HOH:O	2.18	0.55
1:G:485:ALA:HB1	2:H:69:ILE:HD11	1.89	0.55
1:G:492:GLN:NE2	1:G:494:ASN:HD21	2.04	0.55
1:E:326:ARG:HD2	1:E:365:THR:HB	1.89	0.55
1:A:485:ALA:HB1	2:B:69:ILE:HD11	1.88	0.55
1:E:216:SER:OG	2:F:38:LEU:O	2.14	0.55
2:H:12:THR:HG23	2:H:14:LEU:H	1.72	0.55
2:H:52:ILE:O	4:H:203:HOH:O	2.17	0.55
1:A:244:ASN:HB3	1:A:247:ASN:HB2	1.90	0.54
1:E:499:ALA:O	4:E:714:HOH:O	2.18	0.54
1:A:540:GLY:N	4:A:731:HOH:O	2.41	0.54
1:A:311:ASP:OD2	4:A:711:HOH:O	2.17	0.54
2:D:58:ILE:HD12	2:D:85:GLN:HG3	1.89	0.54
1:G:375:ASN:N	4:G:719:HOH:O	2.40	0.54
1:A:182:ASP:OD2	2:B:37:ARG:NH1	2.41	0.54
1:E:452:GLN:HE22	2:F:71:ARG:HG3	1.72	0.54
1:A:23:TYR:CE2	1:A:25:ASN:HB2	2.43	0.54
1:E:5:ILE:HD12	1:E:6:PRO:HD2	1.89	0.54
1:G:258:LEU:HD21	1:G:295:ARG:HB2	1.88	0.54
1:A:199:ASN:O	4:A:712:HOH:O	2.19	0.53
1:C:217:ASN:HB2	3:C:601:C8E:H161	1.90	0.53
2:H:4:LEU:HD23	2:H:5:ARG:H	1.73	0.53
1:A:391:ASN:HB2	3:A:602:C8E:H12	1.90	0.53
1:A:409:LEU:HD23	3:A:604:C8E:H192	1.91	0.53
1:C:4:LEU:HB2	1:C:21:PRO:HG2	1.89	0.53
1:C:233:TYR:HB2	1:C:254:VAL:HB	1.89	0.53
1:E:182:ASP:OD2	2:F:37:ARG:NH1	2.41	0.53
1:C:-1:SER:O	1:C:0:MET:HB2	2.10	0.53
1:E:69:ASP:HA	4:E:701:HOH:O	2.09	0.53
1:E:175:LYS:NZ	4:E:734:HOH:O	2.42	0.53
1:G:377:THR:HA	1:G:380:LEU:HD11	1.91	0.53
1:E:236:ASP:OD2	4:E:715:HOH:O	2.18	0.52
1:G:114:PHE:CE1	1:G:122:GLY:HA3	2.44	0.52
1:A:233:TYR:HB2	1:A:254:VAL:HB	1.90	0.52
1:A:349:ARG:NH2	3:A:602:C8E:H42	2.20	0.52
2:F:65:GLU:OE2	4:F:202:HOH:O	2.19	0.52
1:G:406:LEU:O	4:G:703:HOH:O	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:PRO:HA	1:A:451:GLN:O	2.09	0.52
1:E:66:LEU:HB3	1:E:84:ARG:HB2	1.91	0.51
1:A:333:VAL:HG23	1:A:360:PHE:HE2	1.75	0.51
1:A:346:ARG:O	2:B:141:THR:HG22	2.11	0.51
2:B:71:ARG:NE	4:B:206:HOH:O	2.22	0.51
1:C:150:GLN:NE2	4:C:728:HOH:O	2.38	0.51
1:E:431:ARG:NH2	2:F:105:THR:HG21	2.24	0.51
1:G:239:ALA:N	4:G:717:HOH:O	2.32	0.51
1:A:217:ASN:HB3	1:A:219:TRP:O	2.10	0.51
1:G:27:ALA:HB3	1:G:30:PHE:HB2	1.92	0.51
1:G:496:CYS:SG	1:G:497:CYS:N	2.81	0.51
1:C:493:TYR:HB3	1:C:500:VAL:HG22	1.92	0.51
1:G:415:ILE:HD11	1:G:427:GLN:NE2	2.25	0.51
1:E:0:MET:O	1:E:1:SER:HB2	2.11	0.51
1:A:432:TYR:HA	1:A:454:ILE:O	2.11	0.51
1:A:451:GLN:HE22	2:B:71:ARG:H	1.59	0.51
1:C:481:ALA:HB2	2:D:71:ARG:NH1	2.25	0.51
1:C:445:VAL:HG12	1:C:451:GLN:OE1	2.10	0.51
2:D:88:VAL:HG11	2:D:142:VAL:HG11	1.92	0.51
1:G:307:LEU:HD23	1:G:441:ALA:HA	1.92	0.51
1:A:11:THR:HG22	1:A:523:LYS:HG2	1.92	0.50
2:H:51:ASP:OD1	2:H:51:ASP:N	2.44	0.50
1:A:360:PHE:CE2	3:A:605:C8E:H171	2.46	0.50
1:A:448:PRO:O	1:A:450:TYR:N	2.45	0.50
1:C:333:VAL:HG23	1:C:360:PHE:HE2	1.77	0.50
1:A:509:THR:HG21	1:A:521:ASP:OD2	2.12	0.50
1:E:233:TYR:OH	1:E:325:ASP:OD1	2.29	0.50
1:G:317:ARG:NH2	4:G:715:HOH:O	2.28	0.50
1:E:72:TYR:C	1:E:74:GLY:H	2.14	0.50
3:E:603:C8E:H21	3:G:602:C8E:H111	1.94	0.50
1:G:41:ARG:NH2	4:G:704:HOH:O	2.03	0.50
1:G:333:VAL:HG23	1:G:360:PHE:HE2	1.76	0.50
2:H:4:LEU:HD23	2:H:5:ARG:HG2	1.93	0.50
1:C:42:ARG:HG2	1:C:66:LEU:HD21	1.93	0.50
1:G:84:ARG:NH1	1:G:110:ASP:OD1	2.44	0.50
2:D:15:GLN:O	2:D:42:THR:N	2.41	0.50
2:H:44:VAL:HG21	2:H:52:ILE:HD11	1.94	0.50
2:B:137:ARG:NH2	4:B:209:HOH:O	2.32	0.50
2:D:8:THR:O	2:D:9:GLN:HB2	2.12	0.49
1:E:49:GLU:OE2	1:E:121:TYR:OH	2.31	0.49
1:A:451:GLN:CD	2:B:70:PHE:HB3	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:14:LEU:HD11	2:D:17:LEU:HD23	1.94	0.49
1:E:398:GLY:HA3	3:E:603:C8E:H131	1.95	0.49
1:G:544:MET:O	1:G:547:SER:OG	2.31	0.49
1:G:11:THR:HG22	1:G:523:LYS:HG2	1.95	0.49
1:A:27:ALA:HB3	1:A:30:PHE:HD2	1.78	0.49
1:C:362:ARG:NH1	4:C:738:HOH:O	2.46	0.49
2:D:117:GLU:OE1	4:D:204:HOH:O	2.20	0.49
1:E:125:THR:HB	2:F:75:ALA:HB2	1.95	0.49
1:E:512:ASN:CG	1:E:514:GLN:HG3	2.37	0.49
1:C:115:THR:O	4:C:711:HOH:O	2.20	0.49
1:E:17:GLU:HG2	1:E:39:MET:HG2	1.93	0.49
2:F:10:VAL:N	2:F:11:PRO:HD3	2.27	0.49
1:A:114:PHE:CE1	1:A:122:GLY:HA3	2.48	0.48
1:A:449:ASP:C	1:A:451:GLN:H	2.21	0.48
2:F:91:PRO:HB3	4:F:211:HOH:O	2.14	0.48
1:G:382:TRP:HB2	1:G:402:TYR:HB2	1.94	0.48
1:C:177:ASP:OD1	2:D:37:ARG:NH2	2.46	0.48
1:C:317:ARG:HD3	2:D:126:GLU:OE2	2.13	0.48
1:E:217:ASN:HB3	1:E:219:TRP:O	2.14	0.48
1:G:270:ASP:OD2	2:H:9:GLN:HB3	2.13	0.48
2:H:136:VAL:O	2:H:139:LEU:HB2	2.14	0.48
1:E:14:ASN:ND2	1:E:116:ASP:O	2.35	0.48
2:H:4:LEU:HD23	2:H:5:ARG:N	2.28	0.48
2:D:4:LEU:HD12	2:D:5:ARG:H	1.79	0.48
2:F:54:THR:OG1	2:F:89:LEU:HB2	2.13	0.48
2:H:3:ASN:O	4:H:201:HOH:O	2.20	0.48
3:A:603:C8E:H13	3:A:603:C8E:H41	1.73	0.47
1:G:554:SER:O	4:G:711:HOH:O	2.20	0.47
2:D:54:THR:OG1	2:D:89:LEU:HB2	2.14	0.47
1:E:436:LYS:NZ	4:E:738:HOH:O	2.47	0.47
1:A:356:GLN:HE22	1:A:358:TYR:HB2	1.78	0.47
1:C:509:THR:HG21	1:C:521:ASP:OD2	2.14	0.47
1:G:431:ARG:NH2	2:H:105:THR:HG21	2.30	0.47
2:H:10:VAL:N	2:H:11:PRO:HD3	2.29	0.47
1:G:45:GLN:HG3	1:G:66:LEU:HB2	1.96	0.47
1:A:227:LYS:HD3	1:A:319:ARG:HH22	1.79	0.47
1:C:23:TYR:CE2	1:C:25:ASN:HB2	2.49	0.47
3:C:603:C8E:H72	3:C:603:C8E:H41	1.73	0.47
1:E:442:VAL:HG12	2:F:109:ASN:HD22	1.79	0.47
1:A:45:GLN:HG3	1:A:66:LEU:HB2	1.96	0.47
1:A:56:PRO:HA	1:A:95:MET:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:VAL:O	1:A:285:PRO:HD2	2.15	0.47
1:G:32:ALA:N	4:G:712:HOH:O	2.47	0.47
2:H:128:ARG:NH2	4:H:202:HOH:O	2.16	0.47
1:G:274:ASP:O	1:G:276:ALA:N	2.48	0.46
1:G:499:ALA:O	1:G:528:ILE:HG13	2.15	0.46
3:C:604:C8E:H22	3:C:604:C8E:H52	1.41	0.46
2:H:49:ARG:HH11	2:H:50:LYS:H	1.62	0.46
2:H:53:PRO:HB3	2:H:90:ILE:HG12	1.96	0.46
1:C:37:HIS:CD2	1:C:39:MET:HG3	2.51	0.46
3:C:602:C8E:H51	3:C:602:C8E:H22	1.41	0.46
2:H:116:LYS:HA	2:H:116:LYS:HD3	1.78	0.46
2:H:3:ASN:OD1	2:H:4:LEU:N	2.49	0.46
1:A:438:ILE:HD12	1:A:453:GLY:HA2	1.98	0.46
1:E:199:ASN:O	4:E:717:HOH:O	2.21	0.46
1:G:423:ASP:OD1	1:G:424:ARG:HG3	2.15	0.46
1:A:166:GLN:HB3	4:A:751:HOH:O	2.16	0.46
2:D:8:THR:OG1	2:D:9:GLN:N	2.48	0.46
1:G:360:PHE:CG	3:G:603:C8E:H142	2.51	0.46
3:A:601:C8E:H72	3:A:601:C8E:H42	1.64	0.46
1:E:254:VAL:O	4:E:707:HOH:O	2.21	0.46
1:E:375:ASN:CG	1:E:376:ALA:H	2.24	0.46
1:G:42:ARG:HG2	1:G:66:LEU:HD21	1.96	0.46
1:G:349:ARG:HH22	3:G:601:C8E:H62	1.81	0.46
1:C:485:ALA:HB1	2:D:69:ILE:HD11	1.98	0.45
1:E:236:ASP:OD1	1:E:236:ASP:N	2.44	0.45
1:A:317:ARG:HD3	2:B:126:GLU:OE2	2.16	0.45
1:A:451:GLN:NE2	1:A:451:GLN:HA	2.30	0.45
1:E:150:GLN:HG3	1:E:164:ARG:NE	2.31	0.45
1:A:237:ILE:HD13	1:A:250:LEU:HB2	1.99	0.45
1:E:78:THR:HG22	1:E:79:ASP:N	2.31	0.45
1:E:495:THR:C	1:E:497:CYS:N	2.75	0.45
1:A:209:PRO:HD2	1:A:228:LEU:O	2.17	0.45
1:C:353:SER:HB2	1:C:385:ASP:OD1	2.16	0.45
1:E:84:ARG:NH1	1:E:110:ASP:OD1	2.50	0.45
2:F:142:VAL:O	2:F:145:ALA:HB3	2.17	0.45
1:G:114:PHE:O	4:G:710:HOH:O	2.21	0.45
1:E:544:MET:N	4:E:730:HOH:O	2.48	0.45
1:C:150:GLN:HG2	4:C:728:HOH:O	2.16	0.45
1:C:0:MET:HB3	1:C:1:SER:H	1.35	0.45
1:E:233:TYR:HB2	1:E:254:VAL:HB	1.98	0.45
1:E:317:ARG:HD3	2:F:126:GLU:OE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LEU:HD21	1:A:295:ARG:HB2	1.98	0.45
3:C:602:C8E:H191	3:C:602:C8E:H161	1.69	0.45
1:C:36:PRO:HG3	1:C:46:TRP:CZ3	2.51	0.45
2:F:96:TYR:CD2	2:F:142:VAL:HG22	2.52	0.45
2:F:13:GLU:HG3	2:F:14:LEU:N	2.32	0.44
2:F:136:VAL:O	2:F:139:LEU:HB2	2.16	0.44
1:G:229:LEU:HD21	1:G:319:ARG:NH2	2.31	0.44
1:A:429:ASN:ND2	4:A:721:HOH:O	2.30	0.44
1:C:-1:SER:HB3	1:C:25:ASN:HD21	1.82	0.44
1:C:114:PHE:CE1	1:C:122:GLY:HA3	2.53	0.44
1:E:362:ARG:NH1	1:E:364:ARG:HD3	2.32	0.44
1:A:84:ARG:NH1	1:A:110:ASP:OD1	2.50	0.44
3:A:602:C8E:H161	3:A:602:C8E:H191	1.87	0.44
1:A:451:GLN:NE2	2:B:70:PHE:HB3	2.31	0.44
1:E:27:ALA:HB3	1:E:30:PHE:HB2	1.99	0.44
1:E:44:LEU:O	1:E:67:PRO:HD2	2.17	0.44
2:F:52:ILE:HA	2:F:53:PRO:HD3	1.87	0.44
1:G:317:ARG:NE	4:G:715:HOH:O	2.39	0.44
1:G:512:ASN:HB3	1:G:516:GLN:O	2.17	0.44
1:E:84:ARG:NH2	1:E:116:ASP:OD2	2.39	0.44
1:G:317:ARG:HD3	2:H:126:GLU:OE2	2.17	0.44
1:E:78:THR:HG22	1:E:79:ASP:H	1.83	0.44
1:A:73:THR:O	1:A:79:ASP:HB3	2.17	0.44
1:A:431:ARG:NH2	2:B:105:THR:HG21	2.33	0.44
1:G:445:VAL:HG22	1:G:451:GLN:OE1	2.18	0.44
1:E:23:TYR:CE2	1:E:25:ASN:HB2	2.52	0.44
1:A:308:MET:HE3	1:A:308:MET:HB3	1.81	0.43
1:E:42:ARG:HD2	4:E:768:HOH:O	2.18	0.43
1:G:380:LEU:HD13	1:G:405:ARG:HD3	2.00	0.43
1:C:72:TYR:O	1:C:73:THR:OG1	2.27	0.43
1:E:175:LYS:NZ	4:E:740:HOH:O	2.51	0.43
1:E:199:ASN:HA	1:E:200:PRO:HD3	1.86	0.43
1:A:333:VAL:HG23	1:A:360:PHE:CE2	2.53	0.43
1:C:68:ASN:ND2	4:C:723:HOH:O	2.36	0.43
1:C:169:LEU:O	1:C:188:GLN:HA	2.18	0.43
1:C:450:TYR:N	1:C:450:TYR:CD1	2.82	0.43
1:G:219:TRP:HB3	2:H:8:THR:HG22	2.00	0.43
2:H:18:LEU:HD11	2:H:54:THR:HB	2.00	0.43
1:C:333:VAL:HG21	3:C:607:C8E:H132	2.01	0.43
1:C:466:ALA:CB	1:C:469:TRP:HB2	2.40	0.43
1:C:472:VAL:HG11	1:C:541:THR:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:VAL:HG13	4:A:722:HOH:O	2.19	0.43
3:C:605:C8E:H62	2:D:5:ARG:HG3	2.01	0.43
1:G:308:MET:HE3	1:G:308:MET:HB3	1.88	0.43
3:A:601:C8E:H41	3:A:601:C8E:H13	1.66	0.43
1:E:482:LYS:HD3	4:E:711:HOH:O	2.19	0.43
1:E:509:THR:HG21	1:E:521:ASP:OD2	2.18	0.43
1:G:509:THR:HG21	1:G:521:ASP:OD2	2.19	0.43
1:A:446:TYR:CD1	1:A:447:ASN:N	2.87	0.43
1:C:64:ASP:O	1:C:85:TRP:HA	2.19	0.43
2:F:15:GLN:N	4:F:210:HOH:O	2.51	0.43
1:A:85:TRP:CD1	1:A:109:SER:HB3	2.54	0.43
1:A:356:GLN:HG2	1:A:357:ILE:N	2.34	0.43
1:C:308:MET:HE3	1:C:308:MET:HB3	1.89	0.43
1:G:349:ARG:CZ	3:G:601:C8E:H102	2.49	0.43
2:D:143:HIS:O	2:D:146:GLU:HG2	2.19	0.42
1:C:277:THR:N	4:C:733:HOH:O	2.52	0.42
1:C:549:ILE:HD12	2:D:69:ILE:HD13	2.01	0.42
1:G:85:TRP:CD1	1:G:109:SER:HB3	2.54	0.42
2:D:10:VAL:C	2:D:12:THR:N	2.77	0.42
1:E:209:PRO:HD2	1:E:228:LEU:O	2.19	0.42
2:H:90:ILE:HA	2:H:91:PRO:HD3	1.92	0.42
1:G:492:GLN:OE1	1:G:541:THR:N	2.53	0.42
1:A:495:THR:O	1:A:496:CYS:C	2.63	0.42
1:C:215:LEU:HB3	3:C:601:C8E:H172	2.00	0.42
1:G:267:VAL:O	1:G:285:PRO:HD2	2.20	0.42
2:D:18:LEU:HD23	2:D:44:VAL:HB	2.02	0.42
1:G:5:ILE:HG12	1:G:528:ILE:HG23	2.02	0.42
1:G:282:THR:O	1:G:339:SER:HA	2.19	0.42
1:E:258:LEU:HD21	1:E:295:ARG:HB2	2.01	0.42
1:E:30:PHE:CZ	1:E:54:LEU:HD21	2.55	0.42
1:E:72:TYR:HD2	1:E:79:ASP:OD2	2.02	0.42
1:E:291:TYR:OH	4:E:716:HOH:O	2.20	0.42
1:G:463:TRP:HA	1:G:464:PRO:HD3	1.89	0.42
1:C:70:ARG:NH1	4:C:736:HOH:O	2.45	0.42
1:C:291:TYR:OH	4:C:712:HOH:O	2.21	0.42
2:F:143:HIS:O	2:F:146:GLU:HG2	2.19	0.42
1:G:209:PRO:HD2	1:G:228:LEU:O	2.20	0.42
1:A:5:ILE:HA	1:A:6:PRO:HD3	1.84	0.42
1:A:169:LEU:O	1:A:188:GLN:HA	2.20	0.42
2:B:136:VAL:O	2:B:139:LEU:HB2	2.20	0.42
1:C:32:ALA:HA	1:C:49:GLU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:PHE:CE1	1:E:122:GLY:HA3	2.54	0.42
1:E:208:GLU:HA	1:E:228:LEU:O	2.19	0.42
1:E:485:ALA:HB1	2:F:69:ILE:HD11	2.01	0.42
1:G:129:ALA:HA	4:G:707:HOH:O	2.20	0.42
1:C:196:ASN:HA	1:C:197:PRO:HD3	1.87	0.41
1:C:287:ALA:HB2	3:C:601:C8E:H32	2.02	0.41
1:C:415:ILE:HD13	1:C:555:ALA:HB2	2.02	0.41
2:F:14:LEU:O	2:F:16:LYS:N	2.44	0.41
2:F:50:LYS:HB3	2:F:50:LYS:HE3	1.56	0.41
1:G:326:ARG:HD2	1:G:365:THR:HB	2.01	0.41
1:C:52:TYR:CZ	1:C:59:GLY:HA3	2.55	0.41
1:C:199:ASN:HA	1:C:200:PRO:HD3	1.87	0.41
1:E:495:THR:O	1:E:496:CYS:C	2.63	0.41
1:G:251:LYS:HD2	1:G:251:LYS:HA	1.84	0.41
1:G:305:THR:HG23	1:G:321:TYR:HB3	2.03	0.41
2:H:8:THR:O	2:H:9:GLN:HB3	2.20	0.41
3:A:604:C8E:H41	3:A:604:C8E:H13	1.57	0.41
1:E:85:TRP:CD1	1:E:109:SER:HB3	2.56	0.41
1:G:346:ARG:HA	1:G:346:ARG:HD3	1.75	0.41
1:A:199:ASN:HA	1:A:200:PRO:HD3	1.87	0.41
1:C:45:GLN:HG3	1:C:66:LEU:HB2	2.03	0.41
1:C:61:MET:HE3	1:C:87:TYR:OH	2.20	0.41
1:C:67:PRO:HA	1:C:83:THR:HG23	2.03	0.41
1:E:149:LYS:HB2	1:E:165:ALA:HB3	2.02	0.41
1:E:280:THR:OG1	1:E:346:ARG:NH1	2.43	0.41
1:G:268:VAL:HG13	1:G:284:GLU:HG2	2.01	0.41
1:A:433:ALA:O	1:A:453:GLY:HA3	2.21	0.41
1:C:140:GLU:O	2:D:30:ARG:NH2	2.54	0.41
1:C:267:VAL:O	1:C:285:PRO:HD2	2.21	0.41
1:A:76:ASP:OD1	1:A:76:ASP:N	2.53	0.41
1:A:153:VAL:HG11	1:A:158:GLY:HA3	2.03	0.41
2:D:71:ARG:HH11	2:D:71:ARG:HD3	1.73	0.41
1:E:61:MET:HE3	1:E:87:TYR:OH	2.20	0.41
1:G:4:LEU:HD12	1:G:4:LEU:N	2.35	0.41
1:A:528:ILE:H	1:A:529:GLU:HG2	1.84	0.41
2:B:54:THR:OG1	2:B:89:LEU:HB2	2.21	0.41
2:B:90:ILE:HA	2:B:91:PRO:HD3	1.88	0.41
2:D:116:LYS:HA	2:D:116:LYS:HD3	1.78	0.41
1:E:333:VAL:HG23	1:E:360:PHE:HE2	1.86	0.41
1:G:17:GLU:HG2	1:G:39:MET:HG2	2.02	0.41
2:B:53:PRO:HB3	2:B:90:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:ASP:C	1:C:276:ALA:H	2.29	0.41
1:E:65:TRP:CZ3	1:E:67:PRO:HG3	2.56	0.41
1:E:267:VAL:O	1:E:285:PRO:HD2	2.21	0.41
1:E:436:LYS:HA	1:E:439:GLN:HG2	2.03	0.41
2:F:11:PRO:HB2	2:F:12:THR:H	1.58	0.41
1:G:196:ASN:HA	1:G:197:PRO:HD3	1.94	0.41
1:C:271:ARG:NH2	1:C:281:GLN:OE1	2.54	0.40
1:C:420:LYS:HD3	1:C:421:ASP:OD1	2.19	0.40
1:G:171:MET:SD	4:G:782:HOH:O	2.63	0.40
1:C:308:MET:SD	2:D:119:GLU:HG3	2.60	0.40
1:C:432:TYR:HA	1:C:454:ILE:O	2.21	0.40
1:G:5:ILE:HA	1:G:6:PRO:HD3	1.92	0.40
1:G:476:TYR:OH	4:G:702:HOH:O	1.96	0.40
1:C:45:GLN:OE1	1:C:47:GLN:NE2	2.40	0.40
2:D:9:GLN:O	2:D:10:VAL:CG2	2.68	0.40
2:D:14:LEU:CD1	2:D:17:LEU:HD23	2.52	0.40
1:A:452:GLN:HG3	1:A:453:GLY:N	2.34	0.40
2:B:18:LEU:HB2	2:B:54:THR:HG22	2.04	0.40
1:A:42:ARG:HG2	1:A:66:LEU:HD21	2.02	0.40
1:C:349:ARG:NH2	3:C:602:C8E:H191	2.34	0.40
1:E:70:ARG:NH2	4:E:718:HOH:O	2.21	0.40
1:E:305:THR:HG23	1:E:321:TYR:HB3	2.04	0.40

All (4) 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)
4:A:846:HOH:O	4:C:823:HOH:O[2_746]	1.86	0.34
4:E:774:HOH:O	4:G:778:HOH:O[2_657]	2.12	0.08
4:E:774:HOH:O	4:G:780:HOH:O[2_657]	2.15	0.05
1:A:38:TYR:OH	1:C:40:GLU:OE2[2_846]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	537/577 (93%)	490 (91%)	36 (7%)	11 (2%)	6	10
1	C	535/577 (93%)	491 (92%)	33 (6%)	11 (2%)	5	9
1	E	530/577 (92%)	483 (91%)	33 (6%)	14 (3%)	4	6
1	G	533/577 (92%)	488 (92%)	38 (7%)	7 (1%)	9	16
2	B	137/198 (69%)	123 (90%)	9 (7%)	5 (4%)	2	4
2	D	144/198 (73%)	134 (93%)	7 (5%)	3 (2%)	5	9
2	F	143/198 (72%)	131 (92%)	6 (4%)	6 (4%)	2	2
2	H	145/198 (73%)	135 (93%)	7 (5%)	3 (2%)	5	9
All	All	2704/3100 (87%)	2475 (92%)	169 (6%)	60 (2%)	5	8

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	80	LYS
1	A	445	VAL
1	A	447	ASN
1	A	496	CYS
1	A	497	CYS
2	B	48	MET
2	B	51	ASP
1	C	1	SER
1	C	448	PRO
1	C	450	TYR
1	C	497	CYS
2	D	9	GLN
2	D	10	VAL
1	E	1	SER
1	E	73	THR
1	E	82	ALA
1	E	374	SER
1	E	496	CYS
1	E	497	CYS
1	E	500	VAL
1	E	514	GLN
1	E	542	ALA
2	F	5	ARG

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Mol	Chain	Res	Type
2	F	11	PRO
2	F	13	GLU
2	F	44	VAL
1	G	275	TRP
1	G	443	PRO
1	G	444	LYS
2	H	11	PRO
1	A	0	MET
1	C	0	MET
1	C	76	ASP
1	C	444	LYS
1	E	12	SER
2	F	4	LEU
2	F	48	MET
1	G	2	GLY
1	G	274	ASP
1	A	452	GLN
2	B	16	LYS
2	B	50	LYS
2	B	143	HIS
1	C	80	LYS
1	C	243	ASP
1	C	447	ASN
1	C	498	TRP
1	E	451	GLN
1	G	243	ASP
2	H	5	ARG
2	D	11	PRO
1	E	375	ASN
2	H	8	THR
1	A	449	ASP
1	A	541	THR
1	E	443	PRO
1	G	80	LYS
1	E	74	GLY
1	A	220	GLY

5.3.2 Protein sidechains ⓘ

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	454/487 (93%)	449 (99%)	5 (1%)	65	79
1	C	456/487 (94%)	448 (98%)	8 (2%)	51	69
1	E	449/487 (92%)	443 (99%)	6 (1%)	61	75
1	G	453/487 (93%)	445 (98%)	8 (2%)	51	69
2	B	121/169 (72%)	120 (99%)	1 (1%)	73	83
2	D	123/169 (73%)	119 (97%)	4 (3%)	33	55
2	F	122/169 (72%)	118 (97%)	4 (3%)	33	55
2	H	127/169 (75%)	123 (97%)	4 (3%)	35	57
All	All	2305/2624 (88%)	2265 (98%)	40 (2%)	53	71

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	LYS
1	A	351	ASN
1	A	425	MET
1	A	450	TYR
1	A	451	GLN
2	B	44	VAL
1	C	0	MET
1	C	351	ASN
1	C	450	TYR
1	C	468	ARG
1	C	496	CYS
1	C	500	VAL
1	C	545	LEU
1	C	553	GLN
2	D	44	VAL
2	D	71	ARG
2	D	93	HIS
2	D	147	VAL
1	E	5	ILE
1	E	80	LYS
1	E	236	ASP
1	E	240	SER
1	E	351	ASN
1	E	517	THR

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Mol	Chain	Res	Type
2	F	10	VAL
2	F	22	SER
2	F	44	VAL
2	F	50	LYS
1	G	5	ILE
1	G	26	ILE
1	G	191	LYS
1	G	236	ASP
1	G	351	ASN
1	G	375	ASN
1	G	500	VAL
1	G	528	ILE
2	H	12	THR
2	H	44	VAL
2	H	54	THR
2	H	95	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	451	GLN
1	C	102	ASN
1	C	356	GLN
2	D	85	GLN
2	D	101	ASN
1	E	102	ASN
1	E	288	GLN
1	E	356	GLN
1	E	427	GLN
1	E	501	ASN
1	G	81	ASN
1	G	102	ASN
1	G	159	ASN
1	G	288	GLN
1	G	356	GLN
1	G	427	GLN
1	G	492	GLN
1	G	501	ASN
2	H	9	GLN
2	H	79	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

21 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	$\# Z > 2$
3	C8E	E	603	-	20,20,20	0.38	0	19,19,19	0.36	0
3	C8E	C	608	-	20,20,20	0.39	0	19,19,19	0.36	0
3	C8E	C	604	-	20,20,20	0.38	0	19,19,19	0.36	0
3	C8E	C	602	-	20,20,20	0.38	0	19,19,19	0.38	0
3	C8E	A	604	-	20,20,20	0.38	0	19,19,19	0.47	0
3	C8E	C	603	-	20,20,20	0.39	0	19,19,19	0.37	0
3	C8E	A	602	-	20,20,20	0.38	0	19,19,19	0.36	0
3	C8E	C	605	-	20,20,20	0.41	0	19,19,19	0.33	0
3	C8E	G	603	-	20,20,20	0.38	0	19,19,19	0.36	0
3	C8E	E	602	-	20,20,20	0.39	0	19,19,19	0.31	0
3	C8E	A	603	-	20,20,20	0.38	0	19,19,19	0.36	0
3	C8E	C	607	-	20,20,20	0.38	0	19,19,19	0.40	0
3	C8E	C	609	-	20,20,20	0.39	0	19,19,19	0.37	0
3	C8E	G	602	-	20,20,20	0.39	0	19,19,19	0.32	0
3	C8E	A	601	-	20,20,20	0.40	0	19,19,19	0.32	0
3	C8E	G	601	-	20,20,20	0.37	0	19,19,19	0.43	0
3	C8E	C	601	-	20,20,20	0.39	0	19,19,19	0.32	0
3	C8E	E	601	-	20,20,20	0.36	0	19,19,19	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	C8E	E	604	-	20,20,20	0.41	0	19,19,19	0.35	0
3	C8E	A	605	-	20,20,20	0.37	0	19,19,19	0.52	0
3	C8E	C	606	-	20,20,20	0.38	0	19,19,19	0.39	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
3	C8E	E	603	-	-	14/18/18/18	-
3	C8E	C	608	-	-	14/18/18/18	-
3	C8E	C	604	-	-	10/18/18/18	-
3	C8E	C	602	-	-	15/18/18/18	-
3	C8E	A	604	-	-	14/18/18/18	-
3	C8E	C	603	-	-	10/18/18/18	-
3	C8E	A	602	-	-	15/18/18/18	-
3	C8E	C	605	-	-	11/18/18/18	-
3	C8E	G	603	-	-	13/18/18/18	-
3	C8E	E	602	-	-	11/18/18/18	-
3	C8E	A	603	-	-	10/18/18/18	-
3	C8E	C	607	-	-	10/18/18/18	-
3	C8E	C	609	-	-	14/18/18/18	-
3	C8E	G	602	-	-	12/18/18/18	-
3	C8E	A	601	-	-	13/18/18/18	-
3	C8E	G	601	-	-	12/18/18/18	-
3	C8E	C	601	-	-	12/18/18/18	-
3	C8E	E	601	-	-	10/18/18/18	-
3	C8E	E	604	-	-	12/18/18/18	-
3	C8E	A	605	-	-	11/18/18/18	-
3	C8E	C	606	-	-	13/18/18/18	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (256) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	606	C8E	O12-C13-C14-O15
3	C	608	C8E	O9-C10-C11-O12
3	C	608	C8E	O12-C13-C14-O15
3	E	603	C8E	O9-C10-C11-O12
3	A	601	C8E	O9-C10-C11-O12
3	E	603	C8E	O12-C13-C14-O15
3	E	604	C8E	O12-C13-C14-O15
3	G	601	C8E	O12-C13-C14-O15
3	C	602	C8E	C2-C3-C4-C5
3	C	604	C8E	C2-C3-C4-C5
3	A	605	C8E	O18-C19-C20-O21
3	A	603	C8E	C3-C4-C5-C6
3	E	601	C8E	C2-C3-C4-C5
3	C	605	C8E	O15-C16-C17-O18
3	C	609	C8E	O12-C13-C14-O15
3	A	603	C8E	O9-C10-C11-O12
3	A	601	C8E	O12-C13-C14-O15
3	C	609	C8E	O15-C16-C17-O18
3	E	604	C8E	O15-C16-C17-O18
3	C	603	C8E	O15-C16-C17-O18
3	C	603	C8E	O12-C13-C14-O15
3	A	601	C8E	O18-C19-C20-O21
3	C	604	C8E	O18-C19-C20-O21
3	C	607	C8E	O18-C19-C20-O21
3	C	608	C8E	O18-C19-C20-O21
3	G	601	C8E	O18-C19-C20-O21
3	A	604	C8E	O12-C13-C14-O15
3	A	601	C8E	C4-C5-C6-C7
3	C	606	C8E	O9-C10-C11-O12
3	C	604	C8E	O12-C13-C14-O15
3	C	604	C8E	C4-C5-C6-C7
3	A	602	C8E	O12-C13-C14-O15
3	C	607	C8E	O9-C10-C11-O12
3	C	604	C8E	O9-C10-C11-O12
3	C	604	C8E	C6-C7-C8-O9
3	G	601	C8E	C6-C7-C8-O9
3	E	602	C8E	O12-C13-C14-O15
3	A	604	C8E	O18-C19-C20-O21
3	C	602	C8E	O18-C19-C20-O21
3	C	603	C8E	O18-C19-C20-O21
3	C	606	C8E	O18-C19-C20-O21
3	C	603	C8E	C4-C5-C6-C7
3	C	601	C8E	O12-C13-C14-O15

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Mol	Chain	Res	Type	Atoms
3	C	609	C8E	C6-C7-C8-O9
3	G	601	C8E	O9-C10-C11-O12
3	C	602	C8E	C6-C7-C8-O9
3	A	602	C8E	O18-C19-C20-O21
3	E	604	C8E	O18-C19-C20-O21
3	G	602	C8E	O18-C19-C20-O21
3	E	601	C8E	O15-C16-C17-O18
3	A	604	C8E	O9-C10-C11-O12
3	C	608	C8E	C5-C6-C7-C8
3	C	601	C8E	C3-C4-C5-C6
3	E	603	C8E	C3-C4-C5-C6
3	G	601	C8E	C2-C3-C4-C5
3	C	605	C8E	C2-C3-C4-C5
3	A	605	C8E	O15-C16-C17-O18
3	C	602	C8E	O12-C13-C14-O15
3	E	604	C8E	C3-C4-C5-C6
3	A	602	C8E	C16-C17-O18-C19
3	C	604	C8E	O15-C16-C17-O18
3	C	607	C8E	C3-C4-C5-C6
3	E	602	C8E	C4-C5-C6-C7
3	C	605	C8E	C4-C5-C6-C7
3	A	601	C8E	C6-C7-C8-O9
3	C	608	C8E	C2-C3-C4-C5
3	A	603	C8E	O18-C19-C20-O21
3	C	609	C8E	O18-C19-C20-O21
3	E	602	C8E	O18-C19-C20-O21
3	G	603	C8E	O12-C13-C14-O15
3	A	603	C8E	C2-C3-C4-C5
3	C	604	C8E	C3-C4-C5-C6
3	A	604	C8E	C2-C3-C4-C5
3	C	605	C8E	O12-C13-C14-O15
3	C	607	C8E	C4-C5-C6-C7
3	A	602	C8E	C4-C5-C6-C7
3	G	603	C8E	C2-C3-C4-C5
3	A	602	C8E	C6-C7-C8-O9
3	E	601	C8E	O12-C13-C14-O15
3	C	602	C8E	C16-C17-O18-C19
3	C	606	C8E	C2-C3-C4-C5
3	C	605	C8E	C6-C7-C8-O9
3	A	601	C8E	C2-C3-C4-C5
3	E	602	C8E	C6-C7-C8-O9
3	G	603	C8E	C6-C7-C8-O9

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Mol	Chain	Res	Type	Atoms
3	A	604	C8E	C1-C2-C3-C4
3	C	601	C8E	O18-C19-C20-O21
3	E	601	C8E	O18-C19-C20-O21
3	A	601	C8E	C1-C2-C3-C4
3	C	602	C8E	C4-C5-C6-C7
3	A	602	C8E	C3-C4-C5-C6
3	A	604	C8E	C5-C6-C7-C8
3	A	605	C8E	C3-C4-C5-C6
3	C	608	C8E	O15-C16-C17-O18
3	A	605	C8E	O12-C13-C14-O15
3	C	609	C8E	C3-C4-C5-C6
3	E	601	C8E	C6-C7-C8-O9
3	A	601	C8E	C3-C4-C5-C6
3	G	602	C8E	C2-C3-C4-C5
3	G	603	C8E	O18-C19-C20-O21
3	G	602	C8E	C3-C4-C5-C6
3	E	602	C8E	C2-C3-C4-C5
3	E	604	C8E	C2-C3-C4-C5
3	C	608	C8E	C3-C4-C5-C6
3	A	604	C8E	C6-C7-C8-O9
3	A	605	C8E	C6-C7-C8-O9
3	A	605	C8E	C2-C3-C4-C5
3	C	601	C8E	C5-C6-C7-C8
3	C	602	C8E	C3-C4-C5-C6
3	E	602	C8E	C3-C4-C5-C6
3	C	609	C8E	C1-C2-C3-C4
3	G	601	C8E	C4-C5-C6-C7
3	G	602	C8E	O12-C13-C14-O15
3	A	603	C8E	C1-C2-C3-C4
3	C	607	C8E	C2-C3-C4-C5
3	C	601	C8E	C4-C5-C6-C7
3	C	603	C8E	C2-C3-C4-C5
3	A	605	C8E	C1-C2-C3-C4
3	C	605	C8E	O9-C10-C11-O12
3	E	604	C8E	O9-C10-C11-O12
3	E	602	C8E	C1-C2-C3-C4
3	E	604	C8E	C1-C2-C3-C4
3	C	606	C8E	O15-C16-C17-O18
3	E	603	C8E	C6-C7-C8-O9
3	G	603	C8E	C1-C2-C3-C4
3	A	602	C8E	O15-C16-C17-O18
3	C	601	C8E	O9-C10-C11-O12

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Mol	Chain	Res	Type	Atoms
3	C	606	C8E	C1-C2-C3-C4
3	A	604	C8E	O15-C16-C17-O18
3	G	603	C8E	C3-C4-C5-C6
3	C	608	C8E	C1-C2-C3-C4
3	A	605	C8E	C13-C14-O15-C16
3	C	603	C8E	C14-C13-O12-C11
3	A	603	C8E	C13-C14-O15-C16
3	C	604	C8E	C20-C19-O18-C17
3	E	604	C8E	C20-C19-O18-C17
3	E	604	C8E	C11-C10-O9-C8
3	C	603	C8E	C6-C7-C8-O9
3	A	601	C8E	C20-C19-O18-C17
3	C	601	C8E	C20-C19-O18-C17
3	C	606	C8E	C20-C19-O18-C17
3	C	609	C8E	C17-C16-O15-C14
3	G	601	C8E	C13-C14-O15-C16
3	G	602	C8E	C20-C19-O18-C17
3	C	607	C8E	C20-C19-O18-C17
3	C	608	C8E	C20-C19-O18-C17
3	E	601	C8E	C13-C14-O15-C16
3	A	601	C8E	C10-C11-O12-C13
3	A	602	C8E	C13-C14-O15-C16
3	E	604	C8E	C17-C16-O15-C14
3	G	601	C8E	C14-C13-O12-C11
3	A	602	C8E	C14-C13-O12-C11
3	A	603	C8E	C16-C17-O18-C19
3	C	607	C8E	C14-C13-O12-C11
3	A	603	C8E	C20-C19-O18-C17
3	C	601	C8E	C14-C13-O12-C11
3	C	602	C8E	C17-C16-O15-C14
3	E	603	C8E	O18-C19-C20-O21
3	E	603	C8E	C20-C19-O18-C17
3	G	601	C8E	C17-C16-O15-C14
3	E	603	C8E	C1-C2-C3-C4
3	E	601	C8E	C11-C10-O9-C8
3	G	601	C8E	C10-C11-O12-C13
3	E	603	C8E	C10-C11-O12-C13
3	A	602	C8E	C20-C19-O18-C17
3	A	604	C8E	C14-C13-O12-C11
3	C	602	C8E	C20-C19-O18-C17
3	C	601	C8E	C13-C14-O15-C16
3	E	601	C8E	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
3	C	605	C8E	C7-C8-O9-C10
3	G	601	C8E	C7-C8-O9-C10
3	G	602	C8E	C5-C6-C7-C8
3	A	604	C8E	C4-C5-C6-C7
3	C	602	C8E	C10-C11-O12-C13
3	C	606	C8E	C10-C11-O12-C13
3	E	602	C8E	C5-C6-C7-C8
3	C	608	C8E	C10-C11-O12-C13
3	G	602	C8E	C7-C8-O9-C10
3	E	603	C8E	C13-C14-O15-C16
3	C	608	C8E	C6-C7-C8-O9
3	A	605	C8E	C17-C16-O15-C14
3	C	603	C8E	C3-C4-C5-C6
3	A	602	C8E	C1-C2-C3-C4
3	A	604	C8E	C7-C8-O9-C10
3	E	603	C8E	C7-C8-O9-C10
3	A	602	C8E	C17-C16-O15-C14
3	C	605	C8E	C3-C4-C5-C6
3	A	604	C8E	C3-C4-C5-C6
3	E	603	C8E	C5-C6-C7-C8
3	C	606	C8E	C17-C16-O15-C14
3	C	607	C8E	C1-C2-C3-C4
3	C	609	C8E	C11-C10-O9-C8
3	C	609	C8E	C2-C3-C4-C5
3	C	606	C8E	C3-C4-C5-C6
3	G	602	C8E	C10-C11-O12-C13
3	C	608	C8E	C13-C14-O15-C16
3	E	603	C8E	C17-C16-O15-C14
3	G	603	C8E	C13-C14-O15-C16
3	G	603	C8E	C10-C11-O12-C13
3	C	606	C8E	C16-C17-O18-C19
3	G	603	C8E	C17-C16-O15-C14
3	C	605	C8E	C17-C16-O15-C14
3	A	601	C8E	C7-C8-O9-C10
3	C	608	C8E	C7-C8-O9-C10
3	C	609	C8E	C14-C13-O12-C11
3	G	603	C8E	C14-C13-O12-C11
3	C	609	C8E	C20-C19-O18-C17
3	E	602	C8E	C20-C19-O18-C17
3	A	602	C8E	C7-C8-O9-C10
3	C	606	C8E	C7-C8-O9-C10
3	E	604	C8E	C16-C17-O18-C19

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Mol	Chain	Res	Type	Atoms
3	E	603	C8E	C2-C3-C4-C5
3	C	602	C8E	C1-C2-C3-C4
3	A	605	C8E	O9-C10-C11-O12
3	G	602	C8E	C14-C13-O12-C11
3	C	603	C8E	C20-C19-O18-C17
3	A	605	C8E	C14-C13-O12-C11
3	C	602	C8E	C13-C14-O15-C16
3	E	602	C8E	O15-C16-C17-O18
3	G	601	C8E	C3-C4-C5-C6
3	A	601	C8E	C11-C10-O9-C8
3	E	602	C8E	C17-C16-O15-C14
3	A	603	C8E	O15-C16-C17-O18
3	C	603	C8E	C16-C17-O18-C19
3	C	602	C8E	C14-C13-O12-C11
3	A	601	C8E	O15-C16-C17-O18
3	C	606	C8E	C13-C14-O15-C16
3	C	605	C8E	C13-C14-O15-C16
3	G	602	C8E	C4-C5-C6-C7
3	A	602	C8E	C10-C11-O12-C13
3	A	604	C8E	C20-C19-O18-C17
3	E	603	C8E	C16-C17-O18-C19
3	C	602	C8E	C7-C8-O9-C10
3	E	604	C8E	C10-C11-O12-C13
3	E	601	C8E	C7-C8-O9-C10
3	C	601	C8E	C1-C2-C3-C4
3	G	602	C8E	C1-C2-C3-C4
3	G	603	C8E	O15-C16-C17-O18
3	C	608	C8E	C4-C5-C6-C7
3	G	603	C8E	C20-C19-O18-C17
3	C	609	C8E	C7-C8-O9-C10
3	A	603	C8E	C7-C8-O9-C10
3	C	609	C8E	C13-C14-O15-C16
3	A	604	C8E	C13-C14-O15-C16
3	C	607	C8E	C16-C17-O18-C19
3	C	602	C8E	O15-C16-C17-O18
3	G	602	C8E	O9-C10-C11-O12
3	C	605	C8E	C10-C11-O12-C13
3	C	601	C8E	C7-C8-O9-C10
3	C	604	C8E	C1-C2-C3-C4
3	A	602	C8E	O9-C10-C11-O12
3	E	601	C8E	O9-C10-C11-O12
3	C	601	C8E	O15-C16-C17-O18

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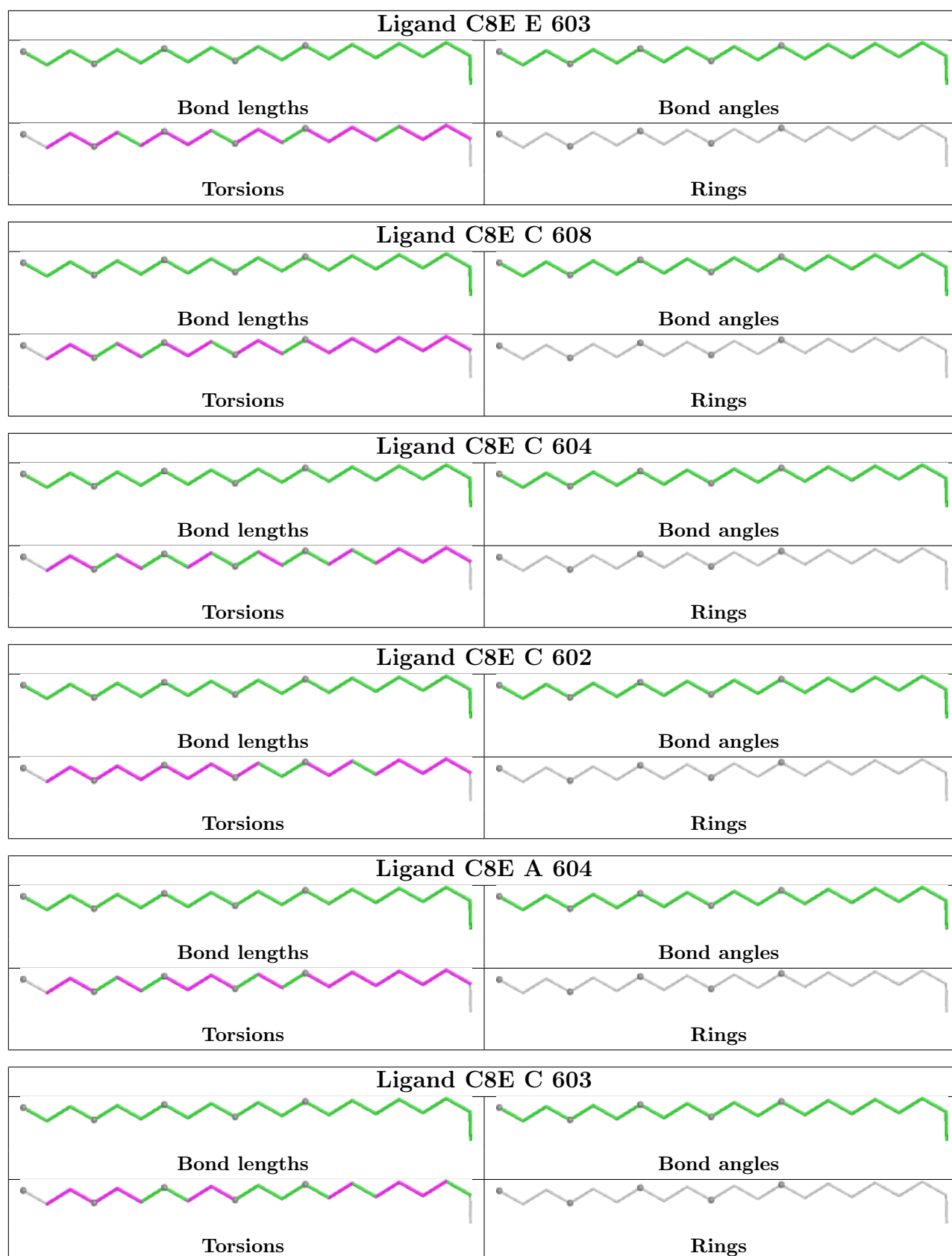
Mol	Chain	Res	Type	Atoms
3	C	609	C8E	O9-C10-C11-O12
3	G	603	C8E	O9-C10-C11-O12
3	C	607	C8E	C17-C16-O15-C14

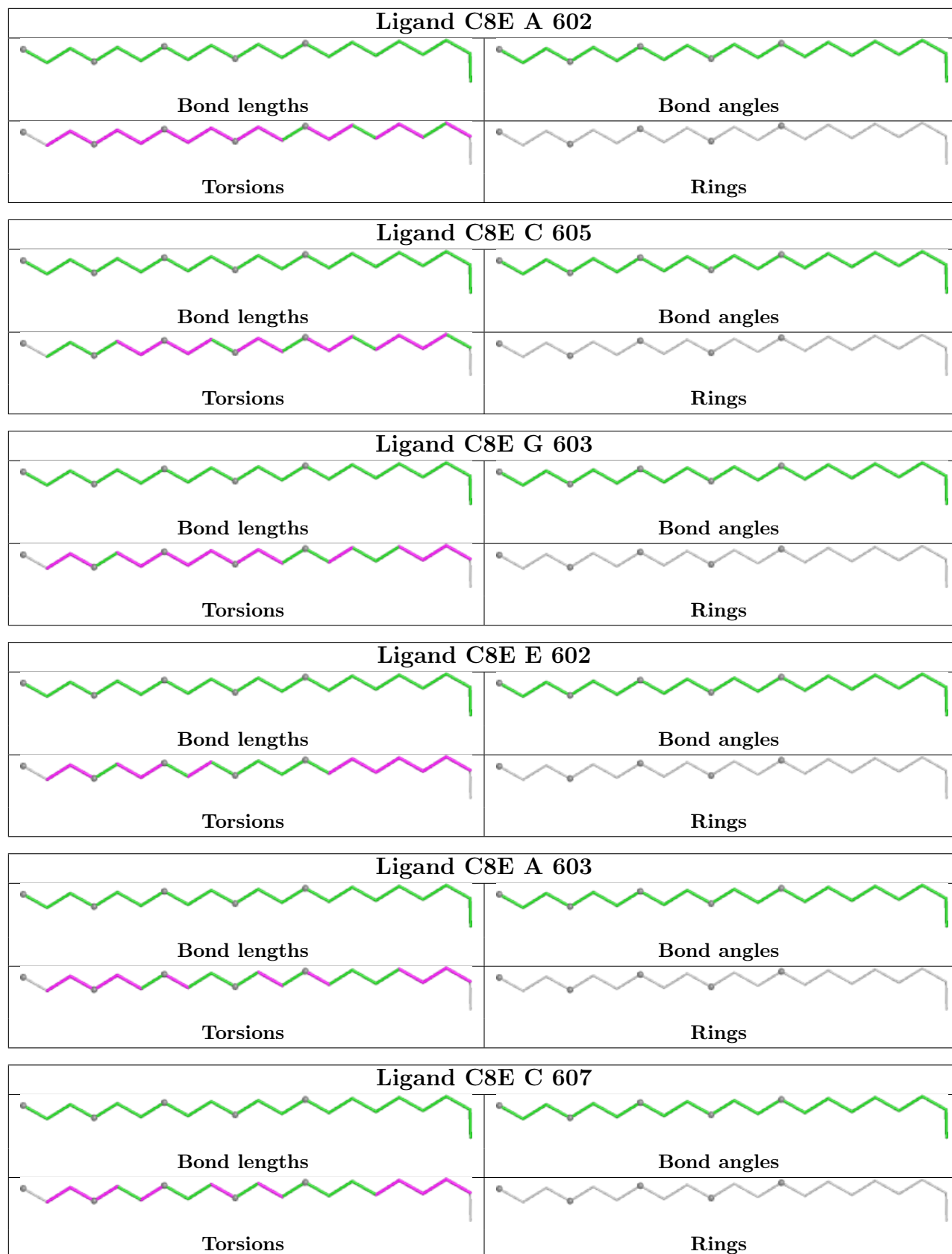
There are no ring outliers.

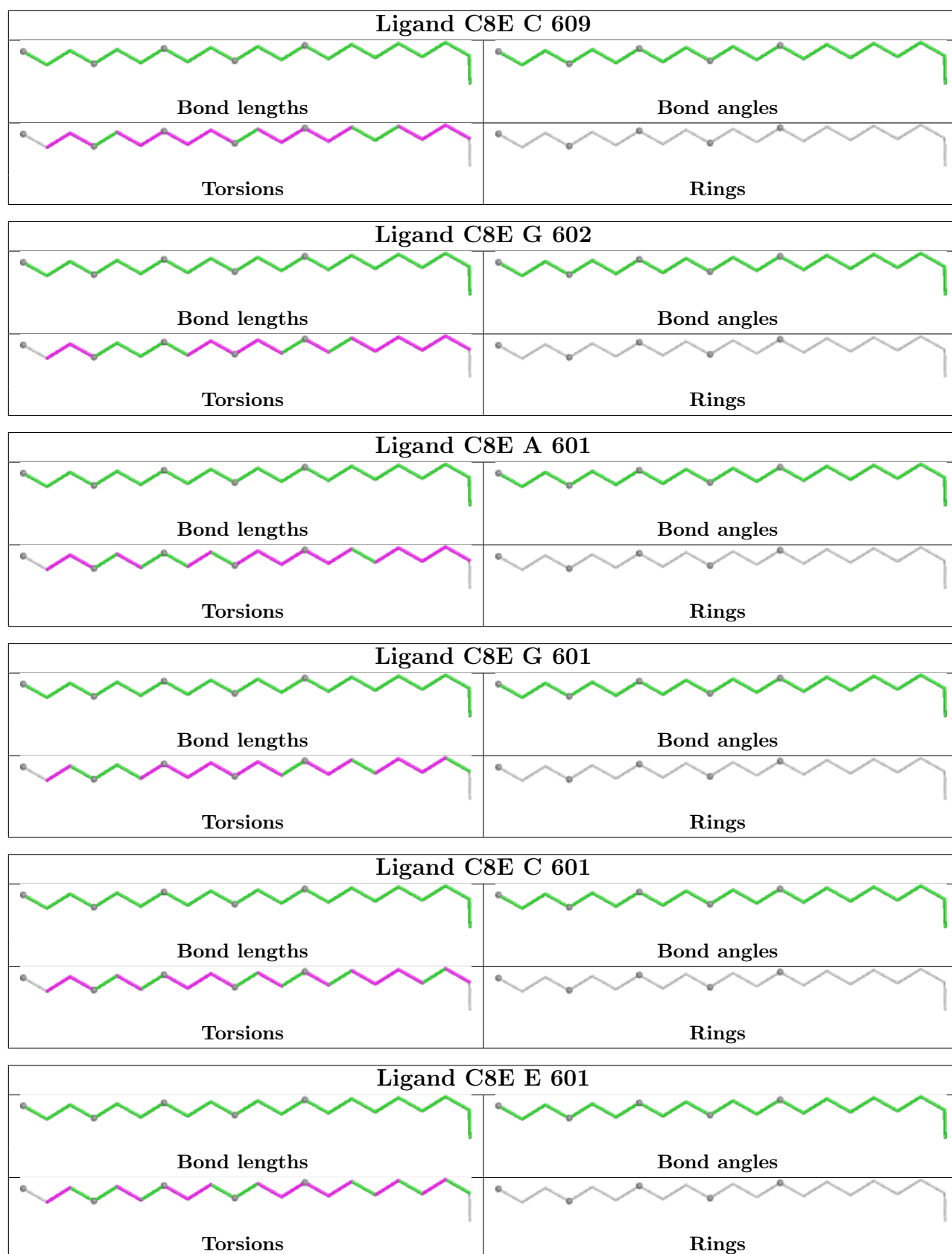
15 monomers are involved in 32 short contacts:

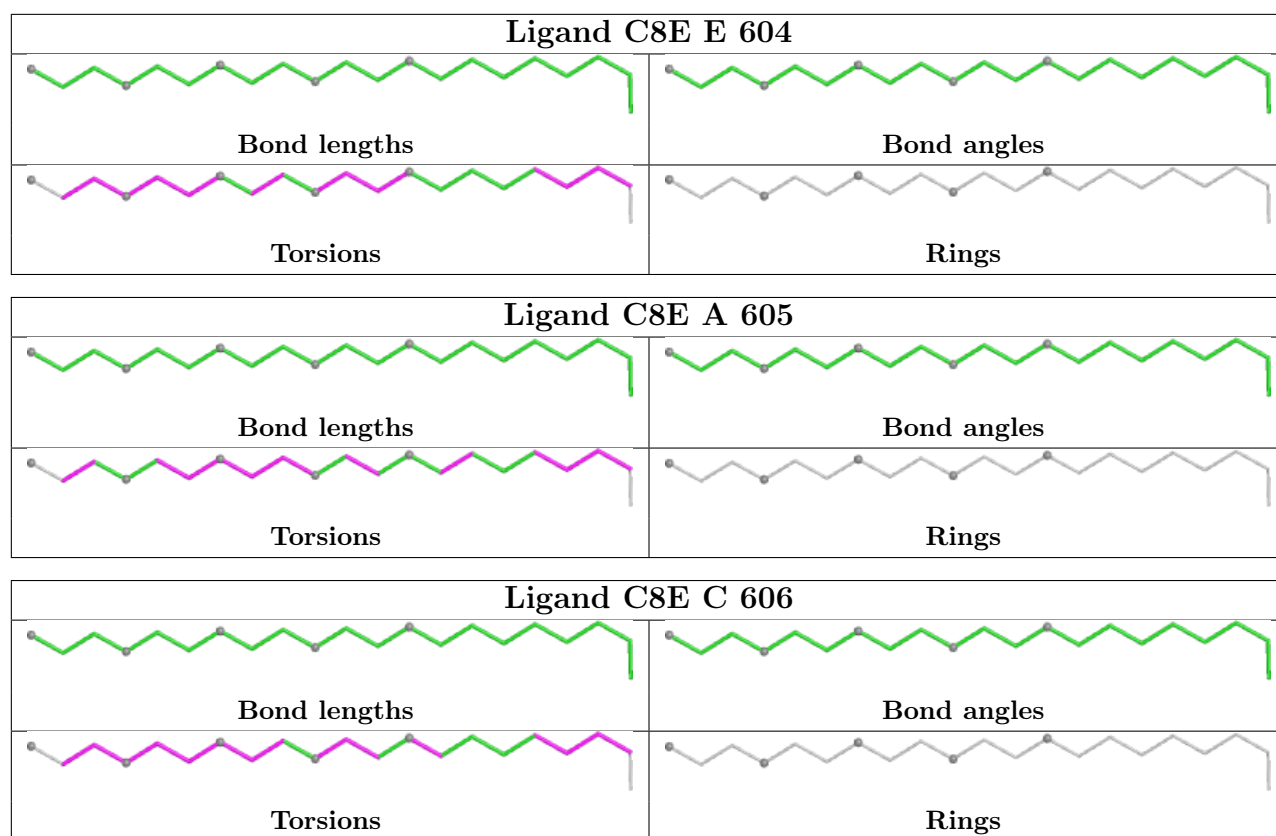
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	603	C8E	2	0
3	C	604	C8E	1	0
3	C	602	C8E	5	0
3	A	604	C8E	2	0
3	C	603	C8E	1	0
3	A	602	C8E	4	0
3	C	605	C8E	1	0
3	G	603	C8E	1	0
3	A	603	C8E	2	0
3	C	607	C8E	1	0
3	G	602	C8E	2	0
3	A	601	C8E	4	0
3	G	601	C8E	2	0
3	C	601	C8E	4	0
3	A	605	C8E	1	0

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	543/577 (94%)	0.17	35 (6%)	25 25	13, 32, 84, 131	0
1	C	541/577 (93%)	0.20	35 (6%)	25 24	11, 33, 89, 128	0
1	E	538/577 (93%)	0.89	83 (15%)	5 5	21, 53, 110, 166	0
1	G	539/577 (93%)	0.54	54 (10%)	12 13	18, 44, 97, 140	0
2	B	141/198 (71%)	0.50	22 (15%)	5 5	14, 36, 102, 127	0
2	D	146/198 (73%)	0.62	27 (18%)	3 3	13, 38, 106, 123	0
2	F	145/198 (73%)	1.13	33 (22%)	2 2	28, 54, 117, 145	0
2	H	147/198 (74%)	0.61	19 (12%)	7 7	19, 45, 101, 124	0
All	All	2740/3100 (88%)	0.51	308 (11%)	10 10	11, 41, 103, 166	0

All (308) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	245	ALA	10.4
2	F	11	PRO	6.5
1	E	500	VAL	6.5
2	F	10	VAL	5.9
1	E	445	VAL	5.8
1	A	446	TYR	5.6
1	C	526	PHE	5.5
1	E	498	TRP	5.5
2	B	142	VAL	5.3
2	D	11	PRO	5.2
2	F	45	ASP	5.2
1	A	445	VAL	5.1
1	A	529	GLU	5.0
1	A	375	ASN	4.9
1	A	498	TRP	4.9
1	C	498	TRP	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	450	TYR	4.8
2	D	10	VAL	4.7
2	D	12	THR	4.7
2	F	12	THR	4.6
2	H	8	THR	4.6
1	A	451	GLN	4.5
1	G	3	PHE	4.5
1	G	76	ASP	4.4
2	H	14	LEU	4.4
1	E	528	ILE	4.4
1	E	22	TYR	4.3
1	E	450	TYR	4.3
1	G	368	THR	4.2
2	B	141	THR	4.2
1	E	369	GLU	4.2
1	E	499	ALA	4.2
1	A	369	GLU	4.2
2	H	7	THR	4.2
1	C	500	VAL	4.2
2	B	2	PHE	4.1
2	F	14	LEU	4.1
2	D	2	PHE	4.1
1	G	445	VAL	4.1
1	G	498	TRP	4.1
1	E	526	PHE	4.0
2	F	9	GLN	4.0
2	F	47	ALA	4.0
1	C	446	TYR	4.0
1	E	10	PHE	4.0
1	G	526	PHE	4.0
2	F	44	VAL	3.9
2	B	9	GLN	3.9
1	G	446	TYR	3.8
1	G	496	CYS	3.8
1	E	495	THR	3.8
1	C	450	TYR	3.7
1	C	448	PRO	3.7
2	F	48	MET	3.7
2	H	92	GLY	3.7
2	F	147	VAL	3.6
1	A	526	PHE	3.6
2	H	2	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	46	ASP	3.5
1	C	422	ALA	3.5
1	E	77	GLY	3.5
2	D	13	GLU	3.5
2	D	9	GLN	3.5
1	A	528	ILE	3.5
1	C	375	ASN	3.5
2	F	51	ASP	3.4
2	H	4	LEU	3.4
2	B	12	THR	3.4
1	A	499	ALA	3.4
2	F	46	ASP	3.4
1	C	445	VAL	3.4
2	F	96	TYR	3.4
1	E	19	LEU	3.4
1	E	32	ALA	3.4
1	G	495	THR	3.3
2	B	14	LEU	3.3
1	C	451	GLN	3.3
1	G	500	VAL	3.3
2	H	13	GLU	3.3
1	E	245	ALA	3.3
1	E	376	ALA	3.3
2	D	147	VAL	3.3
1	E	279	PHE	3.3
1	G	449	ASP	3.3
1	E	475	TYR	3.2
1	C	528	ILE	3.2
2	D	14	LEU	3.2
1	G	448	PRO	3.2
1	E	239	ALA	3.2
1	C	527	ASN	3.2
1	C	78	THR	3.1
1	C	245	ALA	3.1
2	D	48	MET	3.1
1	E	277	THR	3.1
1	E	374	SER	3.1
1	A	0	MET	3.0
1	A	447	ASN	3.0
1	C	449	ASP	3.0
1	E	483	GLN	3.0
1	E	444	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	18	PHE	3.0
1	C	501	ASN	3.0
1	E	527	ASN	3.0
1	E	75	PRO	3.0
2	H	148	LYS	3.0
2	F	71	ARG	3.0
1	E	5	ILE	3.0
2	B	48	MET	2.9
1	C	73	THR	2.9
2	F	8	THR	2.9
1	C	499	ALA	2.9
2	B	144	ALA	2.9
2	D	47	ALA	2.9
2	D	142	VAL	2.9
1	E	39	MET	2.9
1	G	528	ILE	2.9
1	A	368	THR	2.9
2	B	8	THR	2.9
1	A	452	GLN	2.9
2	H	9	GLN	2.9
2	D	141	THR	2.9
1	G	444	LYS	2.9
1	G	451	GLN	2.9
1	E	441	ALA	2.9
1	E	442	VAL	2.9
2	B	15	GLN	2.8
2	D	7	THR	2.8
2	F	142	VAL	2.8
1	G	2	GLY	2.8
1	E	72	TYR	2.8
2	B	47	ALA	2.8
1	A	500	VAL	2.8
1	A	469	TRP	2.8
1	C	469	TRP	2.8
1	E	278	GLY	2.8
2	B	46	ASP	2.8
1	A	422	ALA	2.8
1	C	242	ALA	2.8
1	G	422	ALA	2.8
1	G	30	PHE	2.8
1	G	493	TYR	2.8
2	F	144	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	368	THR	2.8
1	E	422	ALA	2.8
1	E	375	ASN	2.7
1	A	73	THR	2.7
1	A	495	THR	2.7
2	D	51	ASP	2.7
2	F	53	PRO	2.7
1	E	78	THR	2.7
1	E	496	CYS	2.7
1	C	368	THR	2.7
1	G	16	PHE	2.7
1	A	448	PRO	2.7
1	G	466	ALA	2.7
1	E	274	ASP	2.7
1	E	452	GLN	2.6
2	B	143	HIS	2.6
1	E	80	LYS	2.6
1	A	5	ILE	2.6
1	C	465	ILE	2.6
1	E	9	LYS	2.6
2	F	94	ASP	2.6
1	E	34	ILE	2.6
1	E	40	GLU	2.6
1	G	28	PRO	2.6
1	E	547	SER	2.6
1	C	77	GLY	2.6
1	A	496	CYS	2.6
1	G	242	ALA	2.6
1	E	275	TRP	2.5
1	G	5	ILE	2.5
1	C	444	LYS	2.5
2	H	6	GLY	2.5
1	C	452	GLN	2.5
2	F	145	ALA	2.5
1	E	512	ASN	2.5
1	C	79	ASP	2.5
2	D	4	LEU	2.5
1	E	542	ALA	2.5
2	D	144	ALA	2.5
1	C	547	SER	2.5
1	G	443	PRO	2.5
1	E	35	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	F	140	LEU	2.5
2	D	143	HIS	2.5
1	E	15	GLY	2.5
1	E	466	ALA	2.5
1	E	485	ALA	2.5
1	E	83	THR	2.4
2	F	7	THR	2.4
2	D	49	ARG	2.4
1	G	26	ILE	2.4
1	G	243	ASP	2.4
1	G	529	GLU	2.4
1	E	195	VAL	2.4
1	E	3	PHE	2.4
2	B	16	LYS	2.4
2	F	50	LYS	2.4
2	D	145	ALA	2.4
1	E	501	ASN	2.4
2	D	93	HIS	2.4
1	E	24	TRP	2.4
2	H	45	ASP	2.4
2	F	3	ASN	2.4
2	F	93	HIS	2.4
1	A	-1	SER	2.4
1	A	515	GLY	2.4
2	H	10	VAL	2.4
1	C	493	TYR	2.4
1	G	450	TYR	2.4
2	F	90	ILE	2.4
2	D	3	ASN	2.4
1	A	243	ASP	2.4
1	G	546	ASN	2.3
1	C	423	ASP	2.3
1	E	65	TRP	2.3
2	B	49	ARG	2.3
1	G	23	TYR	2.3
1	E	198	THR	2.3
2	H	93	HIS	2.3
1	G	494	ASN	2.3
2	B	45	ASP	2.3
1	G	4	LEU	2.3
1	G	19	LEU	2.3
2	D	140	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	18	LEU	2.3
1	A	546	ASN	2.3
1	C	447	ASN	2.3
1	E	546	ASN	2.3
1	A	246	SER	2.3
1	E	272	SER	2.3
1	G	24	TRP	2.3
1	E	71	ILE	2.3
2	H	47	ALA	2.3
2	B	7	THR	2.3
2	H	12	THR	2.3
1	E	217	ASN	2.3
1	E	12	SER	2.3
1	G	468	ARG	2.3
1	G	441	ALA	2.2
2	B	50	LYS	2.2
1	A	277	THR	2.2
1	A	527	ASN	2.2
2	H	11	PRO	2.2
1	E	0	MET	2.2
1	G	376	ALA	2.2
1	G	497	CYS	2.2
1	G	541	THR	2.2
1	A	1	SER	2.2
2	H	46	ASP	2.2
1	G	18	PHE	2.2
2	B	90	ILE	2.2
1	A	497	CYS	2.2
1	E	497	CYS	2.2
1	A	444	LYS	2.2
1	E	243	ASP	2.2
1	E	548	GLY	2.2
2	F	13	GLU	2.2
2	F	141	THR	2.2
1	E	2	GLY	2.2
1	E	220	GLY	2.2
1	E	55	ALA	2.1
1	C	369	GLU	2.1
1	G	501	ASN	2.1
2	B	4	LEU	2.1
2	F	18	LEU	2.1
1	E	407	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	79	ASP	2.1
1	C	556	PHE	2.1
1	G	469	TRP	2.1
1	C	497	CYS	2.1
1	A	493	TYR	2.1
1	E	43	GLY	2.1
2	D	92	GLY	2.1
1	G	31	ASP	2.1
1	E	276	ALA	2.1
1	G	277	THR	2.1
2	H	48	MET	2.1
1	G	54	LEU	2.1
2	F	4	LEU	2.1
2	F	6	GLY	2.1
1	G	499	ALA	2.1
1	E	511	TRP	2.1
2	D	91	PRO	2.1
1	E	20	LEU	2.1
1	E	50	PHE	2.1
1	E	70	ARG	2.0
1	G	79	ASP	2.0
2	D	45	ASP	2.0
2	F	110	PRO	2.0
1	G	20	LEU	2.0
1	C	524	ILE	2.0
1	E	508	ILE	2.0
1	E	515	GLY	2.0
1	C	274	ASP	2.0
1	G	27	ALA	2.0
1	G	276	ALA	2.0
1	G	421	ASP	2.0
2	B	121	GLU	2.0
1	E	27	ALA	2.0
1	E	481	ALA	2.0
1	G	310	SER	2.0
2	F	54	THR	2.0
1	E	7	ASN	2.0
1	G	34	ILE	2.0
2	B	92	GLY	2.0
2	D	90	ILE	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](#)

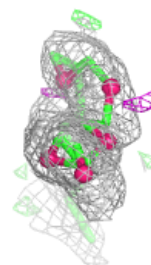
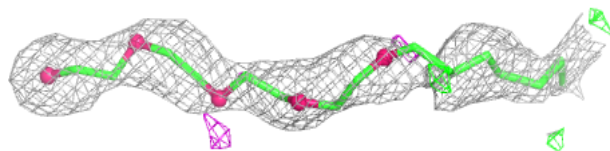
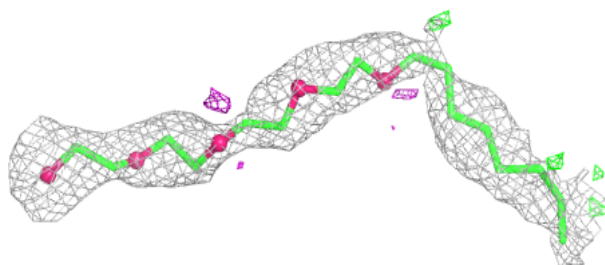
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	C8E	C	608	21/21	0.77	0.23	31,56,78,86	0
3	C8E	C	604	21/21	0.81	0.22	46,65,83,90	0
3	C8E	A	601	21/21	0.81	0.19	24,38,60,74	0
3	C8E	E	601	21/21	0.81	0.22	33,48,86,89	0
3	C8E	G	602	21/21	0.81	0.24	35,55,115,123	0
3	C8E	A	603	21/21	0.82	0.21	31,65,88,99	0
3	C8E	G	603	21/21	0.82	0.23	33,76,105,109	0
3	C8E	E	603	21/21	0.83	0.20	20,47,69,75	0
3	C8E	C	607	21/21	0.84	0.18	26,54,74,94	0
3	C8E	C	605	21/21	0.84	0.18	38,52,71,88	0
3	C8E	A	605	21/21	0.85	0.23	31,57,109,114	0
3	C8E	E	602	21/21	0.86	0.18	24,42,69,82	0
3	C8E	E	604	21/21	0.86	0.19	38,63,85,93	0
3	C8E	C	602	21/21	0.87	0.15	30,47,60,73	0
3	C8E	G	601	21/21	0.87	0.16	21,48,62,73	0
3	C8E	C	609	21/21	0.88	0.21	21,60,103,110	0
3	C8E	C	606	21/21	0.88	0.18	22,48,69,71	0
3	C8E	C	601	21/21	0.88	0.19	29,44,80,96	0
3	C8E	A	602	21/21	0.88	0.15	28,44,65,72	0
3	C8E	C	603	21/21	0.89	0.17	25,47,71,74	0
3	C8E	A	604	21/21	0.92	0.12	22,34,46,49	0

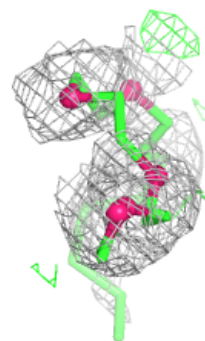
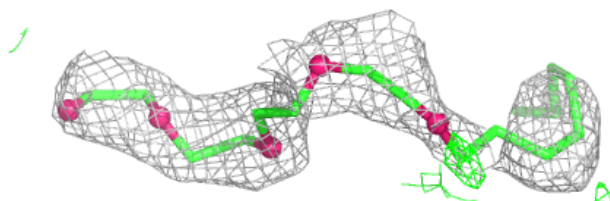
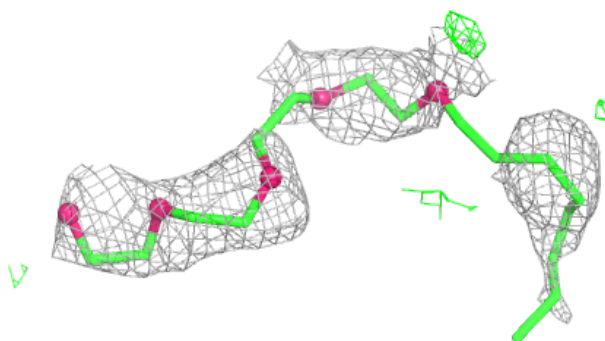
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around C8E C 608:

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

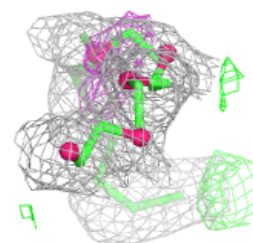
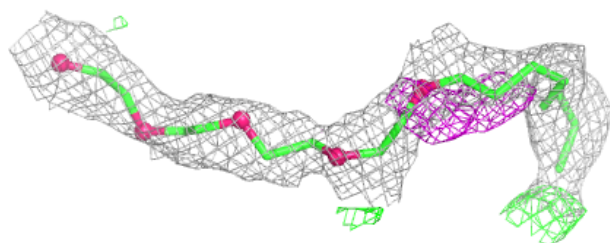
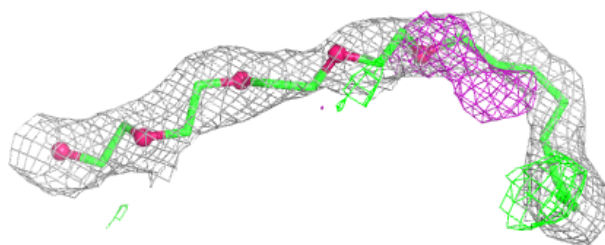
**Electron density around C8E C 604:**

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

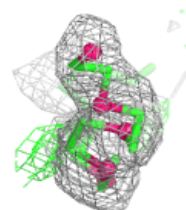
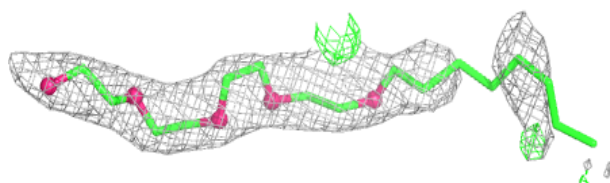
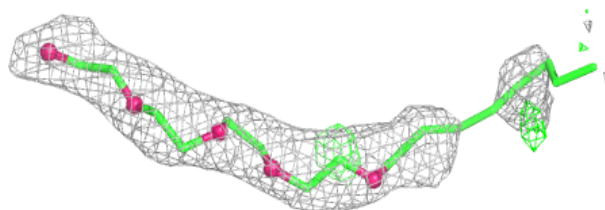


Electron density around C8E A 601:

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

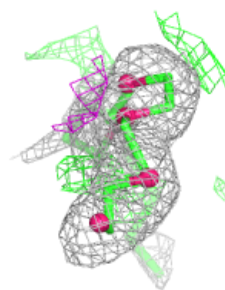
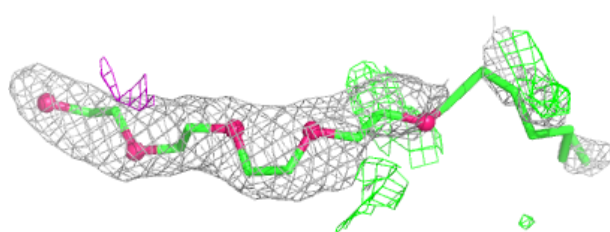
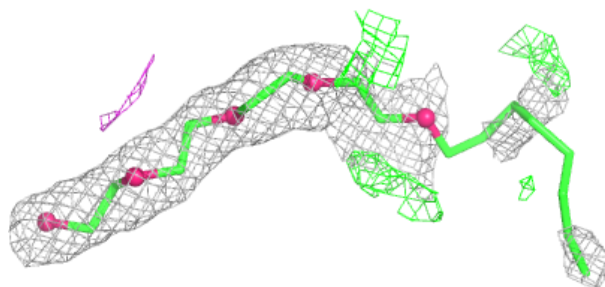
**Electron density around C8E E 601:**

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

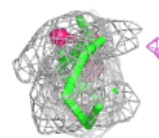
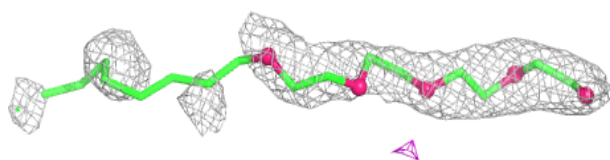
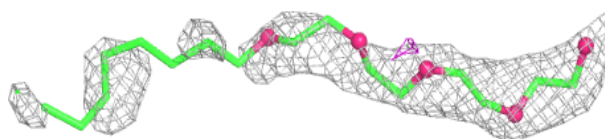


Electron density around C8E G 602:

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

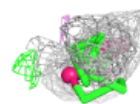
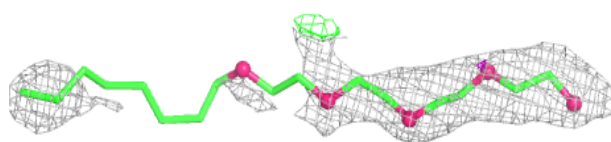
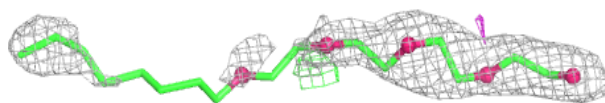
**Electron density around C8E A 603:**

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

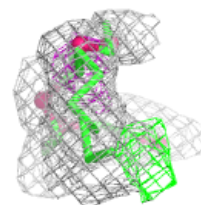
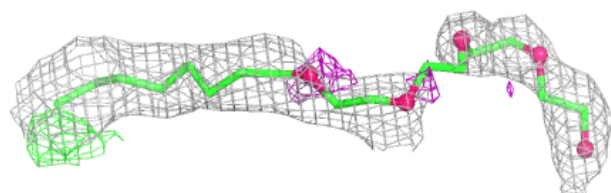
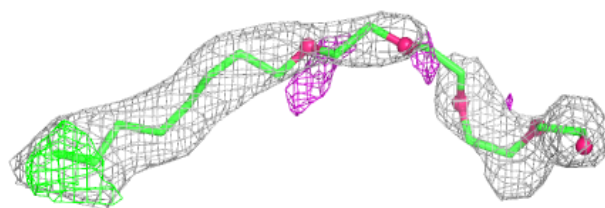


Electron density around C8E G 603:

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

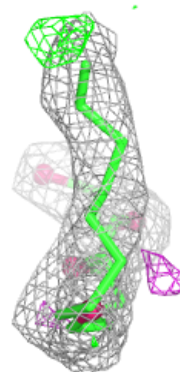
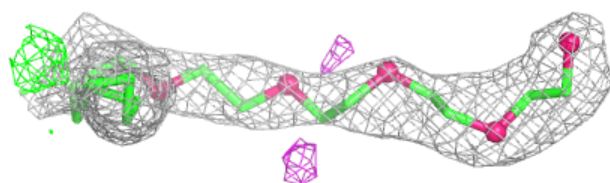
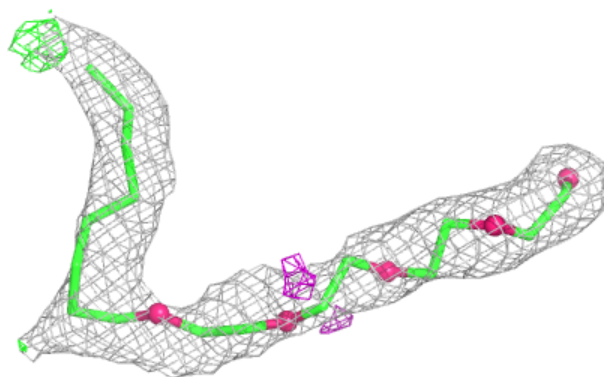
**Electron density around C8E E 603:**

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

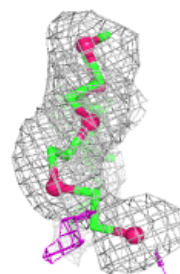
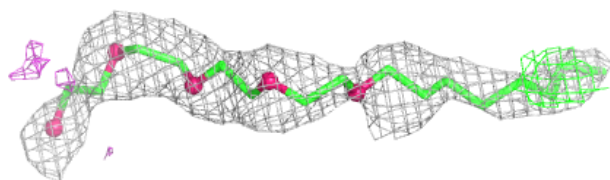
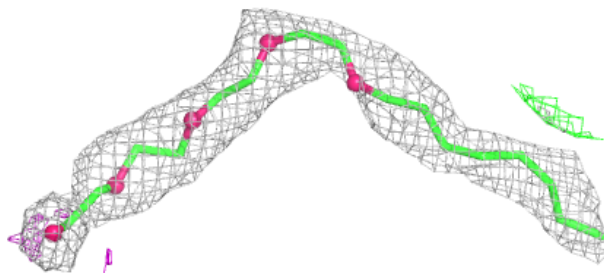


Electron density around C8E C 607:

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

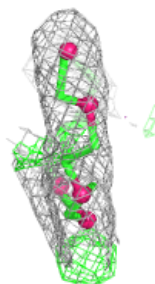
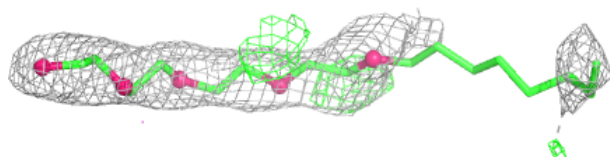
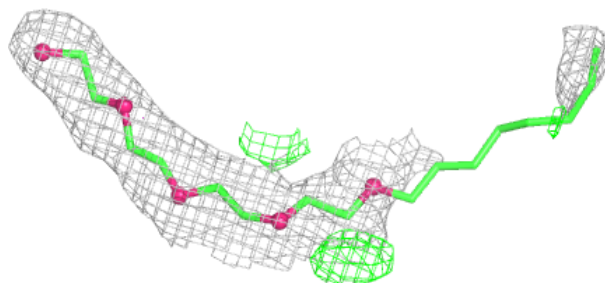
**Electron density around C8E C 605:**

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

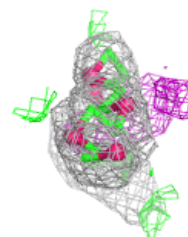
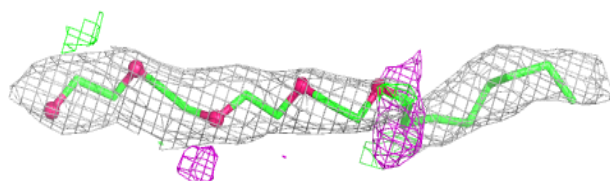
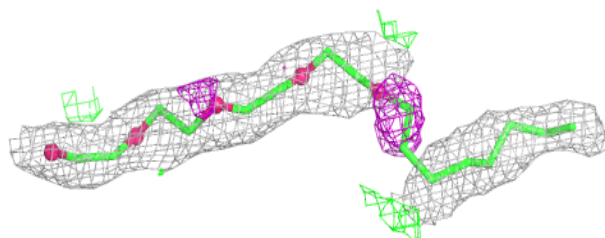


Electron density around C8E A 605:

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

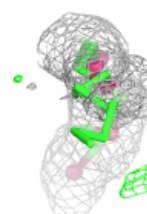
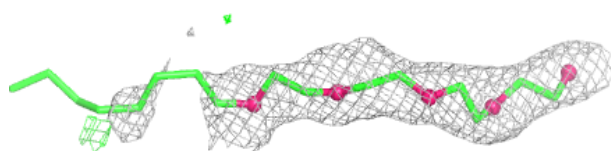
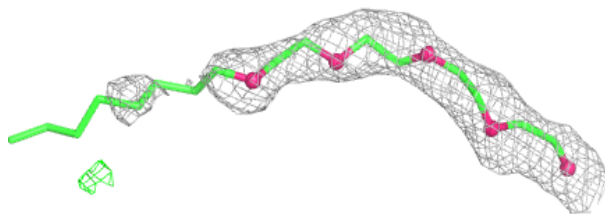
**Electron density around C8E E 602:**

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

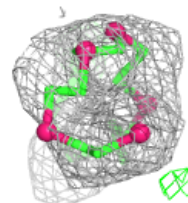
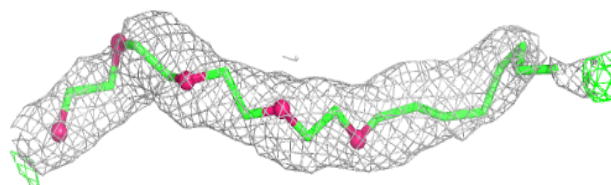
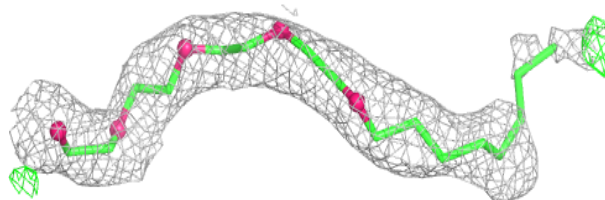


Electron density around C8E E 604:

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

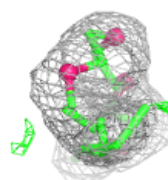
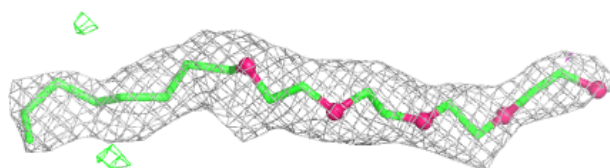
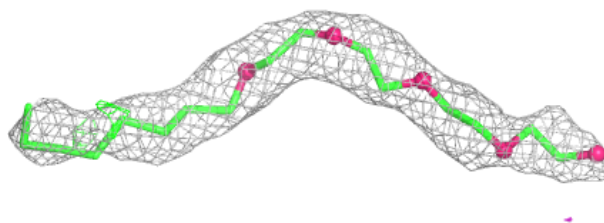
**Electron density around C8E C 602:**

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

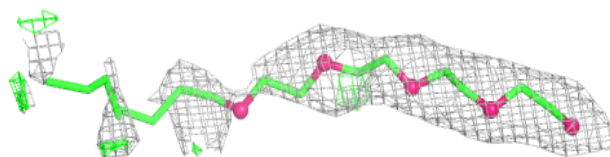
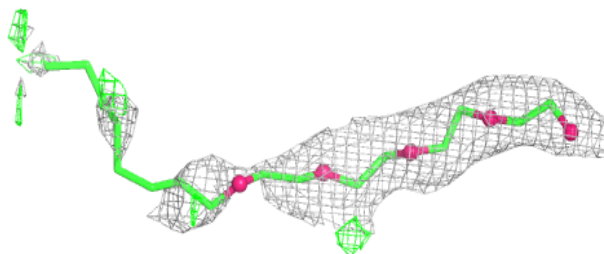


Electron density around C8E G 601:

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

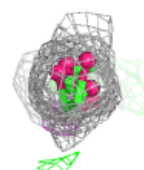
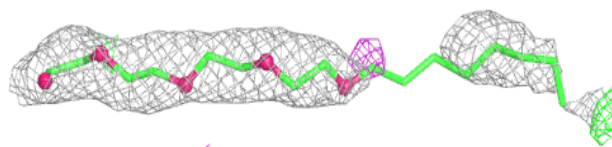
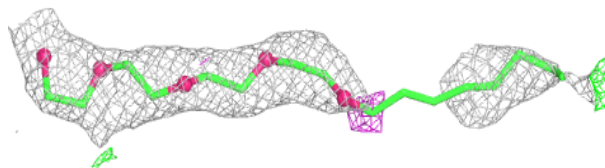
**Electron density around C8E C 609:**

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

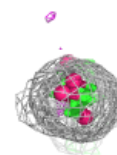
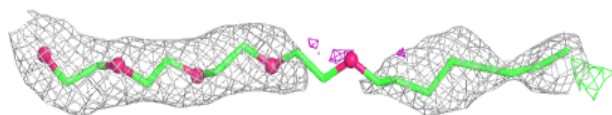
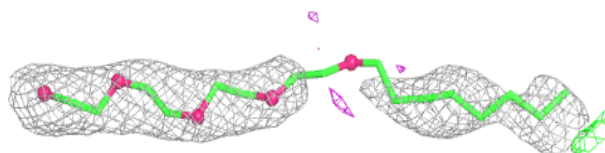


Electron density around C8E C 606:

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

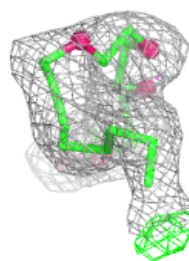
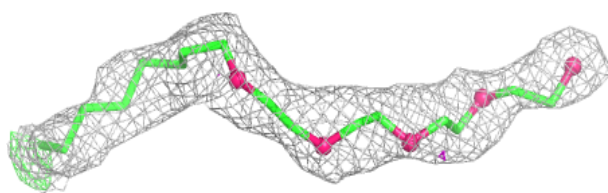
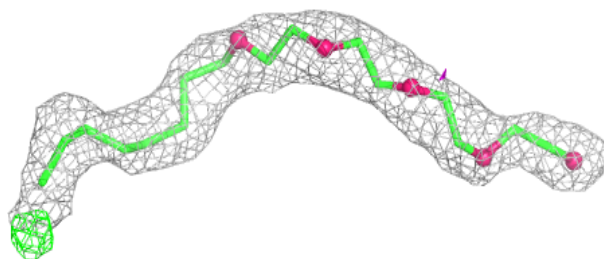
**Electron density around C8E C 601:**

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

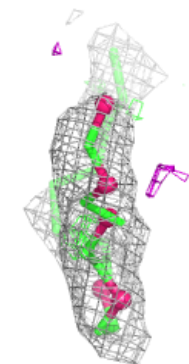
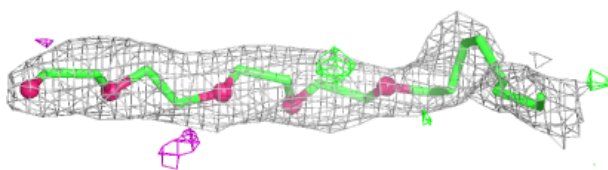
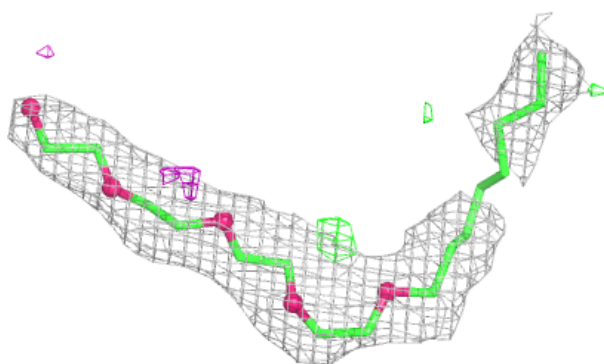


Electron density around C8E A 602:

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

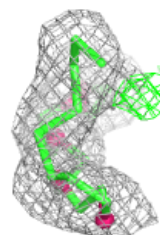
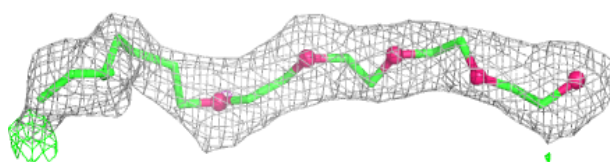
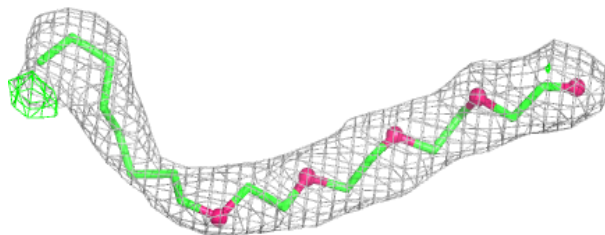
**Electron density around C8E C 603:**

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



Electron density around C8E A 604:

$2mF_o-DF_c$ (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.