



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 04:30 AM BST

PDB ID : 4RPU
Title : Crystal Structure of Human Presequence Protease in Complex with Inhibitor MitoBloCK-60
Authors : Mo, S.M.; Liang, W.G.; King, J.V.; Wijaya, J.; Koehler, C.M.; Tang, W.J.
Deposited on : 2014-10-31
Resolution : 2.27 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 : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

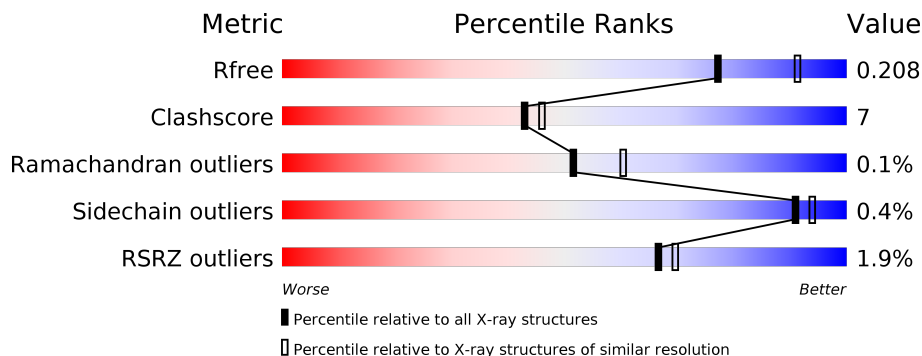
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 on 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	1014	<p>0% 86% 11% ••</p>
2	B	1014	<p>2% 82% 15% •</p>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 17042 atoms, of which 100 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 Presequence protease, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	As	C	N	O	S			
1	A	988	7985	1	5101	1350	1493	40	0	5	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	-	EXPRESSION TAG	UNP Q5JRX3
A	25	HIS	-	EXPRESSION TAG	UNP Q5JRX3
A	26	HIS	-	EXPRESSION TAG	UNP Q5JRX3
A	27	HIS	-	EXPRESSION TAG	UNP Q5JRX3
A	28	HIS	-	EXPRESSION TAG	UNP Q5JRX3
A	29	HIS	-	EXPRESSION TAG	UNP Q5JRX3
A	30	HIS	-	EXPRESSION TAG	UNP Q5JRX3
A	31	ALA	-	EXPRESSION TAG	UNP Q5JRX3
A	32	ALA	-	EXPRESSION TAG	UNP Q5JRX3
A	107	GLN	GLU	ENGINEERED MUTATION	UNP Q5JRX3
A	328	VAL	ILE	SEE REMARK 999	UNP Q5JRX3
A	397	VAL	ALA	SEE REMARK 999	UNP Q5JRX3
A	1037	ARG	GLN	SEE REMARK 999	UNP Q5JRX3

- Molecule 2 is a protein called Presequence protease, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	As	C	N	O	S			
2	B	979	7878	1	5036	1327	1474	40	0	1	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	24	MET	-	EXPRESSION TAG	UNP Q5JRX3
B	25	HIS	-	EXPRESSION TAG	UNP Q5JRX3
B	26	HIS	-	EXPRESSION TAG	UNP Q5JRX3

Continued on next page...

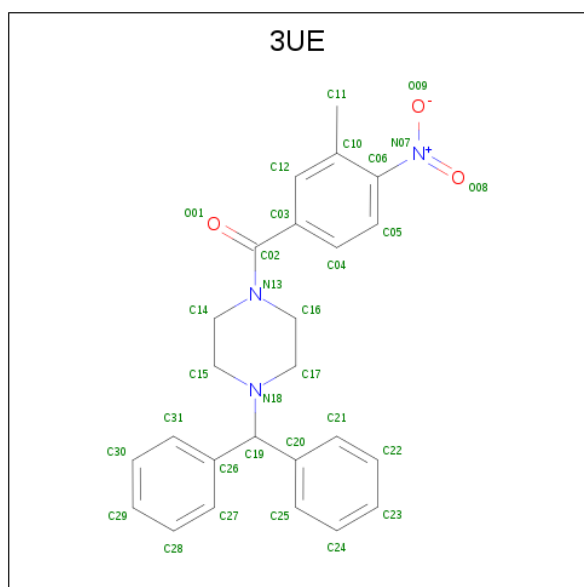
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	27	HIS	-	EXPRESSION TAG	UNP Q5JRX3
B	28	HIS	-	EXPRESSION TAG	UNP Q5JRX3
B	29	HIS	-	EXPRESSION TAG	UNP Q5JRX3
B	30	HIS	-	EXPRESSION TAG	UNP Q5JRX3
B	31	ALA	-	EXPRESSION TAG	UNP Q5JRX3
B	32	ALA	-	EXPRESSION TAG	UNP Q5JRX3
B	107	GLN	GLU	ENGINEERED MUTATION	UNP Q5JRX3
B	328	VAL	ILE	SEE REMARK 999	UNP Q5JRX3
B	397	VAL	ALA	SEE REMARK 999	UNP Q5JRX3
B	1037	ARG	GLN	SEE REMARK 999	UNP Q5JRX3

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Zn 1 1	0	0
3	A	1	Total Zn 1 1	0	0

- Molecule 4 is [4-(diphenylmethyl)piperazin-1-yl](3-methyl-4-nitrophenyl)methanone (three-letter code: 3UE) (formula: C₂₅H₂₅N₃O₃).



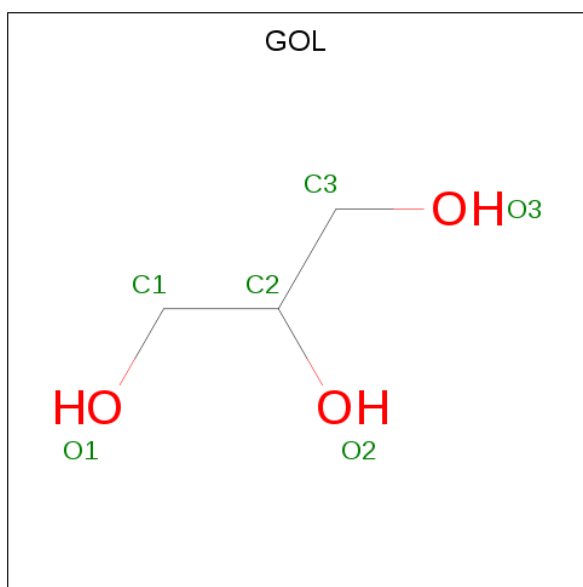
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H N O 56 25 25 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	A	1	Total	C	H	N	O	0	0
			56	25	25	3	3		
4	B	1	Total	C	H	N	O	0	0
			56	25	25	3	3		
4	B	1	Total	C	H	N	O	0	0
			56	25	25	3	3		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



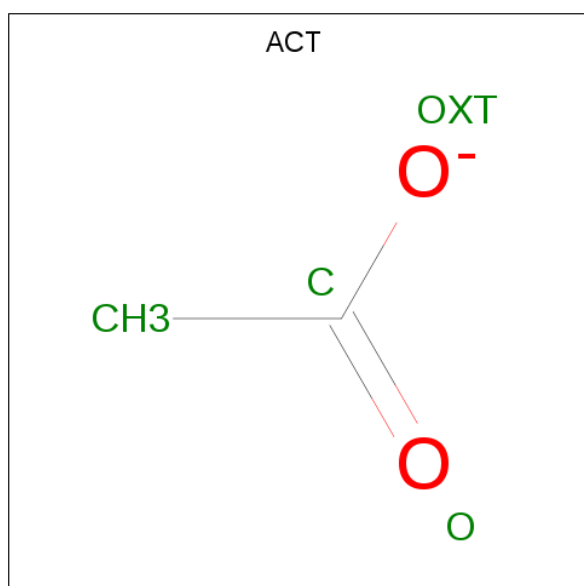
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C O	0	0
			6	3 3		
5	A	1	Total	C O	0	0
			6	3 3		
5	A	1	Total	C O	0	0
			6	3 3		
5	A	1	Total	C O	0	0
			6	3 3		
5	A	1	Total	C O	0	0
			6	3 3		
5	A	1	Total	C O	0	0
			6	3 3		
5	A	1	Total	C O	0	0
			6	3 3		

Continued on next page...

Continued from previous page...

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

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

Continued on next page...

Continued from previous page...

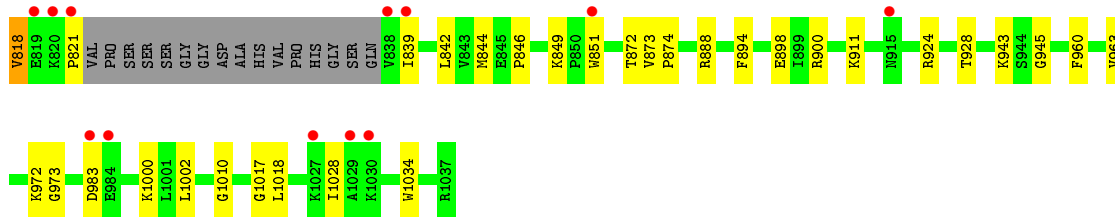
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	2	Total Ca 2 2	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	420	Total O 420 420	0	0
8	B	391	Total O 391 391	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	245.62Å 85.49Å 158.21Å 90.00° 127.53° 90.00°	Depositor
Resolution (Å)	44.85 – 2.27 44.85 – 2.26	Depositor EDS
% Data completeness (in resolution range)	98.5 (44.85-2.27) 93.2 (44.85-2.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.27Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.175 , 0.208 0.179 , 0.208	Depositor DCC
R_{free} test set	1992 reflections (1.67%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtrriage
Anisotropy	0.393	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.015 for -h-2*1,-k,l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17042	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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: GOL, ZN, CAS, CA, 3UE, ACT, MLZ, MLY

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	0.37	0/7776	0.54	4/10565 (0.0%)
2	B	0.35	0/7640	0.51	1/10365 (0.0%)
All	All	0.36	0/15416	0.53	5/20930 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	GLU	CB-CA-C	5.97	122.33	110.40
1	A	894	PHE	N-CA-C	5.81	126.69	111.00
1	A	228	ASP	CB-CA-C	-5.75	98.91	110.40
2	B	928	THR	N-CA-C	5.34	125.42	111.00
1	A	894	PHE	N-CA-CB	-5.29	101.08	110.60

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	7985	0	7877	97	0
2	B	7878	0	7775	112	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	62	50	50	4	0
4	B	62	50	50	2	0
5	A	66	0	88	7	0
5	B	42	0	56	11	0
6	A	12	0	9	0	0
6	B	20	0	15	2	0
7	B	2	0	0	0	0
8	A	420	0	0	6	0
8	B	391	0	0	7	0
All	All	16942	100	15920	217	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 7.

All (217) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:822:VAL:HB	1:A:838:VAL:HG13	1.40	1.00
2:B:380:TYR:HB3	5:B:1105:GOL:H31	1.57	0.87
1:A:248:GLU:OE2	1:A:251:MLY:HH12	1.74	0.86
1:A:326:THR:HG21	1:A:401:ILE:HD11	1.57	0.85
2:B:398:GLU:HG3	2:B:505:ARG:HH21	1.46	0.81
1:A:946:MLY:HG2	1:A:946:MLY:HH22	1.60	0.80
1:A:283:GLU:O	1:A:287:MLY:HE3	1.84	0.78
1:A:272:PRO:HA	5:A:1111:GOL:H2	1.67	0.77
1:A:853:MET:HE1	1:A:1035:ILE:HD11	1.68	0.76
2:B:466:MLY:HG3	5:B:1107:GOL:H32	1.70	0.73
1:A:171:CYS:SG	8:A:1372:HOH:O	2.47	0.72
1:A:915:ASN:ND2	1:A:915:ASN:O	2.23	0.71
1:A:696:GLU:OE2	1:A:759:MLY:HH23	1.89	0.71
2:B:102:VAL:HG13	2:B:103:PRO:HD3	1.72	0.70
1:A:822:VAL:HB	1:A:838:VAL:CG1	2.20	0.69
1:A:367:GLU:HG3	8:A:1439:HOH:O	1.93	0.69
2:B:945:GLY:HA3	2:B:1002:LEU:HD21	1.75	0.68
2:B:973:GLY:H	6:B:1114:ACT:H3	1.58	0.67
1:A:696:GLU:HG3	1:A:758:ILE:HD11	1.78	0.66
2:B:677:LEU:HD21	2:B:792:THR:HA	1.76	0.66
2:B:782:VAL:HG11	2:B:792:THR:HG21	1.77	0.66
2:B:323:SER:HA	8:B:1500:HOH:O	1.94	0.66
2:B:185:GLU:HG2	2:B:199:MLZ:HCM2	1.77	0.66
2:B:582:ASP:OD1	2:B:582:ASP:N	2.30	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:GLU:OE2	1:A:251:MLY:HH23	1.97	0.65
1:A:582:ASP:N	1:A:582:ASP:OD1	2.28	0.64
1:A:782:VAL:HG11	1:A:792:THR:HG21	1.79	0.64
1:A:357:PRO:HA	1:A:362:TYR:CD1	2.33	0.64
2:B:398:GLU:HG3	2:B:505:ARG:NH2	2.14	0.63
1:A:138:PHE:CZ	1:A:145:LEU:HD23	2.32	0.63
1:A:677:LEU:HB3	1:A:678:PRO:HD3	1.81	0.63
1:A:326:THR:HG21	1:A:401:ILE:CD1	2.28	0.63
1:A:328:VAL:HG12	1:A:396:ILE:CD1	2.29	0.62
2:B:326:THR:HG21	2:B:401:ILE:HD11	1.82	0.62
1:A:765:LEU:HB2	1:A:766:PRO:HD3	1.82	0.62
1:A:677:LEU:HD21	1:A:792:THR:HA	1.81	0.62
1:A:111:LEU:HD12	5:A:1106:GOL:H32	1.81	0.62
1:A:853:MET:HE1	1:A:1035:ILE:CD1	2.30	0.61
1:A:794:MLY:HH12	1:A:798:ASP:OD2	2.00	0.61
1:A:740:PHE:O	1:A:745:GLN:HG2	2.00	0.61
2:B:323:SER:N	8:B:1486:HOH:O	2.33	0.60
2:B:720:LEU:HD23	2:B:911:MLY:HH21	1.84	0.60
5:B:1109:GOL:H11	8:B:1323:HOH:O	2.01	0.60
2:B:136:ASN:O	2:B:147:PRO:HD2	2.02	0.59
2:B:174:GLU:OE2	2:B:540:MLY:HH12	2.01	0.59
1:A:946:MLY:CG	1:A:946:MLY:HH22	2.29	0.59
2:B:120:ARG:O	2:B:125:MLZ:HE2	2.02	0.59
1:A:666:VAL:HG21	1:A:772:LEU:HD21	1.84	0.59
1:A:714:ILE:HB	1:A:715:PRO:HD3	1.85	0.59
2:B:759:MLZ:N	2:B:760:PRO:HD2	2.17	0.59
1:A:433:GLU:OE2	1:A:437:MLZ:HCM2	2.03	0.58
2:B:844:MET:HG2	2:B:846:PRO:HD3	1.86	0.58
2:B:496:ASN:O	2:B:499:MLY:HE3	2.03	0.58
6:B:1113:ACT:H1	8:B:1272:HOH:O	2.03	0.58
2:B:509:LYS:O	2:B:513:MLY:HG2	2.04	0.58
2:B:765:LEU:HB2	2:B:766:PRO:HD3	1.84	0.58
1:A:321:ASP:OD1	1:A:321:ASP:N	2.36	0.57
1:A:1017:GLY:C	1:A:1018:LEU:HD12	2.24	0.57
2:B:761:ILE:O	2:B:764:MLZ:HB3	2.04	0.56
2:B:873:VAL:HB	2:B:874:PRO:HD2	1.87	0.56
1:A:342:GLU:OE2	1:A:488:MLY:HH23	2.07	0.55
1:A:283:GLU:O	1:A:287:MLY:CE	2.54	0.55
1:A:102:VAL:HG13	1:A:103:PRO:HD3	1.87	0.55
2:B:102:VAL:CG1	2:B:103:PRO:HD3	2.36	0.55
2:B:97:MET:HE1	2:B:230:THR:HB	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:324:MLZ:HG2	2:B:397:VAL:CG2	2.37	0.55
1:A:155:ASP:HB2	1:A:560:LEU:HD11	1.88	0.55
1:A:898:GLU:OE2	1:A:902:MLY:HH12	2.07	0.54
2:B:740:PHE:O	2:B:745:GLN:HG2	2.06	0.54
1:A:898:GLU:OE1	1:A:902:MLY:HH23	2.08	0.54
1:A:704:MLY:HH12	8:A:1454:HOH:O	2.07	0.54
2:B:216:ILE:HG12	5:B:1104:GOL:H11	1.90	0.53
2:B:714:ILE:HB	2:B:715:PRO:HD3	1.90	0.53
2:B:174:GLU:OE1	2:B:540:MLY:HH23	2.09	0.53
2:B:849:LYS:O	2:B:851:TRP:HE3	1.92	0.53
2:B:782:VAL:CG1	2:B:792:THR:HG21	2.39	0.52
1:A:854:MLY:HH12	1:A:1033:SER:OG	2.08	0.52
2:B:894:PHE:CE1	2:B:898:GLU:HG3	2.45	0.52
2:B:960:PHE:HA	2:B:963:VAL:HG22	1.91	0.52
2:B:900:ARG:HH22	5:B:1106:GOL:H11	1.74	0.52
1:A:659:MET:CE	1:A:872:THR:O	2.58	0.52
2:B:695:GLU:HG3	2:B:698:HIS:HB3	1.92	0.52
1:A:700:MLY:CG	1:A:758:ILE:HG12	2.40	0.51
1:A:94:THR:O	1:A:142:ASP:HA	2.11	0.51
1:A:897:THR:HA	1:A:901:GLU:HB2	1.91	0.51
1:A:208:GLY:HA3	1:A:924:ARG:HD3	1.93	0.50
2:B:943:MLY:HH12	2:B:1010:GLY:HA3	1.93	0.50
1:A:393:LEU:HB2	1:A:396:ILE:HD11	1.92	0.50
2:B:571:VAL:HG13	2:B:983:ASP:OD2	2.12	0.50
1:A:757:ASP:OD1	1:A:759:MLY:HH22	2.12	0.50
2:B:109:THR:O	2:B:112:CAS:HB3	2.11	0.50
1:A:494:LYS:NZ	8:A:1614:HOH:O	2.31	0.50
1:A:174:GLU:OE1	1:A:540:MLY:HH23	2.11	0.50
1:A:946:MLY:HH11	2:B:894:PHE:CD2	2.47	0.49
2:B:324:MLZ:HG2	2:B:397:VAL:HG22	1.94	0.49
2:B:572:THR:HG22	2:B:972:MLY:HH13	1.93	0.49
1:A:136:ASN:O	1:A:147:PRO:HD2	2.12	0.49
2:B:1028:ILE:HG23	2:B:1034:TRP:CG	2.47	0.49
2:B:260:PRO:HB3	2:B:285:LEU:CD2	2.43	0.49
1:A:370:LEU:CD1	1:A:407:LEU:HD12	2.42	0.49
2:B:752:ILE:CG2	2:B:758:ILE:HD11	2.43	0.49
1:A:873:VAL:HB	1:A:874:PRO:HD2	1.94	0.49
2:B:260:PRO:HB3	2:B:285:LEU:HD22	1.93	0.49
1:A:853:MET:CE	1:A:1035:ILE:CD1	2.91	0.49
1:A:111:LEU:HD12	5:A:1106:GOL:C3	2.43	0.48
2:B:1017:GLY:C	2:B:1018:LEU:HD12	2.33	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:THR:HB	5:B:1109:GOL:H31	1.95	0.48
2:B:759:MLZ:O	2:B:763:ARG:HG3	2.12	0.48
1:A:960:PHE:HA	1:A:963:VAL:HG22	1.95	0.48
2:B:138:PHE:CZ	2:B:145:LEU:HD23	2.49	0.48
1:A:102:VAL:CG1	1:A:103:PRO:HD3	2.44	0.48
1:A:367:GLU:OE2	1:A:698:HIS:ND1	2.47	0.48
1:A:410:ARG:O	1:A:414:GLU:HG3	2.14	0.48
2:B:663:GLU:HB2	2:B:842:LEU:HG	1.95	0.48
2:B:229:HIS:CG	2:B:230:THR:H	2.32	0.47
1:A:575:ASP:OD2	5:A:1114:GOL:O1	2.32	0.47
2:B:106:LEU:O	2:B:110:VAL:HG13	2.14	0.47
2:B:357:PRO:HA	2:B:362:TYR:CD1	2.50	0.47
2:B:102:VAL:HG13	2:B:103:PRO:CD	2.44	0.47
2:B:728:ARG:CG	2:B:729:THR:HG23	2.44	0.47
4:B:1102:3UE:C04	4:B:1102:3UE:H12	2.44	0.47
2:B:45:LYS:HE2	8:B:1574:HOH:O	2.14	0.47
1:A:512:GLU:OE1	1:A:512:GLU:N	2.45	0.47
1:A:791:GLN:OE1	1:A:791:GLN:N	2.36	0.47
1:A:759:MLY:O	1:A:763:ARG:HG3	2.15	0.47
5:B:1106:GOL:O3	5:B:1106:GOL:O1	2.31	0.47
2:B:818:VAL:HG11	2:B:844:MET:HE1	1.96	0.46
4:A:1103:3UE:H12	4:A:1103:3UE:C12	2.45	0.46
1:A:229:HIS:CG	1:A:230:THR:H	2.33	0.46
2:B:412:ILE:O	2:B:416:VAL:HG23	2.15	0.46
2:B:595:MET:CE	2:B:671:LEU:HD12	2.45	0.46
1:A:1000:MLZ:HD3	1:A:1000:MLZ:HCM3	1.50	0.46
2:B:71:ASP:O	2:B:290:MLY:HB3	2.16	0.46
2:B:507:ASP:OD2	2:B:513:MLY:HH23	2.15	0.46
2:B:945:GLY:CA	2:B:1002:LEU:HD21	2.43	0.46
2:B:102:VAL:N	2:B:103:PRO:HD2	2.30	0.46
2:B:466:MLY:CG	5:B:1107:GOL:H32	2.43	0.45
2:B:529:LEU:HD22	2:B:533:ASP:HB3	1.99	0.45
1:A:272:PRO:HA	5:A:1111:GOL:C2	2.40	0.45
1:A:102:VAL:N	1:A:103:PRO:HD2	2.31	0.45
1:A:328:VAL:HG12	1:A:396:ILE:HD12	1.98	0.45
1:A:822:VAL:CB	1:A:838:VAL:HG13	2.27	0.45
2:B:550:MLY:HD2	2:B:550:MLY:HH23	1.77	0.45
1:A:821:PRO:HB3	1:A:839:ILE:HD12	1.99	0.45
2:B:696:GLU:OE1	2:B:759:MLZ:HCM2	2.17	0.45
2:B:401:ILE:O	2:B:405:ARG:HG3	2.16	0.45
2:B:900:ARG:NH2	5:B:1106:GOL:H11	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LEU:O	1:A:81:ARG:NH1	2.50	0.44
2:B:1000:MLZ:HCM3	2:B:1000:MLZ:HD3	1.47	0.44
1:A:700:MLY:HG2	1:A:758:ILE:HG12	2.00	0.44
2:B:332:PHE:CE2	2:B:499:MLY:HD2	2.52	0.44
1:A:342:GLU:OE1	1:A:488:MLY:HH12	2.17	0.44
1:A:696:GLU:OE1	1:A:759:MLY:HH12	2.18	0.44
1:A:109:THR:O	1:A:112:CAS:HB3	2.17	0.44
4:A:1102:3UE:C04	4:A:1102:3UE:H12	2.46	0.44
1:A:322:PRO:HA	1:A:506:PRO:HG2	1.99	0.44
1:A:716:ASP:HB2	8:A:1226:HOH:O	2.16	0.44
2:B:789:MET:HB3	2:B:790:PRO:HD3	2.00	0.43
2:B:185:GLU:HB3	2:B:199:MLZ:HD3	2.00	0.43
2:B:75:ARG:NH2	2:B:458:ASP:OD1	2.52	0.43
2:B:821:PRO:HA	2:B:839:ILE:HD13	1.99	0.43
5:A:1112:GOL:H11	8:A:1494:HOH:O	2.18	0.43
2:B:301:THR:HA	2:B:302:PRO:HD3	1.90	0.43
2:B:659:MET:CE	2:B:872:THR:O	2.67	0.43
1:A:370:LEU:HD11	1:A:407:LEU:HD12	2.00	0.43
2:B:260:PRO:CB	2:B:285:LEU:HD22	2.48	0.43
1:A:174:GLU:OE1	1:A:540:MLY:HE3	2.18	0.43
1:A:663:GLU:HB2	1:A:842:LEU:HG	2.00	0.43
1:A:888:ARG:HD2	1:A:888:ARG:HA	1.78	0.43
2:B:728:ARG:HG2	2:B:729:THR:HG23	2.01	0.43
2:B:89:SER:HA	2:B:146:TYR:O	2.18	0.43
1:A:750:MLY:HD3	1:A:750:MLY:HH12	1.66	0.43
1:A:853:MET:CE	1:A:1035:ILE:HD12	2.49	0.43
1:A:106:LEU:HA	1:A:250:LEU:HD11	2.01	0.42
2:B:396:ILE:HD11	2:B:401:ILE:HG12	2.00	0.42
2:B:552:GLN:OE1	8:B:1258:HOH:O	2.21	0.42
2:B:604:LEU:HD23	2:B:772:LEU:HD21	2.01	0.42
1:A:427:ALA:HB1	1:A:640:GLU:HG2	2.00	0.42
1:A:782:VAL:CG1	1:A:792:THR:HG21	2.47	0.42
2:B:278:MLY:HD2	2:B:278:MLY:HH13	1.52	0.42
2:B:334:LEU:HB3	2:B:335:PRO:CD	2.49	0.42
1:A:759:MLY:N	1:A:760:PRO:CD	2.82	0.42
2:B:281:HIS:HA	2:B:285:LEU:HB2	2.02	0.42
1:A:75:ARG:NH2	1:A:458:ASP:OD1	2.51	0.42
1:A:758:ILE:HD12	1:A:758:ILE:C	2.39	0.42
2:B:94:THR:O	2:B:142:ASP:HA	2.20	0.42
2:B:70:ASP:O	2:B:290:MLY:HH12	2.18	0.42
2:B:208:GLY:HA3	2:B:924:ARG:HD3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:HIS:CD2	5:B:1109:GOL:H32	2.54	0.42
2:B:75:ARG:NH1	8:B:1440:HOH:O	2.53	0.42
2:B:436:MET:HG2	2:B:467:LEU:HD12	2.02	0.42
2:B:677:LEU:HB3	2:B:678:PRO:HD3	2.02	0.42
2:B:242:ILE:HB	2:B:243:PRO:HD3	2.02	0.42
1:A:182:TRP:HA	1:A:199:LYS:O	2.21	0.41
4:B:1103:3UE:C12	4:B:1103:3UE:H12	2.50	0.41
2:B:53:GLN:HB3	2:B:66:MLZ:HB3	2.01	0.41
4:A:1103:3UE:C25	4:A:1103:3UE:H13	2.49	0.41
2:B:155:ASP:HB2	2:B:560:LEU:HD11	2.03	0.41
2:B:849:LYS:O	2:B:851:TRP:CE3	2.73	0.41
1:A:95:THR:OG1	5:A:1110:GOL:H32	2.21	0.41
2:B:671:LEU:HD23	2:B:671:LEU:N	2.36	0.41
2:B:466:MLY:HG3	5:B:1107:GOL:C3	2.45	0.41
2:B:604:LEU:HG	2:B:665:GLY:HA2	2.03	0.41
2:B:297:VAL:O	2:B:385:ARG:NH1	2.48	0.41
1:A:888:ARG:HG2	1:A:958:SER:HB3	2.02	0.41
2:B:182:TRP:CE2	2:B:243:PRO:HA	2.56	0.41
1:A:382:GLY:N	4:A:1102:3UE:O08	2.53	0.41
2:B:327:THR:O	2:B:503:SER:HA	2.21	0.41
2:B:41:MLY:HH22	2:B:41:MLY:HD3	1.74	0.40
2:B:512:GLU:N	2:B:512:GLU:OE1	2.47	0.40
2:B:752:ILE:HG23	2:B:758:ILE:HD11	2.03	0.40
2:B:888:ARG:HA	2:B:888:ARG:HD2	1.79	0.40
1:A:89:SER:HA	1:A:146:TYR:O	2.21	0.40
2:B:317:SER:HB2	2:B:318:PHE:CE1	2.56	0.40
1:A:794:MLY:HH23	1:A:794:MLY:HD3	1.90	0.40
1:A:821:PRO:HA	1:A:839:ILE:HD13	2.03	0.40
2:B:844:MET:HE2	2:B:844:MET:HB3	1.83	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	950/1014 (94%)	937 (99%)	12 (1%)	1 (0%)	51 60
2	B	931/1014 (92%)	919 (99%)	11 (1%)	1 (0%)	51 60
All	All	1881/2028 (93%)	1856 (99%)	23 (1%)	2 (0%)	51 60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	147	PRO
1	A	147	PRO

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	848/864 (98%)	842 (99%)	6 (1%)	84 90
2	B	834/862 (97%)	832 (100%)	2 (0%)	93 96
All	All	1682/1726 (98%)	1674 (100%)	8 (0%)	91 92

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	321	ASP
1	A	716	ASP
1	A	728	ARG
1	A	777[A]	ASN
1	A	777[B]	ASN
1	A	811	ARG
2	B	107	GLN
2	B	818	VAL

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

Mol	Chain	Res	Type
1	A	915	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

76 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MLZ	B	125	2	8,9,10	1.06	0	4,9,11	0.65	0
2	MLZ	B	884	2	8,9,10	1.10	0	4,9,11	1.02	0
1	MLY	A	278	1	9,10,11	0.51	0	6,11,13	0.65	0
1	MLY	A	794	1	9,10,11	0.55	0	6,11,13	0.53	0
2	MLY	B	525	2	9,10,11	0.59	0	6,11,13	0.70	0
1	MLY	A	764	1	9,10,11	0.48	0	6,11,13	0.85	0
2	MLZ	B	1013	2	8,9,10	1.18	0	4,9,11	0.68	0
1	MLY	A	854	1	9,10,11	0.61	0	6,11,13	0.65	0
1	MLY	A	466	1	9,10,11	0.47	0	6,11,13	0.85	0
1	MLZ	A	769	1	8,9,10	1.13	0	4,9,11	0.82	0
2	MLZ	B	759	2	8,9,10	1.05	0	4,9,11	0.86	0
1	MLZ	A	884	1	8,9,10	1.14	0	4,9,11	0.87	0
1	MLZ	A	972	1	8,9,10	1.07	0	4,9,11	0.89	0
1	MLY	A	700	1	9,10,11	0.53	0	6,11,13	1.10	0
1	MLZ	A	943	1	8,9,10	1.12	0	4,9,11	0.84	0
2	MLY	B	540	2	9,10,11	0.47	0	6,11,13	0.69	0
2	MLZ	B	490	2	8,9,10	1.20	0	4,9,11	1.03	0
2	MLZ	B	764	2	8,9,10	1.13	0	4,9,11	0.92	0
2	MLY	B	278	2	9,10,11	0.52	0	6,11,13	0.74	0
1	MLY	A	911	1	9,10,11	0.65	0	6,11,13	0.92	0
1	MLZ	A	66	1	8,9,10	1.05	0	4,9,11	0.85	0
2	MLZ	B	199	2	8,9,10	1.11	0	4,9,11	1.02	0
2	MLZ	B	854	2	8,9,10	1.09	0	4,9,11	0.87	0
1	MLZ	A	525	1	8,9,10	1.17	0	4,9,11	1.03	0
1	CAS	A	112	1	5,8,9	1.34	1 (20%)	1,9,11	1.33	0
2	MLY	B	466	2	9,10,11	0.55	0	6,11,13	0.89	0
1	MLY	A	946	1	9,10,11	0.52	0	6,11,13	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	A	513	1	9,10,11	0.56	0	6,11,13	0.79	0
2	MLY	B	550	2	9,10,11	0.55	0	6,11,13	1.02	0
1	MLY	A	704	1	9,10,11	0.63	0	6,11,13	0.78	0
1	MLY	A	488	1	9,10,11	0.51	0	6,11,13	0.60	0
1	MLY	A	287	1	9,10,11	0.44	0	6,11,13	0.63	0
2	MLY	B	911	2	9,10,11	0.55	0	6,11,13	0.89	0
1	MLY	A	251	1	9,10,11	0.61	0	6,11,13	0.90	0
2	MLZ	B	624	2	8,9,10	1.05	0	4,9,11	0.94	0
2	CAS	B	112	2	5,8,9	1.37	0	1,9,11	1.68	0
2	MLY	B	750	2	9,10,11	0.53	0	6,11,13	0.76	0
1	MLY	A	521	1	9,10,11	0.59	0	6,11,13	0.84	0
2	MLZ	B	902	2	8,9,10	1.03	0	4,9,11	0.90	0
1	MLY	A	363	1	9,10,11	0.58	0	6,11,13	0.76	0
1	MLY	A	642	1	9,10,11	0.46	0	6,11,13	0.98	0
1	MLZ	A	1000	1	8,9,10	1.15	1 (12%)	4,9,11	0.86	0
2	MLZ	B	1000	2	8,9,10	1.14	0	4,9,11	1.01	0
1	MLY	A	902	1	9,10,11	0.56	0	6,11,13	0.55	0
1	MLY	A	540	1	9,10,11	0.55	0	6,11,13	0.71	0
1	MLY	A	154	1	9,10,11	0.53	0	6,11,13	0.83	0
1	MLY	A	431	1	9,10,11	0.59	0	6,11,13	1.00	0
2	MLY	B	642	2	9,10,11	0.48	0	6,11,13	0.82	0
1	MLY	A	116	1	9,10,11	0.45	0	6,11,13	1.00	0
2	MLY	B	488	2	9,10,11	0.49	0	6,11,13	0.83	0
2	MLY	B	499	2	9,10,11	0.53	0	6,11,13	0.82	0
2	MLY	B	513	2	9,10,11	0.52	0	6,11,13	0.77	0
2	MLZ	B	324	2	8,9,10	1.14	0	4,9,11	0.65	0
1	MLZ	A	437	1	8,9,10	1.06	0	4,9,11	0.74	0
2	MLZ	B	494	2	8,9,10	1.09	0	4,9,11	0.79	0
2	MLY	B	41	2	9,10,11	0.52	0	6,11,13	0.96	0
1	MLZ	A	207	1	8,9,10	1.08	0	4,9,11	0.80	0
2	MLY	B	363	2	9,10,11	0.69	0	6,11,13	0.64	0
1	MLZ	A	937	1	8,9,10	1.08	0	4,9,11	0.79	0
1	MLY	A	750	1	9,10,11	0.46	0	6,11,13	0.89	0
1	MLY	A	759	1	9,10,11	0.50	0	6,11,13	0.72	0
2	MLY	B	972	2	9,10,11	0.59	0	6,11,13	0.80	0
2	MLY	B	290	2	9,10,11	0.59	0	6,11,13	0.77	0
2	MLY	B	116	2	9,10,11	0.51	0	6,11,13	0.91	0
2	MLZ	B	769	2	8,9,10	1.13	0	4,9,11	0.93	0
2	MLY	B	287	2	9,10,11	0.54	0	6,11,13	0.89	0
2	MLY	B	431	2	9,10,11	0.51	0	6,11,13	1.16	0
1	MLY	A	956	1	9,10,11	0.53	0	6,11,13	1.05	0
2	MLZ	B	937	2	8,9,10	1.02	0	4,9,11	0.71	0
1	MLZ	A	550	1	8,9,10	1.13	0	4,9,11	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MLY	B	946	2	9,10,11	0.46	0	6,11,13	1.00	0
2	MLY	B	943	2	9,10,11	0.62	0	6,11,13	0.77	0
2	MLY	B	986	2	9,10,11	0.49	0	6,11,13	0.71	0
1	MLY	A	290	1	9,10,11	0.59	0	6,11,13	0.74	0
2	MLZ	B	956	2	8,9,10	1.02	0	4,9,11	0.68	0
2	MLZ	B	66	2	8,9,10	0.96	0	4,9,11	0.58	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	MLZ	B	125	2	-	1/7/8/10	-
2	MLZ	B	884	2	-	0/7/8/10	-
1	MLY	A	278	1	-	0/8/9/11	-
1	MLY	A	794	1	-	2/8/9/11	-
2	MLY	B	525	2	-	2/8/9/11	-
1	MLY	A	764	1	-	0/8/9/11	-
2	MLZ	B	1013	2	-	5/7/8/10	-
1	MLY	A	854	1	-	0/8/9/11	-
1	MLY	A	466	1	-	2/8/9/11	-
1	MLZ	A	769	1	-	3/7/8/10	-
2	MLZ	B	759	2	-	0/7/8/10	-
1	MLZ	A	884	1	-	1/7/8/10	-
1	MLZ	A	972	1	-	2/7/8/10	-
1	MLY	A	700	1	-	2/8/9/11	-
1	MLZ	A	943	1	-	2/7/8/10	-
2	MLY	B	540	2	-	2/8/9/11	-
2	MLZ	B	490	2	-	0/7/8/10	-
2	MLZ	B	764	2	-	3/7/8/10	-
2	MLY	B	278	2	-	2/8/9/11	-
1	MLY	A	911	1	-	0/8/9/11	-
1	MLZ	A	66	1	-	3/7/8/10	-
2	MLZ	B	199	2	-	1/7/8/10	-
2	MLZ	B	854	2	-	1/7/8/10	-
1	MLZ	A	525	1	-	2/7/8/10	-
1	CAS	A	112	1	-	0/0/7/9	-
2	MLY	B	466	2	-	3/8/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	946	1	-	0/8/9/11	-
1	MLY	A	513	1	-	0/8/9/11	-
2	MLY	B	550	2	-	0/8/9/11	-
1	MLY	A	704	1	-	0/8/9/11	-
1	MLY	A	488	1	-	2/8/9/11	-
1	MLY	A	287	1	-	0/8/9/11	-
2	MLY	B	911	2	-	0/8/9/11	-
1	MLY	A	251	1	-	0/8/9/11	-
2	MLZ	B	624	2	-	1/7/8/10	-
2	CAS	B	112	2	-	0/0/7/9	-
2	MLY	B	750	2	-	1/8/9/11	-
1	MLY	A	521	1	-	2/8/9/11	-
2	MLZ	B	902	2	-	0/7/8/10	-
1	MLY	A	363	1	-	0/8/9/11	-
1	MLY	A	642	1	-	0/8/9/11	-
1	MLZ	A	1000	1	-	3/7/8/10	-
2	MLZ	B	1000	2	-	3/7/8/10	-
1	MLY	A	902	1	-	2/8/9/11	-
1	MLY	A	540	1	-	2/8/9/11	-
1	MLY	A	154	1	-	0/8/9/11	-
1	MLY	A	431	1	-	1/8/9/11	-
2	MLY	B	642	2	-	0/8/9/11	-
1	MLY	A	116	1	-	0/8/9/11	-
2	MLY	B	488	2	-	0/8/9/11	-
2	MLY	B	499	2	-	1/8/9/11	-
2	MLY	B	513	2	-	2/8/9/11	-
2	MLZ	B	324	2	-	4/7/8/10	-
1	MLZ	A	437	1	-	4/7/8/10	-
2	MLZ	B	494	2	-	0/7/8/10	-
2	MLY	B	41	2	-	0/8/9/11	-
1	MLZ	A	207	1	-	1/7/8/10	-
2	MLY	B	363	2	-	0/8/9/11	-
1	MLZ	A	937	1	-	2/7/8/10	-
1	MLY	A	750	1	-	2/8/9/11	-
1	MLY	A	759	1	-	2/8/9/11	-
2	MLY	B	972	2	-	4/8/9/11	-
2	MLY	B	290	2	-	0/8/9/11	-
2	MLY	B	116	2	-	3/8/9/11	-
2	MLZ	B	769	2	-	3/7/8/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLY	B	287	2	-	0/8/9/11	-
2	MLY	B	431	2	-	1/8/9/11	-
1	MLY	A	956	1	-	1/8/9/11	-
2	MLZ	B	937	2	-	2/7/8/10	-
1	MLZ	A	550	1	-	2/7/8/10	-
2	MLY	B	946	2	-	0/8/9/11	-
2	MLY	B	943	2	-	3/8/9/11	-
2	MLY	B	986	2	-	1/8/9/11	-
1	MLY	A	290	1	-	1/8/9/11	-
2	MLZ	B	956	2	-	1/7/8/10	-
2	MLZ	B	66	2	-	2/7/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1000	MLZ	CA-N	-2.04	1.42	1.48
1	A	112	CAS	O-C	2.03	1.28	1.19

There are no bond angle outliers.

There are no chirality outliers.

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1013	MLZ	N-CA-CB-CG
2	B	1013	MLZ	C-CA-CB-CG
1	A	769	MLZ	C-CA-CB-CG
1	A	1000	MLZ	C-CA-CB-CG
2	B	1000	MLZ	CD-CE-NZ-CM
1	A	437	MLZ	O-C-CA-CB
2	B	324	MLZ	N-CA-CB-CG
2	B	324	MLZ	C-CA-CB-CG
2	B	324	MLZ	O-C-CA-CB
2	B	972	MLY	N-CA-CB-CG
2	B	972	MLY	C-CA-CB-CG
2	B	116	MLY	O-C-CA-CB
2	B	943	MLY	O-C-CA-CB
2	B	66	MLZ	C-CA-CB-CG
2	B	769	MLZ	CG-CD-CE-NZ
2	B	513	MLY	CD-CE-NZ-CH2
2	B	466	MLY	CD-CE-NZ-CH2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	972	MLY	CD-CE-NZ-CH1
2	B	278	MLY	CG-CD-CE-NZ
1	A	972	MLZ	CG-CD-CE-NZ
1	A	1000	MLZ	CD-CE-NZ-CM
1	A	902	MLY	CD-CE-NZ-CH2
2	B	972	MLY	CD-CE-NZ-CH2
2	B	116	MLY	CD-CE-NZ-CH1
2	B	431	MLY	CD-CE-NZ-CH2
1	A	956	MLY	CD-CE-NZ-CH2
1	A	759	MLY	CG-CD-CE-NZ
1	A	550	MLZ	CG-CD-CE-NZ
1	A	750	MLY	CG-CD-CE-NZ
1	A	700	MLY	CD-CE-NZ-CH2
2	B	278	MLY	CD-CE-NZ-CH1
1	A	521	MLY	CD-CE-NZ-CH2
2	B	943	MLY	CD-CE-NZ-CH2
1	A	290	MLY	CD-CE-NZ-CH2
2	B	1013	MLZ	CD-CE-NZ-CM
2	B	199	MLZ	CD-CE-NZ-CM
1	A	488	MLY	CG-CD-CE-NZ
1	A	1000	MLZ	CG-CD-CE-NZ
2	B	324	MLZ	CD-CE-NZ-CM
2	B	769	MLZ	CA-CB-CG-CD
2	B	1000	MLZ	CG-CD-CE-NZ
1	A	540	MLY	CD-CE-NZ-CH1
1	A	759	MLY	CD-CE-NZ-CH2
1	A	794	MLY	CG-CD-CE-NZ
1	A	207	MLZ	CE-CD-CG-CB
1	A	521	MLY	CA-CB-CG-CD
2	B	943	MLY	CD-CE-NZ-CH1
1	A	66	MLZ	CE-CD-CG-CB
2	B	1013	MLZ	CG-CD-CE-NZ
2	B	854	MLZ	CG-CD-CE-NZ
1	A	437	MLZ	CG-CD-CE-NZ
2	B	750	MLY	CE-CD-CG-CB
1	A	937	MLZ	CE-CD-CG-CB
1	A	794	MLY	CE-CD-CG-CB
1	A	66	MLZ	CA-CB-CG-CD
2	B	764	MLZ	CG-CD-CE-NZ
1	A	884	MLZ	CA-CB-CG-CD
1	A	943	MLZ	C-CA-CB-CG
2	B	540	MLY	C-CA-CB-CG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	525	MLY	CD-CE-NZ-CH2
2	B	513	MLY	CD-CE-NZ-CH1
2	B	466	MLY	CD-CE-NZ-CH1
1	A	488	MLY	CD-CE-NZ-CH2
2	B	116	MLY	CD-CE-NZ-CH2
1	A	972	MLZ	CA-CB-CG-CD
2	B	125	MLZ	CG-CD-CE-NZ
2	B	937	MLZ	CG-CD-CE-NZ
1	A	66	MLZ	CG-CD-CE-NZ
1	A	902	MLY	CD-CE-NZ-CH1
2	B	466	MLY	CE-CD-CG-CB
1	A	550	MLZ	CE-CD-CG-CB
2	B	540	MLY	CD-CE-NZ-CH1
2	B	1013	MLZ	CA-CB-CG-CD
1	A	431	MLY	CD-CE-NZ-CH1
1	A	466	MLY	CD-CE-NZ-CH1
2	B	525	MLY	N-CA-CB-CG
1	A	769	MLZ	N-CA-CB-CG
1	A	525	MLZ	N-CA-CB-CG
1	A	750	MLY	N-CA-CB-CG
1	A	700	MLY	C-CA-CB-CG
2	B	956	MLZ	C-CA-CB-CG
2	B	986	MLY	CE-CD-CG-CB
1	A	437	MLZ	CA-CB-CG-CD
2	B	764	MLZ	CE-CD-CG-CB
2	B	66	MLZ	CD-CE-NZ-CM
2	B	937	MLZ	CE-CD-CG-CB
2	B	499	MLY	CE-CD-CG-CB
1	A	943	MLZ	CE-CD-CG-CB
2	B	764	MLZ	C-CA-CB-CG
2	B	1000	MLZ	C-CA-CB-CG
1	A	937	MLZ	CA-CB-CG-CD
1	A	540	MLY	CG-CD-CE-NZ
1	A	437	MLZ	CD-CE-NZ-CM
2	B	624	MLZ	CD-CE-NZ-CM
2	B	769	MLZ	CD-CE-NZ-CM
1	A	525	MLZ	CE-CD-CG-CB
1	A	769	MLZ	CD-CE-NZ-CM
1	A	466	MLY	CG-CD-CE-NZ

There are no ring outliers.

34 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	125	MLZ	1	0
1	A	794	MLY	2	0
1	A	854	MLY	1	0
2	B	759	MLZ	3	0
1	A	700	MLY	2	0
2	B	540	MLY	2	0
2	B	764	MLZ	1	0
2	B	278	MLY	1	0
2	B	199	MLZ	2	0
1	A	112	CAS	1	0
2	B	466	MLY	3	0
1	A	946	MLY	3	0
2	B	550	MLY	1	0
1	A	704	MLY	1	0
1	A	488	MLY	2	0
1	A	287	MLY	2	0
2	B	911	MLY	1	0
1	A	251	MLY	2	0
2	B	112	CAS	1	0
1	A	1000	MLZ	1	0
2	B	1000	MLZ	1	0
1	A	902	MLY	2	0
1	A	540	MLY	2	0
2	B	499	MLY	2	0
2	B	513	MLY	2	0
2	B	324	MLZ	2	0
1	A	437	MLZ	1	0
2	B	41	MLY	1	0
1	A	750	MLY	1	0
1	A	759	MLY	5	0
2	B	972	MLY	1	0
2	B	290	MLY	2	0
2	B	943	MLY	1	0
2	B	66	MLZ	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 4 are monoatomic - leaving 30 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	GOL	A	1112	-	5,5,5	0.32	0	5,5,5	0.31	0
4	3UE	A	1102	-	33,34,34	3.97	11 (33%)	44,47,47	1.16	5 (11%)
5	GOL	B	1108	-	5,5,5	0.38	0	5,5,5	0.39	0
5	GOL	A	1106	-	5,5,5	0.37	0	5,5,5	0.29	0
5	GOL	A	1110	-	5,5,5	0.36	0	5,5,5	0.29	0
5	GOL	A	1114	-	5,5,5	0.42	0	5,5,5	0.24	0
6	ACT	A	1115	-	1,3,3	1.50	0	0,3,3	0.00	-
6	ACT	B	1112	-	1,3,3	1.57	0	0,3,3	0.00	-
5	GOL	A	1108	-	5,5,5	0.43	0	5,5,5	0.30	0
5	GOL	A	1113	-	5,5,5	0.37	0	5,5,5	0.31	0
6	ACT	A	1117	3	1,3,3	1.15	0	0,3,3	0.00	-
5	GOL	B	1109	-	5,5,5	0.40	0	5,5,5	0.27	0
5	GOL	B	1107	-	5,5,5	0.29	0	5,5,5	0.41	0
5	GOL	A	1105	-	5,5,5	0.37	0	5,5,5	0.32	0
6	ACT	B	1115	3	1,3,3	1.58	0	0,3,3	0.00	-
5	GOL	A	1111	-	5,5,5	0.35	0	5,5,5	0.36	0
5	GOL	B	1105	-	5,5,5	0.46	0	5,5,5	0.58	0
5	GOL	A	1107	-	5,5,5	0.35	0	5,5,5	0.27	0
6	ACT	B	1113	-	1,3,3	1.14	0	0,3,3	0.00	-
4	3UE	B	1103	-	33,34,34	3.99	13 (39%)	44,47,47	1.45	6 (13%)
6	ACT	A	1116	-	1,3,3	1.29	0	0,3,3	0.00	-
4	3UE	A	1103	-	33,34,34	3.99	13 (39%)	44,47,47	1.55	9 (20%)
6	ACT	B	1114	-	1,3,3	1.68	0	0,3,3	0.00	-
6	ACT	B	1111	-	1,3,3	1.74	0	0,3,3	0.00	-
4	3UE	B	1102	-	33,34,34	3.92	14 (42%)	44,47,47	1.26	8 (18%)
5	GOL	A	1104	-	5,5,5	0.32	0	5,5,5	0.54	0
5	GOL	B	1106	-	5,5,5	0.35	0	5,5,5	0.41	0
5	GOL	B	1104	-	5,5,5	0.41	0	5,5,5	0.34	0
5	GOL	A	1109	-	5,5,5	0.36	0	5,5,5	0.52	0
5	GOL	B	1110	-	5,5,5	0.39	0	5,5,5	0.29	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
5	GOL	A	1112	-	-	2/4/4/4	-
4	3UE	A	1102	-	-	0/22/34/34	0/4/4/4
5	GOL	B	1108	-	-	2/4/4/4	-
5	GOL	A	1106	-	-	4/4/4/4	-
5	GOL	A	1110	-	-	2/4/4/4	-
5	GOL	A	1114	-	-	4/4/4/4	-
5	GOL	A	1108	-	-	2/4/4/4	-
5	GOL	A	1113	-	-	4/4/4/4	-
5	GOL	B	1109	-	-	0/4/4/4	-
5	GOL	B	1107	-	-	0/4/4/4	-
5	GOL	A	1105	-	-	2/4/4/4	-
5	GOL	A	1111	-	-	3/4/4/4	-
5	GOL	B	1105	-	-	2/4/4/4	-
5	GOL	A	1107	-	-	2/4/4/4	-
4	3UE	B	1103	-	-	0/22/34/34	0/4/4/4
4	3UE	A	1103	-	-	1/22/34/34	0/4/4/4
5	GOL	B	1106	-	-	1/4/4/4	-
4	3UE	B	1102	-	-	0/22/34/34	0/4/4/4
5	GOL	A	1104	-	-	0/4/4/4	-
5	GOL	B	1104	-	-	2/4/4/4	-
5	GOL	A	1109	-	-	2/4/4/4	-
5	GOL	B	1110	-	-	0/4/4/4	-

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1103	3UE	C19-N18	-12.16	1.27	1.48
4	A	1103	3UE	C19-N18	-11.83	1.27	1.48
4	A	1102	3UE	C19-N18	-11.68	1.28	1.48
4	B	1102	3UE	C19-N18	-11.64	1.28	1.48
4	B	1103	3UE	O08-N07	10.99	1.41	1.22
4	A	1103	3UE	O08-N07	10.88	1.41	1.22
4	A	1102	3UE	O08-N07	10.85	1.41	1.22
4	B	1102	3UE	O08-N07	10.54	1.40	1.22
4	B	1102	3UE	C16-N13	-8.74	1.31	1.47
4	A	1102	3UE	C16-N13	-8.59	1.31	1.47
4	B	1103	3UE	C16-N13	-8.56	1.31	1.47
4	A	1103	3UE	C16-N13	-8.40	1.32	1.47
4	A	1103	3UE	C14-N13	-7.58	1.33	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1102	3UE	C14-N13	-7.29	1.34	1.47
4	A	1102	3UE	C14-N13	-7.21	1.34	1.47
4	A	1102	3UE	C02-N13	7.15	1.50	1.34
4	B	1103	3UE	C14-N13	-7.14	1.34	1.47
4	B	1102	3UE	C02-N13	6.87	1.50	1.34
4	B	1103	3UE	C02-N13	6.80	1.49	1.34
4	A	1103	3UE	C02-N13	6.53	1.49	1.34
4	A	1103	3UE	C20-C19	4.36	1.58	1.52
4	A	1102	3UE	C20-C19	4.17	1.58	1.52
4	B	1102	3UE	C20-C19	4.04	1.58	1.52
4	B	1103	3UE	C20-C19	3.69	1.57	1.52
4	A	1103	3UE	C30-C31	3.60	1.46	1.38
4	B	1103	3UE	C30-C31	3.47	1.46	1.38
4	A	1102	3UE	C30-C31	3.39	1.46	1.38
4	B	1102	3UE	C30-C31	3.37	1.46	1.38
4	A	1103	3UE	C26-C19	3.28	1.57	1.52
4	A	1103	3UE	C29-C28	3.22	1.46	1.38
4	A	1102	3UE	C26-C19	3.22	1.57	1.52
4	A	1102	3UE	C29-C28	3.16	1.46	1.38
4	B	1102	3UE	C29-C28	3.09	1.46	1.38
4	B	1103	3UE	C29-C28	3.02	1.46	1.38
4	A	1103	3UE	C17-N18	-2.79	1.41	1.47
4	A	1102	3UE	C03-C02	-2.57	1.45	1.50
4	B	1103	3UE	C17-N18	-2.54	1.42	1.47
4	B	1103	3UE	C26-C19	2.45	1.56	1.52
4	B	1103	3UE	C11-C10	2.42	1.55	1.51
4	A	1102	3UE	C11-C10	2.37	1.55	1.51
4	B	1102	3UE	C11-C10	2.36	1.55	1.51
4	A	1103	3UE	C03-C02	-2.31	1.46	1.50
4	B	1102	3UE	C03-C02	-2.31	1.46	1.50
4	B	1103	3UE	C12-C03	2.29	1.42	1.39
4	A	1103	3UE	C11-C10	2.27	1.55	1.51
4	B	1103	3UE	C05-C04	2.25	1.42	1.38
4	B	1102	3UE	C05-C04	2.22	1.42	1.38
4	B	1102	3UE	C17-N18	-2.12	1.43	1.47
4	B	1102	3UE	C26-C19	2.11	1.55	1.52
4	B	1102	3UE	C21-C20	-2.03	1.35	1.39
4	A	1103	3UE	C31-C26	2.03	1.42	1.39

All (28) bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1103	3UE	C16-N13-C14	6.06	124.29	112.62
4	B	1103	3UE	C16-N13-C14	4.90	122.06	112.62
4	B	1103	3UE	C03-C02-N13	3.46	123.11	118.72
4	A	1103	3UE	C03-C02-N13	3.26	122.86	118.72
4	B	1102	3UE	C16-N13-C14	3.12	118.62	112.62
4	A	1102	3UE	C14-C15-N18	3.02	116.36	110.59
4	A	1102	3UE	C03-C02-N13	2.98	122.50	118.72
4	A	1102	3UE	C16-N13-C14	2.98	118.36	112.62
4	B	1102	3UE	C20-C19-N18	2.93	115.68	111.42
4	B	1103	3UE	C26-C19-C20	-2.91	104.72	112.33
4	A	1103	3UE	C17-N18-C15	-2.61	104.30	109.08
4	A	1102	3UE	C26-C19-C20	-2.47	105.87	112.33
4	B	1102	3UE	C16-C17-N18	2.45	115.29	110.59
4	B	1103	3UE	C17-N18-C15	-2.44	104.62	109.08
4	A	1103	3UE	C20-C19-N18	2.38	114.88	111.42
4	B	1102	3UE	C03-C02-N13	2.36	121.71	118.72
4	B	1102	3UE	C14-C15-N18	2.35	115.08	110.59
4	A	1102	3UE	C16-C17-N18	2.32	115.04	110.59
4	A	1103	3UE	C16-C17-N18	2.29	114.97	110.59
4	B	1102	3UE	C26-C19-C20	-2.29	106.34	112.33
4	B	1102	3UE	C05-C06-N07	2.26	118.89	116.47
4	B	1103	3UE	C31-C26-C27	2.12	120.94	118.29
4	A	1103	3UE	C05-C06-N07	2.11	118.73	116.47
4	A	1103	3UE	C17-C16-N13	2.10	114.93	110.44
4	A	1103	3UE	C26-C19-C20	-2.06	106.94	112.33
4	B	1103	3UE	C15-N18-C19	2.05	115.81	111.66
4	B	1102	3UE	C31-C26-C27	2.02	120.81	118.29
4	A	1103	3UE	C14-N13-C02	-2.02	116.41	122.78

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1112	GOL	O1-C1-C2-C3
5	B	1108	GOL	O1-C1-C2-C3
5	A	1106	GOL	O1-C1-C2-C3
5	A	1106	GOL	C1-C2-C3-O3
5	A	1110	GOL	O1-C1-C2-C3
5	A	1114	GOL	O1-C1-C2-C3
5	A	1108	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	1113	GOL	O1-C1-C2-C3
5	A	1113	GOL	C1-C2-C3-O3
5	A	1105	GOL	O1-C1-C2-O2
5	A	1105	GOL	O1-C1-C2-C3
5	A	1111	GOL	O1-C1-C2-C3
5	B	1104	GOL	O1-C1-C2-C3
5	A	1109	GOL	O1-C1-C2-C3
5	A	1114	GOL	C1-C2-C3-O3
5	B	1105	GOL	O1-C1-C2-C3
5	A	1107	GOL	O1-C1-C2-C3
5	B	1106	GOL	O1-C1-C2-C3
5	A	1106	GOL	O2-C2-C3-O3
5	A	1110	GOL	O1-C1-C2-O2
5	A	1114	GOL	O1-C1-C2-O2
5	A	1111	GOL	O1-C1-C2-O2
5	A	1107	GOL	O1-C1-C2-O2
5	A	1112	GOL	O1-C1-C2-O2
5	B	1108	GOL	O1-C1-C2-O2
5	A	1106	GOL	O1-C1-C2-O2
5	B	1104	GOL	O1-C1-C2-O2
4	A	1103	3UE	C05-C06-N07-O08
5	A	1108	GOL	O1-C1-C2-O2
5	A	1113	GOL	O1-C1-C2-O2
5	B	1105	GOL	O1-C1-C2-O2
5	A	1113	GOL	O2-C2-C3-O3
5	A	1109	GOL	O1-C1-C2-O2
5	A	1114	GOL	O2-C2-C3-O3
5	A	1111	GOL	O2-C2-C3-O3

There are no ring outliers.

16 monomers are involved in 26 short contacts:

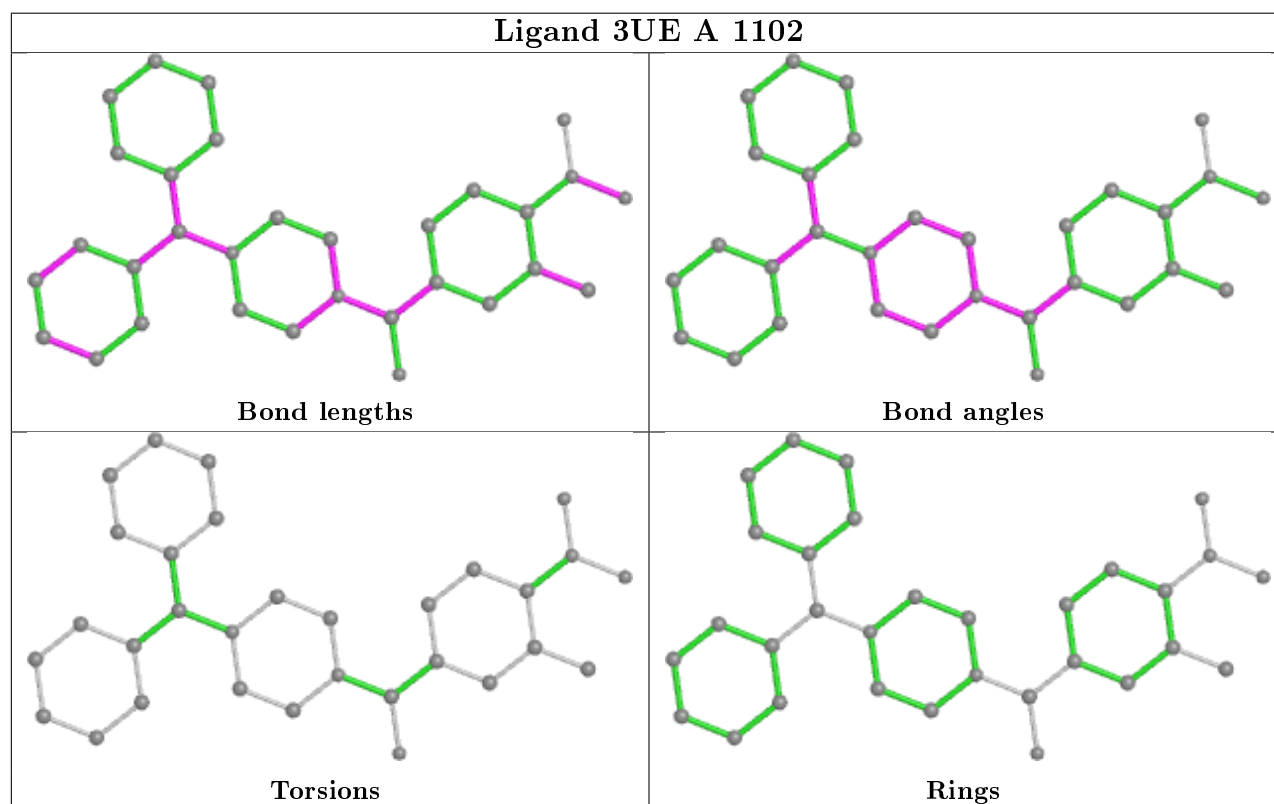
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1112	GOL	1	0
4	A	1102	3UE	2	0
5	A	1106	GOL	2	0
5	A	1110	GOL	1	0
5	A	1114	GOL	1	0
5	B	1109	GOL	3	0
5	B	1107	GOL	3	0
5	A	1111	GOL	2	0
5	B	1105	GOL	1	0

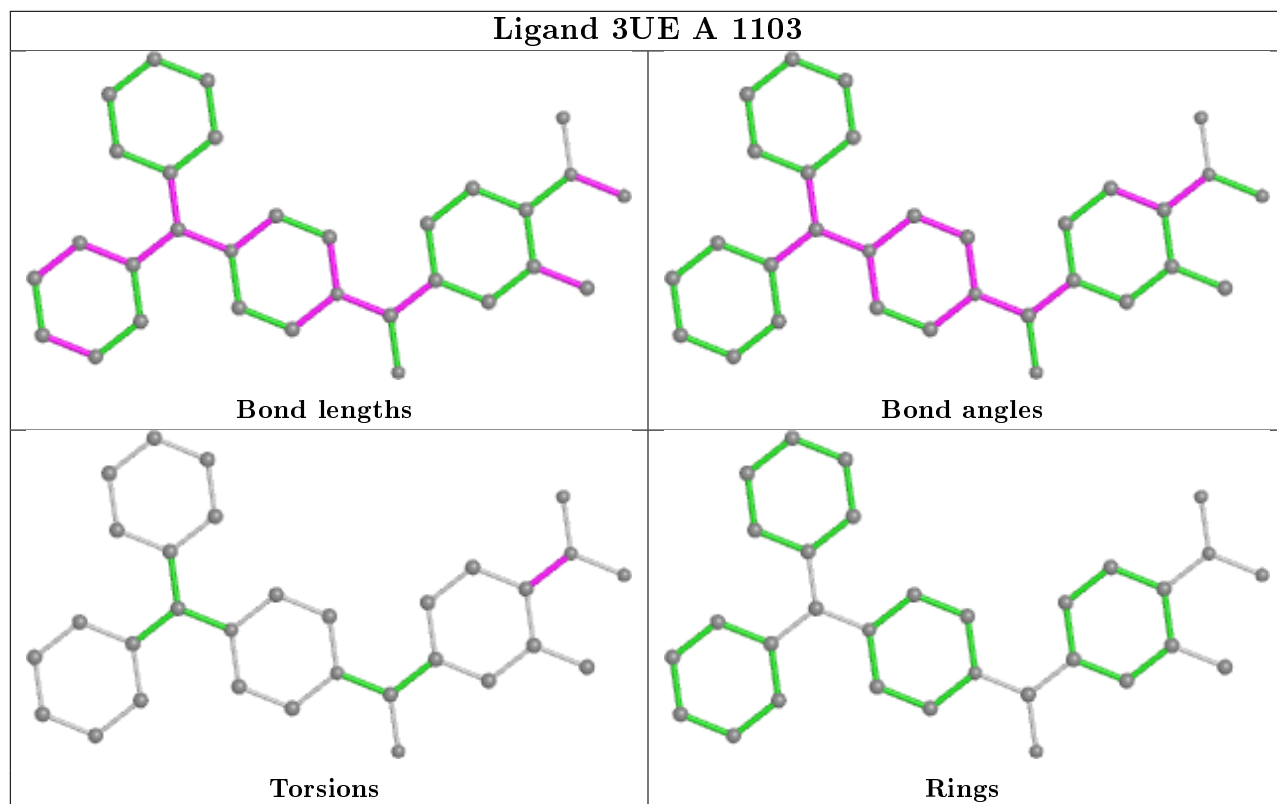
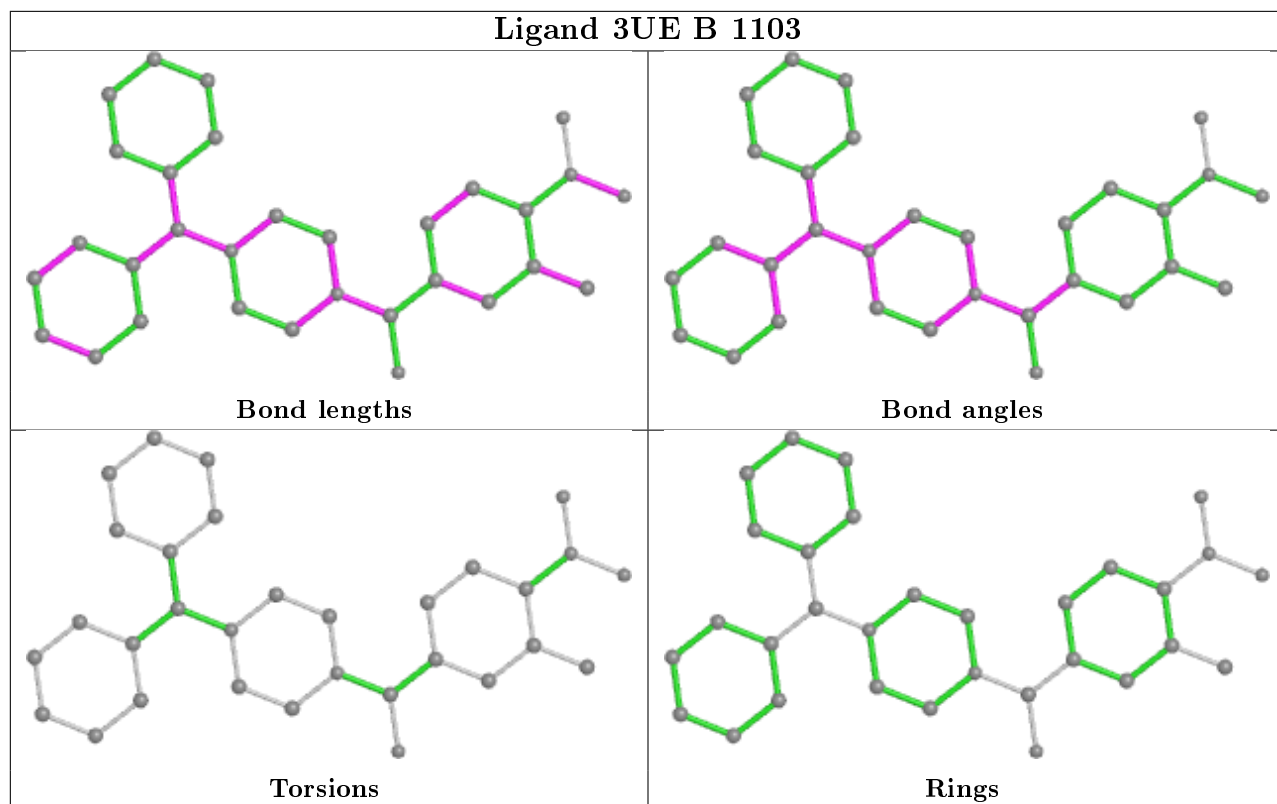
Continued on next page...

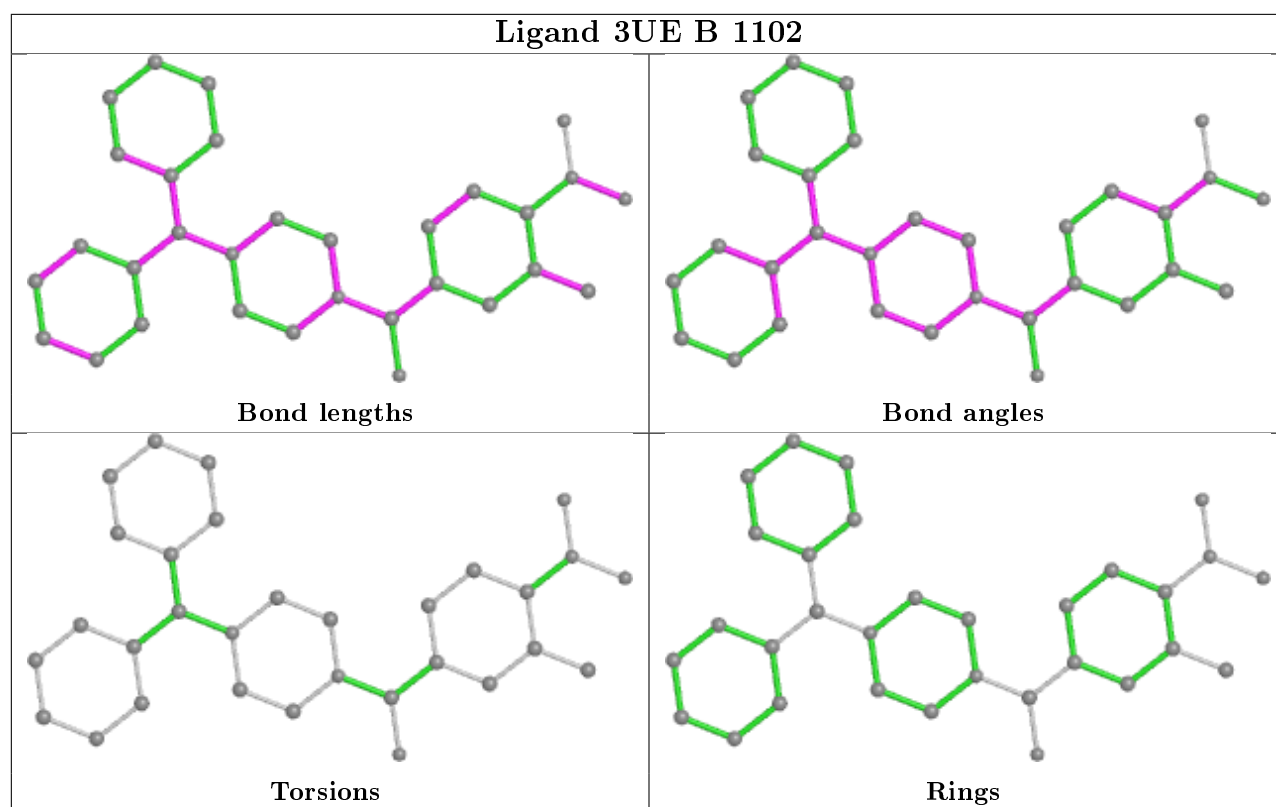
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1113	ACT	1	0
4	B	1103	3UE	1	0
4	A	1103	3UE	2	0
6	B	1114	ACT	1	0
4	B	1102	3UE	1	0
5	B	1106	GOL	3	0
5	B	1104	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	951/1014 (93%)	-0.10	11 (1%) 79 81	27, 32, 51, 83	0
2	B	940/1014 (92%)	-0.12	25 (2%) 54 57	27, 34, 54, 94	0
All	All	1891/2028 (93%)	-0.11	36 (1%) 66 69	27, 33, 53, 94	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	823	PRO	5.0
1	A	838	VAL	3.9
2	B	839	ILE	3.5
2	B	838	VAL	3.4
2	B	1030	LYS	3.2
2	B	851	TRP	3.2
1	A	531	PRO	3.1
2	B	571	VAL	2.9
1	A	571	VAL	2.8
1	A	813	VAL	2.7
2	B	1027	LYS	2.7
1	A	811	ARG	2.7
2	B	582	ASP	2.6
1	A	821	PRO	2.6
2	B	572	THR	2.5
2	B	577	VAL	2.5
2	B	570	PRO	2.4
2	B	323	SER	2.4
2	B	915	ASN	2.4
2	B	819	GLU	2.4
2	B	813	VAL	2.3
1	A	36	ARG	2.3
2	B	821	PRO	2.3
2	B	983	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	984	GLU	2.2
2	B	397	VAL	2.2
2	B	575	ASP	2.2
1	A	42	LEU	2.2
2	B	812	PRO	2.2
2	B	820	LYS	2.1
2	B	1029	ALA	2.1
1	A	193	GLN	2.1
2	B	417	GLU	2.1
2	B	399	LYS	2.0
1	A	814	ARG	2.0
2	B	569	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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	MLZ	B	324	10/11	0.81	0.34	46,61,69,70	0
1	MLY	A	750	11/12	0.90	0.18	31,39,54,57	0
1	MLY	A	521	11/12	0.91	0.24	42,46,60,63	0
1	MLY	A	794	11/12	0.91	0.14	37,51,66,67	0
1	MLY	A	700	11/12	0.91	0.24	31,32,61,61	0
2	MLY	B	513	11/12	0.92	0.22	34,39,47,49	0
2	MLY	B	499	11/12	0.92	0.23	33,41,65,65	0
1	MLY	A	704	11/12	0.92	0.14	30,31,51,53	0
2	MLY	B	750	11/12	0.92	0.16	35,41,47,53	0
2	MLZ	B	494	10/11	0.93	0.25	33,40,54,57	0
2	MLY	B	550	11/12	0.93	0.13	27,32,38,44	0
2	MLY	B	972	11/12	0.93	0.17	32,34,56,59	0
2	MLY	B	287	11/12	0.93	0.16	31,32,41,41	0
1	MLZ	A	972	10/11	0.94	0.15	29,33,49,51	0
2	MLZ	B	1013	10/11	0.94	0.13	40,45,54,58	0
2	MLZ	B	490	10/11	0.94	0.25	32,38,59,60	0
2	MLY	B	911	11/12	0.94	0.15	28,29,41,45	0
2	MLY	B	41	11/12	0.94	0.14	34,35,46,49	0
1	MLY	A	251	11/12	0.94	0.10	31,31,45,46	0
1	MLY	A	759	11/12	0.94	0.21	35,35,41,44	0
2	MLY	B	278	11/12	0.94	0.16	31,35,50,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MLY	B	290	11/12	0.94	0.15	33,37,53,54	0
2	MLZ	B	902	10/11	0.94	0.11	28,33,39,42	0
1	MLY	A	956	11/12	0.94	0.17	27,28,53,55	0
2	MLZ	B	937	10/11	0.94	0.15	28,33,42,47	0
2	MLY	B	986	11/12	0.94	0.23	32,42,54,56	0
2	MLZ	B	66	10/11	0.94	0.16	31,31,47,50	0
2	MLZ	B	199	10/11	0.95	0.15	29,38,49,50	0
1	MLY	A	278	11/12	0.95	0.11	31,32,35,36	0
2	MLZ	B	624	10/11	0.95	0.15	33,34,39,42	0
2	MLY	B	363	11/12	0.95	0.13	33,34,51,55	0
1	MLZ	A	937	10/11	0.95	0.12	28,29,43,44	0
1	MLY	A	513	11/12	0.95	0.16	33,36,44,51	0
2	MLZ	B	769	10/11	0.95	0.13	38,39,42,46	0
2	MLY	B	540	11/12	0.95	0.12	28,29,34,38	0
1	MLY	A	363	11/12	0.95	0.11	30,32,52,56	0
2	MLY	B	116	11/12	0.95	0.14	28,39,47,54	0
1	MLY	A	642	11/12	0.95	0.13	29,31,35,40	0
2	MLY	B	431	11/12	0.95	0.16	31,32,48,56	0
1	MLZ	A	1000	10/11	0.95	0.14	27,31,44,44	0
2	MLZ	B	1000	10/11	0.95	0.15	31,36,54,56	0
1	MLZ	A	66	10/11	0.95	0.12	31,32,42,45	0
1	MLY	A	290	11/12	0.95	0.13	34,37,48,50	0
2	MLZ	B	956	10/11	0.95	0.11	28,31,42,42	0
1	MLZ	A	207	10/11	0.95	0.18	29,29,46,53	0
1	MLZ	A	437	10/11	0.96	0.12	28,29,47,48	0
2	MLZ	B	764	10/11	0.96	0.13	39,43,45,47	0
1	MLY	A	287	11/12	0.96	0.13	31,32,34,38	0
1	MLY	A	854	11/12	0.96	0.12	31,31,38,40	0
1	MLY	A	488	11/12	0.96	0.11	30,30,32,35	0
1	MLY	A	911	11/12	0.96	0.17	27,27,38,46	0
1	MLY	A	466	11/12	0.96	0.12	29,33,44,46	0
1	MLZ	A	884	10/11	0.96	0.10	27,27,29,31	0
2	MLZ	B	884	10/11	0.96	0.12	28,32,43,45	0
2	MLZ	B	854	10/11	0.96	0.11	32,33,36,40	0
1	MLZ	A	525	10/11	0.96	0.18	37,38,44,45	0
2	MLY	B	466	11/12	0.96	0.11	30,31,34,40	0
1	MLY	A	946	11/12	0.96	0.12	26,34,48,48	0
2	MLY	B	525	11/12	0.96	0.10	32,34,42,43	0
1	MLY	A	764	11/12	0.96	0.12	34,34,40,46	0
1	MLY	A	154	11/12	0.96	0.12	28,30,43,43	0
2	MLY	B	946	11/12	0.96	0.13	27,35,47,47	0
2	MLY	B	943	11/12	0.96	0.10	28,31,48,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	MLY	A	431	11/12	0.96	0.12	28,31,52,53	0
2	MLY	B	642	11/12	0.96	0.16	33,34,39,41	0
1	MLY	A	116	11/12	0.96	0.12	29,29,30,37	0
2	MLZ	B	125	10/11	0.96	0.12	27,27,39,41	0
2	MLY	B	488	11/12	0.97	0.15	31,32,37,40	0
1	MLY	A	902	11/12	0.97	0.11	28,29,37,39	0
1	MLZ	A	550	10/11	0.97	0.10	27,30,37,41	0
1	MLZ	A	769	10/11	0.97	0.10	33,34,39,43	0
1	MLY	A	540	11/12	0.97	0.12	30,31,33,35	0
1	MLZ	A	943	10/11	0.97	0.10	27,35,38,42	0
2	CAS	B	112	9/10	0.97	0.12	27,28,60,92	0
2	MLZ	B	759	10/11	0.97	0.18	39,45,47,50	0
1	CAS	A	112	9/10	0.97	0.14	28,32,68,93	0

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
5	GOL	A	1110	6/6	0.68	0.26	51,66,68,69	0
6	ACT	A	1115	4/4	0.76	0.21	56,63,63,67	0
5	GOL	A	1114	6/6	0.77	0.26	54,60,72,80	0
5	GOL	B	1108	6/6	0.78	0.30	69,70,74,75	0
5	GOL	A	1107	6/6	0.79	0.18	48,59,68,72	0
5	GOL	A	1109	6/6	0.82	0.34	54,62,73,77	0
6	ACT	B	1111	4/4	0.83	0.15	41,44,52,53	0
5	GOL	B	1107	6/6	0.83	0.24	53,60,68,75	0
5	GOL	A	1108	6/6	0.84	0.23	51,62,70,72	0
6	ACT	B	1114	4/4	0.84	0.21	41,51,52,59	0
5	GOL	A	1112	6/6	0.84	0.22	32,46,57,63	0
5	GOL	A	1105	6/6	0.84	0.23	50,51,65,72	0
5	GOL	A	1104	6/6	0.85	0.19	38,41,46,48	0
5	GOL	A	1111	6/6	0.85	0.32	35,50,60,67	0
5	GOL	B	1106	6/6	0.88	0.20	51,57,58,61	0

Continued on next page...

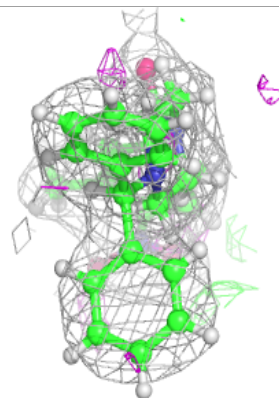
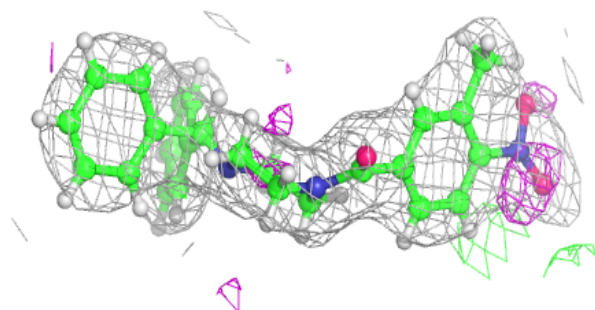
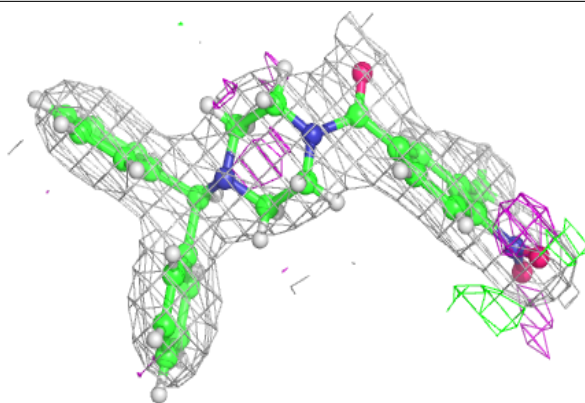
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	A	1113	6/6	0.88	0.22	54,58,61,62	0
5	GOL	B	1104	6/6	0.91	0.15	41,48,52,54	0
5	GOL	B	1105	6/6	0.92	0.21	39,41,49,51	0
6	ACT	B	1112	4/4	0.92	0.25	43,47,52,61	0
5	GOL	A	1106	6/6	0.93	0.24	58,61,65,65	0
4	3UE	B	1102	31/31	0.94	0.12	29,31,36,49	0
6	ACT	B	1113	4/4	0.94	0.21	43,47,49,49	0
4	3UE	A	1102	31/31	0.94	0.13	27,33,45,64	0
5	GOL	B	1109	6/6	0.94	0.14	28,43,48,52	0
4	3UE	B	1103	31/31	0.95	0.11	29,35,40,56	0
4	3UE	A	1103	31/31	0.95	0.13	28,32,39,58	0
5	GOL	B	1110	6/6	0.95	0.12	35,41,46,54	0
6	ACT	A	1116	4/4	0.96	0.15	33,34,39,39	0
7	CA	B	1116	1/1	0.96	0.13	41,41,41,41	0
6	ACT	B	1115	4/4	0.96	0.12	28,42,43,45	0
7	CA	B	1117	1/1	0.97	0.26	54,54,54,54	0
6	ACT	A	1117	4/4	0.98	0.19	28,37,44,46	0
3	ZN	B	1101	1/1	0.99	0.12	42,42,42,42	0
3	ZN	A	1101	1/1	1.00	0.11	38,38,38,38	0

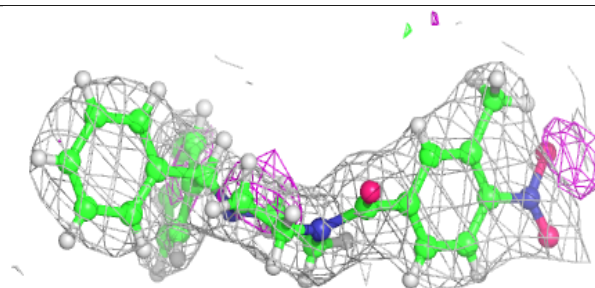
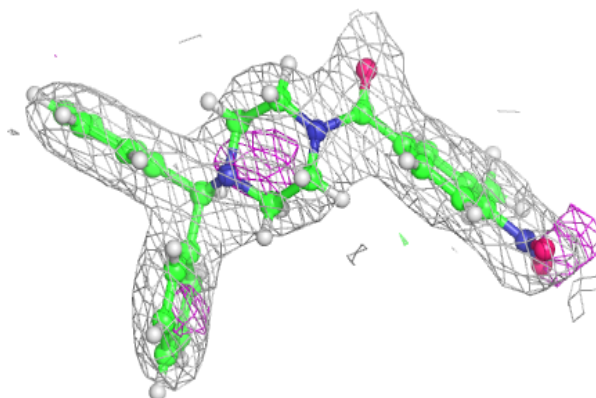
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 3UE B 1102:

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

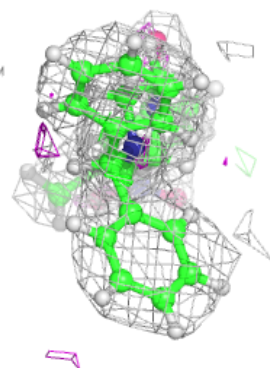
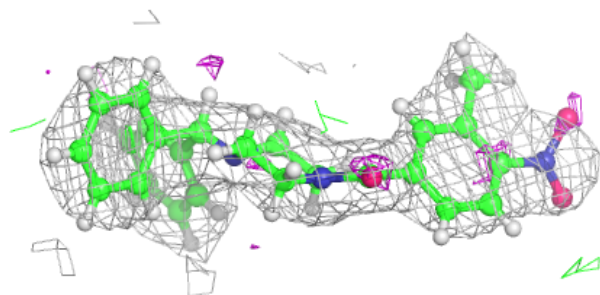
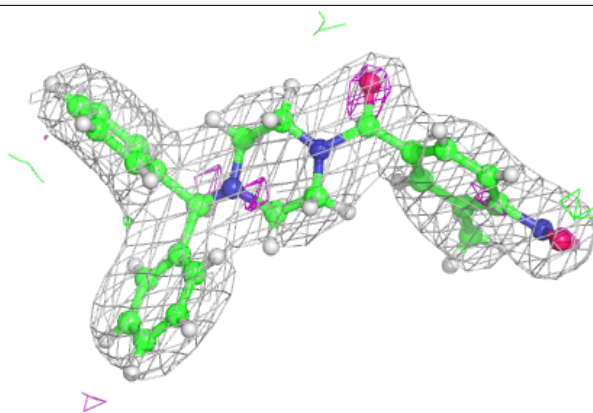
**Electron density around 3UE A 1102:**

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

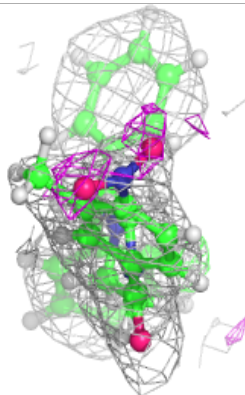
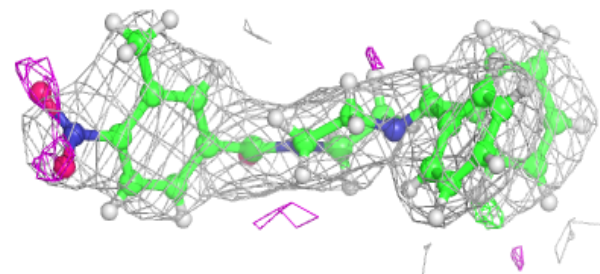
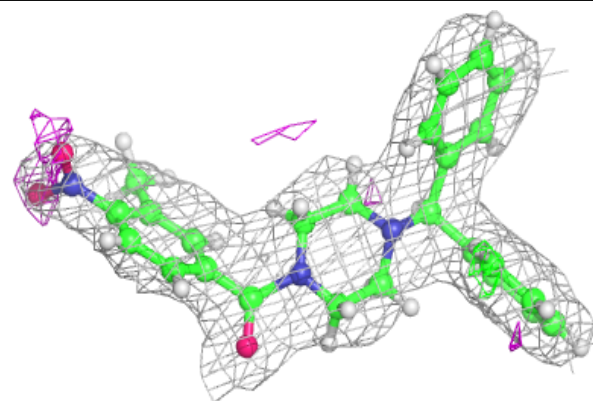


Electron density around 3UE B 1103:

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

**Electron density around 3UE A 1103:**

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



6.5 Other polymers

There are no such residues in this entry.