



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:34 AM UTC

PDB ID : 7Q4X / pdb_00007q4x
Title : Crystal Structure of Equine Serum Albumin in Complex with Cefaclor
Authors : Duszynski, K.; Sekula, B.; Bujacz, A.
Deposited on : 2021-11-02
Resolution : 2.12 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

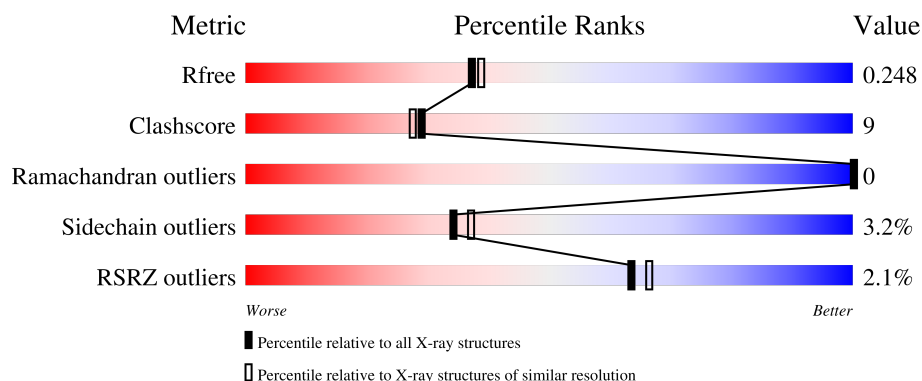
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

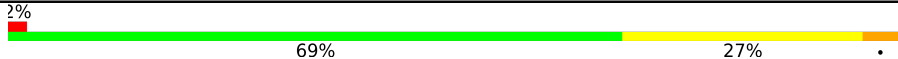
The reported resolution of this entry is 2.12 Å.

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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	580	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	LMR	A	608	-	-	X	-

2 Entry composition [i](#)

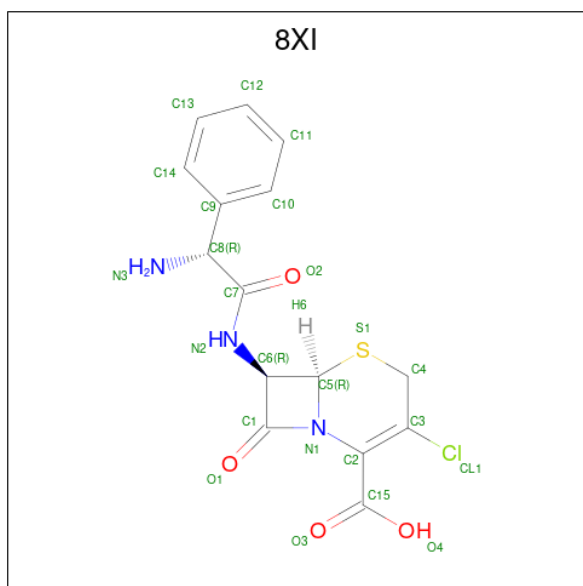
There are 7 unique types of molecules in this entry. The entry contains 4858 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Albumin.

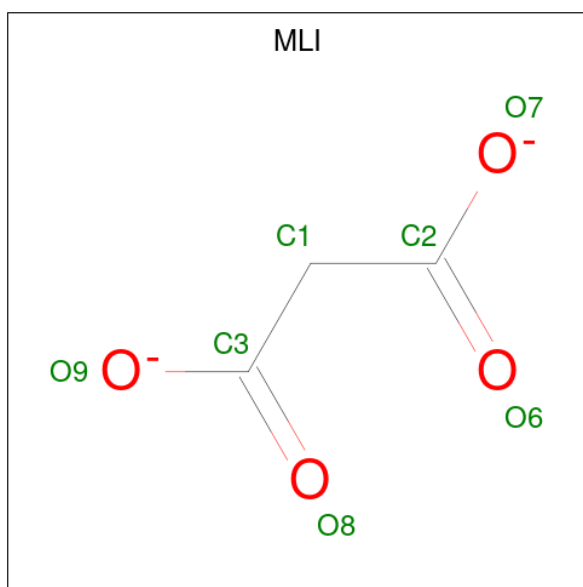
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	580	Total	C	N	O	S	0	8	0
			4598	2911	771	881	35			

- Molecule 2 is Cefaclor (CCD ID: 8XI) (formula: $C_{15}H_{14}ClN_3O_4S$) (labeled as "Ligand of Interest" by depositor).



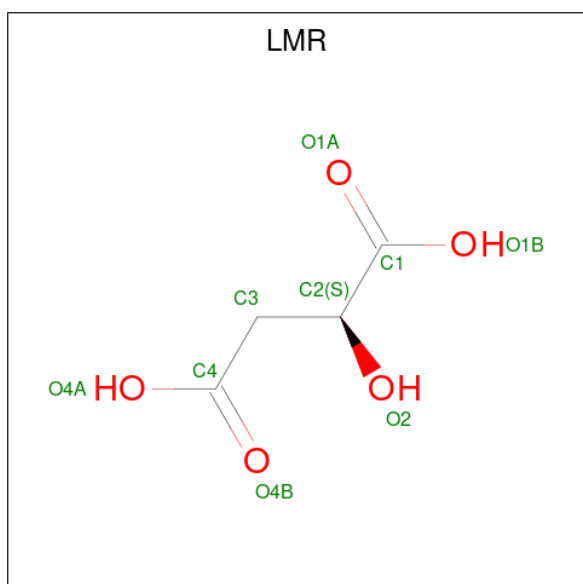
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	0
			24	15	1	3	4	1		
2	A	1	Total	C	Cl	N	O	S	0	0
			24	15	1	3	4	1		

- Molecule 3 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$).



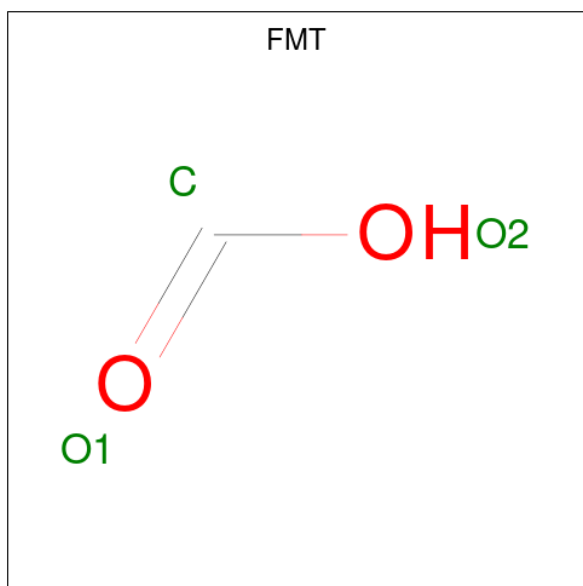
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	3	4		
3	A	1	Total	C	O	0	0
			7	3	4		
3	A	1	Total	C	O	0	0
			7	3	4		
3	A	1	Total	C	O	0	0
			7	3	4		
3	A	1	Total	C	O	0	0
			7	3	4		

- Molecule 4 is (2S)-2-hydroxybutanedioic acid (CCD ID: LMR) (formula: $C_4H_6O_5$).



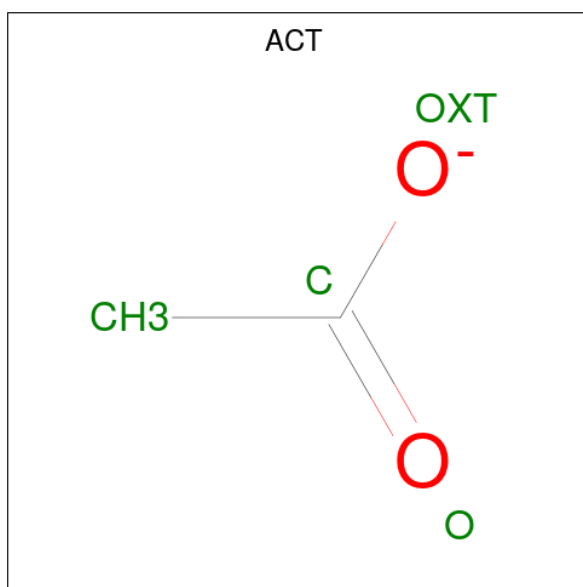
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			9	4	5		

- Molecule 5 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



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

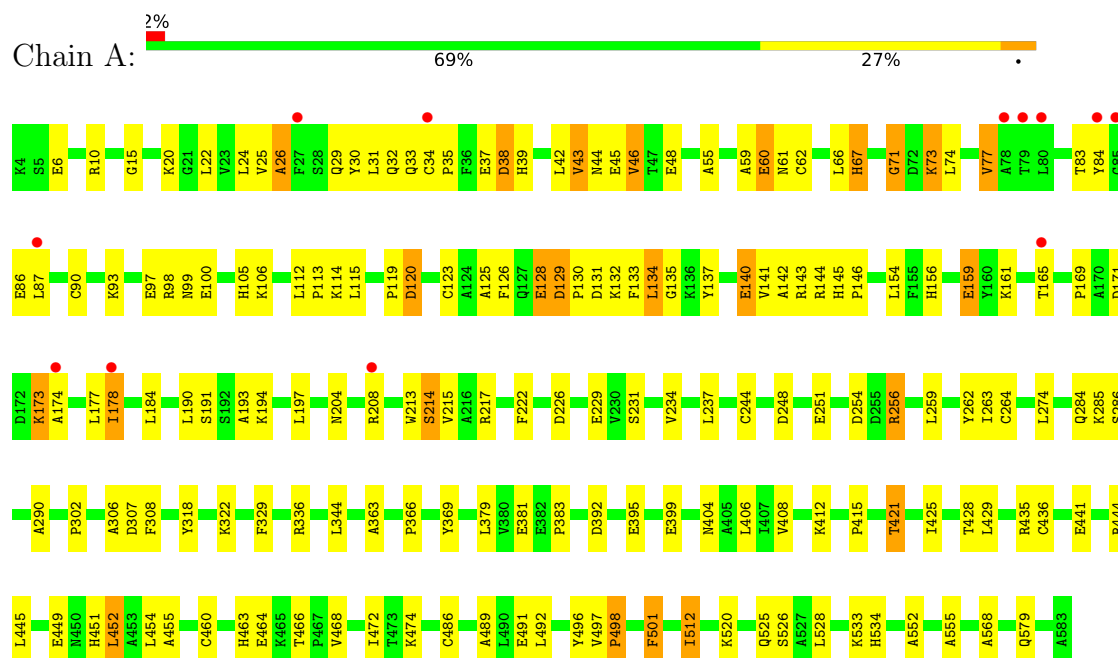
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	139	Total	O	0	0
			139	139		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Albumin



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	94.75Å 94.75Å 142.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.38 – 2.12 47.38 – 2.12	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.38-2.12) 94.5 (47.38-2.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.187 , 0.249 0.187 , 0.248	Depositor DCC
R_{free} test set	2052 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	46.5	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.051 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4858	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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: ACT, LMR, 8XI, MLI, FMT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.63	46/4727 (1.0%)	1.51	45/6376 (0.7%)

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	178	ILE	CA-CB	9.84	1.59	1.54
1	A	145	HIS	C-O	-8.79	1.14	1.24
1	A	229	GLU	CA-C	8.46	1.63	1.52
1	A	520	LYS	CA-C	8.29	1.63	1.52
1	A	264	CYS	C-O	-8.23	1.13	1.24
1	A	445	LEU	N-CA	-7.86	1.40	1.46
1	A	215	VAL	N-CA	6.95	1.54	1.46
1	A	454	LEU	CA-C	6.93	1.61	1.52
1	A	83	THR	CA-C	6.79	1.61	1.52
1	A	99	ASN	C-O	6.70	1.32	1.24
1	A	190	LEU	CA-C	6.70	1.61	1.52
1	A	231	SER	CA-C	-6.54	1.44	1.52
1	A	451	HIS	C-O	-6.52	1.16	1.24
1	A	254	ASP	C-O	6.45	1.31	1.24
1	A	43	VAL	N-CA	-6.39	1.39	1.46
1	A	344	LEU	CA-C	6.36	1.61	1.52
1	A	468	VAL	C-O	-6.21	1.16	1.24
1	A	193	ALA	CA-C	6.00	1.60	1.52
1	A	197	LEU	N-CA	5.79	1.53	1.46
1	A	486	CYS	CA-C	5.74	1.60	1.52
1	A	73	LYS	CA-C	-5.74	1.45	1.52
1	A	48	GLU	N-CA	-5.72	1.39	1.46
1	A	496	TYR	C-N	5.67	1.37	1.32
1	A	307	ASP	CA-C	5.60	1.60	1.52
1	A	20	LYS	C-O	5.56	1.30	1.24
1	A	100	GLU	N-CA	5.48	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	329	PHE	CA-C	5.47	1.59	1.52
1	A	213	TRP	N-CA	5.45	1.52	1.46
1	A	486	CYS	C-O	-5.39	1.17	1.24
1	A	489	ALA	C-O	-5.38	1.17	1.24
1	A	130	PRO	CA-C	5.32	1.60	1.52
1	A	67	HIS	CA-C	-5.31	1.45	1.52
1	A	463	HIS	N-CA	-5.29	1.39	1.46
1	A	194	LYS	N-CA	5.28	1.52	1.46
1	A	26	ALA	CA-C	5.22	1.59	1.52
1	A	15	GLY	C-O	5.19	1.29	1.23
1	A	568	ALA	N-CA	5.18	1.52	1.46
1	A	274	LEU	CA-C	-5.18	1.45	1.52
1	A	392	ASP	C-O	-5.15	1.18	1.24
1	A	213	TRP	CA-CB	5.13	1.61	1.53
1	A	306	ALA	N-CA	-5.13	1.40	1.46
1	A	421	THR	N-CA	5.13	1.52	1.46
1	A	501	PHE	CA-C	5.09	1.59	1.52
1	A	528	LEU	N-CA	5.06	1.52	1.46
1	A	406	LEU	N-CA	5.05	1.52	1.46
1	A	256	ARG	N-CA	-5.04	1.40	1.46

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	GLY	N-CA-C	-8.80	102.29	112.50
1	A	496	TYR	CA-C-N	-7.48	115.20	123.43
1	A	496	TYR	C-N-CA	-7.48	115.20	123.43
1	A	177	LEU	N-CA-C	7.24	120.23	111.40
1	A	105	HIS	N-CA-C	6.87	121.26	113.01
1	A	33	GLN	N-CA-C	6.59	121.54	112.90
1	A	25	VAL	CB-CA-C	6.31	119.70	111.81
1	A	308	PHE	N-CA-C	6.23	121.05	113.38
1	A	129	ASP	CA-C-N	-6.23	112.43	119.28
1	A	129	ASP	C-N-CA	-6.23	112.43	119.28
1	A	263	ILE	N-CA-C	-6.06	104.60	110.72
1	A	363	ALA	N-CA-C	5.97	118.55	111.33
1	A	83	THR	N-CA-C	5.90	117.39	111.07
1	A	226	ASP	N-CA-C	5.87	118.48	110.55
1	A	159	GLU	CA-C-N	5.85	128.12	120.28
1	A	159	GLU	C-N-CA	5.85	128.12	120.28
1	A	141	VAL	CB-CA-C	5.80	119.64	112.04
1	A	520	LYS	N-CA-CB	-5.79	101.60	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	555	ALA	N-CA-C	-5.79	104.97	111.28
1	A	55	ALA	N-CA-C	-5.77	106.37	113.41
1	A	145	HIS	N-CA-C	-5.72	99.38	108.82
1	A	512	ILE	N-CA-C	-5.69	105.33	113.07
1	A	140	GLU	N-CA-C	-5.59	105.27	111.36
1	A	284	GLN	CA-C-N	5.53	127.63	120.44
1	A	284	GLN	C-N-CA	5.53	127.63	120.44
1	A	399	GLU	N-CA-C	5.49	116.94	111.07
1	A	44	ASN	N-CA-C	5.44	117.21	111.28
1	A	254	ASP	N-CA-C	-5.42	105.28	111.14
1	A	214	SER	N-CA-CB	5.33	118.15	110.20
1	A	552	ALA	N-CA-C	-5.31	105.57	111.36
1	A	285	LYS	N-CA-C	-5.28	105.42	111.07
1	A	171	ASP	N-CA-C	5.25	116.69	111.07
1	A	449	GLU	CB-CG-CD	5.25	121.53	112.60
1	A	120	ASP	N-CA-C	5.23	121.95	110.80
1	A	222	PHE	CA-C-N	-5.19	114.47	119.87
1	A	222	PHE	C-N-CA	-5.19	114.47	119.87
1	A	191	SER	N-CA-C	-5.19	105.31	110.97
1	A	474	LYS	CB-CA-C	5.14	118.96	110.88
1	A	34	CYS	CA-C-N	-5.12	114.45	119.92
1	A	34	CYS	C-N-CA	-5.12	114.45	119.92
1	A	25	VAL	N-CA-C	-5.11	105.35	110.30
1	A	204	ASN	N-CA-C	5.10	119.55	113.23
1	A	259	LEU	N-CA-C	5.07	116.50	111.07
1	A	128	GLU	N-CA-C	5.06	121.58	110.80
1	A	428	THR	N-CA-C	-5.03	105.71	111.14

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	4598	0	4540	80	0
2	A	48	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	35	0	10	2	0
4	A	9	0	4	5	0
5	A	21	0	7	2	0
6	A	8	0	6	1	0
7	A	139	0	0	2	0
All	All	4858	0	4567	81	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 9.

All (81) 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:119:PRO:O	1:A:173:LYS:HD3	1.64	0.98
1:A:74:LEU:O	1:A:77:VAL:HG23	1.70	0.90
1:A:290:ALA:HA	4:A:608:LMR:H3A	1.53	0.88
1:A:318:TYR:O	1:A:322[A]:LYS:HG3	1.74	0.87
1:A:421:THR:O	1:A:425[B]:ILE:HG22	1.79	0.83
1:A:429:LEU:HD22	1:A:452[B]:LEU:HD12	1.61	0.81
1:A:526:SER:HB2	5:A:609:FMT:H	1.67	0.77
1:A:129:ASP:OD2	1:A:132:LYS:HB2	1.86	0.74
1:A:381:GLU:HG3	7:A:830:HOH:O	1.87	0.72
1:A:125:ALA:O	1:A:128:GLU:HB3	1.89	0.71
1:A:174:ALA:HB1	1:A:178:ILE:HD12	1.71	0.71
1:A:115:LEU:HD21	1:A:144:ARG:CZ	2.24	0.68
1:A:35:PRO:HD2	1:A:38:ASP:OD2	1.95	0.67
1:A:67:HIS:NE2	1:A:248:ASP:OD1	2.27	0.66
1:A:302:PRO:HD2	1:A:336:ARG:HH22	1.63	0.62
1:A:6:GLU:HG2	1:A:66:LEU:HG	1.81	0.62
1:A:46:VAL:HG23	1:A:73:LYS:HG3	1.81	0.61
1:A:237:LEU:HD13	4:A:608:LMR:H2	1.80	0.61
1:A:31:LEU:O	1:A:39:HIS:NE2	2.32	0.58
1:A:137:TYR:OH	1:A:184:LEU:HD21	2.05	0.57
1:A:237:LEU:CD1	4:A:608:LMR:H2	2.36	0.55
1:A:29:GLN:HG3	1:A:142:ALA:HB1	1.88	0.54
1:A:131:ASP:HB3	2:A:601:8XI:O1	2.08	0.54
1:A:534:HIS:HD2	1:A:579:GLN:OE1	1.91	0.54
1:A:71:GLY:HA3	1:A:98:ARG:NH2	2.23	0.53
1:A:67:HIS:CE1	1:A:248:ASP:OD1	2.63	0.52
1:A:87:LEU:O	1:A:90:CYS:HB2	2.09	0.51
1:A:42:LEU:HD22	1:A:73:LYS:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:ASN:OD1	1:A:525:GLN:HG2	2.11	0.51
1:A:429:LEU:HD21	1:A:455:ALA:HB3	1.93	0.51
1:A:290:ALA:HA	4:A:608:LMR:C3	2.33	0.51
1:A:441:GLU:HA	1:A:444:ARG:HD3	1.92	0.51
1:A:46:VAL:CG2	1:A:73:LYS:HG3	2.42	0.50
1:A:379:LEU:O	1:A:383:PRO:HD2	2.12	0.50
1:A:10:ARG:NH2	1:A:251:GLU:HG3	2.26	0.50
1:A:32:GLN:NE2	1:A:143:ARG:O	2.40	0.49
1:A:208[A]:ARG:HG2	5:A:613:FMT:H	1.94	0.49
1:A:42:LEU:HD11	1:A:77:VAL:HG22	1.93	0.49
1:A:119:PRO:HG2	1:A:174:ALA:HB2	1.94	0.49
1:A:26:ALA:O	1:A:30:TYR:HD1	1.96	0.49
1:A:290:ALA:CA	4:A:608:LMR:H3A	2.34	0.48
1:A:156:HIS:O	1:A:159:GLU:HB2	2.13	0.48
1:A:59:ALA:HB3	1:A:62:CYS:SG	2.54	0.47
1:A:415:PRO:O	1:A:533:LYS:HE2	2.13	0.47
3:A:605:MLI:O7	3:A:605:MLI:O8	2.31	0.47
1:A:119:PRO:O	1:A:123:CYS:HB2	2.15	0.46
1:A:115:LEU:HD21	1:A:144:ARG:NH1	2.31	0.46
1:A:22:LEU:HG	1:A:154:LEU:HD11	1.98	0.45
1:A:134:LEU:HD21	1:A:161:LYS:HB2	1.98	0.45
1:A:466:THR:O	6:A:616:ACT:H3	2.16	0.45
1:A:501:PHE:HB2	1:A:534:HIS:CE1	2.51	0.45
1:A:84:TYR:HB3	1:A:87:LEU:HB2	1.98	0.45
1:A:214:SER:HB2	1:A:234:VAL:HG13	1.99	0.45
1:A:106:LYS:NZ	1:A:146:PRO:O	2.45	0.44
1:A:165:THR:O	1:A:169:PRO:HD2	2.16	0.44
1:A:43:VAL:HG11	2:A:601:8XI:CL1	2.54	0.44
1:A:429:LEU:HD23	1:A:429:LEU:HA	1.70	0.44
1:A:460:CYS:O	1:A:464:GLU:HG3	2.18	0.44
1:A:29:GLN:HG2	1:A:146:PRO:HA	1.99	0.44
1:A:87:LEU:HD12	1:A:87:LEU:HA	1.84	0.43
1:A:93:LYS:NZ	1:A:97:GLU:OE2	2.50	0.42
1:A:408:VAL:O	1:A:412:LYS:HG3	2.19	0.42
1:A:60:GLU:O	1:A:61:ASN:HB2	2.19	0.42
1:A:491:GLU:O	1:A:492:LEU:C	2.62	0.42
1:A:126:PHE:HB2	1:A:133:PHE:CD2	2.54	0.42
1:A:472:ILE:HD13	1:A:472:ILE:HG21	1.77	0.42
1:A:262:TYR:CD2	1:A:262:TYR:C	2.98	0.42
1:A:45:GLU:OE2	1:A:73:LYS:HE3	2.19	0.42
1:A:119:PRO:O	1:A:173:LYS:CD	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:PHE:HB2	1:A:133:PHE:CE2	2.55	0.42
1:A:435:ARG:NH1	7:A:707:HOH:O	2.53	0.41
1:A:366:PRO:HA	1:A:369:TYR:CZ	2.56	0.41
1:A:112:LEU:O	1:A:113:PRO:C	2.62	0.41
1:A:497:VAL:O	1:A:498:PRO:C	2.64	0.41
1:A:24:LEU:HD21	1:A:135:GLY:O	2.21	0.41
1:A:217:ARG:HE	3:A:603:MLI:H11	1.86	0.41
1:A:256:ARG:CZ	1:A:286:SER:HB3	2.51	0.41
1:A:436:CYS:O	1:A:444:ARG:HG2	2.21	0.41
1:A:318:TYR:O	1:A:322[A]:LYS:CG	2.56	0.40
1:A:71:GLY:HA3	1:A:98:ARG:CZ	2.50	0.40
1:A:429:LEU:CD2	1:A:452[B]:LEU:HD12	2.42	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	586/580 (101%)	562 (96%)	24 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	510/502 (102%)	493 (97%)	17 (3%)	33	36

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	38	ASP
1	A	46	VAL
1	A	60	GLU
1	A	77	VAL
1	A	86	GLU
1	A	114	LYS
1	A	120	ASP
1	A	134	LEU
1	A	140	GLU
1	A	173	LYS
1	A	244	CYS
1	A	395	GLU
1	A	452[A]	LEU
1	A	452[B]	LEU
1	A	498	PRO
1	A	512	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	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

17 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$
5	FMT	A	614	-	2,2,2	0.48	0	1,1,1	1.03	0
6	ACT	A	617	-	3,3,3	0.84	0	3,3,3	0.76	0
3	MLI	A	605	-	6,6,6	1.43	1 (16%)	7,7,7	1.07	0
5	FMT	A	615	-	2,2,2	0.77	0	1,1,1	0.67	0
6	ACT	A	616	-	3,3,3	1.05	0	3,3,3	0.60	0
4	LMR	A	608	-	8,8,8	1.14	0	10,10,10	1.54	2 (20%)
5	FMT	A	612	-	2,2,2	0.96	0	1,1,1	0.72	0
2	8XI	A	601	-	22,26,26	2.09	7 (31%)	31,38,38	2.24	8 (25%)
5	FMT	A	609	-	2,2,2	1.16	0	1,1,1	0.31	0
5	FMT	A	610	-	2,2,2	0.90	0	1,1,1	0.27	0
2	8XI	A	602	-	22,26,26	2.01	9 (40%)	31,38,38	2.35	7 (22%)
3	MLI	A	606	-	6,6,6	1.18	0	7,7,7	1.07	0
3	MLI	A	604	-	6,6,6	1.29	0	7,7,7	1.02	0
3	MLI	A	607	-	6,6,6	2.19	2 (33%)	7,7,7	1.05	0
5	FMT	A	613	-	2,2,2	0.64	0	1,1,1	0.57	0
3	MLI	A	603	-	6,6,6	1.87	1 (16%)	7,7,7	0.99	0
5	FMT	A	611	-	2,2,2	0.84	0	1,1,1	0.50	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	MLI	A	605	-	-	0/4/4/4	-
4	LMR	A	608	-	-	2/8/8/8	-
2	8XI	A	601	-	-	3/16/45/45	0/3/3/3
2	8XI	A	602	-	-	2/16/45/45	0/3/3/3
3	MLI	A	606	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MLI	A	604	-	-	2/4/4/4	-
3	MLI	A	607	-	-	2/4/4/4	-
3	MLI	A	603	-	-	2/4/4/4	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	8XI	C9-C8	-4.48	1.47	1.52
2	A	601	8XI	C1-N1	-3.85	1.27	1.38
2	A	602	8XI	C1-N1	-3.82	1.27	1.38
2	A	602	8XI	C9-C8	-3.63	1.48	1.52
2	A	602	8XI	C2-N1	-3.49	1.34	1.41
2	A	601	8XI	C2-N1	-3.40	1.35	1.41
3	A	607	MLI	C1-C2	3.39	1.56	1.51
2	A	601	8XI	C5-S1	-3.21	1.74	1.80
2	A	601	8XI	C4-S1	-3.02	1.76	1.82
2	A	602	8XI	C5-C6	2.99	1.61	1.56
2	A	602	8XI	C6-C1	-2.92	1.47	1.54
3	A	603	MLI	C1-C3	2.70	1.55	1.51
2	A	601	8XI	C6-C1	-2.70	1.48	1.54
3	A	607	MLI	C1-C3	2.59	1.55	1.51
2	A	602	8XI	C10-C9	2.43	1.43	1.39
3	A	605	MLI	O8-C3	2.24	1.29	1.22
2	A	602	8XI	C4-S1	-2.09	1.77	1.82
2	A	601	8XI	O4-C15	-2.07	1.24	1.30
2	A	602	8XI	C12-C13	2.04	1.42	1.38
2	A	602	8XI	C3-CL1	2.02	1.79	1.74

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	602	8XI	C4-S1-C5	8.03	109.08	94.36
2	A	601	8XI	C4-S1-C5	6.71	106.65	94.36
2	A	601	8XI	C5-C6-N2	-5.01	108.11	118.49
2	A	602	8XI	C6-C5-N1	-4.91	81.33	87.26
2	A	602	8XI	C5-C6-N2	-4.62	108.92	118.49
2	A	601	8XI	O1-C1-C6	-4.12	125.62	136.11
2	A	601	8XI	C6-C5-N1	-3.94	82.50	87.26
2	A	601	8XI	C1-N1-C2	-3.91	125.35	133.72
2	A	602	8XI	C1-N1-C2	-3.81	125.57	133.72
2	A	602	8XI	O1-C1-C6	-3.74	126.58	136.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	608	LMR	O1B-C1-C2	3.12	119.33	112.74
4	A	608	LMR	O1A-C1-C2	-2.88	116.85	122.60
2	A	601	8XI	C6-C5-S1	-2.81	111.74	116.74
2	A	602	8XI	C6-C5-S1	-2.58	112.16	116.74
2	A	602	8XI	C5-N1-C1	2.50	99.27	94.87
2	A	601	8XI	S1-C5-N1	-2.27	106.67	110.60
2	A	601	8XI	C5-N1-C1	2.27	98.87	94.87

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	8XI	O4-C15-C2-C3
4	A	608	LMR	C1-C2-C3-C4
4	A	608	LMR	O2-C2-C3-C4
3	A	603	MLI	C3-C1-C2-O6
2	A	602	8XI	N2-C7-C8-N3
2	A	602	8XI	O2-C7-C8-N3
3	A	603	MLI	C3-C1-C2-O7
3	A	604	MLI	C3-C1-C2-O6
3	A	604	MLI	C3-C1-C2-O7
2	A	601	8XI	O4-C15-C2-N1
2	A	601	8XI	C5-C6-N2-C7
3	A	607	MLI	C3-C1-C2-O7
3	A	607	MLI	C3-C1-C2-O6

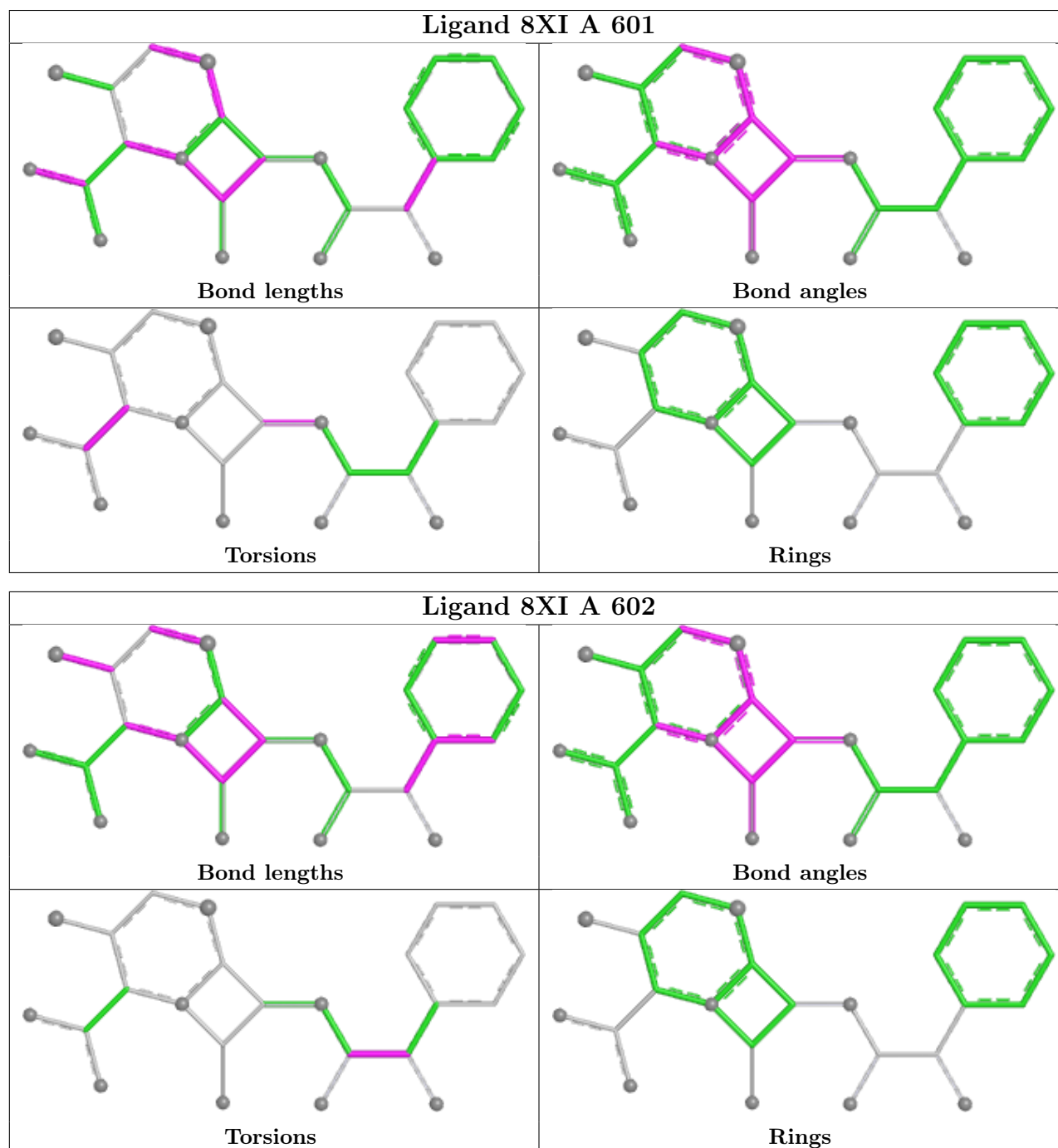
There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	605	MLI	1	0
6	A	616	ACT	1	0
4	A	608	LMR	5	0
2	A	601	8XI	2	0
5	A	609	FMT	1	0
5	A	613	FMT	1	0
3	A	603	MLI	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	580/580 (100%)	-0.07	12 (2%) 63 66	27, 52, 92, 126	8 (1%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	78	ALA	3.5
1	A	80	LEU	3.5
1	A	84	TYR	3.1
1	A	85	GLY	2.5
1	A	87	LEU	2.4
1	A	27	PHE	2.4
1	A	34	CYS	2.3
1	A	178	ILE	2.1
1	A	174	ALA	2.1
1	A	79	THR	2.1
1	A	208[A]	ARG	2.1
1	A	165	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

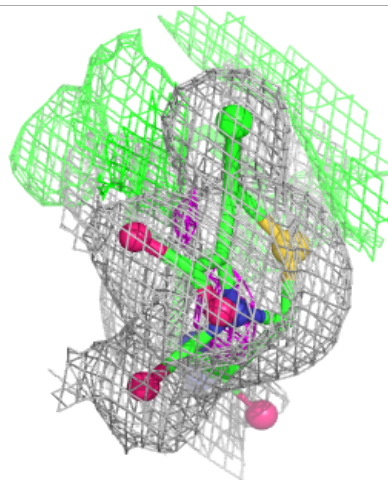
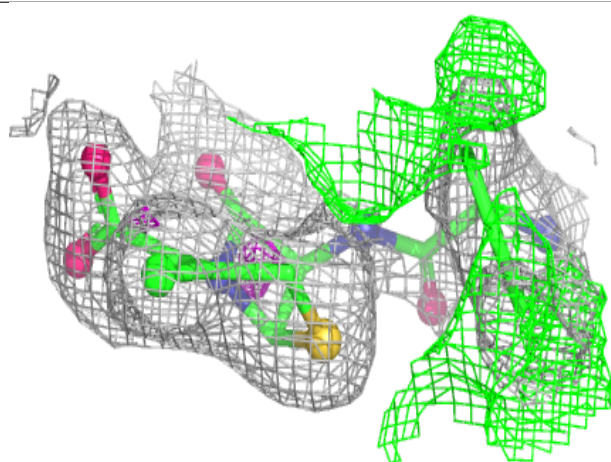
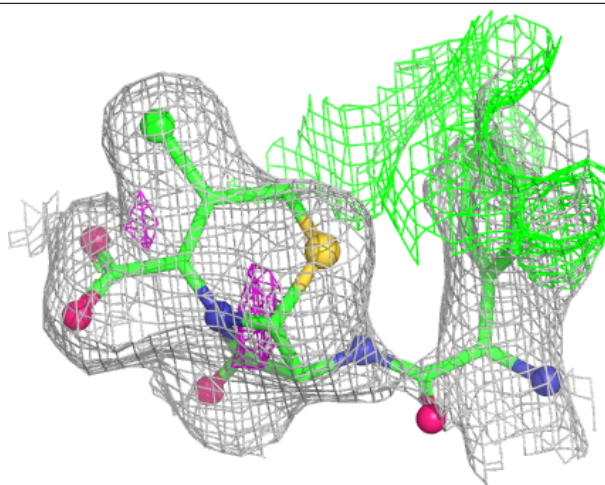
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	FMT	A	613	3/3	0.80	0.15	77,77,86,92	0
2	8XI	A	602	24/24	0.81	0.15	54,76,93,99	0
5	FMT	A	611	3/3	0.83	0.09	74,74,78,85	0
5	FMT	A	610	3/3	0.83	0.18	55,55,61,66	0
3	MLI	A	604	7/7	0.84	0.10	66,69,76,84	0
6	ACT	A	617	4/4	0.84	0.12	69,72,72,73	0
6	ACT	A	616	4/4	0.85	0.15	48,54,72,75	0
3	MLI	A	607	7/7	0.86	0.17	66,77,92,93	0
3	MLI	A	603	7/7	0.86	0.11	55,62,77,83	0
3	MLI	A	605	7/7	0.86	0.15	58,64,71,71	0
3	MLI	A	606	7/7	0.87	0.14	65,71,82,86	0
5	FMT	A	614	3/3	0.87	0.20	72,72,72,80	0
4	LMR	A	608	9/9	0.87	0.14	53,59,67,67	0
5	FMT	A	612	3/3	0.87	0.19	63,63,68,73	0
5	FMT	A	609	3/3	0.89	0.18	53,53,55,65	0
2	8XI	A	601	24/24	0.89	0.13	70,83,94,97	0
5	FMT	A	615	3/3	0.91	0.13	66,66,73,77	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.

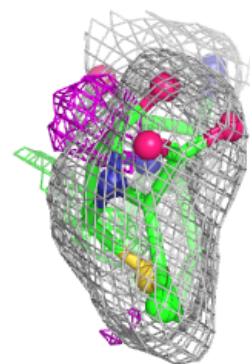
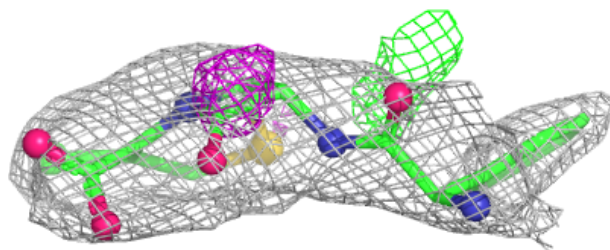
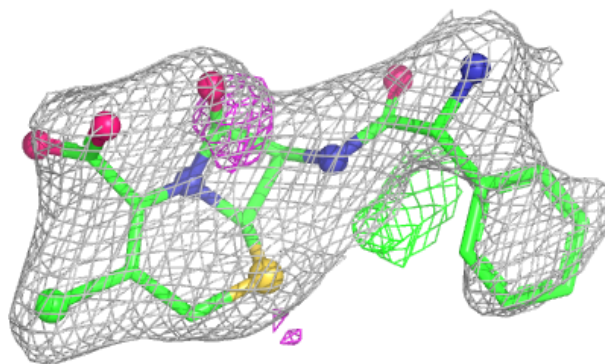
Electron density around 8XI A 602:

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



Electron density around 8XI 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.