



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:59 AM UTC

PDB ID : 4RPU / pdb_00004rpu
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 types of validation reports are described at

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

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

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

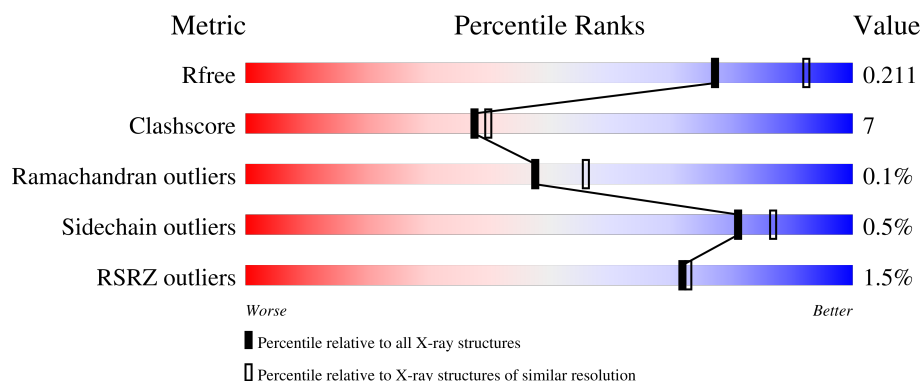
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (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 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	1014	% 84% 12% ..
2	B	1014	2% 81% 15% .

2 Entry composition

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

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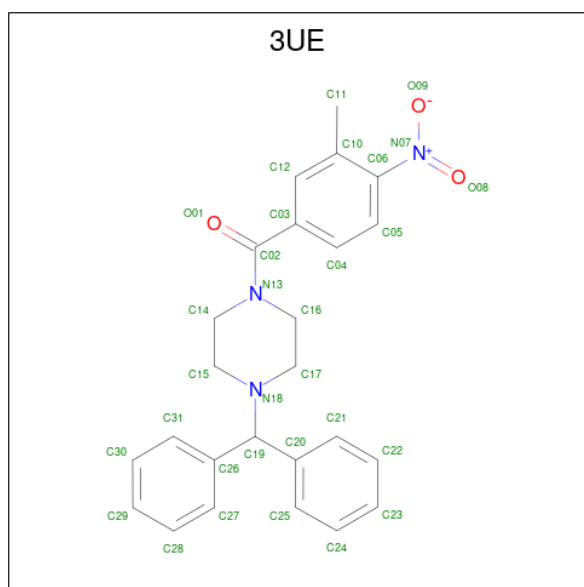
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Chain	Residue	Modelled	Actual	Comment	Reference
B	27	HIS	-	expression tag	UNP Q5JRX3
B	28	HIS	-	expression tag	UNP Q5JRX3
B	29	HIS	-	expression tag	UNP Q5JRX3
B	30	HIS	-	expression tag	UNP Q5JRX3
B	31	ALA	-	expression tag	UNP Q5JRX3
B	32	ALA	-	expression 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 (CCD ID: ZN) (formula: Zn).

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

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



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

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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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



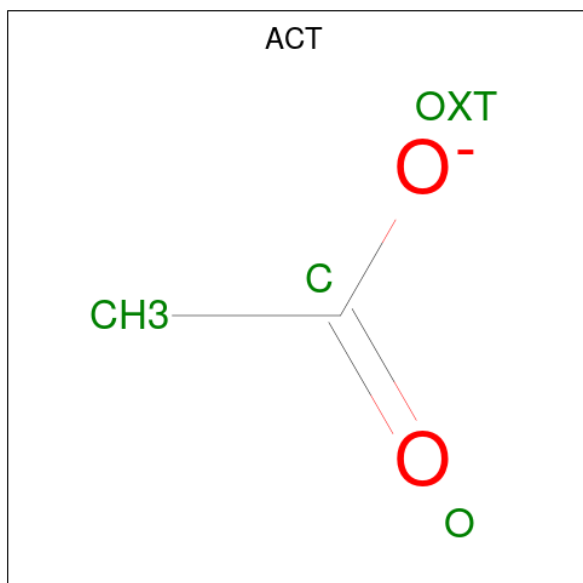
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

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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		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

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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 (CCD ID: CA) (formula: Ca).

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

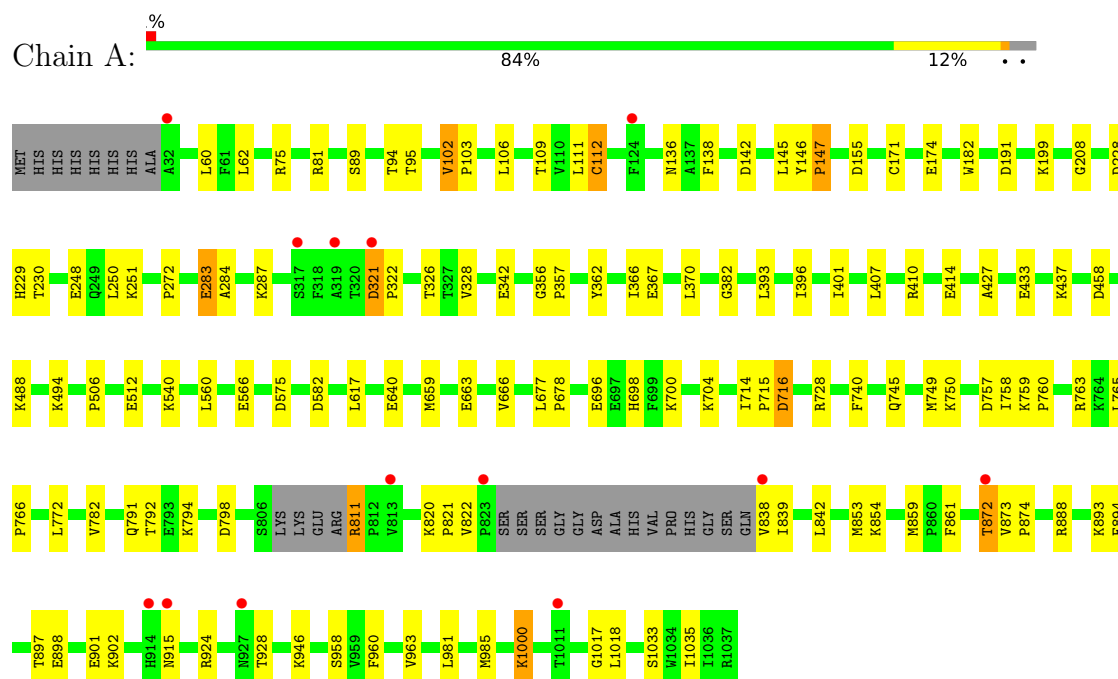
- Molecule 8 is water.

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

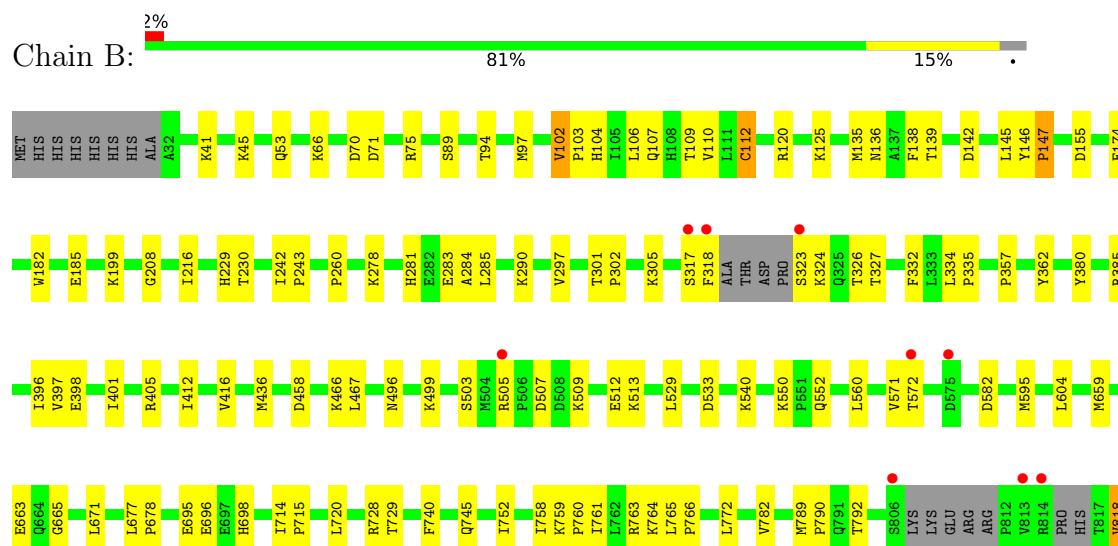
3 Residue-property plots

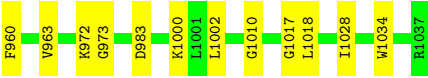
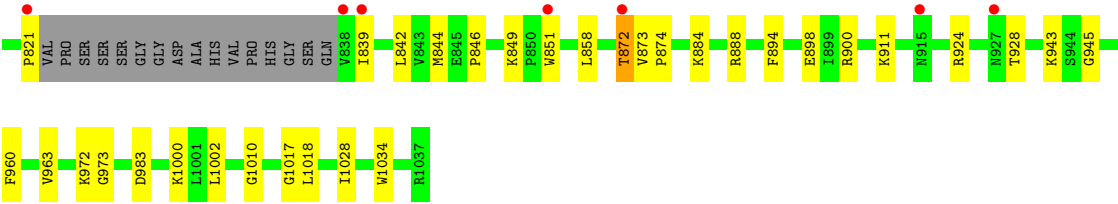
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



- Molecule 2: Presequence protease, mitochondrial





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 – 2.27	Depositor EDS
% Data completeness (in resolution range)	98.5 (44.85-2.27) 93.2 (44.85-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.27Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.175 , 0.208 0.181 , 0.211	Depositor DCC
R_{free} test set	1992 reflections (1.67%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 34.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17042	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage'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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CA, CAS, ACT, ZN, 3UE, MLY, MLZ

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	0.51	1/7776 (0.0%)	0.79	17/10565 (0.2%)
2	B	0.48	1/7640 (0.0%)	0.76	7/10365 (0.1%)
All	All	0.49	2/15416 (0.0%)	0.78	24/20930 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	VAL	CA-CB	5.45	1.57	1.53
2	B	102	VAL	CA-CB	5.24	1.57	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	894	PHE	N-CA-C	10.54	126.69	112.68
2	B	928	THR	N-CA-C	9.84	125.42	113.12
1	A	928	THR	N-CA-C	8.03	123.35	112.68
1	A	191	ASP	CB-CA-C	6.70	119.10	110.13
1	A	283	GLU	CB-CA-C	6.43	122.33	110.56
1	A	228	ASP	CB-CA-C	-6.17	98.91	110.01
2	B	284	ALA	N-CA-C	6.05	120.98	112.93
2	B	872	THR	N-CA-C	-5.95	100.47	108.86
1	A	284	ALA	N-CA-C	5.91	120.22	112.13
1	A	356	GLY	CA-C-N	5.78	126.53	120.12
1	A	356	GLY	C-N-CA	5.78	126.53	120.12
1	A	566	GLU	CA-C-N	5.61	125.28	119.05
1	A	566	GLU	C-N-CA	5.61	125.28	119.05
2	B	283	GLU	CB-CA-C	5.60	120.20	110.79
1	A	894	PHE	N-CA-CB	-5.51	101.08	110.33
1	A	228	ASP	N-CA-C	5.28	119.71	113.16
2	B	305	LYS	CA-C-N	5.21	125.15	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	305	LYS	C-N-CA	5.21	125.15	119.78
1	A	872	THR	N-CA-C	-5.20	101.53	108.34
1	A	811	ARG	CA-C-N	5.16	125.10	119.78
1	A	811	ARG	C-N-CA	5.16	125.10	119.78
1	A	366	ILE	N-CA-C	5.12	115.78	110.82
2	B	283	GLU	N-CA-C	-5.07	105.22	111.40
1	A	893	LYS	CB-CA-C	5.01	119.73	110.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7985	0	7880	102	0
2	B	7878	0	7779	115	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
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	15927	225	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 (225) 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:HH22	1:A:946:MLY:HG2	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
2:B:466:MLY:HG3	5:B:1107:GOL:H32	1.70	0.73
2:B:818:VAL:CG1	2:B:844:MET:HE2	2.18	0.73
1:A:171:CYS:SG	8:A:1372:HOH:O	2.47	0.72
1:A:915:ASN:O	1:A:915:ASN:ND2	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:853:MET:HE1	1:A:1035:ILE:HD11	1.74	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
1:A:248:GLU:OE2	1:A:251:MLY:HH23	1.97	0.65
1:A:582:ASP:OD1	1:A:582:ASP:N	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:494:LYS:NZ	8:A:1614:HOH:O	2.31	0.63
1:A:677:LEU:HB3	1:A:678:PRO:HD3	1.81	0.63
2:B:818:VAL:HG11	2:B:844:MET:HE2	1.80	0.63
2:B:818:VAL:HG12	2:B:844:MET:HE2	1.80	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:1017:GLY:C	1:A:1018:LEU:HD12	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH22	1:A:946:MLY:CG	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
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:853:MET:HE1	1:A:1035:ILE:CD1	2.36	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: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:1017:GLY:C	2:B:1018:LEU:HD12	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:659:MET:HE2	1:A:872:THR:O	2.12	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: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:260:PRO:HB3	2:B:285:LEU:CD2	2.43	0.49
2:B:1028:ILE:HG23	2:B:1034:TRP:CG	2.47	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: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
1:A:758:ILE:C	1:A:758:ILE:HD12	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:45:LYS:HE2	8:B:1574:HOH:O	2.14	0.47
4:B:1102:3UE:C04	4:B:1102:3UE:H12	2.44	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
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:97:MET:HE1	2:B:230:THR:HB	1.97	0.46
1:A:981:LEU:HD12	1:A:985:MET:HE2	1.97	0.46
2:B:507:ASP:OD2	2:B:513:MLY:HH23	2.15	0.46
2:B:102:VAL:N	2:B:103:PRO:HD2	2.30	0.46
2:B:945:GLY:CA	2:B:1002:LEU:HD21	2.43	0.46
1:A:859:MET:HE3	1:A:861:PHE:CZ	2.51	0.45
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
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
1:A:322:PRO:HA	1:A:506:PRO:HG2	1.99	0.44
4:A:1102:3UE:C04	4:A:1102:3UE:H12	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:135:MET:HE2	2:B:135:MET:HB3	1.93	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:HH13	2:B:278:MLY:HD2	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
2:B:70:ASP:O	2:B:290:MLY:HH12	2.18	0.42
2:B:94:THR:O	2:B:142:ASP:HA	2.20	0.42
2:B:208:GLY:HA3	2:B:924:ARG:HD3	2.01	0.42
2:B:75:ARG:NH1	8:B:1440:HOH:O	2.53	0.42
2:B:104:HIS:CD2	5:B:1109:GOL:H32	2.54	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
2:B:53:GLN:HB3	2:B:66:MLZ:HB3	2.01	0.41
4:B:1103:3UE:C12	4:B:1103:3UE:H12	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:62:LEU:HD12	1:A:62:LEU:C	2.45	0.41
1:A:617:LEU:HD13	1:A:749:MET:HE1	2.03	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
2:B:297:VAL:O	2:B:385:ARG:NH1	2.48	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:OE1	2:B:512:GLU:N	2.47	0.40
2:B:595:MET:HE2	2:B:671:LEU:HD12	2.03	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

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%)	48 56
2	B	931/1014 (92%)	919 (99%)	11 (1%)	1 (0%)	48 56
All	All	1881/2028 (93%)	1856 (99%)	23 (1%)	2 (0%)	48 56

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	848/864 (98%)	843 (99%)	5 (1%)	78	84
2	B	834/862 (97%)	831 (100%)	3 (0%)	84	89
All	All	1682/1726 (98%)	1674 (100%)	8 (0%)	81	87

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	811	ARG
1	A	820	LYS
2	B	107	GLN
2	B	818	VAL
2	B	858	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	85	ASN
1	A	204	ASN
1	A	219	GLN
1	A	223	ASN
1	A	252	GLN
1	A	310	GLN
1	A	915	ASN
2	B	52	ASN

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Mol	Chain	Res	Type
2	B	204	ASN
2	B	275	GLN
2	B	880	HIS
2	B	989	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	$\# Z > 2$
1	MLY	A	116	1	9,10,11	0.45	0	6,11,13	0.99	0
2	MLZ	B	759	2	8,9,10	1.05	0	4,9,11	0.86	0
1	MLZ	A	525	1	8,9,10	1.17	0	4,9,11	1.04	0
1	MLY	A	854	1	9,10,11	0.61	0	6,11,13	0.65	0
1	MLY	A	521	1	9,10,11	0.59	0	6,11,13	0.84	0
1	MLZ	A	66	1	8,9,10	1.05	0	4,9,11	0.81	0
1	MLZ	A	884	1	8,9,10	1.13	0	4,9,11	0.85	0
2	MLY	B	431	2	9,10,11	0.51	0	6,11,13	1.16	0
2	MLY	B	642	2	9,10,11	0.48	0	6,11,13	0.82	0
2	MLZ	B	937	2	8,9,10	1.02	0	4,9,11	0.67	0
1	MLY	A	251	1	9,10,11	0.61	0	6,11,13	0.90	0
2	MLZ	B	902	2	8,9,10	1.05	0	4,9,11	0.88	0
1	MLY	A	911	1	9,10,11	0.66	0	6,11,13	0.94	0
2	MLY	B	278	2	9,10,11	0.52	0	6,11,13	0.74	0
2	MLZ	B	1000	2	8,9,10	1.12	0	4,9,11	0.97	0
1	MLZ	A	207	1	8,9,10	1.07	0	4,9,11	0.78	0
1	MLY	A	513	1	9,10,11	0.57	0	6,11,13	0.79	0
1	MLY	A	540	1	9,10,11	0.55	0	6,11,13	0.73	0
1	MLY	A	750	1	9,10,11	0.47	0	6,11,13	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MLY	B	972	2	9,10,11	0.59	0	6,11,13	0.79	0
1	MLZ	A	769	1	8,9,10	1.11	0	4,9,11	0.81	0
1	MLY	A	902	1	9,10,11	0.56	0	6,11,13	0.56	0
2	MLY	B	513	2	9,10,11	0.52	0	6,11,13	0.78	0
2	MLZ	B	854	2	8,9,10	1.10	0	4,9,11	0.84	0
2	MLY	B	363	2	9,10,11	0.69	0	6,11,13	0.64	0
2	MLZ	B	494	2	8,9,10	1.09	0	4,9,11	0.77	0
1	MLY	A	700	1	9,10,11	0.53	0	6,11,13	1.11	0
2	MLZ	B	956	2	8,9,10	1.04	0	4,9,11	0.66	0
1	MLY	A	278	1	9,10,11	0.52	0	6,11,13	0.64	0
1	MLY	A	704	1	9,10,11	0.64	0	6,11,13	0.77	0
1	MLY	A	946	1	9,10,11	0.52	0	6,11,13	0.87	0
1	MLZ	A	1000	1	8,9,10	1.16	1 (12%)	4,9,11	0.86	0
2	MLZ	B	490	2	8,9,10	1.20	0	4,9,11	1.01	0
2	MLY	B	41	2	9,10,11	0.52	0	6,11,13	0.95	0
1	MLY	A	431	1	9,10,11	0.59	0	6,11,13	1.00	0
1	MLY	A	642	1	9,10,11	0.45	0	6,11,13	0.98	0
1	MLZ	A	937	1	8,9,10	1.10	0	4,9,11	0.77	0
2	MLY	B	911	2	9,10,11	0.55	0	6,11,13	0.90	0
2	MLY	B	943	2	9,10,11	0.62	0	6,11,13	0.77	0
1	MLY	A	794	1	9,10,11	0.56	0	6,11,13	0.53	0
1	MLY	A	363	1	9,10,11	0.58	0	6,11,13	0.77	0
1	MLZ	A	972	1	8,9,10	1.07	0	4,9,11	0.87	0
1	MLY	A	759	1	9,10,11	0.50	0	6,11,13	0.72	0
2	MLZ	B	324	2	8,9,10	1.15	0	4,9,11	0.66	0
2	MLY	B	488	2	9,10,11	0.49	0	6,11,13	0.84	0
1	MLY	A	764	1	9,10,11	0.48	0	6,11,13	0.84	0
1	CAS	A	112	1	5,8,9	1.36	1 (20%)	1,9,11	1.17	0
2	MLY	B	116	2	9,10,11	0.52	0	6,11,13	0.90	0
2	MLY	B	986	2	9,10,11	0.49	0	6,11,13	0.71	0
1	MLY	A	956	1	9,10,11	0.54	0	6,11,13	1.05	0
1	MLZ	A	550	1	8,9,10	1.14	0	4,9,11	0.99	0
2	MLY	B	525	2	9,10,11	0.60	0	6,11,13	0.69	0
2	MLY	B	550	2	9,10,11	0.55	0	6,11,13	1.01	0
2	MLZ	B	1013	2	8,9,10	1.18	0	4,9,11	0.66	0
2	MLY	B	466	2	9,10,11	0.55	0	6,11,13	0.89	0
2	MLZ	B	624	2	8,9,10	1.06	0	4,9,11	0.93	0
2	CAS	B	112	2	5,8,9	1.39	1 (20%)	1,9,11	0.55	0
1	MLY	A	290	1	9,10,11	0.60	0	6,11,13	0.74	0
1	MLY	A	154	1	9,10,11	0.54	0	6,11,13	0.83	0
2	MLZ	B	66	2	8,9,10	0.96	0	4,9,11	0.57	0
1	MLY	A	287	1	9,10,11	0.45	0	6,11,13	0.63	0

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	0.63	0
2	MLZ	B	769	2	8,9,10	1.13	0	4,9,11	0.95	0
2	MLY	B	946	2	9,10,11	0.46	0	6,11,13	1.00	0
1	MLZ	A	943	1	8,9,10	1.13	0	4,9,11	0.82	0
2	MLY	B	540	2	9,10,11	0.46	0	6,11,13	0.70	0
2	MLY	B	499	2	9,10,11	0.53	0	6,11,13	0.81	0
1	MLZ	A	437	1	8,9,10	1.07	0	4,9,11	0.74	0
2	MLY	B	290	2	9,10,11	0.60	0	6,11,13	0.77	0
2	MLZ	B	764	2	8,9,10	1.14	0	4,9,11	0.92	0
2	MLY	B	287	2	9,10,11	0.54	0	6,11,13	0.87	0
1	MLY	A	466	1	9,10,11	0.48	0	6,11,13	0.84	0
1	MLY	A	488	1	9,10,11	0.52	0	6,11,13	0.59	0
2	MLZ	B	884	2	8,9,10	1.12	1 (12%)	4,9,11	0.99	0
2	MLY	B	750	2	9,10,11	0.53	0	6,11,13	0.76	0
2	MLZ	B	199	2	8,9,10	1.10	0	4,9,11	0.98	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
1	MLY	A	116	1	-	0/8/9/11	-
2	MLZ	B	759	2	-	1/7/8/10	-
1	MLZ	A	525	1	-	2/7/8/10	-
1	MLY	A	854	1	-	0/8/9/11	-
1	MLY	A	521	1	-	2/8/9/11	-
1	MLZ	A	66	1	-	3/7/8/10	-
1	MLZ	A	884	1	-	1/7/8/10	-
2	MLY	B	431	2	-	1/8/9/11	-
2	MLY	B	642	2	-	0/8/9/11	-
2	MLZ	B	937	2	-	2/7/8/10	-
1	MLY	A	251	1	-	0/8/9/11	-
2	MLZ	B	902	2	-	0/7/8/10	-
1	MLY	A	911	1	-	0/8/9/11	-
2	MLY	B	278	2	-	2/8/9/11	-
2	MLZ	B	1000	2	-	3/7/8/10	-
1	MLZ	A	207	1	-	2/7/8/10	-
1	MLY	A	513	1	-	1/8/9/11	-
1	MLY	A	540	1	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	750	1	-	2/8/9/11	-
2	MLY	B	972	2	-	4/8/9/11	-
1	MLZ	A	769	1	-	2/7/8/10	-
1	MLY	A	902	1	-	2/8/9/11	-
2	MLY	B	513	2	-	2/8/9/11	-
2	MLZ	B	854	2	-	1/7/8/10	-
2	MLY	B	363	2	-	0/8/9/11	-
2	MLZ	B	494	2	-	0/7/8/10	-
1	MLY	A	700	1	-	2/8/9/11	-
2	MLZ	B	956	2	-	1/7/8/10	-
1	MLY	A	278	1	-	0/8/9/11	-
1	MLY	A	704	1	-	0/8/9/11	-
1	MLY	A	946	1	-	0/8/9/11	-
1	MLZ	A	1000	1	-	3/7/8/10	-
2	MLZ	B	490	2	-	0/7/8/10	-
2	MLY	B	41	2	-	0/8/9/11	-
1	MLY	A	431	1	-	1/8/9/11	-
1	MLY	A	642	1	-	0/8/9/11	-
1	MLZ	A	937	1	-	3/7/8/10	-
2	MLY	B	911	2	-	0/8/9/11	-
2	MLY	B	943	2	-	3/8/9/11	-
1	MLY	A	794	1	-	3/8/9/11	-
1	MLY	A	363	1	-	0/8/9/11	-
1	MLZ	A	972	1	-	2/7/8/10	-
1	MLY	A	759	1	-	3/8/9/11	-
2	MLZ	B	324	2	-	4/7/8/10	-
2	MLY	B	488	2	-	0/8/9/11	-
1	MLY	A	764	1	-	0/8/9/11	-
1	CAS	A	112	1	-	0/0/7/9	-
2	MLY	B	116	2	-	3/8/9/11	-
2	MLY	B	986	2	-	1/8/9/11	-
1	MLY	A	956	1	-	1/8/9/11	-
1	MLZ	A	550	1	-	2/7/8/10	-
2	MLY	B	525	2	-	2/8/9/11	-
2	MLY	B	550	2	-	0/8/9/11	-
2	MLZ	B	1013	2	-	5/7/8/10	-
2	MLY	B	466	2	-	3/8/9/11	-
2	MLZ	B	624	2	-	0/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CAS	B	112	2	-	0/0/7/9	-
1	MLY	A	290	1	-	1/8/9/11	-
1	MLY	A	154	1	-	0/8/9/11	-
2	MLZ	B	66	2	-	2/7/8/10	-
1	MLY	A	287	1	-	0/8/9/11	-
2	MLZ	B	125	2	-	1/7/8/10	-
2	MLZ	B	769	2	-	2/7/8/10	-
2	MLY	B	946	2	-	0/8/9/11	-
1	MLZ	A	943	1	-	2/7/8/10	-
2	MLY	B	540	2	-	2/8/9/11	-
2	MLY	B	499	2	-	1/8/9/11	-
1	MLZ	A	437	1	-	4/7/8/10	-
2	MLY	B	290	2	-	0/8/9/11	-
2	MLZ	B	764	2	-	3/7/8/10	-
2	MLY	B	287	2	-	0/8/9/11	-
1	MLY	A	466	1	-	2/8/9/11	-
1	MLY	A	488	1	-	2/8/9/11	-
2	MLZ	B	884	2	-	0/7/8/10	-
2	MLY	B	750	2	-	1/8/9/11	-
2	MLZ	B	199	2	-	2/7/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1000	MLZ	CA-N	-2.17	1.42	1.48
1	A	112	CAS	O-C	2.12	1.28	1.20
2	B	112	CAS	O-C	2.07	1.27	1.20
2	B	884	MLZ	CA-N	-2.01	1.42	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	437	MLZ	O-C-CA-CB
1	A	437	MLZ	CD-CE-NZ-CM
1	A	769	MLZ	C-CA-CB-CG
1	A	1000	MLZ	C-CA-CB-CG
1	A	1000	MLZ	CD-CE-NZ-CM

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Mol	Chain	Res	Type	Atoms
2	B	66	MLZ	C-CA-CB-CG
2	B	66	MLZ	CD-CE-NZ-CM
2	B	116	MLY	O-C-CA-CB
2	B	199	MLZ	CD-CE-NZ-CM
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	324	MLZ	CD-CE-NZ-CM
2	B	943	MLY	O-C-CA-CB
2	B	972	MLY	N-CA-CB-CG
2	B	972	MLY	C-CA-CB-CG
2	B	1000	MLZ	CD-CE-NZ-CM
2	B	1013	MLZ	N-CA-CB-CG
2	B	1013	MLZ	C-CA-CB-CG
2	B	1013	MLZ	CD-CE-NZ-CM
2	B	513	MLY	CD-CE-NZ-CH2
2	B	769	MLZ	CG-CD-CE-NZ
2	B	278	MLY	CG-CD-CE-NZ
1	A	902	MLY	CD-CE-NZ-CH2
1	A	956	MLY	CD-CE-NZ-CH2
2	B	116	MLY	CD-CE-NZ-CH1
2	B	431	MLY	CD-CE-NZ-CH2
2	B	466	MLY	CD-CE-NZ-CH2
2	B	972	MLY	CD-CE-NZ-CH1
2	B	972	MLY	CD-CE-NZ-CH2
1	A	972	MLZ	CG-CD-CE-NZ
1	A	759	MLY	CG-CD-CE-NZ
1	A	550	MLZ	CG-CD-CE-NZ
1	A	290	MLY	CD-CE-NZ-CH2
1	A	521	MLY	CD-CE-NZ-CH2
1	A	700	MLY	CD-CE-NZ-CH2
2	B	278	MLY	CD-CE-NZ-CH1
2	B	943	MLY	CD-CE-NZ-CH2
1	A	750	MLY	CG-CD-CE-NZ
1	A	488	MLY	CG-CD-CE-NZ
1	A	1000	MLZ	CG-CD-CE-NZ
1	A	759	MLY	CD-CE-NZ-CH2
2	B	1000	MLZ	CG-CD-CE-NZ
1	A	794	MLY	CG-CD-CE-NZ
1	A	540	MLY	CD-CE-NZ-CH1
1	A	207	MLZ	CE-CD-CG-CB
2	B	1013	MLZ	CG-CD-CE-NZ

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Mol	Chain	Res	Type	Atoms
1	A	66	MLZ	CE-CD-CG-CB
2	B	769	MLZ	CA-CB-CG-CD
2	B	943	MLY	CD-CE-NZ-CH1
2	B	750	MLY	CE-CD-CG-CB
2	B	854	MLZ	CG-CD-CE-NZ
1	A	937	MLZ	CE-CD-CG-CB
1	A	437	MLZ	CG-CD-CE-NZ
2	B	764	MLZ	CG-CD-CE-NZ
1	A	521	MLY	CA-CB-CG-CD
1	A	794	MLY	CE-CD-CG-CB
1	A	488	MLY	CD-CE-NZ-CH2
2	B	525	MLY	CD-CE-NZ-CH2
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	66	MLZ	CA-CB-CG-CD
2	B	466	MLY	CE-CD-CG-CB
1	A	884	MLZ	CA-CB-CG-CD
1	A	550	MLZ	CE-CD-CG-CB
2	B	540	MLY	CD-CE-NZ-CH1
1	A	972	MLZ	CA-CB-CG-CD
1	A	700	MLY	C-CA-CB-CG
1	A	943	MLZ	C-CA-CB-CG
2	B	540	MLY	C-CA-CB-CG
2	B	764	MLZ	C-CA-CB-CG
2	B	956	MLZ	C-CA-CB-CG
2	B	1000	MLZ	C-CA-CB-CG
2	B	116	MLY	CD-CE-NZ-CH2
2	B	466	MLY	CD-CE-NZ-CH1
2	B	513	MLY	CD-CE-NZ-CH1
1	A	431	MLY	CD-CE-NZ-CH1
1	A	466	MLY	CD-CE-NZ-CH1
1	A	525	MLZ	N-CA-CB-CG
1	A	750	MLY	N-CA-CB-CG
1	A	769	MLZ	N-CA-CB-CG
2	B	525	MLY	N-CA-CB-CG
2	B	986	MLY	CE-CD-CG-CB
1	A	902	MLY	CD-CE-NZ-CH1
2	B	1013	MLZ	CA-CB-CG-CD
2	B	764	MLZ	CE-CD-CG-CB
2	B	937	MLZ	CE-CD-CG-CB
2	B	499	MLY	CE-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
1	A	437	MLZ	CA-CB-CG-CD
1	A	943	MLZ	CE-CD-CG-CB
1	A	540	MLY	CG-CD-CE-NZ
1	A	207	MLZ	C-CA-CB-CG
1	A	513	MLY	C-CA-CB-CG
1	A	759	MLY	C-CA-CB-CG
1	A	794	MLY	C-CA-CB-CG
1	A	937	MLZ	C-CA-CB-CG
2	B	199	MLZ	C-CA-CB-CG
2	B	759	MLZ	C-CA-CB-CG
1	A	937	MLZ	CA-CB-CG-CD
1	A	525	MLZ	CE-CD-CG-CB
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	759	MLZ	3	0
1	A	854	MLY	1	0
1	A	251	MLY	2	0
2	B	278	MLY	1	0
2	B	1000	MLZ	1	0
1	A	540	MLY	2	0
1	A	750	MLY	1	0
2	B	972	MLY	1	0
1	A	902	MLY	2	0
2	B	513	MLY	2	0
1	A	700	MLY	2	0
1	A	704	MLY	1	0
1	A	946	MLY	3	0
1	A	1000	MLZ	1	0
2	B	41	MLY	1	0
2	B	911	MLY	1	0
2	B	943	MLY	1	0
1	A	794	MLY	2	0
1	A	759	MLY	5	0
2	B	324	MLZ	2	0
1	A	112	CAS	1	0
2	B	550	MLY	1	0
2	B	466	MLY	3	0
2	B	112	CAS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	66	MLZ	1	0
1	A	287	MLY	2	0
2	B	125	MLZ	1	0
2	B	540	MLY	2	0
2	B	499	MLY	2	0
1	A	437	MLZ	1	0
2	B	290	MLY	2	0
2	B	764	MLZ	1	0
1	A	488	MLY	2	0
2	B	199	MLZ	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	1114	-	5,5,5	0.42	0	5,5,5	0.27	0
5	GOL	A	1108	-	5,5,5	0.44	0	5,5,5	0.34	0
5	GOL	A	1106	-	5,5,5	0.37	0	5,5,5	0.32	0
5	GOL	B	1110	-	5,5,5	0.40	0	5,5,5	0.33	0
5	GOL	B	1109	-	5,5,5	0.40	0	5,5,5	0.31	0
5	GOL	A	1107	-	5,5,5	0.36	0	5,5,5	0.29	0
6	ACT	A	1115	-	3,3,3	0.86	0	3,3,3	1.39	0
6	ACT	A	1116	-	3,3,3	0.82	0	3,3,3	1.38	0
5	GOL	B	1105	-	5,5,5	0.47	0	5,5,5	0.63	0
4	3UE	A	1102	-	34,34,34	4.03	12 (35%)	44,47,47	1.19	5 (11%)
4	3UE	B	1103	-	34,34,34	4.06	14 (41%)	44,47,47	1.45	7 (15%)
5	GOL	B	1106	-	5,5,5	0.35	0	5,5,5	0.45	0
4	3UE	A	1103	-	34,34,34	4.05	15 (44%)	44,47,47	1.55	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ACT	B	1114	-	3,3,3	0.83	0	3,3,3	1.50	0
5	GOL	A	1109	-	5,5,5	0.36	0	5,5,5	0.57	0
6	ACT	A	1117	3	3,3,3	0.83	0	3,3,3	1.19	0
6	ACT	B	1113	-	3,3,3	0.77	0	3,3,3	1.35	0
6	ACT	B	1112	-	3,3,3	0.80	0	3,3,3	1.35	0
5	GOL	A	1111	-	5,5,5	0.36	0	5,5,5	0.39	0
5	GOL	A	1113	-	5,5,5	0.38	0	5,5,5	0.36	0
6	ACT	B	1115	3	3,3,3	0.77	0	3,3,3	1.39	0
5	GOL	B	1108	-	5,5,5	0.39	0	5,5,5	0.44	0
5	GOL	B	1107	-	5,5,5	0.29	0	5,5,5	0.45	0
5	GOL	B	1104	-	5,5,5	0.42	0	5,5,5	0.38	0
5	GOL	A	1112	-	5,5,5	0.33	0	5,5,5	0.35	0
5	GOL	A	1105	-	5,5,5	0.38	0	5,5,5	0.35	0
4	3UE	B	1102	-	34,34,34	3.99	14 (41%)	44,47,47	1.29	8 (18%)
5	GOL	A	1110	-	5,5,5	0.36	0	5,5,5	0.33	0
5	GOL	A	1104	-	5,5,5	0.32	0	5,5,5	0.58	0
6	ACT	B	1111	-	3,3,3	0.93	0	3,3,3	1.12	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	1114	-	-	4/4/4/4	-
5	GOL	A	1108	-	-	2/4/4/4	-
5	GOL	A	1106	-	-	4/4/4/4	-
5	GOL	B	1110	-	-	0/4/4/4	-
5	GOL	B	1109	-	-	0/4/4/4	-
5	GOL	A	1107	-	-	2/4/4/4	-
5	GOL	B	1105	-	-	2/4/4/4	-
4	3UE	A	1102	-	-	0/22/34/34	0/4/4/4
4	3UE	B	1103	-	-	0/22/34/34	0/4/4/4
5	GOL	B	1106	-	-	1/4/4/4	-
4	3UE	A	1103	-	-	0/22/34/34	0/4/4/4
5	GOL	A	1109	-	-	2/4/4/4	-
5	GOL	A	1111	-	-	3/4/4/4	-
5	GOL	A	1113	-	-	4/4/4/4	-
5	GOL	B	1108	-	-	2/4/4/4	-
5	GOL	B	1107	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	1104	-	-	2/4/4/4	-
5	GOL	A	1112	-	-	2/4/4/4	-
5	GOL	A	1105	-	-	2/4/4/4	-
4	3UE	B	1102	-	-	0/22/34/34	0/4/4/4
5	GOL	A	1110	-	-	2/4/4/4	-
5	GOL	A	1104	-	-	0/4/4/4	-

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1103	3UE	C19-N18	-12.76	1.27	1.48
4	A	1103	3UE	C19-N18	-12.41	1.27	1.48
4	A	1102	3UE	C19-N18	-12.26	1.28	1.48
4	B	1102	3UE	C19-N18	-12.22	1.28	1.48
4	B	1103	3UE	O08-N07	10.82	1.41	1.22
4	A	1103	3UE	O08-N07	10.71	1.41	1.22
4	A	1102	3UE	O08-N07	10.68	1.41	1.22
4	B	1102	3UE	O08-N07	10.37	1.40	1.22
4	B	1102	3UE	C16-N13	-8.68	1.31	1.47
4	A	1102	3UE	C16-N13	-8.53	1.31	1.47
4	B	1103	3UE	C16-N13	-8.50	1.31	1.47
4	A	1103	3UE	C16-N13	-8.34	1.32	1.47
4	A	1102	3UE	C02-N13	7.56	1.50	1.34
4	A	1103	3UE	C14-N13	-7.53	1.33	1.47
4	B	1102	3UE	C02-N13	7.26	1.50	1.34
4	B	1102	3UE	C14-N13	-7.24	1.34	1.47
4	B	1103	3UE	C02-N13	7.18	1.49	1.34
4	A	1102	3UE	C14-N13	-7.16	1.34	1.47
4	B	1103	3UE	C14-N13	-7.09	1.34	1.47
4	A	1103	3UE	C02-N13	6.90	1.49	1.34
4	A	1103	3UE	C30-C31	4.44	1.46	1.38
4	B	1103	3UE	C30-C31	4.29	1.46	1.38
4	A	1102	3UE	C30-C31	4.18	1.46	1.38
4	B	1102	3UE	C30-C31	4.15	1.46	1.38
4	A	1103	3UE	C20-C19	3.93	1.58	1.52
4	A	1103	3UE	C29-C28	3.78	1.46	1.38
4	A	1102	3UE	C20-C19	3.75	1.58	1.52
4	A	1102	3UE	C29-C28	3.70	1.46	1.38
4	B	1102	3UE	C20-C19	3.63	1.58	1.52
4	B	1102	3UE	C29-C28	3.63	1.46	1.38
4	B	1103	3UE	C29-C28	3.54	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1103	3UE	C20-C19	3.32	1.57	1.52
4	A	1103	3UE	C26-C19	2.95	1.57	1.52
4	A	1103	3UE	C17-N18	-2.95	1.41	1.47
4	A	1102	3UE	C26-C19	2.89	1.57	1.52
4	B	1103	3UE	O09-N07	-2.88	1.16	1.35
4	A	1103	3UE	O09-N07	-2.88	1.16	1.35
4	A	1102	3UE	O09-N07	-2.80	1.16	1.35
4	B	1102	3UE	O09-N07	-2.77	1.16	1.35
4	B	1103	3UE	C17-N18	-2.68	1.42	1.47
4	B	1103	3UE	C11-C10	2.60	1.55	1.51
4	A	1102	3UE	C11-C10	2.54	1.55	1.51
4	B	1102	3UE	C11-C10	2.54	1.55	1.51
4	B	1103	3UE	C05-C04	2.49	1.42	1.38
4	A	1102	3UE	C03-C02	-2.47	1.45	1.50
4	B	1102	3UE	C05-C04	2.46	1.42	1.38
4	A	1103	3UE	C11-C10	2.44	1.55	1.51
4	B	1102	3UE	C17-N18	-2.25	1.43	1.47
4	A	1103	3UE	C03-C02	-2.22	1.46	1.50
4	B	1102	3UE	C03-C02	-2.22	1.46	1.50
4	B	1103	3UE	C12-C03	2.21	1.42	1.39
4	B	1103	3UE	C26-C19	2.20	1.56	1.52
4	B	1102	3UE	C21-C20	-2.16	1.35	1.39
4	A	1103	3UE	C31-C26	2.02	1.42	1.39
4	A	1103	3UE	C05-C04	2.01	1.42	1.38

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1103	3UE	C16-N13-C14	5.69	124.29	112.68
4	B	1103	3UE	C16-N13-C14	4.60	122.06	112.68
4	B	1103	3UE	C03-C02-N13	3.56	123.11	118.66
4	A	1103	3UE	C03-C02-N13	3.36	122.86	118.66
4	A	1102	3UE	C14-C15-N18	3.27	116.36	110.61
4	A	1102	3UE	C03-C02-N13	3.08	122.50	118.66
4	B	1103	3UE	C26-C19-C20	-3.00	104.72	112.54
4	B	1102	3UE	C16-N13-C14	2.91	118.62	112.68
4	B	1102	3UE	C20-C19-N18	2.87	115.68	111.50
4	A	1102	3UE	C16-N13-C14	2.78	118.36	112.68
4	B	1102	3UE	C16-C17-N18	2.66	115.29	110.61
4	A	1102	3UE	C26-C19-C20	-2.56	105.87	112.54
4	B	1102	3UE	C14-C15-N18	2.54	115.08	110.61
4	A	1103	3UE	C17-N18-C15	-2.53	104.30	109.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1102	3UE	C16-C17-N18	2.52	115.04	110.61
4	A	1103	3UE	C16-C17-N18	2.48	114.97	110.61
4	B	1102	3UE	C03-C02-N13	2.44	121.71	118.66
4	B	1102	3UE	C26-C19-C20	-2.38	106.34	112.54
4	B	1103	3UE	C17-N18-C15	-2.37	104.62	109.13
4	A	1103	3UE	C20-C19-N18	2.32	114.88	111.50
4	A	1103	3UE	C17-C16-N13	2.27	114.93	110.42
4	B	1102	3UE	C05-C06-N07	2.26	118.89	116.47
4	A	1103	3UE	C26-C19-C20	-2.15	106.94	112.54
4	B	1103	3UE	C31-C26-C27	2.12	120.94	118.30
4	A	1103	3UE	C05-C06-N07	2.11	118.73	116.47
4	B	1103	3UE	C15-N18-C19	2.08	115.81	111.64
4	A	1103	3UE	C14-N13-C02	-2.06	116.41	122.79
4	B	1103	3UE	C14-N13-C02	-2.04	116.47	122.79
4	B	1102	3UE	C31-C26-C27	2.02	120.81	118.30

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1105	GOL	O1-C1-C2-O2
5	A	1105	GOL	O1-C1-C2-C3
5	A	1106	GOL	O1-C1-C2-C3
5	A	1106	GOL	C1-C2-C3-O3
5	A	1108	GOL	O1-C1-C2-C3
5	A	1110	GOL	O1-C1-C2-C3
5	A	1111	GOL	O1-C1-C2-C3
5	A	1112	GOL	O1-C1-C2-C3
5	A	1113	GOL	O1-C1-C2-C3
5	A	1113	GOL	C1-C2-C3-O3
5	A	1114	GOL	O1-C1-C2-C3
5	B	1104	GOL	O1-C1-C2-C3
5	B	1108	GOL	O1-C1-C2-C3
5	A	1107	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	B	1106	GOL	O1-C1-C2-C3
5	A	1106	GOL	O2-C2-C3-O3
5	A	1107	GOL	O1-C1-C2-O2
5	A	1110	GOL	O1-C1-C2-O2
5	A	1111	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	1114	GOL	O1-C1-C2-O2
5	A	1106	GOL	O1-C1-C2-O2
5	A	1112	GOL	O1-C1-C2-O2
5	B	1104	GOL	O1-C1-C2-O2
5	B	1108	GOL	O1-C1-C2-O2
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	1109	GOL	O1-C1-C2-O2
5	A	1113	GOL	O2-C2-C3-O3
5	A	1114	GOL	O2-C2-C3-O3
5	A	1111	GOL	O2-C2-C3-O3

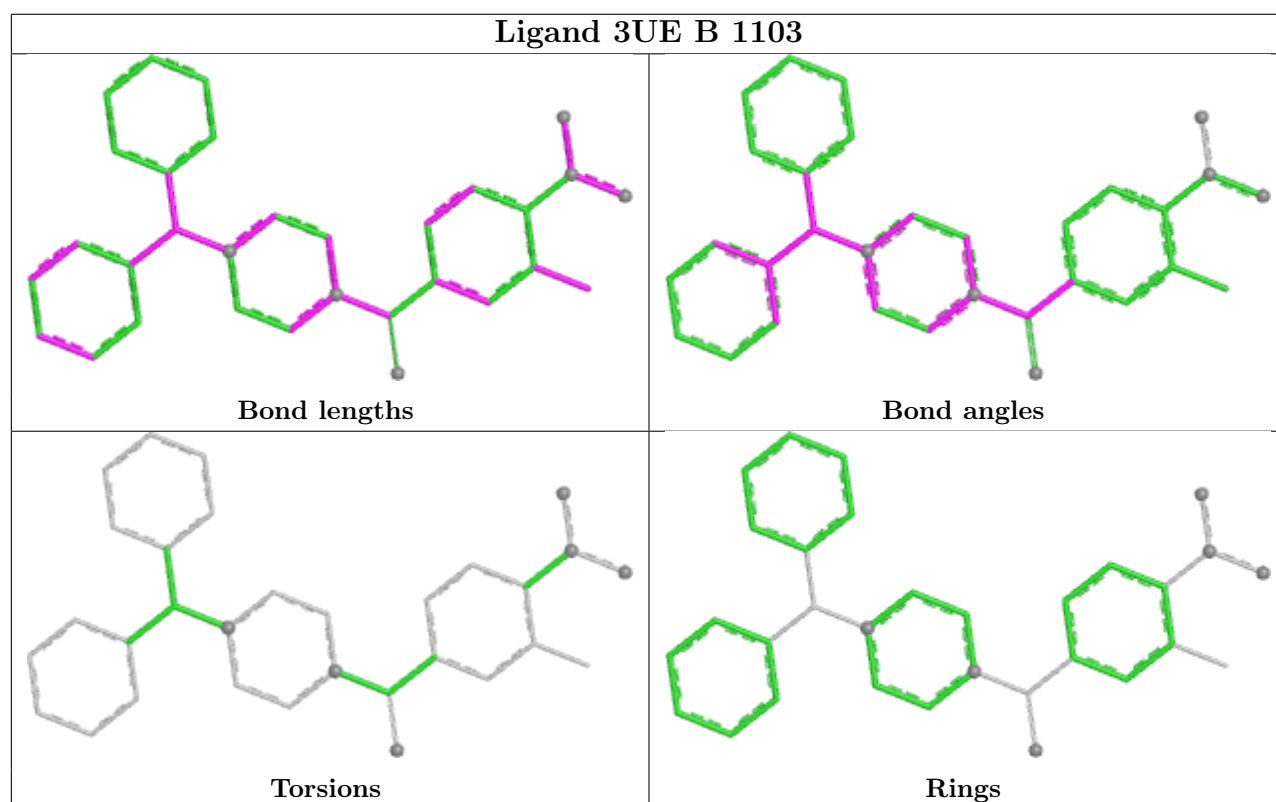
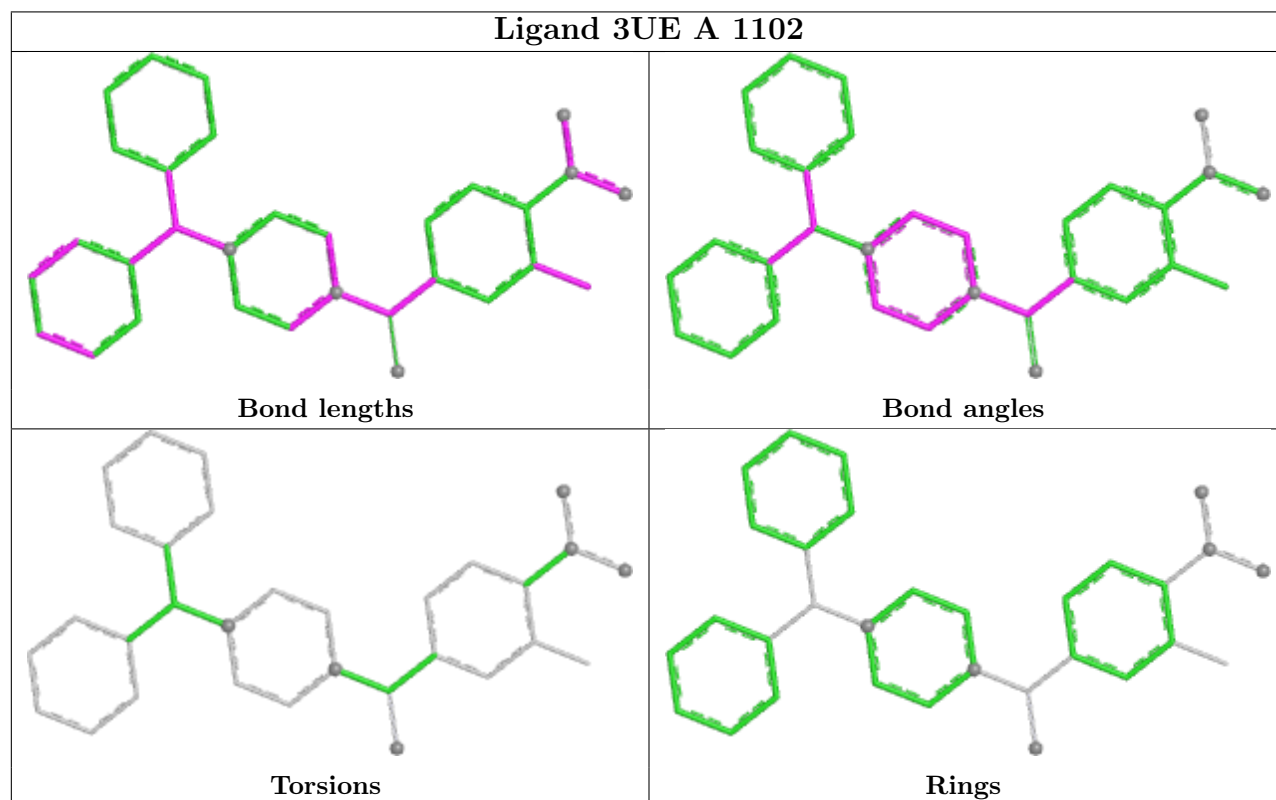
There are no ring outliers.

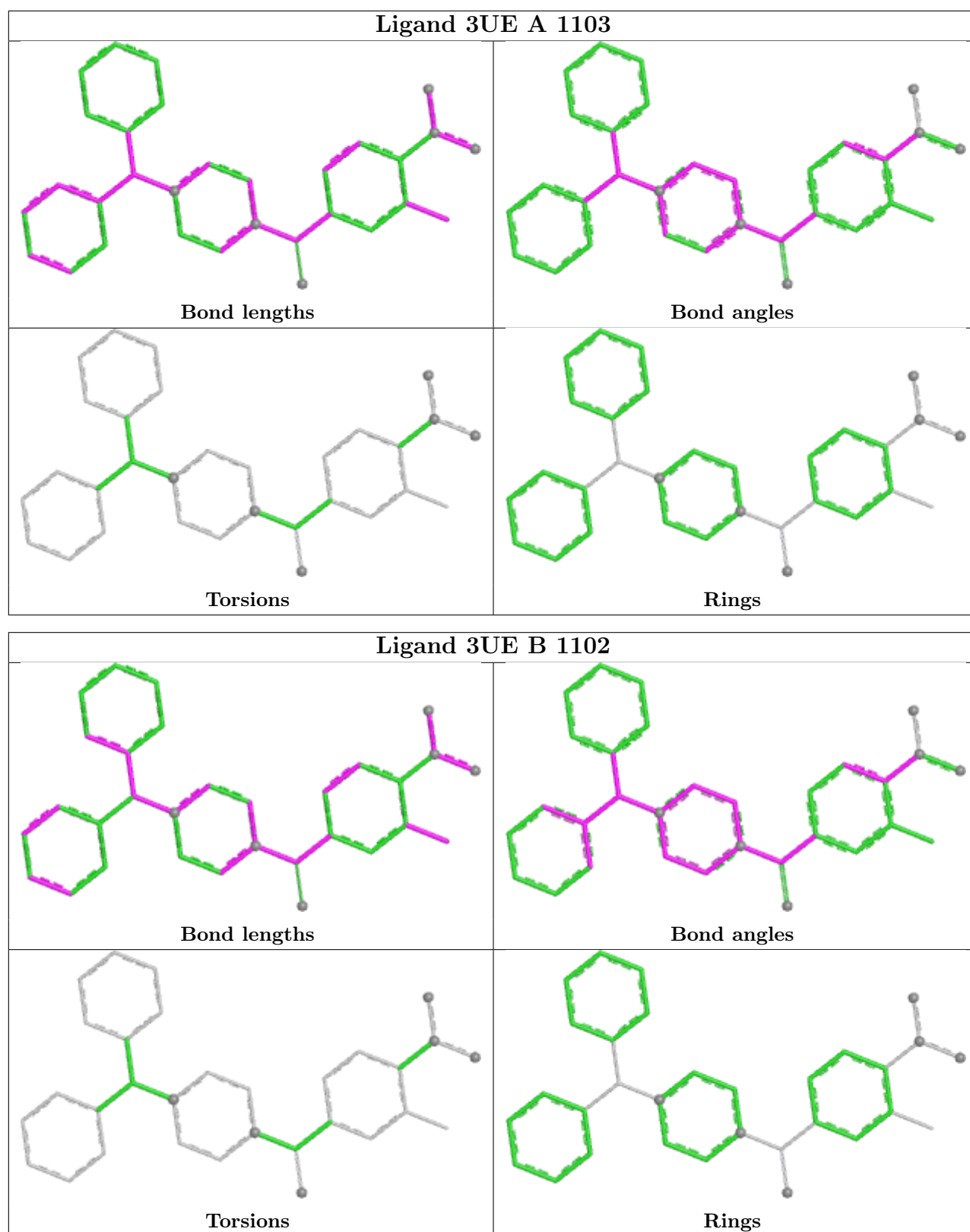
16 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1114	GOL	1	0
5	A	1106	GOL	2	0
5	B	1109	GOL	3	0
5	B	1105	GOL	1	0
4	A	1102	3UE	2	0
4	B	1103	3UE	1	0
5	B	1106	GOL	3	0
4	A	1103	3UE	2	0
6	B	1114	ACT	1	0
6	B	1113	ACT	1	0
5	A	1111	GOL	2	0
5	B	1107	GOL	3	0
5	B	1104	GOL	1	0
5	A	1112	GOL	1	0
4	B	1102	3UE	1	0
5	A	1110	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 ⓘ

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%)	-0.05	13 (1%) 73 74	15, 32, 51, 82	5 (0%)
2	B	940/1014 (92%)	0.02	16 (1%) 69 70	16, 34, 54, 94	1 (0%)
All	All	1891/2028 (93%)	-0.01	29 (1%) 72 73	15, 33, 53, 94	6 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	915	ASN	4.4
2	B	851	TRP	4.3
2	B	318	PHE	3.9
1	A	927	ASN	3.9
1	A	838	VAL	3.8
2	B	813	VAL	3.3
2	B	839	ILE	3.2
2	B	814	ARG	3.1
1	A	823	PRO	3.1
2	B	927	ASN	3.1
1	A	321	ASP	3.0
2	B	323	SER	2.8
2	B	821	PRO	2.7
2	B	505	ARG	2.7
1	A	872	THR	2.6
1	A	1011	THR	2.5
2	B	838	VAL	2.5
2	B	806	SER	2.4
2	B	872	THR	2.3
1	A	813	VAL	2.3
1	A	317	SER	2.3
1	A	319	ALA	2.3
2	B	317	SER	2.2
1	A	32	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	915	ASN	2.1
2	B	575	ASP	2.1
1	A	124	PHE	2.1
2	B	572	THR	2.0
1	A	914	HIS	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(Å ²)	Q<0.9
2	MLZ	B	324	10/11	0.77	0.23	46,61,69,70	0
1	MLY	A	521	11/12	0.81	0.17	42,46,60,63	0
1	MLY	A	794	11/12	0.84	0.17	37,51,66,67	0
1	MLY	A	700	11/12	0.85	0.17	31,32,61,61	0
2	MLY	B	499	11/12	0.85	0.18	33,41,65,65	0
2	MLZ	B	1013	10/11	0.85	0.14	40,45,54,58	0
1	MLY	A	750	11/12	0.86	0.16	31,39,54,57	0
2	MLY	B	513	11/12	0.88	0.12	34,39,47,49	0
2	MLY	B	972	11/12	0.88	0.16	32,34,56,59	0
2	MLZ	B	494	10/11	0.88	0.12	33,40,54,57	0
1	MLY	A	704	11/12	0.89	0.13	30,31,51,53	0
2	MLY	B	750	11/12	0.90	0.12	35,41,47,53	0
2	MLY	B	41	11/12	0.90	0.12	34,35,46,49	0
2	MLY	B	986	11/12	0.90	0.14	32,42,54,56	0
2	MLY	B	290	11/12	0.90	0.13	33,37,53,54	0
1	MLY	A	363	11/12	0.91	0.12	30,32,52,56	0
2	MLZ	B	769	10/11	0.91	0.10	38,39,42,46	0
2	MLZ	B	902	10/11	0.91	0.11	28,33,39,42	0
2	MLY	B	116	11/12	0.91	0.13	28,39,47,54	0
2	MLY	B	287	11/12	0.91	0.11	31,32,41,41	0
1	MLY	A	290	11/12	0.91	0.11	34,37,48,50	0
2	MLZ	B	66	10/11	0.92	0.11	31,31,47,50	0
1	MLY	A	251	11/12	0.92	0.10	31,31,45,46	0
2	MLZ	B	125	10/11	0.92	0.10	27,27,39,41	0
2	MLY	B	550	11/12	0.92	0.11	27,32,38,44	0
2	MLY	B	278	11/12	0.92	0.12	31,35,50,53	0
2	MLZ	B	759	10/11	0.92	0.10	39,45,47,50	0
1	MLY	A	431	11/12	0.92	0.12	28,31,52,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	MLY	A	911	11/12	0.92	0.11	27,27,38,46	0
2	MLY	B	911	11/12	0.92	0.11	28,29,41,45	0
1	MLY	A	466	11/12	0.92	0.11	29,33,44,46	0
2	MLY	B	363	11/12	0.92	0.12	33,34,51,55	0
2	MLZ	B	490	10/11	0.92	0.13	32,38,59,60	0
1	MLY	A	956	11/12	0.93	0.12	27,28,53,55	0
2	MLZ	B	199	10/11	0.93	0.11	29,38,49,50	0
1	MLZ	A	972	10/11	0.93	0.11	29,33,49,51	0
2	MLZ	B	884	10/11	0.93	0.10	28,32,43,45	0
1	MLZ	A	525	10/11	0.93	0.09	37,38,44,45	0
1	MLY	A	759	11/12	0.93	0.10	35,35,41,44	0
2	MLZ	B	937	10/11	0.93	0.10	28,33,42,47	0
2	MLY	B	943	11/12	0.93	0.10	28,31,48,52	0
2	MLZ	B	956	10/11	0.93	0.09	28,31,42,42	0
2	MLY	B	525	11/12	0.93	0.09	32,34,42,43	0
2	MLY	B	540	11/12	0.93	0.09	28,29,34,38	0
1	MLY	A	946	11/12	0.93	0.10	26,34,48,48	0
1	MLZ	A	66	10/11	0.94	0.09	31,32,42,45	0
2	MLZ	B	624	10/11	0.94	0.08	33,34,39,42	0
1	MLY	A	540	11/12	0.94	0.08	30,31,33,35	0
1	MLY	A	642	11/12	0.94	0.09	29,31,35,40	0
2	MLZ	B	764	10/11	0.94	0.08	39,43,45,47	0
1	MLZ	A	437	10/11	0.94	0.09	28,29,47,48	0
2	MLZ	B	854	10/11	0.94	0.08	32,33,36,40	0
2	MLZ	B	1000	10/11	0.94	0.11	31,36,54,56	0
1	MLY	A	902	11/12	0.94	0.10	28,29,37,39	0
1	MLY	A	116	11/12	0.95	0.08	29,29,30,37	0
1	MLY	A	764	11/12	0.95	0.08	34,34,40,46	0
2	MLY	B	431	11/12	0.95	0.10	31,32,48,56	0
2	MLY	B	466	11/12	0.95	0.08	30,31,34,40	0
1	MLZ	A	1000	10/11	0.95	0.08	27,31,44,44	0
1	MLZ	A	769	10/11	0.95	0.08	33,34,39,43	0
1	MLY	A	488	11/12	0.95	0.07	30,30,32,35	0
1	MLY	A	854	11/12	0.95	0.08	31,31,38,40	0
1	MLZ	A	884	10/11	0.95	0.08	27,27,29,31	0
2	MLY	B	946	11/12	0.95	0.10	27,35,47,47	0
1	MLY	A	513	11/12	0.95	0.07	33,36,44,51	0
1	MLY	A	278	11/12	0.95	0.07	31,32,35,36	0
1	MLZ	A	943	10/11	0.95	0.09	27,35,38,42	0
2	MLY	B	642	11/12	0.95	0.09	33,34,39,41	0
1	MLZ	A	207	10/11	0.95	0.10	29,29,46,53	0
1	MLY	A	154	11/12	0.96	0.09	28,30,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	MLY	A	287	11/12	0.96	0.07	31,32,34,38	0
1	MLZ	A	937	10/11	0.96	0.07	28,29,43,44	0
2	CAS	B	112	9/10	0.97	0.10	27,28,60,92	0
1	CAS	A	112	9/10	0.97	0.10	28,32,68,93	0
2	MLY	B	488	11/12	0.97	0.07	31,32,37,40	0
1	MLZ	A	550	10/11	0.97	0.06	27,30,37,41	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

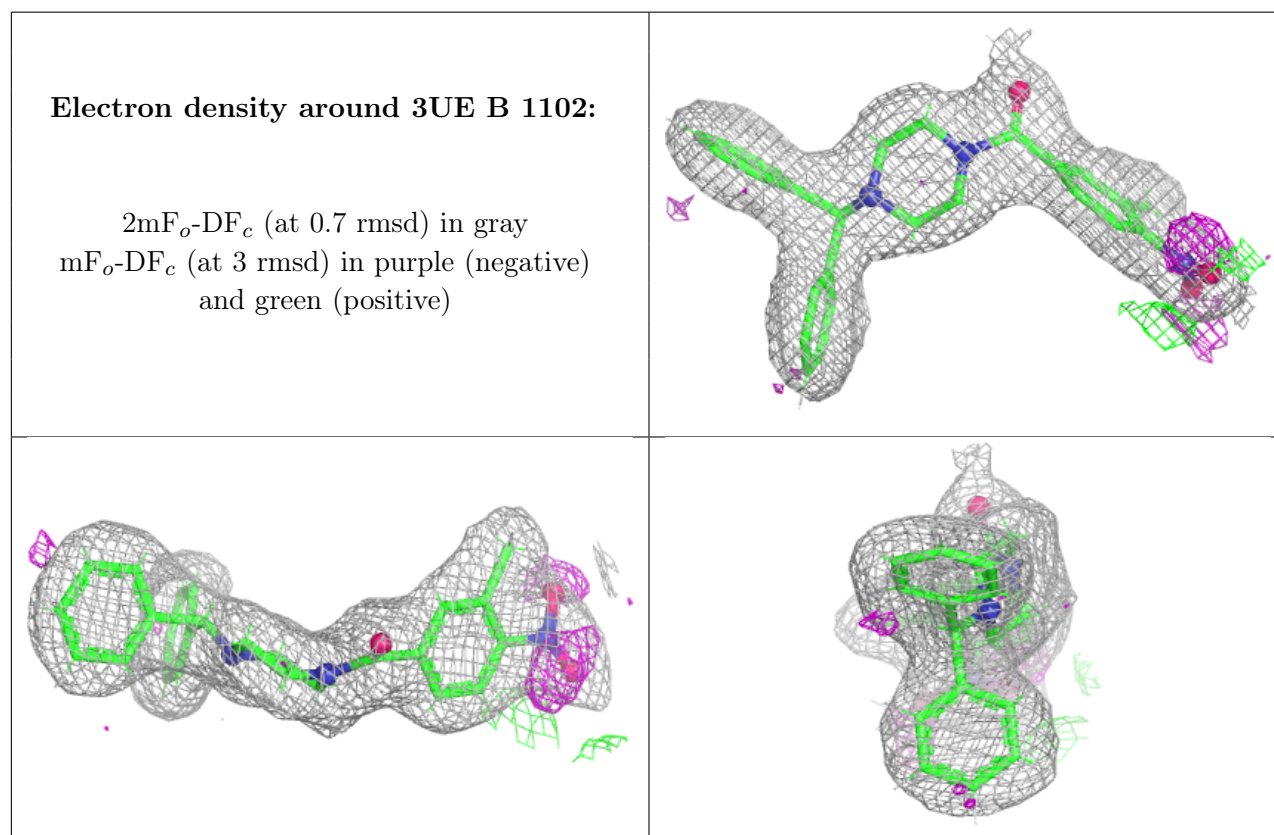
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	ACT	A	1115	4/4	0.67	0.21	56,63,63,67	0
5	GOL	B	1108	6/6	0.77	0.24	69,70,74,75	0
6	ACT	B	1112	4/4	0.77	0.17	43,47,52,61	0
5	GOL	B	1107	6/6	0.80	0.20	53,60,68,75	0
5	GOL	A	1109	6/6	0.80	0.23	54,62,73,77	0
6	ACT	B	1114	4/4	0.80	0.17	41,51,52,59	0
5	GOL	A	1110	6/6	0.82	0.15	51,66,68,69	0
5	GOL	A	1106	6/6	0.82	0.20	58,61,65,65	0
5	GOL	A	1105	6/6	0.82	0.18	50,51,65,72	0
5	GOL	A	1108	6/6	0.84	0.17	51,62,70,72	0
6	ACT	B	1111	4/4	0.84	0.14	41,44,52,53	0
5	GOL	A	1107	6/6	0.85	0.14	48,59,68,72	0
6	ACT	B	1113	4/4	0.85	0.14	43,47,49,49	0
5	GOL	A	1112	6/6	0.85	0.18	32,46,57,63	0
5	GOL	A	1111	6/6	0.86	0.18	35,50,60,67	0
5	GOL	B	1105	6/6	0.87	0.14	39,41,49,51	0
5	GOL	A	1114	6/6	0.87	0.14	54,60,72,80	0
5	GOL	B	1106	6/6	0.88	0.16	51,57,58,61	0
5	GOL	A	1113	6/6	0.88	0.14	54,58,61,62	0
5	GOL	A	1104	6/6	0.90	0.16	38,41,46,48	0
5	GOL	B	1109	6/6	0.91	0.12	28,43,48,52	0
5	GOL	B	1104	6/6	0.91	0.12	41,48,52,54	0

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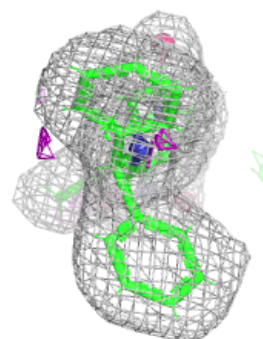
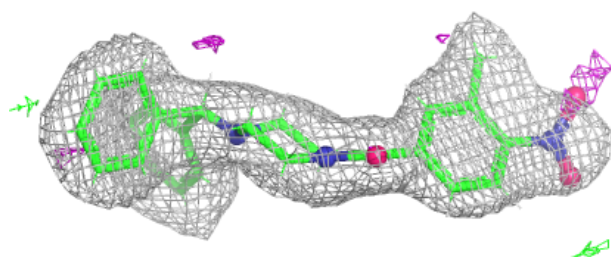
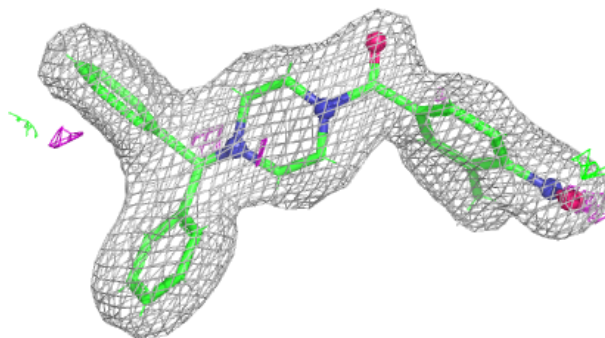
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	ACT	B	1115	4/4	0.92	0.10	28,42,43,45	0
6	ACT	A	1116	4/4	0.93	0.10	33,34,39,39	0
5	GOL	B	1110	6/6	0.93	0.10	35,41,46,54	0
4	3UE	B	1102	31/31	0.93	0.08	29,31,36,49	0
4	3UE	B	1103	31/31	0.94	0.07	29,35,40,56	0
4	3UE	A	1103	31/31	0.94	0.07	28,32,39,58	0
6	ACT	A	1117	4/4	0.95	0.11	28,37,44,46	0
4	3UE	A	1102	31/31	0.95	0.07	27,33,45,64	0
7	CA	B	1116	1/1	0.98	0.07	41,41,41,41	0
7	CA	B	1117	1/1	0.98	0.14	54,54,54,54	0
3	ZN	A	1101	1/1	1.00	0.02	38,38,38,38	0
3	ZN	B	1101	1/1	1.00	0.03	42,42,42,42	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.

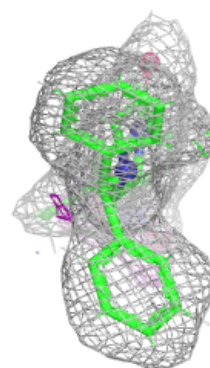
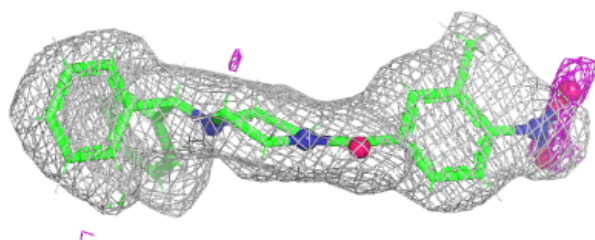
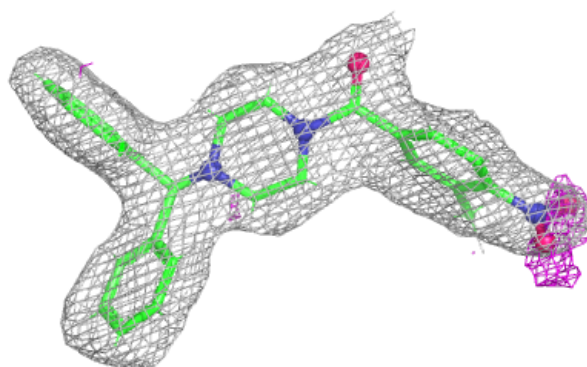


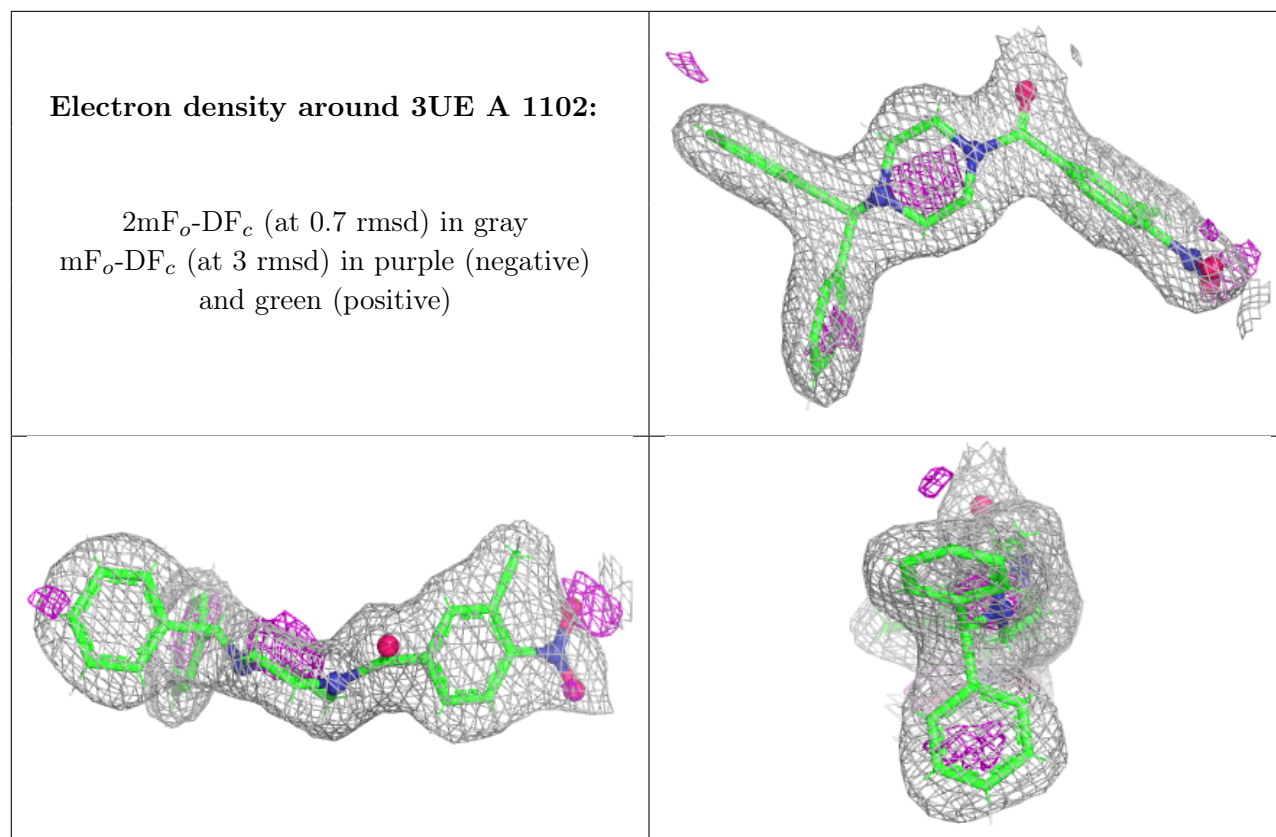
Electron density around 3UE B 1103:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.