



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 20, 2021 – 12:22 AM JST

PDB ID : 7BTK
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.

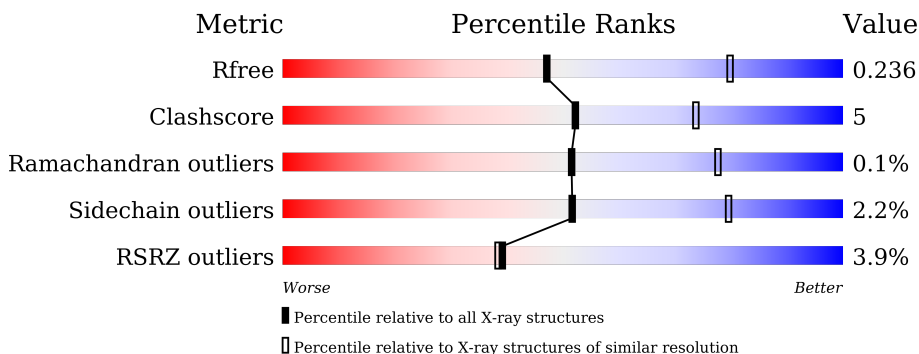
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.18
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) : 2.18

i

X-RAY DIFFRACTION

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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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	<div><div></div><div>3%</div><div>84%</div><div>15%</div></div>	
1	B	1025	<div><div></div><div>4%</div><div>86%</div><div>13%</div></div>	
1	C	1025	<div><div></div><div>4%</div><div>86%</div><div>13%</div></div>	
1	D	1025	<div><div></div><div>5%</div><div>86%</div><div>13%</div></div>	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	F6L	A	1101	-	-	-	X
2	F6L	B	1101	-	-	-	X
2	F6L	C	1101	-	-	-	X
2	F6L	D	1101	-	-	-	X

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.

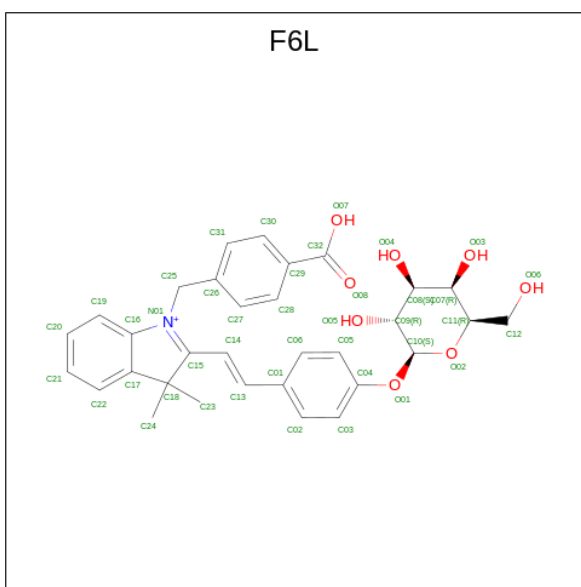
- Molecule 1 is a protein called Beta-galactosidase.

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 (three-letter code: F6L) (formula: C₃₂H₃₄NO₈) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

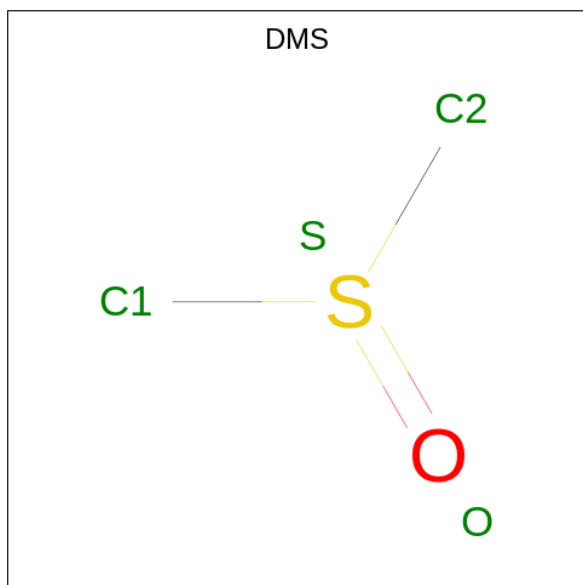
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Na 2 2	0	0

Continued on next page...

Continued from previous page...

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 (three-letter code: 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		

Continued on next page...

Continued from previous page...

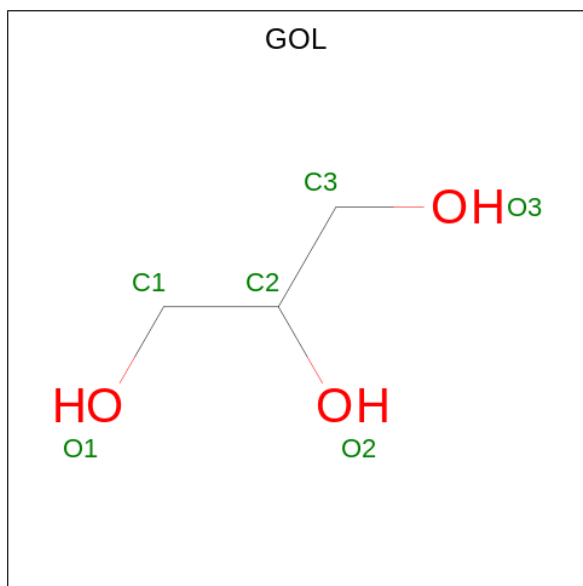
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2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

Continued on next page...

Continued from previous page...

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 (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

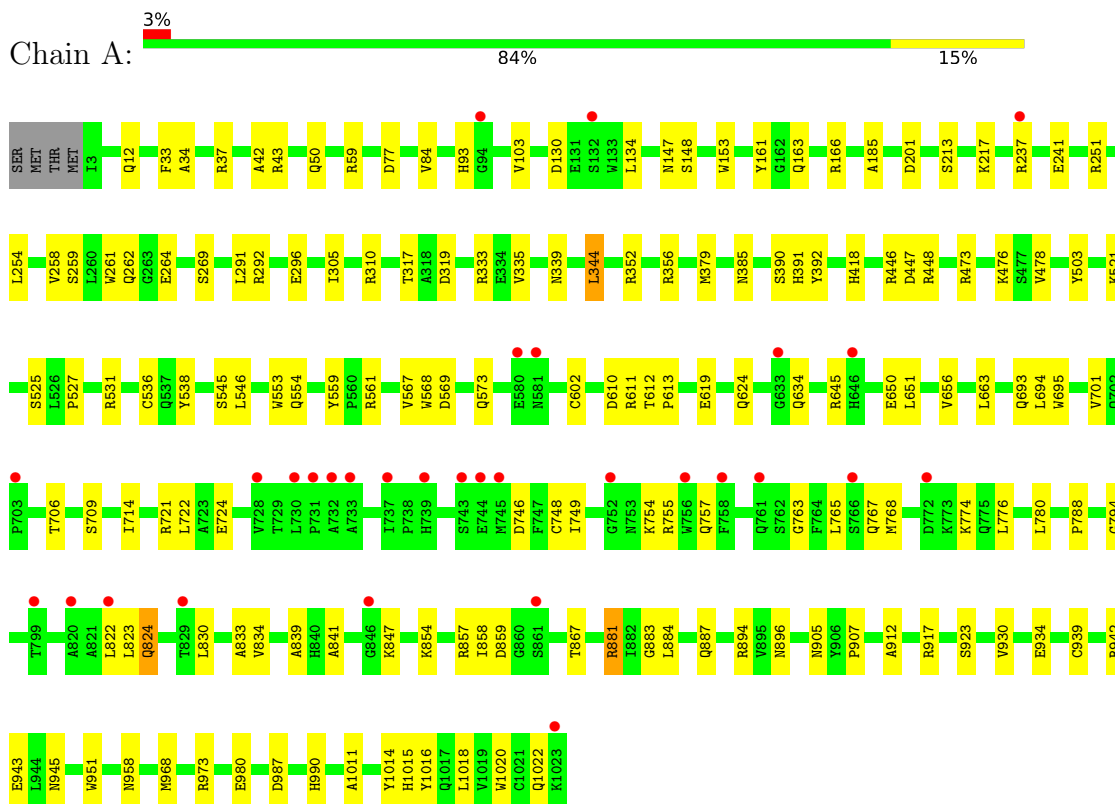
- Molecule 7 is water.

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

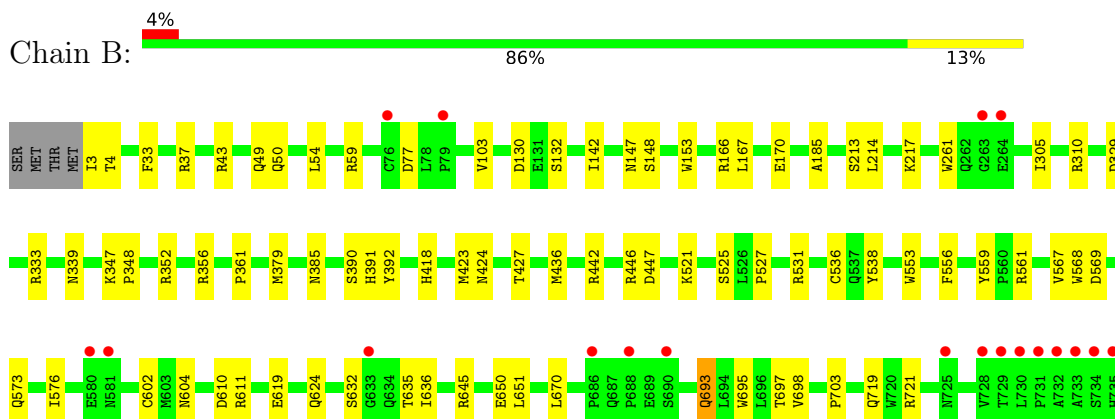
3 Residue-property plots

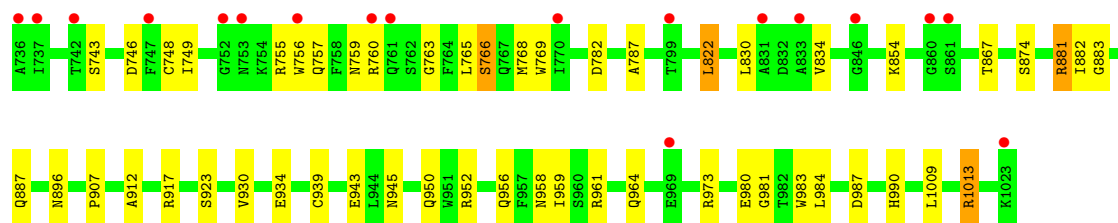
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

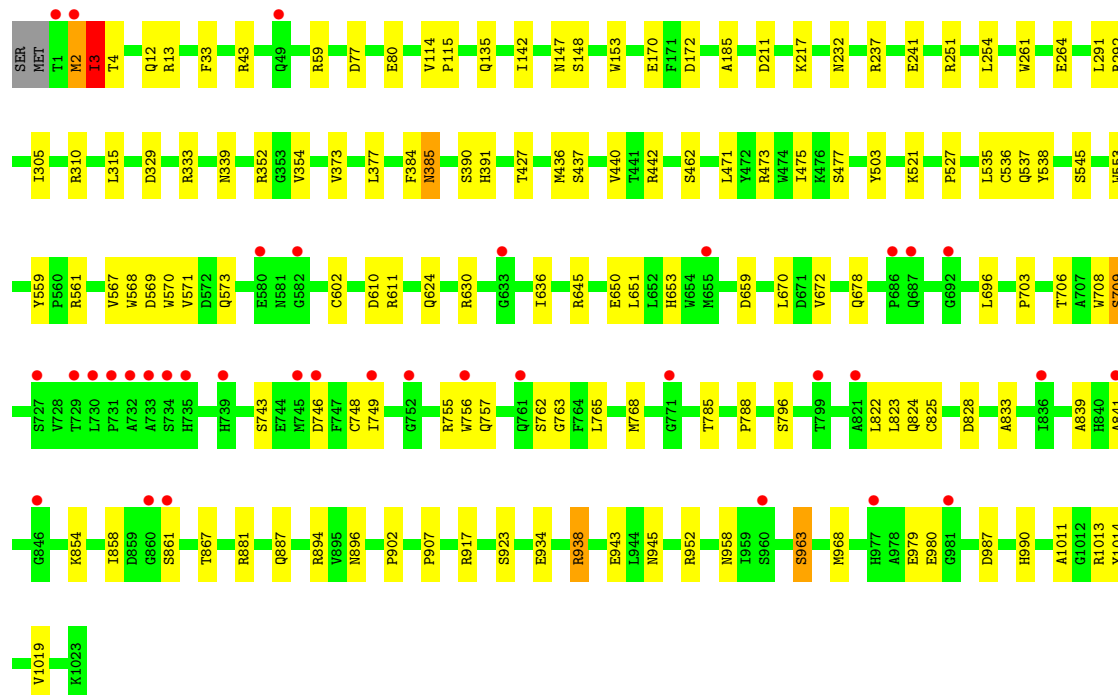
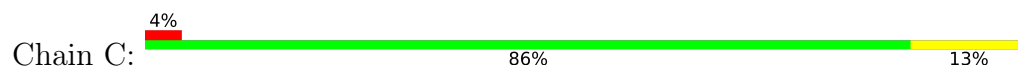


• Molecule 1: Beta-galactosidase

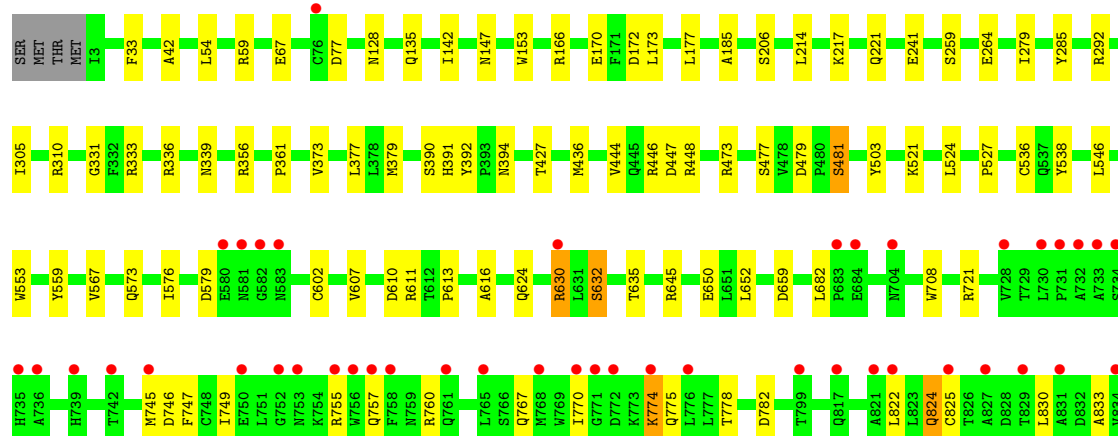
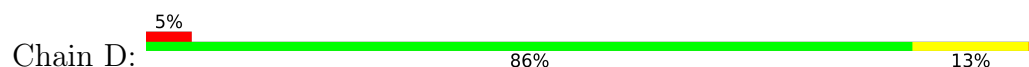


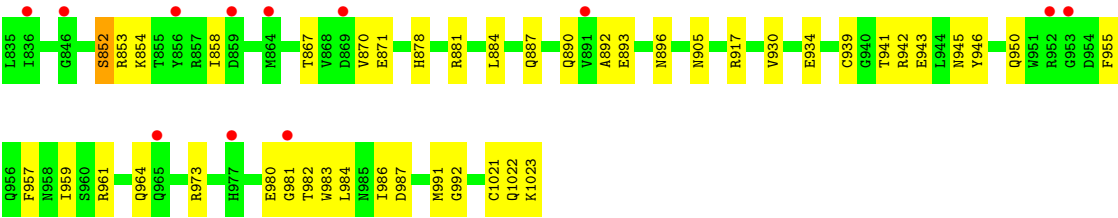


• Molecule 1: Beta-galactosidase



• 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 19.86 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.87-2.70) 99.8 (19.86-2.70)	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 (5.13%)	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 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	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: MG, F6L, DMS, 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	0.43	0/8367	0.56	0/11423
1	B	0.42	0/8329	0.57	0/11380
1	C	0.42	0/8333	0.57	0/11382
1	D	0.41	0/8348	0.58	0/11400
All	All	0.42	0/33377	0.57	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	90	0
1	B	8084	0	7608	87	0
1	C	8092	0	7614	80	0
1	D	8107	0	7675	98	0
2	A	41	0	0	1	0
2	B	41	0	0	0	0
2	C	41	0	0	3	0
2	D	41	0	0	1	0
3	A	2	0	0	0	0

Continued on next page...

Continued from previous page...

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	2	0
5	B	40	0	60	1	0
5	C	32	0	48	0	0
5	D	32	0	48	1	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	6	0
All	All	33869	0	30836	347	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 5.

All (347) 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:B:427:THR:HA	1:B:436:MET:HE1	1.70	0.71
1:C:427:THR:HA	1:C:436:MET:HE1	1.72	0.71
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: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

Continued on next page...

Continued from previous page...

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:D:946:TYR:OH	1:D:982:THR:HG21	1.94	0.67
1:B:1013:ARG:HH21	1:B:1013:ARG:HG2	1.61	0.65
1:D:427:THR:HA	1:D:436: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: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: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: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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:693:GLN:CD	1:B:721:ARG:HD3	2.27	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:A:503:TYR:OH	2:A:1101:F6L:O04	2.20	0.55
1:D:473:ARG:HH21	1:D:477:SER:HB2	1.72	0.55
1:B:1013:ARG:CZ	1:D:942:ARG:HH22	2.19	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:D:503:TYR:HH	2:D:1101:F6L:C08	2.23	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:339:ASN:O	1:D:527:PRO:HB3	2.12	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: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: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: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:331:GLY:H	5:D:1106:DMS:H13	1.77	0.49
1:D:905:ASN:OD1	1:D:939:CYS:HB2	2.13	0.49
1:D:610:ASP:O	1:D:611:ARG:HB2	2.13	0.49
1:D:546:LEU:HD22	1:D:616:ALA:HB1	1.95	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: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:C:503:TYR:OH	2:C:1101:F6L:O04	2.23	0.49
1:A:147:ASN:HA	1:A:148:SER:HA	1.64	0.49
1:B:854:LYS:HA	1:B:867:THR:O	2.13	0.49
5:B:1113:DMS:H22	7:B:1257:HOH:O	2.12	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:610:ASP:O	1:A:611:ARG:HB2	2.14	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:695:TRP:CH2	1:A:721:ARG:HG2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:1015:HIS:H	5:A:1117:DMS:H11	1.78	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:C:917:ARG:NH2	1:C:943:GLU:OE1	2.48	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
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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:610:ASP:O	1:B:611:ARG:HB2	2.15	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: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:D:356:ARG:HD2	1:D:379:MET:CE	2.46	0.45
1:A:645:ARG:HH22	1:A:650:GLU:CD	2.20	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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:670:LEU:HD23	1:C:670:LEU:HA	1.83	0.44
1:A:356:ARG:HD2	1:A:379:MET:CE	2.47	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:822:LEU:HD21	1:C:825:CYS:HB2	2.00	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
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:D:645:ARG:HH22	1:D:650:GLU:CD	2.22	0.43
1:A:237:ARG:HE	1:A:296:GLU:CD	2.21	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:632:SER:O	1:D:635:THR:OG1	2.33	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:B:645:ARG:HH22	1:B:650:GLU:CD	2.21	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
1:D:746:ASP:OD2	1:D:757:GLN:NE2	2.44	0.41
1:D:746:ASP:CG	1:D:757:GLN:HE21	2.23	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:1011:ALA:HB3	1:A:1014:TYR:CZ	2.57	0.40
1:D:356:ARG:HD2	1:D:379:MET:HE3	2.02	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	1019/1025 (99%)	977 (96%)	40 (4%)	2 (0%)	47	73
1	B	1020/1025 (100%)	978 (96%)	42 (4%)	0	100	100
1	C	1021/1025 (100%)	977 (96%)	42 (4%)	2 (0%)	47	73
1	D	1019/1025 (99%)	975 (96%)	44 (4%)	0	100	100
All	All	4079/4100 (100%)	3907 (96%)	168 (4%)	4 (0%)	51	78

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 [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	857/877 (98%)	837 (98%)	20 (2%)	50	78
1	B	844/877 (96%)	830 (98%)	14 (2%)	60	84
1	C	843/877 (96%)	820 (97%)	23 (3%)	44	74
1	D	851/877 (97%)	833 (98%)	18 (2%)	53	80
All	All	3395/3508 (97%)	3320 (98%)	75 (2%)	52	79

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	130	ASP
1	A	213	SER
1	A	259	SER
1	A	262	GLN
1	A	264	GLU
1	A	269	SER
1	A	333	ARG
1	A	344	LEU
1	A	536	CYS
1	A	545	SER
1	A	554	GLN
1	A	634	GLN
1	A	651	LEU
1	A	774	LYS
1	A	824	GLN
1	A	847	LYS
1	A	881	ARG
1	A	894	ARG
1	A	923	SER
1	B	49	GLN
1	B	213	SER
1	B	333	ARG
1	B	423	MET
1	B	536	CYS
1	B	693	GLN
1	B	743	SER
1	B	746	ASP
1	B	766	SER
1	B	822	LEU
1	B	874	SER
1	B	881	ARG
1	B	923	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1013	ARG
1	C	2	MET
1	C	3	ILE
1	C	12	GLN
1	C	13	ARG
1	C	80	GLU
1	C	135	GLN
1	C	291	LEU
1	C	333	ARG
1	C	385	ASN
1	C	535	LEU
1	C	536	CYS
1	C	545	SER
1	C	630	ARG
1	C	659	ASP
1	C	709	SER
1	C	762	SER
1	C	796	SER
1	C	824	GLN
1	C	861	SER
1	C	894	ARG
1	C	923	SER
1	C	938	ARG
1	C	963	SER
1	D	128	ASN
1	D	135	GLN
1	D	259	SER
1	D	264	GLU
1	D	333	ARG
1	D	394	ASN
1	D	481	SER
1	D	536	CYS
1	D	579	ASP
1	D	630	ARG
1	D	632	SER
1	D	652	LEU
1	D	659	ASP
1	D	774	LYS
1	D	824	GLN
1	D	852	SER
1	D	893	GLU
1	D	1021	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	GLN
1	A	624	GLN
1	A	687	GLN
1	A	693	GLN
1	A	761	GLN
1	A	843	GLN
1	B	93	HIS
1	B	558	GLN
1	B	950	GLN
1	B	964	GLN
1	C	385	ASN
1	C	394	ASN
1	C	757	GLN
1	C	878	HIS
1	D	163	GLN
1	D	624	GLN
1	D	634	GLN
1	D	890	GLN
1	D	945	ASN
1	D	965	GLN

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](#)

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	1112	-	3,3,3	0.32	0	3,3,3	0.80	0
5	DMS	C	1107	-	3,3,3	0.27	0	3,3,3	0.93	0
5	DMS	C	1113	-	3,3,3	0.29	0	3,3,3	0.67	0
5	DMS	B	1108	-	3,3,3	0.36	0	3,3,3	0.73	0
5	DMS	A	1109	-	3,3,3	0.28	0	3,3,3	0.72	0
5	DMS	B	1109	-	3,3,3	0.31	0	3,3,3	0.53	0
5	DMS	C	1106	-	3,3,3	0.22	0	3,3,3	1.04	0
5	DMS	C	1111	-	3,3,3	0.36	0	3,3,3	0.79	0
5	DMS	A	1113	-	3,3,3	0.37	0	3,3,3	0.81	0
5	DMS	D	1111	-	3,3,3	0.32	0	3,3,3	0.81	0
5	DMS	D	1113	-	3,3,3	0.29	0	3,3,3	0.84	0
5	DMS	D	1107	-	3,3,3	0.29	0	3,3,3	0.88	0
5	DMS	A	1108	-	3,3,3	0.36	0	3,3,3	1.08	0
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	D	1112	-	3,3,3	0.35	0	3,3,3	0.67	0
5	DMS	B	1107	-	3,3,3	0.16	0	3,3,3	1.10	0
2	F6L	A	1101	3,4	43,45,45	2.57	9 (20%)	62,66,66	2.63	31 (50%)
2	F6L	D	1101	3,4	43,45,45	2.57	9 (20%)	62,66,66	2.90	28 (45%)
5	DMS	A	1117	-	3,3,3	0.43	0	3,3,3	0.95	0
5	DMS	C	1110	-	3,3,3	0.18	0	3,3,3	0.77	0
5	DMS	D	1106	-	3,3,3	0.33	0	3,3,3	0.85	0
6	GOL	B	1114	-	5,5,5	0.30	0	5,5,5	0.45	0
5	DMS	B	1105	-	3,3,3	0.34	0	3,3,3	0.72	0
5	DMS	B	1111	-	3,3,3	0.25	0	3,3,3	0.76	0
5	DMS	B	1113	-	3,3,3	0.48	0	3,3,3	0.50	0
2	F6L	B	1101	3,4	43,45,45	2.60	10 (23%)	62,66,66	2.56	27 (43%)
5	DMS	D	1110	-	3,3,3	0.32	0	3,3,3	0.52	0
5	DMS	C	1109	-	3,3,3	0.31	0	3,3,3	0.86	0
5	DMS	D	1109	-	3,3,3	0.28	0	3,3,3	0.63	0
5	DMS	C	1112	-	3,3,3	0.28	0	3,3,3	0.80	0
5	DMS	A	1116	-	3,3,3	0.23	0	3,3,3	0.78	0
5	DMS	A	1111	-	3,3,3	0.33	0	3,3,3	0.79	0
2	F6L	C	1101	3,4	43,45,45	2.41	8 (18%)	62,66,66	2.41	26 (41%)
5	DMS	B	1110	-	3,3,3	0.37	0	3,3,3	0.75	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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	A	1106	-	3,3,3	0.33	0	3,3,3	1.03	0
5	DMS	B	1106	-	3,3,3	0.31	0	3,3,3	0.75	0
5	DMS	A	1114	-	3,3,3	0.37	0	3,3,3	0.87	0
5	DMS	A	1110	-	3,3,3	0.32	0	3,3,3	0.74	0
5	DMS	B	1104	-	3,3,3	0.25	0	3,3,3	0.80	0
5	DMS	A	1112	-	3,3,3	0.21	0	3,3,3	1.02	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	B	1101	3,4	-	9/15/59/59	0/5/5/5
2	F6L	A	1101	3,4	-	10/15/59/59	0/5/5/5
2	F6L	D	1101	3,4	-	7/15/59/59	0/5/5/5
6	GOL	B	1114	-	-	0/4/4/4	-
2	F6L	C	1101	3,4	-	5/15/59/59	0/5/5/5

All (36) 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	B	1101	F6L	C29-C32	6.71	1.53	1.47
2	C	1101	F6L	C21-C22	6.65	1.52	1.38
2	A	1101	F6L	C29-C32	6.31	1.53	1.47
2	D	1101	F6L	C29-C32	5.70	1.53	1.47
2	C	1101	F6L	C29-C32	5.57	1.52	1.47
2	A	1101	F6L	C07-C11	-3.23	1.46	1.53
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	C	1101	F6L	C07-C11	-2.66	1.47	1.53
2	C	1101	F6L	C15-N01	2.61	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	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	A	1101	F6L	C16-C17	-2.26	1.34	1.38
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	A	1101	F6L	C28-C29	2.13	1.43	1.39
2	C	1101	F6L	O05-C09	2.08	1.47	1.43
2	B	1101	F6L	C28-C29	2.04	1.43	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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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 (31) 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	C01-C13-C14-C15
2	D	1101	F6L	O02-C11-C12-O06
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	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

Continued on next page...

Continued from previous page...

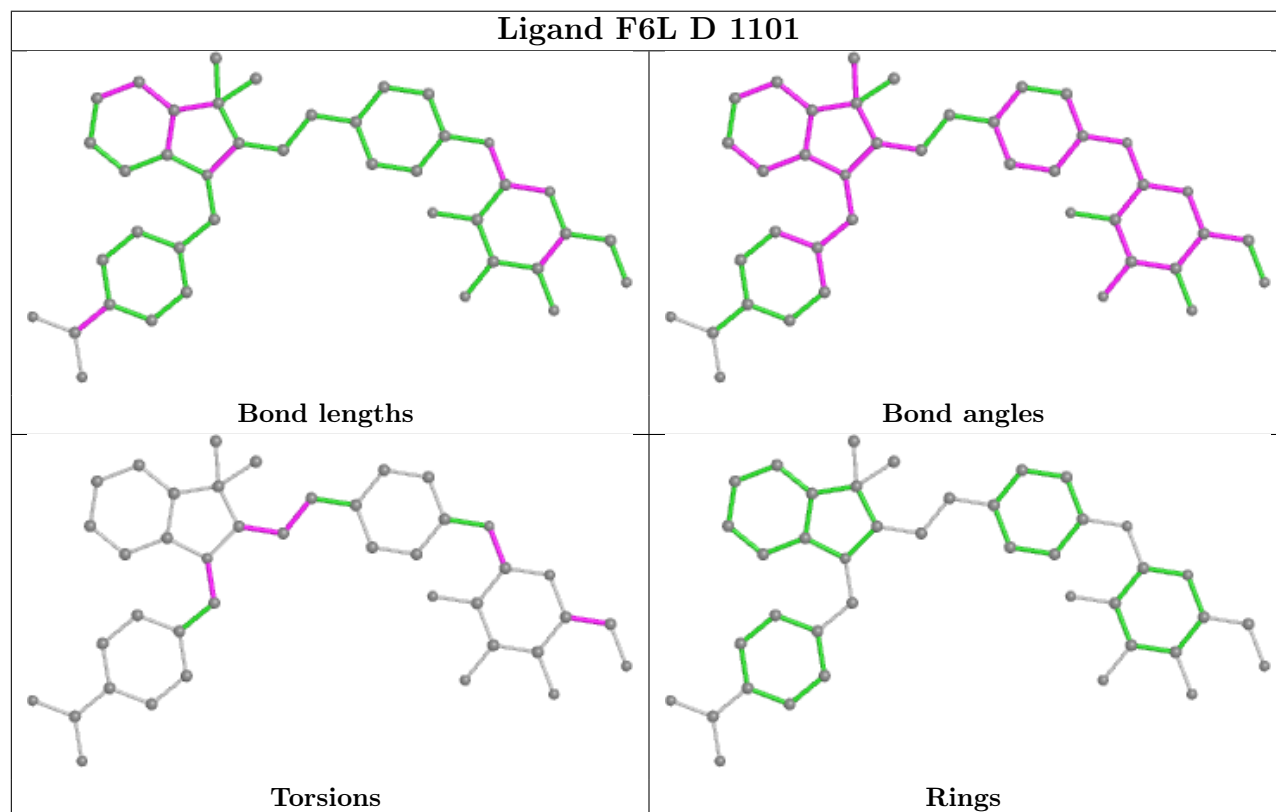
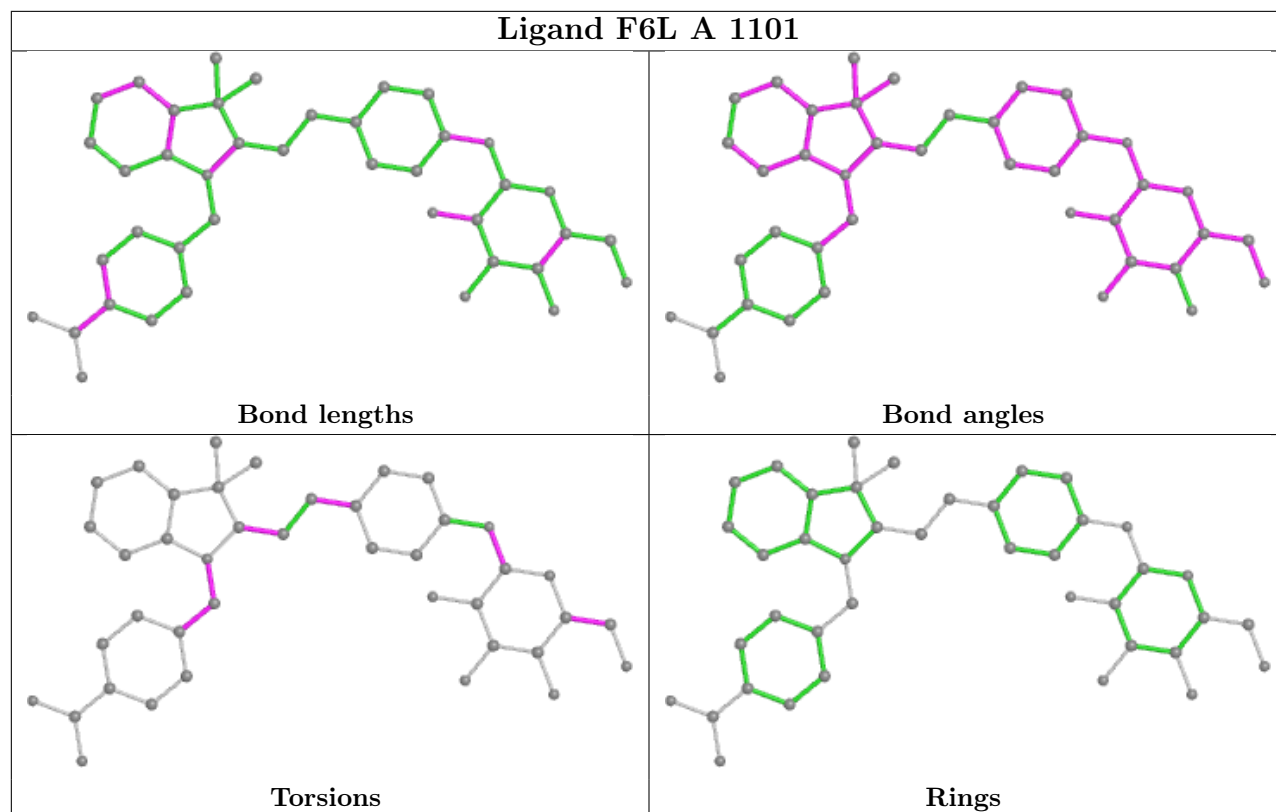
Mol	Chain	Res	Type	Atoms
2	A	1101	F6L	N01-C25-C26-C27

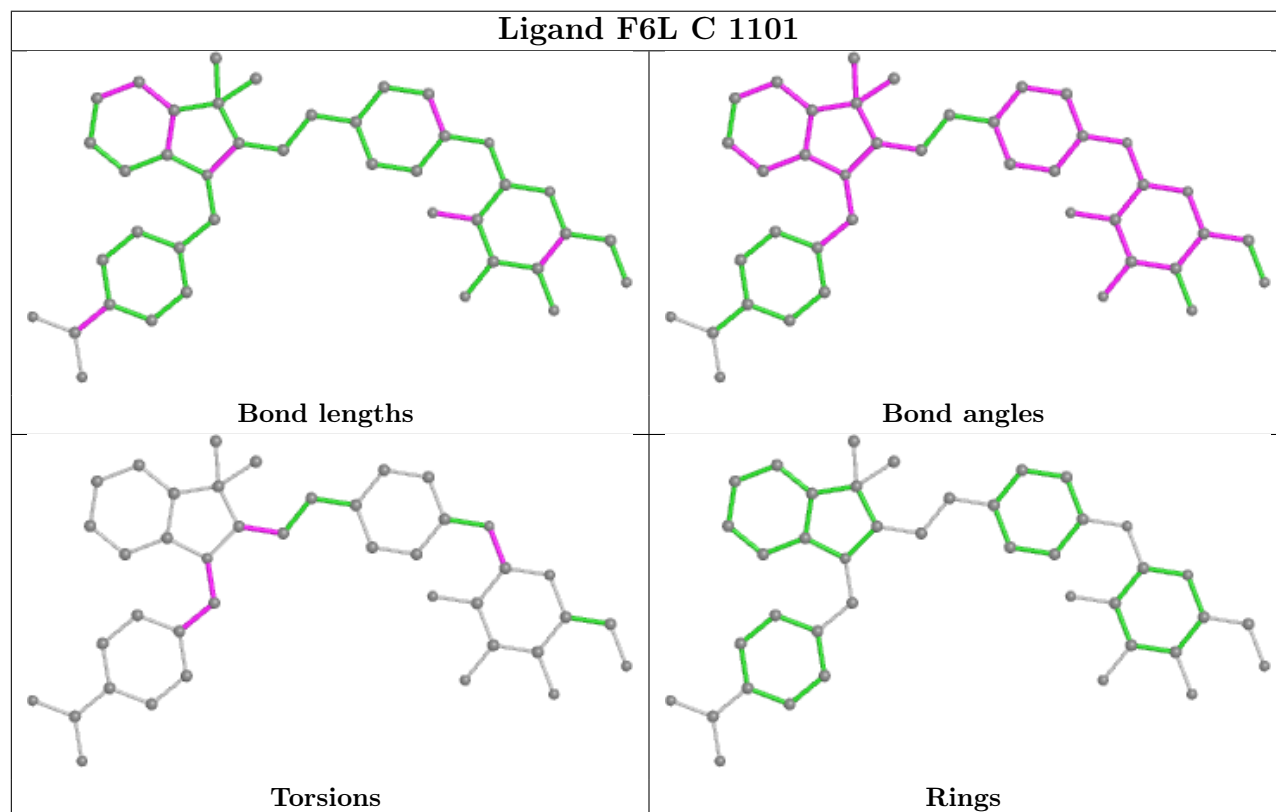
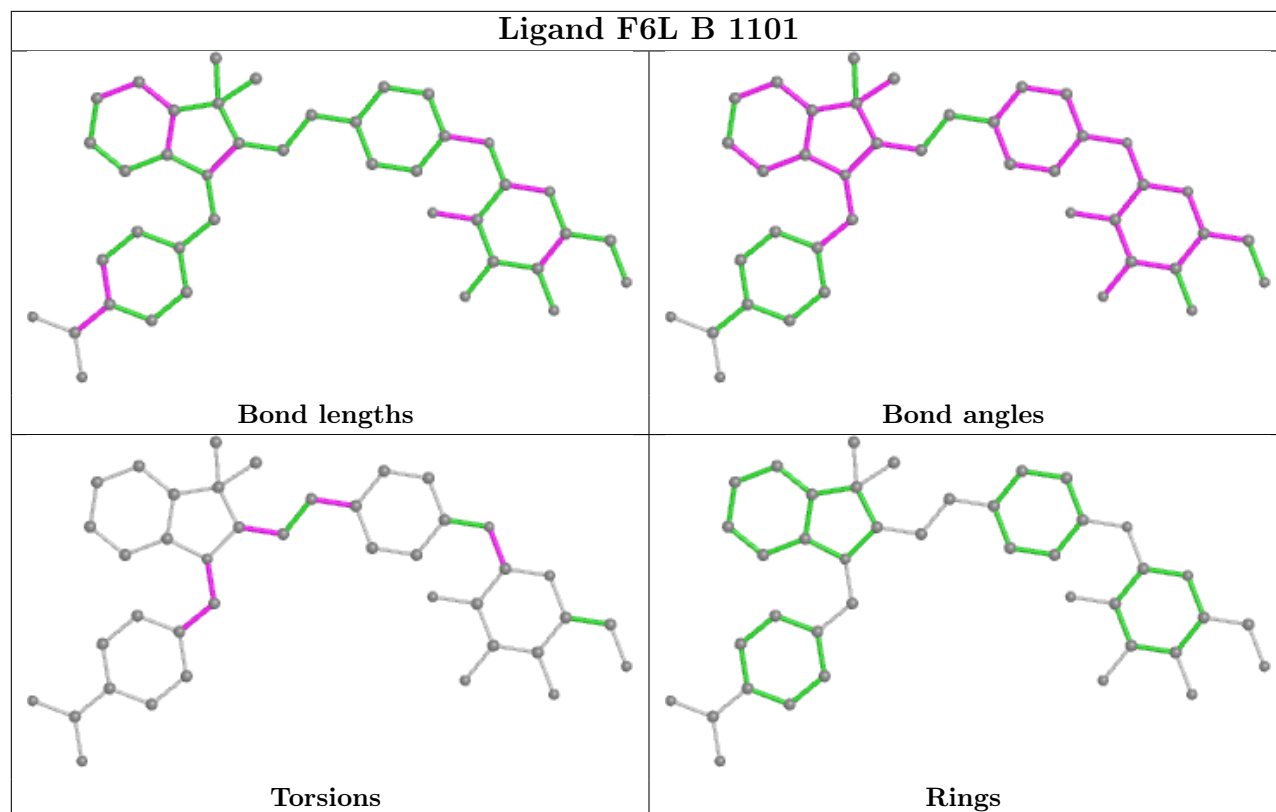
There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	F6L	1	0
2	D	1101	F6L	1	0
5	A	1117	DMS	1	0
5	D	1106	DMS	1	0
5	B	1113	DMS	1	0
2	C	1101	F6L	3	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%)	0.03	31 (3%)	50	51	11, 31, 67, 96	0
1	B	1021/1025 (99%)	0.07	37 (3%)	42	42	12, 32, 70, 134	0
1	C	1023/1025 (99%)	0.09	36 (3%)	44	44	10, 33, 73, 117	0
1	D	1021/1025 (99%)	0.22	56 (5%)	25	24	12, 36, 82, 117	0
All	All	4086/4100 (99%)	0.10	160 (3%)	39	38	10, 33, 74, 134	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	731	PRO	9.0
1	C	1	THR	6.7
1	B	733	ALA	6.2
1	C	732	ALA	5.6
1	D	846	GLY	5.2
1	D	732	ALA	5.1
1	D	731	PRO	5.1
1	D	752	GLY	4.6
1	D	733	ALA	4.5
1	C	731	PRO	4.5
1	D	761	GLN	4.4
1	D	684	GLU	4.4
1	D	756	TRP	4.3
1	D	734	SER	4.3
1	C	580	GLU	4.2
1	B	732	ALA	4.2
1	A	581	ASN	4.2
1	C	734	SER	4.1
1	B	735	HIS	4.0
1	C	846	GLY	3.9
1	C	746	ASP	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	731	PRO	3.8
1	C	735	HIS	3.8
1	C	739	HIS	3.8
1	B	730	LEU	3.7
1	B	831	ALA	3.6
1	D	953	GLY	3.6
1	A	733	ALA	3.5
1	D	730	LEU	3.5
1	B	752	GLY	3.4
1	C	761	GLN	3.4
1	A	580	GLU	3.4
1	A	799	THR	3.3
1	C	771	GLY	3.3
1	A	730	LEU	3.2
1	C	752	GLY	3.2
1	A	633	GLY	3.2
1	B	846	GLY	3.2
1	D	753	ASN	3.2
1	B	861	SER	3.2
1	B	737	ILE	3.1
1	B	580	GLU	3.1
1	C	2	MET	3.1
1	A	772	ASP	3.1
1	D	831	ALA	3.1
1	A	732	ALA	3.1
1	D	825	CYS	3.0
1	C	745	MET	3.0
1	C	756	TRP	3.0
1	C	733	ALA	3.0
1	D	735	HIS	3.0
1	D	772	ASP	3.0
1	D	580	GLU	3.0
1	A	761	GLN	3.0
1	D	581	ASN	3.0
1	D	817	GLN	2.9
1	A	766	SER	2.9
1	B	734	SER	2.9
1	B	688	PRO	2.9
1	A	1023	LYS	2.9
1	D	965	GLN	2.9
1	B	581	ASN	2.9
1	C	730	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	977	HIS	2.8
1	C	799	THR	2.8
1	B	728	VAL	2.7
1	D	750	GLU	2.7
1	A	737	ILE	2.7
1	A	756	TRP	2.7
1	D	736	ALA	2.7
1	C	749	ILE	2.7
1	D	582	GLY	2.7
1	B	969	GLU	2.7
1	D	977	HIS	2.6
1	D	745	MET	2.6
1	C	841	ALA	2.6
1	D	728	VAL	2.6
1	D	758	PHE	2.6
1	D	776	LEU	2.5
1	B	79	PRO	2.5
1	B	1023	LYS	2.5
1	D	630	ARG	2.5
1	B	264	GLU	2.5
1	A	743	SER	2.5
1	A	745	MET	2.5
1	A	820	ALA	2.5
1	D	742	THR	2.5
1	A	758	PHE	2.5
1	A	752	GLY	2.4
1	C	49	GLN	2.4
1	A	94	GLY	2.4
1	D	774	LYS	2.4
1	B	753	ASN	2.4
1	D	755	ARG	2.4
1	A	861	SER	2.4
1	D	583	ASN	2.4
1	D	836	ILE	2.4
1	D	952	ARG	2.4
1	D	864	MET	2.3
1	C	687	GLN	2.3
1	C	861	SER	2.3
1	A	846	GLY	2.3
1	A	829	THR	2.3
1	B	833	ALA	2.3
1	A	728	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	757	GLN	2.3
1	D	76	CYS	2.3
1	D	739	HIS	2.3
1	C	981	GLY	2.3
1	A	646	HIS	2.3
1	D	821	ALA	2.3
1	C	860	GLY	2.3
1	B	747	PHE	2.3
1	B	770	ILE	2.3
1	B	686	PRO	2.2
1	C	655	MET	2.2
1	B	860	GLY	2.2
1	D	891	VAL	2.2
1	D	981	GLY	2.2
1	C	727	SER	2.2
1	C	821	ALA	2.2
1	D	771	GLY	2.2
1	B	756	TRP	2.2
1	D	829	THR	2.2
1	B	725	ASN	2.2
1	B	76	CYS	2.2
1	B	736	ALA	2.2
1	B	263	GLY	2.2
1	D	799	THR	2.2
1	D	834	VAL	2.2
1	A	739	HIS	2.2
1	C	692	GLY	2.2
1	C	960	SER	2.2
1	A	744	GLU	2.1
1	D	770	ILE	2.1
1	D	856	TYR	2.1
1	D	869	ASP	2.1
1	C	686	PRO	2.1
1	D	768	MET	2.1
1	A	822	LEU	2.1
1	B	760	ARG	2.1
1	D	765	LEU	2.1
1	A	703	PRO	2.1
1	D	683	PRO	2.1
1	B	799	THR	2.1
1	A	132	SER	2.1
1	D	859	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	822	LEU	2.1
1	B	729	THR	2.1
1	C	729	THR	2.1
1	B	633	GLY	2.1
1	D	704	ASN	2.0
1	B	742	THR	2.0
1	B	761	GLN	2.0
1	C	836	ILE	2.0
1	C	633	GLY	2.0
1	A	237	ARG	2.0
1	B	690	SER	2.0
1	C	582	GLY	2.0
1	D	827	ALA	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(\AA^2)	Q<0.9
2	F6L	C	1101	41/41	0.59	0.59	56,106,146,152	0
2	F6L	A	1101	41/41	0.66	0.49	47,110,151,152	0
2	F6L	D	1101	41/41	0.68	0.49	68,122,158,162	0
2	F6L	B	1101	41/41	0.70	0.46	49,106,146,153	0
3	MG	C	1103	1/1	0.80	0.13	26,26,26,26	0
5	DMS	A	1117	4/4	0.80	0.27	56,63,69,77	0
5	DMS	D	1108	4/4	0.81	0.32	44,51,55,68	0
5	DMS	A	1113	4/4	0.84	0.29	75,86,86,88	0
5	DMS	A	1114	4/4	0.84	0.25	50,64,66,72	0
5	DMS	C	1111	4/4	0.85	0.27	67,75,76,77	0

Continued on next page...

Continued from previous page...

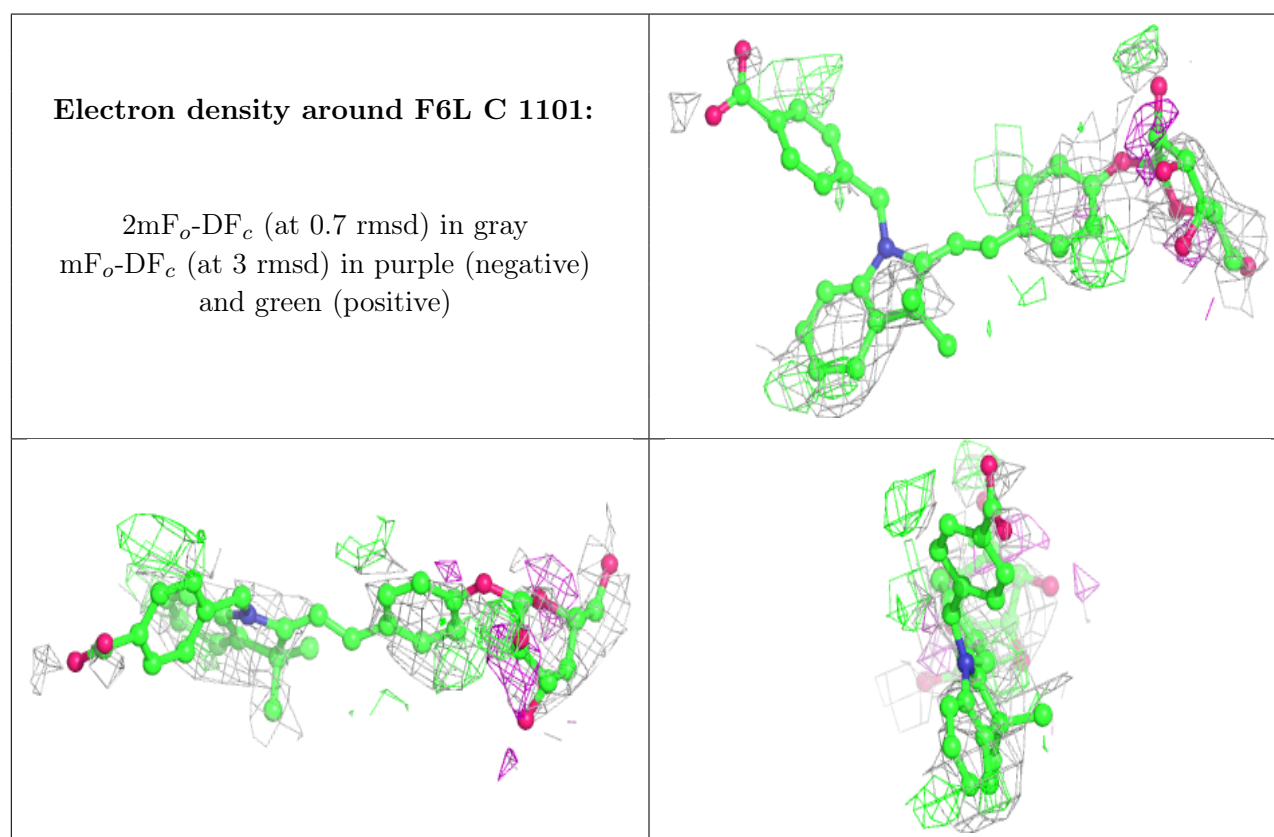
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	DMS	B	1110	4/4	0.86	0.31	56,62,63,77	0
5	DMS	B	1112	4/4	0.86	0.21	74,76,82,84	0
6	GOL	B	1114	6/6	0.86	0.20	39,44,51,56	0
5	DMS	A	1112	4/4	0.87	0.21	56,64,64,66	0
5	DMS	D	1112	4/4	0.87	0.43	87,89,90,95	0
5	DMS	A	1116	4/4	0.87	0.34	52,61,63,67	0
5	DMS	D	1107	4/4	0.88	0.23	59,65,65,68	0
5	DMS	C	1109	4/4	0.88	0.24	61,63,65,70	0
5	DMS	B	1111	4/4	0.88	0.34	69,74,78,79	0
5	DMS	D	1106	4/4	0.88	0.25	47,53,54,59	0
4	NA	C	1104	1/1	0.89	0.27	29,29,29,29	0
5	DMS	C	1110	4/4	0.89	0.20	53,59,60,64	0
5	DMS	D	1111	4/4	0.89	0.26	59,66,67,75	0
5	DMS	A	1107	4/4	0.89	0.21	51,53,57,61	0
5	DMS	B	1113	4/4	0.89	0.27	72,73,74,77	0
5	DMS	A	1110	4/4	0.90	0.24	63,69,70,73	0
5	DMS	B	1107	4/4	0.91	0.20	65,68,70,72	0
5	DMS	B	1109	4/4	0.91	0.22	73,75,78,78	0
5	DMS	D	1110	4/4	0.91	0.23	68,75,75,76	0
5	DMS	A	1115	4/4	0.91	0.34	67,72,72,75	0
4	NA	D	1104	1/1	0.91	0.29	32,32,32,32	0
5	DMS	D	1113	4/4	0.91	0.24	73,79,79,79	0
5	DMS	A	1109	4/4	0.91	0.22	57,60,63,65	0
5	DMS	B	1105	4/4	0.92	0.19	52,57,60,60	0
3	MG	D	1103	1/1	0.92	0.08	32,32,32,32	0
5	DMS	A	1108	4/4	0.92	0.20	49,50,52,52	0
5	DMS	C	1108	4/4	0.92	0.23	55,59,60,63	0
5	DMS	A	1111	4/4	0.92	0.26	54,62,62,64	0
5	DMS	C	1113	4/4	0.93	0.17	75,76,77,77	0
5	DMS	B	1108	4/4	0.93	0.21	62,67,69,71	0
5	DMS	C	1107	4/4	0.93	0.19	47,52,56,58	0
5	DMS	C	1112	4/4	0.93	0.29	72,75,75,76	0
5	DMS	D	1109	4/4	0.93	0.21	56,57,57,60	0
5	DMS	B	1106	4/4	0.94	0.21	51,55,57,60	0
4	NA	D	1105	1/1	0.94	0.08	19,19,19,19	0
3	MG	D	1102	1/1	0.95	0.10	35,35,35,35	0
5	DMS	B	1104	4/4	0.95	0.21	43,47,47,47	0
5	DMS	A	1106	4/4	0.95	0.29	44,45,46,48	0
5	DMS	C	1106	4/4	0.95	0.20	43,48,50,51	0
3	MG	C	1102	1/1	0.95	0.08	37,37,37,37	0
4	NA	C	1105	1/1	0.96	0.09	18,18,18,18	0
4	NA	A	1105	1/1	0.96	0.06	19,19,19,19	0

Continued on next page...

Continued from previous page...

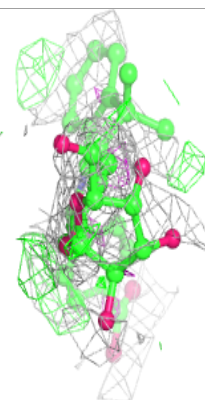
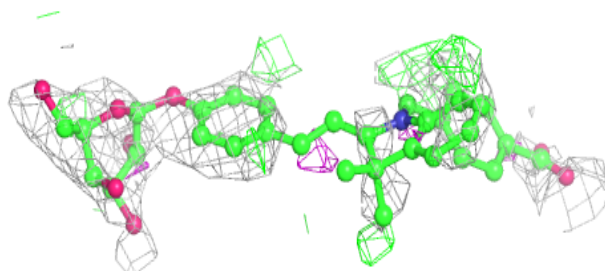
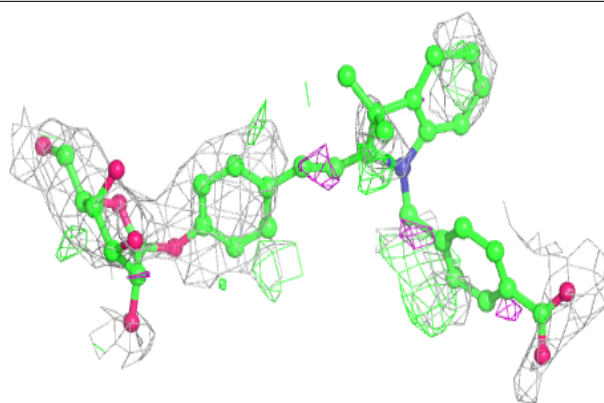
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NA	A	1104	1/1	0.96	0.09	21,21,21,21	0
3	MG	B	1102	1/1	0.97	0.07	26,26,26,26	0
3	MG	A	1102	1/1	0.97	0.11	30,30,30,30	0
4	NA	B	1103	1/1	0.98	0.10	24,24,24,24	0
3	MG	A	1103	1/1	0.98	0.09	19,19,19,19	0

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.

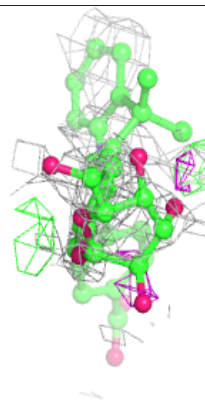
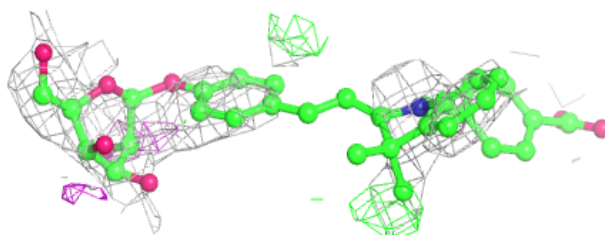
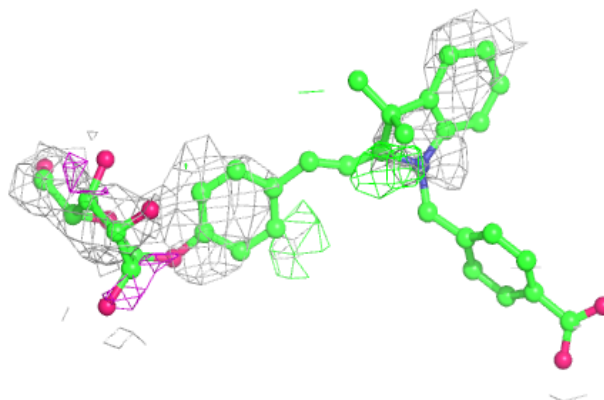


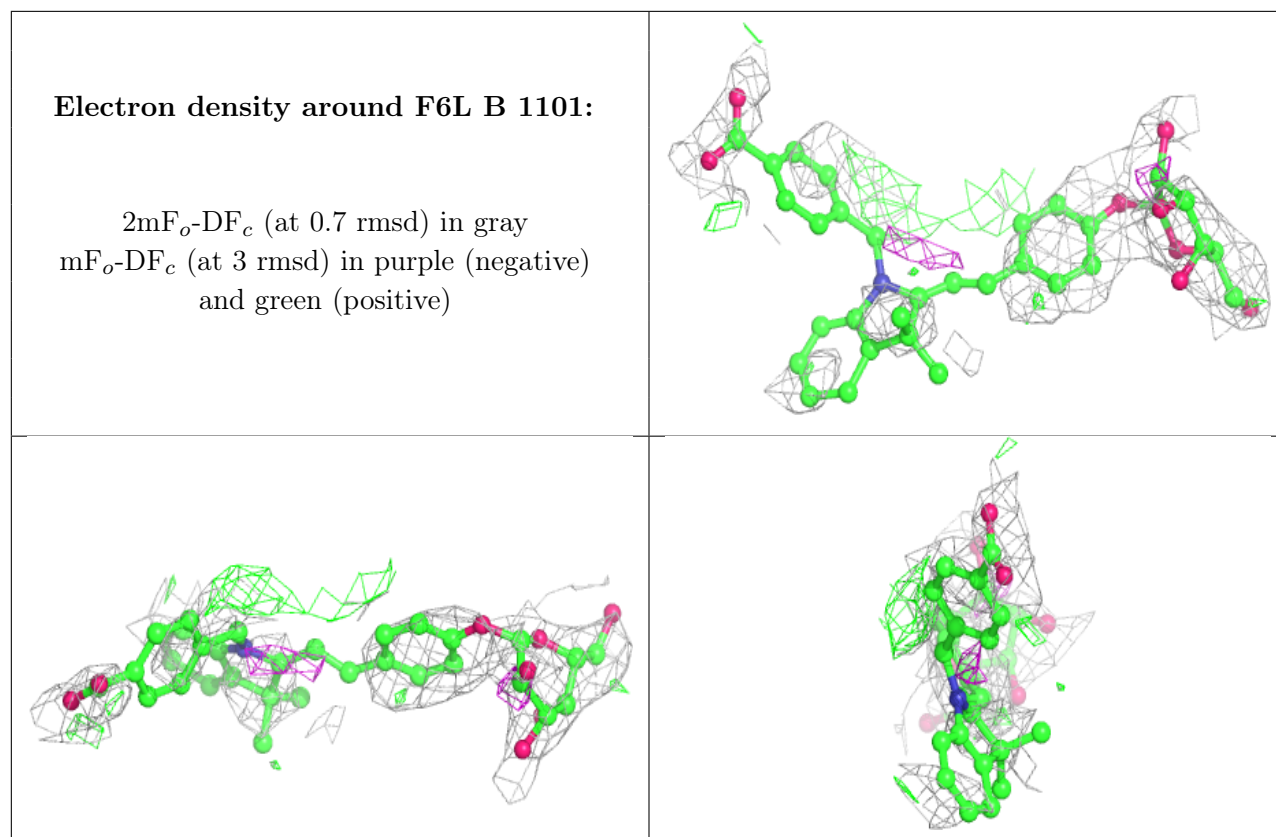
Electron density around F6L A 1101:

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

**Electron density around F6L 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.