



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:43 pm BST

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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

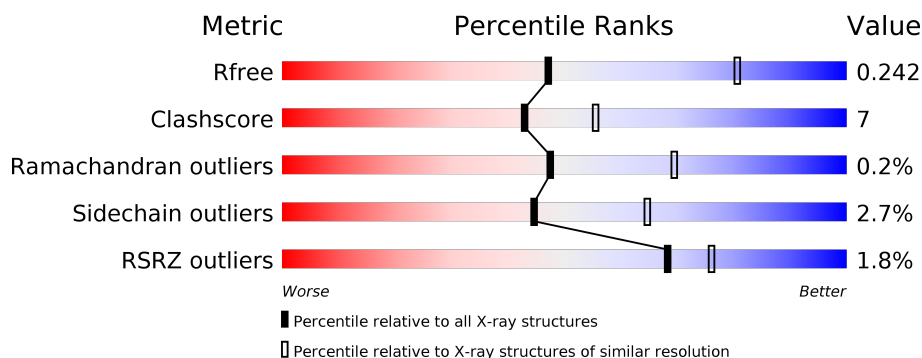
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	1032	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 1%, green 86%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 86% 12% </div> </div>
1	B	1032	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 1%, green 85%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 85% 13% </div> </div>
1	C	1032	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 1%, green 84%, grey 14%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 84% 14% </div> </div>
1	D	1032	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 1%, green 85%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 85% 13% </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	-
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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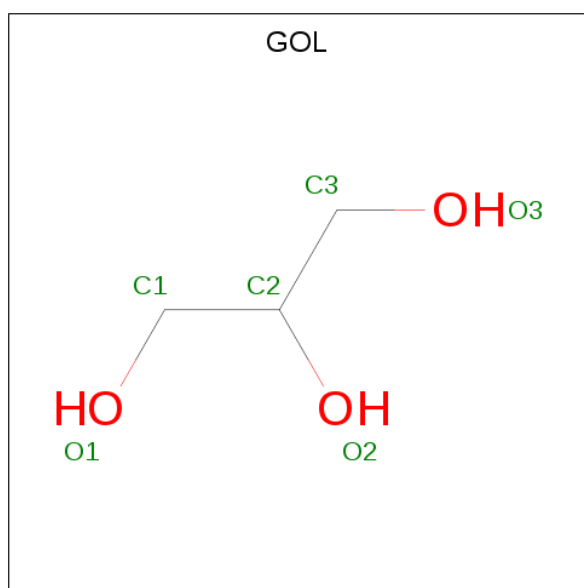
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	ASP	-	EXPRESSION TAG	UNP P00723
D	0	ASP	-	EXPRESSION TAG	UNP P00723
D	1	LYS	-	EXPRESSION TAG	UNP P00723
B	-6	ASP	-	EXPRESSION TAG	UNP P00723
B	-5	TYR	-	EXPRESSION TAG	UNP P00723
B	-4	LYS	-	EXPRESSION 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: C₃H₈O₃).



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

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 ($\text{RSRZ} > 2$). 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.

Chain A: 

Node	Value	Category
F960	100	High
N961	95	High
S965	90	High
D966	85	High
D971	80	High
R981	75	High
D990	70	High
V996	65	High
D1007	60	High
E1025	55	High
T665	50	High
T666	45	High
D667	40	High
D675	35	High
T698	30	High
K712	25	High
T728	20	High
F729	15	High
D730	10	High
T735	5	High
K738	0	High
A739	0	High
A740	0	High
E752	0	High
G755	0	High
L756	0	High
H757	0	High
K762	0	High
S779	0	High
T787	0	High
H804	0	High
H807	0	High
H819	0	High
S825	0	High
H826	0	High
G827	0	High
H841	0	High
V842	0	High
D876	0	High
F877	0	High
H878	0	High
H879	0	High
Q930	0	High
H934	0	High
D937	0	High
E957	0	High
V958	0	High
T959	0	High
P472	0	High
A483	0	High
Q498	0	High
L499	0	High
D517	0	High
I518	0	High
P524	0	High
T525	0	High
F526	0	High
E527	0	High
I528	0	High
M529	0	High
E530	0	High
R531	0	High
M532	0	High
R533	0	High
H536	0	High
E539	0	High
L549	0	High
M556	0	High
G557	0	High
N558	0	High
K574	0	High
F575	0	High
V576	0	High
Q577	0	High
I581	0	High
M582	0	High
E583	0	High
S585	0	High
N587	0	High
S588	0	High
H589	0	High
S595	0	High
T596	0	High
H602	0	High
E613	0	High
I621	0	High
M622	0	High
D623	0	High
G624	0	High
L625	0	High
E629	0	High
Y639	0	High
T643	0	High
Q224	0	High
Q235	0	High
D257	0	High
E265	0	High
N266	0	High
T269	0	High
T270	0	High
E286	0	High
I291	0	High
P296	0	High
T300	0	High
N303	0	High
H326	0	High
H327	0	High
R331	0	High
N339	0	High
I340	0	High
T341	0	High
F349	0	High
R350	0	High
N353	0	High
V385	0	High
R386	0	High
N387	0	High
S388	0	High
H389	0	High
T415	0	High
Q419	0	High
R424	0	High
H425	0	High
M437	0	High
M443	0	High
D459	0	High
Q463	0	High
V469	0	High
M470	0	High
R471	0	High
D221	0	High
Q222	0	High
M221	0	High
R222	0	High
R196	0	High
S178	0	High
D179	0	High
S180	0	High
D220	0	High
R221	0	High
D222	0	High
M221	0	High
R222	0	High
R196	0	High
S178	0	High
D179	0	High
S180	0	High
D220	0	High
R221	0	High
D222	0	High
M221	0	High
R222	0	High
R196	0	High
S178	0	High
D179	0	High
S180	0	High

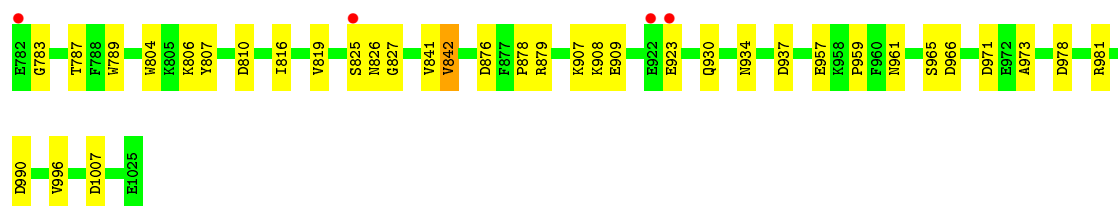
Chain C:

29% 84% 14%

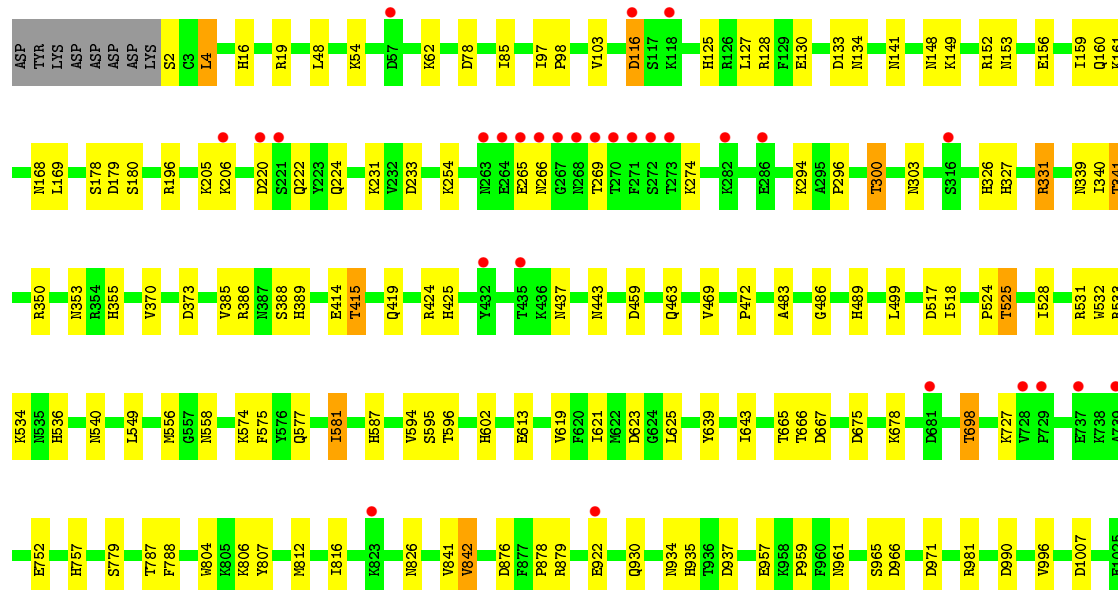
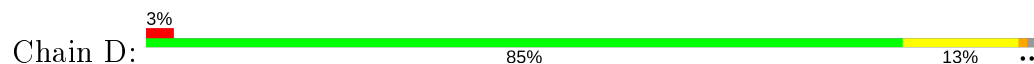
ASP TYR LYS ASP ASP ASP ASP LYS S2 C3 L4 E17 M18 R19 L48 T85 I97 P98 L115 E121 H125 R126 L127 E130 N141 M148 K149 R152 N153 G154 I159 Q160 N168 L169 S178 D179 S180 W189 R196 K206 D220 S231

Q222 Y223 Q224 E264 E265 E266 G267 N268 T269 T270 F271 S272 T273 I277 T281 A295 P296 T300 N303 H326 H327 R331 Q332 V333 N339 I340 T341 V352 N353 H354 R355 D356 V385 R386 N387 S388 H389 E410 G411 K412 L549 G553 M556 G557 N558 K574 F575 Y576 Q577 I581 W582 R583

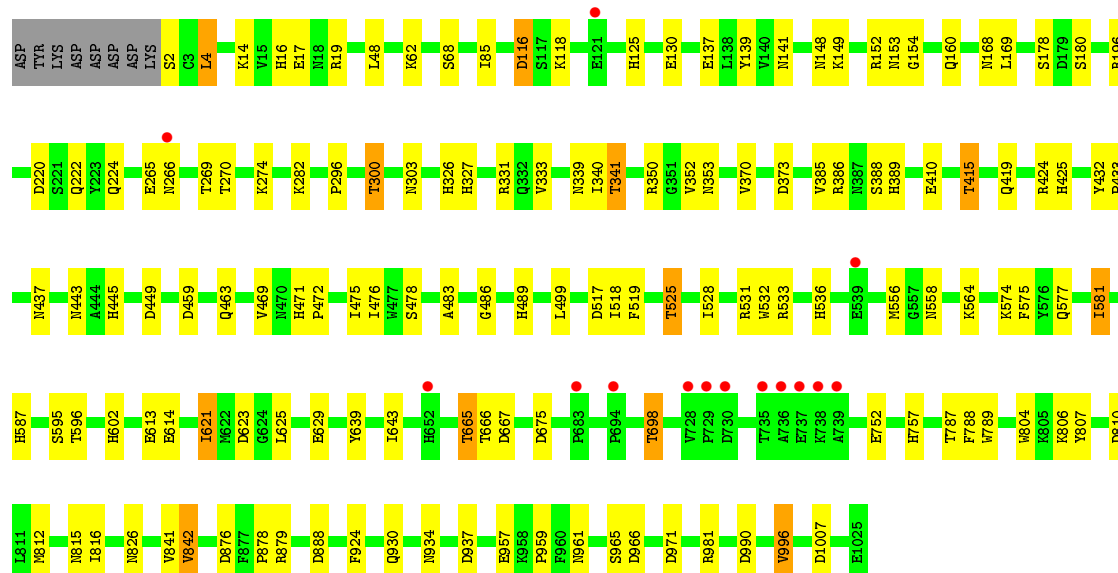
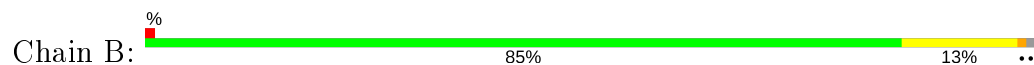
H587 E592 E593 V594 S595 T596 H602 E613 I621 M622 D623 G624 L625 Y639 I643 H647 I657 T665 T666 D667 D675 T676 G677 V691 D696 T697 T698 V703 G714 G717 P729 D730 E737 E752 H757 K762 K766 S779



• 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.77Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.207 , 0.243 0.206 , 0.242	Depositor DCC
R_{free} test set	6092 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 25.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [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 [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	1022/1032 (99%)	978 (96%)	42 (4%)	2 (0%)	47	69
1	B	1022/1032 (99%)	976 (96%)	44 (4%)	2 (0%)	47	69
1	C	1022/1032 (99%)	973 (95%)	47 (5%)	2 (0%)	47	69
1	D	1022/1032 (99%)	974 (95%)	46 (4%)	2 (0%)	47	69
All	All	4088/4128 (99%)	3901 (95%)	179 (4%)	8 (0%)	47	69

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%)	43	63
1	B	905/913 (99%)	881 (97%)	24 (3%)	44	65
1	C	905/913 (99%)	881 (97%)	24 (3%)	44	65
1	D	905/913 (99%)	881 (97%)	24 (3%)	44	65
All	All	3620/3652 (99%)	3523 (97%)	97 (3%)	44	65

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	C	1026	-	5,5,5	0.36	0	5,5,5	0.59	0
3	GOL	A	1026	-	5,5,5	0.47	0	5,5,5	0.09	0
3	GOL	C	1029	-	5,5,5	0.41	0	5,5,5	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	B	1026	-	5,5,5	0.41	0	5,5,5	0.46	0
3	GOL	C	1028	-	5,5,5	0.43	0	5,5,5	0.30	0
3	GOL	D	1026	-	5,5,5	0.44	0	5,5,5	0.28	0
3	GOL	C	1027	-	5,5,5	0.40	0	5,5,5	0.29	0
3	GOL	A	1027	-	5,5,5	0.43	0	5,5,5	0.35	0
3	GOL	B	1027	-	5,5,5	1.35	1 (20%)	5,5,5	0.87	0
3	GOL	D	1027	-	5,5,5	0.40	0	5,5,5	0.46	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	C	1026	-	-	2/4/4/4	-
3	GOL	A	1026	-	-	2/4/4/4	-
3	GOL	C	1029	-	-	2/4/4/4	-
3	GOL	B	1026	-	-	2/4/4/4	-
3	GOL	C	1028	-	-	4/4/4/4	-
3	GOL	D	1026	-	-	2/4/4/4	-
3	GOL	C	1027	-	-	2/4/4/4	-
3	GOL	A	1027	-	-	2/4/4/4	-
3	GOL	B	1027	-	-	4/4/4/4	-
3	GOL	D	1027	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1027	GOL	O2-C2	-2.41	1.36	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1026	GOL	C1-C2-C3-O3
3	C	1026	GOL	O2-C2-C3-O3
3	A	1026	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	B	1026	GOL	O1-C1-C2-O2
3	B	1026	GOL	O1-C1-C2-C3
3	C	1028	GOL	O1-C1-C2-C3
3	C	1028	GOL	C1-C2-C3-O3
3	C	1027	GOL	C1-C2-C3-O3
3	C	1027	GOL	O2-C2-C3-O3
3	B	1027	GOL	C1-C2-C3-O3
3	D	1027	GOL	C1-C2-C3-O3
3	D	1027	GOL	O2-C2-C3-O3
3	C	1029	GOL	O1-C1-C2-C3
3	A	1027	GOL	C1-C2-C3-O3
3	A	1026	GOL	O2-C2-C3-O3
3	C	1028	GOL	O1-C1-C2-O2
3	C	1028	GOL	O2-C2-C3-O3
3	B	1027	GOL	O2-C2-C3-O3
3	B	1027	GOL	O1-C1-C2-O2
3	C	1029	GOL	O1-C1-C2-O2
3	D	1026	GOL	C1-C2-C3-O3
3	A	1027	GOL	O2-C2-C3-O3
3	B	1027	GOL	O1-C1-C2-C3
3	D	1026	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1026	GOL	6	0
3	C	1029	GOL	2	0
3	C	1028	GOL	3	0
3	B	1027	GOL	4	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1024/1032 (99%)	-0.14	7 (0%) 87 91	8, 17, 37, 62	0
1	B	1024/1032 (99%)	-0.15	14 (1%) 75 82	8, 17, 37, 62	0
1	C	1024/1032 (99%)	0.00	23 (2%) 62 70	8, 17, 37, 62	0
1	D	1024/1032 (99%)	-0.04	29 (2%) 53 62	8, 17, 37, 62	0
All	All	4096/4128 (99%)	-0.08	73 (1%) 68 76	8, 17, 37, 62	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	270	THR	11.6
1	D	273	THR	11.3
1	D	266	ASN	10.5
1	C	272	SER	10.4
1	D	267	GLY	9.9
1	C	267	GLY	9.7
1	C	268	ASN	9.3
1	C	273	THR	8.9
1	D	271	PHE	8.2
1	D	268	ASN	8.1
1	C	270	THR	7.9
1	D	272	SER	7.6
1	D	269	THR	7.3
1	C	271	PHE	7.1
1	C	266	ASN	7.0
1	C	269	THR	5.8
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	3.2
1	B	736	ALA	3.2
1	C	206	LYS	3.2
1	B	739	ALA	3.1
1	C	825	SER	3.1
1	D	681	ASP	3.1
1	C	737	GLU	3.0
1	D	206	LYS	3.0
1	A	730	ASP	3.0
1	C	923	GLU	2.9
1	D	282	LYS	2.9
1	B	694	PRO	2.9
1	D	728	VAL	2.9
1	D	729	PRO	2.8
1	C	922	GLU	2.8
1	D	57	ASP	2.8
1	B	738	LYS	2.7
1	B	735	THR	2.7
1	B	730	ASP	2.6
1	B	728	VAL	2.6
1	D	435	THR	2.6
1	D	432	TYR	2.6
1	B	266	ASN	2.6
1	D	263	ASN	2.5
1	C	696	ASP	2.5
1	D	220	ASP	2.5
1	A	728	VAL	2.4
1	D	221	SER	2.4
1	B	539	GLU	2.4
1	B	729	PRO	2.4
1	A	738	LYS	2.4
1	D	739	ALA	2.4
1	B	121	GLU	2.4
1	B	683	PRO	2.4
1	A	291	ILE	2.4
1	D	264	GLU	2.3
1	A	827	GLY	2.3
1	C	540	ASN	2.3
1	B	737	GLU	2.3
1	C	730	ASP	2.3
1	D	116	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	121	GLU	2.2
1	C	277	ILE	2.2
1	C	677	GLY	2.2
1	D	922	GLU	2.2
1	D	118	LYS	2.2
1	D	823	LYS	2.1
1	C	782	GLU	2.1
1	A	266	ASN	2.1
1	D	316	SER	2.1
1	D	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	D	1026	6/6	0.57	0.47	49,50,51,51	0
3	GOL	C	1026	6/6	0.83	0.32	25,26,29,30	0
3	GOL	A	1026	6/6	0.91	0.22	29,29,30,30	0
3	GOL	B	1027	6/6	0.92	0.17	12,15,16,18	0
3	GOL	C	1028	6/6	0.93	0.20	17,19,19,19	0
3	GOL	C	1027	6/6	0.94	0.14	16,16,16,18	0
3	GOL	C	1029	6/6	0.94	0.15	10,10,11,11	0
3	GOL	B	1026	6/6	0.95	0.15	22,23,23,24	0
3	GOL	D	1027	6/6	0.96	0.15	10,11,12,14	0
3	GOL	A	1027	6/6	0.97	0.13	21,22,22,23	0
2	MN3	C	2001	1/1	0.97	0.09	8,8,8,8	0
2	MN3	D	2001	1/1	0.98	0.09	11,11,11,11	0
2	MN3	A	2001	1/1	0.99	0.09	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MN3	B	2001	1/1	0.99	0.09	8,8,8,8	0

6.5 Other polymers [i](#)

There are no such residues in this entry.