



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:55 am GMT

PDB ID : 3OB8
Title : Structure of the beta-galactosidase from Kluyveromyces lactis in complex with galactose
Authors : Fernandez-Leiro, R.; Pereira-Rodriguez, A.; Becerra, M.; Gonzalez-Siso, I.; Cerdan, M.E.; Sanz-Aparicio, J.
Deposited on : 2010-08-06
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (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

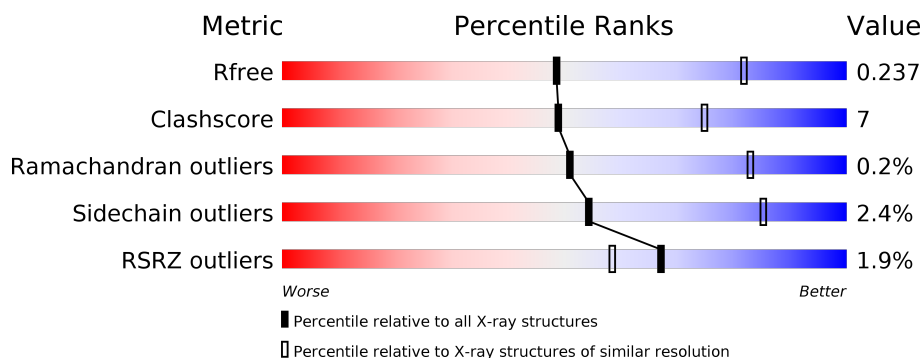
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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 13%, green 85%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 85% 13% .. </div> </div>
1	B	1032	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 13%, green 85%, grey 8%);"></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 2%, yellow 12%, green 86%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 86% 12% .. </div> </div>
1	D	1032	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 13%, green 85%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 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	MG	A	3001	-	-	-	X
3	MG	B	3001	-	-	-	X
4	NA	B	3002	-	-	-	X
4	NA	D	3002	-	-	-	X
4	NA	D	3006	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 34419 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	B	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	C	1024	Total	C	N	O	S	0	0	0
			8325	5335	1388	1587	15			

There are 32 discrepancies between the modelled and reference sequences:

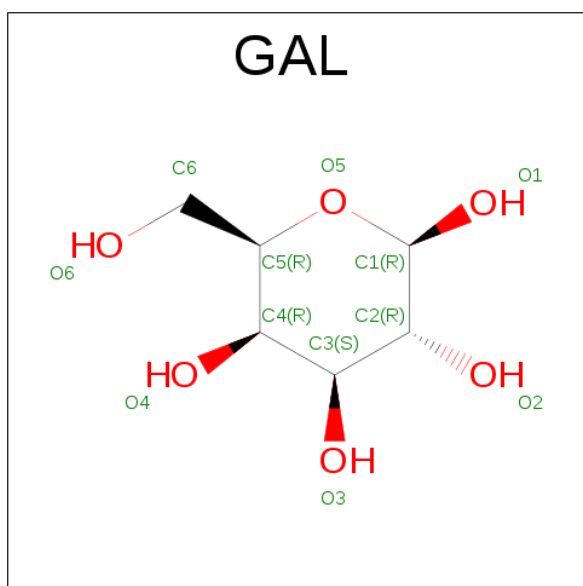
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ASP	-	EXPRESSION TAG	UNP P00723
A	-5	TYR	-	EXPRESSION TAG	UNP P00723
A	-4	LYS	-	EXPRESSION TAG	UNP P00723
A	-3	ASP	-	EXPRESSION TAG	UNP P00723
A	-2	ASP	-	EXPRESSION TAG	UNP P00723
A	-1	ASP	-	EXPRESSION TAG	UNP P00723
A	0	ASP	-	EXPRESSION TAG	UNP P00723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

Continued on next page...

Continued from previous page...

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
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

- Molecule 2 is SUGAR (BETA-D-GALACTOSE) (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		
2	D	1	Total	C	O	0	0
			12	6	6		
2	C	1	Total	C	O	0	0
			12	6	6		

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

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	4	Total Na 4 4	0	0
4	A	4	Total Na 4 4	0	0
4	D	4	Total Na 4 4	0	0
4	C	4	Total Na 4 4	0	0

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	231	Total O 231 231	0	0
6	B	293	Total O 293 293	0	0
6	D	253	Total O 253 253	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	270	Total	O	0	0
			270	270		

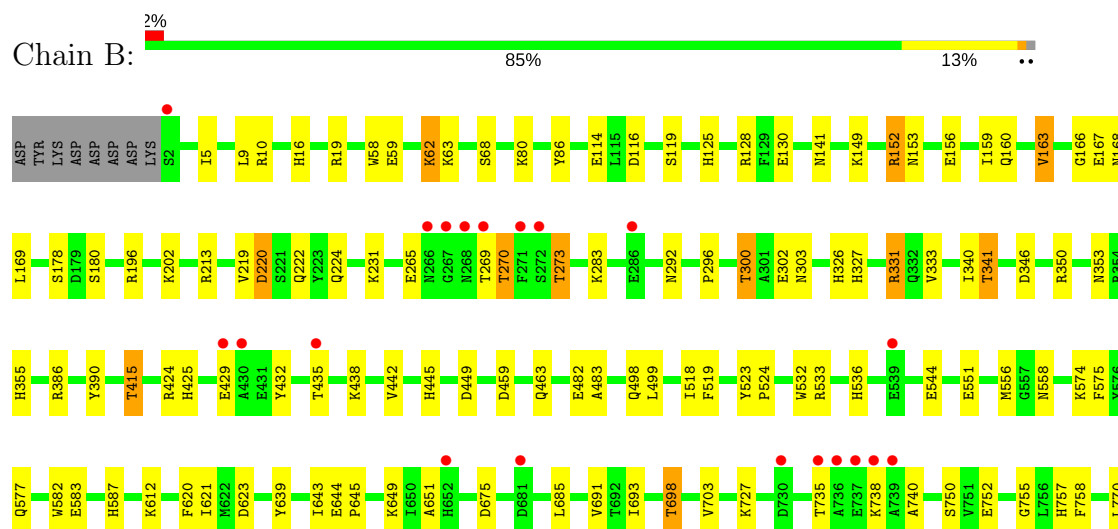
3 Residue-property plots [i](#)

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

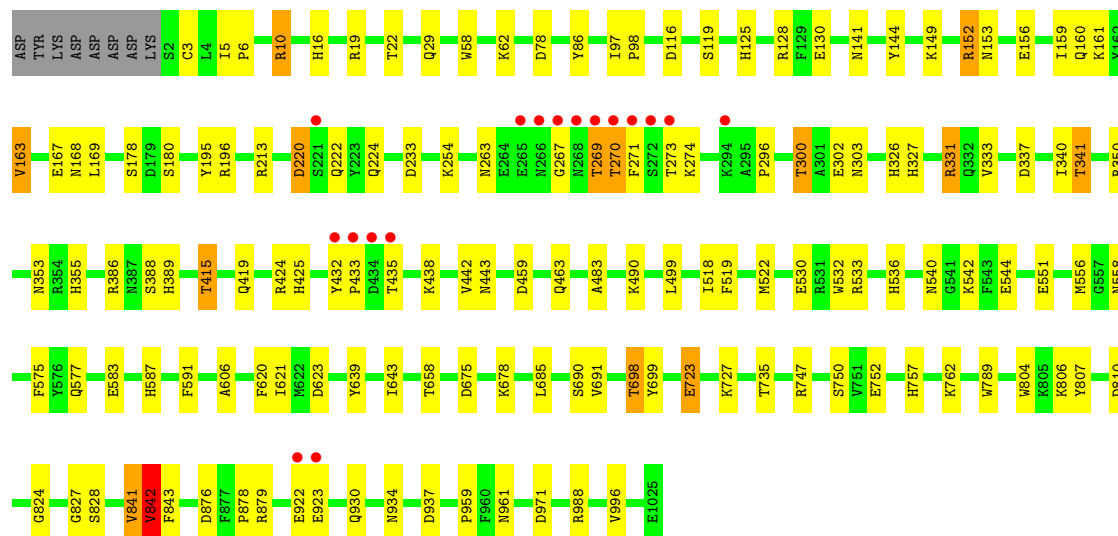
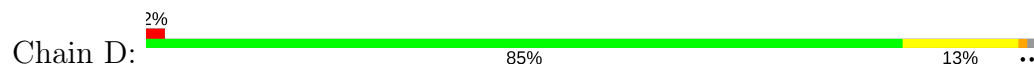


• Molecule 1: Beta-galactosidase

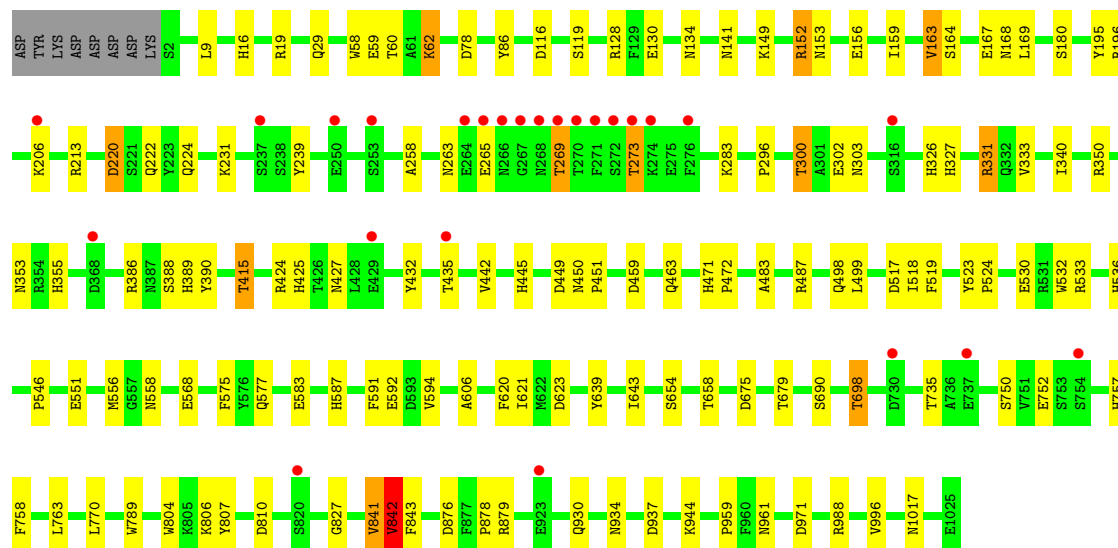
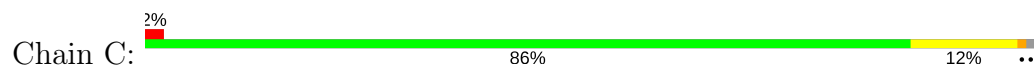




• Molecule 1: Beta-galactosidase



• Molecule 1: Beta-galactosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	140.38Å 153.45Å 217.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.30 – 2.80 49.30 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.30-2.80) 99.9 (49.30-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.35 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.214 , 0.246 0.209 , 0.237	Depositor DCC
R_{free} test set	5800 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	34419	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MG, MN, GAL

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	0.49	5/8561 (0.1%)	0.56	1/11614 (0.0%)
1	B	0.50	5/8561 (0.1%)	0.56	0/11614
1	C	0.51	5/8561 (0.1%)	0.57	0/11614
1	D	0.51	5/8561 (0.1%)	0.56	0/11614
All	All	0.50	20/34244 (0.1%)	0.56	1/46456 (0.0%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	843	PHE	CD2-CE2	-5.80	1.27	1.39
1	B	843	PHE	CD2-CE2	-5.80	1.27	1.39
1	A	843	PHE	CD2-CE2	-5.79	1.27	1.39
1	D	843	PHE	CD2-CE2	-5.78	1.27	1.39
1	B	843	PHE	CD1-CE1	-5.48	1.28	1.39
1	D	843	PHE	CD1-CE1	-5.48	1.28	1.39
1	C	843	PHE	CD1-CE1	-5.48	1.28	1.39
1	A	843	PHE	CD1-CE1	-5.48	1.28	1.39
1	D	843	PHE	CE2-CZ	-5.31	1.27	1.37
1	B	843	PHE	CE2-CZ	-5.29	1.27	1.37
1	A	843	PHE	CE2-CZ	-5.27	1.27	1.37
1	C	843	PHE	CE2-CZ	-5.25	1.27	1.37
1	D	841	VAL	CB-CG1	-5.08	1.42	1.52
1	C	841	VAL	CB-CG1	-5.05	1.42	1.52
1	B	841	VAL	CB-CG2	-5.04	1.42	1.52
1	A	841	VAL	CB-CG1	-5.04	1.42	1.52
1	A	841	VAL	CB-CG2	-5.04	1.42	1.52
1	C	841	VAL	CB-CG2	-5.03	1.42	1.52
1	B	841	VAL	CB-CG1	-5.03	1.42	1.52
1	D	841	VAL	CB-CG2	-5.03	1.42	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	ASP	CB-CG-OD2	5.07	122.87	118.30

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	119	0
1	B	8325	0	7972	126	0
1	C	8325	0	7972	112	1
1	D	8325	0	7972	120	1
2	A	12	0	12	1	0
2	B	12	0	12	1	0
2	C	12	0	11	1	0
2	D	12	0	11	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	231	0	0	19	0
6	B	293	0	0	34	0
6	C	270	0	0	28	0
6	D	253	0	0	32	0
All	All	34419	0	31934	446	1

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 (446) 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:587:HIS:HB2	1:C:621:ILE:HG13	1.28	1.11
1:D:587:HIS:HB2	1:D:621:ILE:HG13	1.27	1.09
1:B:587:HIS:HB2	1:B:621:ILE:HG13	1.29	1.07
1:A:587:HIS:HB2	1:A:621:ILE:HG13	1.29	1.06
1:B:841:VAL:O	1:B:842:VAL:HG13	1.56	1.06
1:C:841:VAL:O	1:C:842:VAL:HG13	1.56	1.05
1:D:841:VAL:O	1:D:842:VAL:HG13	1.56	1.05
1:A:841:VAL:O	1:A:842:VAL:HG13	1.56	1.04
1:C:164:SER:HB2	6:C:1127:HOH:O	1.56	1.03
1:D:691:VAL:HB	6:D:1141:HOH:O	1.56	1.02
1:A:712:LYS:HD2	6:A:1074:HOH:O	1.61	1.00
1:A:340:ILE:H	1:A:577:GLN:HE22	1.13	0.96
1:D:340:ILE:H	1:D:577:GLN:HE22	1.07	0.93
1:D:540:ASN:HA	6:D:1079:HOH:O	1.68	0.92
1:C:340:ILE:H	1:C:577:GLN:HE22	1.07	0.92
1:D:438:LYS:HG3	6:D:1271:HOH:O	1.72	0.89
1:D:270:THR:HG21	6:D:1200:HOH:O	1.71	0.88
1:B:340:ILE:H	1:B:577:GLN:HE22	1.12	0.88
1:B:612:LYS:HE2	6:B:1204:HOH:O	1.73	0.86
1:D:29:GLN:HG3	6:D:1032:HOH:O	1.75	0.85
1:B:544:GLU:HG2	6:B:1130:HOH:O	1.75	0.85
1:A:596:THR:HG21	6:A:1086:HOH:O	1.78	0.83
6:A:1181:HOH:O	1:B:114:GLU:HG3	1.80	0.82
1:D:271:PHE:HB3	6:D:1185:HOH:O	1.80	0.81
1:B:283:LYS:HE2	6:B:1238:HOH:O	1.79	0.80
1:A:153:ASN:HB3	1:A:463:GLN:HG2	1.64	0.80
1:C:841:VAL:O	1:C:842:VAL:CG1	2.30	0.79
1:A:841:VAL:O	1:A:842:VAL:CG1	2.30	0.79
1:D:841:VAL:C	1:D:842:VAL:CG1	2.51	0.79
1:B:649:LYS:HE2	6:B:1162:HOH:O	1.81	0.79
1:B:841:VAL:C	1:B:842:VAL:CG1	2.51	0.79
1:D:490:LYS:HE3	6:D:1203:HOH:O	1.80	0.79
1:A:841:VAL:C	1:A:842:VAL:CG1	2.51	0.78
1:B:841:VAL:O	1:B:842:VAL:CG1	2.30	0.78
1:C:841:VAL:C	1:C:842:VAL:CG1	2.51	0.78
1:B:498:GLN:HG2	6:B:1099:HOH:O	1.82	0.78
1:B:740:ALA:HB3	6:B:1194:HOH:O	1.83	0.78
1:C:592:GLU:HG2	6:C:1199:HOH:O	1.82	0.77
1:D:841:VAL:O	1:D:842:VAL:CG1	2.30	0.77
1:B:153:ASN:HB3	1:B:463:GLN:HG2	1.68	0.76
1:D:153:ASN:HB3	1:D:463:GLN:HG2	1.66	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:957:GLU:HB3	6:B:1132:HOH:O	1.86	0.76
1:C:153:ASN:HB3	1:C:463:GLN:HG2	1.67	0.76
1:D:340:ILE:N	1:D:577:GLN:HE22	1.84	0.74
1:B:752:GLU:HG2	1:B:757:HIS:CD2	2.23	0.74
1:B:340:ILE:N	1:B:577:GLN:HE22	1.86	0.74
1:A:752:GLU:HG2	1:A:757:HIS:CD2	2.24	0.73
1:B:80:LYS:HE3	6:B:1272:HOH:O	1.89	0.73
1:B:848:GLU:HG3	6:B:1128:HOH:O	1.88	0.72
1:B:341:THR:HG22	6:B:1127:HOH:O	1.89	0.71
1:C:340:ILE:N	1:C:577:GLN:HE22	1.84	0.71
1:B:425:HIS:HE1	6:B:1093:HOH:O	1.73	0.71
1:B:346:ASP:O	1:B:346:ASP:OD1	2.09	0.70
1:B:934:ASN:HD21	1:B:961:ASN:HB3	1.56	0.70
1:A:340:ILE:N	1:A:577:GLN:HE22	1.87	0.70
1:C:752:GLU:HG2	1:C:757:HIS:CD2	2.27	0.70
1:D:536:HIS:HE1	6:D:1124:HOH:O	1.75	0.70
1:B:58:TRP:O	1:B:62:LYS:HB2	1.92	0.69
1:B:231:LYS:HE2	6:B:1116:HOH:O	1.90	0.69
1:C:265:GLU:HG2	6:C:1172:HOH:O	1.91	0.69
1:C:415:THR:HG21	6:C:1249:HOH:O	1.92	0.68
1:C:679:THR:HG21	6:C:1228:HOH:O	1.92	0.68
1:D:752:GLU:HG2	1:D:757:HIS:CD2	2.28	0.68
1:D:271:PHE:HZ	6:D:1226:HOH:O	1.77	0.68
1:B:842:VAL:CG2	1:B:842:VAL:O	2.42	0.68
1:A:934:ASN:HD21	1:A:961:ASN:HB3	1.58	0.67
1:B:551:GLU:OE1	2:B:2001:GAL:H1	1.94	0.67
1:C:58:TRP:O	1:C:62:LYS:HB2	1.94	0.67
1:C:934:ASN:HD21	1:C:961:ASN:HB3	1.58	0.67
1:A:842:VAL:CG2	1:A:842:VAL:O	2.42	0.67
1:D:934:ASN:HD21	1:D:961:ASN:HB3	1.60	0.67
1:B:438:LYS:HB2	6:B:1282:HOH:O	1.93	0.67
1:A:58:TRP:O	1:A:62:LYS:HB2	1.94	0.67
1:C:842:VAL:CG2	1:C:842:VAL:O	2.42	0.66
1:C:60:THR:HG23	6:C:1132:HOH:O	1.94	0.66
1:D:213:ARG:NH2	1:D:499:LEU:O	2.29	0.66
1:D:842:VAL:CG2	1:D:842:VAL:O	2.42	0.66
1:C:220:ASP:OD2	1:C:222:GLN:HG2	1.95	0.66
1:B:888:ASP:HB3	6:B:1273:HOH:O	1.96	0.66
1:A:116:ASP:H	1:B:270:THR:HG21	1.61	0.66
1:A:116:ASP:HB2	1:B:270:THR:HG21	1.77	0.66
1:A:755:GLY:HA2	1:D:78:ASP:OD1	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ASP:HB2	1:B:270:THR:CG2	2.27	0.65
1:B:213:ARG:NH2	1:B:499:LEU:O	2.30	0.64
1:A:213:ARG:NH2	1:A:499:LEU:O	2.30	0.64
1:C:533:ARG:HG3	1:C:575:PHE:CD2	2.32	0.64
1:C:587:HIS:CB	1:C:621:ILE:HG13	2.18	0.64
1:A:568:GLU:HG3	6:A:1202:HOH:O	1.97	0.64
1:D:267:GLY:HA2	6:D:1208:HOH:O	1.97	0.64
1:C:675:ASP:OD2	1:C:698:THR:HB	1.98	0.64
1:C:213:ARG:NH2	1:C:499:LEU:O	2.31	0.63
1:C:558:ASN:H	1:C:930:GLN:NE2	1.97	0.63
1:D:58:TRP:O	1:D:62:LYS:HB2	1.98	0.63
1:D:842:VAL:HG23	1:D:842:VAL:O	1.99	0.63
1:A:842:VAL:HG23	1:A:842:VAL:O	1.99	0.63
1:B:842:VAL:HG23	1:B:842:VAL:O	1.99	0.63
1:D:116:ASP:HB2	6:D:1090:HOH:O	1.99	0.63
1:D:587:HIS:CB	1:D:621:ILE:HG13	2.17	0.63
1:C:1017:ASN:HB3	6:C:1138:HOH:O	1.98	0.62
1:B:587:HIS:CB	1:B:621:ILE:HG13	2.18	0.62
1:B:533:ARG:HG3	1:B:575:PHE:CD2	2.34	0.62
1:C:842:VAL:HG23	1:C:842:VAL:O	1.99	0.62
1:D:533:ARG:HG3	1:D:575:PHE:CD2	2.35	0.62
1:B:841:VAL:C	1:B:842:VAL:HG12	2.19	0.62
1:D:220:ASP:OD2	1:D:222:GLN:HG2	1.99	0.62
1:D:841:VAL:C	1:D:842:VAL:HG12	2.19	0.62
1:D:639:TYR:O	1:D:643:ILE:HG12	2.00	0.62
1:A:533:ARG:HG3	1:A:575:PHE:CD2	2.35	0.62
1:A:841:VAL:C	1:A:842:VAL:HG12	2.19	0.62
1:B:639:TYR:O	1:B:643:ILE:HG12	2.01	0.61
1:C:841:VAL:C	1:C:842:VAL:HG12	2.19	0.61
1:A:220:ASP:OD2	1:A:222:GLN:HG2	2.00	0.61
1:A:273:THR:HG21	1:B:166:GLY:HA2	1.82	0.61
1:B:220:ASP:OD2	1:B:222:GLN:HG2	2.00	0.61
1:D:341:THR:HG22	6:D:1137:HOH:O	2.00	0.61
1:A:664:ILE:HA	6:A:1219:HOH:O	1.99	0.61
1:C:29:GLN:HB2	6:C:1264:HOH:O	2.00	0.61
1:C:639:TYR:O	1:C:643:ILE:HG12	2.01	0.60
1:A:587:HIS:CB	1:A:621:ILE:HG13	2.19	0.60
1:C:283:LYS:HE2	6:C:1107:HOH:O	2.01	0.60
1:B:823:LYS:HE2	6:B:1172:HOH:O	2.01	0.60
1:C:415:THR:HB	1:C:483:ALA:HA	1.84	0.60
1:D:415:THR:HB	1:D:483:ALA:HA	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:ARG:O	1:D:806:LYS:HE2	2.02	0.59
1:C:340:ILE:H	1:C:577:GLN:NE2	1.90	0.59
1:A:300:THR:HG22	1:A:302:GLU:H	1.68	0.59
1:B:425:HIS:HD2	1:D:807:TYR:OH	1.86	0.59
1:B:59:GLU:CB	6:B:1182:HOH:O	2.50	0.58
1:B:675:ASP:OD2	1:B:698:THR:HB	2.03	0.58
1:D:340:ILE:H	1:D:577:GLN:NE2	1.90	0.58
1:D:556:MET:HA	1:D:623:ASP:HA	1.85	0.58
1:A:340:ILE:H	1:A:577:GLN:NE2	1.94	0.57
1:A:415:THR:HB	1:A:483:ALA:HA	1.85	0.57
1:A:424:ARG:O	1:C:806:LYS:HE2	2.05	0.57
1:A:675:ASP:OD2	1:A:698:THR:HB	2.04	0.57
1:C:141:ASN:ND2	1:C:169:LEU:H	2.03	0.57
1:D:153:ASN:CB	1:D:463:GLN:HG2	2.33	0.57
1:D:551:GLU:OE1	2:D:2001:GAL:H1	2.05	0.57
1:A:728:VAL:HG23	6:A:1079:HOH:O	2.04	0.56
1:C:239:TYR:HE2	6:C:1290:HOH:O	1.87	0.56
1:C:300:THR:HG22	1:C:302:GLU:H	1.70	0.56
1:A:274:LYS:HD3	6:A:1245:HOH:O	2.04	0.56
1:C:757:HIS:HB3	6:C:1045:HOH:O	2.05	0.56
1:C:263:ASN:HA	6:C:1073:HOH:O	2.05	0.56
1:C:463:GLN:NE2	6:C:1244:HOH:O	2.39	0.56
1:D:128:ARG:HB2	1:D:156:GLU:HG2	1.87	0.56
1:C:331:ARG:C	1:C:331:ARG:HD3	2.26	0.56
1:A:806:LYS:HE2	1:C:424:ARG:O	2.05	0.56
1:B:556:MET:HA	1:B:623:ASP:HA	1.87	0.56
1:B:651:ALA:HA	6:B:1149:HOH:O	2.06	0.56
1:A:556:MET:HA	1:A:623:ASP:HA	1.89	0.55
1:A:739:ALA:HB1	6:A:1143:HOH:O	2.06	0.55
1:D:29:GLN:HB3	6:D:1028:HOH:O	2.05	0.55
1:B:300:THR:HG22	1:B:302:GLU:H	1.72	0.55
1:B:219:VAL:HG12	6:B:1098:HOH:O	2.06	0.55
1:D:300:THR:HG22	1:D:303:ASN:H	1.71	0.55
1:D:675:ASP:OD2	1:D:698:THR:HB	2.07	0.55
1:A:153:ASN:CB	1:A:463:GLN:HG2	2.35	0.55
1:C:355:HIS:HE1	6:C:1065:HOH:O	1.88	0.55
1:C:556:MET:HA	1:C:623:ASP:HA	1.87	0.55
1:B:727:LYS:HE3	6:B:1124:HOH:O	2.06	0.54
1:B:86:TYR:CE1	1:B:621:ILE:HD13	2.42	0.54
1:D:350:ARG:HD3	1:D:643:ILE:O	2.06	0.54
1:B:340:ILE:H	1:B:577:GLN:NE2	1.93	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:THR:HB	1:B:483:ALA:HA	1.90	0.54
1:D:141:ASN:ND2	1:D:169:LEU:H	2.05	0.54
1:D:263:ASN:HA	6:D:1123:HOH:O	2.07	0.54
1:D:331:ARG:HD3	1:D:331:ARG:C	2.27	0.54
1:B:346:ASP:OD2	1:B:574:LYS:HE2	2.07	0.54
1:A:804:TRP:CE3	1:A:878:PRO:HG3	2.43	0.53
1:D:558:ASN:H	1:D:930:GLN:NE2	2.06	0.53
1:A:341:THR:HG22	6:A:1126:HOH:O	2.08	0.53
1:B:153:ASN:CB	1:B:463:GLN:HG2	2.37	0.53
1:A:270:THR:HG21	1:B:116:ASP:H	1.72	0.53
1:B:128:ARG:HB2	1:B:156:GLU:HG2	1.91	0.53
1:B:353:ASN:OD1	1:B:386:ARG:HD3	2.08	0.53
1:C:153:ASN:CB	1:C:463:GLN:HG2	2.36	0.53
1:A:300:THR:HG22	1:A:303:ASN:H	1.73	0.53
1:A:300:THR:HG22	1:A:302:GLU:N	2.24	0.53
1:C:415:THR:O	1:C:415:THR:CG2	2.56	0.53
1:D:415:THR:O	1:D:415:THR:CG2	2.57	0.53
1:D:161:LYS:HE2	6:D:1263:HOH:O	2.09	0.53
1:D:300:THR:HG22	1:D:302:GLU:N	2.24	0.53
1:B:738:LYS:HE3	6:B:1047:HOH:O	2.09	0.53
1:B:152:ARG:HD2	1:B:152:ARG:N	2.25	0.52
1:D:300:THR:HG22	1:D:302:GLU:H	1.73	0.52
1:B:558:ASN:H	1:B:930:GLN:NE2	2.07	0.52
1:B:300:THR:HG22	1:B:303:ASN:H	1.73	0.52
1:C:331:ARG:O	1:C:331:ARG:HD3	2.09	0.52
6:B:1207:HOH:O	1:C:594:VAL:HG21	2.09	0.52
1:D:141:ASN:HD21	1:D:168:ASN:HA	1.75	0.52
1:B:63:LYS:HE3	6:B:1095:HOH:O	2.09	0.52
1:C:128:ARG:HB2	1:C:156:GLU:HG2	1.91	0.52
1:C:141:ASN:HD21	1:C:168:ASN:HA	1.74	0.52
1:A:415:THR:CG2	1:A:415:THR:O	2.59	0.51
1:B:331:ARG:HD3	1:B:331:ARG:C	2.30	0.51
1:A:331:ARG:C	1:A:331:ARG:HD3	2.31	0.51
1:C:532:TRP:O	1:C:536:HIS:HD2	1.94	0.51
1:C:944:LYS:HE2	6:C:1150:HOH:O	2.09	0.51
1:D:337:ASP:HB3	6:D:1199:HOH:O	2.10	0.51
1:D:583:GLU:OE1	1:D:587:HIS:NE2	2.36	0.51
1:B:806:LYS:HE2	1:D:424:ARG:O	2.11	0.51
1:B:19:ARG:NH2	1:B:459:ASP:OD1	2.42	0.51
1:C:130:GLU:HB2	1:C:196:ARG:HB3	1.92	0.51
1:D:270:THR:CG2	6:D:1200:HOH:O	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:HIS:CD2	1:A:19:ARG:H	2.29	0.51
1:B:415:THR:CG2	1:B:415:THR:O	2.58	0.51
1:B:425:HIS:CD2	1:D:807:TYR:OH	2.63	0.51
1:A:128:ARG:HB2	1:A:156:GLU:HG2	1.91	0.51
1:A:432:TYR:HB2	1:A:435:THR:HG22	1.92	0.51
1:B:935:HIS:HE1	6:B:1101:HOH:O	1.94	0.51
1:B:752:GLU:HG2	1:B:757:HIS:HD2	1.74	0.51
1:D:544:GLU:HG3	6:D:1193:HOH:O	2.10	0.51
1:B:130:GLU:HB2	1:B:196:ARG:HB3	1.92	0.51
1:B:300:THR:HG22	1:B:302:GLU:N	2.25	0.50
1:C:789:TRP:CE3	1:C:810:ASP:HB3	2.46	0.50
1:C:152:ARG:HD2	1:C:152:ARG:N	2.27	0.50
1:A:130:GLU:HB2	1:A:196:ARG:HB3	1.94	0.50
1:A:752:GLU:HG2	1:A:757:HIS:HD2	1.76	0.50
1:B:804:TRP:CE3	1:B:878:PRO:HG3	2.46	0.50
1:A:558:ASN:H	1:A:930:GLN:NE2	2.09	0.50
1:D:331:ARG:O	1:D:331:ARG:HD3	2.12	0.50
1:C:353:ASN:OD1	1:C:386:ARG:HD3	2.11	0.50
1:C:350:ARG:HD3	1:C:643:ILE:O	2.12	0.50
1:B:789:TRP:CE3	1:B:810:ASP:HB3	2.47	0.49
1:C:224:GLN:O	1:C:296:PRO:HD2	2.12	0.49
1:D:130:GLU:HB2	1:D:196:ARG:HB3	1.93	0.49
1:B:141:ASN:HD21	1:B:168:ASN:HA	1.76	0.49
1:B:265:GLU:HB2	6:B:1190:HOH:O	2.12	0.49
1:C:879:ARG:NE	1:C:988:ARG:HD3	2.28	0.49
1:D:152:ARG:HD2	1:D:152:ARG:N	2.27	0.49
1:A:270:THR:CG2	1:B:116:ASP:HB2	2.43	0.49
1:B:59:GLU:HB2	6:B:1182:HOH:O	2.12	0.49
1:D:922:GLU:HB2	6:D:1172:HOH:O	2.13	0.49
1:A:929:PRO:HA	6:A:1246:HOH:O	2.13	0.49
1:B:149:LYS:HD3	1:B:180:SER:HB2	1.95	0.49
1:D:269:THR:HG22	6:D:1156:HOH:O	2.13	0.49
1:D:3:CYS:HA	6:D:1230:HOH:O	2.12	0.49
1:D:86:TYR:CE1	1:D:621:ILE:HD13	2.48	0.49
1:B:141:ASN:ND2	1:B:169:LEU:H	2.11	0.49
1:A:806:LYS:HE3	1:C:427:ASN:ND2	2.28	0.49
1:A:935:HIS:HE1	6:A:1121:HOH:O	1.96	0.48
1:B:879:ARG:NE	1:B:988:ARG:HD3	2.28	0.48
1:D:159:ILE:HG22	1:D:163:VAL:HG23	1.95	0.48
1:D:353:ASN:OD1	1:D:386:ARG:HD3	2.13	0.48
1:B:429:GLU:HG2	6:B:1262:HOH:O	2.11	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ASN:HD21	1:A:168:ASN:HA	1.79	0.48
1:C:432:TYR:HB2	1:C:435:THR:HG22	1.95	0.48
1:D:727:LYS:HE3	6:D:1076:HOH:O	2.13	0.48
1:A:435:THR:HG23	6:A:1078:HOH:O	2.13	0.48
1:A:639:TYR:O	1:A:643:ILE:HG12	2.12	0.48
1:B:5:ILE:HG13	1:B:10:ARG:HD3	1.96	0.48
1:D:923:GLU:HB2	6:D:1064:HOH:O	2.13	0.48
1:B:16:HIS:CD2	1:B:19:ARG:H	2.31	0.48
1:B:224:GLN:O	1:B:296:PRO:HD2	2.13	0.48
1:D:432:TYR:HB2	1:D:435:THR:HG22	1.94	0.48
1:A:141:ASN:ND2	1:A:169:LEU:H	2.11	0.48
1:C:300:THR:HG22	1:C:302:GLU:N	2.28	0.48
1:D:879:ARG:NE	1:D:988:ARG:HD3	2.28	0.48
1:A:551:GLU:OE1	2:A:2001:GAL:H1	2.14	0.47
1:B:432:TYR:HB2	1:B:435:THR:HG22	1.95	0.47
1:B:532:TRP:O	1:B:536:HIS:HD2	1.97	0.47
1:A:270:THR:HG21	1:B:116:ASP:HB2	1.97	0.47
1:D:224:GLN:O	1:D:296:PRO:HD2	2.14	0.47
1:D:518:ILE:HG22	1:D:519:PHE:O	2.14	0.47
1:A:603:LYS:HE2	6:A:1067:HOH:O	2.13	0.47
1:A:879:ARG:NE	1:A:988:ARG:HD3	2.29	0.47
1:D:532:TRP:O	1:D:536:HIS:HD2	1.96	0.47
1:D:698:THR:HG22	6:D:1051:HOH:O	2.14	0.47
1:D:789:TRP:CE3	1:D:810:ASP:HB3	2.50	0.47
1:A:19:ARG:NH2	1:A:459:ASP:OD1	2.48	0.47
1:A:350:ARG:HD3	1:A:643:ILE:O	2.15	0.47
1:A:22:THR:OG1	1:A:463:GLN:NE2	2.48	0.47
1:B:805:LYS:HE2	6:B:1250:HOH:O	2.14	0.47
1:B:350:ARG:HD3	1:B:643:ILE:O	2.15	0.47
1:C:789:TRP:CD2	1:C:810:ASP:HB3	2.50	0.47
1:A:152:ARG:N	1:A:152:ARG:HD2	2.30	0.46
1:A:326:HIS:CG	1:A:327:HIS:H	2.33	0.46
1:B:435:THR:HG23	6:B:1072:HOH:O	2.13	0.46
1:C:265:GLU:HB2	6:C:1084:HOH:O	2.14	0.46
1:C:206:LYS:HD2	6:C:1087:HOH:O	2.15	0.46
1:C:300:THR:HG22	1:C:303:ASN:H	1.80	0.46
1:A:353:ASN:OD1	1:A:386:ARG:HD3	2.15	0.46
1:A:86:TYR:CE1	1:A:621:ILE:HD13	2.50	0.46
1:C:86:TYR:CE1	1:C:621:ILE:HD13	2.51	0.46
1:D:16:HIS:CD2	1:D:19:ARG:H	2.33	0.46
1:A:789:TRP:CE3	1:A:810:ASP:HB3	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:937:ASP:HA	1:A:959:PRO:HB2	1.96	0.46
1:B:807:TYR:OH	1:D:425:HIS:HD2	1.97	0.46
1:D:149:LYS:HD3	1:D:180:SER:HB2	1.97	0.46
1:D:19:ARG:NH2	1:D:459:ASP:OD1	2.48	0.46
1:A:149:LYS:HD3	1:A:180:SER:HB2	1.96	0.46
1:C:116:ASP:HB3	1:C:119:SER:H	1.80	0.46
1:D:804:TRP:CE3	1:D:878:PRO:HG3	2.50	0.46
1:A:427:ASN:ND2	1:C:806:LYS:HE3	2.30	0.46
1:B:758:PHE:HD1	1:B:770:LEU:HD13	1.81	0.46
1:D:937:ASP:HA	1:D:959:PRO:HB2	1.97	0.46
1:B:879:ARG:HE	1:B:988:ARG:HD3	1.81	0.46
1:D:530:GLU:HG2	6:D:1219:HOH:O	2.16	0.46
1:A:178:SER:OG	1:A:180:SER:HB3	2.16	0.45
1:B:755:GLY:N	1:C:78:ASP:OD2	2.37	0.45
1:B:937:ASP:HA	1:B:959:PRO:HB2	1.98	0.45
1:C:16:HIS:CD2	1:C:19:ARG:H	2.34	0.45
1:C:220:ASP:HB3	6:C:1041:HOH:O	2.16	0.45
1:C:265:GLU:HG3	6:C:1067:HOH:O	2.17	0.45
1:C:879:ARG:HE	1:C:988:ARG:HD3	1.81	0.45
1:D:233:ASP:HB2	6:D:1122:HOH:O	2.16	0.45
1:D:326:HIS:CG	1:D:327:HIS:H	2.34	0.45
1:D:22:THR:OG1	1:D:463:GLN:NE2	2.50	0.45
1:B:116:ASP:HB3	1:B:119:SER:H	1.81	0.45
1:A:300:THR:CG2	1:A:302:GLU:H	2.29	0.45
1:A:804:TRP:CD2	1:A:878:PRO:HG3	2.52	0.45
1:C:326:HIS:CG	1:C:327:HIS:H	2.35	0.45
1:C:530:GLU:OE2	1:C:533:ARG:NH1	2.50	0.45
1:C:804:TRP:CE3	1:C:878:PRO:HG3	2.52	0.45
1:A:735:THR:HB	1:A:827:GLY:HA3	1.98	0.45
1:D:415:THR:O	1:D:415:THR:HG23	2.17	0.45
1:A:629:GLU:HG3	6:A:1071:HOH:O	2.16	0.44
1:B:1014:GLN:HB2	6:B:1026:HOH:O	2.17	0.44
1:B:292:ASN:HB2	6:B:1283:HOH:O	2.17	0.44
1:C:415:THR:O	1:C:415:THR:HG23	2.17	0.44
1:C:735:THR:HB	1:C:827:GLY:HA3	1.99	0.44
1:A:102:THR:HG22	1:C:763:LEU:HD12	1.99	0.44
1:D:125:HIS:HD2	1:D:160:GLN:OE1	2.00	0.44
1:D:699:TYR:HB2	6:D:1051:HOH:O	2.17	0.44
1:A:658:THR:HG23	1:A:690:SER:HB3	1.99	0.44
1:B:789:TRP:CD2	1:B:810:ASP:HB3	2.51	0.44
1:D:153:ASN:CG	1:D:463:GLN:HG2	2.38	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:ARG:CD	1:D:331:ARG:C	2.86	0.44
1:A:425:HIS:CD2	1:C:807:TYR:OH	2.71	0.44
1:D:723:GLU:HG3	6:D:1142:HOH:O	2.17	0.44
1:A:116:ASP:HB3	1:A:119:SER:H	1.82	0.44
1:A:879:ARG:HE	1:A:988:ARG:HD3	1.83	0.44
1:A:159:ILE:HG22	1:A:163:VAL:HG23	1.99	0.44
1:B:685:LEU:HD21	1:B:691:VAL:HG23	1.99	0.44
1:B:891:GLU:CD	6:B:1135:HOH:O	2.56	0.44
1:C:331:ARG:C	1:C:331:ARG:CD	2.86	0.44
1:D:735:THR:HB	1:D:827:GLY:HA3	2.00	0.44
1:A:806:LYS:HE3	1:C:427:ASN:HD21	1.83	0.44
1:A:738:LYS:HA	6:A:1110:HOH:O	2.18	0.44
1:A:532:TRP:O	1:A:536:HIS:HD2	2.01	0.43
1:B:755:GLY:HA2	1:C:78:ASP:OD1	2.17	0.43
1:C:19:ARG:NH2	1:C:459:ASP:OD1	2.48	0.43
1:D:5:ILE:HG13	1:D:10:ARG:HD3	2.00	0.43
1:D:178:SER:OG	1:D:180:SER:HB3	2.18	0.43
1:C:518:ILE:HG22	1:C:519:PHE:O	2.18	0.43
1:C:937:ASP:HA	1:C:959:PRO:HB2	1.99	0.43
1:C:355:HIS:HD2	1:C:390:TYR:OH	2.02	0.43
1:D:583:GLU:OE2	1:D:623:ASP:OD1	2.34	0.43
1:D:685:LEU:HD21	1:D:691:VAL:HG23	2.00	0.43
1:A:355:HIS:HD2	1:A:390:TYR:OH	2.02	0.43
1:A:386:ARG:HG3	1:A:408:ILE:HB	2.01	0.43
1:D:116:ASP:HB3	1:D:119:SER:H	1.83	0.43
1:D:879:ARG:HE	1:D:988:ARG:HD3	1.84	0.43
1:B:326:HIS:CG	1:B:327:HIS:H	2.36	0.43
1:A:388:SER:HA	1:A:389:HIS:HA	1.78	0.43
1:A:5:ILE:HG13	1:A:10:ARG:HD3	2.00	0.43
1:A:814:GLN:HG3	1:A:838:ILE:HG12	1.99	0.43
1:C:591:PHE:CD2	1:C:606:ALA:HB2	2.53	0.43
1:B:583:GLU:OE2	1:B:623:ASP:OD1	2.36	0.43
1:C:498:GLN:HG2	6:C:1170:HOH:O	2.18	0.43
1:A:270:THR:HG23	1:B:202:LYS:HZ1	1.84	0.43
1:B:300:THR:CG2	1:B:302:GLU:H	2.32	0.43
1:B:355:HIS:HD2	1:B:390:TYR:OH	2.02	0.43
1:B:621:ILE:HA	1:B:621:ILE:HD12	1.94	0.43
1:D:678:LYS:HD3	6:D:1136:HOH:O	2.19	0.43
1:B:178:SER:OG	1:B:180:SER:HB3	2.18	0.42
1:A:33:GLU:HA	1:B:265:GLU:OE1	2.19	0.42
1:B:735:THR:HB	1:B:827:GLY:HA3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:THR:HG23	1:A:415:THR:O	2.19	0.42
1:D:300:THR:CG2	1:D:302:GLU:H	2.32	0.42
1:D:355:HIS:HE1	6:D:1087:HOH:O	2.02	0.42
1:D:97:ILE:HA	1:D:98:PRO:HA	1.84	0.42
1:A:224:GLN:O	1:A:296:PRO:HD2	2.20	0.42
1:A:166:GLY:HA2	1:B:273:THR:HG21	2.01	0.42
1:A:363:ARG:HD3	6:A:1030:HOH:O	2.20	0.42
1:A:583:GLU:OE1	1:A:587:HIS:NE2	2.38	0.42
1:A:795:ASN:HB3	6:A:1049:HOH:O	2.19	0.42
1:B:415:THR:HG23	1:B:415:THR:O	2.19	0.42
1:B:445:HIS:HA	1:B:449:ASP:HB3	2.01	0.42
1:A:755:GLY:N	1:D:78:ASP:OD2	2.45	0.42
1:A:152:ARG:HG3	1:A:195:TYR:OH	2.19	0.42
1:B:482:GLU:HA	6:B:1078:HOH:O	2.19	0.42
1:C:149:LYS:HD3	1:C:180:SER:HB2	2.01	0.42
1:D:419:GLN:NE2	1:D:443:ASN:HB2	2.35	0.42
1:D:658:THR:HG23	1:D:690:SER:HB3	2.00	0.42
1:C:152:ARG:HG3	1:C:195:TYR:OH	2.20	0.42
1:D:254:LYS:HG2	6:D:1153:HOH:O	2.19	0.42
1:D:542:LYS:HD3	6:D:1052:HOH:O	2.20	0.42
1:A:530:GLU:OE2	1:A:533:ARG:NH1	2.53	0.42
1:C:388:SER:HA	1:C:389:HIS:HA	1.79	0.42
1:C:546:PRO:CB	1:C:577:GLN:HE21	2.33	0.42
1:D:388:SER:HA	1:D:389:HIS:HA	1.80	0.42
1:D:747:ARG:O	1:D:762:LYS:HB2	2.20	0.42
1:D:789:TRP:CD2	1:D:810:ASP:HB3	2.55	0.42
1:C:258:ALA:HB3	6:C:1237:HOH:O	2.20	0.42
1:C:551:GLU:OE1	2:C:2001:GAL:H1	2.19	0.42
1:D:591:PHE:CD2	1:D:606:ALA:HB2	2.55	0.42
1:A:115:LEU:HD23	1:A:115:LEU:HA	1.94	0.41
1:C:568:GLU:HG2	6:C:1074:HOH:O	2.19	0.41
1:A:355:HIS:HE1	6:A:1235:HOH:O	2.02	0.41
1:B:582:TRP:CD1	1:B:583:GLU:HB2	2.55	0.41
1:B:807:TYR:OH	1:D:425:HIS:CD2	2.73	0.41
1:C:269:THR:HG21	6:C:1084:HOH:O	2.19	0.41
1:D:432:TYR:HA	1:D:433:PRO:HD3	1.95	0.41
1:C:583:GLU:OE2	1:C:623:ASP:OD1	2.38	0.41
1:C:231:LYS:HG2	6:C:1047:HOH:O	2.20	0.41
1:C:517:ASP:O	1:C:518:ILE:HD13	2.20	0.41
1:C:758:PHE:HD1	1:C:770:LEU:HD13	1.85	0.41
1:B:125:HIS:HD2	1:B:160:GLN:OE1	2.04	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ILE:HG22	1:B:163:VAL:HG23	2.01	0.41
1:C:487:ARG:HB2	6:C:1211:HOH:O	2.20	0.41
1:D:5:ILE:HA	1:D:6:PRO:HD3	1.96	0.41
1:A:257:ASP:OD2	1:B:68:SER:HB2	2.21	0.41
1:C:450:ASN:HA	1:C:451:PRO:HD3	1.95	0.41
1:C:498:GLN:HG3	6:C:1062:HOH:O	2.21	0.41
1:A:523:TYR:N	1:A:524:PRO:HD3	2.36	0.41
1:B:523:TYR:N	1:B:524:PRO:HD3	2.36	0.41
1:C:658:THR:HG23	1:C:690:SER:HB3	2.02	0.41
1:A:425:HIS:HD2	1:C:807:TYR:OH	2.02	0.41
1:C:159:ILE:HG22	1:C:163:VAL:HG23	2.02	0.41
1:D:824:GLY:HA3	1:D:828:SER:O	2.20	0.41
1:A:897:GLY:O	1:A:913:PHE:HA	2.20	0.41
1:B:644:GLU:HA	1:B:645:PRO:HD3	1.99	0.41
1:C:59:GLU:HB2	6:C:1206:HOH:O	2.20	0.41
1:A:331:ARG:NH2	1:A:474:ILE:O	2.54	0.40
1:A:583:GLU:OE2	1:A:623:ASP:OD1	2.39	0.40
1:A:685:LEU:HD21	1:A:691:VAL:HG23	2.02	0.40
1:A:755:GLY:HA3	6:A:1169:HOH:O	2.21	0.40
1:A:789:TRP:CD2	1:A:810:ASP:HB3	2.55	0.40
1:C:445:HIS:HA	1:C:449:ASP:HB3	2.03	0.40
1:C:471:HIS:HA	1:C:472:PRO:HD2	1.95	0.40
1:A:419:GLN:NE2	1:A:443:ASN:HB2	2.36	0.40
1:B:518:ILE:HG22	1:B:519:PHE:O	2.21	0.40
1:B:795:ASN:HB3	6:B:1110:HOH:O	2.21	0.40
1:B:59:GLU:HG3	6:B:1182:HOH:O	2.21	0.40
1:C:220:ASP:CB	6:C:1041:HOH:O	2.70	0.40
1:C:523:TYR:N	1:C:524:PRO:HD3	2.37	0.40
1:A:755:GLY:HA2	1:D:78:ASP:CG	2.42	0.40
1:A:807:TYR:OH	1:C:425:HIS:CD2	2.74	0.40
1:B:691:VAL:HG12	1:B:693:ILE:HG13	2.03	0.40
1:D:152:ARG:HG3	1:D:195:TYR:OH	2.22	0.40
1:D:419:GLN:HE22	1:D:443:ASN:HB2	1.87	0.40
1:D:5:ILE:O	1:D:10:ARG:NH1	2.52	0.40
1:A:350:ARG:HG2	1:A:643:ILE:HB	2.03	0.40
1:A:445:HIS:HA	1:A:449:ASP:HB3	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:TYR:O	1:C:273:THR:OG1[3_545]	1.80	0.40

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%)	971 (95%)	48 (5%)	3 (0%)	44	77
1	B	1022/1032 (99%)	971 (95%)	49 (5%)	2 (0%)	51	83
1	C	1022/1032 (99%)	973 (95%)	47 (5%)	2 (0%)	51	83
1	D	1022/1032 (99%)	971 (95%)	49 (5%)	2 (0%)	51	83
All	All	4088/4128 (99%)	3886 (95%)	193 (5%)	9 (0%)	51	83

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	842	VAL
1	B	842	VAL
1	D	842	VAL
1	C	842	VAL
1	A	62	LYS
1	A	274	LYS
1	D	274	LYS
1	C	62	LYS
1	B	62	LYS

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	905/913 (99%)	883 (98%)	22 (2%)	54	85
1	B	905/913 (99%)	883 (98%)	22 (2%)	54	85
1	C	905/913 (99%)	884 (98%)	21 (2%)	56	86
1	D	905/913 (99%)	882 (98%)	23 (2%)	53	84
All	All	3620/3652 (99%)	3532 (98%)	88 (2%)	54	85

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	152	ARG
1	A	167	GLU
1	A	220	ASP
1	A	269	THR
1	A	270	THR
1	A	273	THR
1	A	300	THR
1	A	331	ARG
1	A	333	VAL
1	A	341	THR
1	A	415	THR
1	A	442	VAL
1	A	620	PHE
1	A	698	THR
1	A	703	VAL
1	A	723	GLU
1	A	750	SER
1	A	842	VAL
1	A	876	ASP
1	A	971	ASP
1	A	996	VAL
1	B	9	LEU
1	B	152	ARG
1	B	163	VAL
1	B	167	GLU
1	B	220	ASP
1	B	269	THR
1	B	270	THR
1	B	273	THR
1	B	300	THR
1	B	331	ARG
1	B	333	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	341	THR
1	B	415	THR
1	B	442	VAL
1	B	620	PHE
1	B	698	THR
1	B	703	VAL
1	B	750	SER
1	B	842	VAL
1	B	876	ASP
1	B	971	ASP
1	B	996	VAL
1	D	10	ARG
1	D	152	ARG
1	D	163	VAL
1	D	167	GLU
1	D	220	ASP
1	D	269	THR
1	D	270	THR
1	D	273	THR
1	D	300	THR
1	D	331	ARG
1	D	333	VAL
1	D	341	THR
1	D	415	THR
1	D	442	VAL
1	D	522	MET
1	D	620	PHE
1	D	698	THR
1	D	723	GLU
1	D	750	SER
1	D	842	VAL
1	D	876	ASP
1	D	971	ASP
1	D	996	VAL
1	C	9	LEU
1	C	134	ASN
1	C	152	ARG
1	C	163	VAL
1	C	167	GLU
1	C	220	ASP
1	C	269	THR
1	C	273	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	300	THR
1	C	331	ARG
1	C	333	VAL
1	C	415	THR
1	C	442	VAL
1	C	620	PHE
1	C	654	SER
1	C	698	THR
1	C	750	SER
1	C	842	VAL
1	C	876	ASP
1	C	971	ASP
1	C	996	VAL

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	29	GLN
1	A	125	HIS
1	A	134	ASN
1	A	141	ASN
1	A	266	ASN
1	A	355	HIS
1	A	387	ASN
1	A	392	ASN
1	A	419	GLN
1	A	423	ASN
1	A	425	HIS
1	A	427	ASN
1	A	463	GLN
1	A	489	HIS
1	A	536	HIS
1	A	567	GLN
1	A	577	GLN
1	A	757	HIS
1	A	817	HIS
1	A	861	ASN
1	A	930	GLN
1	A	934	ASN
1	A	935	HIS
1	A	955	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	16	HIS
1	B	125	HIS
1	B	134	ASN
1	B	141	ASN
1	B	224	GLN
1	B	266	ASN
1	B	355	HIS
1	B	387	ASN
1	B	392	ASN
1	B	419	GLN
1	B	423	ASN
1	B	425	HIS
1	B	427	ASN
1	B	443	ASN
1	B	463	GLN
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
1	D	16	HIS
1	D	125	HIS
1	D	134	ASN
1	D	141	ASN
1	D	266	ASN
1	D	339	ASN
1	D	355	HIS
1	D	387	ASN
1	D	392	ASN
1	D	419	GLN
1	D	423	ASN
1	D	425	HIS
1	D	443	ASN
1	D	463	GLN
1	D	489	HIS
1	D	536	HIS
1	D	567	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	577	GLN
1	D	757	HIS
1	D	861	ASN
1	D	930	GLN
1	D	934	ASN
1	D	935	HIS
1	D	955	GLN
1	C	16	HIS
1	C	125	HIS
1	C	134	ASN
1	C	141	ASN
1	C	266	ASN
1	C	355	HIS
1	C	387	ASN
1	C	392	ASN
1	C	419	GLN
1	C	423	ASN
1	C	425	HIS
1	C	427	ASN
1	C	443	ASN
1	C	463	GLN
1	C	489	HIS
1	C	536	HIS
1	C	567	GLN
1	C	577	GLN
1	C	647	HIS
1	C	757	HIS
1	C	930	GLN
1	C	934	ASN
1	C	935	HIS
1	C	955	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 28 ligands modelled in this entry, 24 are monoatomic - leaving 4 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	$\# Z > 2$
2	GAL	A	2001	4	12,12,12	0.56	0	17,17,17	1.02	1 (5%)
2	GAL	B	2001	4	12,12,12	0.54	0	17,17,17	0.66	0
2	GAL	C	2001	4	12,12,12	0.52	0	17,17,17	1.32	1 (5%)
2	GAL	D	2001	4	12,12,12	0.47	0	17,17,17	1.10	1 (5%)

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
2	GAL	A	2001	4	-	0/2/22/22	0/1/1/1
2	GAL	B	2001	4	-	0/2/22/22	0/1/1/1
2	GAL	C	2001	4	-	0/2/22/22	0/1/1/1
2	GAL	D	2001	4	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	GAL	C1-O5-C5	2.72	118.30	113.39
2	D	2001	GAL	C1-O5-C5	2.78	118.40	113.39
2	C	2001	GAL	C1-O5-C5	3.48	119.67	113.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	GAL	1	0
2	B	2001	GAL	1	0
2	C	2001	GAL	1	0
2	D	2001	GAL	1	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%)	-0.23	14 (1%) 75 69	28, 34, 42, 50	0
1	B	1024/1032 (99%)	-0.18	20 (1%) 65 56	28, 34, 42, 50	0
1	C	1024/1032 (99%)	-0.07	25 (2%) 59 49	28, 34, 42, 50	0
1	D	1024/1032 (99%)	-0.16	17 (1%) 70 63	28, 34, 42, 50	0
All	All	4096/4128 (99%)	-0.16	76 (1%) 67 58	28, 34, 42, 50	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	272	SER	9.4
1	D	273	THR	9.2
1	C	270	THR	9.2
1	D	270	THR	8.6
1	C	269	THR	8.4
1	D	269	THR	8.2
1	D	271	PHE	7.9
1	C	268	ASN	7.4
1	C	267	GLY	7.1
1	C	266	ASN	6.6
1	C	272	SER	6.4
1	C	271	PHE	6.1
1	D	268	ASN	6.0
1	D	267	GLY	5.9
1	C	273	THR	5.8
1	D	266	ASN	5.2
1	A	272	SER	4.8
1	B	430	ALA	4.6
1	C	923	GLU	4.5
1	A	273	THR	4.4
1	A	271	PHE	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	735	THR	3.9
1	B	735	THR	3.8
1	D	923	GLU	3.7
1	D	922	GLU	3.6
1	C	264	GLU	3.5
1	B	737	GLU	3.5
1	B	266	ASN	3.4
1	C	435	THR	3.4
1	D	435	THR	3.3
1	B	739	ALA	3.3
1	C	265	GLU	3.2
1	B	272	SER	3.2
1	C	274	LYS	3.1
1	C	754	SER	3.0
1	B	736	ALA	3.0
1	A	737	GLU	2.8
1	B	681	ASP	2.8
1	B	730	ASP	2.8
1	A	266	ASN	2.7
1	B	429	GLU	2.7
1	C	276	PHE	2.7
1	B	267	GLY	2.7
1	B	268	ASN	2.7
1	D	265	GLU	2.6
1	B	271	PHE	2.6
1	C	250	GLU	2.6
1	B	738	LYS	2.5
1	C	429	GLU	2.5
1	A	730	ASP	2.5
1	B	652	HIS	2.5
1	D	434	ASP	2.4
1	B	269	THR	2.4
1	B	2	SER	2.4
1	A	268	ASN	2.4
1	A	738	LYS	2.4
1	A	734	GLU	2.3
1	C	237	SER	2.3
1	D	432	TYR	2.3
1	A	2	SER	2.3
1	D	294	LYS	2.3
1	B	539	GLU	2.2
1	A	435	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	435	THR	2.2
1	A	826	ASN	2.2
1	C	253	SER	2.2
1	C	368	ASP	2.1
1	C	820	SER	2.1
1	D	221	SER	2.1
1	C	730	ASP	2.1
1	C	316	SER	2.1
1	D	433	PRO	2.0
1	C	206	LYS	2.0
1	C	737	GLU	2.0
1	B	286	GLU	2.0
1	A	270	THR	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	MG	B	3001	1/1	0.95	0.34	8.38	30,30,30,30	0
3	MG	A	3001	1/1	0.92	0.28	7.47	22,22,22,22	0
4	NA	D	3002	1/1	0.97	0.23	5.87	9,9,9,9	0
4	NA	B	3002	1/1	0.98	0.21	3.03	2,2,2,2	0
4	NA	D	3006	1/1	0.65	0.22	2.29	36,36,36,36	0
4	NA	B	3004	1/1	0.96	0.22	1.98	5,5,5,5	0
4	NA	C	3002	1/1	0.97	0.20	1.83	11,11,11,11	0
2	GAL	D	2001	12/12	0.93	0.17	1.25	41,44,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NA	C	3006	1/1	0.88	0.23	1.10	33,33,33,33	0
2	GAL	B	2001	12/12	0.89	0.17	0.57	35,38,39,41	0
4	NA	C	3004	1/1	0.98	0.17	0.37	13,13,13,13	0
2	GAL	C	2001	12/12	0.90	0.17	0.08	39,45,45,46	0
2	GAL	A	2001	12/12	0.92	0.15	0.02	39,41,42,42	0
3	MG	C	3001	1/1	0.94	0.16	0.01	38,38,38,38	0
4	NA	D	3003	1/1	0.97	0.15	-0.67	20,20,20,20	0
4	NA	A	3002	1/1	0.97	0.14	-1.36	2,2,2,2	0
4	NA	A	3003	1/1	0.98	0.11	-1.65	19,19,19,19	0
4	NA	D	3004	1/1	0.98	0.10	-1.88	5,5,5,5	0
4	NA	A	3004	1/1	0.99	0.07	-2.70	2,2,2,2	0
5	MN	B	3005	1/1	0.99	0.07	-2.71	30,30,30,30	0
5	MN	C	3005	1/1	0.99	0.05	-2.88	30,30,30,30	0
4	NA	B	3003	1/1	0.94	0.11	-2.94	13,13,13,13	0
4	NA	B	3006	1/1	0.95	0.11	-2.95	19,19,19,19	0
3	MG	D	3001	1/1	0.98	0.11	-3.43	23,23,23,23	0
4	NA	A	3006	1/1	0.95	0.07	-3.58	22,22,22,22	0
5	MN	A	3005	1/1	0.99	0.05	-5.22	24,24,24,24	0
4	NA	C	3003	1/1	0.98	0.07	-5.30	18,18,18,18	0
5	MN	D	3005	1/1	0.96	0.06	-6.22	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.