



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 02:13 PM BST

PDB ID : 3A3Y  
Title : Crystal structure of the sodium-potassium pump with bound potassium and ouabain  
Authors : Ogawa, H.; Shinoda, T.; Cornelius, F.; Toyoshima, C.  
Deposited on : 2009-06-23  
Resolution : 2.80 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

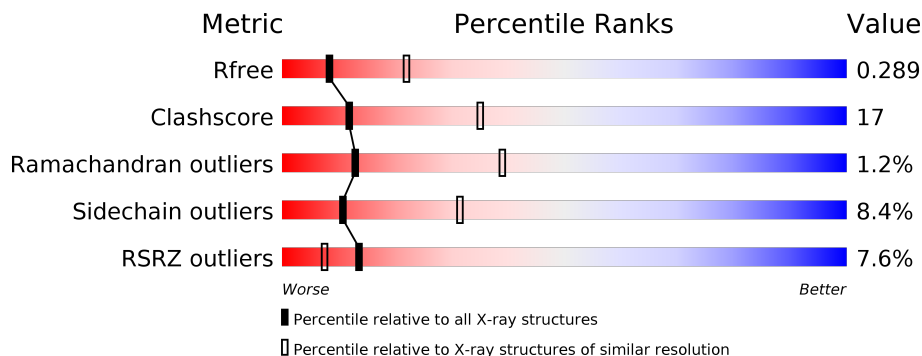
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	1028	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 61%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 32%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">7% 61% 32% . .</p>
2	B	305	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 50%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 32%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">10% 50% 32% 5% 13%</p>
3	G	74	<div style="display: flex; align-items: center;"> <div style="width: 32%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 49%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">32% 19% 49%</p>

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 10308 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Na, K-ATPase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	992	7675	4886	1290	1453	46	0	0	0

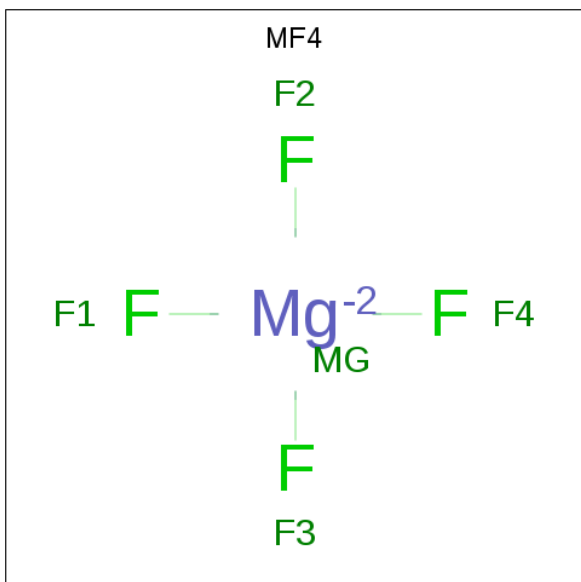
- Molecule 2 is a protein called NA<sup>+</sup>,K<sup>+</sup>-ATPASE BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	265	2151	1392	356	392	11	0	0	0

- Molecule 3 is a protein called Phospholemman-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	38	296	195	49	51	1	0	0	0

- Molecule 4 is TETRAFLUOROMAGNESATE(2-) (three-letter code: MF4) (formula: F<sub>4</sub>Mg).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	F	Mg	0	0
			5	4	1		

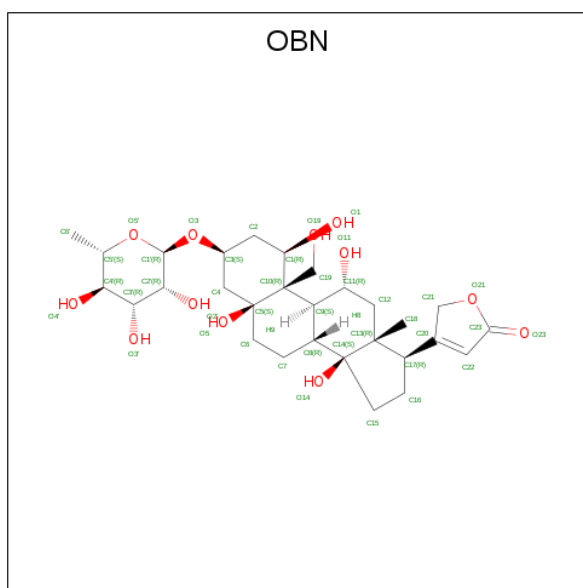
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

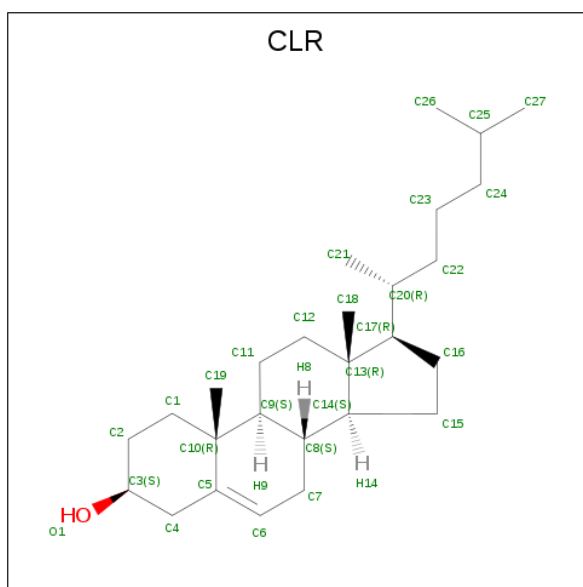
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	K	0	0
			3	3		

- Molecule 7 is OUABAIN (three-letter code: OBN) (formula: C<sub>29</sub>H<sub>44</sub>O<sub>12</sub>).



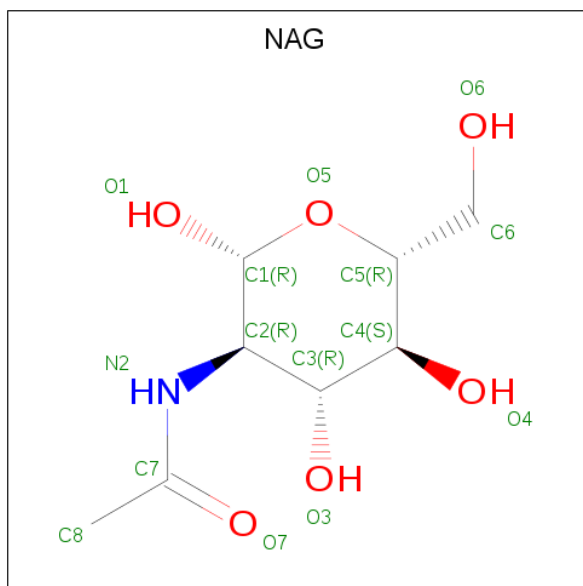
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			41	29	12		

- Molecule 8 is CHOLESTEROL (three-letter code: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			28	27	1		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
9	B	1	14	8	1	5	0	0

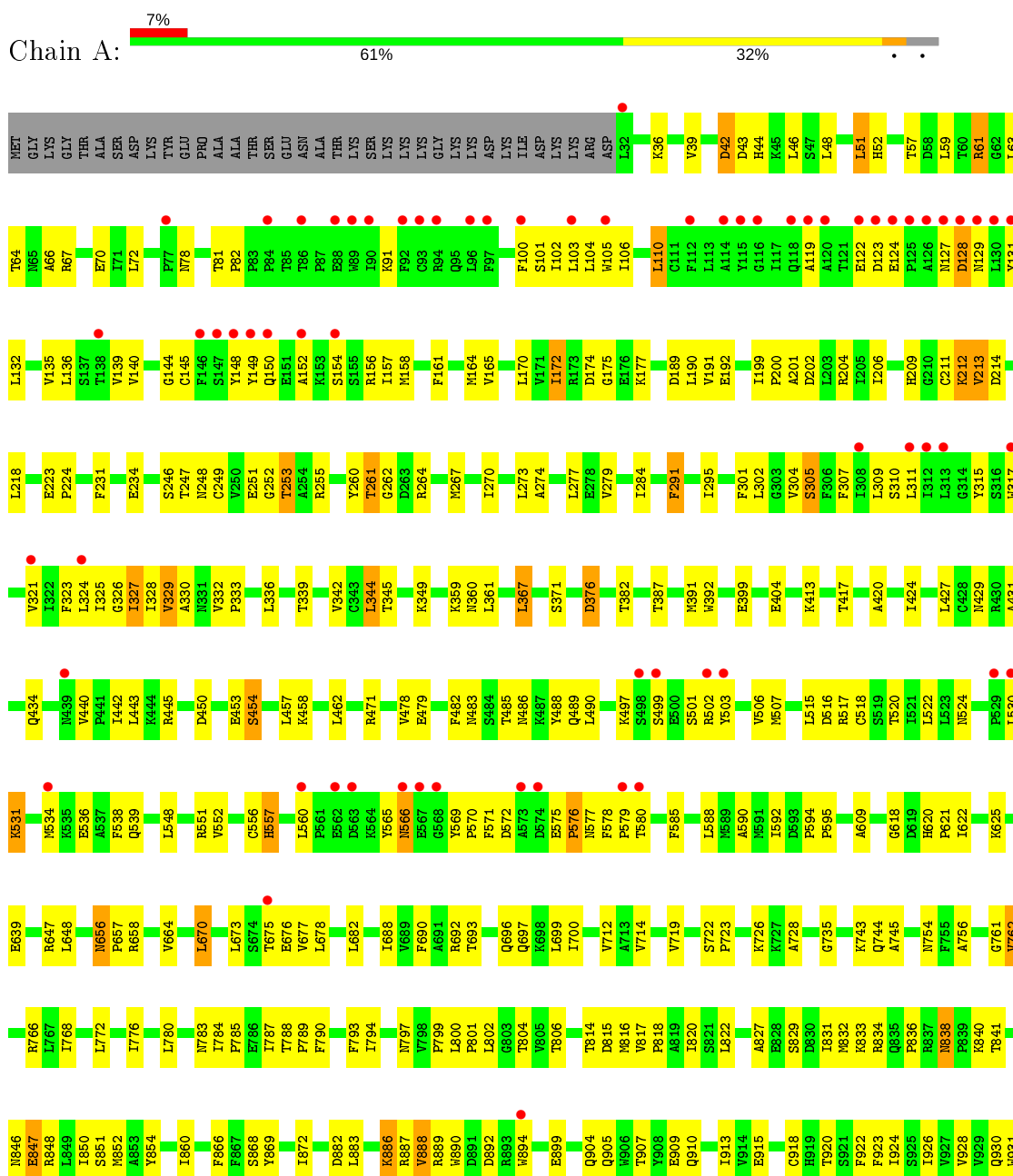
- Molecule 10 is water.

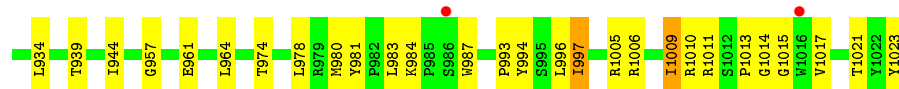
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	65	Total	O	0	0
			65	65		
10	G	1	Total	O	0	0
			1	1		

### 3 Residue-property plots

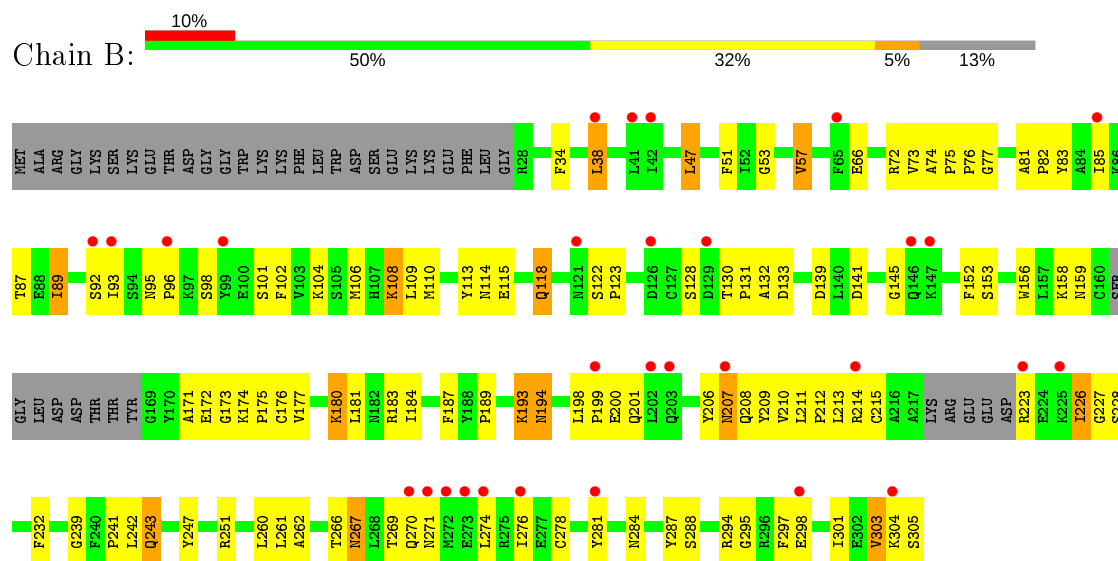
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

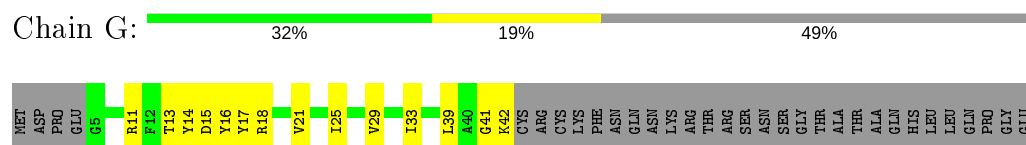




- Molecule 2:  $\text{Na}^+$ ,  $\text{K}^+$ -ATPASE BETA SUBUNIT



- Molecule 3: Phospholemman-like protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	222.88Å 50.72Å 163.34Å 90.00° 104.63° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 43.58 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-2.80) 99.9 (43.58-2.80)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.41 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.247 , 0.293 0.245 , 0.289	Depositor DCC
$R_{free}$ test set	1342 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.5	Xtrriage
Anisotropy	0.362	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 72.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10308	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OBN, MG, NAG, K, MF4, CLR

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	0/7825	0.55	0/10616
2	B	0.35	0/2205	0.54	0/2970
3	G	0.39	0/300	0.53	0/407
All	All	0.37	0/10330	0.55	0/13993

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1015	GLY	Peptide

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7675	0	7700	270	0
2	B	2151	0	2127	81	0
3	G	296	0	312	11	0
4	A	5	0	0	1	0
5	A	1	0	0	0	0
6	A	3	0	0	0	0
7	A	41	0	44	7	0
8	B	28	0	46	2	0
9	B	42	0	39	3	0
10	A	65	0	0	3	0
10	G	1	0	0	0	0
All	All	10308	0	10268	355	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 17.

All (355) 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:905:GLN:HE21	2:B:183:ARG:H	1.13	0.96
1:A:328:ILE:HG13	1:A:329:VAL:H	1.30	0.94
1:A:102:ILE:HA	1:A:105:TRP:HD1	1.32	0.94
1:A:44:HIS:H	1:A:44:HIS:CD2	1.83	0.93
1:A:894:TRP:HB2	2:B:83:TYR:HE1	1.38	0.88
1:A:905:GLN:NE2	2:B:183:ARG:H	1.71	0.88
1:A:714:VAL:HG23	1:A:728:ALA:HB2	1.56	0.86
1:A:450:ASP:OD1	1:A:453:GLU:HB2	1.80	0.82
1:A:329:VAL:HB	7:A:6000:OBN:O21	1.80	0.82
2:B:271:ASN:HD21	2:B:305:SER:H	1.25	0.82
1:A:78:ASN:HA	1:A:261:THR:HG23	1.63	0.80
2:B:171:ALA:HB3	2:B:175:PRO:HA	1.62	0.80
1:A:246:SER:OG	1:A:267:MET:HG3	1.82	0.79
1:A:806:THR:CG2	1:A:923:PHE:HB2	2.13	0.78
1:A:78:ASN:HD22	1:A:262:GLY:H	1.29	0.77
1:A:102:ILE:HA	1:A:105:TRP:CD1	2.20	0.76
1:A:61:ARG:HB3	1:A:61:ARG:HH11	1.51	0.75
1:A:344:LEU:HB3	1:A:361:LEU:HG	1.68	0.75
1:A:656:ASN:HD22	1:A:657:PRO:HD2	1.51	0.74
2:B:174:LYS:HB3	2:B:266:THR:HA	1.67	0.74
1:A:483:ASN:HB2	1:A:486:ASN:HB2	1.71	0.73
2:B:271:ASN:ND2	2:B:305:SER:H	1.85	0.73
1:A:61:ARG:CB	1:A:61:ARG:HH11	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:ALA:HB3	2:B:75:PRO:HD3	1.71	0.72
7:A:6000:OBN:H212	7:A:6000:OBN:H181	1.70	0.72
1:A:52:HIS:CE1	1:A:59:LEU:HA	2.24	0.71
7:A:6000:OBN:H1	7:A:6000:OBN:O11	1.90	0.71
1:A:301:PHE:O	1:A:305:SER:HB2	1.91	0.70
1:A:994:TYR:HA	1:A:997:ILE:HG22	1.74	0.70
1:A:328:ILE:HG13	1:A:329:VAL:N	2.06	0.70
1:A:572:ASP:HB3	1:A:577:ASN:HB2	1.72	0.69
1:A:61:ARG:CG	1:A:61:ARG:HH11	2.05	0.69
2:B:232:PHE:HB2	2:B:262:ALA:HB3	1.72	0.69
1:A:100:PHE:HE1	1:A:295:ILE:HG21	1.58	0.69
2:B:81:ALA:HB2	2:B:109:LEU:HD23	1.74	0.69
1:A:330:ALA:HB1	1:A:787:ILE:HG12	1.74	0.69
1:A:780:LEU:O	1:A:783:ASN:HB2	1.93	0.69
1:A:497:LYS:HE2	1:A:499:SER:HB2	1.75	0.68
2:B:270:GLN:HG3	2:B:271:ASN:HD22	1.58	0.68
1:A:806:THR:HG22	1:A:923:PHE:HB2	1.76	0.68
1:A:48:LEU:H	1:A:48:LEU:HD12	1.60	0.67
1:A:894:TRP:HD1	2:B:83:TYR:HH	1.42	0.67
1:A:100:PHE:HA	1:A:103:LEU:HD12	1.77	0.67
1:A:722:SER:OG	1:A:723:PRO:HD3	1.94	0.66
1:A:838:ASN:HD21	1:A:840:LYS:HG2	1.60	0.66
1:A:924:ILE:HD12	1:A:983:LEU:HD12	1.76	0.66
2:B:82:PRO:HG2	2:B:177:VAL:HG22	1.77	0.66
1:A:488:TYR:HE1	1:A:490:LEU:HD23	1.61	0.65
1:A:342:VAL:HB	1:A:820:ILE:HD12	1.77	0.65
1:A:907:THR:OG1	1:A:910:GLN:HG3	1.96	0.65
1:A:994:TYR:HA	1:A:997:ILE:CG2	2.27	0.65
1:A:102:ILE:CA	1:A:105:TRP:HD1	2.09	0.64
1:A:625:LYS:HD2	1:A:664:VAL:HG21	1.80	0.64
1:A:78:ASN:ND2	1:A:262:GLY:H	1.95	0.64
1:A:127:ASN:O	1:A:131:TYR:HB2	1.97	0.64
1:A:892:ASP:OD1	1:A:894:TRP:CD1	2.51	0.64
1:A:261:THR:HG22	1:A:264:ARG:NH2	2.13	0.63
2:B:131:PRO:HA	2:B:243:GLN:HE21	1.63	0.63
1:A:714:VAL:CG2	1:A:728:ALA:HB2	2.26	0.63
1:A:330:ALA:H	7:A:6000:OBN:C23	2.12	0.63
1:A:565:TYR:OH	1:A:579:PRO:HD3	1.99	0.63
2:B:213:LEU:HD23	2:B:261:LEU:HD13	1.80	0.63
1:A:622:ILE:HG12	10:A:5056:HOH:O	1.98	0.62
3:G:41:GLY:O	3:G:42:LYS:HB3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:GLY:HA2	2:B:295:GLY:H	1.65	0.62
1:A:325:ILE:O	1:A:328:ILE:HG12	1.99	0.62
1:A:44:HIS:H	1:A:44:HIS:HD2	1.44	0.62
1:A:656:ASN:HD22	1:A:657:PRO:CD	2.12	0.62
1:A:417:THR:HA	1:A:522:LEU:HD22	1.81	0.61
2:B:89:ILE:HG22	2:B:102:PHE:CE2	2.36	0.61
2:B:214:ARG:HD3	2:B:281:TYR:OH	2.01	0.61
1:A:838:ASN:HD22	1:A:840:LYS:H	1.48	0.61
1:A:502:ARG:CG	1:A:503:TYR:H	2.14	0.61
2:B:171:ALA:HB1	2:B:173:GLY:O	2.00	0.61
1:A:202:ASP:HB2	1:A:260:TYR:HB2	1.83	0.60
1:A:772:LEU:O	1:A:776:ILE:HG12	2.01	0.60
1:A:61:ARG:HB3	1:A:61:ARG:NH1	2.15	0.60
1:A:170:LEU:HD23	1:A:192:GLU:HB3	1.83	0.60
1:A:261:THR:HG21	10:A:5028:HOH:O	2.01	0.60
1:A:301:PHE:HD2	1:A:302:LEU:HD23	1.65	0.60
1:A:304:VAL:HG12	1:A:324:LEU:HD11	1.83	0.60
1:A:851:SER:HA	8:B:3001:CLR:H72	1.81	0.60
2:B:132:ALA:O	2:B:209:TYR:HB3	2.02	0.60
2:B:226:ILE:HG22	2:B:269:THR:HB	1.84	0.60
1:A:846:ASN:ND2	1:A:848:ARG:HB2	2.17	0.59
2:B:53:GLY:O	2:B:57:VAL:HG13	2.03	0.59
1:A:214:ASP:O	1:A:247:THR:HB	2.03	0.59
1:A:172:ILE:HG13	1:A:190:LEU:HD23	1.84	0.58
1:A:621:PRO:HD2	10:A:5056:HOH:O	2.02	0.58
1:A:431:ALA:O	1:A:471:ARG:NH2	2.36	0.58
1:A:64:THR:HG22	1:A:66:ALA:H	1.68	0.58
1:A:814:THR:HB	1:A:961:GLU:HG3	1.85	0.58
1:A:838:ASN:ND2	1:A:840:LYS:H	2.01	0.58
1:A:502:ARG:CD	1:A:503:TYR:H	2.17	0.58
1:A:291:PHE:CZ	1:A:336:LEU:HD23	2.39	0.58
1:A:905:GLN:HE21	2:B:183:ARG:N	1.93	0.57
1:A:323:PHE:CD1	1:A:790:PHE:HZ	2.22	0.57
1:A:783:ASN:O	1:A:787:ILE:HG13	2.04	0.57
1:A:122:GLU:O	1:A:124:GLU:HG2	2.04	0.57
1:A:392:TRP:HB3	1:A:588:LEU:HB2	1.85	0.57
1:A:106:ILE:HG22	1:A:325:ILE:HD13	1.87	0.57
1:A:61:ARG:HG3	1:A:61:ARG:HH11	1.70	0.56
1:A:333:PRO:HB2	1:A:336:LEU:HB2	1.87	0.56
1:A:44:HIS:N	1:A:44:HIS:CD2	2.65	0.56
1:A:67:ARG:NH1	1:A:70:GLU:OE1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ASP:HB2	1:A:46:LEU:HD12	1.88	0.56
1:A:866:PHE:O	1:A:869:TYR:HB3	2.06	0.56
1:A:442:ILE:O	1:A:445:ARG:HG2	2.06	0.56
1:A:565:TYR:HD2	1:A:569:TYR:CE2	2.23	0.56
1:A:939:THR:O	1:A:1006:ARG:NH1	2.39	0.56
1:A:766:ARG:HD2	1:A:832:MET:CE	2.36	0.56
1:A:502:ARG:HD2	1:A:503:TYR:N	2.21	0.55
1:A:261:THR:HG22	1:A:264:ARG:HH21	1.70	0.55
1:A:497:LYS:O	1:A:501:SER:N	2.40	0.55
1:A:888:VAL:O	1:A:892:ASP:HB2	2.06	0.55
2:B:241:PRO:HB2	2:B:243:GLN:HG3	1.89	0.55
1:A:64:THR:HA	1:A:174:ASP:OD1	2.07	0.55
2:B:74:ALA:CB	2:B:75:PRO:HD3	2.37	0.55
1:A:502:ARG:HD2	1:A:503:TYR:H	1.70	0.54
1:A:145:CYS:O	1:A:149:TYR:HB2	2.07	0.54
1:A:429:ASN:HA	1:A:453:GLU:OE1	2.07	0.54
1:A:129:ASN:HA	1:A:132:LEU:HB3	1.89	0.54
1:A:974:THR:HG23	1:A:978:LEU:HD12	1.90	0.54
1:A:838:ASN:C	1:A:838:ASN:HD22	2.12	0.53
1:A:894:TRP:HB2	2:B:83:TYR:CE1	2.30	0.53
1:A:52:HIS:CE1	1:A:59:LEU:CA	2.91	0.53
1:A:52:HIS:HE1	1:A:59:LEU:HA	1.70	0.53
1:A:578:PHE:HB2	1:A:579:PRO:HD2	1.89	0.53
3:G:29:VAL:O	3:G:33:ILE:HG12	2.09	0.53
1:A:860:ILE:HG12	2:B:47:LEU:HD11	1.91	0.53
1:A:59:LEU:HG	1:A:206:ILE:HD12	1.91	0.53
2:B:213:LEU:HD11	2:B:278:CYS:HB3	1.90	0.53
1:A:673:LEU:HD22	1:A:677:VAL:HG11	1.91	0.53
2:B:132:ALA:H	2:B:243:GLN:HG2	1.73	0.53
2:B:114:ASN:O	2:B:118:GLN:HG3	2.09	0.53
1:A:103:LEU:HA	1:A:106:ILE:HD12	1.91	0.52
1:A:100:PHE:CE1	1:A:295:ILE:HG21	2.42	0.52
1:A:790:PHE:O	1:A:794:ILE:HG13	2.09	0.52
1:A:784:ILE:HG13	1:A:854:TYR:HA	1.90	0.52
1:A:696:GLN:O	1:A:700:ILE:HG12	2.10	0.52
1:A:920:THR:HG21	1:A:981:TYR:O	2.09	0.52
2:B:93:ILE:H	2:B:305:SER:HB2	1.73	0.52
1:A:571:PHE:HA	1:A:577:ASN:HD22	1.75	0.52
2:B:128:SER:HB3	2:B:130:THR:O	2.09	0.52
1:A:63:LEU:HD22	1:A:189:ASP:HB3	1.92	0.52
1:A:676:GLU:H	1:A:676:GLU:CD	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ILE:CG1	1:A:329:VAL:H	2.11	0.52
1:A:693:THR:HA	1:A:697:GLN:HE21	1.74	0.52
1:A:974:THR:HG22	1:A:980:MET:HB2	1.91	0.51
1:A:894:TRP:HD1	2:B:83:TYR:OH	1.94	0.51
2:B:212:PRO:HG2	2:B:281:TYR:HB2	1.92	0.51
1:A:1005:ARG:HH21	1:A:1021:THR:HB	1.76	0.51
1:A:61:ARG:CG	1:A:61:ARG:NH1	2.73	0.51
2:B:193:LYS:HA	2:B:207:ASN:HD21	1.76	0.51
1:A:36:LYS:O	1:A:696:GLN:HG2	2.11	0.51
2:B:106:MET:O	2:B:110:MET:HG2	2.11	0.51
1:A:1011:ARG:O	1:A:1013:PRO:HD3	2.11	0.50
1:A:101:SER:O	1:A:105:TRP:CD1	2.64	0.50
1:A:212:LYS:HG2	1:A:224:PRO:HB2	1.93	0.50
1:A:754:ASN:HD21	1:A:756:ALA:HB3	1.75	0.50
1:A:790:PHE:CE2	1:A:794:ILE:HD11	2.45	0.50
1:A:818:PRO:HB3	1:A:934:LEU:HD22	1.93	0.50
2:B:171:ALA:CB	2:B:175:PRO:HA	2.39	0.50
1:A:735:GLY:O	1:A:743:LYS:HE3	2.12	0.50
1:A:192:GLU:OE1	1:A:255:ARG:HD2	2.12	0.50
2:B:101:SER:O	2:B:104:LYS:HB3	2.12	0.50
1:A:291:PHE:HZ	1:A:336:LEU:HD23	1.75	0.50
1:A:531:LYS:HE3	1:A:534:MET:HG2	1.92	0.50
1:A:345:THR:O	1:A:349:LYS:HG2	2.11	0.50
1:A:110:LEU:HD22	1:A:325:ILE:HG21	1.94	0.49
1:A:993:PRO:O	1:A:997:ILE:HG22	2.12	0.49
2:B:76:PRO:HG3	2:B:184:ILE:HD12	1.94	0.49
1:A:518:CYS:SG	1:A:585:PHE:HB2	2.52	0.49
1:A:693:THR:HA	1:A:697:GLN:NE2	2.27	0.49
2:B:180:LYS:HG2	2:B:181:LEU:N	2.27	0.49
2:B:95:ASN:HB2	2:B:98:SER:HB2	1.93	0.49
1:A:458:LYS:O	1:A:462:LEU:HB2	2.13	0.49
1:A:784:ILE:HD11	1:A:854:TYR:CG	2.47	0.49
1:A:572:ASP:CB	1:A:577:ASN:HB2	2.42	0.49
1:A:785:PRO:HB2	1:A:926:ILE:HD12	1.93	0.49
1:A:212:LYS:HB2	1:A:251:GLU:HG2	1.94	0.49
1:A:502:ARG:HG2	1:A:503:TYR:H	1.77	0.49
1:A:534:MET:C	1:A:536:GLU:H	2.15	0.49
2:B:113:TYR:CE1	2:B:260:LEU:HD11	2.48	0.49
1:A:790:PHE:O	1:A:793:PHE:HB3	2.13	0.49
1:A:150:GLN:HA	1:A:361:LEU:HB2	1.95	0.48
1:A:376:ASP:OD2	4:A:2001:MF4:F4	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:GLU:OE2	1:A:647:ARG:NH1	2.46	0.48
1:A:852:MET:HG2	1:A:1021:THR:HG22	1.95	0.48
1:A:868:SER:O	1:A:872:ILE:HG12	2.13	0.48
2:B:104:LYS:HE2	2:B:108:LYS:NZ	2.28	0.48
1:A:170:LEU:HD21	1:A:177:LYS:HD3	1.95	0.48
2:B:34:PHE:CE2	2:B:38:LEU:HD12	2.48	0.48
1:A:420:ALA:HB1	1:A:557:HIS:CE1	2.49	0.48
1:A:887:ARG:HA	1:A:890:TRP:HB3	1.94	0.48
1:A:61:ARG:HA	1:A:175:GLY:HA2	1.95	0.48
1:A:424:ILE:HG23	1:A:506:VAL:HB	1.96	0.48
1:A:48:LEU:O	1:A:52:HIS:HD2	1.97	0.48
3:G:18:ARG:HG2	3:G:18:ARG:HH11	1.79	0.48
1:A:209:HIS:HB3	1:A:253:THR:HG22	1.96	0.47
2:B:194:ASN:HD22	2:B:194:ASN:N	2.11	0.47
2:B:92:SER:HA	2:B:304:LYS:O	2.14	0.47
1:A:832:MET:HA	1:A:832:MET:HE2	1.95	0.47
1:A:502:ARG:HD3	1:A:560:LEU:O	2.14	0.47
1:A:797:ASN:C	1:A:887:ARG:HG2	2.35	0.47
1:A:274:ALA:O	1:A:726:LYS:HE2	2.15	0.47
1:A:670:LEU:HD23	1:A:678:LEU:CD2	2.45	0.47
1:A:618:GLY:O	1:A:692:ARG:HD2	2.15	0.47
2:B:215:CYS:HA	2:B:278:CYS:HA	1.96	0.47
1:A:592:ILE:O	1:A:594:PRO:HD3	2.14	0.47
2:B:210:VAL:HG13	2:B:239:GLY:HA3	1.95	0.47
1:A:152:ALA:O	1:A:360:ASN:ND2	2.47	0.47
1:A:135:VAL:O	1:A:139:VAL:HG23	2.15	0.47
1:A:994:TYR:CA	1:A:997:ILE:HG22	2.44	0.47
1:A:132:LEU:O	1:A:136:LEU:HG	2.15	0.46
1:A:831:ILE:HG22	1:A:834:ARG:CZ	2.45	0.46
2:B:288:SER:HB2	2:B:294:ARG:HH11	1.79	0.46
1:A:788:THR:N	1:A:789:PRO:HD2	2.31	0.46
2:B:194:ASN:HA	2:B:198:LEU:HD11	1.97	0.46
2:B:81:ALA:HB2	2:B:109:LEU:CD2	2.42	0.46
3:G:25:ILE:O	3:G:29:VAL:HG23	2.15	0.46
1:A:846:ASN:ND2	1:A:1023:TYR:OXT	2.49	0.46
2:B:227:GLY:HA2	2:B:267:ASN:CB	2.46	0.46
3:G:15:ASP:OD2	3:G:18:ARG:HG3	2.14	0.46
2:B:209:TYR:HA	2:B:242:LEU:HD22	1.96	0.46
2:B:270:GLN:CG	2:B:271:ASN:HD22	2.27	0.46
1:A:310:SER:O	1:A:315:TYR:HD2	1.99	0.46
1:A:503:TYR:CE1	1:A:571:PHE:HE1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LEU:HB2	1:A:726:LYS:HD2	1.98	0.46
1:A:883:LEU:HA	1:A:886:LYS:HZ3	1.80	0.46
1:A:100:PHE:HB3	1:A:332:VAL:CG1	2.46	0.46
1:A:52:HIS:NE2	1:A:59:LEU:HD12	2.31	0.46
1:A:156:ARG:HB2	1:A:744:GLN:OE1	2.15	0.45
2:B:159:ASN:HD21	9:B:4021:NAG:C1	2.28	0.45
1:A:815:ASP:CG	1:A:930:GLN:HE21	2.20	0.45
1:A:367:LEU:O	1:A:762:VAL:HB	2.17	0.45
1:A:915:GLU:O	1:A:918:CYS:HB2	2.16	0.45
2:B:122:SER:HA	2:B:123:PRO:HA	1.78	0.45
1:A:399:GLU:O	1:A:399:GLU:HG3	2.16	0.45
2:B:189:PRO:HB2	2:B:211:LEU:HD13	1.98	0.45
2:B:87:THR:HB	2:B:298:GLU:O	2.17	0.45
1:A:551:ARG:O	1:A:590:ALA:HA	2.17	0.45
1:A:909:GLU:O	1:A:913:ILE:HG12	2.17	0.45
2:B:187:PHE:CZ	2:B:284:ASN:HB3	2.52	0.45
1:A:367:LEU:HD23	1:A:761:GLY:HA3	1.99	0.45
1:A:387:THR:HB	1:A:594:PRO:HG3	2.00	0.45
1:A:211:CYS:HA	1:A:252:GLY:HA3	1.98	0.44
1:A:846:ASN:HD22	1:A:848:ARG:HB2	1.80	0.44
1:A:939:THR:OG1	1:A:1006:ARG:NH1	2.50	0.44
1:A:575:GLU:O	1:A:577:ASN:N	2.50	0.44
1:A:827:ALA:HB1	1:A:829:SER:O	2.17	0.44
2:B:297:PHE:O	2:B:298:GLU:HG2	2.18	0.44
1:A:91:LYS:HB3	1:A:148:TYR:HE1	1.82	0.44
1:A:154:SER:HB3	1:A:359:LYS:HE3	1.99	0.44
1:A:61:ARG:HG3	1:A:61:ARG:NH1	2.32	0.44
1:A:816:MET:O	1:A:820:ILE:HG12	2.18	0.44
2:B:158:LYS:HB2	2:B:232:PHE:CD2	2.52	0.44
1:A:277:LEU:HB2	1:A:726:LYS:CD	2.48	0.44
1:A:295:ILE:HA	1:A:295:ILE:HD13	1.81	0.44
1:A:802:LEU:CD1	1:A:922:PHE:HB3	2.48	0.44
1:A:838:ASN:ND2	1:A:840:LYS:HG2	2.30	0.44
2:B:74:ALA:HB3	2:B:75:PRO:CD	2.44	0.44
1:A:321:VAL:O	1:A:325:ILE:HG22	2.17	0.44
1:A:326:GLY:O	7:A:6000:OBN:C22	2.66	0.44
1:A:42:ASP:HB3	1:A:43:ASP:H	1.49	0.43
3:G:17:TYR:O	3:G:21:VAL:HG23	2.19	0.43
1:A:984:LYS:HG2	3:G:14:TYR:CZ	2.53	0.43
2:B:228:SER:HB3	2:B:267:ASN:HA	2.00	0.43
2:B:93:ILE:HD11	2:B:303:VAL:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1009:ILE:HG22	1:A:1010:ARG:N	2.33	0.43
1:A:799:PRO:HD2	1:A:869:TYR:OH	2.18	0.43
1:A:899:GLU:HA	1:A:904:GLN:O	2.19	0.43
9:B:4001:NAG:O4	9:B:4002:NAG:N2	2.44	0.43
1:A:536:GLU:HA	1:A:539:GLN:HB2	2.00	0.43
2:B:115:GLU:OE2	2:B:153:SER:HA	2.18	0.43
1:A:140:VAL:O	1:A:144:GLY:N	2.51	0.43
1:A:191:VAL:HG11	1:A:200:PRO:HG2	2.00	0.43
1:A:566:ASN:N	1:A:569:TYR:HB2	2.33	0.43
2:B:227:GLY:HA2	2:B:267:ASN:HB2	1.99	0.43
1:A:273:LEU:HD21	1:A:699:LEU:HD23	2.00	0.43
2:B:118:GLN:HE22	2:B:152:PHE:H	1.66	0.43
2:B:174:LYS:H	2:B:303:VAL:HG11	1.82	0.43
2:B:66:GLU:OE2	3:G:11:ARG:CZ	2.66	0.43
1:A:51:LEU:HD13	1:A:204:ARG:HG3	2.01	0.43
1:A:327:ILE:HG22	1:A:327:ILE:O	2.19	0.43
1:A:479:GLU:HB2	1:A:490:LEU:O	2.18	0.43
1:A:52:HIS:HD1	1:A:57:THR:HG23	1.84	0.43
1:A:785:PRO:HB2	1:A:926:ILE:CD1	2.49	0.43
2:B:206:TYR:O	2:B:208:GLN:N	2.52	0.43
3:G:18:ARG:CG	3:G:18:ARG:HH11	2.32	0.43
1:A:569:TYR:CE2	1:A:570:PRO:O	2.72	0.43
7:A:6000:OBN:H212	7:A:6000:OBN:C18	2.44	0.43
1:A:517:ARG:HD3	1:A:580:THR:O	2.19	0.42
1:A:658:ARG:HA	1:A:658:ARG:NE	2.34	0.42
1:A:43:ASP:HB2	1:A:46:LEU:CD1	2.49	0.42
2:B:72:ARG:HA	2:B:72:ARG:HD3	1.79	0.42
1:A:688:ILE:HG21	1:A:690:PHE:CE1	2.54	0.42
1:A:928:VAL:O	1:A:931:TRP:HB2	2.19	0.42
1:A:382:THR:HA	1:A:595:PRO:HA	2.00	0.42
1:A:502:ARG:CG	1:A:503:TYR:N	2.82	0.42
1:A:576:PRO:C	1:A:578:PHE:H	2.22	0.42
1:A:620:HIS:HA	1:A:621:PRO:HD3	1.81	0.42
1:A:850:ILE:O	1:A:854:TYR:HB2	2.20	0.42
1:A:48:LEU:HD23	1:A:206:ILE:HB	2.01	0.42
1:A:450:ASP:O	1:A:454:SER:OG	2.38	0.42
1:A:860:ILE:HG12	2:B:47:LEU:CD1	2.50	0.42
9:B:4001:NAG:O6	9:B:4002:NAG:H5	2.20	0.42
1:A:800:LEU:HA	1:A:801:PRO:HD3	1.77	0.42
2:B:159:ASN:HA	2:B:159:ASN:HD22	1.70	0.42
2:B:95:ASN:HA	2:B:96:PRO:HD3	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:39:LEU:HD23	3:G:42:LYS:HA	2.02	0.42
1:A:507:MET:HG2	1:A:556:CYS:SG	2.60	0.41
1:A:609:ALA:O	1:A:836:PRO:HD3	2.19	0.41
1:A:482:PHE:HB2	1:A:489:GLN:HB2	2.02	0.41
1:A:328:ILE:O	1:A:329:VAL:C	2.58	0.41
1:A:565:TYR:CD2	1:A:569:TYR:CE2	3.06	0.41
2:B:133:ASP:O	2:B:243:GLN:HA	2.20	0.41
1:A:1009:ILE:HG13	1:A:1017:VAL:HG12	2.01	0.41
1:A:488:TYR:CE1	1:A:490:LEU:HD23	2.49	0.41
1:A:882:ASP:O	1:A:886:LYS:NZ	2.53	0.41
1:A:161:PHE:HA	1:A:164:MET:HE2	2.01	0.41
1:A:345:THR:HA	1:A:361:LEU:HD11	2.02	0.41
1:A:478:VAL:HG21	1:A:571:PHE:HB2	2.02	0.41
1:A:223:GLU:HA	1:A:224:PRO:HD2	1.89	0.41
1:A:44:HIS:HE1	1:A:234:GLU:O	2.04	0.41
1:A:847:GLU:H	1:A:847:GLU:CD	2.24	0.41
1:A:924:ILE:HD12	1:A:983:LEU:CD1	2.48	0.41
2:B:269:THR:HG23	2:B:274:LEU:HD11	2.02	0.41
2:B:89:ILE:HG13	2:B:301:ILE:HG22	2.02	0.41
3:G:14:TYR:HB3	3:G:16:TYR:CE1	2.55	0.41
1:A:63:LEU:HD13	1:A:189:ASP:HA	2.03	0.41
1:A:790:PHE:CG	7:A:6000:OBN:H161	2.56	0.41
2:B:153:SER:HB2	2:B:156:TRP:CD1	2.55	0.41
2:B:183:ARG:HD2	2:B:247:TYR:CE2	2.55	0.41
1:A:534:MET:C	1:A:536:GLU:N	2.74	0.41
1:A:570:PRO:O	1:A:577:ASN:ND2	2.54	0.41
1:A:802:LEU:HD13	1:A:922:PHE:HB3	2.03	0.41
1:A:199:ILE:HG22	1:A:201:ALA:O	2.21	0.41
1:A:851:SER:HB3	8:B:3001:CLR:C4	2.51	0.41
1:A:817:VAL:HG12	1:A:957:GLY:HA2	2.03	0.41
2:B:270:GLN:HG3	2:B:271:ASN:ND2	2.32	0.41
1:A:150:GLN:HA	1:A:361:LEU:CB	2.51	0.40
1:A:136:LEU:O	1:A:139:VAL:HB	2.20	0.40
1:A:339:THR:HG23	1:A:820:ILE:HD13	2.04	0.40
1:A:367:LEU:HD12	1:A:367:LEU:HA	1.84	0.40
1:A:157:ILE:HD11	1:A:745:ALA:HA	2.02	0.40
1:A:81:THR:HA	1:A:82:PRO:HD2	1.78	0.40
1:A:82:PRO:HA	1:A:158:MET:HG2	2.04	0.40
1:A:218:LEU:HD12	1:A:218:LEU:N	2.37	0.40
1:A:48:LEU:O	1:A:52:HIS:CD2	2.75	0.40
1:A:503:TYR:CD1	1:A:571:PHE:CE1	3.10	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LEU:O	1:A:59:LEU:HD23	2.22	0.40
1:A:994:TYR:OH	2:B:51:PHE:HA	2.22	0.40
1:A:213:VAL:HG23	1:A:249:CYS:HA	2.04	0.40
1:A:443:LEU:HA	1:A:458:LYS:HD3	2.04	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	990/1028 (96%)	902 (91%)	78 (8%)	10 (1%)	15	44
2	B	259/305 (85%)	216 (83%)	37 (14%)	6 (2%)	6	21
3	G	36/74 (49%)	32 (89%)	4 (11%)	0	100	100
All	All	1285/1407 (91%)	1150 (90%)	119 (9%)	16 (1%)	13	39

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	ASP
1	A	329	VAL
1	A	566	ASN
1	A	576	PRO
2	B	85	ILE
2	B	201	GLN
2	B	207	ASN
1	A	128	ASP
1	A	327	ILE
1	A	404	GLU
2	B	118	GLN
1	A	119	ALA
2	B	199	PRO

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Mol	Chain	Res	Type
1	A	1014	GLY
2	B	145	GLY
1	A	279	VAL

### 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	840/869 (97%)	770 (92%)	70 (8%)	11	32
2	B	232/266 (87%)	210 (90%)	22 (10%)	8	25
3	G	31/62 (50%)	30 (97%)	1 (3%)	39	73
All	All	1103/1197 (92%)	1010 (92%)	93 (8%)	11	31

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	VAL
1	A	42	ASP
1	A	51	LEU
1	A	61	ARG
1	A	72	LEU
1	A	104	LEU
1	A	110	LEU
1	A	128	ASP
1	A	165	VAL
1	A	172	ILE
1	A	212	LYS
1	A	213	VAL
1	A	231	PHE
1	A	248	ASN
1	A	253	THR
1	A	261	THR
1	A	270	ILE
1	A	284	ILE
1	A	291	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	305	SER
1	A	307	PHE
1	A	309	LEU
1	A	311	LEU
1	A	317	TRP
1	A	344	LEU
1	A	367	LEU
1	A	371	SER
1	A	376	ASP
1	A	391	MET
1	A	413	LYS
1	A	427	LEU
1	A	434	GLN
1	A	440	VAL
1	A	454	SER
1	A	457	LEU
1	A	485	THR
1	A	515	LEU
1	A	516	ASP
1	A	520	THR
1	A	524	ASN
1	A	530	LEU
1	A	531	LYS
1	A	538	PHE
1	A	548	LEU
1	A	552	VAL
1	A	557	HIS
1	A	648	LEU
1	A	656	ASN
1	A	670	LEU
1	A	675	THR
1	A	682	LEU
1	A	712	VAL
1	A	719	VAL
1	A	762	VAL
1	A	768	ILE
1	A	804	THR
1	A	822	LEU
1	A	833	LYS
1	A	838	ASN
1	A	841	THR
1	A	847	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	886	LYS
1	A	888	VAL
1	A	889	ARG
1	A	944	ILE
1	A	964	LEU
1	A	987	TRP
1	A	996	LEU
1	A	997	ILE
1	A	1009	ILE
2	B	38	LEU
2	B	47	LEU
2	B	57	VAL
2	B	73	VAL
2	B	89	ILE
2	B	108	LYS
2	B	139	ASP
2	B	141	ASP
2	B	172	GLU
2	B	176	CYS
2	B	180	LYS
2	B	193	LYS
2	B	194	ASN
2	B	200	GLU
2	B	223	ARG
2	B	226	ILE
2	B	243	GLN
2	B	251	ARG
2	B	267	ASN
2	B	276	ILE
2	B	287	TYR
2	B	303	VAL
3	G	13	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	44	HIS
1	A	52	HIS
1	A	78	ASN
1	A	118	GLN
1	A	168	GLN
1	A	434	GLN

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Mol	Chain	Res	Type
1	A	524	ASN
1	A	557	HIS
1	A	577	ASN
1	A	656	ASN
1	A	697	GLN
1	A	754	ASN
1	A	838	ASN
1	A	846	ASN
1	A	904	GLN
1	A	905	GLN
1	A	1019	GLN
2	B	70	GLN
2	B	80	HIS
2	B	95	ASN
2	B	118	GLN
2	B	194	ASN
2	B	201	GLN
2	B	203	GLN
2	B	207	ASN
2	B	243	GLN
2	B	267	ASN
2	B	271	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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
9	NAG	B	4002	-	14,14,15	0.58	0	17,19,21	1.08	1 (5%)
7	OBN	A	6000	-	44,46,46	0.75	1 (2%)	66,76,76	1.63	11 (16%)
9	NAG	B	4001	-	14,14,15	0.55	0	17,19,21	0.95	1 (5%)
9	NAG	B	4021	-	14,14,15	0.50	0	17,19,21	0.89	0
4	MF4	A	2001	-	0,4,4	0.00	-	-		
8	CLR	B	3001	-	31,31,31	0.48	0	48,48,48	1.31	6 (12%)

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
7	OBN	A	6000	-	-	4/11/116/116	0/6/6/6
9	NAG	B	4001	-	-	0/6/23/26	0/1/1/1
9	NAG	B	4021	-	-	0/6/23/26	0/1/1/1
9	NAG	B	4002	-	-	2/6/23/26	0/1/1/1
8	CLR	B	3001	-	-	1/10/68/68	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	6000	OBN	O21-C23	3.49	1.45	1.36

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	6000	OBN	C15-C14-C13	6.08	108.11	103.37
7	A	6000	OBN	C16-C17-C13	4.48	110.01	104.98
8	B	3001	CLR	C7-C8-C9	3.91	114.45	109.71
7	A	6000	OBN	C15-C14-C8	-3.62	110.98	116.05
7	A	6000	OBN	C12-C11-C9	-3.58	107.69	112.60
7	A	6000	OBN	C18-C13-C12	-3.33	106.52	111.11
7	A	6000	OBN	C17-C20-C22	-3.21	120.30	128.84
8	B	3001	CLR	C3-C4-C5	-3.02	106.90	112.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	3001	CLR	C14-C8-C9	-2.95	105.14	109.09
8	B	3001	CLR	C15-C14-C13	2.86	107.29	103.84
8	B	3001	CLR	C1-C2-C3	2.77	114.02	110.47
7	A	6000	OBN	C16-C17-C20	-2.50	108.77	113.68
9	B	4001	NAG	C3-C4-C5	2.45	114.61	110.24
9	B	4002	NAG	C4-C3-C2	2.44	114.59	111.02
7	A	6000	OBN	C13-C14-C8	2.40	116.95	113.83
7	A	6000	OBN	O23-C23-C22	-2.39	125.98	130.81
7	A	6000	OBN	C21-C20-C22	2.32	113.85	108.57
8	B	3001	CLR	C4-C5-C10	2.29	119.46	116.42
7	A	6000	OBN	C1'-O5'-C5'	2.05	117.19	113.67

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	6000	OBN	O5'-C1'-O3-C3
9	B	4002	NAG	C4-C5-C6-O6
9	B	4002	NAG	O5-C5-C6-O6
7	A	6000	OBN	C1-C10-C19-O19
7	A	6000	OBN	C9-C10-C19-O19
8	B	3001	CLR	C22-C23-C24-C25
7	A	6000	OBN	C16-C17-C20-C21

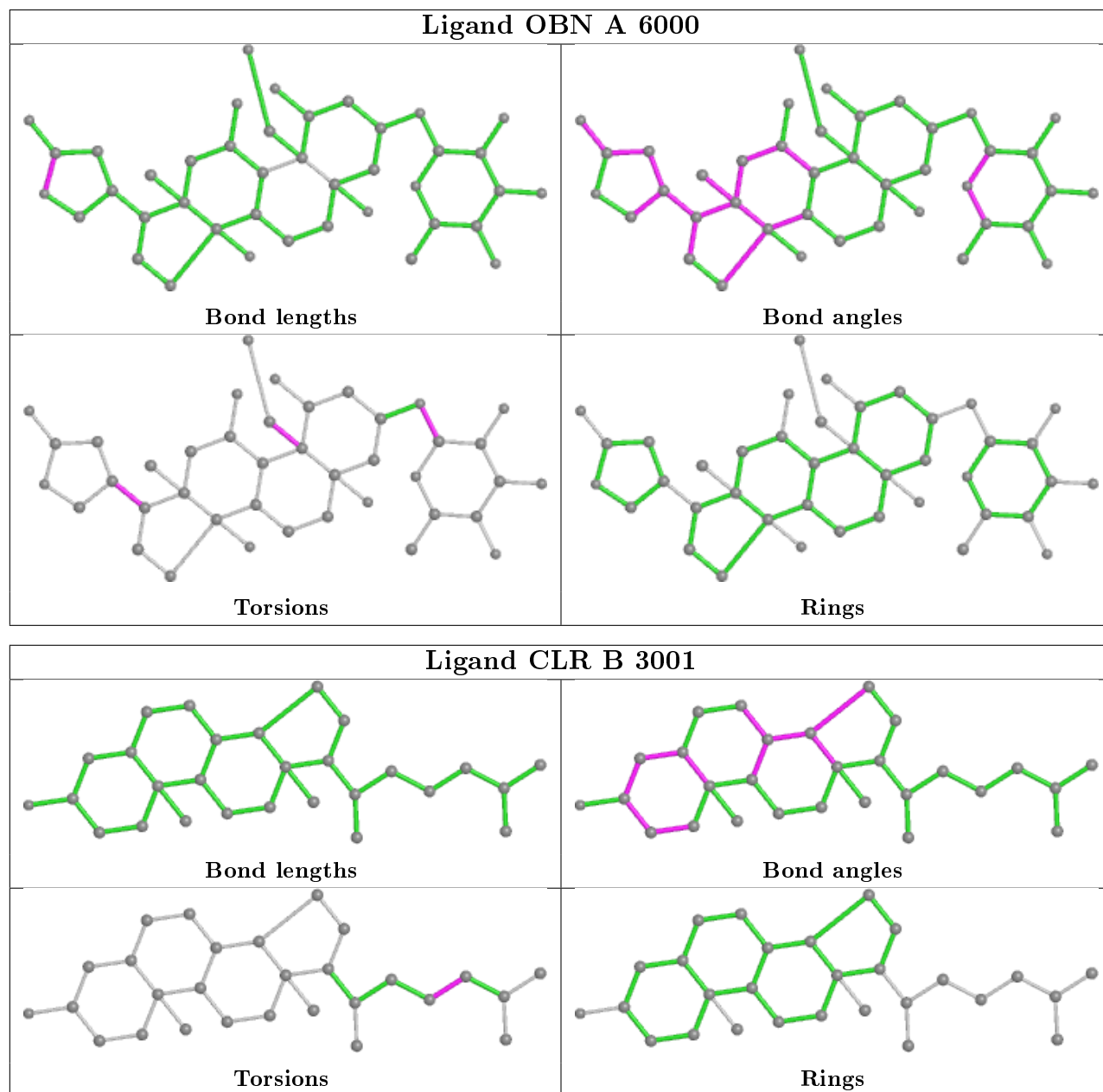
There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	4002	NAG	2	0
7	A	6000	OBN	7	0
9	B	4001	NAG	2	0
9	B	4021	NAG	1	0
4	A	2001	MF4	1	0
8	B	3001	CLR	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	992/1028 (96%)	0.27	69 (6%) 16   9	23, 48, 111, 161	0
2	B	265/305 (86%)	0.66	30 (11%) 5   3	45, 86, 120, 127	0
3	G	38/74 (51%)	-0.22	0 100   100	37, 46, 85, 89	0
All	All	1295/1407 (92%)	0.33	99 (7%) 13   7	23, 54, 116, 161	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	116	GLY	6.9
1	A	131	TYR	6.3
1	A	317	TRP	6.3
1	A	90	ILE	6.3
1	A	313	LEU	6.2
1	A	125	PRO	5.5
1	A	119	ALA	5.1
1	A	112	PHE	5.1
2	B	199	PRO	5.0
1	A	115	TYR	4.8
1	A	146	PHE	4.8
1	A	130	LEU	4.7
1	A	96	LEU	4.6
1	A	312	ILE	4.5
1	A	499	SER	4.4
2	B	225	LYS	4.3
1	A	579	PRO	4.3
2	B	270	GLN	4.2
1	A	498	SER	4.2
2	B	121	ASN	4.1
2	B	214	ARG	4.0
1	A	86	THR	3.8
1	A	123	ASP	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	42	ILE	3.7
1	A	563	ASP	3.7
1	A	126	ALA	3.7
1	A	567	GLU	3.6
1	A	308	ILE	3.6
2	B	38	LEU	3.6
2	B	93	ILE	3.6
1	A	89	TRP	3.5
2	B	99	TYR	3.5
1	A	92	PHE	3.3
1	A	100	PHE	3.3
2	B	202	LEU	3.3
1	A	530	LEU	3.2
2	B	41	LEU	3.2
1	A	573	ALA	3.2
1	A	127	ASN	3.2
1	A	321	VAL	3.2
2	B	85	ILE	3.2
1	A	150	GLN	3.2
1	A	324	LEU	3.1
2	B	273	GLU	3.1
2	B	207	ASN	3.0
1	A	114	ALA	3.0
2	B	203	GLN	3.0
1	A	562	GLU	3.0
1	A	675	THR	3.0
1	A	129	ASN	2.9
1	A	580	THR	2.8
1	A	503	TYR	2.8
1	A	529	PRO	2.7
1	A	986	SER	2.7
1	A	439	ASN	2.7
1	A	566	ASN	2.7
2	B	96	PRO	2.7
1	A	138	THR	2.6
1	A	560	LEU	2.6
2	B	271	ASN	2.6
1	A	122	GLU	2.6
1	A	574	ASP	2.5
1	A	120	ALA	2.5
2	B	129	ASP	2.5
1	A	84	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	894	TRP	2.5
2	B	281	TYR	2.5
2	B	92	SER	2.5
1	A	128	ASP	2.5
1	A	88	GLU	2.4
1	A	154	SER	2.4
1	A	32	LEU	2.4
1	A	97	PHE	2.4
2	B	272	MET	2.4
1	A	502	ARG	2.4
1	A	148	TYR	2.3
2	B	298	GLU	2.3
2	B	65	PHE	2.3
1	A	93	CYS	2.3
1	A	534	MET	2.3
1	A	1016	TRP	2.3
1	A	77	PRO	2.2
1	A	124	GLU	2.2
2	B	304	LYS	2.2
2	B	276	ILE	2.2
2	B	274	LEU	2.2
2	B	146	GLN	2.2
1	A	118	GLN	2.2
1	A	149	TYR	2.2
2	B	147	LYS	2.1
1	A	105	TRP	2.1
1	A	152	ALA	2.1
1	A	94	ARG	2.1
1	A	147	SER	2.1
2	B	126	ASP	2.1
1	A	103	LEU	2.0
2	B	223	ARG	2.0
1	A	568	GLY	2.0
1	A	311	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates

There are no monosaccharides in this entry.

### 6.4 Ligands

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, 95<sup>th</sup> 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.

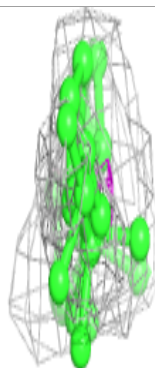
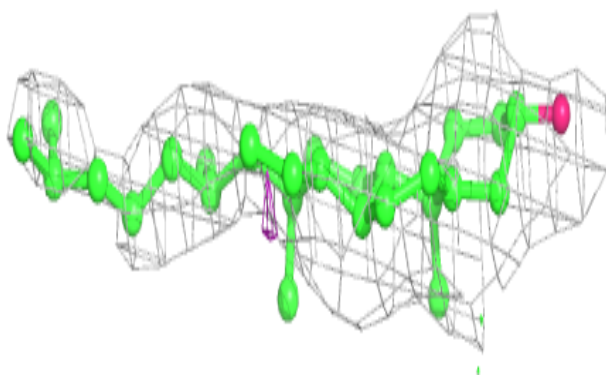
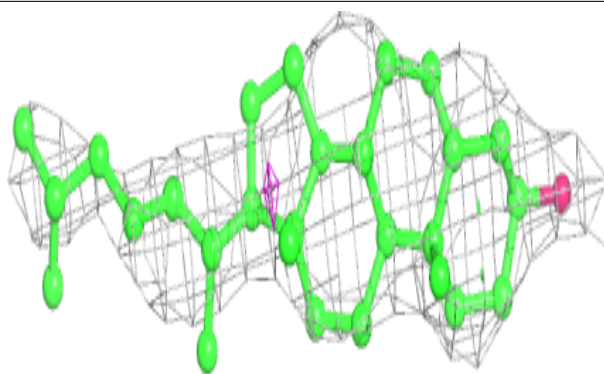
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	NAG	B	4021	14/15	0.48	0.39	116,117,117,117	0
9	NAG	B	4002	14/15	0.63	0.32	109,110,111,111	0
8	CLR	B	3001	28/28	0.81	0.34	86,88,89,89	0
7	OBN	A	6000	41/41	0.84	0.19	93,95,98,98	0
9	NAG	B	4001	14/15	0.87	0.22	101,102,102,102	0
4	MF4	A	2001	5/5	0.94	0.24	23,23,24,27	0
6	K	A	2005	1/1	0.94	0.10	76,76,76,76	0
6	K	A	2004	1/1	0.95	0.10	72,72,72,72	0
5	MG	A	2002	1/1	0.97	0.19	25,25,25,25	0
6	K	A	2003	1/1	0.97	0.14	50,50,50,50	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.

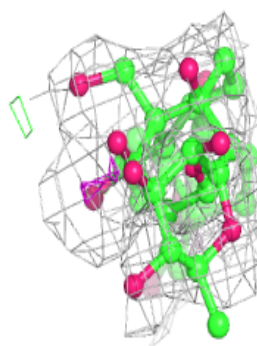
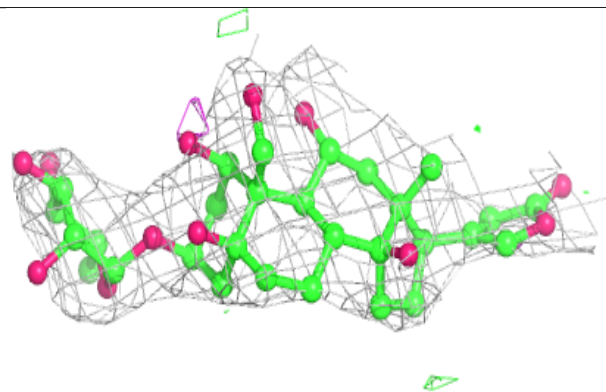
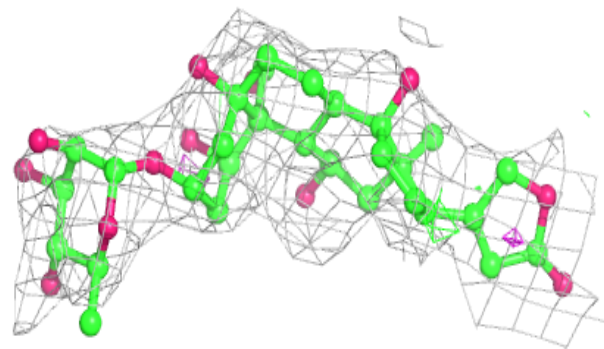


**Electron density around CLR B 3001:**

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

**Electron density around OBN A 6000:**

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



## 6.5 Other polymers

There are no such residues in this entry.