



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 08:42 AM EDT

PDB ID : 3KVN
Title : Crystal structure of the full-length autotransporter EstA from *Pseudomonas aeruginosa*
Authors : van den Berg, B.
Deposited on : 2009-11-30
Resolution : 2.50 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

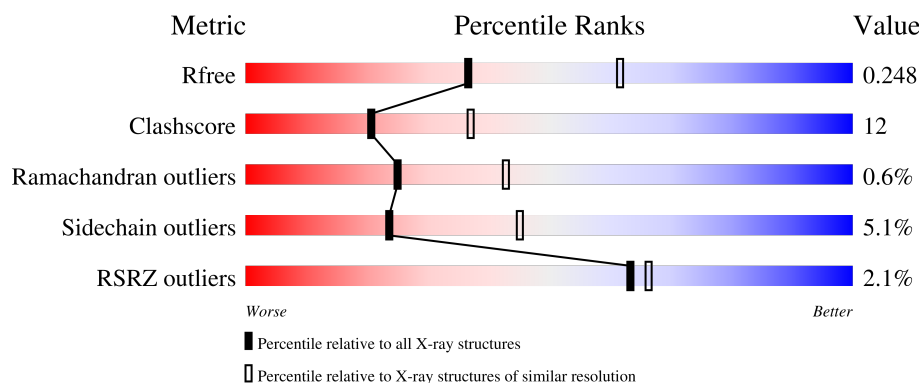
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

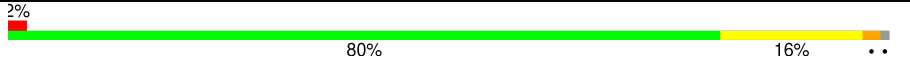

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	632	
1	X	632	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10102 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.

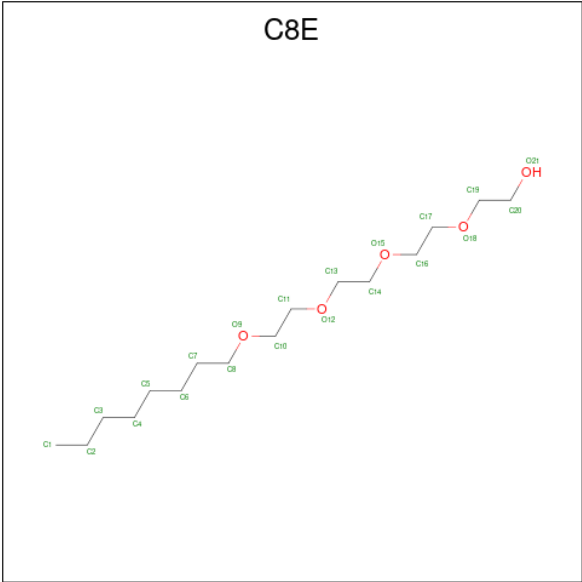
- Molecule 1 is a protein called Esterase estA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	628	Total	C	N	O	S	0	0	0
			4798	2998	839	952	9			
1	A	627	Total	C	N	O	S	0	0	0
			4793	2995	838	951	9			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	-9	MET	-	EXPRESSION TAG	UNP O33407
X	-8	HIS	-	EXPRESSION TAG	UNP O33407
X	-7	HIS	-	EXPRESSION TAG	UNP O33407
X	-6	HIS	-	EXPRESSION TAG	UNP O33407
X	-5	HIS	-	EXPRESSION TAG	UNP O33407
X	-4	HIS	-	EXPRESSION TAG	UNP O33407
X	-3	HIS	-	EXPRESSION TAG	UNP O33407
X	-2	HIS	-	EXPRESSION TAG	UNP O33407
X	-1	LEU	-	EXPRESSION TAG	UNP O33407
X	0	GLU	-	EXPRESSION TAG	UNP O33407
A	-9	MET	-	EXPRESSION TAG	UNP O33407
A	-8	HIS	-	EXPRESSION TAG	UNP O33407
A	-7	HIS	-	EXPRESSION TAG	UNP O33407
A	-6	HIS	-	EXPRESSION TAG	UNP O33407
A	-5	HIS	-	EXPRESSION TAG	UNP O33407
A	-4	HIS	-	EXPRESSION TAG	UNP O33407
A	-3	HIS	-	EXPRESSION TAG	UNP O33407
A	-2	HIS	-	EXPRESSION TAG	UNP O33407
A	-1	LEU	-	EXPRESSION TAG	UNP O33407
A	0	GLU	-	EXPRESSION TAG	UNP O33407

- Molecule 2 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C₁₆H₃₄O₅).

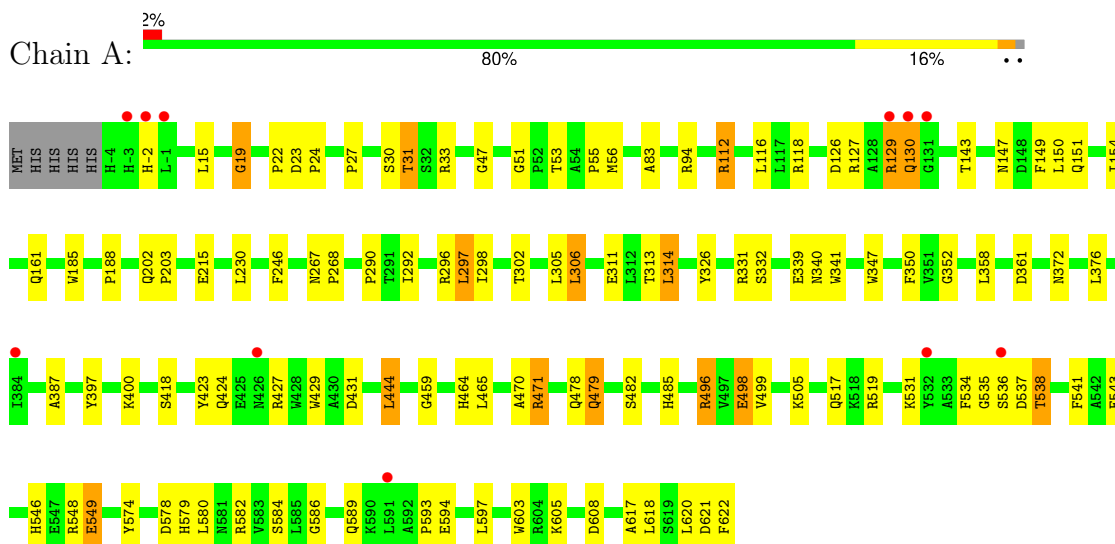
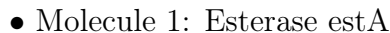


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	X	1	Total C O 18 14 4	0	0
2	X	1	Total C 6 6	0	0
2	A	1	Total C O 20 15 5	0	0
2	A	1	Total C 6 6	0	0
2	A	1	Total C 6 6	0	0
2	A	1	Total C 6 6	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	X	228	Total O 228 228	0	0
3	A	221	Total O 221 221	0	0

- Molecule 1: Esterase estA



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	143.83Å 143.83Å 186.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.18 – 2.50 39.18 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (39.18-2.50) 98.6 (39.18-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.204 , 0.255 0.200 , 0.248	Depositor DCC
R_{free} test set	1978 reflections (2.93%)	wwPDB-VP
Wilson B-factor (Å ²)	40.1	Xtriage
Anisotropy	0.594	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10102	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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: 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	0.39	0/4908	0.55	0/6675
1	X	0.45	3/4913 (0.1%)	0.55	1/6682 (0.0%)
All	All	0.42	3/9821 (0.0%)	0.55	1/13357 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	347	TRP	C-O	-6.91	1.10	1.23
1	X	345	GLY	C-O	-6.47	1.13	1.23
1	X	347	TRP	CG-CD1	-6.22	1.28	1.36

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	345	GLY	N-CA-C	5.68	127.29	113.10

There are no chirality outliers.

There are no planarity outliers.

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	4793	0	4516	111	0
1	X	4798	0	4518	120	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	38	0	62	9	0
2	X	24	0	35	4	0
3	A	221	0	0	8	0
3	X	228	0	0	7	0
All	All	10102	0	9131	231	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (231) 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:129:ARG:HG3	1:A:129:ARG:HH11	1.07	1.18
1:A:479:GLN:HG3	1:A:482:SER:HB2	1.29	1.15
1:X:342:GLN:HG3	1:X:346:GLN:O	1.45	1.13
1:X:161:GLN:HG2	1:X:215:GLU:HG3	1.51	0.90
1:A:31:THR:HG22	1:A:33:ARG:HH12	1.38	0.88
1:A:129:ARG:HG3	1:A:129:ARG:NH1	1.87	0.87
1:A:161:GLN:HG2	1:A:215:GLU:HG3	1.56	0.86
1:X:31:THR:HG22	1:X:33:ARG:HH12	1.40	0.84
1:X:496:ARG:HG3	1:X:496:ARG:HH11	1.43	0.83
1:X:53:THR:HG23	1:X:55:PRO:HD2	1.60	0.83
1:A:53:THR:HG23	1:A:55:PRO:HD2	1.61	0.82
1:A:479:GLN:CG	1:A:482:SER:HB2	2.09	0.81
1:X:496:ARG:HG3	1:X:496:ARG:NH1	1.97	0.80
1:A:496:ARG:HG3	1:A:496:ARG:HH11	1.45	0.79
1:X:479:GLN:HG3	1:X:482:SER:HB2	1.64	0.78
1:A:496:ARG:HG3	1:A:496:ARG:NH1	1.97	0.77
1:X:464:HIS:NE2	1:X:498:GLU:HG2	1.99	0.77
1:A:129:ARG:HH11	1:A:129:ARG:CG	1.94	0.76
1:X:313:THR:HG21	1:X:574:TYR:H	1.52	0.75
1:X:-2:HIS:ND1	1:X:361:ASP:HB3	2.02	0.74
1:A:464:HIS:NE2	1:A:498:GLU:HG2	2.01	0.74
1:A:19:GLY:HA3	1:A:31:THR:HG23	1.71	0.73
1:A:331:ARG:HD3	1:A:471:ARG:HH22	1.54	0.73
1:A:479:GLN:HG3	1:A:482:SER:CB	2.15	0.72
1:X:331:ARG:HD3	1:X:471:ARG:HH22	1.55	0.71
1:X:464:HIS:HD2	3:X:755:HOH:O	1.74	0.71
1:A:112:ARG:HD2	2:A:626:C8E:H31	1.73	0.70
1:X:19:GLY:HA3	1:X:31:THR:HG23	1.74	0.70
1:A:313:THR:HG21	1:A:574:TYR:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:THR:HA	1:A:517:GLN:OE1	1.94	0.67
1:X:161:GLN:CG	1:X:215:GLU:HG3	2.24	0.67
1:A:51:GLY:HA3	3:A:766:HOH:O	1.94	0.67
1:A:538:THR:HB	1:A:589:GLN:OE1	1.96	0.67
1:A:129:ARG:HB2	3:A:844:HOH:O	1.95	0.66
1:A:147:ASN:OD1	2:A:623:C8E:H192	1.96	0.66
1:X:313:THR:HA	1:X:517:GLN:OE1	1.96	0.65
1:X:346:GLN:O	1:X:346:GLN:HG3	1.97	0.65
1:X:538:THR:HB	1:X:589:GLN:OE1	1.97	0.65
1:X:-2:HIS:ND1	1:X:361:ASP:CB	2.61	0.64
1:X:313:THR:CG2	1:X:574:TYR:H	2.11	0.64
1:A:161:GLN:CG	1:A:215:GLU:HG3	2.28	0.63
1:X:147:ASN:OD1	2:X:623:C8E:H171	1.98	0.63
1:A:129:ARG:NH1	1:A:130:GLN:HB2	2.13	0.62
1:X:341:TRP:CH2	1:X:424:GLN:HG2	2.35	0.62
1:A:15:LEU:HD11	2:A:623:C8E:H132	1.81	0.62
1:X:313:THR:HG21	1:X:574:TYR:N	2.14	0.62
1:A:429:TRP:HZ3	1:A:471:ARG:HD3	1.64	0.61
1:A:341:TRP:CH2	1:A:424:GLN:HG2	2.34	0.61
1:A:331:ARG:HD3	1:A:471:ARG:NH2	2.14	0.61
1:X:31:THR:HG22	1:X:33:ARG:NH1	2.15	0.60
1:A:150:LEU:HD12	2:A:623:C8E:H191	1.81	0.60
1:X:331:ARG:HD3	1:X:471:ARG:HH12	1.66	0.60
1:X:331:ARG:HD3	1:X:471:ARG:NH2	2.15	0.60
1:X:534:PHE:HB2	1:X:538:THR:HG23	1.84	0.60
1:A:19:GLY:HA3	1:A:31:THR:CG2	2.32	0.60
1:X:27:PRO:HG3	1:X:47:GLY:O	2.01	0.60
1:X:15:LEU:HD11	2:X:623:C8E:H112	1.82	0.60
1:A:331:ARG:HD3	1:A:471:ARG:HH12	1.66	0.60
1:X:496:ARG:HH11	1:X:496:ARG:CG	2.12	0.59
1:A:593:PRO:O	1:A:594:GLU:HB2	2.03	0.58
1:A:534:PHE:HB2	1:A:538:THR:HG23	1.86	0.58
1:X:342:GLN:HG3	1:X:346:GLN:HG3	1.83	0.58
1:A:498:GLU:O	1:A:498:GLU:HG3	2.03	0.58
1:A:531:LYS:HB3	1:A:541:PHE:HB3	1.86	0.58
1:X:479:GLN:CG	1:X:482:SER:HB2	2.31	0.58
1:X:429:TRP:HZ3	1:X:471:ARG:HD3	1.68	0.58
1:A:31:THR:HG22	1:A:33:ARG:NH1	2.13	0.58
1:X:531:LYS:HB3	1:X:541:PHE:HB3	1.85	0.57
1:X:19:GLY:HA3	1:X:31:THR:CG2	2.33	0.57
1:A:313:THR:HG21	1:A:574:TYR:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:578:ASP:OD1	1:X:579:HIS:HD2	1.88	0.57
1:A:313:THR:CG2	1:A:574:TYR:H	2.18	0.57
1:A:27:PRO:HD2	1:A:30:SER:OG	2.04	0.57
1:X:27:PRO:HD2	1:X:30:SER:OG	2.05	0.56
1:A:341:TRP:CZ2	1:A:424:GLN:HG2	2.41	0.56
1:A:429:TRP:CZ3	1:A:471:ARG:HD3	2.40	0.56
1:X:498:GLU:HG3	1:X:498:GLU:O	2.06	0.56
1:X:347:TRP:HB2	1:X:622:PHE:HB2	1.88	0.55
1:X:112:ARG:O	1:X:115:THR:HG23	2.05	0.55
1:X:593:PRO:O	1:X:594:GLU:HB2	2.07	0.55
1:A:129:ARG:O	1:A:130:GLN:CB	2.55	0.55
1:A:578:ASP:OD1	1:A:579:HIS:HD2	1.89	0.54
1:X:531:LYS:CB	1:X:541:PHE:HB3	2.38	0.54
1:A:496:ARG:HH11	1:A:496:ARG:CG	2.12	0.54
1:X:331:ARG:HD3	1:X:471:ARG:NH1	2.23	0.54
1:A:112:ARG:NH1	2:A:626:C8E:H51	2.23	0.54
1:A:331:ARG:HD3	1:A:471:ARG:NH1	2.23	0.54
1:X:478:GLN:N	1:X:479:GLN:HG2	2.23	0.54
1:A:464:HIS:HD2	3:A:687:HOH:O	1.91	0.53
1:A:427:ARG:HD2	1:A:478:GLN:HA	1.89	0.53
1:A:-2:HIS:ND1	1:A:361:ASP:HB3	2.24	0.53
1:X:458:LYS:HD2	3:X:853:HOH:O	2.10	0.52
1:A:31:THR:CG2	1:A:33:ARG:HH12	2.18	0.52
1:A:331:ARG:CG	1:A:471:ARG:HH12	2.22	0.52
1:A:27:PRO:HG3	1:A:47:GLY:O	2.10	0.52
1:X:23:ASP:HB3	1:X:30:SER:HB3	1.90	0.52
1:A:541:PHE:CE1	1:A:586:GLY:HA3	2.44	0.52
1:X:535:GLY:O	1:X:537:ASP:N	2.43	0.51
1:A:535:GLY:O	1:A:537:ASP:N	2.43	0.51
1:X:541:PHE:CE1	1:X:586:GLY:HA3	2.45	0.51
1:A:546:HIS:HE1	1:A:579:HIS:ND1	2.08	0.51
1:A:531:LYS:CB	1:A:541:PHE:HB3	2.40	0.51
1:X:477:ALA:HB1	1:X:479:GLN:HG3	1.92	0.51
1:A:23:ASP:HB3	1:A:30:SER:HB3	1.92	0.51
1:A:297:LEU:HD12	3:A:628:HOH:O	2.09	0.51
1:X:546:HIS:HE1	1:X:579:HIS:ND1	2.08	0.51
1:A:202:GLN:HB3	1:A:203:PRO:HD3	1.93	0.50
1:X:429:TRP:CZ3	1:X:471:ARG:HD3	2.46	0.50
1:A:331:ARG:CD	1:A:471:ARG:HH12	2.25	0.50
1:A:150:LEU:CD1	2:A:623:C8E:H191	2.41	0.50
1:A:112:ARG:HH11	2:A:626:C8E:H51	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ARG:CD	1:A:478:GLN:HA	2.42	0.49
1:X:341:TRP:CZ2	1:X:424:GLN:HG2	2.47	0.49
1:A:331:ARG:HD2	1:A:543:GLU:OE2	2.12	0.49
1:X:546:HIS:CE1	1:X:579:HIS:ND1	2.81	0.49
1:X:202:GLN:HB3	1:X:203:PRO:HD3	1.93	0.49
1:X:429:TRP:HE1	1:X:487:SER:HG	1.61	0.49
1:A:19:GLY:CA	1:A:31:THR:HG23	2.40	0.49
1:A:546:HIS:CE1	1:A:579:HIS:ND1	2.81	0.48
1:X:331:ARG:CG	1:X:471:ARG:HH12	2.25	0.48
1:A:290:PRO:HG3	2:A:623:C8E:H72	1.94	0.48
1:A:302:THR:HG22	1:A:306:LEU:HD22	1.94	0.48
1:X:331:ARG:HD2	1:X:543:GLU:OE2	2.14	0.47
1:X:19:GLY:CA	1:X:31:THR:HG23	2.43	0.47
1:X:143:THR:HG22	1:X:185:TRP:CG	2.48	0.47
1:X:331:ARG:CD	1:X:471:ARG:HH12	2.27	0.47
1:X:549:GLU:HG3	3:X:665:HOH:O	2.14	0.47
1:A:143:THR:HG22	1:A:185:TRP:CG	2.50	0.47
1:X:143:THR:HG22	1:X:185:TRP:CD1	2.50	0.47
1:X:603:TRP:CZ2	1:X:605:LYS:HB2	2.50	0.47
1:A:116:LEU:HD11	1:A:118:ARG:O	2.15	0.47
1:X:342:GLN:CG	1:X:346:GLN:O	2.39	0.47
1:A:431:ASP:OD2	1:A:471:ARG:HD2	2.15	0.46
1:A:603:TRP:CZ2	1:A:605:LYS:HB2	2.50	0.46
1:A:465:LEU:C	1:A:465:LEU:HD12	2.35	0.46
1:X:201:LEU:HA	3:X:770:HOH:O	2.14	0.46
1:X:484:TRP:HB3	1:X:532:TYR:CD1	2.50	0.46
1:A:597:LEU:HD12	1:A:617:ALA:O	2.15	0.46
1:X:161:GLN:HG2	1:X:215:GLU:CG	2.36	0.46
1:X:302:THR:HG22	1:X:306:LEU:HD22	1.96	0.46
1:X:352:GLY:O	1:X:376:LEU:HD12	2.15	0.46
1:X:342:GLN:CG	1:X:346:GLN:HG3	2.45	0.46
1:X:543:GLU:HG2	1:X:584:SER:HB2	1.98	0.46
1:A:31:THR:CG2	1:A:33:ARG:NH1	2.78	0.46
1:X:94:ARG:HD3	1:X:151:GLN:OE1	2.16	0.45
1:X:347:TRP:HA	1:X:381:SER:O	2.16	0.45
1:X:549:GLU:HB2	1:X:578:ASP:HA	1.99	0.45
1:X:201:LEU:HD23	3:X:770:HOH:O	2.15	0.45
1:X:350:PHE:HA	1:X:618:LEU:O	2.16	0.45
1:X:481:ASP:OD2	1:X:481:ASP:N	2.50	0.45
1:X:113:ASP:O	1:X:115:THR:HG22	2.17	0.45
1:X:128:ALA:C	1:X:130:GLN:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:31:THR:CG2	1:X:33:ARG:NH1	2.79	0.45
1:A:543:GLU:HG2	1:A:584:SER:HB2	1.98	0.45
1:X:465:LEU:C	1:X:465:LEU:HD12	2.37	0.45
1:X:161:GLN:CB	1:X:215:GLU:HG3	2.46	0.44
1:X:289:HIS:HA	1:X:290:PRO:HD3	1.74	0.44
1:A:188:PRO:HG2	2:A:623:C8E:H102	1.98	0.44
1:A:143:THR:HG22	1:A:185:TRP:CD1	2.53	0.44
1:X:31:THR:CG2	1:X:33:ARG:HH12	2.19	0.44
1:X:620:LEU:HG	1:X:621:ASP:N	2.31	0.44
1:A:-2:HIS:HE1	1:A:608:ASP:OD1	2.00	0.44
1:X:22:PRO:O	1:X:24:PRO:HD3	2.18	0.44
1:X:431:ASP:OD2	1:X:471:ARG:HD2	2.18	0.44
1:A:185:TRP:CZ2	1:A:298:ILE:HD13	2.52	0.44
1:A:331:ARG:HD3	1:A:471:ARG:CZ	2.48	0.44
1:A:331:ARG:HG3	1:A:471:ARG:HH12	1.83	0.44
1:A:387:ALA:O	1:A:423:TYR:HA	2.18	0.44
1:A:431:ASP:O	1:A:470:ALA:HA	2.18	0.44
1:A:593:PRO:O	1:A:594:GLU:CB	2.64	0.43
1:X:331:ARG:HD3	1:X:471:ARG:CZ	2.48	0.43
1:A:94:ARG:HD3	1:A:151:GLN:OE1	2.18	0.43
1:X:597:LEU:HD12	1:X:617:ALA:O	2.19	0.43
1:A:350:PHE:HA	1:A:618:LEU:O	2.18	0.43
1:X:313:THR:HG23	1:X:574:TYR:HB2	2.01	0.43
1:X:292:ILE:O	1:X:296:ARG:HG3	2.18	0.43
1:X:-3:HIS:HE1	1:X:-1:LEU:HD22	1.84	0.43
1:A:267:ASN:HA	1:A:268:PRO:HD3	1.91	0.43
1:X:593:PRO:O	1:X:594:GLU:CB	2.67	0.43
1:A:517:GLN:HB2	3:A:703:HOH:O	2.19	0.43
1:X:-1:LEU:HD12	1:X:-1:LEU:HA	1.81	0.42
1:A:347:TRP:HB2	1:A:622:PHE:HB2	2.01	0.42
1:X:523:ARG:HA	1:X:548:ARG:O	2.19	0.42
1:A:427:ARG:NE	1:A:478:GLN:HA	2.34	0.42
1:X:149:PHE:CD2	1:X:154:ILE:HD12	2.54	0.42
1:X:594:GLU:O	1:X:620:LEU:HA	2.19	0.42
1:A:431:ASP:HB2	1:A:471:ARG:HG3	2.01	0.42
1:A:292:ILE:O	1:A:296:ARG:HG3	2.20	0.42
1:A:372:ASN:O	1:A:400:LYS:HG2	2.19	0.42
1:A:549:GLU:HB2	1:A:578:ASP:HA	2.00	0.42
1:A:505:LYS:HE3	3:A:690:HOH:O	2.18	0.42
1:A:127:ARG:C	1:A:129:ARG:N	2.73	0.42
1:A:161:GLN:CB	1:A:215:GLU:HG3	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:GLU:O	1:A:314:LEU:HB2	2.20	0.42
1:X:57:LEU:HD13	1:X:296:ARG:HG2	2.02	0.42
1:X:118:ARG:HG2	1:X:119:SER:N	2.35	0.42
1:X:311:GLU:O	1:X:314:LEU:HB2	2.20	0.42
1:A:246:PHE:HB3	1:A:297:LEU:HD21	2.02	0.42
1:A:339:GLU:HG3	1:A:485:HIS:CE1	2.55	0.42
1:A:149:PHE:CD2	1:A:154:ILE:HD12	2.55	0.41
1:X:431:ASP:HB2	1:X:471:ARG:HG3	2.02	0.41
1:X:431:ASP:O	1:X:470:ALA:HA	2.20	0.41
1:X:343:ASN:O	1:X:346:GLN:HG2	2.20	0.41
1:X:7:THR:HA	1:X:64:ILE:HD12	2.02	0.41
1:A:22:PRO:O	1:A:24:PRO:HD3	2.20	0.41
1:A:126:ASP:O	1:A:129:ARG:HB3	2.19	0.41
1:A:326:TYR:HA	1:A:397:TYR:OH	2.20	0.41
1:X:75:PRO:O	1:X:79:GLN:HG3	2.21	0.41
1:X:194:PRO:HB2	1:X:287:SER:HA	2.03	0.41
1:X:246:PHE:HA	1:X:451:GLY:HA3	2.03	0.41
1:X:185:TRP:CZ2	1:X:298:ILE:HD13	2.54	0.41
1:X:290:PRO:HG3	2:X:623:C8E:H52	2.02	0.41
1:X:372:ASN:O	1:X:400:LYS:HG2	2.20	0.41
1:A:83:ALA:HA	3:A:779:HOH:O	2.20	0.41
1:X:146:GLY:HA3	2:X:623:C8E:H131	2.03	0.41
1:X:243:PRO:HD2	3:X:721:HOH:O	2.21	0.41
1:X:326:TYR:HA	1:X:397:TYR:OH	2.21	0.41
1:X:331:ARG:HG3	1:X:471:ARG:HH12	1.86	0.41
1:X:387:ALA:O	1:X:423:TYR:HA	2.21	0.41
1:A:129:ARG:O	1:A:130:GLN:HB3	2.21	0.41
1:A:424:GLN:HG3	3:A:785:HOH:O	2.21	0.41
1:A:594:GLU:O	1:A:620:LEU:HA	2.20	0.41
1:X:444:LEU:HD22	1:X:460:ASP:HA	2.04	0.40
1:A:53:THR:HG22	1:A:56:MET:SD	2.61	0.40
1:X:262:ASN:ND2	3:X:731:HOH:O	2.42	0.40
1:X:354:GLY:HA3	1:X:614:VAL:O	2.22	0.40
1:A:352:GLY:O	1:A:376:LEU:HD12	2.21	0.40
1:X:191:GLY:HA2	1:X:196:THR:OG1	2.21	0.40
1:X:446:ARG:O	1:X:456:SER:HA	2.22	0.40
1:X:587:PHE:CE2	1:X:599:GLY:HA3	2.56	0.40
1:A:444:LEU:HB2	1:A:459:GLY:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	625/632 (99%)	602 (96%)	19 (3%)	4 (1%)	25	43
1	X	626/632 (99%)	605 (97%)	18 (3%)	3 (0%)	29	48
All	All	1251/1264 (99%)	1207 (96%)	37 (3%)	7 (1%)	25	43

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	340	ASN
1	X	536	SER
1	A	340	ASN
1	A	536	SER
1	X	19	GLY
1	A	130	GLN
1	A	19	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	488/493 (99%)	464 (95%)	24 (5%)	25	47
1	X	488/493 (99%)	462 (95%)	26 (5%)	22	43
All	All	976/986 (99%)	926 (95%)	50 (5%)	24	45

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	-1	LEU
1	X	31	THR
1	X	115	THR
1	X	207	GLN
1	X	230	LEU
1	X	297	LEU
1	X	305	LEU
1	X	306	LEU
1	X	314	LEU
1	X	332	SER
1	X	346	GLN
1	X	358	LEU
1	X	365	SER
1	X	418	SER
1	X	444	LEU
1	X	471	ARG
1	X	479	GLN
1	X	496	ARG
1	X	498	GLU
1	X	499	VAL
1	X	519	ARG
1	X	538	THR
1	X	548	ARG
1	X	549	GLU
1	X	580	LEU
1	X	582	ARG
1	A	31	THR
1	A	112	ARG
1	A	129	ARG
1	A	230	LEU
1	A	297	LEU
1	A	305	LEU
1	A	306	LEU
1	A	314	LEU
1	A	332	SER
1	A	358	LEU
1	A	418	SER
1	A	444	LEU
1	A	471	ARG
1	A	479	GLN
1	A	496	ARG
1	A	498	GLU
1	A	499	VAL

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Mol	Chain	Res	Type
1	A	519	ARG
1	A	538	THR
1	A	548	ARG
1	A	549	GLU
1	A	580	LEU
1	A	582	ARG
1	A	621	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	546	HIS
1	A	-2	HIS
1	A	546	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	C8E	A	624	-	5,5,20	0.37	0	4,4,19	0.25	0
2	C8E	A	623	-	19,19,20	0.39	0	18,18,19	0.50	0
2	C8E	A	625	-	5,5,20	0.32	0	4,4,19	0.33	0
2	C8E	X	623	-	17,17,20	0.45	0	16,16,19	0.27	0
2	C8E	A	626	-	5,5,20	0.33	0	4,4,19	0.38	0
2	C8E	X	624	-	5,5,20	0.41	0	4,4,19	0.10	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	C8E	A	624	-	-	2/3/3/18	-
2	C8E	A	623	-	-	7/17/17/18	-
2	C8E	A	625	-	-	3/3/3/18	-
2	C8E	X	623	-	-	5/15/15/18	-
2	C8E	A	626	-	-	2/3/3/18	-
2	C8E	X	624	-	-	1/3/3/18	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	623	C8E	O12-C13-C14-O15
2	A	623	C8E	O18-C19-C20-O21
2	X	623	C8E	O12-C13-C14-O15
2	X	624	C8E	C2-C3-C4-C5
2	A	626	C8E	C1-C2-C3-C4
2	A	625	C8E	C2-C3-C4-C5
2	A	623	C8E	C5-C6-C7-C8
2	A	623	C8E	C2-C3-C4-C5
2	A	625	C8E	C1-C2-C3-C4
2	X	623	C8E	C16-C17-O18-C19
2	X	623	C8E	C17-C16-O15-C14
2	A	624	C8E	C3-C4-C5-C6
2	A	625	C8E	C3-C4-C5-C6
2	A	624	C8E	C2-C3-C4-C5

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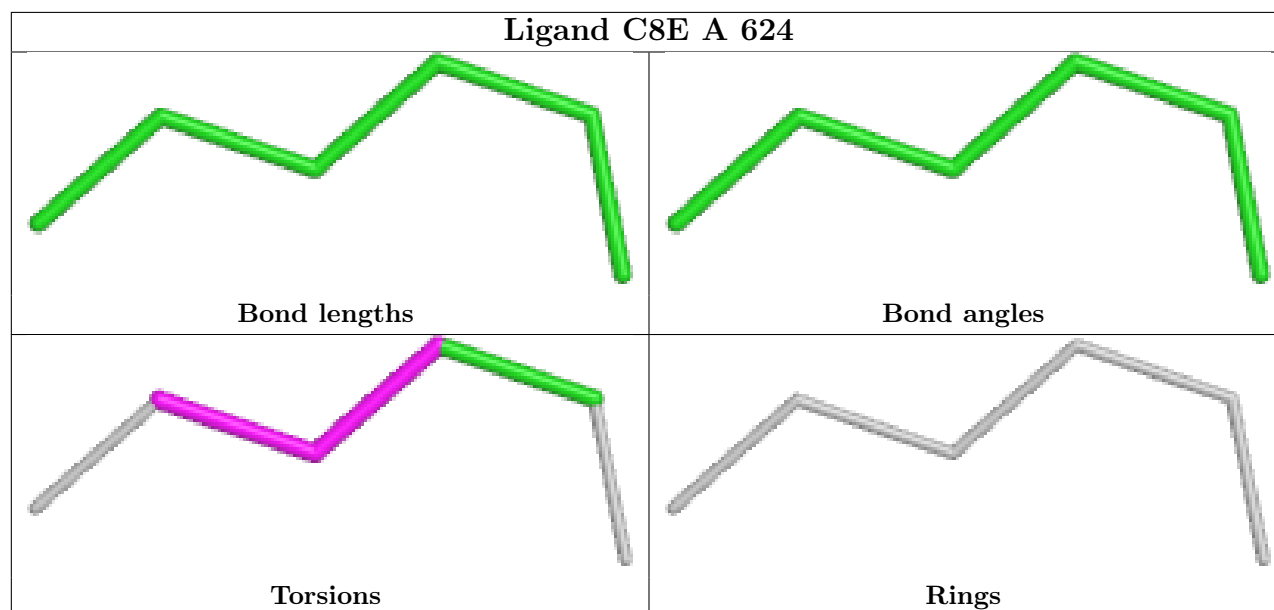
Mol	Chain	Res	Type	Atoms
2	X	623	C8E	C7-C8-O9-C10
2	A	626	C8E	C2-C3-C4-C5
2	A	623	C8E	C16-C17-O18-C19
2	X	623	C8E	O15-C16-C17-O18
2	A	623	C8E	C20-C19-O18-C17
2	A	623	C8E	O15-C16-C17-O18

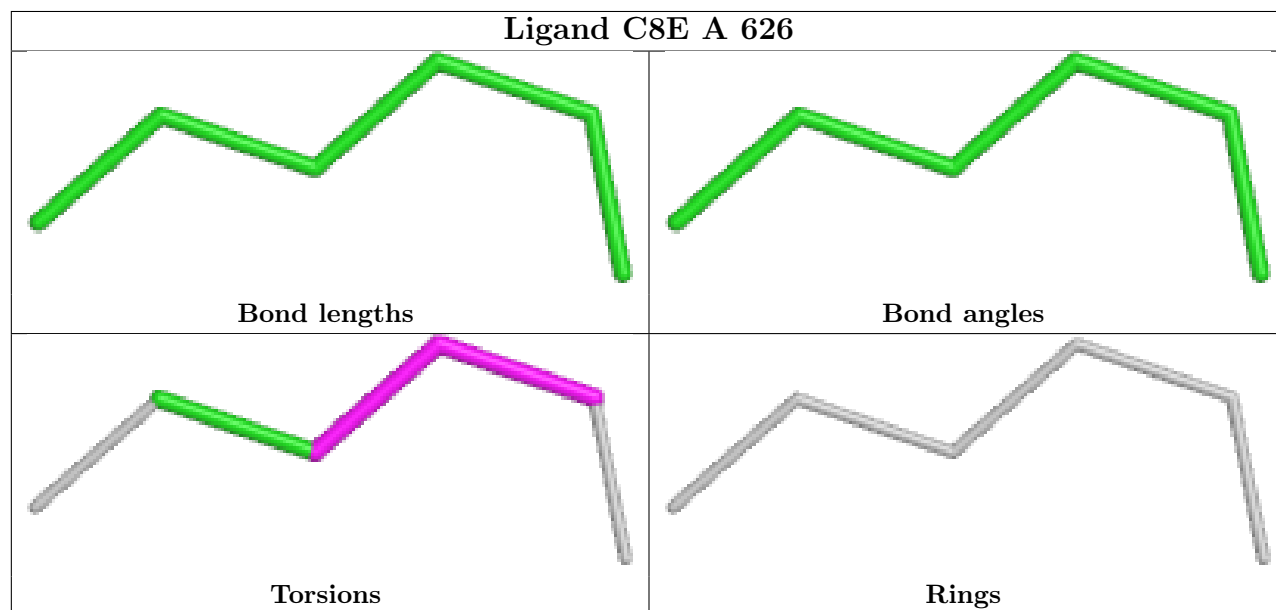
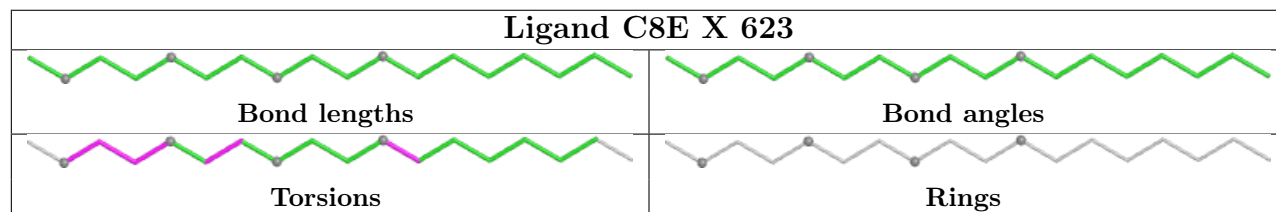
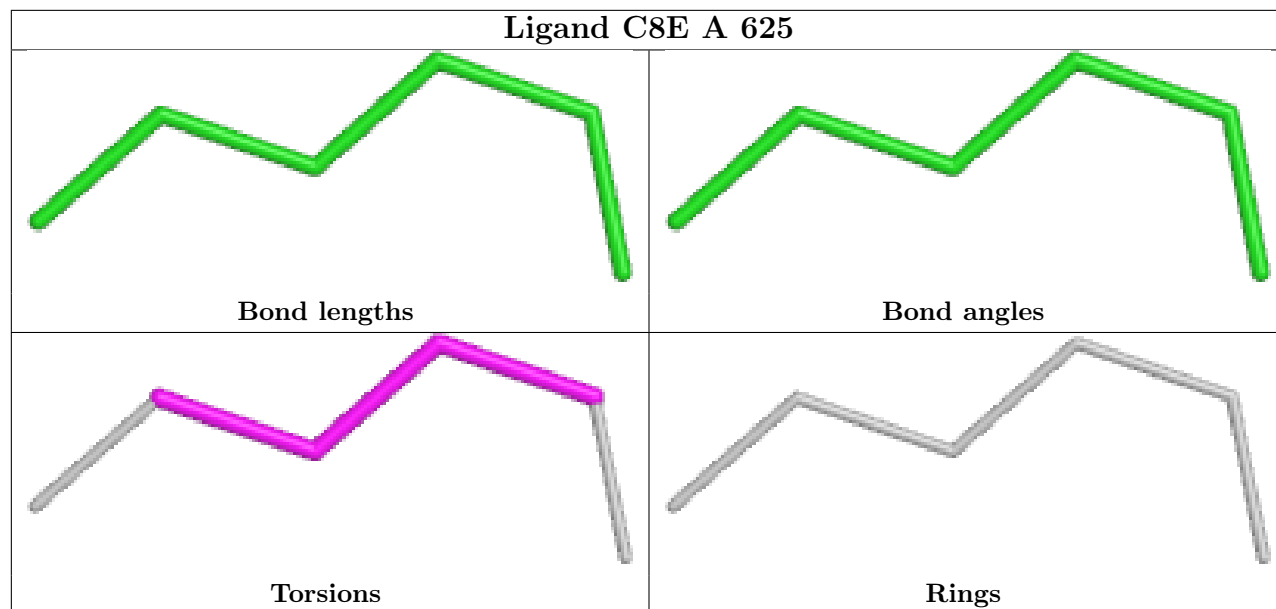
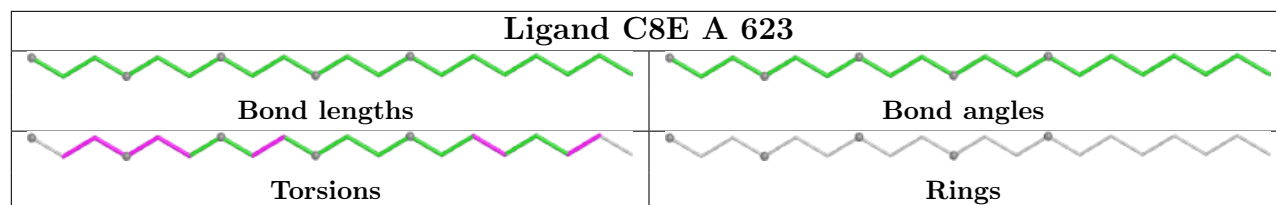
There are no ring outliers.

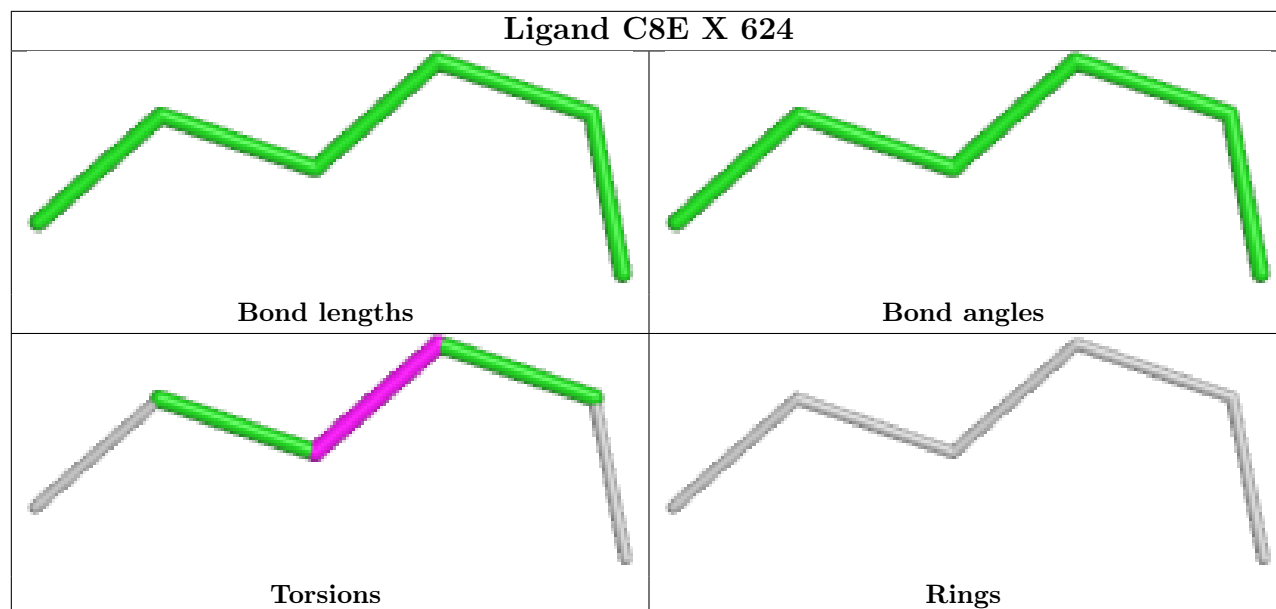
3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	623	C8E	6	0
2	X	623	C8E	4	0
2	A	626	C8E	3	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	627/632 (99%)	-0.19	11 (1%) 68 71	23, 46, 78, 130	0
1	X	628/632 (99%)	-0.08	15 (2%) 59 62	22, 45, 78, 100	0
All	All	1255/1264 (99%)	-0.13	26 (2%) 63 66	22, 45, 78, 130	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	346	GLN	4.4
1	X	428	TRP	4.0
1	A	-3	HIS	3.8
1	X	81	GLY	3.7
1	X	388	TRP	3.2
1	X	384	ILE	3.0
1	A	131	GLY	3.0
1	A	536	SER	2.9
1	X	594	GLU	2.8
1	X	82	ILE	2.6
1	X	535	GLY	2.6
1	A	384	ILE	2.6
1	A	-2	HIS	2.6
1	A	129	ARG	2.6
1	X	550	TYR	2.4
1	A	-1	LEU	2.4
1	A	591	LEU	2.4
1	A	130	GLN	2.4
1	A	426	ASN	2.3
1	X	-1	LEU	2.3
1	X	-3	HIS	2.3
1	X	592	ALA	2.3
1	X	536	SER	2.2
1	A	532	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	X	382	TYR	2.0
1	X	546	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

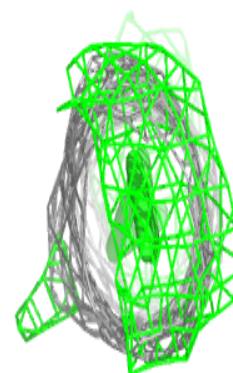
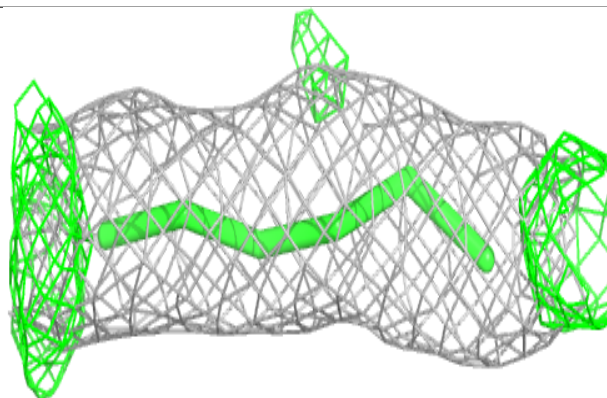
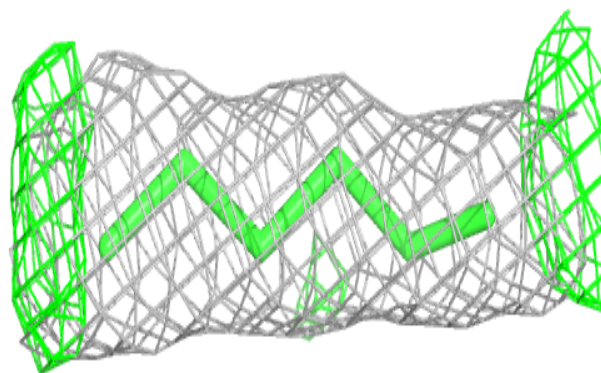
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	C8E	A	624	6/21	0.81	0.19	27,48,54,57	0
2	C8E	A	626	6/21	0.88	0.27	38,46,51,51	0
2	C8E	A	625	6/21	0.90	0.18	41,49,57,57	0
2	C8E	X	624	6/21	0.91	0.26	32,34,49,52	0
2	C8E	X	623	18/21	0.92	0.26	24,42,72,75	0
2	C8E	A	623	20/21	0.96	0.21	28,44,62,75	0

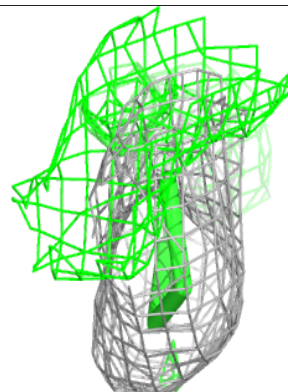
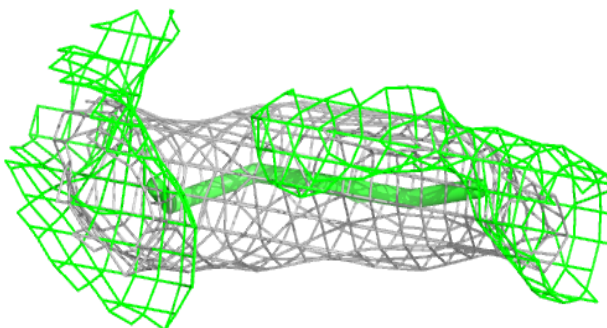
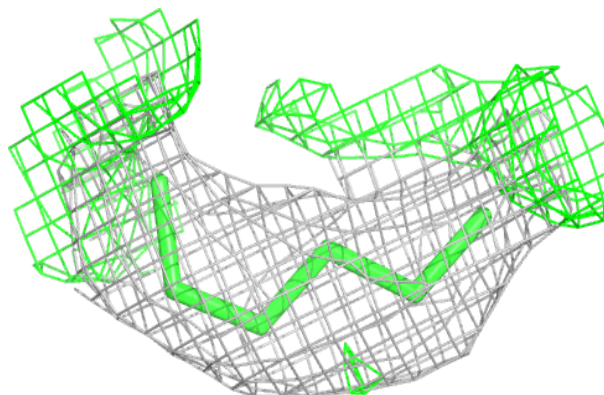
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around C8E A 624:

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

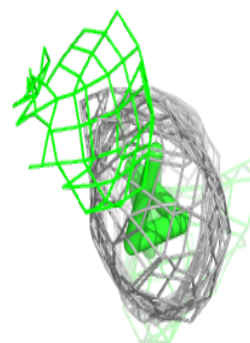
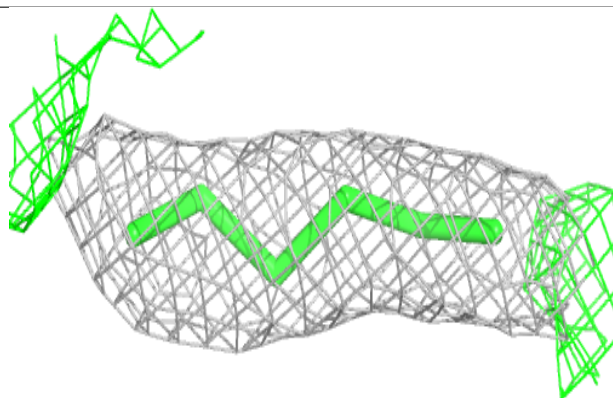
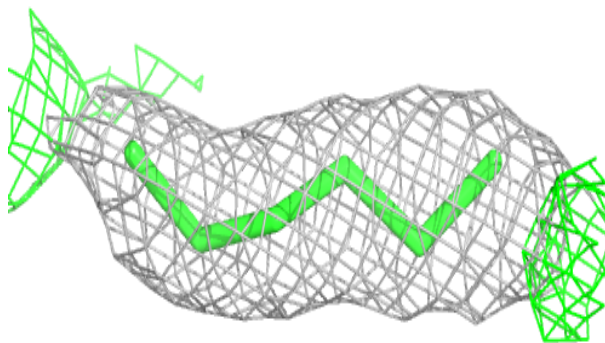
**Electron density around C8E A 626:**

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

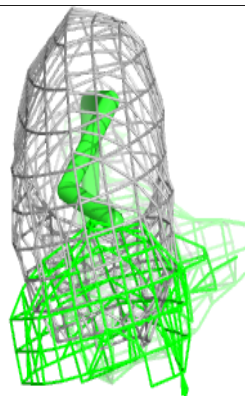
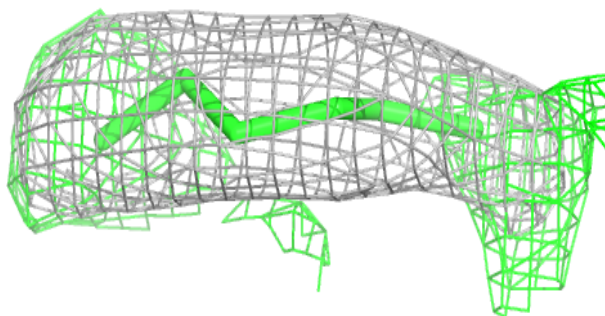
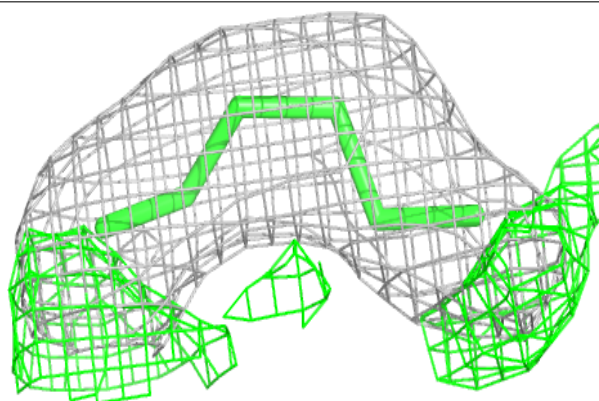


Electron density around C8E A 625:

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

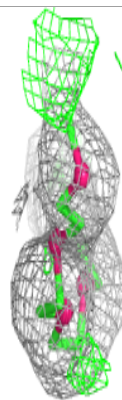
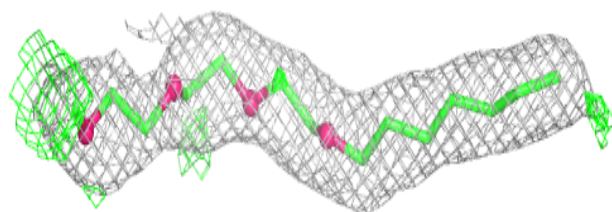
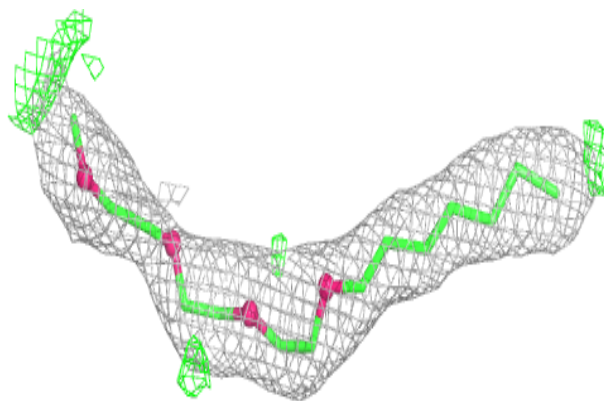
**Electron density around C8E X 624:**

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

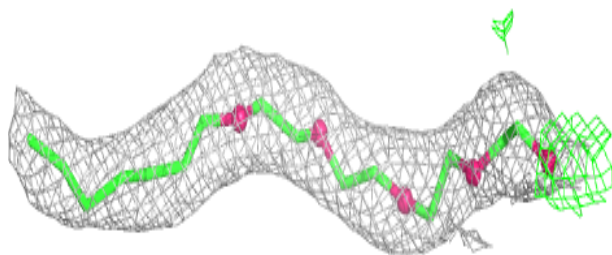
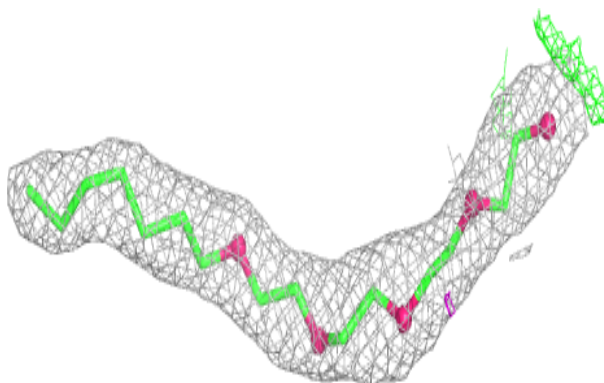


Electron density around C8E X 623:

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

**Electron density around C8E A 623:**

$2mF_o-DF_c$ (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.