



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:51 am GMT

PDB ID : 3OBA  
Title : Structure of the beta-galactosidase from Kluyveromyces lactis  
Authors : Fernandez-Leiro, R.; Pereira-Rodriguez, A.; Becerra, M.; Gonzalez-Siso, I.; Cerdan, M.E.; Sanz-Aparicio, J.  
Deposited on : 2010-08-06  
Resolution : 2.75 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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

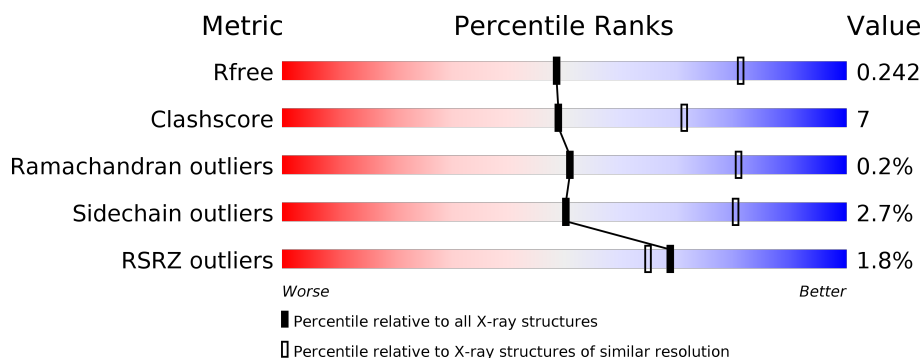
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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))
$R_{free}$	100719	3666 (2.80-2.72)
Clashscore	112137	4174 (2.80-2.72)
Ramachandran outliers	110173	4103 (2.80-2.72)
Sidechain outliers	110143	4106 (2.80-2.72)
RSRZ outliers	101464	3697 (2.80-2.72)

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. 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	1032	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 12%, green 86%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>86%</span> <span>12% ..</span> </div> </div>
1	B	1032	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 13%, green 85%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>85%</span> <span>13% ..</span> </div> </div>
1	C	1032	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 14%, green 84%, grey 14%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>84%</span> <span>14% ..</span> </div> </div>
1	D	1032	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 3%, yellow 13%, green 85%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>85%</span> <span>13% ..</span> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	1027	-	-	X	-
3	GOL	C	1026	-	-	X	X
3	GOL	D	1026	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 35030 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 Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1024	Total	C	N	O	S	0	0	0
			8325	5335	1388	1587	15			
1	C	1024	Total	C	N	O	S	0	0	0
			8325	5335	1388	1587	15			
1	D	1024	Total	C	N	O	S	0	0	0
			8325	5335	1388	1587	15			
1	B	1024	Total	C	N	O	S	0	0	0
			8325	5335	1388	1587	15			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ASP	-	EXPRESSION TAG	UNP P00723
A	-5	TYR	-	EXPRESSION TAG	UNP P00723
A	-4	LYS	-	EXPRESSION TAG	UNP P00723
A	-3	ASP	-	EXPRESSION TAG	UNP P00723
A	-2	ASP	-	EXPRESSION TAG	UNP P00723
A	-1	ASP	-	EXPRESSION TAG	UNP P00723
A	0	ASP	-	EXPRESSION TAG	UNP P00723
A	1	LYS	-	EXPRESSION TAG	UNP P00723
C	-6	ASP	-	EXPRESSION TAG	UNP P00723
C	-5	TYR	-	EXPRESSION TAG	UNP P00723
C	-4	LYS	-	EXPRESSION TAG	UNP P00723
C	-3	ASP	-	EXPRESSION TAG	UNP P00723
C	-2	ASP	-	EXPRESSION TAG	UNP P00723
C	-1	ASP	-	EXPRESSION TAG	UNP P00723
C	0	ASP	-	EXPRESSION TAG	UNP P00723
C	1	LYS	-	EXPRESSION TAG	UNP P00723
D	-6	ASP	-	EXPRESSION TAG	UNP P00723
D	-5	TYR	-	EXPRESSION TAG	UNP P00723
D	-4	LYS	-	EXPRESSION TAG	UNP P00723
D	-3	ASP	-	EXPRESSION TAG	UNP P00723
D	-2	ASP	-	EXPRESSION TAG	UNP P00723

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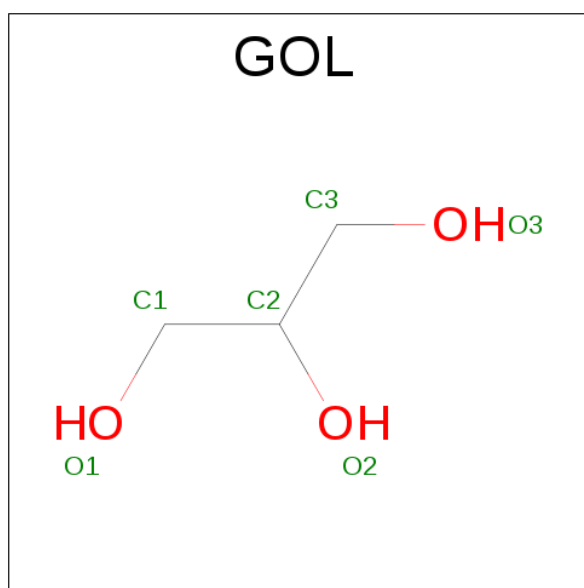
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	ASP	-	EXPRESSION TAG	UNP P00723
D	0	ASP	-	EXPRESSION TAG	UNP P00723
D	1	LYS	-	EXPRESSION TAG	UNP P00723
B	-6	ASP	-	EXPRESSION TAG	UNP P00723
B	-5	TYR	-	EXPRESSION TAG	UNP P00723
B	-4	LYS	-	EXPRESSION TAG	UNP P00723
B	-3	ASP	-	EXPRESSION TAG	UNP P00723
B	-2	ASP	-	EXPRESSION TAG	UNP P00723
B	-1	ASP	-	EXPRESSION TAG	UNP P00723
B	0	ASP	-	EXPRESSION TAG	UNP P00723
B	1	LYS	-	EXPRESSION TAG	UNP P00723

- Molecule 2 is MANGANESE (III) ION (three-letter code: MN3) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mn 1 1	0	0
2	A	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

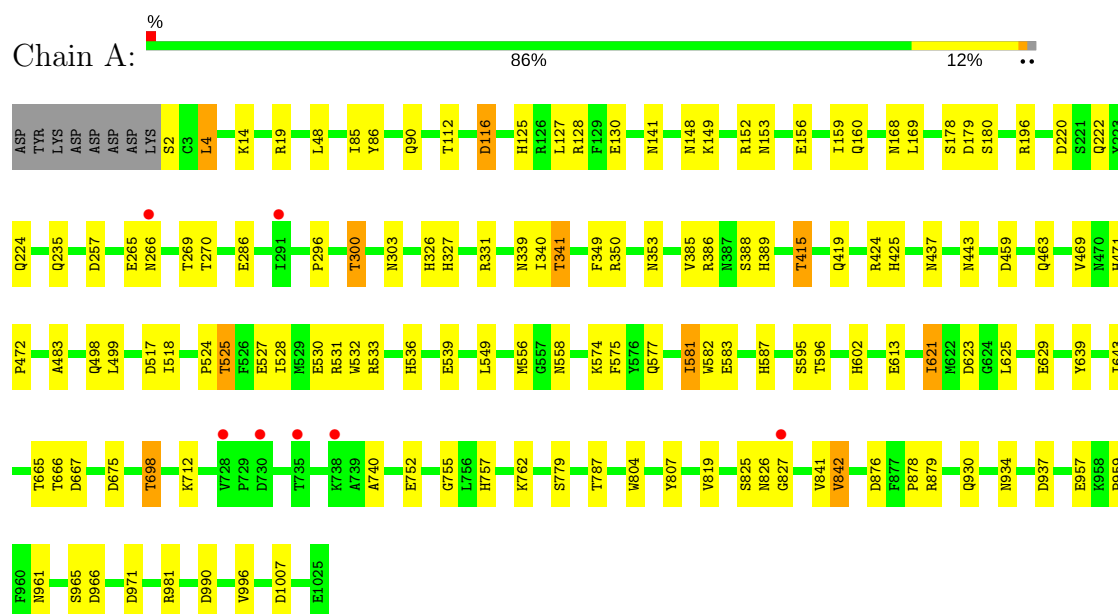
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	426	Total O 426 426	0	0
4	C	436	Total O 436 436	0	0
4	D	396	Total O 396 396	0	0
4	B	408	Total O 408 408	0	0

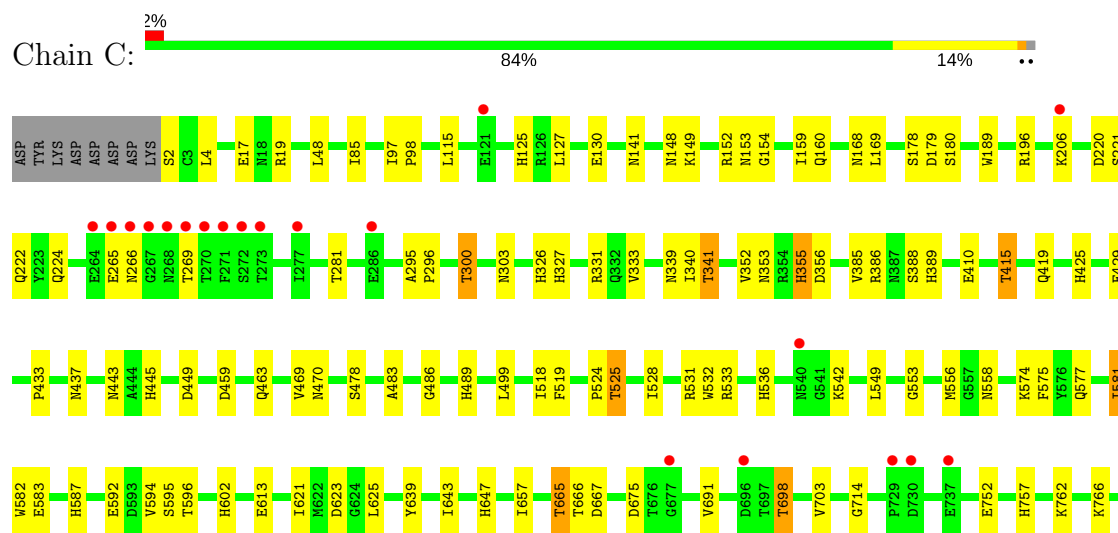
### 3 Residue-property plots

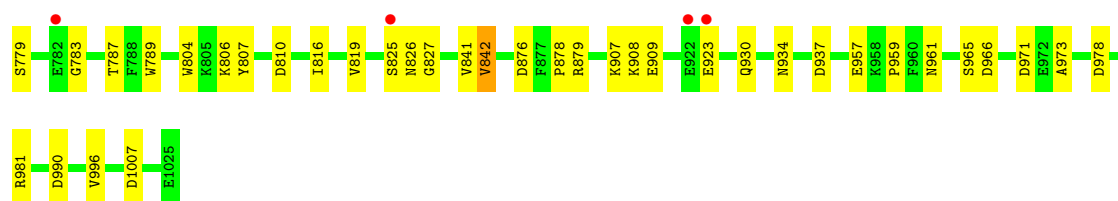
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

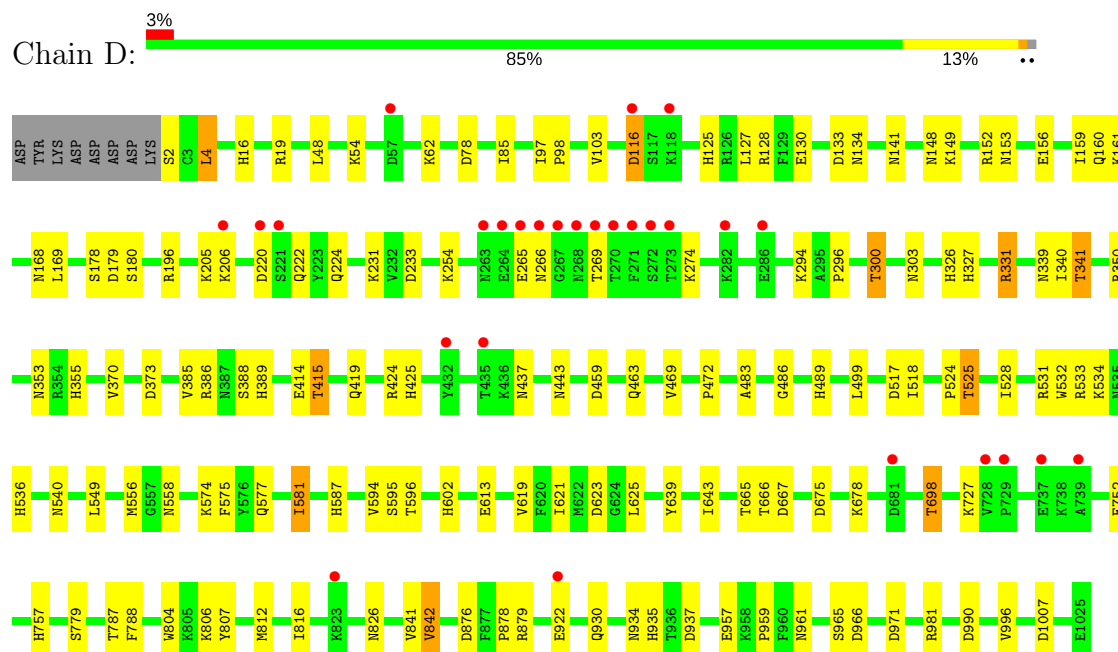


#### • Molecule 1: Beta-galactosidase

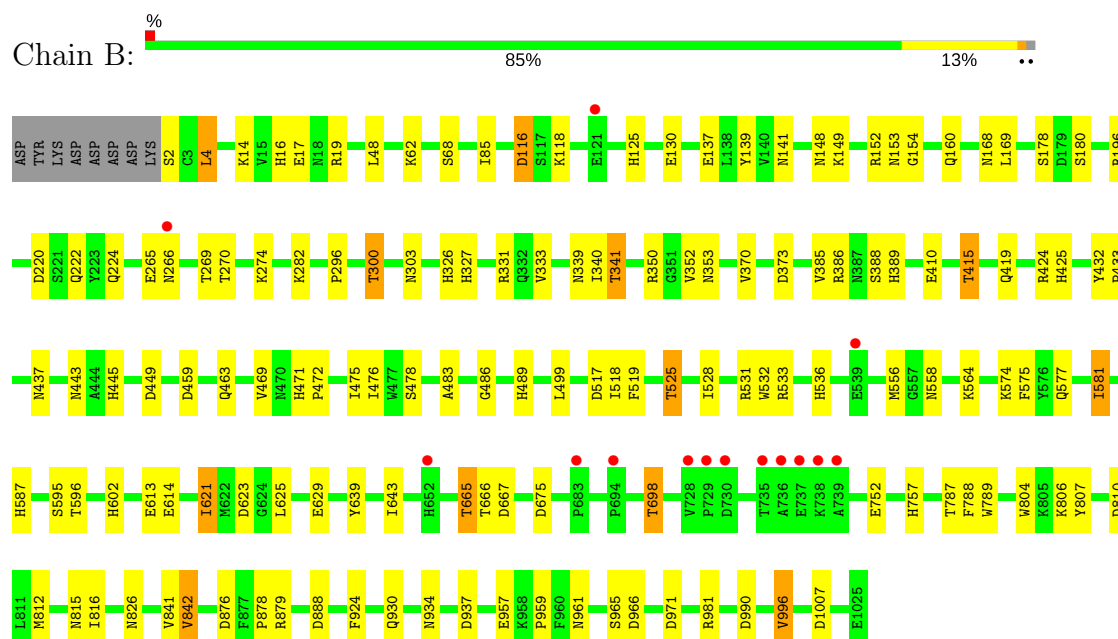




• Molecule 1: Beta-galactosidase



• Molecule 1: Beta-galactosidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.03Å 153.34Å 216.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.57 – 2.75 62.53 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (62.57-2.75) 99.9 (62.53-2.75)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.22 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.207 , 0.243 0.206 , 0.242	Depositor DCC
$R_{free}$ test set	6092 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.0	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 25.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	35030	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% 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, MN3

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	0.43	1/8561 (0.0%)	0.55	0/11614
1	B	0.41	0/8561	0.55	0/11614
1	C	0.42	0/8561	0.56	0/11614
1	D	0.42	0/8561	0.56	0/11614
All	All	0.42	1/34244 (0.0%)	0.55	0/46456

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	349	PHE	CD1-CE1	-5.03	1.29	1.39

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	8325	0	7972	103	0
1	B	8325	0	7972	110	0
1	C	8325	0	7972	128	0
1	D	8325	0	7972	123	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	12	0	16	0	0
3	B	12	0	14	4	0
3	C	24	0	32	11	0
3	D	12	0	16	0	0
4	A	426	0	0	13	0
4	B	408	0	0	16	0
4	C	436	0	0	28	0
4	D	396	0	0	27	0
All	All	35030	0	31966	441	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 (441) 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:C:356:ASP:O	3:C:1026:GOL:H11	1.36	1.26
1:B:265:GLU:HB3	1:B:266:ASN:HB2	1.30	1.09
1:A:265:GLU:HB3	1:A:266:ASN:HB2	1.35	1.05
1:C:265:GLU:HB3	1:C:266:ASN:HB2	1.34	1.04
1:D:265:GLU:HB3	1:D:266:ASN:HB2	1.37	1.04
1:C:340:ILE:H	1:C:577:GLN:HE22	1.07	1.00
1:D:665:THR:HG22	1:D:667:ASP:H	1.27	1.00
1:A:340:ILE:H	1:A:577:GLN:HE22	1.10	1.00
1:B:665:THR:HG22	1:B:667:ASP:H	1.28	0.98
1:C:665:THR:HG22	1:C:667:ASP:H	1.28	0.98
1:A:665:THR:HG22	1:A:667:ASP:H	1.28	0.94
1:B:14:LYS:HE2	4:B:1186:HOH:O	1.68	0.94
1:B:340:ILE:H	1:B:577:GLN:HE22	1.05	0.94
1:D:103:VAL:HB	3:B:1027:GOL:H32	1.50	0.93
1:D:340:ILE:H	1:D:577:GLN:HE22	1.11	0.91
1:A:116:ASP:HB2	1:B:270:THR:HG21	1.53	0.90
1:C:221:SER:HB2	4:C:1048:HOH:O	1.74	0.87
1:D:254:LYS:HE3	4:D:1065:HOH:O	1.76	0.84
1:C:356:ASP:O	3:C:1026:GOL:C1	2.25	0.82
1:C:19:ARG:HH11	1:C:148:ASN:ND2	1.76	0.82
1:A:581:ILE:HD11	1:A:625:LEU:HG	1.63	0.81
1:B:19:ARG:HH11	1:B:148:ASN:ND2	1.79	0.80
1:D:19:ARG:HH11	1:D:148:ASN:ND2	1.78	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:LYS:HE3	4:D:1605:HOH:O	1.81	0.79
1:A:19:ARG:HH11	1:A:148:ASN:ND2	1.82	0.78
1:B:340:ILE:N	1:B:577:GLN:HE22	1.81	0.77
1:D:54:LYS:HD2	4:D:1064:HOH:O	1.85	0.76
1:A:116:ASP:HB2	1:B:270:THR:CG2	2.15	0.76
1:D:581:ILE:HD11	1:D:625:LEU:HG	1.68	0.75
1:A:525:THR:HB	1:A:528:ILE:HD12	1.67	0.75
1:A:787:THR:OG1	1:A:879:ARG:NH2	2.20	0.75
1:C:879:ARG:NH1	1:C:990:ASP:OD1	2.20	0.74
1:C:787:THR:OG1	1:C:879:ARG:NH2	2.20	0.74
1:A:879:ARG:NH1	1:A:990:ASP:OD1	2.21	0.74
1:D:787:THR:OG1	1:D:879:ARG:NH2	2.20	0.74
1:A:340:ILE:N	1:A:577:GLN:HE22	1.86	0.73
1:D:525:THR:HG21	4:D:1069:HOH:O	1.87	0.73
1:B:525:THR:HB	1:B:528:ILE:HD12	1.70	0.73
1:D:340:ILE:N	1:D:577:GLN:HE22	1.86	0.73
1:B:787:THR:OG1	1:B:879:ARG:NH2	2.23	0.72
1:C:581:ILE:HD11	1:C:625:LEU:HG	1.70	0.72
1:B:581:ILE:HD11	1:B:625:LEU:HG	1.70	0.72
1:C:525:THR:HB	1:C:528:ILE:HD12	1.72	0.71
1:D:879:ARG:NH1	1:D:990:ASP:OD1	2.25	0.70
1:C:536:HIS:HE1	4:C:1082:HOH:O	1.74	0.70
1:B:300:THR:HG22	1:B:303:ASN:H	1.55	0.69
1:C:691:VAL:HB	4:C:1347:HOH:O	1.92	0.69
1:C:340:ILE:N	1:C:577:GLN:HE22	1.84	0.69
1:D:533:ARG:HG3	1:D:575:PHE:CD2	2.28	0.69
1:C:153:ASN:HB3	1:C:463:GLN:HG2	1.74	0.69
1:C:594:VAL:HG22	4:C:1136:HOH:O	1.92	0.69
1:A:265:GLU:CB	1:A:266:ASN:HB2	2.18	0.69
1:B:265:GLU:CB	1:B:266:ASN:HB2	2.15	0.69
1:D:153:ASN:HB3	1:D:463:GLN:HG2	1.74	0.69
1:A:300:THR:HG22	1:A:303:ASN:H	1.58	0.69
1:C:533:ARG:HG3	1:C:575:PHE:CD2	2.28	0.69
1:A:14:LYS:HE3	4:A:1295:HOH:O	1.91	0.69
1:C:265:GLU:CB	1:C:266:ASN:HB2	2.18	0.69
1:D:265:GLU:CB	1:D:266:ASN:HB2	2.20	0.68
1:C:281:THR:HG22	4:C:1296:HOH:O	1.92	0.68
1:D:300:THR:HG22	1:D:303:ASN:H	1.57	0.68
1:D:274:LYS:HA	4:D:1186:HOH:O	1.93	0.68
1:A:153:ASN:HB3	1:A:463:GLN:HG2	1.75	0.68
1:C:281:THR:CG2	4:C:1296:HOH:O	2.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:ARG:HG3	1:A:575:PHE:CD2	2.28	0.68
1:B:153:ASN:HB3	1:B:463:GLN:HG2	1.76	0.68
1:C:300:THR:HG22	1:C:303:ASN:H	1.59	0.67
1:D:525:THR:HB	1:D:528:ILE:HD12	1.75	0.67
1:B:533:ARG:HG3	1:B:575:PHE:CD2	2.30	0.67
1:D:54:LYS:CD	4:D:1064:HOH:O	2.41	0.67
1:D:265:GLU:HG3	4:D:1116:HOH:O	1.94	0.66
1:A:270:THR:HG21	1:B:116:ASP:HB2	1.78	0.66
1:B:341:THR:HG22	4:B:1045:HOH:O	1.95	0.66
1:C:594:VAL:HG21	4:B:1209:HOH:O	1.96	0.65
1:B:879:ARG:NH1	1:B:990:ASP:OD1	2.30	0.65
1:C:189:TRP:HD1	3:C:1026:GOL:H32	1.60	0.64
1:D:415:THR:HB	1:D:483:ALA:HA	1.78	0.64
1:D:540:ASN:HA	4:D:1159:HOH:O	1.97	0.64
1:D:525:THR:HG22	1:D:528:ILE:H	1.62	0.64
1:D:161:LYS:HE2	4:D:1089:HOH:O	1.98	0.64
1:D:4:LEU:HD13	1:B:816:ILE:HG22	1.79	0.63
1:A:178:SER:OG	1:A:180:SER:HB3	1.99	0.63
1:A:675:ASP:OD2	1:A:698:THR:HB	1.99	0.63
1:C:909:GLU:H	3:C:1028:GOL:H11	1.63	0.63
1:A:415:THR:HB	1:A:483:ALA:HA	1.80	0.63
1:A:530:GLU:HG2	4:A:1241:HOH:O	1.99	0.63
1:A:539:GLU:HA	4:A:1640:HOH:O	1.97	0.63
1:B:340:ILE:H	1:B:577:GLN:NE2	1.89	0.63
1:B:564:LYS:HE3	4:B:1452:HOH:O	1.99	0.63
1:A:525:THR:HG21	4:A:1396:HOH:O	1.97	0.62
1:C:415:THR:HB	1:C:483:ALA:HA	1.80	0.61
1:C:558:ASN:H	1:C:930:GLN:NE2	1.97	0.61
1:B:675:ASP:OD2	1:B:698:THR:HB	2.01	0.61
1:A:286:GLU:HG2	4:A:1272:HOH:O	2.00	0.61
1:D:341:THR:HG22	4:D:1198:HOH:O	2.00	0.61
1:A:331:ARG:HH11	1:A:331:ARG:HG2	1.66	0.61
1:B:558:ASN:H	1:B:930:GLN:NE2	1.99	0.61
1:C:934:ASN:HD21	1:C:961:ASN:HB3	1.66	0.60
1:A:19:ARG:NH2	1:A:459:ASP:OD1	2.34	0.60
1:A:19:ARG:HD3	1:A:148:ASN:HD22	1.67	0.60
1:A:525:THR:HG22	1:A:528:ILE:H	1.66	0.60
1:A:712:LYS:HD2	4:A:1175:HOH:O	2.01	0.60
1:B:415:THR:HB	1:B:483:ALA:HA	1.83	0.60
1:B:339:ASN:HD21	1:B:574:LYS:HG2	1.66	0.60
1:B:19:ARG:NH2	1:B:459:ASP:OD1	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:614:GLU:HG2	4:B:1297:HOH:O	1.99	0.60
1:D:934:ASN:HD21	1:D:961:ASN:HB3	1.67	0.60
1:D:103:VAL:CB	3:B:1027:GOL:H32	2.27	0.60
1:D:339:ASN:HD21	1:D:574:LYS:HG2	1.66	0.59
1:C:19:ARG:HD3	1:C:148:ASN:HD22	1.67	0.59
1:C:339:ASN:HD21	1:C:574:LYS:HG2	1.67	0.59
1:B:525:THR:HG22	1:B:528:ILE:H	1.68	0.59
1:C:581:ILE:HG22	4:C:1421:HOH:O	2.02	0.59
1:D:816:ILE:HG22	1:B:4:LEU:HD13	1.84	0.59
1:C:19:ARG:NH2	1:C:459:ASP:OD1	2.34	0.59
1:A:934:ASN:HD21	1:A:961:ASN:HB3	1.67	0.59
1:B:581:ILE:HG12	1:B:625:LEU:HD11	1.84	0.59
1:D:178:SER:OG	1:D:180:SER:HB3	2.03	0.59
1:D:331:ARG:HG2	1:D:331:ARG:HH11	1.67	0.59
1:C:415:THR:HG21	4:C:1069:HOH:O	2.03	0.58
1:D:665:THR:CG2	1:D:666:THR:N	2.66	0.58
1:D:19:ARG:NH2	1:D:459:ASP:OD1	2.35	0.58
1:A:755:GLY:HA2	1:D:78:ASP:OD1	2.03	0.58
1:B:934:ASN:HD21	1:B:961:ASN:HB3	1.66	0.58
1:C:525:THR:HG22	1:C:528:ILE:H	1.67	0.58
1:C:581:ILE:HG12	1:C:625:LEU:HD11	1.85	0.58
1:B:815:ASN:OD1	3:B:1027:GOL:O3	2.20	0.58
1:A:339:ASN:HD21	1:A:574:LYS:HG2	1.69	0.58
1:D:141:ASN:HD21	1:D:168:ASN:HA	1.68	0.58
1:A:270:THR:CG2	1:B:116:ASP:HB2	2.34	0.58
1:A:558:ASN:H	1:A:930:GLN:NE2	2.01	0.58
1:C:189:TRP:CD1	3:C:1026:GOL:H32	2.39	0.57
1:C:675:ASP:OD2	1:C:698:THR:HB	2.04	0.57
1:B:274:LYS:NZ	4:B:1060:HOH:O	2.32	0.57
1:D:675:ASP:OD2	1:D:698:THR:HB	2.05	0.57
1:A:740:ALA:HB3	4:A:1335:HOH:O	2.04	0.57
1:C:331:ARG:HH11	1:C:331:ARG:HG2	1.70	0.57
1:B:752:GLU:HG2	1:B:757:HIS:HD2	1.69	0.57
1:B:178:SER:OG	1:B:180:SER:HB3	2.05	0.56
1:C:141:ASN:HD21	1:C:168:ASN:HA	1.69	0.56
1:A:752:GLU:HG2	1:A:757:HIS:HD2	1.70	0.56
1:A:19:ARG:HD3	1:A:148:ASN:ND2	2.20	0.56
1:A:966:ASP:HB3	1:A:981:ARG:HH11	1.70	0.56
1:C:19:ARG:HD3	1:C:148:ASN:ND2	2.21	0.56
1:D:806:LYS:HD3	1:B:424:ARG:HB3	1.88	0.56
1:A:966:ASP:HB3	1:A:981:ARG:NH1	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:807:TYR:OH	1:B:425:HIS:HD2	1.89	0.56
1:D:807:TYR:OH	1:B:425:HIS:CD2	2.59	0.56
1:C:908:LYS:H	3:C:1028:GOL:C1	2.19	0.55
1:D:19:ARG:HD3	1:D:148:ASN:HD22	1.71	0.55
1:C:178:SER:OG	1:C:180:SER:HB3	2.07	0.55
1:B:639:TYR:O	1:B:643:ILE:HG12	2.06	0.55
1:D:581:ILE:HG12	1:D:625:LEU:HD11	1.89	0.55
1:C:752:GLU:HG2	1:C:757:HIS:HD2	1.71	0.55
1:D:558:ASN:H	1:D:930:GLN:NE2	2.05	0.55
1:A:665:THR:CG2	1:A:666:THR:N	2.70	0.55
1:C:966:ASP:HB3	1:C:981:ARG:HH11	1.71	0.55
1:C:433:PRO:HD3	4:C:1084:HOH:O	2.06	0.55
1:D:639:TYR:O	1:D:643:ILE:HG12	2.07	0.55
1:C:556:MET:HA	1:C:623:ASP:HA	1.89	0.55
1:B:141:ASN:HD21	1:B:168:ASN:HA	1.72	0.54
1:C:966:ASP:HB3	1:C:981:ARG:NH1	2.22	0.54
1:A:581:ILE:HG12	1:A:625:LEU:HD11	1.90	0.54
1:B:331:ARG:HH11	1:B:331:ARG:HG2	1.71	0.54
1:B:966:ASP:HB3	1:B:981:ARG:HH11	1.71	0.54
1:B:19:ARG:HD3	1:B:148:ASN:HD22	1.72	0.54
1:B:556:MET:HA	1:B:623:ASP:HA	1.90	0.53
1:A:141:ASN:HD21	1:A:168:ASN:HA	1.72	0.53
1:B:62:LYS:HE3	4:B:1094:HOH:O	2.07	0.53
1:C:265:GLU:HG3	4:C:1203:HOH:O	2.08	0.53
1:B:966:ASP:HB3	1:B:981:ARG:NH1	2.24	0.53
1:D:141:ASN:ND2	1:D:169:LEU:H	2.07	0.53
1:A:425:HIS:CD2	1:C:807:TYR:OH	2.62	0.53
1:D:556:MET:HA	1:D:623:ASP:HA	1.91	0.53
1:D:752:GLU:HG2	1:D:757:HIS:HD2	1.74	0.52
1:B:665:THR:CG2	1:B:666:THR:N	2.72	0.52
1:C:141:ASN:ND2	1:C:169:LEU:H	2.08	0.52
1:C:639:TYR:O	1:C:643:ILE:HG12	2.10	0.52
1:C:657:ILE:HB	4:C:1347:HOH:O	2.10	0.52
1:C:665:THR:CG2	1:C:666:THR:N	2.71	0.52
1:C:907:LYS:HA	3:C:1028:GOL:H12	1.92	0.52
1:C:19:ARG:HH11	1:C:148:ASN:HD21	1.56	0.52
1:D:922:GLU:HG2	4:D:1083:HOH:O	2.09	0.52
1:C:340:ILE:H	1:C:577:GLN:NE2	1.91	0.51
1:A:141:ASN:ND2	1:A:169:LEU:H	2.08	0.51
1:A:130:GLU:HB2	1:A:196:ARG:HB3	1.92	0.51
1:B:19:ARG:HD3	1:B:148:ASN:ND2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:996:VAL:HA	4:B:1138:HOH:O	2.10	0.51
1:C:592:GLU:HG2	4:C:1105:HOH:O	2.10	0.51
1:D:19:ARG:HH11	1:D:148:ASN:HD21	1.58	0.51
1:A:556:MET:HA	1:A:623:ASP:HA	1.92	0.51
1:D:424:ARG:HB3	1:B:806:LYS:HD3	1.91	0.51
1:C:553:GLY:HA3	4:C:1421:HOH:O	2.09	0.51
1:C:130:GLU:HB2	1:C:196:ARG:HB3	1.92	0.51
1:C:923:GLU:HB2	4:C:1129:HOH:O	2.09	0.51
1:A:424:ARG:HB3	1:C:806:LYS:HD3	1.93	0.51
1:A:879:ARG:HH11	1:A:990:ASP:CG	2.14	0.51
1:D:153:ASN:CB	1:D:463:GLN:HG2	2.41	0.50
1:D:19:ARG:HD3	1:D:148:ASN:ND2	2.25	0.50
1:D:206:LYS:HG2	4:D:1086:HOH:O	2.11	0.50
1:A:419:GLN:NE2	1:A:443:ASN:HD22	2.08	0.50
1:A:752:GLU:HG2	1:A:757:HIS:CD2	2.46	0.50
1:B:888:ASP:HB2	4:B:1077:HOH:O	2.10	0.50
1:D:665:THR:HG22	1:D:667:ASP:N	2.11	0.50
1:D:125:HIS:HD2	1:D:160:GLN:OE1	1.95	0.50
1:D:966:ASP:HB3	1:D:981:ARG:NH1	2.26	0.50
1:D:4:LEU:HD13	1:B:816:ILE:CG2	2.42	0.50
1:B:141:ASN:ND2	1:B:169:LEU:H	2.09	0.50
1:C:783:GLY:HA2	3:C:1029:GOL:H12	1.93	0.50
1:B:804:TRP:CE3	1:B:878:PRO:HG3	2.47	0.50
1:C:415:THR:O	1:C:415:THR:CG2	2.60	0.50
1:C:581:ILE:CG2	4:C:1421:HOH:O	2.58	0.50
1:D:130:GLU:HB2	1:D:196:ARG:HB3	1.93	0.50
1:C:532:TRP:O	1:C:536:HIS:HD2	1.95	0.49
1:D:85:ILE:HG23	1:D:613:GLU:HG2	1.93	0.49
1:D:804:TRP:CE3	1:D:878:PRO:HG3	2.47	0.49
1:B:125:HIS:HD2	1:B:160:GLN:OE1	1.96	0.49
1:A:937:ASP:HA	1:A:959:PRO:HB2	1.95	0.49
1:C:206:LYS:HB2	4:C:1276:HOH:O	2.12	0.49
1:C:341:THR:HG22	4:C:1135:HOH:O	2.13	0.49
1:D:532:TRP:O	1:D:536:HIS:HD2	1.95	0.49
1:B:532:TRP:O	1:B:536:HIS:HD2	1.96	0.49
1:C:189:TRP:HB2	3:C:1026:GOL:H31	1.94	0.49
1:C:153:ASN:CB	1:C:463:GLN:HG2	2.41	0.49
1:B:341:THR:CG2	4:B:1045:HOH:O	2.57	0.49
1:C:752:GLU:HG2	1:C:757:HIS:CD2	2.48	0.49
4:A:1130:HOH:O	1:D:594:VAL:HG21	2.12	0.49
1:A:220:ASP:OD2	1:A:222:GLN:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:VAL:HG21	3:B:1027:GOL:H12	1.95	0.49
1:C:429:GLU:HG2	4:C:1066:HOH:O	2.12	0.49
1:D:841:VAL:O	1:D:842:VAL:HB	2.13	0.49
1:C:266:ASN:HB3	1:C:269:THR:OG1	2.13	0.48
1:C:879:ARG:HH11	1:C:990:ASP:CG	2.16	0.48
1:A:331:ARG:NH1	1:A:331:ARG:HG2	2.28	0.48
1:B:536:HIS:HE1	4:B:1048:HOH:O	1.96	0.48
1:D:966:ASP:HB3	1:D:981:ARG:HH11	1.77	0.48
1:D:816:ILE:CG2	1:B:4:LEU:HD13	2.44	0.48
1:C:149:LYS:NZ	1:C:179:ASP:OD1	2.43	0.48
1:A:532:TRP:O	1:A:536:HIS:HD2	1.96	0.48
1:B:282:LYS:HD2	4:B:1533:HOH:O	2.13	0.48
1:D:965:SER:OG	1:D:966:ASP:N	2.45	0.48
1:A:257:ASP:OD2	1:B:68:SER:HB2	2.13	0.48
1:D:665:THR:HG22	1:D:666:THR:N	2.28	0.48
1:D:678:LYS:HB2	4:D:1091:HOH:O	2.13	0.48
1:A:90:GLN:HB2	1:C:842:VAL:HG22	1.95	0.48
1:D:341:THR:CG2	4:D:1198:HOH:O	2.60	0.48
1:D:752:GLU:HG2	1:D:757:HIS:CD2	2.49	0.48
1:B:153:ASN:CB	1:B:463:GLN:HG2	2.43	0.48
1:B:752:GLU:HG2	1:B:757:HIS:CD2	2.47	0.48
1:A:425:HIS:HD2	1:C:807:TYR:OH	1.97	0.48
1:D:419:GLN:NE2	1:D:443:ASN:HD22	2.11	0.48
1:A:125:HIS:HD2	1:A:160:GLN:OE1	1.97	0.48
1:B:130:GLU:HB2	1:B:196:ARG:HB3	1.95	0.47
1:C:595:SER:HB2	1:C:602:HIS:HD2	1.79	0.47
1:A:341:THR:HG22	4:A:1029:HOH:O	2.14	0.47
1:B:220:ASP:OD2	1:B:222:GLN:HG2	2.13	0.47
1:C:224:GLN:O	1:C:296:PRO:HD2	2.15	0.47
1:D:536:HIS:HE1	4:D:1054:HOH:O	1.97	0.47
1:C:804:TRP:CE3	1:C:878:PRO:HG3	2.49	0.47
1:D:353:ASN:OD1	1:D:386:ARG:HD3	2.14	0.47
1:A:415:THR:HG21	4:A:1216:HOH:O	2.14	0.47
1:A:415:THR:CG2	1:A:415:THR:O	2.62	0.47
1:A:804:TRP:CE3	1:A:878:PRO:HG3	2.50	0.47
1:A:807:TYR:OH	1:C:425:HIS:CD2	2.67	0.47
1:D:879:ARG:HH11	1:D:990:ASP:CG	2.17	0.47
1:B:517:ASP:O	1:B:518:ILE:HD13	2.14	0.47
1:D:388:SER:HA	1:D:389:HIS:HA	1.74	0.47
1:C:766:LYS:HE2	4:C:1204:HOH:O	2.14	0.47
1:A:149:LYS:NZ	1:A:179:ASP:OD1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ASN:CB	1:A:463:GLN:HG2	2.43	0.47
1:A:419:GLN:HE22	1:A:443:ASN:HD22	1.63	0.46
1:A:353:ASN:OD1	1:A:386:ARG:HD3	2.15	0.46
1:B:937:ASP:HA	1:B:959:PRO:HB2	1.96	0.46
1:D:414:GLU:OE2	4:D:1686:HOH:O	2.21	0.46
1:B:353:ASN:OD1	1:B:386:ARG:HD3	2.15	0.46
1:B:587:HIS:HB2	1:B:621:ILE:HD12	1.97	0.46
1:D:224:GLN:O	1:D:296:PRO:HD2	2.15	0.46
1:D:326:HIS:CG	1:D:327:HIS:H	2.34	0.46
1:B:352:VAL:HG12	1:B:581:ILE:HG13	1.97	0.46
1:A:388:SER:HA	1:A:389:HIS:HA	1.75	0.46
1:A:841:VAL:O	1:A:842:VAL:HB	2.15	0.46
1:C:85:ILE:HG23	1:C:613:GLU:HG2	1.97	0.46
1:D:231:LYS:HE2	4:D:1068:HOH:O	2.15	0.46
1:B:965:SER:OG	1:B:966:ASP:N	2.43	0.46
1:D:19:ARG:HH11	1:D:148:ASN:HD22	1.62	0.46
1:A:639:TYR:O	1:A:643:ILE:HG12	2.15	0.46
1:C:19:ARG:HH11	1:C:148:ASN:HD22	1.62	0.46
1:C:326:HIS:CG	1:C:327:HIS:H	2.34	0.46
1:C:937:ASP:HA	1:C:959:PRO:HB2	1.98	0.46
1:D:937:ASP:HA	1:D:959:PRO:HB2	1.98	0.46
1:B:415:THR:CG2	1:B:415:THR:O	2.63	0.46
1:A:85:ILE:HG23	1:A:613:GLU:HG2	1.97	0.45
1:A:517:ASP:O	1:A:518:ILE:HD13	2.16	0.45
1:B:19:ARG:HH11	1:B:148:ASN:HD21	1.60	0.45
1:C:17:GLU:HG3	4:C:1246:HOH:O	2.16	0.45
1:C:965:SER:OG	1:C:966:ASP:N	2.47	0.45
1:D:425:HIS:CD2	1:B:807:TYR:OH	2.70	0.45
1:C:220:ASP:OD2	1:C:222:GLN:HG2	2.16	0.45
1:D:331:ARG:NH1	1:D:331:ARG:HG2	2.30	0.45
1:D:340:ILE:H	1:D:577:GLN:NE2	1.95	0.45
1:D:595:SER:HB2	1:D:602:HIS:HD2	1.81	0.45
1:A:4:LEU:HD13	1:C:816:ILE:HG22	1.98	0.45
1:C:388:SER:HA	1:C:389:HIS:HA	1.75	0.45
1:C:841:VAL:O	1:C:842:VAL:HB	2.16	0.45
1:D:355:HIS:HE1	4:D:1689:HOH:O	1.99	0.45
1:C:125:HIS:HD2	1:C:160:GLN:OE1	1.99	0.45
1:C:189:TRP:HB2	3:C:1026:GOL:C3	2.47	0.45
1:D:149:LYS:NZ	1:D:179:ASP:OD1	2.48	0.45
1:D:233:ASP:HB2	4:D:1068:HOH:O	2.17	0.45
1:A:629:GLU:HG3	4:A:1037:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:934:ASN:ND2	4:C:1047:HOH:O	2.49	0.45
1:D:340:ILE:HG12	1:D:518:ILE:HD11	1.98	0.45
1:D:149:LYS:HD3	1:D:180:SER:HB2	1.99	0.45
1:D:350:ARG:HD3	1:D:643:ILE:O	2.17	0.45
1:B:533:ARG:NH2	4:B:1263:HOH:O	2.50	0.45
1:C:331:ARG:NH1	1:C:331:ARG:HG2	2.32	0.45
1:C:340:ILE:HG12	1:C:518:ILE:HD11	1.99	0.45
1:D:205:LYS:HB3	4:D:1184:HOH:O	2.17	0.45
1:C:463:GLN:NE2	4:C:1090:HOH:O	2.50	0.44
1:A:340:ILE:HG12	1:A:518:ILE:HD11	1.99	0.44
1:C:647:HIS:HE1	4:C:1289:HOH:O	2.01	0.44
1:D:16:HIS:CD2	1:D:19:ARG:H	2.36	0.44
1:B:118:LYS:HE2	4:B:1602:HOH:O	2.16	0.44
1:B:410:GLU:HG3	1:B:478:SER:HB3	1.99	0.44
1:C:97:ILE:HA	1:C:98:PRO:HA	1.85	0.44
1:D:266:ASN:HB3	1:D:269:THR:OG1	2.18	0.44
1:D:556:MET:CE	1:D:619:VAL:HG13	2.47	0.44
1:A:127:LEU:HG	1:A:159:ILE:HG13	1.99	0.44
1:B:300:THR:HG22	1:B:303:ASN:N	2.29	0.44
1:C:353:ASN:OD1	1:C:386:ARG:HD3	2.17	0.44
1:B:475:ILE:HG13	1:B:476:ILE:HG13	1.99	0.43
1:B:85:ILE:HG23	1:B:613:GLU:HG2	1.99	0.43
1:A:149:LYS:HD3	1:A:180:SER:HB2	1.99	0.43
1:A:350:ARG:HD3	1:A:643:ILE:O	2.18	0.43
1:B:266:ASN:HB3	1:B:269:THR:OG1	2.18	0.43
1:D:116:ASP:HB2	4:D:1330:HOH:O	2.18	0.43
1:A:159:ILE:HA	1:A:159:ILE:HD13	1.86	0.43
1:A:581:ILE:HD11	1:A:625:LEU:CG	2.43	0.43
1:A:757:HIS:HB3	4:A:1370:HOH:O	2.17	0.43
1:C:355:HIS:HE1	4:C:1680:HOH:O	2.01	0.43
1:C:415:THR:HB	1:C:483:ALA:CA	2.48	0.43
1:C:415:THR:O	1:C:415:THR:HG23	2.19	0.43
1:B:595:SER:HB2	1:B:602:HIS:HD2	1.83	0.43
1:A:965:SER:OG	1:A:966:ASP:N	2.44	0.43
1:B:486:GLY:H	1:B:489:HIS:HD2	1.66	0.43
1:D:415:THR:O	1:D:415:THR:CG2	2.66	0.43
1:A:595:SER:HB2	1:A:602:HIS:HD2	1.84	0.43
1:B:340:ILE:HG12	1:B:518:ILE:HD11	2.01	0.43
1:B:388:SER:HA	1:B:389:HIS:HA	1.77	0.43
1:C:419:GLN:NE2	1:C:443:ASN:HD22	2.17	0.43
1:C:410:GLU:HG3	1:C:478:SER:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:470:ASN:HB2	4:C:1076:HOH:O	2.19	0.43
1:D:127:LEU:HG	1:D:159:ILE:HG13	2.00	0.43
1:A:326:HIS:CG	1:A:327:HIS:H	2.36	0.43
1:D:425:HIS:HD2	1:B:807:TYR:OH	2.00	0.43
1:C:762:LYS:HG2	1:C:819:VAL:HG11	2.00	0.43
1:D:300:THR:HG22	1:D:303:ASN:N	2.30	0.43
1:A:340:ILE:H	1:A:577:GLN:NE2	1.94	0.42
1:B:924:PHE:HA	4:B:1167:HOH:O	2.18	0.42
1:D:587:HIS:HB2	1:D:621:ILE:HD12	2.01	0.42
1:C:542:LYS:HD2	4:C:1576:HOH:O	2.19	0.42
1:C:825:SER:O	1:C:827:GLY:N	2.52	0.42
1:D:486:GLY:H	1:D:489:HIS:HD2	1.67	0.42
1:A:224:GLN:O	1:A:296:PRO:HD2	2.19	0.42
1:B:471:HIS:HA	1:B:472:PRO:HD2	1.91	0.42
1:A:471:HIS:HA	1:A:472:PRO:HD2	1.92	0.42
1:B:326:HIS:CG	1:B:327:HIS:H	2.37	0.42
1:C:352:VAL:HG12	1:C:581:ILE:HG13	2.01	0.42
1:A:4:LEU:HD13	1:C:816:ILE:CG2	2.50	0.42
1:A:762:LYS:HG2	1:A:819:VAL:HG11	2.00	0.42
1:B:331:ARG:NH1	1:B:331:ARG:HG2	2.34	0.42
1:B:419:GLN:NE2	1:B:443:ASN:HD22	2.18	0.42
1:C:300:THR:HB	4:C:1223:HOH:O	2.18	0.42
1:B:841:VAL:O	1:B:842:VAL:HB	2.19	0.42
1:C:789:TRP:CE3	1:C:810:ASP:HB3	2.54	0.42
1:D:524:PRO:HG3	1:D:549:LEU:HD22	2.01	0.42
1:A:587:HIS:HB2	1:A:621:ILE:HD12	2.02	0.42
1:A:825:SER:O	1:A:827:GLY:N	2.53	0.42
1:B:16:HIS:CD2	1:B:19:ARG:H	2.38	0.42
1:B:788:PHE:CE2	1:B:812:MET:HG2	2.55	0.42
1:C:149:LYS:HD3	1:C:180:SER:HB2	2.01	0.42
1:C:595:SER:HB2	1:C:602:HIS:CD2	2.54	0.42
1:C:703:VAL:HG13	1:C:714:GLY:HA2	2.02	0.42
1:D:419:GLN:HE22	1:D:443:ASN:HD22	1.66	0.42
1:B:14:LYS:NZ	1:B:17:GLU:OE1	2.53	0.42
1:B:224:GLN:O	1:B:296:PRO:HD2	2.19	0.42
1:B:789:TRP:CE3	1:B:810:ASP:HB3	2.55	0.42
1:C:973:ALA:HB1	1:C:978:ASP:HB2	2.02	0.42
1:A:128:ARG:HB2	1:A:156:GLU:HG2	2.02	0.41
1:A:582:TRP:HA	1:A:583:GLU:HA	1.85	0.41
1:B:137:GLU:HG3	1:B:139:TYR:HE1	1.84	0.41
1:C:783:GLY:O	3:C:1029:GOL:H11	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:595:SER:HB2	1:D:602:HIS:CD2	2.55	0.41
1:B:595:SER:HB2	1:B:602:HIS:CD2	2.56	0.41
1:C:333:VAL:HA	1:C:341:THR:O	2.20	0.41
1:C:445:HIS:HA	1:C:449:ASP:HB3	2.01	0.41
1:D:254:LYS:HA	4:D:1312:HOH:O	2.19	0.41
1:D:220:ASP:OD2	1:D:222:GLN:HG2	2.21	0.41
1:A:266:ASN:HB3	1:A:269:THR:OG1	2.20	0.41
1:C:486:GLY:H	1:C:489:HIS:HD2	1.69	0.41
1:D:331:ARG:HE	1:D:472:PRO:HA	1.86	0.41
1:D:534:LYS:HE2	4:D:1490:HOH:O	2.21	0.41
1:C:154:GLY:O	1:C:463:GLN:NE2	2.53	0.41
1:C:524:PRO:HG3	1:C:549:LEU:HD22	2.01	0.41
1:C:582:TRP:HA	1:C:583:GLU:HA	1.89	0.41
1:D:54:LYS:HD3	4:D:1064:HOH:O	2.16	0.41
1:A:415:THR:HB	1:A:483:ALA:CA	2.50	0.41
1:B:154:GLY:O	1:B:463:GLN:NE2	2.54	0.41
1:C:127:LEU:HG	1:C:159:ILE:HG13	2.02	0.41
1:D:97:ILE:HA	1:D:98:PRO:HA	1.86	0.41
1:A:524:PRO:HG3	1:A:549:LEU:HD22	2.03	0.41
1:B:518:ILE:HG22	1:B:519:PHE:O	2.21	0.41
1:D:415:THR:HB	1:D:483:ALA:CA	2.47	0.41
1:D:788:PHE:CE2	1:D:812:MET:HG2	2.56	0.41
1:B:804:TRP:CD2	1:B:878:PRO:HG3	2.56	0.41
1:D:370:VAL:O	1:D:373:ASP:HB2	2.21	0.41
1:A:149:LYS:NZ	1:A:179:ASP:OD2	2.52	0.40
1:A:525:THR:HG23	1:A:527:GLU:OE1	2.21	0.40
1:B:149:LYS:HD3	1:B:180:SER:HB2	2.03	0.40
1:D:517:ASP:O	1:D:518:ILE:HD13	2.21	0.40
1:A:595:SER:HB2	1:A:602:HIS:CD2	2.56	0.40
1:B:331:ARG:NH1	1:B:333:VAL:HG12	2.36	0.40
1:B:370:VAL:O	1:B:373:ASP:HB2	2.21	0.40
1:C:587:HIS:HB2	1:C:621:ILE:HD12	2.03	0.40
1:D:133:ASP:HA	1:D:134:ASN:HA	1.92	0.40
1:D:294:LYS:HB2	4:D:1515:HOH:O	2.22	0.40
1:D:727:LYS:HB2	4:D:1246:HOH:O	2.20	0.40
1:A:112:THR:HA	1:A:168:ASN:O	2.20	0.40
1:A:19:ARG:HH11	1:A:148:ASN:HD21	1.64	0.40
1:B:445:HIS:HA	1:B:449:ASP:HB3	2.03	0.40
1:B:629:GLU:HG3	4:B:1067:HOH:O	2.20	0.40
1:B:350:ARG:HD3	1:B:643:ILE:O	2.21	0.40
1:A:86:TYR:CD2	1:A:621:ILE:HG12	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:ALA:HB2	4:C:1288:HOH:O	2.21	0.40
1:C:518:ILE:HG22	1:C:519:PHE:O	2.21	0.40
1:D:935:HIS:HE1	4:D:1203:HOH:O	2.03	0.40
1:A:498:GLN:HB3	4:A:1094:HOH:O	2.21	0.40
1:B:432:TYR:HA	1:B:433:PRO:HD3	1.98	0.40
1:C:115:LEU:HD23	1:C:115:LEU:HA	1.98	0.40
1:D:128:ARG:HB2	1:D:156:GLU:HG2	2.04	0.40
1:D:804:TRP:CD2	1:D:878:PRO:HG3	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	1022/1032 (99%)	978 (96%)	42 (4%)	2 (0%)	51	81
1	B	1022/1032 (99%)	976 (96%)	44 (4%)	2 (0%)	51	81
1	C	1022/1032 (99%)	973 (95%)	47 (5%)	2 (0%)	51	81
1	D	1022/1032 (99%)	974 (95%)	46 (4%)	2 (0%)	51	81
All	All	4088/4128 (99%)	3901 (95%)	179 (4%)	8 (0%)	51	81

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	826	ASN
1	A	842	VAL
1	C	826	ASN
1	C	842	VAL
1	D	826	ASN
1	D	842	VAL
1	B	826	ASN

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Mol	Chain	Res	Type
1	B	842	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	905/913 (99%)	880 (97%)	25 (3%)	49	79
1	B	905/913 (99%)	881 (97%)	24 (3%)	50	80
1	C	905/913 (99%)	881 (97%)	24 (3%)	50	80
1	D	905/913 (99%)	881 (97%)	24 (3%)	50	80
All	All	3620/3652 (99%)	3523 (97%)	97 (3%)	50	80

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	4	LEU
1	A	48	LEU
1	A	116	ASP
1	A	152	ARG
1	A	235	GLN
1	A	300	THR
1	A	341	THR
1	A	385	VAL
1	A	415	THR
1	A	437	ASN
1	A	469	VAL
1	A	499	LEU
1	A	525	THR
1	A	531	ARG
1	A	581	ILE
1	A	596	THR
1	A	621	ILE
1	A	698	THR
1	A	779	SER

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Mol	Chain	Res	Type
1	A	876	ASP
1	A	957	GLU
1	A	971	ASP
1	A	996	VAL
1	A	1007	ASP
1	C	2	SER
1	C	4	LEU
1	C	48	LEU
1	C	152	ARG
1	C	300	THR
1	C	341	THR
1	C	355	HIS
1	C	385	VAL
1	C	415	THR
1	C	437	ASN
1	C	469	VAL
1	C	499	LEU
1	C	525	THR
1	C	531	ARG
1	C	581	ILE
1	C	596	THR
1	C	665	THR
1	C	698	THR
1	C	779	SER
1	C	876	ASP
1	C	957	GLU
1	C	971	ASP
1	C	996	VAL
1	C	1007	ASP
1	D	2	SER
1	D	4	LEU
1	D	48	LEU
1	D	116	ASP
1	D	152	ARG
1	D	300	THR
1	D	331	ARG
1	D	341	THR
1	D	385	VAL
1	D	415	THR
1	D	437	ASN
1	D	469	VAL
1	D	499	LEU

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Mol	Chain	Res	Type
1	D	525	THR
1	D	531	ARG
1	D	581	ILE
1	D	596	THR
1	D	698	THR
1	D	779	SER
1	D	876	ASP
1	D	957	GLU
1	D	971	ASP
1	D	996	VAL
1	D	1007	ASP
1	B	2	SER
1	B	4	LEU
1	B	48	LEU
1	B	116	ASP
1	B	152	ARG
1	B	300	THR
1	B	341	THR
1	B	385	VAL
1	B	415	THR
1	B	437	ASN
1	B	469	VAL
1	B	499	LEU
1	B	525	THR
1	B	531	ARG
1	B	581	ILE
1	B	596	THR
1	B	621	ILE
1	B	665	THR
1	B	698	THR
1	B	876	ASP
1	B	957	GLU
1	B	971	ASP
1	B	996	VAL
1	B	1007	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	125	HIS
1	A	134	ASN

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Mol	Chain	Res	Type
1	A	141	ASN
1	A	148	ASN
1	A	208	HIS
1	A	235	GLN
1	A	339	ASN
1	A	355	HIS
1	A	387	ASN
1	A	419	GLN
1	A	423	ASN
1	A	425	HIS
1	A	427	ASN
1	A	489	HIS
1	A	536	HIS
1	A	567	GLN
1	A	577	GLN
1	A	647	HIS
1	A	652	HIS
1	A	861	ASN
1	A	930	GLN
1	A	934	ASN
1	A	935	HIS
1	A	955	GLN
1	A	1014	GLN
1	C	16	HIS
1	C	125	HIS
1	C	134	ASN
1	C	141	ASN
1	C	148	ASN
1	C	188	GLN
1	C	208	HIS
1	C	339	ASN
1	C	355	HIS
1	C	387	ASN
1	C	419	GLN
1	C	423	ASN
1	C	425	HIS
1	C	427	ASN
1	C	489	HIS
1	C	536	HIS
1	C	567	GLN
1	C	577	GLN
1	C	647	HIS

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Mol	Chain	Res	Type
1	C	757	HIS
1	C	861	ASN
1	C	930	GLN
1	C	934	ASN
1	C	955	GLN
1	D	16	HIS
1	D	125	HIS
1	D	134	ASN
1	D	141	ASN
1	D	148	ASN
1	D	208	HIS
1	D	235	GLN
1	D	339	ASN
1	D	355	HIS
1	D	387	ASN
1	D	419	GLN
1	D	423	ASN
1	D	425	HIS
1	D	489	HIS
1	D	536	HIS
1	D	567	GLN
1	D	577	GLN
1	D	647	HIS
1	D	757	HIS
1	D	817	HIS
1	D	861	ASN
1	D	930	GLN
1	D	934	ASN
1	D	935	HIS
1	D	955	GLN
1	B	16	HIS
1	B	125	HIS
1	B	134	ASN
1	B	141	ASN
1	B	148	ASN
1	B	208	HIS
1	B	235	GLN
1	B	339	ASN
1	B	355	HIS
1	B	387	ASN
1	B	419	GLN
1	B	423	ASN

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Mol	Chain	Res	Type
1	B	425	HIS
1	B	489	HIS
1	B	536	HIS
1	B	567	GLN
1	B	577	GLN
1	B	647	HIS
1	B	861	ASN
1	B	930	GLN
1	B	934	ASN
1	B	935	HIS
1	B	955	GLN

### 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 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	$\# Z  > 2$
3	GOL	A	1026	-	5,5,5	0.45	0	5,5,5	0.07	0
3	GOL	A	1027	-	5,5,5	0.42	0	5,5,5	0.30	0
3	GOL	B	1026	-	5,5,5	0.40	0	5,5,5	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	B	1027	-	5,5,5	1.40	1 (20%)	5,5,5	0.78	0
3	GOL	C	1026	-	5,5,5	0.31	0	5,5,5	0.60	0
3	GOL	C	1027	-	5,5,5	0.39	0	5,5,5	0.26	0
3	GOL	C	1028	-	5,5,5	0.40	0	5,5,5	0.31	0
3	GOL	C	1029	-	5,5,5	0.38	0	5,5,5	0.42	0
3	GOL	D	1026	-	5,5,5	0.42	0	5,5,5	0.25	0
3	GOL	D	1027	-	5,5,5	0.40	0	5,5,5	0.42	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
3	GOL	A	1026	-	-	0/4/4/4	0/0/0/0
3	GOL	A	1027	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1026	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1027	-	-	0/4/4/4	0/0/0/0
3	GOL	C	1026	-	-	0/4/4/4	0/0/0/0
3	GOL	C	1027	-	-	0/4/4/4	0/0/0/0
3	GOL	C	1028	-	-	0/4/4/4	0/0/0/0
3	GOL	C	1029	-	-	0/4/4/4	0/0/0/0
3	GOL	D	1026	-	-	0/4/4/4	0/0/0/0
3	GOL	D	1027	-	-	0/4/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1027	GOL	O2-C2	-2.45	1.36	1.43

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1027	GOL	4	0
3	C	1026	GOL	6	0
3	C	1028	GOL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1029	GOL	2	0

## 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	1024/1032 (99%)	-0.13	7 (0%) 87 85	8, 17, 37, 62	0
1	B	1024/1032 (99%)	-0.15	14 (1%) 75 72	8, 17, 37, 62	0
1	C	1024/1032 (99%)	0.00	24 (2%) 61 56	8, 17, 37, 62	0
1	D	1024/1032 (99%)	-0.04	28 (2%) 55 49	8, 17, 37, 62	0
All	All	4096/4128 (99%)	-0.08	73 (1%) 69 65	8, 17, 37, 62	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	270	THR	11.5
1	D	273	THR	11.2
1	D	266	ASN	10.5
1	C	272	SER	10.4
1	D	267	GLY	10.1
1	C	267	GLY	9.7
1	C	268	ASN	9.3
1	C	273	THR	9.0
1	D	271	PHE	8.1
1	D	268	ASN	8.1
1	C	270	THR	7.8
1	D	272	SER	7.5
1	D	269	THR	7.4
1	C	271	PHE	7.1
1	C	266	ASN	7.0
1	C	269	THR	5.9
1	C	265	GLU	4.6
1	C	729	PRO	4.1
1	D	265	GLU	3.9
1	B	652	HIS	3.8
1	C	264	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	737	GLU	3.3
1	A	735	THR	3.3
1	C	206	LYS	3.2
1	B	736	ALA	3.2
1	B	739	ALA	3.2
1	C	825	SER	3.1
1	D	681	ASP	3.1
1	C	737	GLU	3.1
1	D	206	LYS	3.0
1	A	730	ASP	3.0
1	C	923	GLU	2.9
1	D	728	VAL	2.9
1	B	694	PRO	2.9
1	D	282	LYS	2.9
1	D	729	PRO	2.8
1	D	57	ASP	2.8
1	C	922	GLU	2.8
1	B	738	LYS	2.7
1	B	735	THR	2.7
1	B	730	ASP	2.7
1	D	435	THR	2.6
1	B	266	ASN	2.6
1	B	728	VAL	2.6
1	D	432	TYR	2.6
1	C	696	ASP	2.5
1	D	263	ASN	2.5
1	D	220	ASP	2.5
1	D	221	SER	2.4
1	A	738	LYS	2.4
1	A	728	VAL	2.4
1	B	729	PRO	2.4
1	D	739	ALA	2.4
1	B	539	GLU	2.4
1	B	121	GLU	2.4
1	B	683	PRO	2.4
1	A	291	ILE	2.4
1	A	827	GLY	2.3
1	D	264	GLU	2.3
1	C	540	ASN	2.3
1	C	730	ASP	2.3
1	D	116	ASP	2.3
1	B	737	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	121	GLU	2.2
1	C	277	ILE	2.2
1	D	922	GLU	2.2
1	D	823	LYS	2.2
1	D	118	LYS	2.2
1	C	677	GLY	2.2
1	C	782	GLU	2.1
1	A	266	ASN	2.1
1	D	286	GLU	2.0
1	C	286	GLU	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. 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<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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	C	1026	6/6	0.83	0.32	6.61	25,26,29,30	0
3	GOL	D	1026	6/6	0.56	0.48	3.15	49,50,51,51	0
3	GOL	C	1028	6/6	0.93	0.20	1.54	17,19,19,19	0
3	GOL	B	1027	6/6	0.92	0.17	0.31	12,15,16,18	0
3	GOL	A	1026	6/6	0.91	0.22	0.24	29,29,30,30	0
3	GOL	B	1026	6/6	0.95	0.15	0.08	22,23,23,24	0
3	GOL	D	1027	6/6	0.96	0.15	0.07	10,11,12,14	0
3	GOL	C	1027	6/6	0.94	0.14	-0.38	16,16,16,18	0
3	GOL	A	1027	6/6	0.97	0.13	-0.42	21,22,22,23	0
3	GOL	C	1029	6/6	0.94	0.15	-0.53	10,10,11,11	0
2	MN3	B	2001	1/1	0.99	0.09	-1.15	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MN3	C	2001	1/1	0.97	0.09	-1.48	8,8,8,8	0
2	MN3	D	2001	1/1	0.98	0.09	-1.73	11,11,11,11	0
2	MN3	A	2001	1/1	0.99	0.09	-2.11	8,8,8,8	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.