



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 2, 2026 – 11:06 PM JST

PDB ID : 7BTK / pdb_00007btk
Title : E.coli beta-galactosidase (E537Q) in complex with fluorescent probe KSA01
Authors : Chen, X.; Hu, Y.L.; Liu, Q.M.; Gao, Y.; Yuan, R.; Guo, Y.
Deposited on : 2020-04-01
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

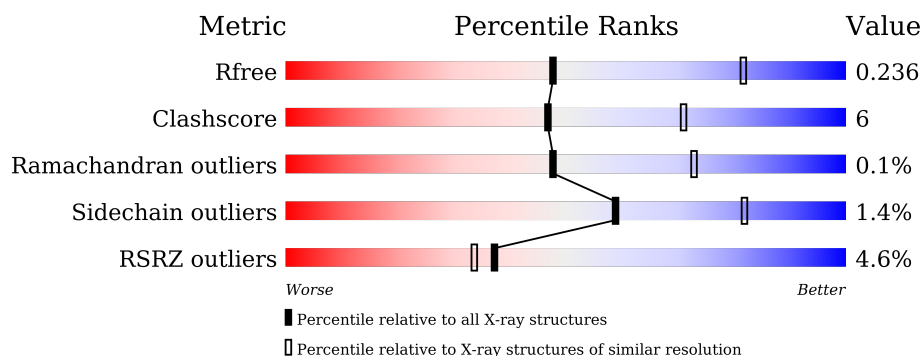
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1025	3% 85% 15%
1	B	1025	4% 86% 13%
1	C	1025	4% 86% 13%
1	D	1025	8% 86% 13%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 33869 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.

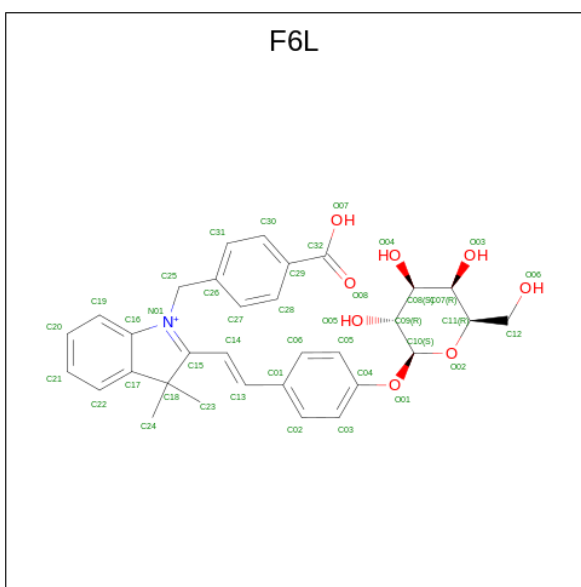
- Molecule 1 is a protein called Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1021	Total	C	N	O	S	0	0	0
			8126	5147	1438	1503	38			
1	B	1021	Total	C	N	O	S	0	1	0
			8084	5120	1434	1493	37			
1	C	1023	Total	C	N	O	S	0	0	0
			8092	5122	1436	1496	38			
1	D	1021	Total	C	N	O	S	0	0	0
			8107	5136	1439	1495	37			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP P00722
A	537	GLN	GLU	engineered mutation	UNP P00722
B	-1	SER	-	expression tag	UNP P00722
B	537	GLN	GLU	engineered mutation	UNP P00722
C	-1	SER	-	expression tag	UNP P00722
C	537	GLN	GLU	engineered mutation	UNP P00722
D	-1	SER	-	expression tag	UNP P00722
D	537	GLN	GLU	engineered mutation	UNP P00722

- Molecule 2 is 4-[[2-[(E)-2-[4-[(2S,3R,4S,5R,6R)-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxyphenyl]ethenyl]-3,3-dimethyl-2H-indol-1-yl]methyl]benzoic acid (CCD ID: F6L) (formula: C₃₂H₃₄NO₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			41	32	1	8		
2	B	1	Total	C	N	O	0	0
			41	32	1	8		
2	C	1	Total	C	N	O	0	0
			41	32	1	8		
2	D	1	Total	C	N	O	0	0
			41	32	1	8		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	1	Total	Mg	0	0
			1	1		
3	C	2	Total	Mg	0	0
			2	2		
3	D	2	Total	Mg	0	0
			2	2		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

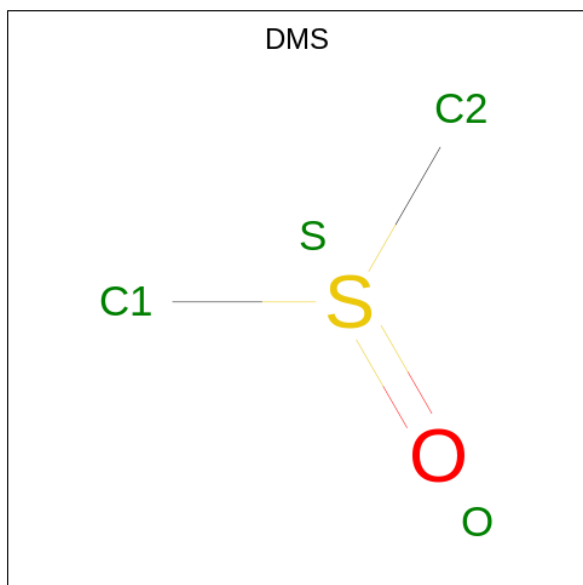
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Na	0	0
			2	2		

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

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



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

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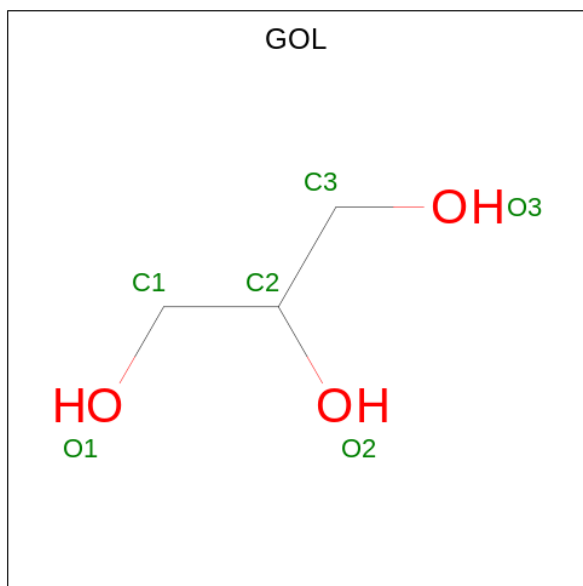
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		

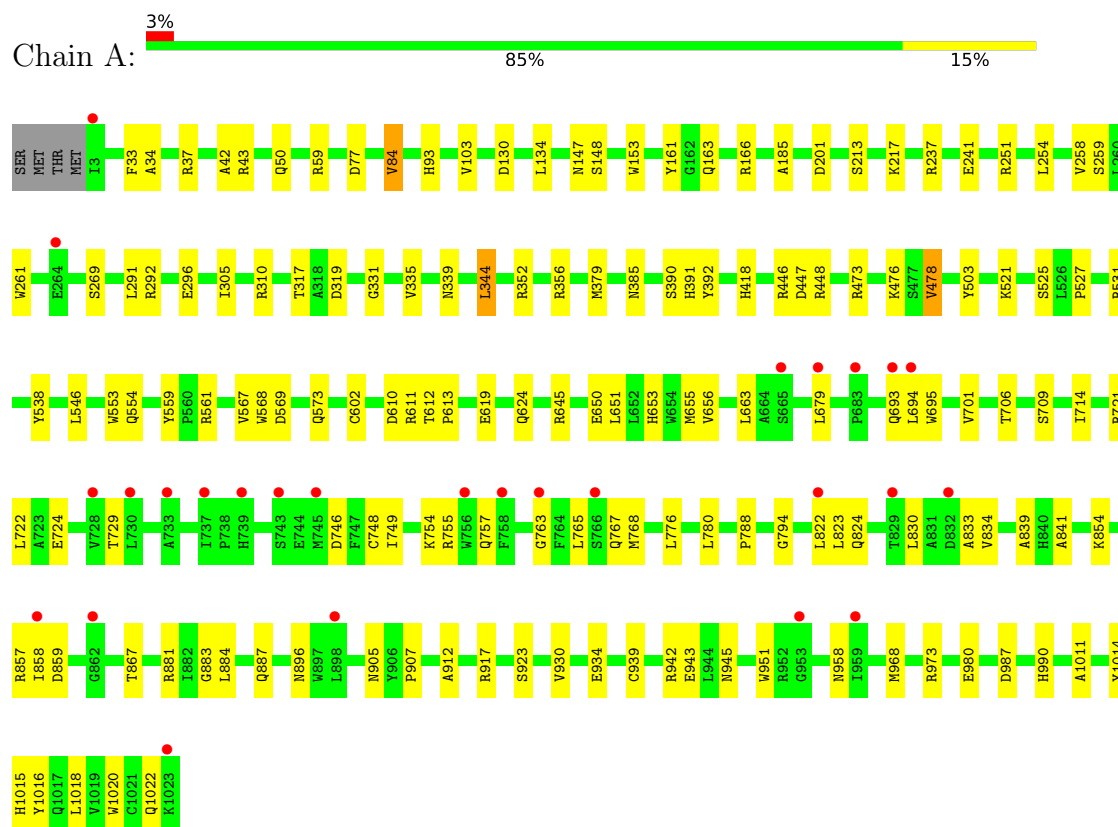
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	293	Total 293	O 293	0	0
7	B	297	Total 297	O 297	0	0
7	C	281	Total 281	O 281	0	0
7	D	253	Total 253	O 253	0	0

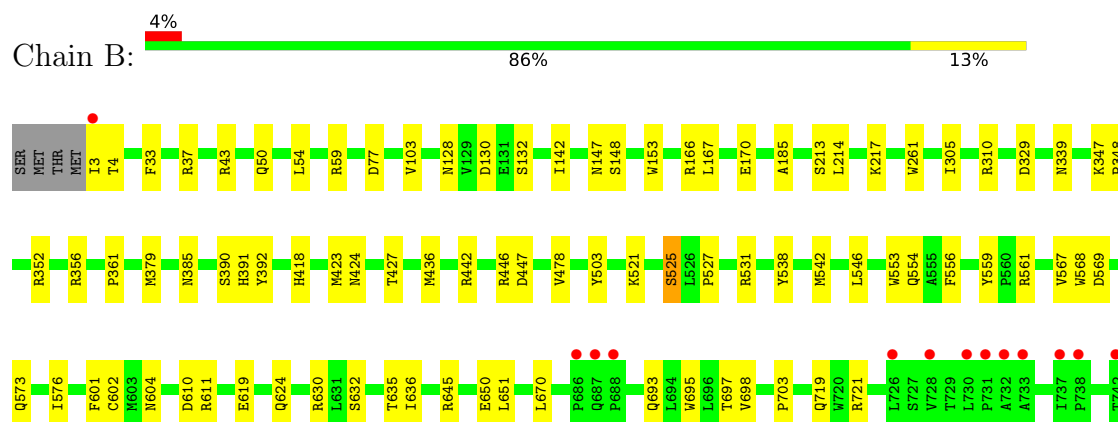
3 Residue-property plots

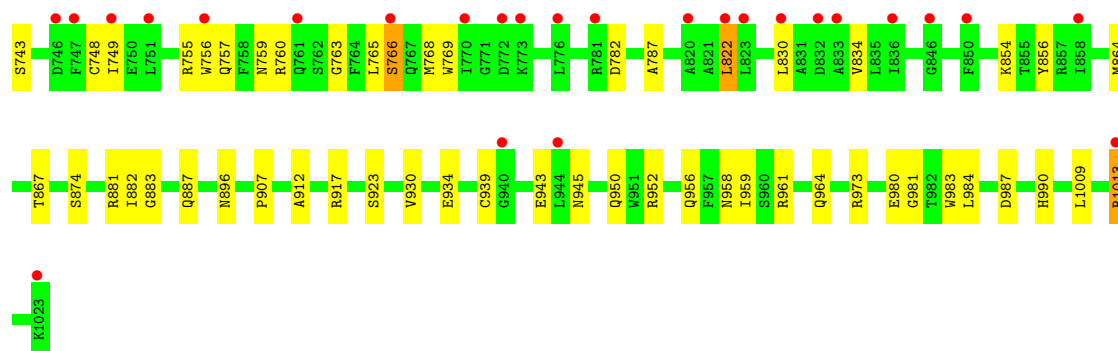
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Beta-galactosidase

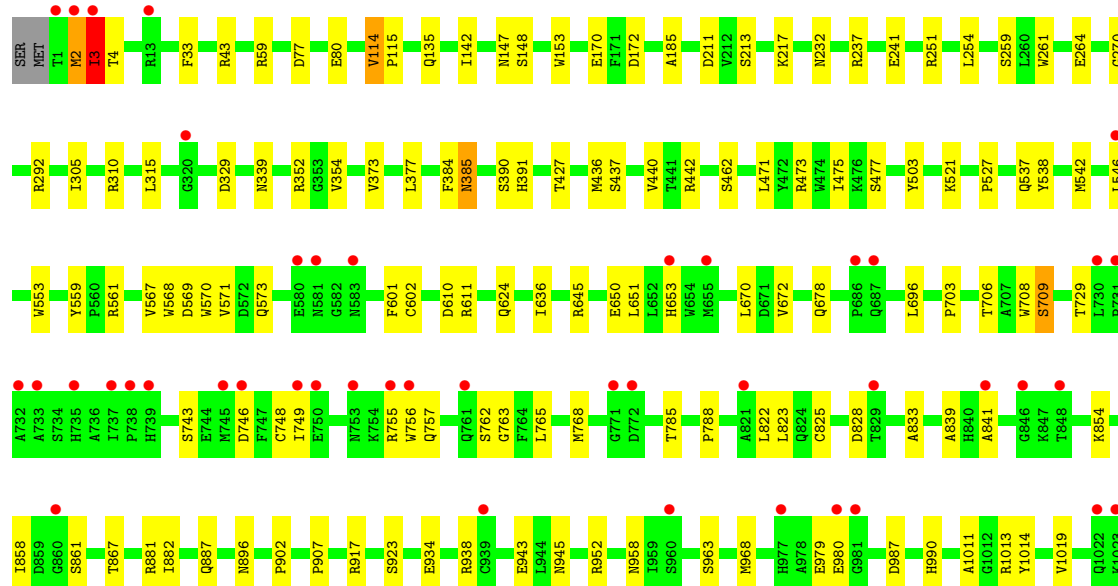
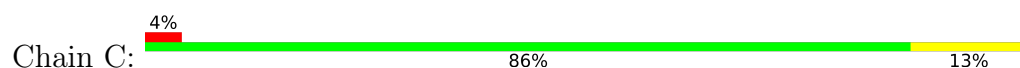


• Molecule 1: Beta-galactosidase

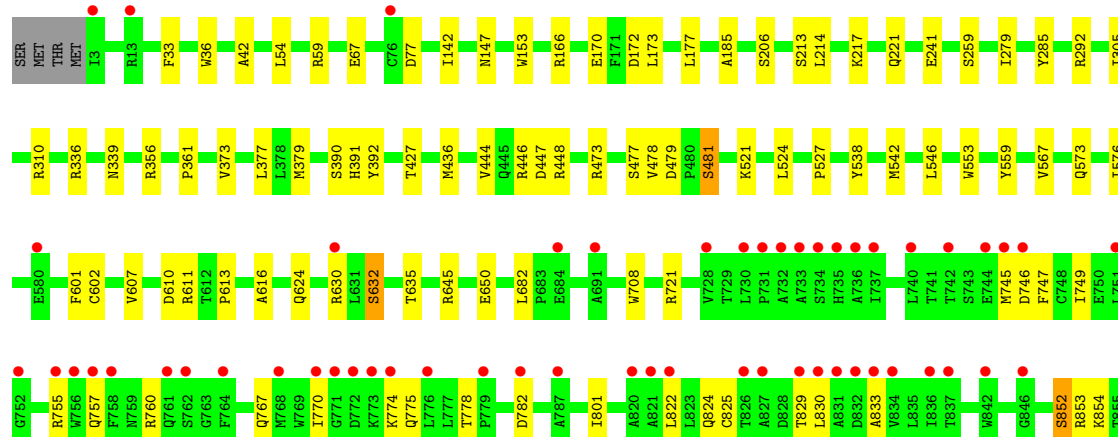
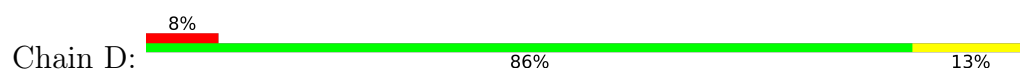


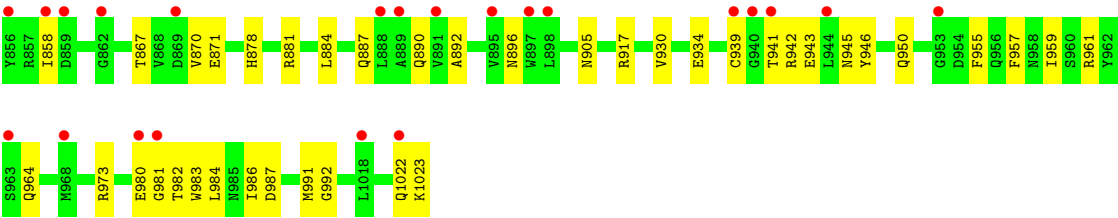


• Molecule 1: Beta-galactosidase



• Molecule 1: Beta-galactosidase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	249.83Å 85.45Å 243.31Å 90.00° 94.15° 90.00°	Depositor
Resolution (Å)	19.87 – 2.70 19.87 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.87-2.70) 99.5 (19.87-2.70)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.218 , 0.233 0.222 , 0.236	Depositor DCC
R_{free} test set	7202 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.7	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	0.91	EDS
Total number of atoms	33869	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.51% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: F6L, DMS, MG, GOL, NA

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	0.65	0/8367	0.70	0/11423
1	B	0.65	0/8329	0.70	0/11380
1	C	0.64	0/8333	0.70	0/11382
1	D	0.64	0/8348	0.71	0/11400
All	All	0.64	0/33377	0.70	0/45585

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8126	0	7703	95	0
1	B	8084	0	7608	94	0
1	C	8092	0	7614	83	0
1	D	8107	0	7675	98	0
2	A	41	0	0	1	0
2	B	41	0	0	1	0
2	C	41	0	0	3	0
2	D	41	0	0	0	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	48	0	72	4	0
5	B	40	0	60	1	0
5	C	32	0	48	1	0
5	D	32	0	48	2	0
6	B	6	0	8	0	0
7	A	293	0	0	6	0
7	B	297	0	0	6	0
7	C	281	0	0	5	0
7	D	253	0	0	7	0
All	All	33869	0	30836	363	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 6.

All (363) 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:C:352:ARG:H	1:C:385:ASN:HD21	0.91	0.89
1:C:352:ARG:H	1:C:385:ASN:ND2	1.70	0.88
1:C:352:ARG:N	1:C:385:ASN:HD21	1.73	0.85
1:A:857:ARG:HH11	1:A:859:ASP:HB3	1.48	0.79
1:D:747:PHE:CE2	1:D:760:ARG:HD3	2.19	0.77
1:A:857:ARG:NH1	1:A:859:ASP:HB3	2.01	0.76
1:C:749:ILE:HD13	1:C:858:ILE:HD13	1.67	0.76
1:B:765:LEU:HD21	1:B:768:MET:SD	2.28	0.73
1:D:887:GLN:NE2	1:D:980:GLU:O	2.22	0.72
1:C:305:ILE:HD11	1:C:645:ARG:HB3	1.71	0.72
1:D:721:ARG:NH2	7:D:1205:HOH:O	2.24	0.70
2:C:1101:F6L:C24	7:C:1248:HOH:O	2.40	0.69
1:A:356:ARG:HD2	1:A:379:MET:HE1	1.74	0.69
1:B:887:GLN:NE2	1:B:980:GLU:O	2.26	0.69
1:D:54:LEU:HD21	1:D:214:LEU:HG	1.75	0.69
1:A:887:GLN:NE2	1:A:980:GLU:O	2.27	0.68
1:B:765:LEU:HD22	1:B:864:MET:HE1	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:ILE:HD11	1:D:645:ARG:HB3	1.77	0.67
1:B:427:THR:HA	1:B:436:MET:HE1	1.77	0.67
1:D:946:TYR:OH	1:D:982:THR:HG21	1.94	0.67
1:A:653:HIS:HE2	1:A:655:MET:HE3	1.60	0.66
1:B:1013:ARG:HH21	1:B:1013:ARG:HG2	1.61	0.65
1:C:427:THR:HA	1:C:436:MET:HE1	1.78	0.65
1:D:356:ARG:HD2	1:D:379:MET:HE1	1.78	0.65
1:D:760:ARG:HG3	1:D:760:ARG:HH11	1.61	0.64
1:A:525:SER:HB2	7:A:1251:HOH:O	1.97	0.64
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.79	0.64
1:C:902:PRO:O	1:C:938:ARG:NH1	2.31	0.64
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.78	0.64
1:B:356:ARG:HD2	1:B:379:MET:HE1	1.80	0.63
1:A:161:TYR:OH	1:A:163:GLN:NE2	2.21	0.63
1:B:305:ILE:HD11	1:B:645:ARG:HB3	1.80	0.63
1:A:746:ASP:OD2	1:A:757:GLN:NE2	2.32	0.62
1:B:1013:ARG:NH1	1:D:942:ARG:HH22	1.97	0.62
1:C:887:GLN:NE2	1:C:980:GLU:O	2.28	0.62
1:B:645:ARG:NH2	1:B:650:GLU:OE1	2.32	0.62
1:D:427:THR:HA	1:D:436:MET:HE1	1.81	0.62
1:A:645:ARG:NH2	1:A:650:GLU:OE1	2.33	0.61
1:D:336:ARG:HG2	1:D:336:ARG:HH11	1.66	0.61
1:B:424:ASN:ND2	7:B:1209:HOH:O	2.34	0.61
1:D:778:THR:HG22	1:D:887:GLN:HB3	1.83	0.61
1:B:759:ASN:HB2	1:B:766:SER:OG	2.00	0.61
1:A:884:LEU:HD13	1:A:1016:TYR:OH	2.01	0.60
1:C:3:ILE:HG22	1:C:4:THR:HG23	1.82	0.60
1:D:241:GLU:HG2	1:D:292:ARG:HG2	1.83	0.60
1:D:630:ARG:NH1	7:D:1217:HOH:O	2.35	0.60
1:A:763:GLY:HA3	1:A:822:LEU:HD13	1.83	0.60
1:C:645:ARG:NH2	1:C:650:GLU:OE1	2.35	0.60
1:B:693:GLN:CD	1:B:721:ARG:HD3	2.27	0.60
1:D:645:ARG:NH2	1:D:650:GLU:OE1	2.35	0.59
1:A:251:ARG:HB2	1:A:254:LEU:HD23	1.84	0.59
1:A:503:TYR:OH	2:A:1101:F6L:O04	2.20	0.59
1:B:568:TRP:HE1	1:B:604:ASN:HD22	1.50	0.59
1:B:525:SER:HB2	7:B:1275:HOH:O	2.01	0.59
1:C:636:ILE:HD11	1:C:696:LEU:HD21	1.85	0.59
1:D:770:ILE:HD11	1:D:1022:GLN:HG2	1.85	0.59
1:C:765:LEU:HD21	1:C:768:MET:SD	2.44	0.58
1:A:59:ARG:HD3	1:A:77:ASP:OD1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:939:CYS:HA	1:B:956:GLN:HG3	1.84	0.58
1:C:672:VAL:HG12	1:C:678:GLN:HB2	1.84	0.58
1:C:785:THR:O	1:C:881:ARG:NH1	2.35	0.57
1:D:767:GLN:NE2	1:D:774:LYS:HB2	2.19	0.57
1:B:130:ASP:OD2	1:B:132:SER:HB3	2.05	0.57
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.86	0.56
1:A:656:VAL:HG12	1:A:694:LEU:HD22	1.87	0.56
1:A:1015:HIS:HB2	7:A:1216:HOH:O	2.05	0.56
1:C:881:ARG:NH2	1:C:934:GLU:OE2	2.38	0.56
1:D:767:GLN:NE2	1:D:774:LYS:HD3	2.21	0.56
1:C:503:TYR:OH	2:C:1101:F6L:O04	2.23	0.56
1:B:787:ALA:H	1:B:964:GLN:HE21	1.54	0.56
1:D:984:LEU:HD11	1:D:986:ILE:HG13	1.87	0.56
1:C:3:ILE:HG22	1:C:4:THR:N	2.21	0.55
1:C:59:ARG:HD3	1:C:77:ASP:OD2	2.06	0.55
1:A:33:PHE:CD2	1:A:217:LYS:HE3	2.42	0.55
1:D:521:LYS:HD2	1:D:559:TYR:CZ	2.42	0.55
1:D:881:ARG:HD3	1:D:987:ASP:OD1	2.06	0.55
1:C:952:ARG:HB2	1:C:1019:VAL:HG22	1.88	0.55
1:C:241:GLU:HG2	1:C:292:ARG:HG2	1.89	0.55
1:D:473:ARG:HH21	1:D:477:SER:HB2	1.72	0.55
1:B:503:TYR:OH	2:B:1101:F6L:O04	2.25	0.54
1:B:1013:ARG:CZ	1:D:942:ARG:HH22	2.19	0.54
1:D:542:MET:HE3	1:D:601:PHE:HA	1.90	0.54
1:D:770:ILE:CD1	1:D:1022:GLN:HG2	2.37	0.54
1:B:59:ARG:HD3	1:B:77:ASP:OD1	2.08	0.53
1:A:573:GLN:HB2	1:A:602:CYS:O	2.07	0.53
1:D:961:ARG:HD2	1:D:982:THR:HG22	1.91	0.53
1:D:984:LEU:CD1	1:D:986:ILE:HG13	2.38	0.53
1:B:763:GLY:HA3	1:B:822:LEU:CD1	2.39	0.53
1:B:854:LYS:HE2	7:B:1210:HOH:O	2.09	0.53
1:D:42:ALA:O	1:D:310:ARG:NH1	2.43	0.53
1:A:335:VAL:HG22	1:A:344:LEU:HD12	1.91	0.52
1:D:941:THR:HG21	1:D:957:PHE:HE1	1.74	0.52
1:A:521:LYS:HD2	1:A:559:TYR:CZ	2.44	0.52
1:A:884:LEU:CD1	1:A:1016:TYR:OH	2.56	0.52
1:C:573:GLN:HB2	1:C:602:CYS:O	2.09	0.52
1:A:823:LEU:HD11	1:A:841:ALA:HB2	1.92	0.52
1:C:251:ARG:H	1:C:254:LEU:HD12	1.75	0.52
1:D:896:ASN:HB3	1:D:945:ASN:HB2	1.92	0.52
1:B:756:TRP:CD1	1:B:768:MET:HG2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:959:ILE:HD13	1:B:984:LEU:HD13	1.91	0.51
1:D:573:GLN:HB2	1:D:602:CYS:O	2.10	0.51
1:B:310:ARG:NH1	1:B:329:ASP:OD1	2.37	0.51
1:D:775:GLN:HA	1:D:890:GLN:HE22	1.76	0.51
1:C:743:SER:HB2	1:C:746:ASP:H	1.74	0.51
1:B:573:GLN:HB2	1:B:602:CYS:O	2.09	0.51
1:A:896:ASN:HB3	1:A:945:ASN:HB2	1.92	0.51
5:D:1108:DMS:H22	7:D:1354:HOH:O	2.11	0.51
1:A:448:ARG:HD3	7:A:1320:HOH:O	2.09	0.51
1:D:172:ASP:OD2	7:D:1201:HOH:O	2.20	0.51
1:C:542:MET:HE3	1:C:601:PHE:HA	1.93	0.50
1:B:339:ASN:O	1:D:527:PRO:HB3	2.12	0.50
1:B:856:TYR:CD2	1:B:864:MET:HE2	2.47	0.50
1:B:881:ARG:NH1	1:B:987:ASP:OD2	2.44	0.50
1:C:651:LEU:HG	1:C:703:PRO:HG3	1.93	0.50
1:A:1015:HIS:H	5:A:1117:DMS:H12	1.76	0.50
1:A:930:VAL:HA	1:A:973:ARG:HD3	1.93	0.50
1:B:881:ARG:NH2	1:B:934:GLU:OE2	2.42	0.50
1:B:961:ARG:HD2	1:B:981:GLY:O	2.12	0.50
1:B:856:TYR:HD2	1:B:864:MET:HE2	1.77	0.50
1:D:444:VAL:O	1:D:448:ARG:HB2	2.11	0.50
1:D:854:LYS:HA	1:D:867:THR:O	2.12	0.50
1:B:896:ASN:HB3	1:B:945:ASN:HB2	1.94	0.50
1:A:645:ARG:HH22	1:A:650:GLU:CD	2.20	0.50
1:A:951:TRP:HD1	1:A:1018:LEU:HD21	1.77	0.50
1:A:473:ARG:NH1	1:A:476:LYS:HB2	2.26	0.50
1:C:473:ARG:NH2	1:C:477:SER:OG	2.43	0.50
1:A:881:ARG:NH2	1:A:934:GLU:OE2	2.43	0.49
1:C:114:VAL:HG13	1:C:115:PRO:HD2	1.94	0.49
1:B:950:GLN:HE22	1:B:952:ARG:HH11	1.60	0.49
1:A:934:GLU:OE2	1:A:958:ASN:ND2	2.45	0.49
1:B:37:ARG:NH1	1:B:50:GLN:HG2	2.28	0.49
1:D:905:ASN:OD1	1:D:939:CYS:HB2	2.13	0.49
1:D:546:LEU:HD22	1:D:616:ALA:HB1	1.95	0.49
1:D:610:ASP:O	1:D:611:ARG:HB2	2.13	0.49
1:A:854:LYS:HA	1:A:867:THR:O	2.13	0.49
1:B:521:LYS:HD2	1:B:559:TYR:CZ	2.47	0.49
1:D:36:TRP:HH2	5:D:1108:DMS:H23	1.78	0.49
1:D:822:LEU:HD11	1:D:824:GLN:O	2.12	0.49
1:A:352:ARG:H	1:A:385:ASN:HB2	1.77	0.49
1:A:147:ASN:HA	1:A:148:SER:HA	1.64	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:854:LYS:HA	1:B:867:THR:O	2.13	0.49
1:A:905:ASN:OD1	1:A:939:CYS:HB2	2.13	0.48
1:B:553:TRP:CZ2	1:B:624:GLN:HG2	2.48	0.48
1:C:254:LEU:HD22	1:C:315:LEU:HD11	1.95	0.48
1:A:531:ARG:O	1:A:561:ARG:NH1	2.43	0.48
1:A:251:ARG:HB2	1:A:254:LEU:CD2	2.43	0.48
1:A:292:ARG:HH12	5:A:1112:DMS:H22	1.78	0.48
1:D:775:GLN:OE1	1:D:890:GLN:NE2	2.46	0.48
1:D:852:SER:HB2	1:D:870:VAL:HG22	1.95	0.48
1:A:34:ALA:HB2	5:A:1114:DMS:C2	2.44	0.48
1:A:237:ARG:HE	1:A:296:GLU:CD	2.21	0.48
1:A:695:TRP:CH2	1:A:721:ARG:HG2	2.48	0.48
1:B:950:GLN:NE2	1:B:952:ARG:HH11	2.11	0.48
1:C:3:ILE:CG2	1:C:4:THR:N	2.77	0.48
1:A:749:ILE:O	1:A:755:ARG:HA	2.14	0.48
1:A:317:THR:OG1	1:A:319:ASP:HB2	2.14	0.48
1:A:610:ASP:O	1:A:611:ARG:HB2	2.14	0.48
1:A:546:LEU:HA	7:A:1364:HOH:O	2.14	0.47
1:A:748:CYS:O	1:A:749:ILE:HD13	2.14	0.47
1:D:941:THR:HG21	1:D:957:PHE:CE1	2.49	0.47
1:A:446:ARG:NE	1:A:447:ASP:OD1	2.47	0.47
1:A:883:GLY:HA3	1:A:987:ASP:HA	1.96	0.47
1:B:147:ASN:HA	1:B:148:SER:HA	1.65	0.47
1:C:310:ARG:NH1	1:C:329:ASP:OD1	2.42	0.47
1:C:570:TRP:CD1	1:C:571:VAL:HG22	2.50	0.47
1:B:934:GLU:HG2	1:B:964:GLN:HE22	1.79	0.47
1:C:610:ASP:O	1:C:611:ARG:HB2	2.15	0.47
1:B:749:ILE:HD12	1:B:834:VAL:HG11	1.96	0.47
1:C:896:ASN:HB3	1:C:945:ASN:HB2	1.96	0.47
1:C:561:ARG:HG3	7:C:1373:HOH:O	2.14	0.47
1:B:934:GLU:OE2	1:B:958:ASN:ND2	2.48	0.47
1:C:952:ARG:HB2	1:C:1019:VAL:CG2	2.44	0.47
1:B:787:ALA:H	1:B:964:GLN:NE2	2.13	0.47
1:C:437:SER:HB3	1:C:471:LEU:HD21	1.97	0.47
1:A:706:THR:OG1	1:A:709:SER:N	2.48	0.47
1:B:645:ARG:HH22	1:B:650:GLU:CD	2.21	0.47
1:C:917:ARG:NH2	1:C:943:GLU:OE1	2.48	0.47
1:D:645:ARG:HH22	1:D:650:GLU:CD	2.22	0.47
1:A:37:ARG:NH1	1:A:50:GLN:HG2	2.29	0.47
1:A:701:VAL:HG22	1:A:714:ILE:HD12	1.96	0.46
1:C:211:ASP:HB3	7:C:1355:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:881:ARG:NH1	1:A:987:ASP:OD2	2.48	0.46
1:B:446:ARG:NE	1:B:447:ASP:OD1	2.45	0.46
1:C:854:LYS:HA	1:C:867:THR:O	2.14	0.46
1:B:166:ARG:HG3	1:B:392:TYR:HB2	1.96	0.46
1:B:619:GLU:HA	1:B:912:ALA:HB2	1.96	0.46
1:C:788:PRO:HD2	1:C:968:MET:HG3	1.96	0.46
1:D:166:ARG:HG3	1:D:392:TYR:HB2	1.97	0.46
1:D:746:ASP:CG	1:D:757:GLN:HE21	2.23	0.46
1:C:264:GLU:O	1:C:264:GLU:HG3	2.14	0.46
1:A:527:PRO:HB3	1:C:339:ASN:O	2.16	0.46
1:C:763:GLY:HA3	1:C:822:LEU:HD22	1.96	0.46
1:D:59:ARG:HD3	1:D:77:ASP:OD2	2.15	0.46
1:D:632:SER:O	1:D:635:THR:OG1	2.33	0.46
1:D:917:ARG:NH2	1:D:943:GLU:OE1	2.48	0.46
1:A:754:LYS:NZ	1:A:1022:GLN:OE1	2.47	0.46
1:C:147:ASN:HA	1:C:148:SER:HA	1.66	0.46
1:A:331:GLY:H	5:A:1110:DMS:H21	1.78	0.46
1:D:941:THR:OG1	1:D:955:PHE:O	2.31	0.46
1:A:942:ARG:HH12	1:C:1013:ARG:NH2	2.14	0.46
1:B:361:PRO:HB2	1:B:576:ILE:HG12	1.97	0.46
1:C:706:THR:OG1	1:C:709:SER:N	2.48	0.46
1:C:756:TRP:CD1	1:C:768:MET:HG2	2.51	0.46
1:D:749:ILE:O	1:D:755:ARG:HA	2.16	0.46
1:A:153:TRP:HB2	1:A:185:ALA:HB3	1.97	0.46
1:B:33:PHE:CD2	1:B:217:LYS:HE3	2.51	0.46
1:B:352:ARG:H	1:B:385:ASN:HB2	1.81	0.46
1:A:788:PRO:HD2	1:A:968:MET:HG3	1.98	0.46
1:D:361:PRO:HB2	1:D:576:ILE:HG13	1.97	0.46
1:D:945:ASN:ND2	1:D:950:GLN:HG3	2.31	0.46
1:A:42:ALA:O	1:A:310:ARG:NH1	2.46	0.45
1:A:521:LYS:O	7:A:1201:HOH:O	2.21	0.45
1:B:610:ASP:O	1:B:611:ARG:HB2	2.15	0.45
1:B:651:LEU:CD1	1:B:703:PRO:HG3	2.47	0.45
1:C:934:GLU:OE2	1:C:958:ASN:ND2	2.49	0.45
1:D:279:ILE:HD12	1:D:285:TYR:CD2	2.51	0.45
1:A:619:GLU:HA	1:A:912:ALA:HB2	1.99	0.45
1:A:103:VAL:HG22	1:A:418:HIS:CE1	2.52	0.45
1:B:749:ILE:O	1:B:755:ARG:HA	2.16	0.45
1:B:907:PRO:HG2	1:B:990:HIS:O	2.17	0.45
1:A:693:GLN:HE21	1:A:724:GLU:HB2	1.82	0.45
1:C:442:ARG:NH2	7:C:1231:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:749:ILE:O	1:C:755:ARG:HA	2.16	0.45
1:D:221:GLN:OE1	7:D:1202:HOH:O	2.21	0.45
1:D:822:LEU:HD21	1:D:825:CYS:HB2	1.97	0.45
1:B:153:TRP:HB2	1:B:185:ALA:HB3	1.98	0.45
1:B:538:TYR:O	1:B:567:VAL:HA	2.17	0.45
1:D:356:ARG:HD2	1:D:379:MET:CE	2.46	0.45
1:D:153:TRP:HB2	1:D:185:ALA:HB3	1.99	0.45
1:D:760:ARG:HG3	1:D:760:ARG:NH1	2.30	0.45
1:A:538:TYR:O	1:A:567:VAL:HA	2.17	0.45
1:A:780:LEU:HD22	1:A:1020:TRP:HZ3	1.81	0.45
1:A:830:LEU:HB2	1:C:828:ASP:OD1	2.17	0.45
1:B:930:VAL:HA	1:B:973:ARG:HD3	1.98	0.45
1:C:373:VAL:O	1:C:377:LEU:HG	2.17	0.45
1:D:991:MET:HG2	1:D:992:GLY:O	2.17	0.45
1:A:241:GLU:HG2	1:A:292:ARG:HG2	2.00	0.44
1:A:553:TRP:CZ2	1:A:624:GLN:HG2	2.52	0.44
5:B:1113:DMS:H12	7:B:1448:HOH:O	2.16	0.44
1:C:670:LEU:HD23	1:C:670:LEU:HA	1.83	0.44
1:B:883:GLY:HA3	1:B:987:ASP:HA	1.99	0.44
1:C:33:PHE:CD2	1:C:217:LYS:HE3	2.52	0.44
1:C:172:ASP:OD2	7:C:1201:HOH:O	2.20	0.44
1:A:765:LEU:HD21	1:A:768:MET:SD	2.57	0.44
1:C:521:LYS:HD2	1:C:559:TYR:CZ	2.52	0.44
1:C:645:ARG:HH22	1:C:650:GLU:CD	2.25	0.44
1:C:822:LEU:HD21	1:C:825:CYS:HB2	2.00	0.44
1:B:542:MET:HE3	1:B:601:PHE:HA	2.00	0.44
1:C:270:GLY:HA3	5:C:1108:DMS:H13	1.98	0.44
1:C:963:SER:HB3	1:C:979:GLU:OE2	2.18	0.44
1:B:103:VAL:HG22	1:B:418:HIS:CE1	2.53	0.44
1:A:907:PRO:HG2	1:A:990:HIS:O	2.18	0.44
1:B:352:ARG:HG2	1:B:553:TRP:CH2	2.53	0.44
1:D:67:GLU:OE1	7:D:1203:HOH:O	2.21	0.44
1:B:556:PHE:O	7:B:1201:HOH:O	2.20	0.44
1:B:950:GLN:NE2	1:B:952:ARG:NH1	2.66	0.44
1:B:917:ARG:NH2	1:B:943:GLU:OE1	2.51	0.43
1:D:782:ASP:HA	1:D:884:LEU:HD23	2.00	0.43
1:A:166:ARG:HG3	1:A:392:TYR:HB2	2.00	0.43
1:B:527:PRO:HB3	1:D:339:ASN:O	2.17	0.43
1:C:390:SER:HA	1:C:391:HIS:HA	1.81	0.43
1:D:778:THR:HG22	1:D:887:GLN:CB	2.48	0.43
1:D:479:ASP:OD1	1:D:481:SER:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:745:MET:O	1:D:760:ARG:HB2	2.18	0.43
1:B:390:SER:HA	1:B:391:HIS:HA	1.81	0.43
1:D:279:ILE:HD12	1:D:285:TYR:CE2	2.53	0.43
1:A:258:VAL:HG23	1:A:291:LEU:HD13	2.01	0.43
1:B:43:ARG:HD2	1:B:261:TRP:CD2	2.53	0.43
1:B:748:CYS:O	1:B:749:ILE:HD13	2.19	0.43
1:C:538:TYR:O	1:C:567:VAL:HA	2.19	0.43
1:A:794:GLY:HA3	7:A:1323:HOH:O	2.17	0.43
1:D:930:VAL:HA	1:D:973:ARG:HD3	1.99	0.43
1:C:153:TRP:HB2	1:C:185:ALA:HB3	1.99	0.43
1:D:892:ALA:HB3	1:D:946:TYR:CE1	2.54	0.43
1:A:84:VAL:HG13	1:A:93:HIS:CE1	2.54	0.43
1:B:167:LEU:HD23	1:B:167:LEU:HA	1.92	0.43
1:B:531:ARG:O	1:B:561:ARG:NH1	2.46	0.43
1:B:636:ILE:HD13	1:B:698:VAL:HG11	2.00	0.43
1:B:670:LEU:HD12	1:B:670:LEU:HA	1.78	0.43
1:B:959:ILE:HD12	1:B:983:TRP:O	2.18	0.43
1:C:142:ILE:HG12	1:C:170:GLU:HG2	2.00	0.43
1:C:823:LEU:HD11	1:C:841:ALA:HB2	2.01	0.43
1:D:538:TYR:O	1:D:567:VAL:HA	2.19	0.43
1:B:142:ILE:HG12	1:B:170:GLU:HG2	2.00	0.42
1:C:553:TRP:CZ2	1:C:624:GLN:HG2	2.54	0.42
1:D:630:ARG:HA	1:D:630:ARG:HD2	1.64	0.42
1:A:134:LEU:HA	1:A:134:LEU:HD23	1.81	0.42
1:B:3:ILE:HG23	1:B:4:THR:H	1.84	0.42
1:B:442:ARG:HD3	7:B:1344:HOH:O	2.18	0.42
1:D:878:HIS:HA	7:D:1333:HOH:O	2.20	0.42
1:D:934:GLU:HG2	1:D:964:GLN:HE22	1.83	0.42
1:A:833:ALA:HB1	1:A:858:ILE:O	2.19	0.42
1:D:142:ILE:HG12	1:D:170:GLU:HG2	2.02	0.42
1:C:653:HIS:CD2	1:C:653:HIS:N	2.88	0.42
1:D:336:ARG:HH11	1:D:336:ARG:CG	2.32	0.42
1:A:749:ILE:CD1	1:A:834:VAL:HG11	2.49	0.42
1:B:356:ARG:HD2	1:B:379:MET:CE	2.49	0.42
1:B:568:TRP:CD2	1:B:569:ASP:HB3	2.55	0.42
1:C:907:PRO:HG2	1:C:990:HIS:O	2.19	0.42
1:A:917:ARG:NH2	1:A:943:GLU:OE1	2.53	0.42
1:B:782:ASP:OD2	1:B:854:LYS:NZ	2.50	0.42
1:D:778:THR:HG21	1:D:983:TRP:CH2	2.55	0.42
1:D:373:VAL:O	1:D:377:LEU:HG	2.19	0.42
1:C:833:ALA:HB1	1:C:858:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:746:ASP:OD2	1:D:757:GLN:NE2	2.44	0.41
1:D:853:ARG:NH1	1:D:871:GLU:OE1	2.44	0.41
1:B:882:ILE:HG13	1:B:1009:LEU:HD13	2.02	0.41
1:C:748:CYS:SG	1:C:757:GLN:HG3	2.60	0.41
1:D:833:ALA:HB1	1:D:858:ILE:O	2.20	0.41
1:A:693:GLN:HE22	1:A:721:ARG:HB3	1.85	0.41
1:C:43:ARG:HD2	1:C:261:TRP:CD2	2.56	0.41
1:D:881:ARG:NH2	1:D:934:GLU:CG	2.83	0.41
1:A:43:ARG:HD2	1:A:261:TRP:CD2	2.55	0.41
1:A:663:LEU:HD12	1:A:694:LEU:HD21	2.02	0.41
1:B:347:LYS:HA	1:B:348:PRO:HD3	1.94	0.41
1:B:697:THR:OG1	1:B:719:GLN:OE1	2.31	0.41
1:B:1013:ARG:HH21	1:B:1013:ARG:CG	2.32	0.41
1:D:553:TRP:CZ2	1:D:624:GLN:HG2	2.55	0.41
1:D:961:ARG:NE	1:D:981:GLY:O	2.54	0.41
1:A:473:ARG:HH11	1:A:476:LYS:HB2	1.86	0.41
1:C:354:VAL:HB	1:C:384:PHE:CE1	2.55	0.41
1:C:440:VAL:HG13	1:C:475:ILE:HD11	2.03	0.41
1:C:822:LEU:HD12	1:C:839:ALA:O	2.20	0.41
1:A:339:ASN:O	1:C:527:PRO:HB3	2.20	0.41
1:A:701:VAL:HG22	1:A:714:ILE:CD1	2.51	0.41
1:B:525:SER:HB3	1:D:524:LEU:HB3	2.02	0.41
1:B:830:LEU:HD21	1:D:830:LEU:HD21	2.03	0.41
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.56	0.41
1:D:607:VAL:HG12	1:D:613:PRO:HA	2.02	0.41
1:A:448:ARG:NH2	1:A:478:VAL:HG13	2.36	0.41
1:B:54:LEU:HD11	1:B:214:LEU:HG	2.02	0.41
1:B:632:SER:O	1:B:635:THR:HG22	2.20	0.41
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.55	0.41
1:A:612:THR:HA	1:A:613:PRO:HD3	1.97	0.41
1:A:824:GLN:HB3	1:A:839:ALA:HB3	2.03	0.41
1:C:537:GLN:NE2	2:C:1101:F6L:O03	2.52	0.41
1:C:881:ARG:HD3	1:C:987:ASP:OD1	2.21	0.41
1:D:390:SER:HA	1:D:391:HIS:HA	1.79	0.41
1:A:767:GLN:HA	1:A:776:LEU:HD12	2.02	0.41
1:B:554:GLN:C	1:B:554:GLN:CD	2.89	0.41
1:B:1013:ARG:HG2	1:B:1013:ARG:NH2	2.30	0.41
1:C:232:ASN:ND2	1:C:237:ARG:HG2	2.36	0.41
1:D:446:ARG:NE	1:D:447:ASP:OD1	2.53	0.41
1:D:521:LYS:HD2	1:D:559:TYR:CE1	2.55	0.41
1:D:1023:LYS:HE2	1:D:1023:LYS:HB3	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ARG:HD2	1:A:379:MET:CE	2.47	0.40
1:A:1011:ALA:HB3	1:A:1014:TYR:CZ	2.57	0.40
1:D:427:THR:HA	1:D:436:MET:CE	2.50	0.40
1:D:33:PHE:CD2	1:D:217:LYS:HE3	2.55	0.40
1:A:653:HIS:NE2	1:A:655:MET:HE3	2.33	0.40
1:D:147:ASN:HB3	1:D:206:SER:HA	2.02	0.40
1:D:173:LEU:HB3	1:D:177:LEU:HD13	2.04	0.40
1:D:682:LEU:HD23	1:D:682:LEU:HA	1.90	0.40
1:A:568:TRP:CD2	1:A:569:ASP:HB3	2.56	0.40
1:A:754:LYS:HZ2	1:A:754:LYS:HG2	1.53	0.40
1:A:390:SER:HA	1:A:391:HIS:HA	1.80	0.40
1:B:693:GLN:HG2	1:B:695:TRP:NE1	2.36	0.40
1:B:757:GLN:NE2	1:B:769:TRP:HH2	2.20	0.40
1:B:760:ARG:HE	1:B:760:ARG:HB3	1.71	0.40
1:B:1013:ARG:CG	1:B:1013:ARG:NH2	2.84	0.40
1:C:427:THR:HA	1:C:436:MET:CE	2.49	0.40
1:C:427:THR:HG21	1:C:462:SER:HB3	2.02	0.40
1:D:959:ILE:HG13	1:D:984:LEU:HD23	2.03	0.40

There are no symmetry-related clashes.

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	1019/1025 (99%)	977 (96%)	40 (4%)	2 (0%)	43	68
1	B	1020/1025 (100%)	978 (96%)	42 (4%)	0	100	100
1	C	1021/1025 (100%)	977 (96%)	42 (4%)	2 (0%)	43	68
1	D	1019/1025 (99%)	975 (96%)	44 (4%)	0	100	100
All	All	4079/4100 (100%)	3907 (96%)	168 (4%)	4 (0%)	48	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	3	ILE
1	A	722	LEU
1	C	2	MET
1	A	201	ASP

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	857/877 (98%)	845 (99%)	12 (1%)	59	82
1	B	844/877 (96%)	831 (98%)	13 (2%)	57	81
1	C	843/877 (96%)	828 (98%)	15 (2%)	51	78
1	D	851/877 (97%)	843 (99%)	8 (1%)	70	87
All	All	3395/3508 (97%)	3347 (99%)	48 (1%)	59	82

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	VAL
1	A	130	ASP
1	A	213	SER
1	A	259	SER
1	A	269	SER
1	A	344	LEU
1	A	478	VAL
1	A	554	GLN
1	A	651	LEU
1	A	679	LEU
1	A	729	THR
1	A	923	SER
1	B	128	ASN
1	B	213	SER
1	B	423	MET
1	B	478	VAL
1	B	525	SER
1	B	546	LEU

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Mol	Chain	Res	Type
1	B	630	ARG
1	B	743	SER
1	B	766	SER
1	B	822	LEU
1	B	874	SER
1	B	923	SER
1	B	1013	ARG
1	C	2	MET
1	C	3	ILE
1	C	80	GLU
1	C	114	VAL
1	C	135	GLN
1	C	213	SER
1	C	259	SER
1	C	385	ASN
1	C	546	LEU
1	C	709	SER
1	C	729	THR
1	C	762	SER
1	C	861	SER
1	C	882	ILE
1	C	923	SER
1	D	213	SER
1	D	259	SER
1	D	478	VAL
1	D	481	SER
1	D	632	SER
1	D	801	ILE
1	D	829	THR
1	D	852	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	460	ASN
1	A	634	GLN
1	A	687	GLN
1	A	693	GLN
1	A	702	GLN
1	A	761	GLN
1	A	843	GLN
1	B	93	HIS

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Mol	Chain	Res	Type
1	B	128	ASN
1	B	460	ASN
1	B	583	ASN
1	B	624	GLN
1	B	704	ASN
1	B	824	GLN
1	B	950	GLN
1	B	956	GLN
1	B	964	GLN
1	B	1015	HIS
1	C	12	GLN
1	C	49	GLN
1	C	163	GLN
1	C	339	ASN
1	C	385	ASN
1	C	653	HIS
1	C	704	ASN
1	C	844	HIS
1	C	878	HIS
1	C	1022	GLN
1	D	50	GLN
1	D	163	GLN
1	D	363	HIS
1	D	460	ASN
1	D	554	GLN
1	D	614	HIS
1	D	624	GLN
1	D	634	GLN
1	D	890	GLN
1	D	945	ASN
1	D	950	GLN
1	D	965	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 57 ligands modelled in this entry, 14 are monoatomic - leaving 43 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	DMS	B	1105	-	3,3,3	0.34	0	3,3,3	0.72	0
5	DMS	A	1116	-	3,3,3	0.23	0	3,3,3	0.78	0
5	DMS	A	1112	-	3,3,3	0.21	0	3,3,3	1.02	0
5	DMS	D	1106	-	3,3,3	0.33	0	3,3,3	0.85	0
2	F6L	A	1101	3,4	45,45,45	2.39	9 (20%)	65,66,66	2.58	31 (47%)
2	F6L	C	1101	3,4	45,45,45	2.26	10 (22%)	65,66,66	2.36	26 (40%)
5	DMS	D	1107	-	3,3,3	0.29	0	3,3,3	0.88	0
5	DMS	C	1107	-	3,3,3	0.27	0	3,3,3	0.93	0
5	DMS	B	1106	-	3,3,3	0.31	0	3,3,3	0.75	0
5	DMS	B	1111	-	3,3,3	0.25	0	3,3,3	0.76	0
5	DMS	D	1110	-	3,3,3	0.32	0	3,3,3	0.52	0
5	DMS	C	1113	-	3,3,3	0.29	0	3,3,3	0.67	0
2	F6L	B	1101	3,4	45,45,45	2.40	10 (22%)	65,66,66	2.51	27 (41%)
5	DMS	C	1108	-	3,3,3	0.38	0	3,3,3	0.71	0
5	DMS	A	1115	-	3,3,3	0.26	0	3,3,3	0.82	0
5	DMS	B	1110	-	3,3,3	0.37	0	3,3,3	0.75	0
5	DMS	A	1113	-	3,3,3	0.37	0	3,3,3	0.81	0
5	DMS	C	1111	-	3,3,3	0.36	0	3,3,3	0.79	0
5	DMS	D	1108	-	3,3,3	0.19	0	3,3,3	0.80	0
5	DMS	A	1107	-	3,3,3	0.30	0	3,3,3	0.88	0
5	DMS	A	1109	-	3,3,3	0.28	0	3,3,3	0.72	0
5	DMS	A	1106	-	3,3,3	0.33	0	3,3,3	1.03	0
5	DMS	D	1109	-	3,3,3	0.28	0	3,3,3	0.63	0
5	DMS	B	1104	-	3,3,3	0.25	0	3,3,3	0.80	0
5	DMS	C	1106	-	3,3,3	0.22	0	3,3,3	1.04	0
5	DMS	A	1117	-	3,3,3	0.43	0	3,3,3	0.95	0
5	DMS	B	1107	-	3,3,3	0.16	0	3,3,3	1.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	B	1109	-	3,3,3	0.31	0	3,3,3	0.53	0
5	DMS	A	1108	-	3,3,3	0.36	0	3,3,3	1.08	0
2	F6L	D	1101	3,4	45,45,45	2.41	10 (22%)	65,66,66	2.85	28 (43%)
5	DMS	A	1111	-	3,3,3	0.33	0	3,3,3	0.79	0
5	DMS	D	1112	-	3,3,3	0.35	0	3,3,3	0.67	0
6	GOL	B	1114	-	5,5,5	0.30	0	5,5,5	0.45	0
5	DMS	B	1112	-	3,3,3	0.32	0	3,3,3	0.80	0
5	DMS	B	1113	-	3,3,3	0.48	0	3,3,3	0.50	0
5	DMS	A	1110	-	3,3,3	0.32	0	3,3,3	0.74	0
5	DMS	C	1109	-	3,3,3	0.31	0	3,3,3	0.86	0
5	DMS	C	1112	-	3,3,3	0.28	0	3,3,3	0.80	0
5	DMS	D	1113	-	3,3,3	0.29	0	3,3,3	0.84	0
5	DMS	D	1111	-	3,3,3	0.32	0	3,3,3	0.81	0
5	DMS	A	1114	-	3,3,3	0.37	0	3,3,3	0.87	0
5	DMS	C	1110	-	3,3,3	0.18	0	3,3,3	0.77	0
5	DMS	B	1108	-	3,3,3	0.36	0	3,3,3	0.73	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	F6L	C	1101	3,4	-	9/19/59/59	0/5/5/5
2	F6L	D	1101	3,4	-	11/19/59/59	0/5/5/5
6	GOL	B	1114	-	-	0/4/4/4	-
2	F6L	B	1101	3,4	-	13/19/59/59	0/5/5/5
2	F6L	A	1101	3,4	-	14/19/59/59	0/5/5/5

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1101	F6L	C22-C17	10.80	1.54	1.39
2	B	1101	F6L	C22-C17	10.60	1.53	1.39
2	A	1101	F6L	C22-C17	10.50	1.53	1.39
2	C	1101	F6L	C22-C17	9.92	1.52	1.39
2	D	1101	F6L	C21-C22	7.04	1.53	1.38
2	B	1101	F6L	C21-C22	7.01	1.53	1.38
2	A	1101	F6L	C21-C22	6.94	1.53	1.38
2	C	1101	F6L	C21-C22	6.65	1.52	1.38
2	A	1101	F6L	C07-C11	-3.23	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	F6L	C07-C11	-2.95	1.46	1.53
2	A	1101	F6L	C15-N01	2.85	1.43	1.35
2	B	1101	F6L	C15-N01	2.78	1.42	1.35
2	C	1101	F6L	C16-C17	-2.76	1.33	1.38
2	A	1101	F6L	C28-C29	2.67	1.43	1.39
2	C	1101	F6L	C07-C11	-2.66	1.47	1.53
2	C	1101	F6L	C15-N01	2.61	1.42	1.35
2	D	1101	F6L	C15-N01	2.58	1.42	1.35
2	B	1101	F6L	C16-C17	-2.56	1.34	1.38
2	B	1101	F6L	C28-C29	2.55	1.43	1.39
2	D	1101	F6L	C16-C17	-2.48	1.34	1.38
2	B	1101	F6L	O05-C09	2.46	1.48	1.43
2	D	1101	F6L	C18-C17	2.45	1.55	1.51
2	A	1101	F6L	O05-C09	2.43	1.48	1.43
2	D	1101	F6L	C07-C11	-2.42	1.47	1.53
2	D	1101	F6L	O01-C10	2.40	1.44	1.41
2	A	1101	F6L	O01-C04	-2.33	1.33	1.38
2	B	1101	F6L	O02-C10	2.32	1.47	1.41
2	B	1101	F6L	O01-C04	-2.28	1.33	1.38
2	D	1101	F6L	O07-C32	-2.27	1.23	1.30
2	A	1101	F6L	C16-C17	-2.26	1.34	1.38
2	C	1101	F6L	O07-C32	-2.24	1.23	1.30
2	C	1101	F6L	C05-C04	2.22	1.43	1.38
2	D	1101	F6L	O02-C10	2.22	1.47	1.41
2	D	1101	F6L	C30-C29	2.16	1.43	1.39
2	B	1101	F6L	C29-C32	2.11	1.53	1.49
2	C	1101	F6L	O05-C09	2.08	1.47	1.43
2	C	1101	F6L	C30-C29	2.08	1.42	1.39
2	C	1101	F6L	C28-C29	2.08	1.42	1.39
2	A	1101	F6L	C30-C29	2.05	1.42	1.39

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1101	F6L	C26-C25-N01	12.19	131.30	113.02
2	A	1101	F6L	C04-O01-C10	7.43	128.68	117.79
2	D	1101	F6L	C04-O01-C10	7.02	128.09	117.79
2	D	1101	F6L	C25-N01-C16	6.45	134.57	124.35
2	C	1101	F6L	C09-C08-C07	6.42	122.03	110.82
2	B	1101	F6L	C04-O01-C10	5.92	126.47	117.79
2	D	1101	F6L	C18-C15-N01	-5.88	100.94	109.04
2	A	1101	F6L	O02-C10-C09	5.86	122.75	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	F6L	C09-C08-C07	5.83	121.00	110.82
2	B	1101	F6L	O02-C10-C09	5.81	122.65	110.35
2	A	1101	F6L	C09-C08-C07	5.74	120.85	110.82
2	B	1101	F6L	O02-C11-C07	-5.44	99.81	109.69
2	A	1101	F6L	O02-C11-C07	-5.18	100.29	109.69
2	C	1101	F6L	O02-C10-C09	5.13	121.21	110.35
2	C	1101	F6L	C26-C25-N01	5.11	120.67	113.02
2	A	1101	F6L	C26-C25-N01	5.08	120.64	113.02
2	C	1101	F6L	C04-O01-C10	5.07	125.23	117.79
2	C	1101	F6L	O05-C09-C08	4.91	121.69	110.35
2	B	1101	F6L	C26-C25-N01	4.74	120.13	113.02
2	C	1101	F6L	O02-C11-C07	-4.63	101.28	109.69
2	B	1101	F6L	C06-C01-C02	4.62	124.47	117.64
2	A	1101	F6L	C06-C01-C02	4.54	124.36	117.64
2	B	1101	F6L	O05-C09-C08	4.34	120.37	110.35
2	C	1101	F6L	C06-C01-C02	4.33	124.05	117.64
2	D	1101	F6L	O02-C11-C12	4.29	117.11	106.44
2	A	1101	F6L	O05-C09-C08	4.25	120.17	110.35
2	B	1101	F6L	C05-C04-C03	4.10	126.50	120.18
2	A	1101	F6L	C05-C04-C03	4.08	126.47	120.18
2	D	1101	F6L	C09-C08-C07	3.96	117.73	110.82
2	B	1101	F6L	C20-C19-C16	3.94	125.32	118.61
2	C	1101	F6L	C05-C04-C03	3.82	126.06	120.18
2	D	1101	F6L	O02-C10-C09	3.70	118.18	110.35
2	A	1101	F6L	C20-C19-C16	3.66	124.84	118.61
2	D	1101	F6L	O02-C11-C07	-3.62	103.13	109.69
2	D	1101	F6L	C20-C19-C16	3.59	124.72	118.61
2	A	1101	F6L	C25-N01-C16	3.57	130.00	124.35
2	D	1101	F6L	O02-C10-O01	3.53	117.27	108.29
2	C	1101	F6L	O04-C08-C09	-3.50	102.25	110.35
2	B	1101	F6L	C25-N01-C16	3.49	129.88	124.35
2	B	1101	F6L	O02-C10-O01	3.46	117.09	108.29
2	D	1101	F6L	C17-C18-C15	-3.42	96.17	101.17
2	C	1101	F6L	C20-C19-C16	3.34	124.30	118.61
2	B	1101	F6L	C18-C15-N01	-3.29	104.50	109.04
2	B	1101	F6L	C08-C07-C11	3.29	116.10	110.24
2	A	1101	F6L	C23-C18-C17	3.25	115.47	110.53
2	B	1101	F6L	O04-C08-C09	-3.21	102.92	110.35
2	D	1101	F6L	C12-C11-C07	-3.20	105.52	113.00
2	A	1101	F6L	O02-C11-C12	3.19	114.37	106.44
2	A	1101	F6L	C12-C11-C07	-3.18	105.56	113.00
2	C	1101	F6L	C21-C22-C17	-3.17	114.19	119.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	F6L	O02-C11-C12	3.17	114.31	106.44
2	A	1101	F6L	O02-C10-O01	3.15	116.30	108.29
2	A	1101	F6L	C08-C07-C11	3.12	115.81	110.24
2	D	1101	F6L	C06-C01-C02	2.99	122.07	117.64
2	C	1101	F6L	C25-N01-C16	2.99	129.09	124.35
2	A	1101	F6L	C21-C22-C17	-2.98	114.54	119.96
2	B	1101	F6L	C19-C16-C17	-2.97	119.58	123.20
2	C	1101	F6L	C23-C18-C17	2.89	114.93	110.53
2	D	1101	F6L	O01-C10-C09	2.87	111.30	107.14
2	D	1101	F6L	C23-C18-C17	2.84	114.85	110.53
2	C	1101	F6L	C06-C05-C04	-2.79	116.33	119.73
2	C	1101	F6L	C03-C02-C01	-2.78	117.63	121.25
2	A	1101	F6L	C03-C02-C01	-2.74	117.67	121.25
2	B	1101	F6L	C21-C22-C17	-2.74	114.98	119.96
2	C	1101	F6L	O04-C08-C07	-2.73	104.05	110.35
2	A	1101	F6L	C18-C15-N01	-2.71	105.31	109.04
2	A	1101	F6L	C06-C05-C04	-2.71	116.42	119.73
2	D	1101	F6L	C18-C15-C14	2.70	133.82	128.94
2	D	1101	F6L	C16-N01-C15	-2.70	107.82	111.18
2	A	1101	F6L	C24-C18-C17	-2.69	106.45	110.53
2	D	1101	F6L	C21-C22-C17	-2.67	115.10	119.96
2	B	1101	F6L	C03-C02-C01	-2.67	117.76	121.25
2	B	1101	F6L	C05-C06-C01	-2.64	117.80	121.25
2	A	1101	F6L	O04-C08-C07	-2.61	104.31	110.35
2	C	1101	F6L	C14-C15-N01	2.59	125.84	121.61
2	D	1101	F6L	C25-C26-C27	-2.56	115.78	120.58
2	C	1101	F6L	O02-C11-C12	2.55	112.79	106.44
2	B	1101	F6L	C06-C05-C04	-2.53	116.64	119.73
2	C	1101	F6L	C18-C15-N01	-2.52	105.56	109.04
2	C	1101	F6L	C24-C18-C17	-2.52	106.71	110.53
2	C	1101	F6L	O02-C10-O01	2.51	114.68	108.29
2	D	1101	F6L	C05-C04-C03	2.51	124.04	120.18
2	B	1101	F6L	O01-C04-C03	-2.50	107.77	119.93
2	D	1101	F6L	C23-C18-C15	2.49	116.45	111.37
2	A	1101	F6L	C19-C16-C17	-2.48	120.18	123.20
2	A	1101	F6L	C05-C06-C01	-2.47	118.03	121.25
2	D	1101	F6L	C17-C16-N01	-2.43	106.27	108.59
2	A	1101	F6L	O01-C04-C03	-2.40	108.26	119.93
2	B	1101	F6L	C02-C03-C04	-2.39	116.81	119.73
2	C	1101	F6L	C19-C16-C17	-2.33	120.35	123.20
2	C	1101	F6L	O01-C04-C03	-2.32	108.66	119.93
2	C	1101	F6L	C18-C17-C16	2.31	112.12	109.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	F6L	C16-N01-C15	-2.30	108.31	111.18
2	B	1101	F6L	C14-C15-N01	2.26	125.31	121.61
2	C	1101	F6L	C22-C17-C18	-2.26	127.49	130.65
2	A	1101	F6L	C18-C17-C16	2.26	112.06	109.49
2	C	1101	F6L	C05-C06-C01	-2.26	118.30	121.25
2	D	1101	F6L	C25-C26-C31	2.24	124.80	120.58
2	D	1101	F6L	C03-C02-C01	-2.21	118.37	121.25
2	A	1101	F6L	C02-C03-C04	-2.20	117.04	119.73
2	D	1101	F6L	O04-C08-C09	-2.20	105.26	110.35
2	B	1101	F6L	C24-C18-C17	-2.20	107.20	110.53
2	B	1101	F6L	O04-C08-C07	-2.19	105.28	110.35
2	A	1101	F6L	O06-C12-C11	2.18	118.78	111.29
2	D	1101	F6L	C19-C16-C17	-2.17	120.56	123.20
2	D	1101	F6L	C08-C07-C11	2.13	114.03	110.24
2	A	1101	F6L	C17-C18-C15	-2.12	98.06	101.17
2	A	1101	F6L	C23-C18-C15	2.12	115.69	111.37
2	D	1101	F6L	C14-C15-N01	2.12	125.06	121.61
2	B	1101	F6L	C16-N01-C15	-2.05	108.62	111.18
2	B	1101	F6L	C18-C17-C16	2.05	111.83	109.49
2	A	1101	F6L	C14-C15-N01	2.01	124.89	121.61

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	F6L	C13-C14-C15-N01
2	A	1101	F6L	C09-C10-O01-C04
2	B	1101	F6L	C13-C14-C15-N01
2	B	1101	F6L	C09-C10-O01-C04
2	C	1101	F6L	C13-C14-C15-N01
2	C	1101	F6L	C09-C10-O01-C04
2	D	1101	F6L	C26-C25-N01-C15
2	D	1101	F6L	C26-C25-N01-C16
2	D	1101	F6L	C09-C10-O01-C04
2	D	1101	F6L	C30-C29-C32-O08
2	D	1101	F6L	C28-C29-C32-O07
2	D	1101	F6L	C28-C29-C32-O08
2	D	1101	F6L	C30-C29-C32-O07
2	C	1101	F6L	C28-C29-C32-O07
2	C	1101	F6L	C28-C29-C32-O08
2	C	1101	F6L	C30-C29-C32-O07
2	C	1101	F6L	C30-C29-C32-O08

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Mol	Chain	Res	Type	Atoms
2	D	1101	F6L	C01-C13-C14-C15
2	B	1101	F6L	C28-C29-C32-O08
2	B	1101	F6L	C28-C29-C32-O07
2	B	1101	F6L	C30-C29-C32-O08
2	D	1101	F6L	O02-C11-C12-O06
2	B	1101	F6L	C30-C29-C32-O07
2	D	1101	F6L	C07-C11-C12-O06
2	A	1101	F6L	C13-C14-C15-C18
2	B	1101	F6L	C13-C14-C15-C18
2	C	1101	F6L	C13-C14-C15-C18
2	A	1101	F6L	C28-C29-C32-O07
2	A	1101	F6L	C28-C29-C32-O08
2	A	1101	F6L	C30-C29-C32-O07
2	A	1101	F6L	C30-C29-C32-O08
2	D	1101	F6L	C13-C14-C15-C18
2	C	1101	F6L	C26-C25-N01-C15
2	A	1101	F6L	O02-C11-C12-O06
2	A	1101	F6L	C26-C25-N01-C16
2	B	1101	F6L	N01-C25-C26-C31
2	A	1101	F6L	C02-C01-C13-C14
2	A	1101	F6L	N01-C25-C26-C31
2	B	1101	F6L	C02-C01-C13-C14
2	A	1101	F6L	C26-C25-N01-C15
2	B	1101	F6L	C26-C25-N01-C15
2	B	1101	F6L	C06-C01-C13-C14
2	B	1101	F6L	C26-C25-N01-C16
2	A	1101	F6L	C06-C01-C13-C14
2	B	1101	F6L	N01-C25-C26-C27
2	C	1101	F6L	N01-C25-C26-C31
2	A	1101	F6L	N01-C25-C26-C27

There are no ring outliers.

10 monomers are involved in 13 short contacts:

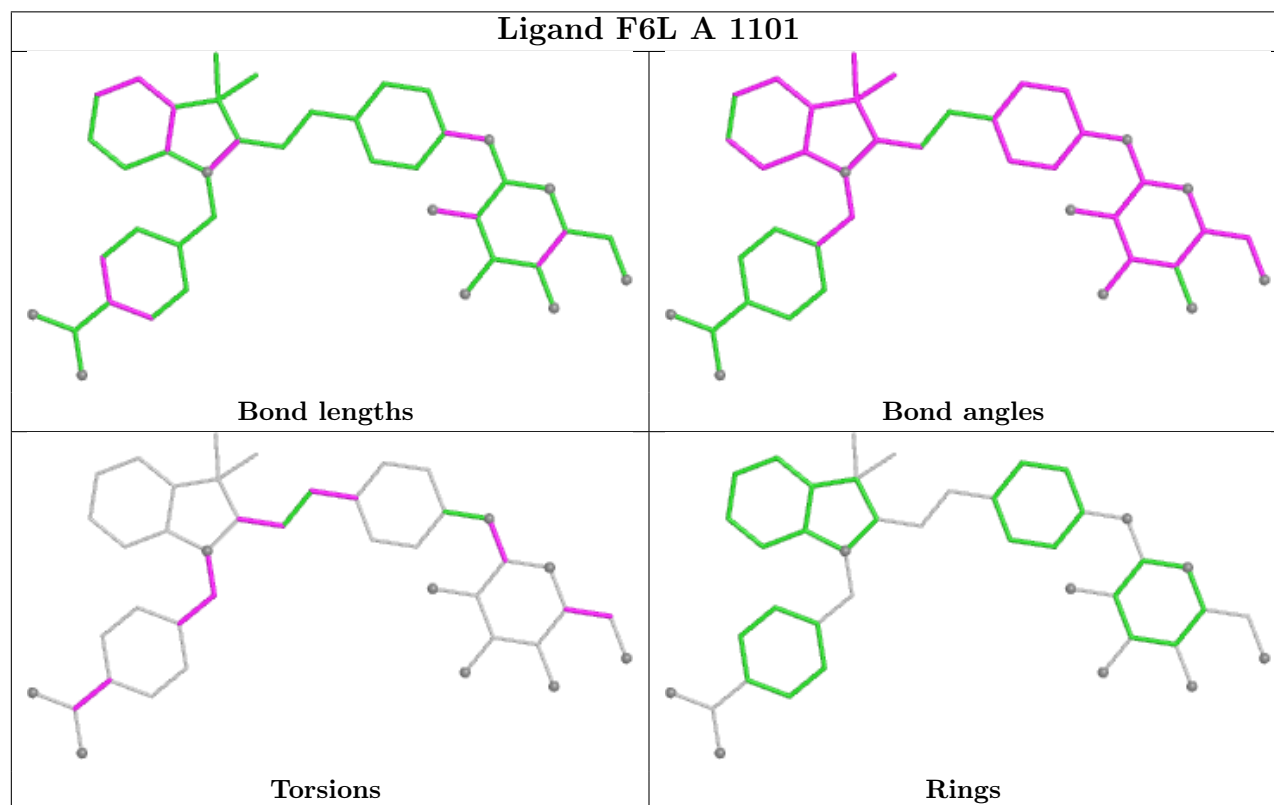
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1112	DMS	1	0
2	A	1101	F6L	1	0
2	C	1101	F6L	3	0
2	B	1101	F6L	1	0
5	C	1108	DMS	1	0
5	D	1108	DMS	2	0
5	A	1117	DMS	1	0

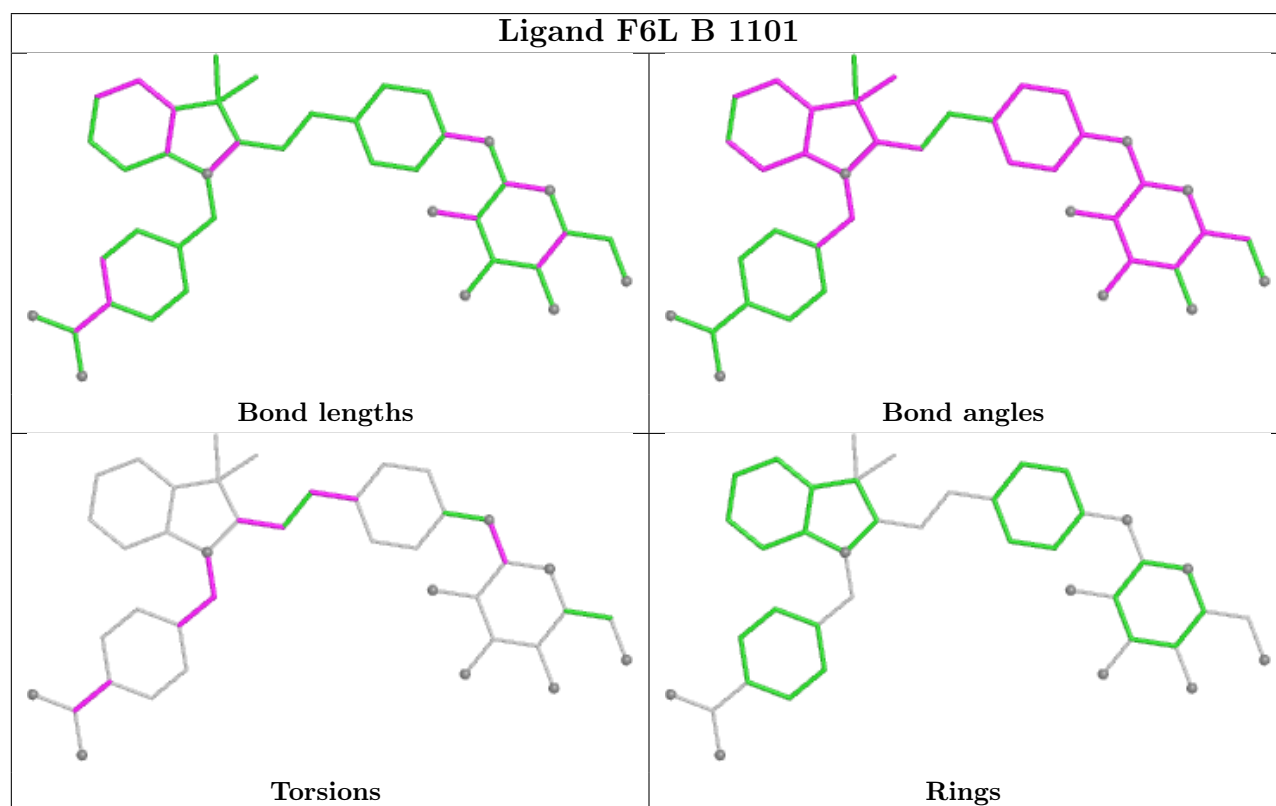
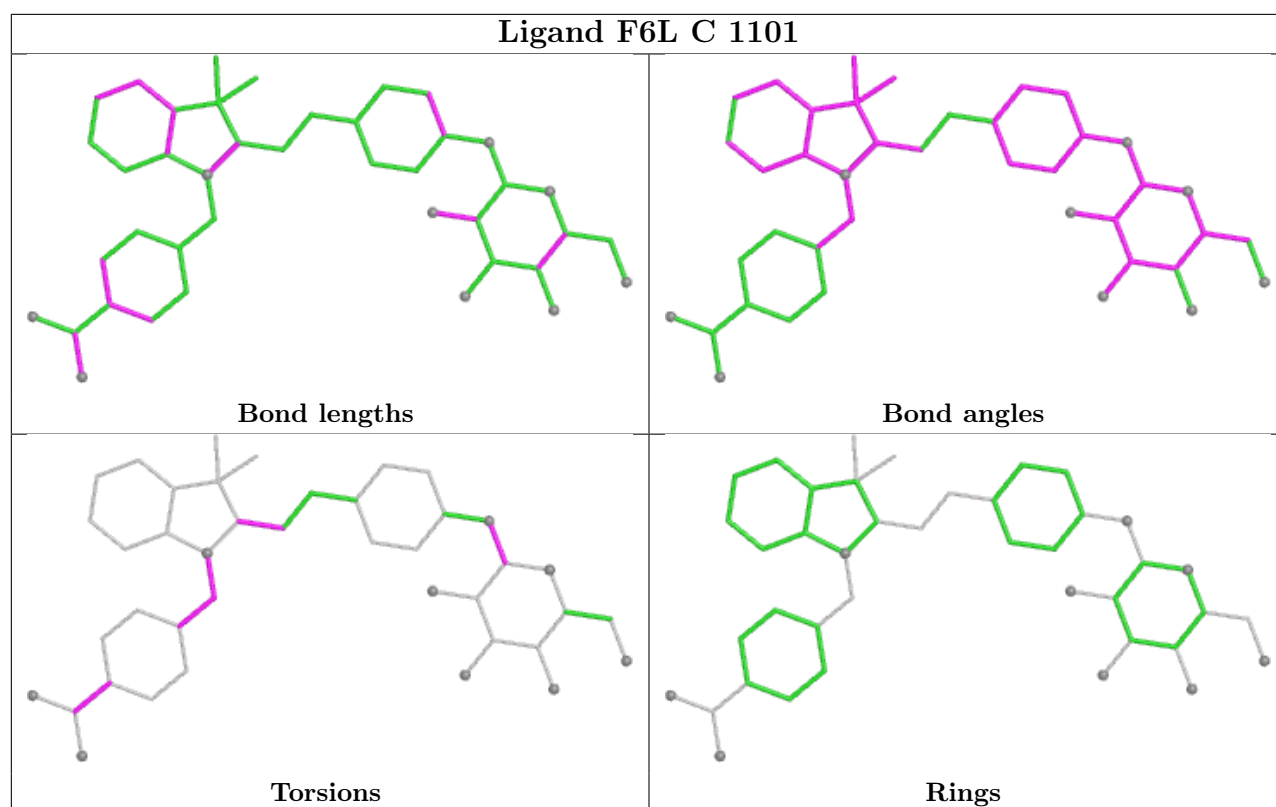
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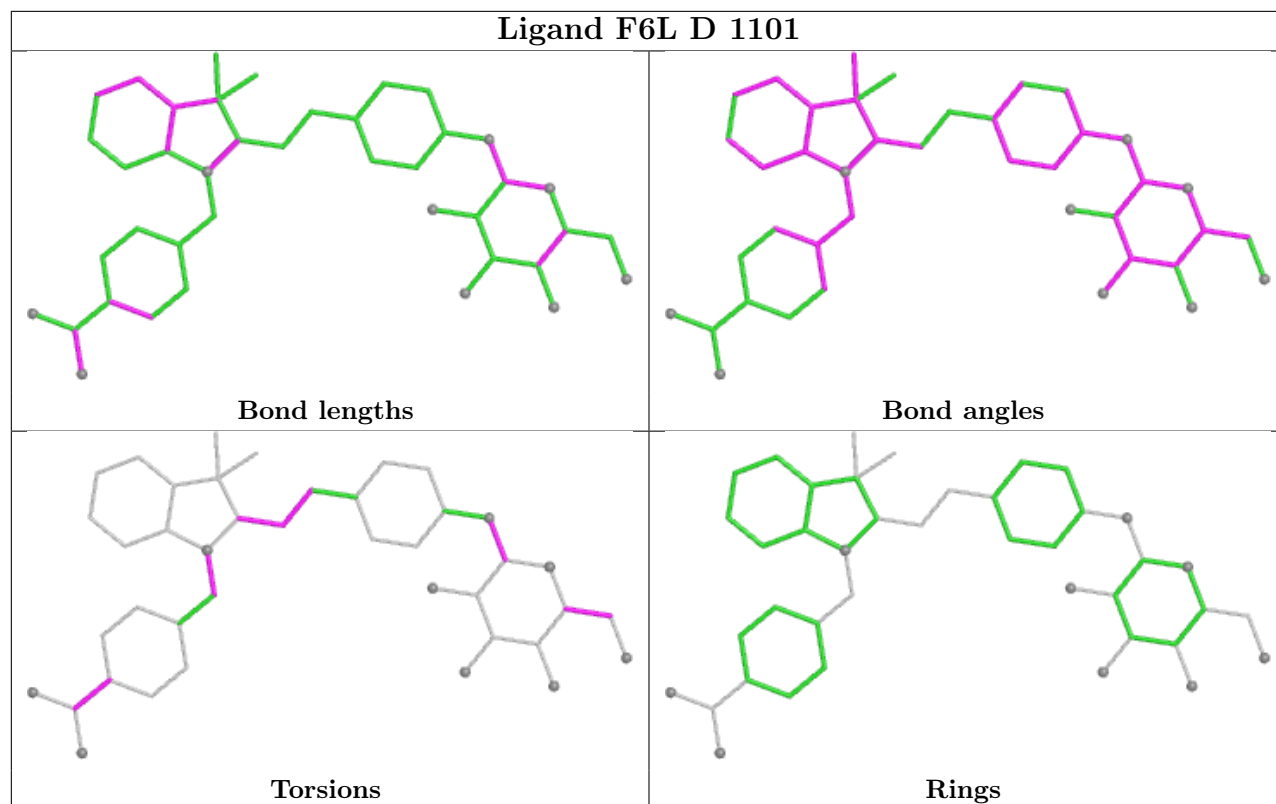
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1113	DMS	1	0
5	A	1110	DMS	1	0
5	A	1114	DMS	1	0

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	1021/1025 (99%)	0.19	27 (2%) 57 54	11, 31, 67, 96	0
1	B	1021/1025 (99%)	0.25	39 (3%) 44 40	12, 32, 70, 134	1 (0%)
1	C	1023/1025 (99%)	0.27	44 (4%) 40 36	10, 33, 73, 117	0
1	D	1021/1025 (99%)	0.42	77 (7%) 20 17	12, 36, 82, 117	0
All	All	4086/4100 (99%)	0.28	187 (4%) 37 34	10, 33, 74, 134	1 (0%)

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	766	SER	5.2
1	D	756	TRP	4.4
1	B	731	PRO	4.2
1	C	731	PRO	3.9
1	B	737	ILE	3.9
1	B	733	ALA	3.9
1	C	580	GLU	3.8
1	D	827	ALA	3.8
1	C	841	ALA	3.8
1	D	733	ALA	3.6
1	D	846	GLY	3.5
1	D	3	ILE	3.5
1	D	737	ILE	3.5
1	C	655	MET	3.5
1	B	832	ASP	3.4
1	D	732	ALA	3.4
1	A	3	ILE	3.4
1	D	730	LEU	3.4
1	A	743	SER	3.3
1	D	953	GLY	3.3
1	A	822	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	830	LEU	3.2
1	C	772	ASP	3.2
1	C	2	MET	3.2
1	C	756	TRP	3.2
1	D	829	THR	3.1
1	D	755	ARG	3.1
1	C	1	THR	3.1
1	B	858	ILE	3.1
1	A	1023	LYS	3.1
1	D	834	VAL	3.1
1	C	686	PRO	3.1
1	C	960	SER	3.1
1	C	733	ALA	3.0
1	D	822	LEU	3.0
1	C	737	ILE	2.9
1	D	770	ILE	2.9
1	D	774	LYS	2.9
1	A	756	TRP	2.9
1	C	755	ARG	2.9
1	D	746	ASP	2.9
1	D	772	ASP	2.9
1	D	859	ASP	2.9
1	A	733	ALA	2.9
1	D	782	ASP	2.8
1	D	981	GLY	2.8
1	B	732	ALA	2.8
1	D	742	THR	2.8
1	D	731	PRO	2.8
1	D	776	LEU	2.8
1	D	764	PHE	2.8
1	B	688	PRO	2.8
1	D	833	ALA	2.8
1	B	749	ILE	2.8
1	D	888	LEU	2.8
1	A	693	GLN	2.7
1	C	687	GLN	2.7
1	C	735	HIS	2.7
1	C	739	HIS	2.7
1	A	959	ILE	2.7
1	B	770	ILE	2.7
1	D	758	PHE	2.7
1	A	745	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	736	ALA	2.7
1	C	738	PRO	2.7
1	A	953	GLY	2.6
1	D	734	SER	2.6
1	B	746	ASP	2.6
1	B	726	LEU	2.6
1	D	773	LYS	2.6
1	D	728	VAL	2.6
1	D	821	ALA	2.6
1	D	684	GLU	2.6
1	D	836	ILE	2.5
1	C	581	ASN	2.5
1	D	740	LEU	2.5
1	C	653	HIS	2.5
1	D	771	GLY	2.5
1	D	940	GLY	2.5
1	C	732	ALA	2.5
1	B	766	SER	2.5
1	A	737	ILE	2.5
1	C	730	LEU	2.5
1	A	730	LEU	2.5
1	C	846	GLY	2.5
1	B	730	LEU	2.4
1	A	665	SER	2.4
1	C	746	ASP	2.4
1	D	580	GLU	2.4
1	B	738	PRO	2.4
1	C	860	GLY	2.4
1	C	1023	LYS	2.4
1	C	1022	GLN	2.4
1	B	751	LEU	2.4
1	A	739	HIS	2.4
1	C	939	CYS	2.4
1	B	747	PHE	2.4
1	A	694	LEU	2.4
1	D	837	THR	2.3
1	D	744	GLU	2.3
1	D	832	ASP	2.3
1	D	963	SER	2.3
1	D	895	VAL	2.3
1	B	823	LEU	2.3
1	D	735	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	941	THR	2.3
1	D	980	GLU	2.3
1	D	762	SER	2.3
1	D	891	VAL	2.3
1	B	820	ALA	2.3
1	D	826	THR	2.3
1	C	753	ASN	2.3
1	A	832	ASP	2.3
1	B	686	PRO	2.3
1	D	869	ASP	2.3
1	A	763	GLY	2.3
1	C	981	GLY	2.3
1	D	76	CYS	2.3
1	D	1018	LEU	2.3
1	A	858	ILE	2.3
1	D	858	ILE	2.3
1	C	750	GLU	2.3
1	B	846	GLY	2.3
1	D	862	GLY	2.3
1	D	751	LEU	2.3
1	B	836	ILE	2.2
1	C	821	ALA	2.2
1	D	745	MET	2.2
1	D	968	MET	2.2
1	A	829	THR	2.2
1	B	761	GLN	2.2
1	B	756	TRP	2.2
1	A	728	VAL	2.2
1	B	822	LEU	2.2
1	B	1023	LYS	2.2
1	D	889	ALA	2.2
1	B	742	THR	2.2
1	D	779	PRO	2.2
1	B	940	GLY	2.2
1	C	848	THR	2.2
1	B	776	LEU	2.2
1	C	771	GLY	2.2
1	D	898	LEU	2.2
1	C	745	MET	2.2
1	C	829	THR	2.2
1	D	630	ARG	2.2
1	B	687	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	546	LEU	2.2
1	D	944	LEU	2.2
1	B	772	ASP	2.2
1	B	833	ALA	2.1
1	D	939	CYS	2.1
1	C	761	GLN	2.1
1	C	320	GLY	2.1
1	D	820	ALA	2.1
1	C	980	GLU	2.1
1	A	683	PRO	2.1
1	D	761	GLN	2.1
1	D	1022	GLN	2.1
1	A	679	LEU	2.1
1	A	898	LEU	2.1
1	C	977	HIS	2.1
1	B	850	PHE	2.1
1	B	781	ARG	2.1
1	D	897	TRP	2.1
1	D	757	GLN	2.1
1	D	768	MET	2.1
1	D	856	TYR	2.1
1	A	758	PHE	2.1
1	D	13	ARG	2.1
1	D	691	ALA	2.1
1	B	944	LEU	2.1
1	C	583	ASN	2.1
1	D	752	GLY	2.1
1	C	3	ILE	2.1
1	C	749	ILE	2.1
1	B	830	LEU	2.0
1	A	862	GLY	2.0
1	B	728	VAL	2.0
1	A	264	GLU	2.0
1	B	773	LYS	2.0
1	D	787	ALA	2.0
1	D	831	ALA	2.0
1	D	842	TRP	2.0
1	B	3	ILE	2.0
1	B	1013	ARG	2.0
1	C	13	ARG	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
2	F6L	C	1101	41/41	0.63	0.34	56,106,146,152	0
2	F6L	A	1101	41/41	0.69	0.33	47,110,151,152	0
2	F6L	B	1101	41/41	0.72	0.29	49,106,146,153	0
2	F6L	D	1101	41/41	0.73	0.30	68,122,158,162	0
5	DMS	A	1117	4/4	0.73	0.23	56,63,69,77	0
5	DMS	B	1112	4/4	0.73	0.23	74,76,82,84	0
5	DMS	A	1115	4/4	0.79	0.22	67,72,72,75	0
5	DMS	D	1108	4/4	0.80	0.21	44,51,55,68	0
5	DMS	B	1107	4/4	0.81	0.20	65,68,70,72	0
5	DMS	B	1111	4/4	0.83	0.20	69,74,78,79	0
5	DMS	A	1114	4/4	0.83	0.22	50,64,66,72	0
5	DMS	D	1107	4/4	0.83	0.17	59,65,65,68	0
5	DMS	B	1110	4/4	0.83	0.21	56,62,63,77	0
5	DMS	D	1113	4/4	0.83	0.21	73,79,79,79	0
5	DMS	C	1109	4/4	0.84	0.21	61,63,65,70	0
5	DMS	A	1113	4/4	0.84	0.21	75,86,86,88	0
5	DMS	A	1112	4/4	0.85	0.19	56,64,64,66	0
5	DMS	A	1116	4/4	0.85	0.20	52,61,63,67	0
5	DMS	D	1110	4/4	0.85	0.18	68,75,75,76	0
5	DMS	C	1111	4/4	0.85	0.19	67,75,76,77	0
5	DMS	C	1112	4/4	0.86	0.17	72,75,75,76	0
5	DMS	D	1106	4/4	0.86	0.15	47,53,54,59	0
5	DMS	C	1110	4/4	0.86	0.18	53,59,60,64	0
6	GOL	B	1114	6/6	0.87	0.10	39,44,51,56	0
5	DMS	B	1109	4/4	0.88	0.17	73,75,78,78	0
5	DMS	B	1113	4/4	0.89	0.19	72,73,74,77	0
5	DMS	A	1111	4/4	0.89	0.16	54,62,62,64	0

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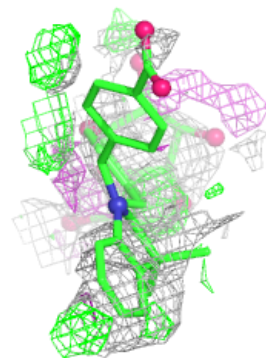
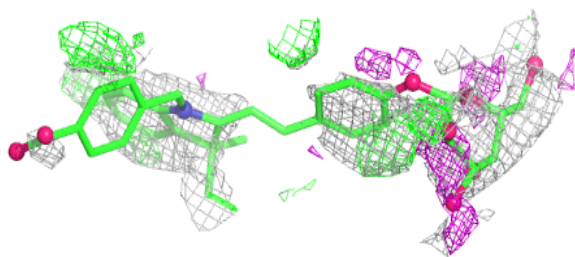
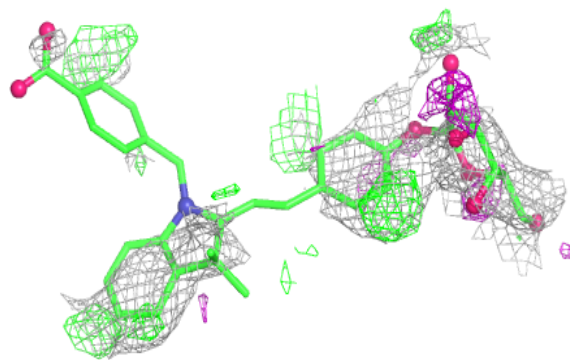
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	C	1103	1/1	0.89	0.10	26,26,26,26	0
5	DMS	A	1107	4/4	0.89	0.15	51,53,57,61	0
5	DMS	A	1110	4/4	0.89	0.18	63,69,70,73	0
5	DMS	C	1113	4/4	0.89	0.16	75,76,77,77	0
5	DMS	D	1112	4/4	0.90	0.17	87,89,90,95	0
4	NA	C	1104	1/1	0.90	0.16	29,29,29,29	0
5	DMS	B	1108	4/4	0.90	0.15	62,67,69,71	0
5	DMS	D	1111	4/4	0.91	0.19	59,66,67,75	0
5	DMS	B	1105	4/4	0.91	0.16	52,57,60,60	0
5	DMS	B	1106	4/4	0.91	0.15	51,55,57,60	0
5	DMS	A	1109	4/4	0.91	0.16	57,60,63,65	0
5	DMS	D	1109	4/4	0.92	0.12	56,57,57,60	0
3	MG	C	1102	1/1	0.92	0.06	37,37,37,37	0
5	DMS	C	1107	4/4	0.92	0.15	47,52,56,58	0
5	DMS	C	1108	4/4	0.93	0.13	55,59,60,63	0
5	DMS	A	1108	4/4	0.93	0.15	49,50,52,52	0
4	NA	D	1104	1/1	0.93	0.18	32,32,32,32	0
5	DMS	B	1104	4/4	0.94	0.14	43,47,47,47	0
5	DMS	C	1106	4/4	0.94	0.12	43,48,50,51	0
3	MG	D	1103	1/1	0.95	0.05	32,32,32,32	0
5	DMS	A	1106	4/4	0.95	0.12	44,45,46,48	0
3	MG	D	1102	1/1	0.97	0.04	35,35,35,35	0
3	MG	A	1102	1/1	0.97	0.05	30,30,30,30	0
4	NA	A	1104	1/1	0.97	0.07	21,21,21,21	0
3	MG	B	1102	1/1	0.97	0.04	26,26,26,26	0
4	NA	C	1105	1/1	0.98	0.04	18,18,18,18	0
4	NA	B	1103	1/1	0.98	0.05	24,24,24,24	0
4	NA	D	1105	1/1	0.98	0.06	19,19,19,19	0
3	MG	A	1103	1/1	0.99	0.02	19,19,19,19	0
4	NA	A	1105	1/1	0.99	0.03	19,19,19,19	0

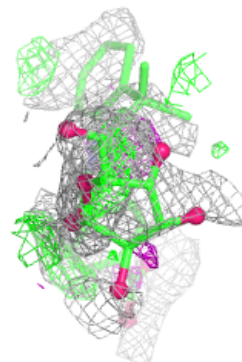
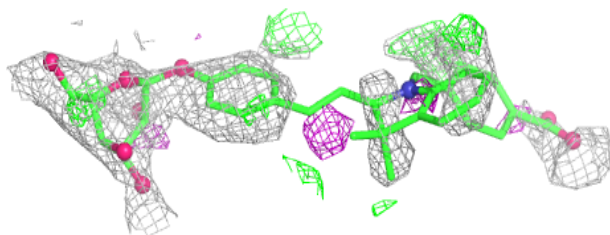
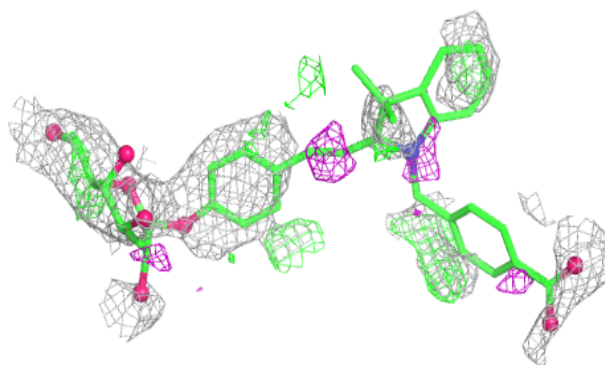
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around F6L C 1101:

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

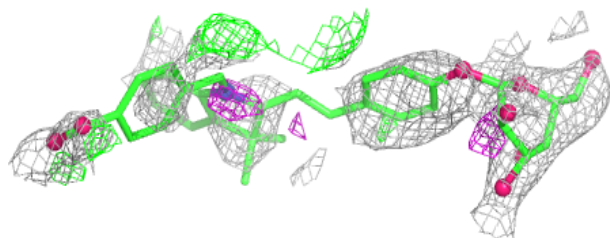
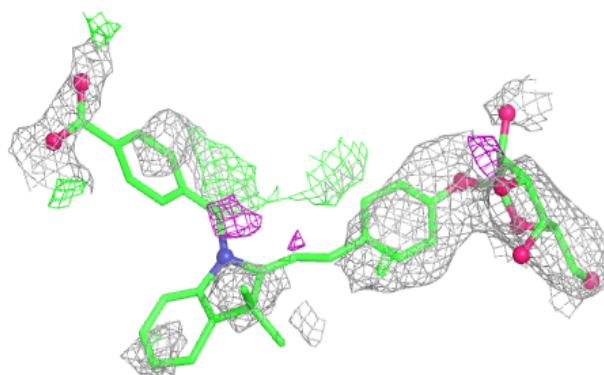
**Electron density around F6L A 1101:**

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

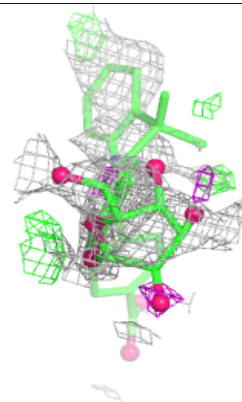
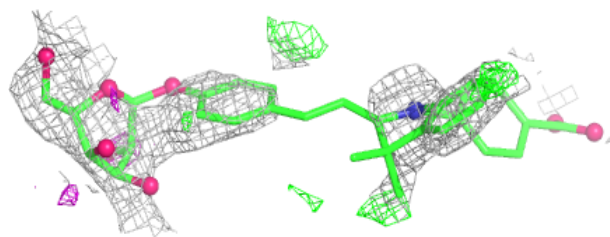
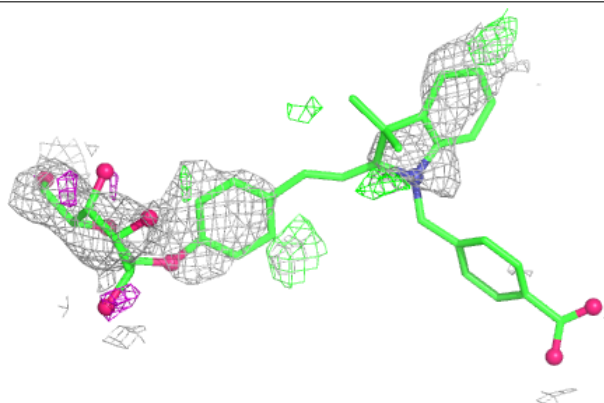


Electron density around F6L B 1101:

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

**Electron density around F6L D 1101:**

$2mF_o-DF_c$ (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.