



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:34 am BST

PDB ID : 1N52  
Title : Cap Binding Complex  
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Deposited on : 2002-11-04  
Resolution : 2.11 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 : 2.11  
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) : 2.11



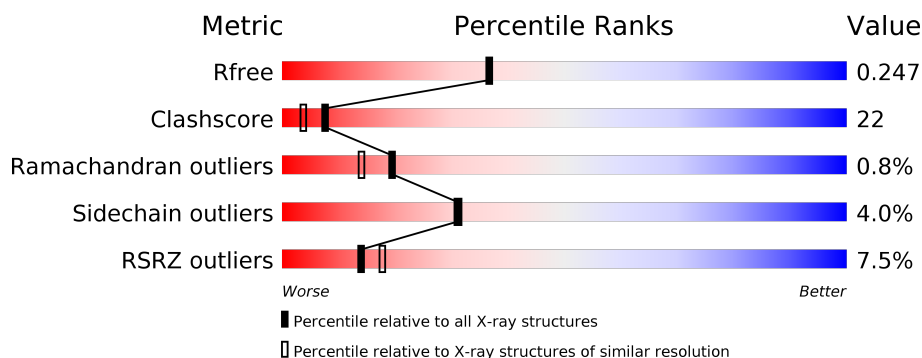
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.11 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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	790	<div> <div>8%</div> <div> <div></div> <div>56%</div> <div>35%</div> <div>• 7%</div> </div> </div>
2	B	156	<div> <div>4%</div> <div> <div></div> <div>61%</div> <div>29%</div> <div>• • 5%</div> </div> </div>

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



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PG4	A	3000	-	-	X	-
5	GOL	A	1555	-	X	-	-
5	GOL	A	1556	-	X	-	-
5	GOL	A	1557	-	X	-	-
5	GOL	A	1560	-	X	-	-
5	GOL	A	1561	-	X	-	-
5	GOL	A	1564	-	X	-	-
5	GOL	A	1565	-	X	-	-
5	GOL	A	1566	-	X	-	-
5	GOL	A	1569	-	X	-	-
5	GOL	A	1572	-	X	-	-
5	GOL	A	1573	-	X	-	-
5	GOL	B	1558	-	X	-	-
5	GOL	B	1568	-	X	-	-
5	GOL	B	1570	-	X	-	-
5	GOL	B	1571	-	X	X	-
5	GOL	B	1574	-	X	X	-



## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7699 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 80 kDa nuclear cap binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	732	Total	C	N	O	S	0	0	0
			5991	3863	1008	1082	38			

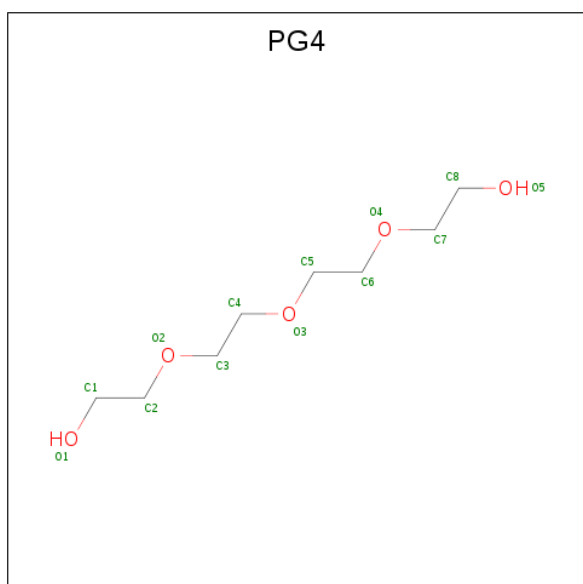
- Molecule 2 is a protein called 20 kDa nuclear cap binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	148	Total	C	N	O	S	0	0	0
			1208	752	216	234	6			

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

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

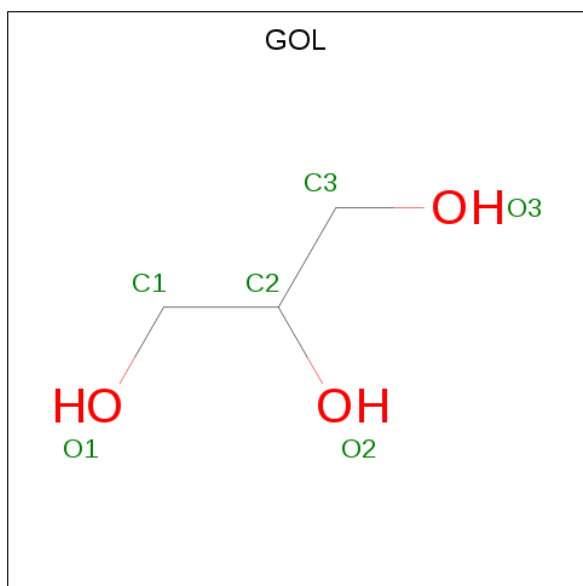
- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	8	5		

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



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

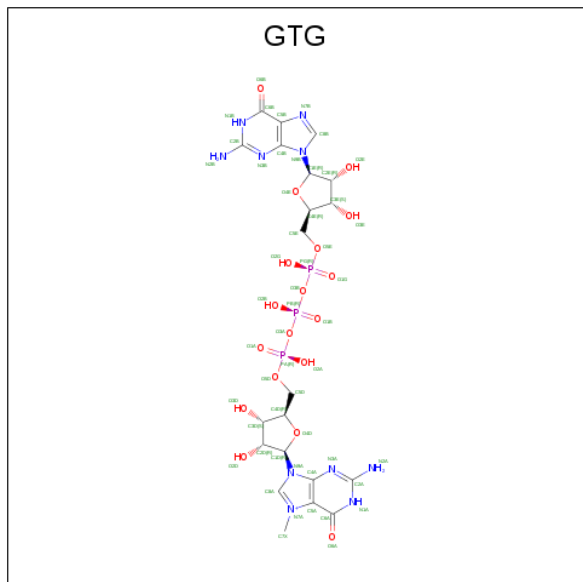
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is 7-METHYL-GUANOSINE-5'-TRIPHOSPHATE-5'-GUANOSINE (three-letter code: GTG) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>10</sub>O<sub>18</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			52	21	10	18	3		

- Molecule 7 is water.

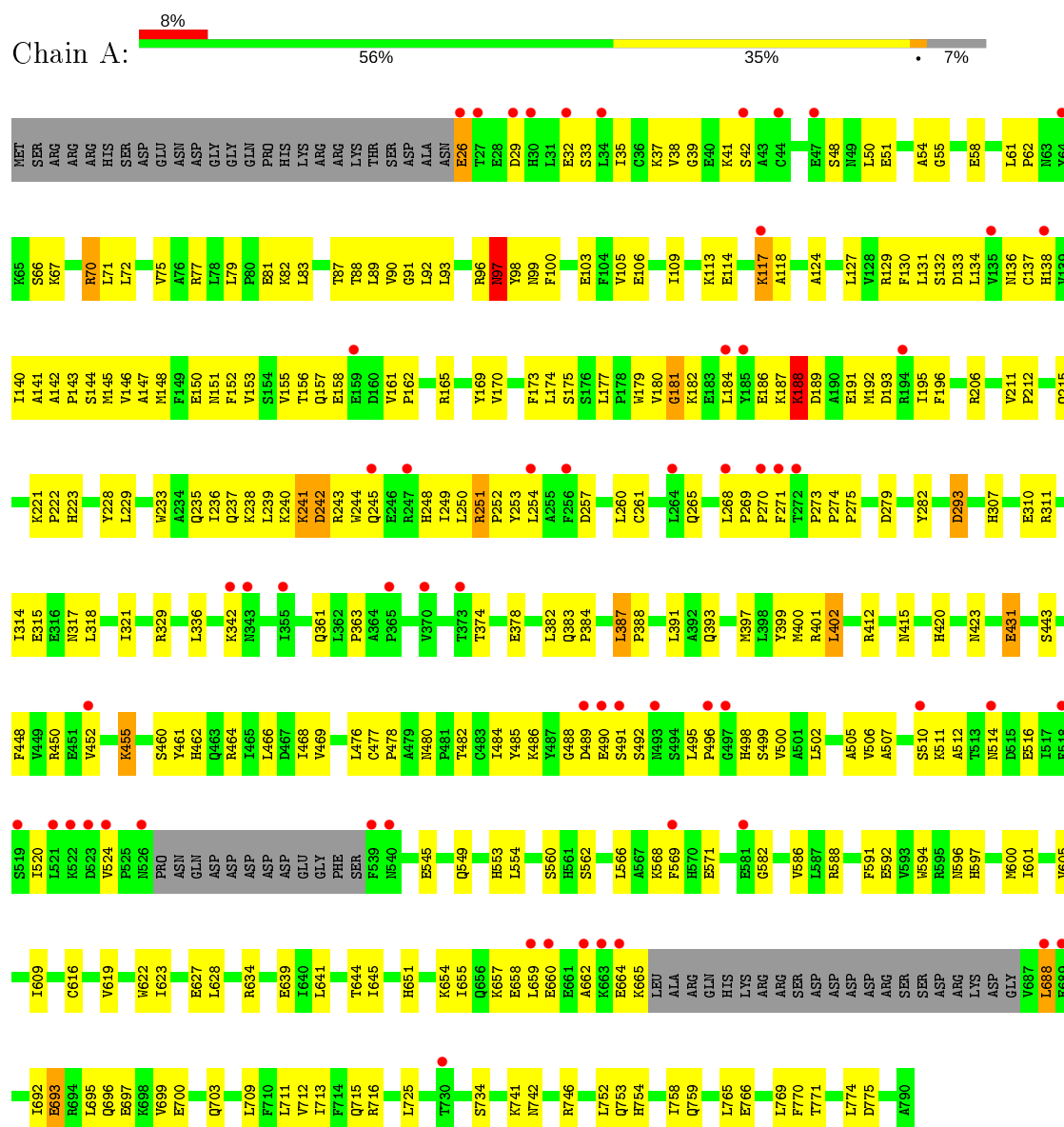
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	254	Total	O	0	0
			254	254		
7	B	84	Total	O	0	0
			84	84		



### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

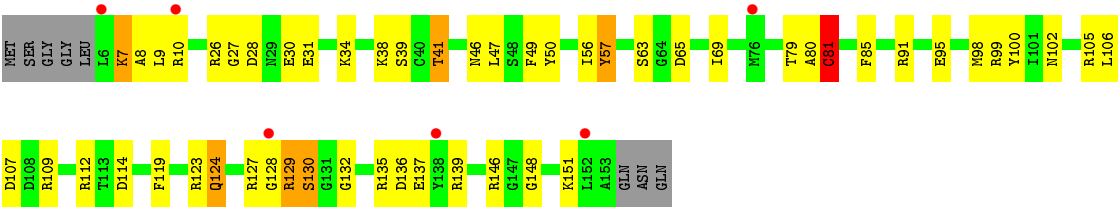
- Molecule 1: 80 kDa nuclear cap binding protein



- Molecule 2: 20 kDa nuclear cap binding protein









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.68Å 111.68Å 177.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.54 – 2.11 37.45 – 2.00	Depositor EDS
% Data completeness (in resolution range)	55.6 (24.54-2.11) 89.4 (37.45-2.00)	Depositor EDS
$R_{merge}$	0.33	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.223 , 0.246 0.223 , 0.247	Depositor DCC
$R_{free}$ test set	3961 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.2	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7699	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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: GOL, PG4, MG, GTG

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	0.38	0/6143	0.58	0/8335
2	B	0.46	1/1228 (0.1%)	0.70	0/1638
All	All	0.40	1/7371 (0.0%)	0.60	0/9973

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	81	CYS	CB-SG	-5.62	1.72	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5991	0	5976	259	0
2	B	1208	0	1165	62	0
3	A	1	0	0	0	0
4	A	13	0	17	7	0
5	A	66	0	44	6	0
5	B	30	0	20	13	0
6	B	52	0	26	3	0
7	A	254	0	0	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	84	0	0	3	0
All	All	7699	0	7248	321	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 22.

All (321) 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)
2:B:80:ALA:H	5:B:1571:GOL:H11	1.15	1.03
1:A:188:LYS:HA	1:A:188:LYS:NZ	1.77	0.98
1:A:180:VAL:HA	7:A:6172:HOH:O	1.64	0.98
1:A:235:GLN:HA	7:A:6164:HOH:O	1.62	0.97
1:A:180:VAL:HG22	1:A:184:LEU:HB2	1.48	0.96
2:B:80:ALA:H	5:B:1571:GOL:C1	1.81	0.93
1:A:238:LYS:HG3	1:A:241:LYS:HZ1	1.31	0.93
1:A:238:LYS:HG3	1:A:241:LYS:NZ	1.85	0.91
2:B:7:LYS:HA	2:B:7:LYS:HE3	1.56	0.86
2:B:27:GLY:CA	2:B:31:GLU:OE1	2.24	0.85
2:B:129:ARG:HD3	2:B:129:ARG:H	1.40	0.85
1:A:140:ILE:HD13	1:A:268:LEU:HD21	1.57	0.84
1:A:188:LYS:HA	1:A:188:LYS:HZ3	1.42	0.84
1:A:363:PRO:HB3	1:A:752:LEU:HD22	1.58	0.83
1:A:146:VAL:O	1:A:150:GLU:HG3	1.81	0.81
2:B:129:ARG:CD	2:B:129:ARG:H	1.89	0.79
2:B:129:ARG:HG2	2:B:137:GLU:HG3	1.65	0.79
1:A:93:LEU:HD23	1:A:100:PHE:HE2	1.47	0.79
1:A:136:ASN:ND2	7:A:6172:HOH:O	2.14	0.77
2:B:80:ALA:N	5:B:1571:GOL:H11	1.97	0.77
2:B:10:ARG:HH11	2:B:10:ARG:HB2	1.47	0.77
1:A:187:LYS:HD2	1:A:188:LYS:H	1.50	0.76
2:B:119:PHE:HE1	2:B:124:GLN:HG3	1.51	0.76
1:A:238:LYS:HA	1:A:241:LYS:HD2	1.67	0.76
1:A:431:GLU:CD	1:A:431:GLU:H	1.89	0.76
2:B:135:ARG:HD2	5:B:1570:GOL:H11	1.67	0.76
2:B:27:GLY:HA3	2:B:31:GLU:OE1	1.85	0.76
1:A:484:ILE:HD11	1:A:596:ASN:ND2	2.02	0.75
1:A:665:LYS:HB3	1:A:688:LEU:HD21	1.69	0.75
1:A:99:ASN:O	1:A:103:GLU:HG3	1.87	0.74
2:B:129:ARG:HH22	5:B:1574:GOL:H12	1.53	0.74
2:B:129:ARG:CD	2:B:129:ARG:N	2.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:GLU:O	1:A:117:LYS:HG3	1.87	0.73
2:B:107:ASP:OD2	5:B:1568:GOL:H11	1.89	0.73
2:B:10:ARG:NH1	2:B:10:ARG:HB2	2.04	0.72
2:B:119:PHE:CE1	2:B:124:GLN:HG3	2.24	0.72
1:A:243:ARG:HB2	1:A:245:GLN:HE21	1.53	0.72
1:A:374:THR:HG21	2:B:100:TYR:O	1.90	0.71
1:A:502:LEU:O	1:A:506:VAL:HG23	1.91	0.71
2:B:98:MET:HE1	2:B:114:ASP:HA	1.72	0.71
1:A:665:LYS:CB	1:A:688:LEU:HD21	2.20	0.70
1:A:188:LYS:HA	1:A:188:LYS:HZ2	1.55	0.69
1:A:716:ARG:HH11	1:A:716:ARG:HA	1.55	0.69
1:A:195:ILE:HB	7:A:6247:HOH:O	1.92	0.69
1:A:400:MET:HE3	7:A:6165:HOH:O	1.92	0.69
1:A:415:ASN:HD21	1:A:455:LYS:NZ	1.91	0.69
2:B:46:ASN:O	2:B:109:ARG:HD3	1.93	0.69
1:A:616:CYS:HB3	7:A:6006:HOH:O	1.92	0.68
1:A:117:LYS:HE2	1:A:118:ALA:HB2	1.76	0.68
1:A:696:GLN:O	1:A:700:GLU:HG2	1.94	0.67
1:A:29:ASP:O	1:A:32:GLU:HG2	1.94	0.67
2:B:57:TYR:CD2	2:B:69:ILE:HD12	2.30	0.67
2:B:130:SER:OG	2:B:151:LYS:HG2	1.95	0.66
1:A:109:ILE:O	1:A:113:LYS:HG3	1.95	0.66
1:A:32:GLU:HB2	2:B:7:LYS:HD2	1.78	0.65
1:A:754:HIS:O	1:A:758:ILE:HG13	1.96	0.65
1:A:554:LEU:HB3	5:A:1564:GOL:H11	1.76	0.65
1:A:484:ILE:HD11	1:A:596:ASN:HD21	1.59	0.65
2:B:26:ARG:HG2	7:B:2192:HOH:O	1.97	0.65
1:A:93:LEU:HD23	1:A:100:PHE:CE2	2.30	0.65
2:B:41:THR:HG22	7:B:2197:HOH:O	1.97	0.65
1:A:488:GLY:C	1:A:490:GLU:H	2.00	0.64
2:B:129:ARG:NH2	5:B:1574:GOL:H12	2.11	0.64
1:A:138:HIS:HB3	1:A:265:GLN:NE2	2.12	0.64
1:A:490:GLU:HG2	1:A:492:SER:HB2	1.80	0.64
1:A:77:ARG:HB3	1:A:127:LEU:HD21	1.80	0.64
1:A:191:GLU:O	1:A:195:ILE:HG12	1.97	0.64
1:A:654:LYS:O	1:A:657:LYS:HG2	1.98	0.63
1:A:153:VAL:HG21	1:A:195:ILE:HG23	1.79	0.63
2:B:26:ARG:HH11	2:B:26:ARG:HG3	1.62	0.63
1:A:97:ASN:HD22	1:A:97:ASN:C	2.02	0.63
1:A:152:PHE:O	1:A:155:VAL:HG23	1.99	0.63
1:A:307:HIS:O	7:A:6164:HOH:O	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LEU:HD11	1:A:130:PHE:HA	1.80	0.62
1:A:67:LYS:HE3	1:A:71:LEU:HD21	1.82	0.62
2:B:27:GLY:HA2	2:B:31:GLU:OE1	2.00	0.62
1:A:26:GLU:O	1:A:29:ASP:HB3	2.00	0.61
2:B:47:LEU:HD22	2:B:106:LEU:HD23	1.81	0.61
1:A:141:ALA:HB3	1:A:144:SER:HB2	1.81	0.61
1:A:657:LYS:O	1:A:660:GLU:HB3	2.01	0.61
1:A:33:SER:O	1:A:37:LYS:HD3	2.01	0.61
1:A:420:HIS:NE2	4:A:3000:PG4:H51	2.16	0.61
1:A:105:VAL:O	1:A:109:ILE:HG12	2.00	0.60
1:A:448:PHE:O	1:A:452:VAL:HG23	2.01	0.60
1:A:634:ARG:HH21	1:A:634:ARG:HG2	1.64	0.60
1:A:399:TYR:HA	1:A:402:LEU:HD22	1.84	0.60
2:B:91:ARG:O	2:B:95:GLU:HG3	2.02	0.60
1:A:310:GLU:O	1:A:314:ILE:HG13	2.03	0.59
1:A:514:ASN:ND2	1:A:571:GLU:HB3	2.17	0.59
1:A:145:MET:HE3	1:A:145:MET:HA	1.83	0.59
1:A:420:HIS:CE1	4:A:3000:PG4:H42	2.37	0.59
2:B:129:ARG:HH21	5:B:1574:GOL:C3	2.16	0.59
1:A:146:VAL:HG23	1:A:184:LEU:HD11	1.85	0.59
1:A:129:ARG:HD3	1:A:179:TRP:CZ3	2.37	0.59
1:A:48:SER:O	1:A:51:GLU:HB3	2.02	0.59
1:A:490:GLU:C	1:A:492:SER:H	2.07	0.58
2:B:28:ASP:N	2:B:31:GLU:OE1	2.36	0.58
1:A:662:ALA:O	1:A:692:ILE:HD11	2.03	0.58
4:A:3000:PG4:O1	7:A:6002:HOH:O	2.14	0.58
1:A:582:GLY:O	1:A:586:VAL:HG23	2.03	0.58
1:A:490:GLU:CG	1:A:492:SER:HB2	2.32	0.58
1:A:138:HIS:HB3	1:A:265:GLN:HE21	1.68	0.58
1:A:415:ASN:HD21	1:A:455:LYS:HZ2	1.52	0.58
1:A:187:LYS:CD	1:A:188:LYS:H	2.17	0.58
1:A:150:GLU:HG2	1:A:195:ILE:HD11	1.85	0.58
1:A:485:TYR:HB2	1:A:553:HIS:CD2	2.39	0.58
2:B:10:ARG:CB	2:B:10:ARG:HH11	2.15	0.57
1:A:180:VAL:HG23	7:A:6172:HOH:O	2.03	0.57
1:A:142:ALA:HB3	1:A:143:PRO:HD3	1.87	0.57
1:A:498:HIS:CD2	1:A:502:LEU:HD11	2.39	0.57
1:A:387:LEU:HB3	1:A:388:PRO:HD3	1.86	0.57
1:A:466:LEU:HD23	1:A:477:CYS:SG	2.45	0.57
1:A:709:LEU:O	1:A:713:ILE:HG13	2.05	0.56
1:A:609:ILE:CD1	1:A:644:THR:HG23	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ASN:O	1:A:321:ILE:HG13	2.04	0.56
1:A:393:GLN:O	1:A:397:MET:HG3	2.06	0.56
5:A:1572:GOL:O2	7:A:6014:HOH:O	2.17	0.56
1:A:41:LYS:O	1:A:41:LYS:HG3	2.05	0.56
2:B:129:ARG:N	2:B:129:ARG:HD3	2.13	0.56
2:B:46:ASN:HA	2:B:135:ARG:HH12	1.71	0.56
1:A:211:VAL:O	1:A:215:GLN:HG3	2.06	0.56
1:A:759:GLN:HG2	5:A:1569:GOL:O2	2.06	0.56
1:A:490:GLU:OE1	1:A:495:LEU:HD12	2.06	0.55
1:A:659:LEU:HA	1:A:695:LEU:HD13	1.89	0.55
1:A:188:LYS:HE3	1:A:191:GLU:OE1	2.06	0.55
1:A:250:LEU:HD21	1:A:342:LYS:HA	1.89	0.55
1:A:609:ILE:HD11	1:A:619:VAL:HG21	1.87	0.55
1:A:147:ALA:O	1:A:151:ASN:ND2	2.39	0.55
1:A:153:VAL:HG21	1:A:195:ILE:CG2	2.37	0.54
1:A:151:ASN:ND2	7:A:6064:HOH:O	2.39	0.54
2:B:129:ARG:NH2	5:B:1574:GOL:C3	2.70	0.54
2:B:136:ASP:OD1	2:B:139:ARG:HD3	2.07	0.54
1:A:137:CYS:O	1:A:260:LEU:HD22	2.07	0.54
1:A:510:SER:O	1:A:511:LYS:HB2	2.06	0.54
1:A:153:VAL:O	1:A:156:THR:HG23	2.08	0.53
1:A:155:VAL:HG21	1:A:169:TYR:CD2	2.43	0.53
1:A:243:ARG:HB2	1:A:245:GLN:NE2	2.22	0.53
1:A:252:PRO:C	1:A:254:LEU:H	2.12	0.53
1:A:248:HIS:O	1:A:342:LYS:HE3	2.09	0.53
1:A:391:LEU:HG	4:A:3000:PG4:H52	1.91	0.53
1:A:480:ASN:HD22	1:A:482:THR:HG23	1.72	0.53
1:A:248:HIS:O	1:A:342:LYS:HB2	2.09	0.53
1:A:498:HIS:O	1:A:502:LEU:HG	2.09	0.52
1:A:92:LEU:H	1:A:92:LEU:CD2	2.22	0.52
1:A:488:GLY:C	1:A:490:GLU:N	2.62	0.52
1:A:486:LYS:O	1:A:490:GLU:CD	2.47	0.52
2:B:50:TYR:HB2	5:B:1568:GOL:O1	2.09	0.52
1:A:233:TRP:O	1:A:237:GLN:HG2	2.09	0.52
2:B:135:ARG:O	2:B:139:ARG:HG3	2.08	0.52
1:A:187:LYS:HG3	1:A:188:LYS:N	2.25	0.52
1:A:92:LEU:H	1:A:92:LEU:HD22	1.74	0.52
1:A:480:ASN:ND2	1:A:482:THR:HG23	2.24	0.52
1:A:38:VAL:HG23	1:A:39:GLY:N	2.25	0.52
1:A:269:PRO:HG3	7:A:6180:HOH:O	2.10	0.52
1:A:741:LYS:HE2	7:A:6049:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LYS:HG3	1:A:241:LYS:HZ2	1.73	0.51
1:A:141:ALA:O	1:A:144:SER:N	2.43	0.51
1:A:420:HIS:CD2	4:A:3000:PG4:H71	2.46	0.51
1:A:712:VAL:O	1:A:716:ARG:HG2	2.09	0.51
1:A:693:GLU:O	1:A:697:GLU:HG3	2.09	0.51
1:A:238:LYS:HB3	7:A:6164:HOH:O	2.11	0.51
2:B:39:SER:O	2:B:91:ARG:HG3	2.10	0.51
1:A:619:VAL:O	1:A:623:ILE:HG12	2.11	0.51
1:A:173:PHE:CE1	1:A:177:LEU:HD21	2.46	0.51
1:A:741:LYS:NZ	7:A:6227:HOH:O	2.45	0.50
1:A:766:GLU:HG2	7:A:6130:HOH:O	2.11	0.50
2:B:49:PHE:HE1	2:B:81:CYS:O	1.94	0.50
1:A:88:THR:HG22	1:A:92:LEU:CD2	2.41	0.50
1:A:187:LYS:CG	1:A:188:LYS:N	2.74	0.50
1:A:588:ARG:HD3	1:A:627:GLU:OE1	2.11	0.50
1:A:588:ARG:O	1:A:592:GLU:HG2	2.11	0.50
1:A:609:ILE:HD13	1:A:644:THR:HG23	1.93	0.50
1:A:657:LYS:HG3	1:A:658:GLU:N	2.24	0.50
1:A:488:GLY:O	1:A:490:GLU:N	2.27	0.50
1:A:51:GLU:O	1:A:54:ALA:HB3	2.10	0.50
1:A:711:LEU:O	1:A:715:GLN:HG3	2.11	0.50
1:A:591:PHE:HB2	1:A:622:TRP:HZ2	1.75	0.50
1:A:92:LEU:HD22	1:A:92:LEU:N	2.27	0.50
2:B:26:ARG:HG3	2:B:26:ARG:NH1	2.26	0.50
1:A:382:LEU:C	1:A:384:PRO:HD3	2.31	0.50
1:A:177:LEU:HA	1:A:181:GLY:H	1.77	0.49
1:A:468:ILE:HG13	1:A:469:VAL:N	2.26	0.49
1:A:420:HIS:NE2	4:A:3000:PG4:H42	2.27	0.49
1:A:657:LYS:CG	1:A:658:GLU:N	2.74	0.49
1:A:270:PRO:HA	7:A:6166:HOH:O	2.12	0.49
1:A:206:ARG:CZ	1:A:229:LEU:HD12	2.42	0.49
1:A:211:VAL:HB	1:A:212:PRO:HD3	1.93	0.49
1:A:88:THR:HG22	1:A:92:LEU:HD21	1.94	0.49
1:A:311:ARG:O	1:A:315:GLU:HG3	2.13	0.48
1:A:480:ASN:HD22	1:A:482:THR:CG2	2.26	0.48
2:B:123:ARG:NH1	2:B:123:ARG:HB3	2.27	0.48
1:A:742:ASN:O	1:A:746:ARG:HG2	2.13	0.48
1:A:490:GLU:HG2	1:A:492:SER:O	2.13	0.48
2:B:139:ARG:NH2	2:B:148:GLY:O	2.44	0.48
1:A:161:VAL:HB	1:A:165:ARG:HD3	1.94	0.48
1:A:129:ARG:NH2	1:A:175:SER:HB2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:LEU:O	1:A:645:ILE:HG13	2.14	0.48
1:A:251:ARG:HD3	1:A:253:TYR:OH	2.13	0.48
1:A:188:LYS:O	1:A:192:MET:HB2	2.14	0.48
1:A:129:ARG:HH21	1:A:175:SER:HB2	1.78	0.48
1:A:187:LYS:CG	1:A:188:LYS:H	2.27	0.47
1:A:742:ASN:HB2	7:A:6152:HOH:O	2.13	0.47
1:A:136:ASN:HD22	1:A:136:ASN:N	2.11	0.47
1:A:191:GLU:C	1:A:193:ASP:H	2.15	0.47
1:A:651:HIS:CE1	1:A:655:ILE:HD11	2.49	0.47
1:A:72:LEU:HA	1:A:75:VAL:HG22	1.96	0.47
1:A:257:ASP:O	1:A:261:CYS:HB2	2.14	0.47
1:A:665:LYS:HB2	1:A:688:LEU:HD21	1.93	0.47
1:A:196:PHE:HZ	1:A:244:TRP:HH2	1.63	0.47
1:A:699:VAL:HG12	1:A:703:GLN:HE21	1.79	0.47
1:A:192:MET:C	7:A:6247:HOH:O	2.53	0.47
2:B:49:PHE:CE1	2:B:81:CYS:O	2.67	0.47
1:A:195:ILE:N	7:A:6247:HOH:O	2.46	0.47
1:A:206:ARG:NH1	1:A:229:LEU:HB2	2.30	0.47
1:A:170:VAL:HG12	1:A:174:LEU:HD13	1.97	0.47
1:A:423:ASN:HA	2:B:105:ARG:HG3	1.97	0.46
1:A:753:GLN:CG	7:A:6117:HOH:O	2.62	0.46
1:A:329:ARG:HG3	1:A:378:GLU:HG3	1.97	0.46
1:A:490:GLU:O	1:A:491:SER:HB2	2.15	0.46
1:A:516:GLU:O	1:A:520:ILE:HG12	2.15	0.46
1:A:660:GLU:O	1:A:664:GLU:HG2	2.15	0.46
1:A:639:GLU:HG3	5:A:1556:GOL:C3	2.45	0.46
1:A:634:ARG:HG2	1:A:634:ARG:NH2	2.30	0.46
1:A:765:LEU:HD23	1:A:769:LEU:HD12	1.98	0.46
1:A:89:LEU:O	1:A:93:LEU:HD13	2.16	0.46
2:B:123:ARG:HH11	2:B:123:ARG:HB3	1.80	0.46
1:A:753:GLN:HG3	7:A:6117:HOH:O	2.15	0.46
1:A:61:LEU:N	1:A:62:PRO:CD	2.79	0.46
1:A:499:SER:HA	1:A:502:LEU:HD12	1.98	0.46
1:A:50:LEU:O	1:A:54:ALA:HB2	2.16	0.45
1:A:238:LYS:O	1:A:242:ASP:HB2	2.15	0.45
1:A:66:SER:C	1:A:70:ARG:HE	2.20	0.45
1:A:254:LEU:HD23	1:A:254:LEU:C	2.37	0.45
1:A:725:LEU:HD13	1:A:775:ASP:CG	2.36	0.45
1:A:90:VAL:HG12	1:A:90:VAL:O	2.16	0.45
1:A:182:LYS:HA	1:A:244:TRP:CB	2.46	0.45
1:A:148:MET:HG3	1:A:271:PHE:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:ARG:NH2	5:B:1570:GOL:O3	2.50	0.45
2:B:79:THR:HA	5:B:1571:GOL:H12	1.97	0.45
1:A:450:ARG:HG2	5:A:1572:GOL:C3	2.47	0.45
1:A:478:PRO:HA	5:A:1572:GOL:O1	2.17	0.45
1:A:88:THR:CG2	1:A:92:LEU:HD21	2.47	0.45
1:A:131:LEU:O	1:A:134:LEU:HB2	2.17	0.45
1:A:274:PRO:HA	1:A:275:PRO:HD3	1.86	0.45
1:A:81:GLU:HG2	1:A:82:LYS:HD2	1.98	0.45
1:A:273:PRO:HA	1:A:274:PRO:HD3	1.88	0.45
1:A:486:LYS:O	1:A:490:GLU:OE1	2.35	0.45
1:A:490:GLU:C	1:A:492:SER:N	2.70	0.44
1:A:507:ALA:HB1	1:A:512:ALA:HB2	1.99	0.44
1:A:771:THR:O	1:A:774:LEU:HB2	2.16	0.44
1:A:26:GLU:O	1:A:29:ASP:N	2.51	0.44
1:A:500:VAL:HG11	1:A:524:VAL:CG2	2.48	0.44
1:A:601:ILE:O	1:A:605:VAL:HG23	2.17	0.44
2:B:136:ASP:HA	2:B:139:ARG:HD3	1.98	0.44
1:A:399:TYR:O	1:A:402:LEU:HB2	2.17	0.44
1:A:248:HIS:C	1:A:342:LYS:HE3	2.38	0.44
1:A:485:TYR:HB2	1:A:553:HIS:HD2	1.81	0.44
1:A:79:LEU:HA	1:A:79:LEU:HD23	1.79	0.44
1:A:415:ASN:HD21	1:A:455:LYS:HZ3	1.64	0.44
1:A:568:LYS:HD3	1:A:569:PHE:CE1	2.52	0.44
1:A:594:TRP:CD2	1:A:600:MET:HG2	2.53	0.44
2:B:95:GLU:O	2:B:99:ARG:HG3	2.18	0.44
1:A:443:SER:HB3	7:A:6016:HOH:O	2.17	0.44
1:A:500:VAL:HG11	1:A:524:VAL:HG22	1.98	0.44
1:A:450:ARG:HG3	1:A:476:LEU:O	2.17	0.43
2:B:38:LYS:HG2	2:B:38:LYS:O	2.18	0.43
1:A:162:PRO:O	1:A:165:ARG:HB3	2.19	0.43
1:A:143:PRO:HG3	1:A:187:LYS:HG2	2.00	0.43
1:A:87:THR:HG21	1:A:133:ASP:HB3	2.00	0.43
1:A:223:HIS:HE1	1:A:293:ASP:HB3	1.84	0.43
1:A:651:HIS:NE2	1:A:655:ILE:HD11	2.34	0.43
1:A:165:ARG:HD2	1:A:282:TYR:OH	2.19	0.43
1:A:397:MET:HE3	1:A:401:ARG:NH2	2.32	0.42
1:A:770:PHE:HA	1:A:774:LEU:HD22	2.01	0.42
6:B:2137:GTG:N7B	5:B:1574:GOL:C3	2.82	0.42
1:A:103:GLU:O	1:A:106:GLU:HB2	2.19	0.42
2:B:123:ARG:NH1	6:B:2137:GTG:O3D	2.52	0.42
1:A:361:GLN:O	1:A:412:ARG:NH1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:LEU:HD21	1:A:696:GLN:HE22	1.84	0.42
1:A:124:ALA:O	1:A:127:LEU:N	2.50	0.42
1:A:134:LEU:HD12	1:A:140:ILE:HD11	2.02	0.42
1:A:623:ILE:HA	1:A:628:LEU:HD12	2.02	0.42
2:B:30:GLU:OE1	2:B:34:LYS:HE3	2.19	0.42
2:B:128:GLY:HA3	2:B:132:GLY:O	2.19	0.42
1:A:495:LEU:HA	1:A:496:PRO:HD3	1.85	0.42
1:A:505:ALA:HA	1:A:554:LEU:HD11	2.01	0.42
2:B:85:PHE:HZ	2:B:123:ARG:HH12	1.67	0.42
1:A:221:LYS:HA	1:A:222:PRO:C	2.39	0.42
1:A:55:GLY:O	1:A:58:GLU:N	2.53	0.42
1:A:32:GLU:HA	1:A:71:LEU:HD13	2.01	0.42
1:A:170:VAL:CG1	1:A:174:LEU:HD13	2.50	0.42
1:A:383:GLN:HB2	1:A:387:LEU:HB2	2.00	0.41
1:A:695:LEU:O	1:A:699:VAL:HG23	2.20	0.41
1:A:38:VAL:HG23	1:A:39:GLY:H	1.84	0.41
1:A:480:ASN:ND2	1:A:482:THR:CG2	2.83	0.41
1:A:96:ARG:O	1:A:97:ASN:HB2	2.19	0.41
1:A:241:LYS:C	1:A:241:LYS:HD3	2.40	0.41
1:A:460:SER:OG	1:A:461:TYR:N	2.53	0.41
2:B:135:ARG:HB2	7:B:2162:HOH:O	2.21	0.41
1:A:146:VAL:HG12	1:A:150:GLU:OE1	2.21	0.41
1:A:35:ILE:O	1:A:38:VAL:HG22	2.20	0.41
1:A:545:GLU:O	1:A:549:GLN:HB2	2.20	0.41
1:A:88:THR:O	1:A:91:GLY:N	2.46	0.41
2:B:7:LYS:O	2:B:9:LEU:N	2.54	0.41
1:A:236:ILE:O	1:A:239:LEU:HB3	2.21	0.41
2:B:7:LYS:CE	2:B:7:LYS:HA	2.38	0.41
1:A:170:VAL:O	1:A:174:LEU:HD13	2.20	0.41
1:A:189:ASP:HA	1:A:192:MET:HB2	2.03	0.41
1:A:391:LEU:HG	4:A:3000:PG4:C5	2.50	0.41
1:A:562:SER:O	1:A:566:LEU:HG	2.19	0.41
1:A:240:LYS:C	1:A:242:ASP:H	2.24	0.41
2:B:127:ARG:HD2	6:B:2137:GTG:O2B	2.21	0.41
1:A:462:HIS:CD2	1:A:480:ASN:HA	2.56	0.40
2:B:102:ASN:OD1	2:B:112:ARG:HA	2.21	0.40
2:B:56:ILE:HG22	2:B:69:ILE:HD13	2.03	0.40
1:A:490:GLU:OE1	1:A:495:LEU:CD1	2.70	0.40
1:A:241:LYS:HG2	1:A:241:LYS:O	2.22	0.40
1:A:97:ASN:O	1:A:98:TYR:C	2.60	0.40
1:A:131:LEU:O	1:A:132:SER:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:GLN:O	1:A:158:GLU:C	2.60	0.40
1:A:314:ILE:O	1:A:318:LEU:HG	2.20	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	726/790 (92%)	660 (91%)	60 (8%)	6 (1%)	19	14
2	B	146/156 (94%)	139 (95%)	6 (4%)	1 (1%)	22	17
All	All	872/946 (92%)	799 (92%)	66 (8%)	7 (1%)	19	14

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	LYS
2	B	8	ALA
1	A	97	ASN
1	A	249	ILE
1	A	489	ASP
1	A	181	GLY
1	A	688	LEU

### 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	672/724 (93%)	649 (97%)	23 (3%)	37	38
2	B	124/130 (95%)	115 (93%)	9 (7%)	14	10
All	All	796/854 (93%)	764 (96%)	32 (4%)	31	31

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	42	SER
1	A	70	ARG
1	A	97	ASN
1	A	117	LYS
1	A	186	GLU
1	A	188	LYS
1	A	228	TYR
1	A	241	LYS
1	A	242	ASP
1	A	251	ARG
1	A	279	ASP
1	A	293	ASP
1	A	336	LEU
1	A	387	LEU
1	A	402	LEU
1	A	431	GLU
1	A	455	LYS
1	A	464	ARG
1	A	560	SER
1	A	597	HIS
1	A	693	GLU
1	A	734	SER
2	B	7	LYS
2	B	41	THR
2	B	57	TYR
2	B	63	SER
2	B	65	ASP
2	B	81	CYS
2	B	124	GLN
2	B	129	ARG
2	B	130	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	97	ASN
1	A	120	ASN
1	A	136	ASN
1	A	245	GLN
1	A	265	GLN
1	A	367	HIS
1	A	415	ASN
1	A	425	GLN
1	A	439	GLN
1	A	462	HIS
1	A	480	ASN
1	A	498	HIS
1	A	514	ASN
1	A	553	HIS
1	A	561	HIS
1	A	596	ASN
1	A	612	GLN
1	A	649	ASN
1	A	696	GLN
1	A	703	GLN
1	A	706	GLN
1	A	753	GLN
1	A	760	GLN
2	B	29	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 for Mogul analysis.



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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
5	GOL	B	1568	-	5,5,5	4.41	5 (100%)	5,5,5	5.88	3 (60%)
5	GOL	B	1570	-	5,5,5	4.52	5 (100%)	5,5,5	5.84	3 (60%)
5	GOL	B	1558	-	5,5,5	4.47	5 (100%)	5,5,5	5.79	3 (60%)
4	PG4	A	3000	-	12,12,12	1.22	1 (8%)	11,11,11	1.70	3 (27%)
5	GOL	A	1557	-	5,5,5	4.48	5 (100%)	5,5,5	5.80	3 (60%)
6	GTG	B	2137	-	46,57,57	2.83	21 (45%)	51,90,90	3.78	21 (41%)
5	GOL	A	1569	-	5,5,5	4.49	5 (100%)	5,5,5	5.79	3 (60%)
5	GOL	A	1561	-	5,5,5	4.52	5 (100%)	5,5,5	5.78	3 (60%)
5	GOL	A	1566	-	5,5,5	4.55	5 (100%)	5,5,5	5.77	3 (60%)
5	GOL	A	1555	-	5,5,5	4.56	5 (100%)	5,5,5	5.78	3 (60%)
5	GOL	A	1565	-	5,5,5	4.55	5 (100%)	5,5,5	5.79	3 (60%)
5	GOL	A	1572	-	5,5,5	4.54	5 (100%)	5,5,5	5.84	3 (60%)
5	GOL	B	1571	-	5,5,5	4.61	5 (100%)	5,5,5	5.83	3 (60%)
5	GOL	A	1573	-	5,5,5	4.48	5 (100%)	5,5,5	5.82	3 (60%)
5	GOL	A	1560	-	5,5,5	4.49	5 (100%)	5,5,5	5.78	3 (60%)
5	GOL	A	1556	-	5,5,5	4.47	5 (100%)	5,5,5	5.83	3 (60%)
5	GOL	A	1564	-	5,5,5	4.47	5 (100%)	5,5,5	5.80	3 (60%)
5	GOL	B	1574	-	5,5,5	4.34	5 (100%)	5,5,5	5.95	3 (60%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	1568	-	-	2/4/4/4	-
5	GOL	B	1570	-	-	3/4/4/4	-
5	GOL	B	1558	-	-	2/4/4/4	-
4	PG4	A	3000	-	-	6/10/10/10	-
5	GOL	A	1557	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GTG	B	2137	-	-	11/24/64/64	0/6/6/6
5	GOL	A	1569	-	-	3/4/4/4	-
5	GOL	A	1561	-	-	3/4/4/4	-
5	GOL	A	1566	-	-	2/4/4/4	-
5	GOL	A	1555	-	-	3/4/4/4	-
5	GOL	A	1565	-	-	3/4/4/4	-
5	GOL	A	1572	-	-	3/4/4/4	-
5	GOL	B	1571	-	-	3/4/4/4	-
5	GOL	A	1573	-	-	3/4/4/4	-
5	GOL	A	1560	-	-	2/4/4/4	-
5	GOL	A	1556	-	-	2/4/4/4	-
5	GOL	A	1564	-	-	2/4/4/4	-
5	GOL	B	1574	-	-	2/4/4/4	-

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	2137	GTG	O4E-C1E	10.58	1.55	1.41
5	A	1555	GOL	C3-C2	-7.58	1.20	1.51
5	A	1566	GOL	C3-C2	-7.44	1.21	1.51
5	A	1569	GOL	C3-C2	-7.43	1.21	1.51
5	A	1565	GOL	C3-C2	-7.40	1.21	1.51
5	A	1572	GOL	C3-C2	-7.37	1.21	1.51
5	A	1561	GOL	C3-C2	-7.37	1.21	1.51
5	B	1570	GOL	C3-C2	-7.32	1.21	1.51
5	A	1560	GOL	C3-C2	-7.28	1.21	1.51
5	B	1558	GOL	C3-C2	-7.25	1.21	1.51
5	A	1573	GOL	C3-C2	-7.25	1.21	1.51
5	A	1564	GOL	C3-C2	-7.21	1.22	1.51
5	B	1571	GOL	C3-C2	-7.17	1.22	1.51
5	A	1556	GOL	C3-C2	-7.16	1.22	1.51
5	A	1557	GOL	C3-C2	-7.11	1.22	1.51
5	B	1568	GOL	C3-C2	-7.10	1.22	1.51
5	B	1574	GOL	C3-C2	-6.93	1.23	1.51
6	B	2137	GTG	O4E-C4E	5.89	1.58	1.45
5	A	1557	GOL	O1-C1	4.74	1.62	1.42
5	A	1564	GOL	O1-C1	4.66	1.62	1.42
5	A	1556	GOL	O1-C1	4.64	1.62	1.42
5	A	1565	GOL	O1-C1	4.62	1.61	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	2137	GTG	C8B-N7B	-4.62	1.26	1.34
5	B	1571	GOL	O1-C1	4.61	1.61	1.42
5	A	1566	GOL	O1-C1	4.59	1.61	1.42
5	A	1560	GOL	O1-C1	4.58	1.61	1.42
5	A	1561	GOL	O1-C1	4.53	1.61	1.42
5	A	1572	GOL	O1-C1	4.52	1.61	1.42
6	B	2137	GTG	C6A-N1A	4.50	1.40	1.33
5	B	1558	GOL	O1-C1	4.46	1.61	1.42
5	A	1555	GOL	O1-C1	4.44	1.61	1.42
6	B	2137	GTG	C2E-C1E	-4.42	1.47	1.53
5	A	1573	GOL	O1-C1	4.39	1.60	1.42
5	B	1570	GOL	O1-C1	4.36	1.60	1.42
5	B	1568	GOL	O1-C1	4.32	1.60	1.42
5	A	1569	GOL	O1-C1	4.30	1.60	1.42
6	B	2137	GTG	C6B-N1B	4.20	1.40	1.33
6	B	2137	GTG	C5E-C4E	-4.20	1.38	1.51
5	B	1574	GOL	O1-C1	4.12	1.59	1.42
6	B	2137	GTG	PG-O5E	4.12	1.76	1.59
5	A	1557	GOL	O3-C3	3.66	1.57	1.42
5	B	1574	GOL	O3-C3	3.62	1.57	1.42
5	A	1556	GOL	O3-C3	3.57	1.57	1.42
5	B	1568	GOL	O3-C3	3.54	1.57	1.42
5	B	1571	GOL	O3-C3	3.48	1.57	1.42
5	A	1565	GOL	O3-C3	3.47	1.57	1.42
5	A	1564	GOL	O3-C3	3.47	1.57	1.42
5	A	1573	GOL	O3-C3	3.46	1.57	1.42
5	B	1571	GOL	C1-C2	-3.46	1.37	1.51
5	A	1560	GOL	O3-C3	3.46	1.57	1.42
5	B	1558	GOL	O3-C3	3.45	1.57	1.42
5	A	1561	GOL	O3-C3	3.43	1.56	1.42
5	A	1566	GOL	O3-C3	3.39	1.56	1.42
5	A	1572	GOL	O3-C3	3.30	1.56	1.42
6	B	2137	GTG	O3E-C3E	-3.29	1.35	1.43
5	B	1570	GOL	O3-C3	3.28	1.56	1.42
5	A	1555	GOL	O3-C3	3.24	1.56	1.42
5	A	1569	GOL	O3-C3	3.20	1.55	1.42
5	B	1570	GOL	C1-C2	-3.17	1.38	1.51
5	B	1574	GOL	C1-C2	-3.17	1.38	1.51
5	A	1572	GOL	O2-C2	-3.13	1.34	1.43
5	B	1571	GOL	O2-C2	-3.08	1.34	1.43
5	A	1573	GOL	C1-C2	-2.97	1.39	1.51
5	A	1569	GOL	C1-C2	-2.96	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1570	GOL	O2-C2	-2.95	1.34	1.43
6	B	2137	GTG	C3E-C4E	2.90	1.60	1.53
6	B	2137	GTG	C2D-C1D	-2.90	1.49	1.53
5	A	1555	GOL	C1-C2	-2.90	1.39	1.51
5	B	1558	GOL	C1-C2	-2.86	1.40	1.51
5	A	1561	GOL	C1-C2	-2.85	1.40	1.51
5	A	1569	GOL	O2-C2	-2.84	1.34	1.43
5	B	1568	GOL	O2-C2	-2.84	1.34	1.43
5	A	1565	GOL	O2-C2	-2.83	1.34	1.43
5	A	1566	GOL	C1-C2	-2.80	1.40	1.51
5	A	1566	GOL	O2-C2	-2.79	1.35	1.43
5	A	1555	GOL	O2-C2	-2.78	1.35	1.43
5	A	1572	GOL	C1-C2	-2.78	1.40	1.51
5	A	1560	GOL	O2-C2	-2.77	1.35	1.43
5	A	1561	GOL	O2-C2	-2.76	1.35	1.43
5	B	1568	GOL	C1-C2	-2.76	1.40	1.51
5	A	1573	GOL	O2-C2	-2.74	1.35	1.43
5	A	1565	GOL	C1-C2	-2.74	1.40	1.51
6	B	2137	GTG	O5E-C5E	-2.74	1.34	1.44
5	A	1556	GOL	O2-C2	-2.72	1.35	1.43
5	B	1558	GOL	O2-C2	-2.71	1.35	1.43
5	A	1564	GOL	C1-C2	-2.68	1.40	1.51
5	A	1560	GOL	C1-C2	-2.68	1.40	1.51
5	A	1557	GOL	O2-C2	-2.68	1.35	1.43
5	A	1564	GOL	O2-C2	-2.67	1.35	1.43
5	A	1556	GOL	C1-C2	-2.66	1.40	1.51
6	B	2137	GTG	C2B-N1B	2.58	1.40	1.35
5	A	1557	GOL	C1-C2	-2.58	1.41	1.51
6	B	2137	GTG	PA-O5D	2.56	1.69	1.59
6	B	2137	GTG	O4D-C1D	2.46	1.44	1.41
6	B	2137	GTG	C8A-N9A	2.43	1.37	1.33
5	B	1574	GOL	O2-C2	-2.42	1.36	1.43
6	B	2137	GTG	C2A-N1A	2.37	1.39	1.35
6	B	2137	GTG	C6B-C5B	2.27	1.45	1.41
6	B	2137	GTG	PB-O1B	-2.24	1.43	1.50
6	B	2137	GTG	C4B-N3B	2.23	1.39	1.35
6	B	2137	GTG	C4A-N3A	2.21	1.39	1.35
4	A	3000	PG4	C7-C8	-2.07	1.38	1.49

All (72) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1574	GOL	O3-C3-C2	11.11	163.48	110.20
5	A	1572	GOL	O3-C3-C2	10.78	161.91	110.20
5	B	1568	GOL	O3-C3-C2	10.70	161.53	110.20
5	B	1570	GOL	O3-C3-C2	10.67	161.37	110.20
5	A	1555	GOL	O3-C3-C2	10.64	161.19	110.20
5	A	1556	GOL	O3-C3-C2	10.62	161.14	110.20
5	A	1573	GOL	O3-C3-C2	10.60	161.03	110.20
5	A	1569	GOL	O3-C3-C2	10.57	160.90	110.20
5	B	1558	GOL	O3-C3-C2	10.54	160.72	110.20
5	A	1557	GOL	O3-C3-C2	10.53	160.67	110.20
5	A	1564	GOL	O3-C3-C2	10.52	160.62	110.20
5	A	1565	GOL	O3-C3-C2	10.51	160.58	110.20
5	A	1560	GOL	O3-C3-C2	10.48	160.46	110.20
5	A	1566	GOL	O3-C3-C2	10.47	160.39	110.20
5	A	1561	GOL	O3-C3-C2	10.44	160.27	110.20
5	B	1571	GOL	O3-C3-C2	10.43	160.19	110.20
6	B	2137	GTG	C5E-C4E-C3E	-10.27	76.70	115.18
6	B	2137	GTG	C5B-C6B-N1B	-8.44	111.88	123.43
6	B	2137	GTG	C5A-C6A-N1A	-7.51	113.15	123.43
6	B	2137	GTG	C2E-C3E-C4E	7.26	116.74	102.64
6	B	2137	GTG	O5E-C5E-C4E	7.24	133.93	108.99
5	B	1571	GOL	O2-C2-C3	7.10	140.38	109.12
5	A	1573	GOL	O2-C2-C3	6.91	139.54	109.12
5	B	1570	GOL	O2-C2-C3	6.85	139.29	109.12
5	A	1569	GOL	O2-C2-C3	6.82	139.18	109.12
5	A	1561	GOL	O2-C2-C3	6.82	139.16	109.12
5	A	1557	GOL	O2-C2-C3	6.80	139.09	109.12
5	B	1558	GOL	O2-C2-C3	6.77	138.93	109.12
5	A	1564	GOL	O2-C2-C3	6.77	138.93	109.12
5	A	1565	GOL	O2-C2-C3	6.77	138.93	109.12
5	A	1566	GOL	O2-C2-C3	6.76	138.88	109.12
5	A	1560	GOL	O2-C2-C3	6.75	138.86	109.12
5	B	1568	GOL	O2-C2-C3	6.74	138.81	109.12
5	B	1574	GOL	O2-C2-C3	6.72	138.72	109.12
5	A	1556	GOL	O2-C2-C3	6.72	138.70	109.12
5	A	1555	GOL	O2-C2-C3	6.66	138.44	109.12
5	A	1572	GOL	O2-C2-C3	6.64	138.35	109.12
6	B	2137	GTG	PG-O5E-C5E	6.50	159.80	121.68
6	B	2137	GTG	C6B-N1B-C2B	6.44	126.16	115.93
6	B	2137	GTG	C6A-N1A-C2A	6.17	125.74	115.93
6	B	2137	GTG	O4E-C4E-C3E	-5.93	93.38	105.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	2137	GTG	O2A-PA-O5D	-5.34	82.93	107.75
6	B	2137	GTG	O5E-PG-O1G	-5.18	88.84	109.07
6	B	2137	GTG	O5D-PA-O1A	-4.98	89.60	109.07
6	B	2137	GTG	N3A-C2A-N1A	-4.70	120.95	127.22
6	B	2137	GTG	C3E-C2E-C1E	4.64	107.97	100.98
6	B	2137	GTG	N3B-C2B-N1B	-4.40	121.36	127.22
5	B	1568	GOL	O1-C1-C2	3.53	127.13	110.20
5	A	1564	GOL	O1-C1-C2	3.36	126.31	110.20
5	A	1556	GOL	O1-C1-C2	3.36	126.29	110.20
6	B	2137	GTG	O2G-PG-O5E	-3.33	92.26	107.75
5	A	1561	GOL	O1-C1-C2	3.33	126.15	110.20
5	A	1560	GOL	O1-C1-C2	3.31	126.09	110.20
5	A	1566	GOL	O1-C1-C2	3.30	126.02	110.20
5	A	1557	GOL	O1-C1-C2	3.28	125.95	110.20
5	A	1565	GOL	O1-C1-C2	3.28	125.93	110.20
5	B	1571	GOL	O1-C1-C2	3.28	125.91	110.20
5	B	1558	GOL	O1-C1-C2	3.22	125.64	110.20
5	A	1572	GOL	O1-C1-C2	3.11	125.13	110.20
5	A	1555	GOL	O1-C1-C2	3.07	124.90	110.20
5	B	1570	GOL	O1-C1-C2	3.02	124.69	110.20
6	B	2137	GTG	O5D-C5D-C4D	3.01	119.36	108.99
5	A	1569	GOL	O1-C1-C2	2.97	124.45	110.20
5	A	1573	GOL	O1-C1-C2	2.95	124.36	110.20
5	B	1574	GOL	O1-C1-C2	2.85	123.86	110.20
4	A	3000	PG4	O3-C5-C6	2.69	122.53	110.39
4	A	3000	PG4	O4-C6-C5	2.66	122.38	110.39
4	A	3000	PG4	O4-C7-C8	2.63	121.61	110.07
6	B	2137	GTG	C2D-C3D-C4D	2.57	107.64	102.64
6	B	2137	GTG	C6A-C5A-C4A	-2.50	118.41	120.80
6	B	2137	GTG	N2A-C2A-N3A	2.12	121.25	117.79
6	B	2137	GTG	C3D-C2D-C1D	2.05	104.06	100.98

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1568	GOL	O1-C1-C2-O2
5	B	1568	GOL	C1-C2-C3-O3
5	B	1570	GOL	C1-C2-C3-O3
5	B	1558	GOL	C1-C2-C3-O3
5	B	1571	GOL	O1-C1-C2-C3
5	B	1571	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	A	1557	GOL	C1-C2-C3-O3
6	B	2137	GTG	C5D-O5D-PA-O1A
6	B	2137	GTG	C5D-O5D-PA-O2A
6	B	2137	GTG	C5E-O5E-PG-O3B
6	B	2137	GTG	C5E-O5E-PG-O1G
6	B	2137	GTG	C5E-O5E-PG-O2G
6	B	2137	GTG	C4E-C5E-O5E-PG
5	A	1561	GOL	O1-C1-C2-C3
5	A	1561	GOL	C1-C2-C3-O3
5	A	1566	GOL	C1-C2-C3-O3
5	A	1565	GOL	O1-C1-C2-C3
5	A	1565	GOL	C1-C2-C3-O3
5	A	1572	GOL	O1-C1-C2-C3
5	A	1572	GOL	C1-C2-C3-O3
5	A	1555	GOL	C1-C2-C3-O3
5	A	1569	GOL	O1-C1-C2-C3
5	A	1569	GOL	C1-C2-C3-O3
5	A	1573	GOL	C1-C2-C3-O3
5	A	1560	GOL	O1-C1-C2-C3
5	A	1560	GOL	C1-C2-C3-O3
5	A	1556	GOL	O1-C1-C2-C3
5	A	1556	GOL	C1-C2-C3-O3
5	A	1564	GOL	O1-C1-C2-C3
5	A	1564	GOL	C1-C2-C3-O3
5	B	1574	GOL	C1-C2-C3-O3
4	A	3000	PG4	O4-C7-C8-O5
5	A	1566	GOL	O1-C1-C2-O2
6	B	2137	GTG	O4D-C4D-C5D-O5D
6	B	2137	GTG	C3D-C4D-C5D-O5D
4	A	3000	PG4	O3-C5-C6-O4
5	B	1558	GOL	O1-C1-C2-O2
5	A	1557	GOL	O1-C1-C2-O2
5	B	1574	GOL	O1-C1-C2-O2
5	B	1571	GOL	O1-C1-C2-O2
5	A	1565	GOL	O1-C1-C2-O2
5	A	1555	GOL	O1-C1-C2-O2
5	A	1569	GOL	O1-C1-C2-O2
6	B	2137	GTG	PB-O3B-PG-O5E
5	B	1570	GOL	O1-C1-C2-O2
5	A	1572	GOL	O1-C1-C2-O2
5	A	1573	GOL	O1-C1-C2-O2
5	A	1555	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	A	3000	PG4	C3-C4-O3-C5
6	B	2137	GTG	C3E-C4E-C5E-O5E
4	A	3000	PG4	C6-C5-O3-C4
4	A	3000	PG4	C8-C7-O4-C6
5	B	1570	GOL	O1-C1-C2-C3
5	A	1573	GOL	O1-C1-C2-C3
4	A	3000	PG4	C5-C6-O4-C7
6	B	2137	GTG	C5D-O5D-PA-O3A
5	A	1561	GOL	O1-C1-C2-O2

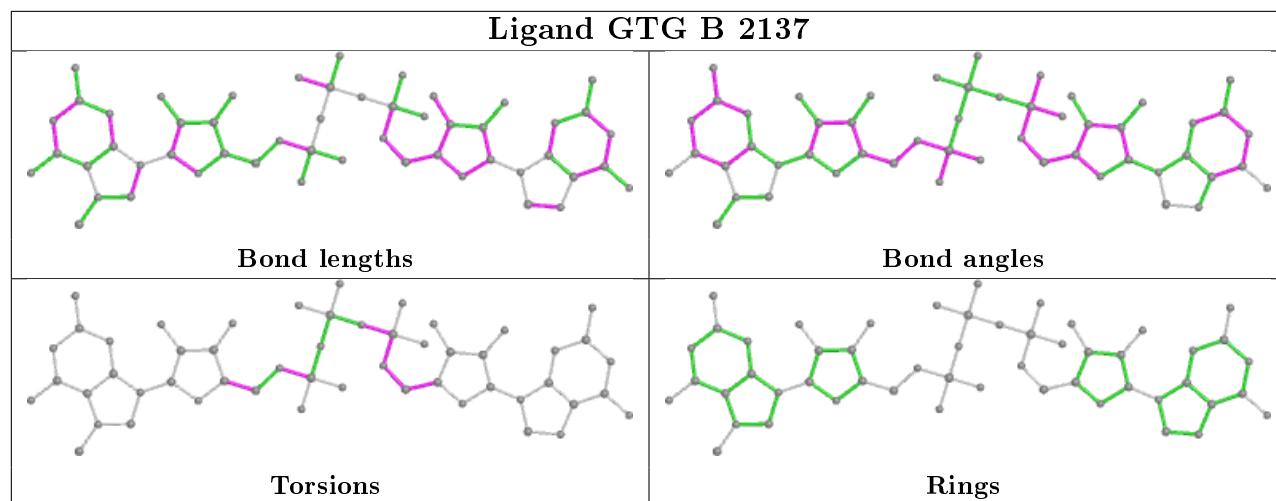
There are no ring outliers.

10 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1568	GOL	2	0
5	B	1570	GOL	2	0
4	A	3000	PG4	7	0
6	B	2137	GTG	3	0
5	A	1569	GOL	1	0
5	A	1572	GOL	3	0
5	B	1571	GOL	4	0
5	A	1556	GOL	1	0
5	A	1564	GOL	1	0
5	B	1574	GOL	5	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	732/790 (92%)	0.55	60 (8%) 11 14	25, 48, 74, 90	0
2	B	148/156 (94%)	0.27	6 (4%) 37 43	28, 42, 63, 73	0
All	All	880/946 (93%)	0.50	66 (7%) 14 18	25, 47, 73, 90	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	664	GLU	5.0
1	A	271	PHE	5.0
1	A	29	ASP	4.8
1	A	519	SER	4.6
2	B	6	LEU	4.5
2	B	138	TYR	3.8
1	A	489	ASP	3.8
1	A	270	PRO	3.8
1	A	491	SER	3.5
2	B	152	LEU	3.4
1	A	44	CYS	3.4
1	A	185	TYR	3.3
1	A	343	ASN	3.3
1	A	521	LEU	3.3
1	A	490	GLU	3.2
1	A	138	HIS	3.2
1	A	663	LYS	3.1
1	A	660	GLU	3.0
1	A	245	GLN	3.0
2	B	76	MET	2.9
1	A	272	THR	2.8
1	A	256	PHE	2.7
1	A	264	LEU	2.7
1	A	662	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	514	ASN	2.7
1	A	526	ASN	2.7
1	A	184	LEU	2.7
1	A	524	VAL	2.6
1	A	30	HIS	2.6
1	A	540	ASN	2.6
2	B	10	ARG	2.5
1	A	27	THR	2.5
1	A	730	THR	2.5
1	A	373	THR	2.4
1	A	42	SER	2.4
1	A	496	PRO	2.4
1	A	510	SER	2.4
1	A	342	LYS	2.3
1	A	194	ARG	2.3
1	A	254	LEU	2.3
1	A	26	GLU	2.3
1	A	159	GLU	2.3
1	A	32	GLU	2.3
1	A	688	LEU	2.2
1	A	518	PHE	2.2
1	A	581	GLU	2.2
1	A	268	LEU	2.2
1	A	522	LYS	2.2
1	A	135	VAL	2.2
1	A	370	VAL	2.2
1	A	689	GLU	2.1
1	A	34	LEU	2.1
1	A	452	VAL	2.1
1	A	355	ILE	2.1
2	B	128	GLY	2.1
1	A	117	LYS	2.1
1	A	47	GLU	2.1
1	A	539	PHE	2.1
1	A	493	ASN	2.1
1	A	659	LEU	2.1
1	A	365	PRO	2.0
1	A	247	ARG	2.0
1	A	569	PHE	2.0
1	A	523	ASP	2.0
1	A	64	TYR	2.0
1	A	497	GLY	2.0



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

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

## 6.3 Carbohydrates [i](#)

There are no 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. 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.

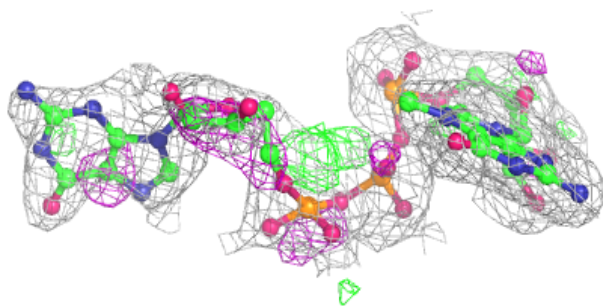
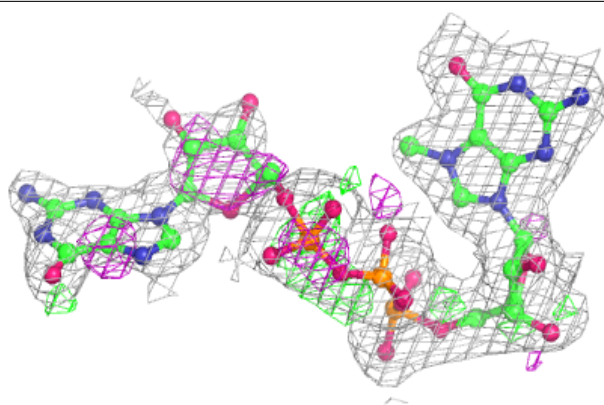
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	A	1560	6/6	0.56	0.23	76,76,76,77	0
5	GOL	A	1564	6/6	0.61	0.36	72,73,74,74	0
5	GOL	A	1556	6/6	0.67	0.36	71,74,74,75	0
5	GOL	A	1572	6/6	0.68	0.24	62,64,65,65	0
5	GOL	A	1557	6/6	0.71	0.18	57,61,62,62	0
5	GOL	A	1565	6/6	0.71	0.22	74,76,76,77	0
5	GOL	B	1568	6/6	0.77	0.16	59,60,61,62	0
4	PG4	A	3000	13/13	0.77	0.27	49,52,55,55	0
5	GOL	A	1566	6/6	0.78	0.20	83,84,84,86	0
5	GOL	A	1561	6/6	0.78	0.31	81,82,82,83	0
5	GOL	B	1558	6/6	0.80	0.23	67,69,70,71	0
5	GOL	A	1573	6/6	0.81	0.17	67,67,68,68	0
5	GOL	A	1569	6/6	0.82	0.22	68,68,69,69	0
5	GOL	B	1571	6/6	0.84	0.13	49,51,52,54	0
5	GOL	A	1555	6/6	0.86	0.22	51,54,55,56	0
5	GOL	B	1574	6/6	0.89	0.28	59,61,61,62	0
5	GOL	B	1570	6/6	0.90	0.27	55,61,63,68	0
6	GTG	B	2137	52/52	0.91	0.18	30,55,78,79	0
3	MG	A	6000	1/1	0.97	0.06	32,32,32,32	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 GTG B 2137:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.