Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:41 PM GMT

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
http://wwpdb.org/validation/2016/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:

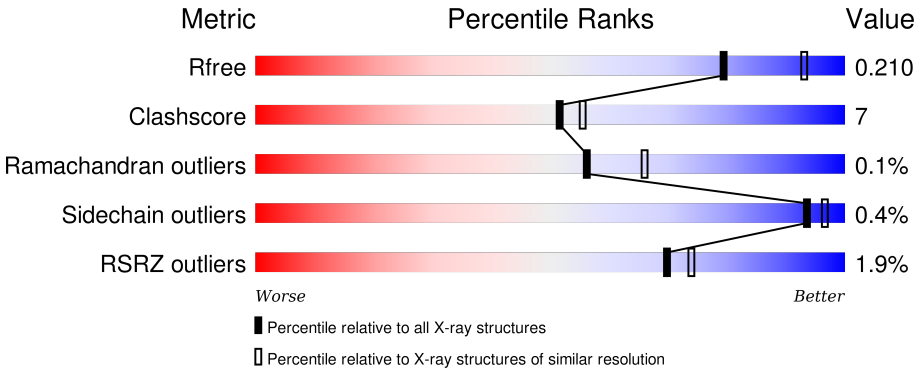
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

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}	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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. 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 <=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	86% 11%
2	B	1014	2% 82% 15%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	A	1104	-	-	-	X
5	GOL	A	1105	-	-	-	X
5	GOL	A	1106	-	-	-	X
5	GOL	A	1109	-	-	-	X
5	GOL	A	1110	-	-	-	X
5	GOL	A	1111	-	-	-	X
5	GOL	A	1112	-	-	-	X
5	GOL	B	1105	-	-	-	X
5	GOL	B	1106	-	-	-	X
5	GOL	B	1107	-	-	-	X
6	ACT	A	1115	-	-	-	X
6	ACT	B	1111	-	-	-	X
6	ACT	B	1113	-	-	-	X
7	CA	B	1117	-	-	-	X

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
1	A	988	Total	As	C	N	O	S	0	5	0
			7985	1	5101	1350	1493	40			

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
2	B	979	Total	As	C	N	O	S	0	1	0
			7878	1	5036	1327	1474	40			

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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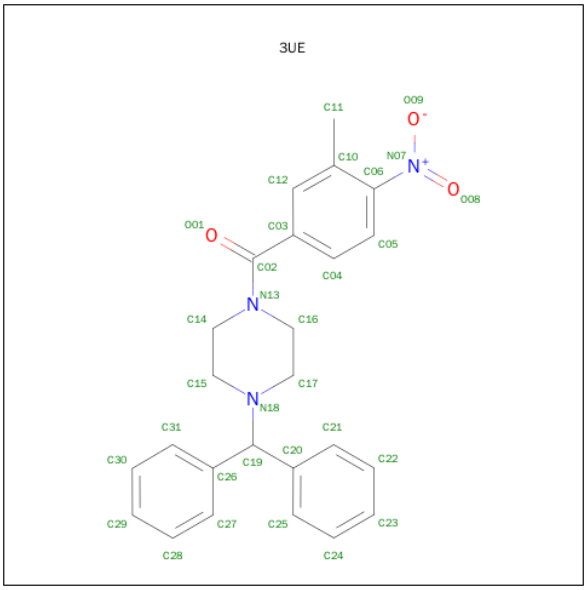
Chain	Residue	Modelled	Actual	Comment	Reference
B	27	HIS	-	EXPRESSION TAG	UNP Q5JRX3
B	28	HIS	-	EXPRESSION TAG	UNP Q5JRX3
B	29	HIS	-	EXPRESSION TAG	UNP Q5JRX3
B	30	HIS	-	EXPRESSION TAG	UNP Q5JRX3
B	31	ALA	-	EXPRESSION TAG	UNP Q5JRX3
B	32	ALA	-	EXPRESSION TAG	UNP Q5JRX3
B	107	GLN	GLU	ENGINEERED MUTATION	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: $C_{25}H_{25}N_3O_3$).



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

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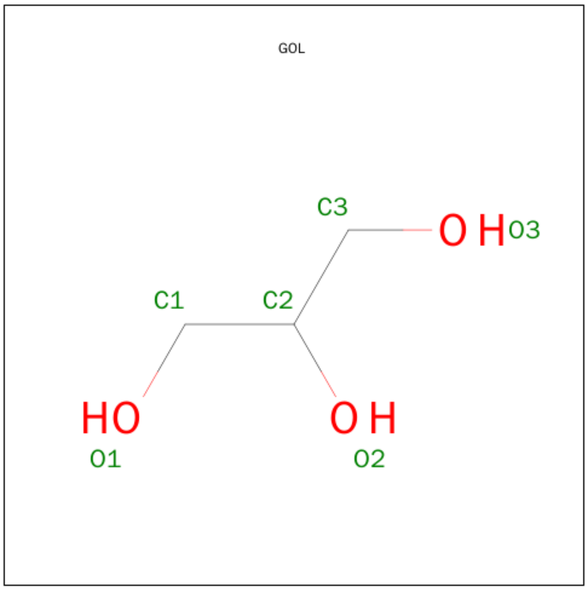
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H N O 56 25 25 3 3	0	0
4	B	1	Total C H N O 56 25 25 3 3	0	0
4	B	1	Total C H N O 56 25 25 3 3	0	0

- 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 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0

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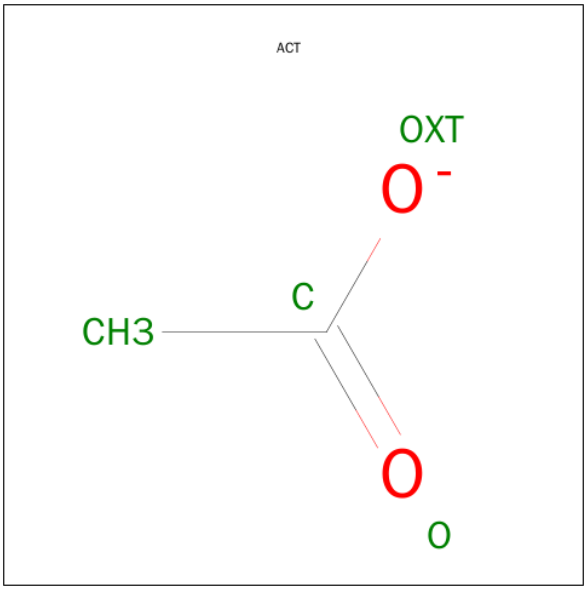
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

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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 (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.

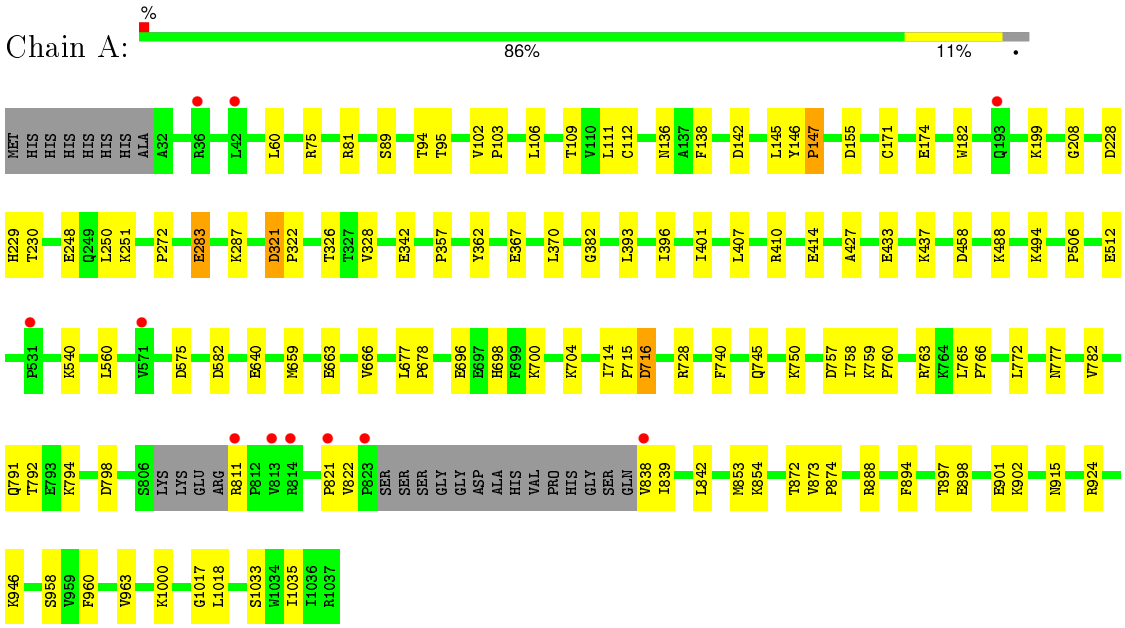
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	420	Total O 420 420	0	0
8	B	391	Total O 391 391	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

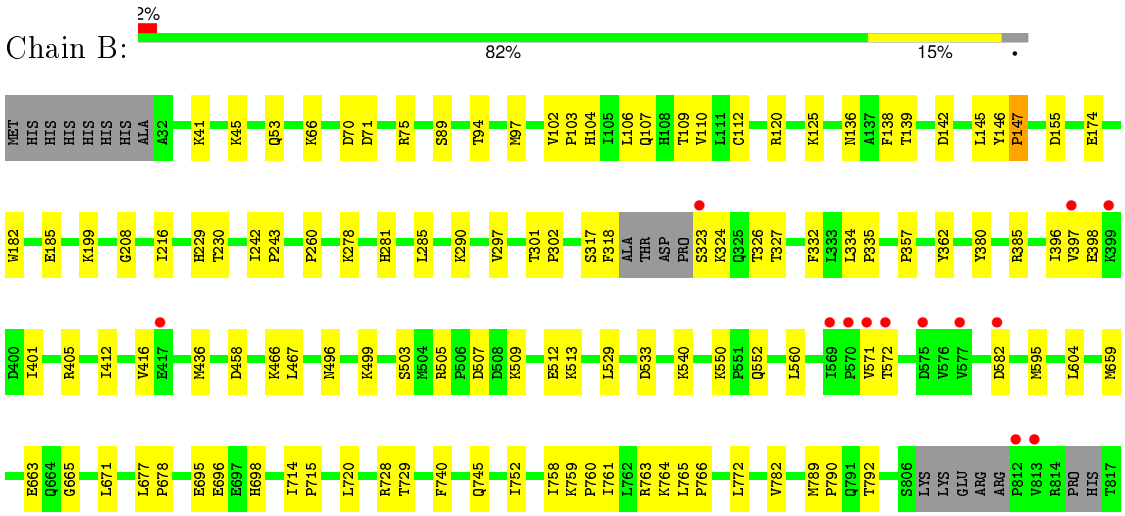
- Molecule 1: Presequence protease, mitochondrial

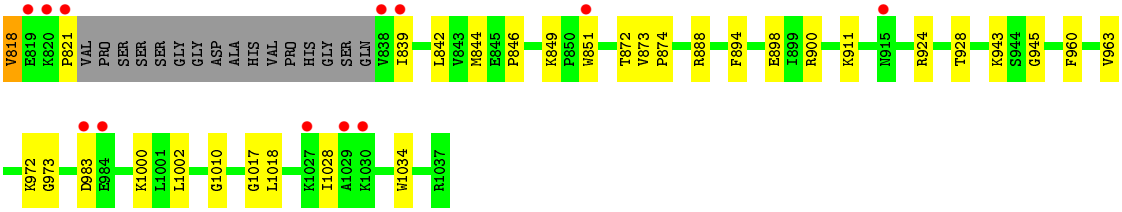
Chain A:



- Molecule 2: Presequence protease, mitochondrial

Chain B:




V818
E819
K820
P821
VAL
PRO
SER
SER
SER
GLY
GLY
ASP
ALA
HIS
VAL
PRO
HIS
GLY
SER
GLN
V838
I839
L842
V843
M844
E845
P846
K849
P850
W851
T872
V873
P874
R888
F894
E898
I899
R900
K911
N915
R924
T928
K943
S944
G945
F960
V963
K972
G973
D983
E984
K1000
L1001
L1002
G1010
G1017
L1018
K1027
I1028
A1029
K1030
W1034
R1037

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.44 (at 2.27Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.175 , 0.208 0.184 , 0.210	Depositor DCC
R_{free} test set	1992 reflections (1.80%)	DCC
Wilson B-factor (Å^2)	33.9	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 38.6	EDS
Estimated twinning fraction	0.013 for -h-2*l,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 119317 reflections (0.001%)	Xtriage
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

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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, 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(^{o})	Ideal(^{o})
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

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

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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

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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:677:LEU:HB3	1:A:678:PRO:HD3	1.81	0.63
1:A:138:PHE:CZ	1:A:145:LEU:HD23	2.32	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
2:B:759:MLZ:N	2:B:760:PRO:HD2	2.17	0.59
1:A:714:ILE:HB	1:A:715:PRO:HD3	1.85	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:765:LEU:HB2	2:B:766:PRO:HD3	1.84	0.58
2:B:509:LYS:O	2:B:513:MLY:HG2	2.04	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

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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
2:B:752:ILE:CG2	2:B:758:ILE:HD11	2.43	0.49
1:A:370:LEU:CD1	1:A:407:LEU:HD12	2.42	0.49
2:B:260:PRO:HB3	2:B:285:LEU:HD22	1.93	0.49
1:A:873:VAL:HB	1:A:874:PRO:HD2	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:759:MLZ:O	2:B:763:ARG:HG3	2.12	0.48
2:B:1017:GLY:C	2:B:1018:LEU:HD12	2.33	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:791:GLN:OE1	1:A:791:GLN:N	2.36	0.47
1:A:512:GLU:OE1	1:A:512:GLU:N	2.45	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
2:B:595:MET:CE	2:B:671:LEU:HD12	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
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: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
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:328:VAL:HG12	1:A:396:ILE:HD12	1.98	0.45
1:A:102:VAL:N	1:A:103:PRO:HD2	2.31	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

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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:696:GLU:OE1	1:A:759:MLY:HH12	2.18	0.44
1:A:342:GLU:OE1	1:A:488:MLY:HH12	2.17	0.44
4:A:1102:3UE:C04	4:A:1102:3UE:H12	2.46	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
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:659:MET:CE	2:B:872:THR:O	2.67	0.43
2:B:301:THR:HA	2:B:302:PRO:HD3	1.90	0.43
2:B:260:PRO:CB	2:B:285:LEU:HD22	2.48	0.43
1:A:370:LEU:HD11	1:A:407:LEU:HD12	2.00	0.43
1:A:174:GLU:OE1	1:A:540:MLY:HE3	2.18	0.43
2:B:728:ARG:HG2	2:B:729:THR:HG23	2.01	0.43
1:A:663:GLU:HB2	1:A:842:LEU:HG	2.00	0.43
1:A:888:ARG:HA	1:A:888:ARG:HD2	1.78	0.43
2:B:89:SER:HA	2:B:146:TYR:O	2.18	0.43
1:A:853:MET:CE	1:A:1035:ILE:HD12	2.49	0.43
1:A:750:MLY:HD3	1:A:750:MLY:HH12	1.66	0.43
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
1:A:106:LEU:HA	1:A:250:LEU:HD11	2.01	0.42
2:B:604:LEU:HD23	2:B:772:LEU:HD21	2.01	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:427:ALA:HB1	1:A:640:GLU:HG2	2.00	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:758:ILE:HD12	1:A:758:ILE:C	2.39	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:208:GLY:HA3	2:B:924:ARG:HD3	2.01	0.42
2:B:94:THR:O	2:B:142:ASP:HA	2.20	0.42

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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:677:LEU:HB3	2:B:678:PRO:HD3	2.02	0.42
2:B:436:MET:HG2	2:B:467:LEU:HD12	2.02	0.42
2:B:242:ILE:HB	2:B:243:PRO:HD3	2.02	0.42
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
1:A:182:TRP:HA	1:A:199:LYS:O	2.21	0.41
2:B:849:LYS:O	2:B:851:TRP:CE3	2.73	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:671:LEU:HD23	2:B:671:LEU:N	2.36	0.41
1:A:95:THR:OG1	5:A:1110:GOL:H32	2.21	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: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: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
2:B:512:GLU:N	2:B:512:GLU:OE1	2.47	0.40
2:B:41:MLY:HH22	2:B:41:MLY:HD3	1.74	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
2:B:844:MET:HE2	2:B:844:MET:HB3	1.83	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%)	56 66
2	B	931/1014 (92%)	919 (99%)	11 (1%)	1 (0%)	56 66
All	All	1881/2028 (93%)	1856 (99%)	23 (1%)	2 (0%)	56 66

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%)	88 93
2	B	834/862 (97%)	832 (100%)	2 (0%)	95 98
All	All	1682/1726 (98%)	1674 (100%)	8 (0%)	93 95

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

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	MLZ	A	1000	1	7,9,10	1.21	1 (14%)	7,9,11	1.14	1 (14%)
1	CAS	A	112	1	4,8,9	1.25	0	2,9,11	2.06	1 (50%)
1	MLY	A	116	1	8,10,11	0.40	0	9,11,13	1.06	0
1	MLY	A	154	1	8,10,11	0.46	0	9,11,13	0.88	0
1	MLZ	A	207	1	7,9,10	1.20	1 (14%)	7,9,11	0.99	0
1	MLY	A	251	1	8,10,11	0.57	0	9,11,13	0.95	0
1	MLY	A	278	1	8,10,11	0.46	0	9,11,13	0.86	1 (11%)
1	MLY	A	287	1	8,10,11	0.38	0	9,11,13	0.86	1 (11%)
1	MLY	A	290	1	8,10,11	0.57	0	9,11,13	0.87	0
1	MLY	A	363	1	8,10,11	0.54	0	9,11,13	0.91	0
1	MLY	A	431	1	8,10,11	0.57	0	9,11,13	0.99	0
1	MLZ	A	437	1	7,9,10	1.17	1 (14%)	7,9,11	1.21	1 (14%)
1	MLY	A	466	1	8,10,11	0.46	0	9,11,13	0.94	0
1	MLY	A	488	1	8,10,11	0.47	0	9,11,13	0.80	0
1	MLY	A	513	1	8,10,11	0.45	0	9,11,13	0.93	0
1	MLY	A	521	1	8,10,11	0.57	0	9,11,13	0.94	0
1	MLZ	A	525	1	7,9,10	1.25	1 (14%)	7,9,11	1.28	1 (14%)
1	MLY	A	540	1	8,10,11	0.53	0	9,11,13	0.86	0
1	MLZ	A	550	1	7,9,10	1.23	1 (14%)	7,9,11	1.34	1 (14%)
1	MLY	A	642	1	8,10,11	0.45	0	9,11,13	1.07	1 (11%)
1	MLZ	A	66	1	7,9,10	1.14	0	7,9,11	1.11	1 (14%)
1	MLY	A	700	1	8,10,11	0.49	0	9,11,13	1.12	0
1	MLY	A	704	1	8,10,11	0.54	0	9,11,13	0.98	1 (11%)
1	MLY	A	750	1	8,10,11	0.39	0	9,11,13	1.03	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	MLY	A	759	1	8,10,11	0.45	0	9,11,13	0.89	1 (11%)
1	MLY	A	764	1	8,10,11	0.43	0	9,11,13	0.95	0
1	MLZ	A	769	1	7,9,10	1.27	1 (14%)	7,9,11	1.02	0
1	MLY	A	794	1	8,10,11	0.51	0	9,11,13	0.79	0
1	MLY	A	854	1	8,10,11	0.57	0	9,11,13	0.88	1 (11%)
1	MLZ	A	884	1	7,9,10	1.29	1 (14%)	7,9,11	1.17	1 (14%)
1	MLY	A	902	1	8,10,11	0.54	0	9,11,13	0.79	0
1	MLY	A	911	1	8,10,11	0.60	0	9,11,13	1.00	0
1	MLZ	A	937	1	7,9,10	1.15	1 (14%)	7,9,11	1.08	1 (14%)
1	MLZ	A	943	1	7,9,10	1.21	1 (14%)	7,9,11	1.25	1 (14%)
1	MLY	A	946	1	8,10,11	0.50	0	9,11,13	0.91	0
1	MLY	A	956	1	8,10,11	0.48	0	9,11,13	1.10	1 (11%)
1	MLZ	A	972	1	7,9,10	1.16	0	7,9,11	1.06	0
2	MLZ	B	1000	2	7,9,10	1.27	0	7,9,11	1.10	0
2	MLZ	B	1013	2	7,9,10	1.25	0	7,9,11	1.12	1 (14%)
2	CAS	B	112	2	4,8,9	1.26	0	2,9,11	2.18	1 (50%)
2	MLY	B	116	2	8,10,11	0.47	0	9,11,13	0.98	0
2	MLZ	B	125	2	7,9,10	1.19	0	7,9,11	1.31	1 (14%)
2	MLZ	B	199	2	7,9,10	1.23	1 (14%)	7,9,11	1.20	1 (14%)
2	MLY	B	278	2	8,10,11	0.48	0	9,11,13	0.95	1 (11%)
2	MLY	B	287	2	8,10,11	0.48	0	9,11,13	1.00	0
2	MLY	B	290	2	8,10,11	0.53	0	9,11,13	0.91	0
2	MLZ	B	324	2	7,9,10	1.20	1 (14%)	7,9,11	1.09	1 (14%)
2	MLY	B	363	2	8,10,11	0.63	0	9,11,13	0.86	1 (11%)
2	MLY	B	41	2	8,10,11	0.49	0	9,11,13	1.08	1 (11%)
2	MLY	B	431	2	8,10,11	0.45	0	9,11,13	1.12	0
2	MLY	B	466	2	8,10,11	0.50	0	9,11,13	0.98	0
2	MLY	B	488	2	8,10,11	0.47	0	9,11,13	0.94	0
2	MLZ	B	490	2	7,9,10	1.30	1 (14%)	7,9,11	1.24	0
2	MLZ	B	494	2	7,9,10	1.17	0	7,9,11	1.14	1 (14%)
2	MLY	B	499	2	8,10,11	0.51	0	9,11,13	0.89	0
2	MLY	B	513	2	8,10,11	0.50	0	9,11,13	0.89	0
2	MLY	B	525	2	8,10,11	0.49	0	9,11,13	0.84	0
2	MLY	B	540	2	8,10,11	0.44	0	9,11,13	0.88	0
2	MLY	B	550	2	8,10,11	0.50	0	9,11,13	1.11	1 (11%)
2	MLZ	B	624	2	7,9,10	1.16	1 (14%)	7,9,11	1.29	1 (14%)
2	MLY	B	642	2	8,10,11	0.46	0	9,11,13	0.98	1 (11%)
2	MLZ	B	66	2	7,9,10	1.07	0	7,9,11	1.02	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MLY	B	750	2	8,10,11	0.51	0	9,11,13	0.93	0
2	MLZ	B	759	2	7,9,10	1.22	1 (14%)	7,9,11	1.27	1 (14%)
2	MLZ	B	764	2	7,9,10	1.24	1 (14%)	7,9,11	1.24	1 (14%)
2	MLZ	B	769	2	7,9,10	1.27	1 (14%)	7,9,11	1.20	0
2	MLZ	B	854	2	7,9,10	1.17	1 (14%)	7,9,11	1.24	1 (14%)
2	MLZ	B	884	2	7,9,10	1.18	1 (14%)	7,9,11	1.21	1 (14%)
2	MLZ	B	902	2	7,9,10	1.10	0	7,9,11	1.05	0
2	MLY	B	911	2	8,10,11	0.55	0	9,11,13	0.96	0
2	MLZ	B	937	2	7,9,10	1.09	0	7,9,11	1.06	1 (14%)
2	MLY	B	943	2	8,10,11	0.62	0	9,11,13	0.92	0
2	MLY	B	946	2	8,10,11	0.45	0	9,11,13	1.00	0
2	MLZ	B	956	2	7,9,10	1.13	0	7,9,11	1.03	1 (14%)
2	MLY	B	972	2	8,10,11	0.55	0	9,11,13	0.89	0
2	MLY	B	986	2	8,10,11	0.45	0	9,11,13	0.88	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	MLZ	A	1000	1	-	0/6/8/10	0/0/0/0
1	CAS	A	112	1	-	0/0/7/9	0/0/0/0
1	MLY	A	116	1	-	0/7/9/11	0/0/0/0
1	MLY	A	154	1	-	0/7/9/11	0/0/0/0
1	MLZ	A	207	1	-	0/6/8/10	0/0/0/0
1	MLY	A	251	1	-	0/7/9/11	0/0/0/0
1	MLY	A	278	1	-	0/7/9/11	0/0/0/0
1	MLY	A	287	1	-	0/7/9/11	0/0/0/0
1	MLY	A	290	1	-	0/7/9/11	0/0/0/0
1	MLY	A	363	1	-	0/7/9/11	0/0/0/0
1	MLY	A	431	1	-	0/7/9/11	0/0/0/0
1	MLZ	A	437	1	-	0/6/8/10	0/0/0/0
1	MLY	A	466	1	-	0/7/9/11	0/0/0/0
1	MLY	A	488	1	-	0/7/9/11	0/0/0/0
1	MLY	A	513	1	-	0/7/9/11	0/0/0/0
1	MLY	A	521	1	-	0/7/9/11	0/0/0/0
1	MLZ	A	525	1	-	0/6/8/10	0/0/0/0
1	MLY	A	540	1	-	0/7/9/11	0/0/0/0
1	MLZ	A	550	1	-	0/6/8/10	0/0/0/0
1	MLY	A	642	1	-	0/7/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLZ	A	66	1	-	0/6/8/10	0/0/0/0
1	MLY	A	700	1	-	0/7/9/11	0/0/0/0
1	MLY	A	704	1	-	0/7/9/11	0/0/0/0
1	MLY	A	750	1	-	0/7/9/11	0/0/0/0
1	MLY	A	759	1	-	0/7/9/11	0/0/0/0
1	MLY	A	764	1	-	0/7/9/11	0/0/0/0
1	MLZ	A	769	1	-	0/6/8/10	0/0/0/0
1	MLY	A	794	1	-	0/7/9/11	0/0/0/0
1	MLY	A	854	1	-	0/7/9/11	0/0/0/0
1	MLZ	A	884	1	-	0/6/8/10	0/0/0/0
1	MLY	A	902	1	-	0/7/9/11	0/0/0/0
1	MLY	A	911	1	-	0/7/9/11	0/0/0/0
1	MLZ	A	937	1	-	0/6/8/10	0/0/0/0
1	MLZ	A	943	1	-	0/6/8/10	0/0/0/0
1	MLY	A	946	1	-	0/7/9/11	0/0/0/0
1	MLY	A	956	1	-	0/7/9/11	0/0/0/0
1	MLZ	A	972	1	-	0/6/8/10	0/0/0/0
2	MLZ	B	1000	2	-	0/6/8/10	0/0/0/0
2	MLZ	B	1013	2	-	0/6/8/10	0/0/0/0
2	CAS	B	112	2	-	0/0/7/9	0/0/0/0
2	MLY	B	116	2	-	0/7/9/11	0/0/0/0
2	MLZ	B	125	2	-	0/6/8/10	0/0/0/0
2	MLZ	B	199	2	-	0/6/8/10	0/0/0/0
2	MLY	B	278	2	-	0/7/9/11	0/0/0/0
2	MLY	B	287	2	-	0/7/9/11	0/0/0/0
2	MLY	B	290	2	-	0/7/9/11	0/0/0/0
2	MLZ	B	324	2	-	0/6/8/10	0/0/0/0
2	MLY	B	363	2	-	0/7/9/11	0/0/0/0
2	MLY	B	41	2	-	0/7/9/11	0/0/0/0
2	MLY	B	431	2	-	0/7/9/11	0/0/0/0
2	MLY	B	466	2	-	0/7/9/11	0/0/0/0
2	MLY	B	488	2	-	0/7/9/11	0/0/0/0
2	MLZ	B	490	2	-	0/6/8/10	0/0/0/0
2	MLZ	B	494	2	-	0/6/8/10	0/0/0/0
2	MLY	B	499	2	-	0/7/9/11	0/0/0/0
2	MLY	B	513	2	-	0/7/9/11	0/0/0/0
2	MLY	B	525	2	-	0/7/9/11	0/0/0/0
2	MLY	B	540	2	-	0/7/9/11	0/0/0/0
2	MLY	B	550	2	-	0/7/9/11	0/0/0/0
2	MLZ	B	624	2	-	0/6/8/10	0/0/0/0
2	MLY	B	642	2	-	0/7/9/11	0/0/0/0
2	MLZ	B	66	2	-	0/6/8/10	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLY	B	750	2	-	0/7/9/11	0/0/0/0
2	MLZ	B	759	2	-	0/6/8/10	0/0/0/0
2	MLZ	B	764	2	-	0/6/8/10	0/0/0/0
2	MLZ	B	769	2	-	0/6/8/10	0/0/0/0
2	MLZ	B	854	2	-	0/6/8/10	0/0/0/0
2	MLZ	B	884	2	-	0/6/8/10	0/0/0/0
2	MLZ	B	902	2	-	0/6/8/10	0/0/0/0
2	MLY	B	911	2	-	0/7/9/11	0/0/0/0
2	MLZ	B	937	2	-	0/6/8/10	0/0/0/0
2	MLY	B	943	2	-	0/7/9/11	0/0/0/0
2	MLY	B	946	2	-	0/7/9/11	0/0/0/0
2	MLZ	B	956	2	-	0/6/8/10	0/0/0/0
2	MLY	B	972	2	-	0/7/9/11	0/0/0/0
2	MLY	B	986	2	-	0/7/9/11	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	769	MLZ	CM-NZ	-2.20	1.42	1.47
1	A	884	MLZ	CM-NZ	-2.19	1.42	1.47
2	B	764	MLZ	CM-NZ	-2.16	1.42	1.47
1	A	769	MLZ	CM-NZ	-2.16	1.42	1.47
2	B	490	MLZ	CM-NZ	-2.15	1.42	1.47
1	A	1000	MLZ	CM-NZ	-2.15	1.42	1.47
2	B	884	MLZ	CM-NZ	-2.14	1.42	1.47
1	A	207	MLZ	CM-NZ	-2.11	1.43	1.47
1	A	943	MLZ	CM-NZ	-2.10	1.43	1.47
1	A	550	MLZ	CM-NZ	-2.09	1.43	1.47
2	B	759	MLZ	CM-NZ	-2.08	1.43	1.47
2	B	199	MLZ	CM-NZ	-2.08	1.43	1.47
1	A	437	MLZ	CM-NZ	-2.08	1.43	1.47
1	A	525	MLZ	CM-NZ	-2.08	1.43	1.47
2	B	624	MLZ	CM-NZ	-2.05	1.43	1.47
1	A	937	MLZ	CM-NZ	-2.03	1.43	1.47
2	B	854	MLZ	CM-NZ	-2.01	1.43	1.47
2	B	324	MLZ	CM-NZ	-2.00	1.43	1.47

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	125	MLZ	O-C-CA	-2.62	118.69	125.72
2	B	624	MLZ	O-C-CA	-2.54	118.92	125.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	112	CAS	O-C-CA	-2.50	119.03	125.72
2	B	854	MLZ	O-C-CA	-2.49	119.05	125.72
1	A	943	MLZ	O-C-CA	-2.45	119.14	125.72
2	B	112	CAS	O-C-CA	-2.40	119.29	125.72
1	A	550	MLZ	O-C-CA	-2.39	119.32	125.72
2	B	759	MLZ	O-C-CA	-2.31	119.52	125.72
1	A	437	MLZ	O-C-CA	-2.30	119.56	125.72
1	A	66	MLZ	O-C-CA	-2.29	119.57	125.72
2	B	324	MLZ	O-C-CA	-2.25	119.69	125.72
2	B	1013	MLZ	O-C-CA	-2.23	119.73	125.72
1	A	704	MLY	O-C-CA	-2.21	119.81	125.72
2	B	278	MLY	O-C-CA	-2.19	119.84	125.72
2	B	41	MLY	O-C-CA	-2.19	119.85	125.72
2	B	937	MLZ	O-C-CA	-2.18	119.88	125.72
2	B	956	MLZ	O-C-CA	-2.17	119.91	125.72
2	B	199	MLZ	O-C-CA	-2.17	119.92	125.72
2	B	642	MLY	O-C-CA	-2.14	119.97	125.72
1	A	937	MLZ	O-C-CA	-2.14	119.98	125.72
2	B	494	MLZ	O-C-CA	-2.14	119.99	125.72
1	A	750	MLY	O-C-CA	-2.13	120.00	125.72
1	A	884	MLZ	O-C-CA	-2.13	120.02	125.72
1	A	642	MLY	O-C-CA	-2.10	120.08	125.72
1	A	525	MLZ	CM-NZ-CE	-2.08	107.66	111.78
2	B	764	MLZ	O-C-CA	-2.07	120.18	125.72
2	B	884	MLZ	O-C-CA	-2.05	120.22	125.72
2	B	550	MLY	O-C-CA	-2.04	120.25	125.72
1	A	854	MLY	O-C-CA	-2.03	120.27	125.72
1	A	1000	MLZ	O-C-CA	-2.03	120.27	125.72
2	B	363	MLY	O-C-CA	-2.03	120.27	125.72
1	A	956	MLY	O-C-CA	-2.03	120.27	125.72
1	A	759	MLY	O-C-CA	-2.02	120.29	125.72
1	A	278	MLY	O-C-CA	-2.02	120.31	125.72
1	A	287	MLY	O-C-CA	-2.02	120.31	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

34 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1000	MLZ	1	0

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

5.5 Carbohydrates (i)

There are no carbohydrates 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	$\#\|Z\| > 2$
4	3UE	A	1102	-	32,34,34	3.99	11 (34%)	42,47,47	1.13	5 (11%)
4	3UE	A	1103	-	32,34,34	4.01	13 (40%)	42,47,47	1.56	6 (14%)
5	GOL	A	1104	-	5,5,5	0.31	0	5,5,5	0.48	0
5	GOL	A	1105	-	5,5,5	0.37	0	5,5,5	0.24	0
5	GOL	A	1106	-	5,5,5	0.36	0	5,5,5	0.24	0
5	GOL	A	1107	-	5,5,5	0.34	0	5,5,5	0.25	0
5	GOL	A	1108	-	5,5,5	0.43	0	5,5,5	0.18	0
5	GOL	A	1109	-	5,5,5	0.34	0	5,5,5	0.47	0
5	GOL	A	1110	-	5,5,5	0.34	0	5,5,5	0.27	0
5	GOL	A	1111	-	5,5,5	0.33	0	5,5,5	0.35	0
5	GOL	A	1112	-	5,5,5	0.30	0	5,5,5	0.27	0
5	GOL	A	1113	-	5,5,5	0.37	0	5,5,5	0.19	0
5	GOL	A	1114	-	5,5,5	0.41	0	5,5,5	0.21	0
6	ACT	A	1115	-	0,3,3	0.00	-	0,3,3	0.00	-
6	ACT	A	1116	-	0,3,3	0.00	-	0,3,3	0.00	-
6	ACT	A	1117	3	0,3,3	0.00	-	0,3,3	0.00	-
4	3UE	B	1102	-	32,34,34	3.93	13 (40%)	42,47,47	1.20	6 (14%)
4	3UE	B	1103	-	32,34,34	3.99	13 (40%)	42,47,47	1.46	6 (14%)
5	GOL	B	1104	-	5,5,5	0.41	0	5,5,5	0.25	0
5	GOL	B	1105	-	5,5,5	0.47	0	5,5,5	0.44	0
5	GOL	B	1106	-	5,5,5	0.34	0	5,5,5	0.34	0
5	GOL	B	1107	-	5,5,5	0.27	0	5,5,5	0.34	0
5	GOL	B	1108	-	5,5,5	0.38	0	5,5,5	0.30	0
5	GOL	B	1109	-	5,5,5	0.39	0	5,5,5	0.19	0
5	GOL	B	1110	-	5,5,5	0.37	0	5,5,5	0.17	0
6	ACT	B	1111	-	0,3,3	0.00	-	0,3,3	0.00	-
6	ACT	B	1112	-	0,3,3	0.00	-	0,3,3	0.00	-
6	ACT	B	1113	-	0,3,3	0.00	-	0,3,3	0.00	-
6	ACT	B	1114	-	0,3,3	0.00	-	0,3,3	0.00	-
6	ACT	B	1115	3	0,3,3	0.00	-	0,3,3	0.00	-

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
4	3UE	A	1102	-	-	0/23/34/34	0/4/4/4
4	3UE	A	1103	-	-	0/23/34/34	0/4/4/4
5	GOL	A	1104	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1105	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1106	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1107	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1108	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1109	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1110	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1111	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1112	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1113	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1114	-	-	0/4/4/4	0/0/0/0
6	ACT	A	1115	-	-	0/0/0/0	0/0/0/0
6	ACT	A	1116	-	-	0/0/0/0	0/0/0/0
6	ACT	A	1117	3	-	0/0/0/0	0/0/0/0
4	3UE	B	1102	-	-	0/23/34/34	0/4/4/4
4	3UE	B	1103	-	-	0/23/34/34	0/4/4/4
5	GOL	B	1104	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1105	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1106	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1107	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1108	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1109	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1110	-	-	0/4/4/4	0/0/0/0
6	ACT	B	1111	-	-	0/0/0/0	0/0/0/0
6	ACT	B	1112	-	-	0/0/0/0	0/0/0/0
6	ACT	B	1113	-	-	0/0/0/0	0/0/0/0
6	ACT	B	1114	-	-	0/0/0/0	0/0/0/0
6	ACT	B	1115	3	-	0/0/0/0	0/0/0/0

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1103	3UE	C19-N18	-12.37	1.27	1.48
4	A	1103	3UE	C19-N18	-12.02	1.27	1.48
4	A	1102	3UE	C19-N18	-11.88	1.28	1.48
4	B	1102	3UE	C19-N18	-11.84	1.28	1.48
4	B	1102	3UE	C16-N13	-8.64	1.31	1.47
4	A	1102	3UE	C16-N13	-8.48	1.31	1.47
4	B	1103	3UE	C16-N13	-8.46	1.31	1.47
4	A	1103	3UE	C16-N13	-8.30	1.32	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1103	3UE	C14-N13	-7.49	1.33	1.47
4	B	1102	3UE	C14-N13	-7.20	1.34	1.47
4	A	1102	3UE	C14-N13	-7.12	1.34	1.47
4	B	1103	3UE	C14-N13	-7.05	1.34	1.47
4	A	1102	3UE	C03-C02	-2.66	1.45	1.50
4	A	1103	3UE	C17-N18	-2.62	1.41	1.47
4	A	1103	3UE	C03-C02	-2.40	1.46	1.50
4	B	1102	3UE	C03-C02	-2.40	1.46	1.50
4	B	1103	3UE	C17-N18	-2.38	1.42	1.47
4	B	1102	3UE	C21-C20	-2.03	1.35	1.39
4	A	1103	3UE	C31-C26	2.01	1.42	1.39
4	B	1102	3UE	C05-C04	2.03	1.42	1.38
4	B	1103	3UE	C05-C04	2.05	1.42	1.38
4	A	1103	3UE	C11-C10	2.29	1.55	1.51
4	B	1103	3UE	C12-C03	2.32	1.42	1.39
4	B	1102	3UE	C11-C10	2.38	1.55	1.51
4	A	1102	3UE	C11-C10	2.39	1.55	1.51
4	B	1103	3UE	C11-C10	2.45	1.55	1.51
4	B	1102	3UE	C26-C19	2.69	1.55	1.52
4	B	1103	3UE	C26-C19	3.10	1.56	1.52
4	B	1103	3UE	C29-C28	3.22	1.46	1.38
4	B	1102	3UE	C29-C28	3.29	1.46	1.38
4	A	1102	3UE	C29-C28	3.36	1.46	1.38
4	A	1103	3UE	C29-C28	3.43	1.46	1.38
4	B	1102	3UE	C30-C31	3.64	1.46	1.38
4	A	1102	3UE	C30-C31	3.67	1.46	1.38
4	B	1103	3UE	C30-C31	3.76	1.46	1.38
4	A	1103	3UE	C30-C31	3.90	1.46	1.38
4	A	1102	3UE	C26-C19	4.06	1.57	1.52
4	A	1103	3UE	C26-C19	4.14	1.57	1.52
4	B	1103	3UE	C20-C19	4.65	1.57	1.52
4	B	1102	3UE	C20-C19	5.07	1.58	1.52
4	A	1102	3UE	C20-C19	5.24	1.58	1.52
4	A	1103	3UE	C20-C19	5.48	1.58	1.52
4	A	1103	3UE	C02-N13	6.44	1.49	1.34
4	B	1103	3UE	C02-N13	6.70	1.49	1.34
4	B	1102	3UE	C02-N13	6.77	1.50	1.34
4	A	1102	3UE	C02-N13	7.05	1.50	1.34
4	B	1102	3UE	O08-N07	9.05	1.40	1.22
4	A	1102	3UE	O08-N07	9.32	1.41	1.22
4	A	1103	3UE	O08-N07	9.35	1.41	1.22
4	B	1103	3UE	O08-N07	9.44	1.41	1.22

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1103	3UE	C20-C19-C26	-2.70	104.72	112.17
4	A	1103	3UE	C17-N18-C15	-2.65	104.30	109.14
4	B	1103	3UE	C17-N18-C15	-2.48	104.62	109.14
4	A	1102	3UE	C20-C19-C26	-2.28	105.87	112.17
4	A	1103	3UE	C14-N13-C02	-2.15	116.41	122.86
4	B	1103	3UE	C14-N13-C02	-2.13	116.47	122.86
4	B	1102	3UE	C20-C19-C26	-2.11	106.34	112.17
4	A	1102	3UE	C16-C17-N18	2.01	115.04	110.65
4	B	1102	3UE	C14-C15-N18	2.03	115.08	110.65
4	B	1103	3UE	C31-C26-C27	2.08	120.94	118.30
4	B	1102	3UE	C16-C17-N18	2.13	115.29	110.65
4	A	1103	3UE	C17-C16-N13	2.13	114.93	110.44
4	A	1103	3UE	C20-C19-N18	2.16	114.88	111.56
4	B	1102	3UE	C03-C02-N13	2.22	121.71	118.77
4	A	1102	3UE	C14-C15-N18	2.62	116.36	110.65
4	B	1102	3UE	C20-C19-N18	2.68	115.68	111.56
4	A	1102	3UE	C03-C02-N13	2.82	122.50	118.77
4	A	1103	3UE	C03-C02-N13	3.08	122.86	118.77
4	A	1102	3UE	C16-N13-C14	3.16	118.36	112.57
4	B	1103	3UE	C03-C02-N13	3.28	123.11	118.77
4	B	1102	3UE	C16-N13-C14	3.30	118.62	112.57
4	B	1103	3UE	C16-N13-C14	5.18	122.06	112.57
4	A	1103	3UE	C16-N13-C14	6.40	124.29	112.57

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1102	3UE	2	0
4	A	1103	3UE	2	0
5	A	1106	GOL	2	0
5	A	1110	GOL	1	0
5	A	1111	GOL	2	0
5	A	1112	GOL	1	0
5	A	1114	GOL	1	0
4	B	1102	3UE	1	0
4	B	1103	3UE	1	0
5	B	1104	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1105	GOL	1	0
5	B	1106	GOL	3	0
5	B	1107	GOL	3	0
5	B	1109	GOL	3	0
6	B	1113	ACT	1	0
6	B	1114	ACT	1	0

5.7 Other polymers

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, 95^{th} 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%)	81	83	27, 32, 51, 83	0
2	B	940/1014 (92%)	-0.12	25 (2%)	58	62	27, 34, 54, 94	0
All	All	1891/2028 (93%)	-0.11	36 (1%)	70	74	27, 33, 53, 94	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	823	PRO	5.1
1	A	838	VAL	4.0
2	B	839	ILE	3.5
2	B	838	VAL	3.4
2	B	1030	LYS	3.2
2	B	851	TRP	3.1
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
1	A	821	PRO	2.6
2	B	582	ASP	2.6
2	B	572	THR	2.5
2	B	577	VAL	2.5
2	B	915	ASN	2.4
2	B	323	SER	2.4
2	B	570	PRO	2.4
2	B	813	VAL	2.4
2	B	819	GLU	2.3
1	A	36	ARG	2.3
2	B	821	PRO	2.3
2	B	984	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	983	ASP	2.2
2	B	397	VAL	2.2
2	B	575	ASP	2.2
2	B	812	PRO	2.2
1	A	42	LEU	2.2
2	B	1029	ALA	2.1
1	A	193	GLN	2.1
2	B	820	LYS	2.1
2	B	417	GLU	2.1
1	A	814	ARG	2.0
2	B	399	LYS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	MLZ	B	125	10/11	0.96	0.12	-	27,27,39,41	0
2	MLZ	B	884	10/11	0.96	0.12	-	28,32,43,45	0
1	MLY	A	278	11/12	0.95	0.11	-	31,32,35,36	0
1	MLY	A	794	11/12	0.91	0.14	-	37,51,66,67	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
2	MLZ	B	1013	10/11	0.94	0.13	-	40,45,54,58	0
1	MLY	A	854	11/12	0.96	0.12	-	31,31,38,40	0
1	MLY	A	466	11/12	0.96	0.12	-	29,33,44,46	0
1	MLZ	A	769	10/11	0.97	0.10	-	33,34,39,43	0
2	MLZ	B	759	10/11	0.97	0.18	-	39,45,47,50	0
1	MLZ	A	884	10/11	0.96	0.10	-	27,27,29,31	0
1	MLZ	A	972	10/11	0.94	0.15	-	29,33,49,51	0
1	MLY	A	700	11/12	0.91	0.24	-	31,32,61,61	0
1	MLZ	A	943	10/11	0.97	0.10	-	27,35,38,42	0
2	MLY	B	540	11/12	0.95	0.12	-	28,29,34,38	0
2	MLZ	B	490	10/11	0.94	0.25	-	32,38,59,60	0
2	MLZ	B	764	10/11	0.96	0.13	-	39,43,45,47	0
2	MLY	B	278	11/12	0.94	0.16	-	31,35,50,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	MLY	A	911	11/12	0.96	0.17	-	27,27,38,46	0
1	MLZ	A	66	10/11	0.95	0.12	-	31,32,42,45	0
2	MLZ	B	199	10/11	0.96	0.15	-	29,38,49,50	0
2	MLY	B	513	11/12	0.92	0.22	-	34,39,47,49	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
1	CAS	A	112	9/10	0.97	0.14	-	28,32,68,93	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
1	MLY	A	513	11/12	0.95	0.16	-	33,36,44,51	0
2	MLY	B	550	11/12	0.93	0.13	-	27,32,38,44	0
1	MLY	A	704	11/12	0.92	0.14	-	30,31,51,53	0
1	MLZ	A	207	10/11	0.95	0.18	-	29,29,46,53	0
1	MLY	A	287	11/12	0.96	0.13	-	31,32,34,38	0
2	MLY	B	911	11/12	0.94	0.15	-	28,29,41,45	0
1	MLY	A	251	11/12	0.94	0.10	-	31,31,45,46	0
2	MLZ	B	624	10/11	0.95	0.15	-	33,34,39,42	0
2	CAS	B	112	9/10	0.97	0.12	-	27,28,60,92	0
2	MLY	B	750	11/12	0.92	0.16	-	35,41,47,53	0
2	MLZ	B	769	10/11	0.95	0.13	-	38,39,42,46	0
2	MLZ	B	902	10/11	0.94	0.11	-	28,33,39,42	0
1	MLY	A	363	11/12	0.95	0.11	-	30,32,52,56	0
1	MLY	A	642	11/12	0.95	0.13	-	29,31,35,40	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	MLY	A	902	11/12	0.97	0.11	-	28,29,37,39	0
1	MLY	A	521	11/12	0.91	0.24	-	42,46,60,63	0
1	MLY	A	540	11/12	0.97	0.12	-	30,31,33,35	0
1	MLY	A	154	11/12	0.96	0.13	-	28,30,43,43	0
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	MLY	B	488	11/12	0.97	0.15	-	31,32,37,40	0
2	MLY	B	499	11/12	0.92	0.23	-	33,41,65,65	0
1	MLZ	A	437	10/11	0.96	0.12	-	28,29,47,48	0
2	MLZ	B	324	10/11	0.81	0.34	-	46,61,69,70	0
2	MLZ	B	494	10/11	0.93	0.25	-	33,40,54,57	0
2	MLY	B	41	11/12	0.94	0.14	-	34,35,46,49	0
1	MLY	A	488	11/12	0.96	0.11	-	30,30,32,35	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	750	11/12	0.90	0.18	-	31,39,54,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	MLY	A	759	11/12	0.94	0.21	-	35,35,41,44	0
2	MLY	B	972	11/12	0.93	0.17	-	32,34,56,59	0
2	MLY	B	290	11/12	0.94	0.15	-	33,37,53,54	0
2	MLY	B	116	11/12	0.95	0.14	-	28,39,47,54	0
2	MLY	B	287	11/12	0.93	0.16	-	31,32,41,41	0
2	MLY	B	431	11/12	0.95	0.16	-	31,32,48,56	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
1	MLZ	A	550	10/11	0.97	0.10	-	27,30,37,41	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
2	MLY	B	986	11/12	0.94	0.23	-	32,42,54,56	0
1	MLY	A	290	11/12	0.95	0.14	-	34,37,48,50	0
2	MLZ	B	956	10/11	0.95	0.11	-	28,31,42,42	0
2	MLZ	B	66	10/11	0.94	0.16	-	31,31,47,50	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
5	GOL	A	1109	6/6	0.82	0.34	11.53	54,62,73,77	0
5	GOL	B	1107	6/6	0.83	0.24	10.92	53,60,68,75	0
5	GOL	A	1110	6/6	0.68	0.26	10.63	51,66,68,69	0
5	GOL	A	1104	6/6	0.84	0.19	9.29	38,41,46,48	0
5	GOL	B	1105	6/6	0.92	0.21	8.65	39,41,49,51	0
6	ACT	A	1115	4/4	0.75	0.21	7.28	56,63,63,67	0
7	CA	B	1117	1/1	0.97	0.26	6.45	54,54,54,54	0
6	ACT	B	1113	4/4	0.94	0.22	5.66	43,47,49,49	0
5	GOL	A	1106	6/6	0.93	0.24	4.24	58,61,65,65	0
5	GOL	A	1105	6/6	0.84	0.22	3.81	50,51,65,72	0
5	GOL	A	1112	6/6	0.84	0.22	3.52	32,46,57,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	GOL	A	1111	6/6	0.85	0.32	2.90	35,50,60,67	0
5	GOL	B	1106	6/6	0.88	0.20	2.61	51,57,58,61	0
6	ACT	B	1111	4/4	0.83	0.15	2.21	41,44,52,53	0
5	GOL	A	1108	6/6	0.84	0.22	1.98	51,62,70,72	0
6	ACT	A	1117	4/4	0.98	0.19	1.74	28,37,44,46	0
5	GOL	A	1107	6/6	0.79	0.18	1.40	48,59,68,72	0
6	ACT	A	1116	4/4	0.96	0.15	1.17	33,34,39,39	0
5	GOL	B	1104	6/6	0.91	0.15	0.89	41,48,52,54	0
6	ACT	B	1114	4/4	0.84	0.22	0.88	41,51,52,59	0
7	CA	B	1116	1/1	0.96	0.13	0.41	41,41,41,41	0
4	3UE	A	1103	31/31	0.95	0.13	0.41	28,32,39,58	0
5	GOL	B	1110	6/6	0.95	0.12	0.37	35,41,46,54	0
4	3UE	A	1102	31/31	0.94	0.13	0.00	27,33,45,64	0
5	GOL	B	1109	6/6	0.94	0.14	-0.53	28,43,48,52	0
4	3UE	B	1102	31/31	0.94	0.12	-0.78	29,31,36,49	0
4	3UE	B	1103	31/31	0.95	0.11	-0.97	29,35,40,56	0
3	ZN	B	1101	1/1	0.99	0.12	-1.04	42,42,42,42	0
6	ACT	B	1115	4/4	0.96	0.12	-1.29	28,42,43,45	0
3	ZN	A	1101	1/1	1.00	0.11	-3.00	38,38,38,38	0
6	ACT	B	1112	4/4	0.92	0.25	-	43,47,52,61	0
5	GOL	B	1108	6/6	0.78	0.30	-	69,70,74,75	0
5	GOL	A	1113	6/6	0.88	0.22	-	54,58,61,62	0
5	GOL	A	1114	6/6	0.77	0.26	-	54,60,72,80	0

6.5 Other polymers (i)

There are no such residues in this entry.