



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 02:04 PM UTC

PDB ID : 3D3I / pdb_00003d3i
Title : Crystal structural of Escherichia coli K12 YgjK, a glucosidase belonging to glycoside hydrolase family 63
Authors : Kurakata, Y.; Uechi, A.; Yoshida, H.; Kamitori, S.; Sakano, Y.; Nishikawa, A.; Tonozuka, T.
Deposited on : 2008-05-12
Resolution : 1.78 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

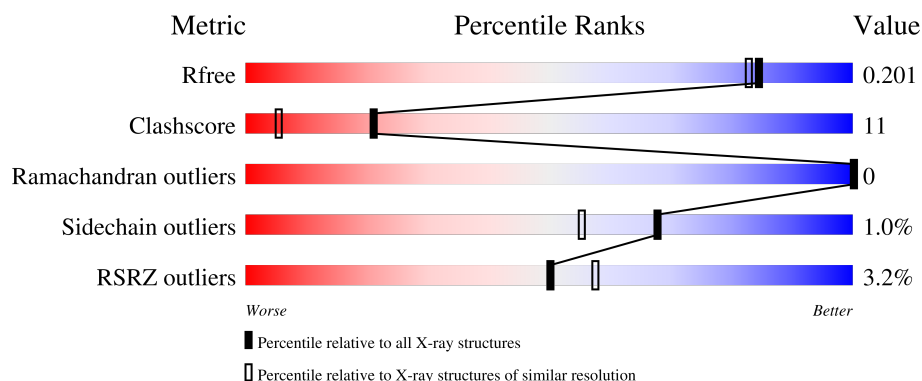
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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}	180053	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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 of 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	761	2% 78% 20% .
1	B	761	4% 78% 19% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14136 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.

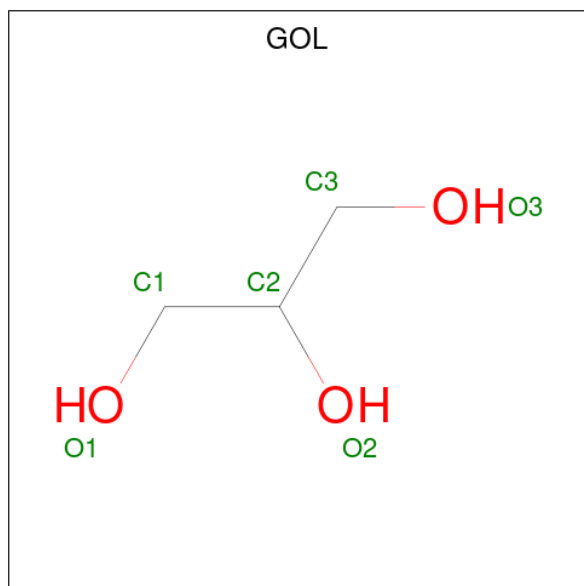
- Molecule 1 is a protein called Uncharacterized protein ygjK.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	758	Total	C	N	O	S	Se	0	0	0
			6053	3847	1038	1151	2	15			
1	B	758	Total	C	N	O	S	Se	0	0	0
			6053	3847	1038	1151	2	15			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		

- Molecule 3 is GLYCEROL (CCD ID: 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	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

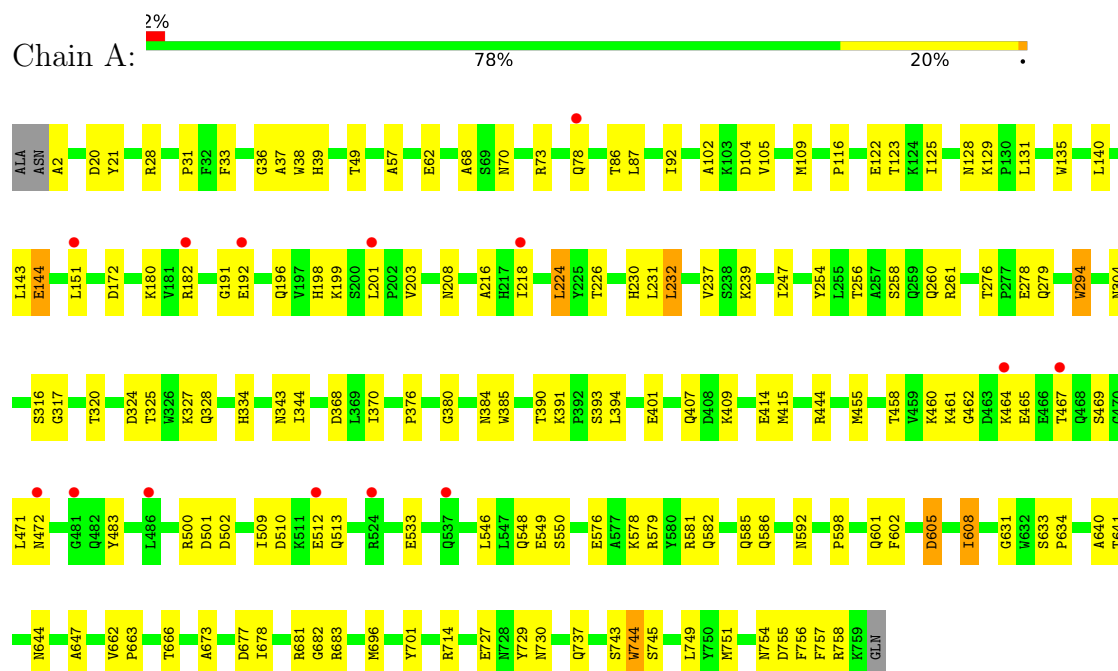
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	995	Total O 995 995	0	0
4	B	1009	Total O 1009 1009	0	0

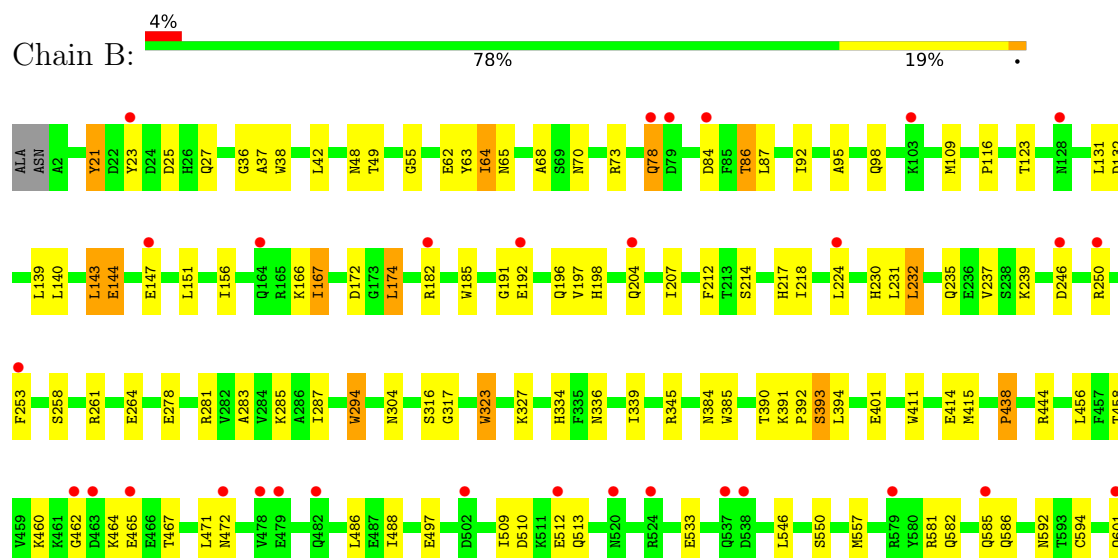
3 Residue-property plots

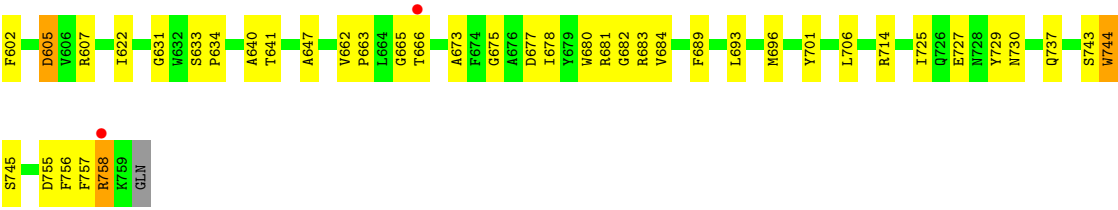
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Uncharacterized protein ygiK



• Molecule 1: Uncharacterized protein ygiK





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.69Å 138.55Å 87.54Å 90.00° 96.60° 90.00°	Depositor
Resolution (Å)	50.00 – 1.78 50.00 – 1.78	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-1.78) 99.8 (50.00-1.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.15 (at 1.78Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.169 , 0.201 0.169 , 0.201	Depositor DCC
R_{free} test set	13914 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å ²)	12.0	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 57.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14136	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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: CA, GOL

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	0.33	0/6204	0.87	27/8409 (0.3%)
1	B	0.33	0/6204	0.88	28/8409 (0.3%)
All	All	0.33	0/12408	0.88	55/16818 (0.3%)

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	21	TYR	N-CA-C	7.58	120.78	110.55
1	A	546	LEU	N-CA-C	-7.16	100.40	110.50
1	B	743	SER	N-CA-C	7.11	118.67	111.07
1	B	143	LEU	N-CA-C	6.98	120.24	111.24
1	B	546	LEU	N-CA-C	-6.74	100.31	110.28
1	A	92	ILE	N-CA-C	-6.55	101.61	109.01
1	A	393	SER	N-CA-C	6.52	119.34	108.20
1	A	143	LEU	N-CA-C	6.51	119.63	111.24
1	A	641	THR	N-CA-C	-6.50	101.78	110.55
1	B	92	ILE	N-CA-C	-6.49	101.67	109.01
1	B	394	LEU	N-CA-C	-6.42	102.82	111.87
1	A	743	SER	N-CA-C	6.37	118.75	111.11
1	A	21	TYR	N-CA-C	6.29	119.83	110.52
1	B	393	SER	N-CA-C	6.26	118.91	108.20
1	A	87	LEU	N-CA-C	6.19	119.56	109.59
1	A	304	ASN	N-CA-C	-6.16	101.82	110.50
1	A	663	PRO	N-CA-C	6.10	120.56	111.41
1	A	755	ASP	N-CA-C	6.06	120.87	112.45
1	B	316	SER	N-CA-C	6.05	117.91	109.31
1	A	662	VAL	N-CA-C	-6.05	95.81	108.88
1	A	608	ILE	N-CA-C	-5.98	97.88	106.55
1	A	444	ARG	N-CA-C	-5.97	100.27	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	641	THR	N-CA-C	-5.94	102.53	110.55
1	A	727	GLU	N-CA-C	5.88	120.63	112.45
1	A	501	ASP	N-CA-C	5.76	120.04	113.19
1	A	394	LEU	N-CA-C	-5.74	103.64	111.56
1	B	444	ARG	N-CA-C	-5.73	100.64	109.76
1	B	594	CYS	N-CA-C	5.71	120.38	112.45
1	B	727	GLU	N-CA-C	5.69	120.36	112.45
1	B	663	PRO	N-CA-C	5.67	119.91	111.41
1	B	86	THR	N-CA-C	-5.59	100.58	109.59
1	A	745	SER	N-CA-C	-5.58	105.28	111.36
1	B	144	GLU	N-CA-C	5.57	117.86	109.23
1	A	730	ASN	N-CA-C	-5.56	101.32	109.50
1	B	605	ASP	N-CA-C	-5.55	103.58	110.41
1	B	745	SER	N-CA-C	-5.52	105.34	111.36
1	B	191	GLY	N-CA-C	-5.48	107.55	115.27
1	A	86	THR	N-CA-C	-5.47	101.25	109.95
1	B	662	VAL	CA-C-N	5.47	125.44	120.03
1	B	662	VAL	C-N-CA	5.47	125.44	120.03
1	B	232	LEU	N-CA-C	5.45	119.93	113.28
1	B	662	VAL	N-CA-C	-5.42	97.16	108.88
1	B	730	ASN	N-CA-C	-5.42	101.53	109.50
1	A	316	SER	N-CA-C	5.40	116.98	109.31
1	B	438	PRO	N-CA-C	5.39	119.69	111.34
1	A	605	ASP	N-CA-C	-5.29	103.54	110.53
1	A	232	LEU	N-CA-C	5.25	119.69	113.28
1	B	87	LEU	N-CA-C	5.25	118.29	109.95
1	B	755	ASP	N-CA-C	5.24	119.73	112.45
1	B	304	ASN	N-CA-C	-5.21	103.15	110.50
1	A	144	GLU	N-CA-C	5.20	117.29	109.23
1	B	95	ALA	N-CA-C	5.12	116.30	108.42
1	A	749	LEU	N-CA-C	-5.08	105.82	111.36
1	A	756	PHE	N-CA-C	5.07	120.99	114.56
1	A	191	GLY	N-CA-C	-5.00	108.21	115.27

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	6053	0	5792	122	0
1	B	6053	0	5792	137	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	12	0	16	1	0
3	B	12	0	16	1	0
4	A	995	0	0	17	0
4	B	1009	0	0	26	0
All	All	14136	0	11616	261	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 11.

All (261) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:THR:HG23	1:A:682:GLY:H	1.12	1.15
1:B:666:THR:HG23	1:B:682:GLY:H	1.19	1.07
1:A:549:GLU:HG3	1:A:608:ILE:HD11	1.36	1.07
1:A:509:ILE:HA	1:A:681:ARG:NH1	1.73	1.03
1:B:673:ALA:HB1	1:B:681:ARG:HH11	1.26	1.01
1:B:27:GLN:HG3	1:B:64:ILE:HD12	1.41	1.00
1:B:509:ILE:HA	1:B:681:ARG:NH1	1.78	0.99
1:A:509:ILE:HA	1:A:681:ARG:HH12	1.31	0.94
1:A:460:LYS:HD3	1:A:465:GLU:HG2	1.52	0.91
1:A:123:THR:HG22	1:A:125:ILE:HD11	1.56	0.86
1:B:509:ILE:HA	1:B:681:ARG:HH12	1.37	0.86
1:A:414:GLU:HG2	1:A:415:MSE:HE3	1.58	0.84
1:B:246:ASP:HB3	4:B:3861:HOH:O	1.77	0.84
1:B:411:TRP:CZ3	1:B:415:MSE:HE3	2.14	0.83
1:A:258:SER:HA	1:A:261:ARG:HH12	1.44	0.83
1:B:666:THR:CG2	1:B:682:GLY:H	1.93	0.82
1:A:666:THR:HG22	1:A:683:ARG:O	1.79	0.82
1:A:666:THR:HG23	1:A:682:GLY:N	1.93	0.81
1:B:607:ARG:HG3	1:B:622:ILE:HD11	1.61	0.81
1:B:460:LYS:HD3	1:B:465:GLU:HG2	1.63	0.80
1:B:673:ALA:HB1	1:B:681:ARG:NH1	1.95	0.80
1:B:336:ASN:OD1	1:B:339:ILE:HD13	1.83	0.79
1:B:706:LEU:HD22	1:B:758:ARG:HD3	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:MSE:HG2	1:A:701:TYR:HB2	1.64	0.77
1:A:673:ALA:HB1	1:A:681:ARG:HH11	1.47	0.77
1:B:393:SER:HB3	4:B:3872:HOH:O	1.85	0.76
1:B:414:GLU:CD	1:B:415:MSE:HE2	2.11	0.76
1:B:607:ARG:HG3	1:B:622:ILE:CD1	2.16	0.76
1:B:666:THR:HG23	1:B:682:GLY:N	1.99	0.76
1:B:250:ARG:HB3	1:B:253:PHE:HD2	1.50	0.76
1:B:283:ALA:O	1:B:287:ILE:HD13	1.85	0.75
1:A:757:PHE:O	1:A:758:ARG:HD2	1.87	0.74
1:A:576:GLU:HG2	1:A:579:ARG:NH2	2.02	0.74
1:B:756:PHE:C	1:B:758:ARG:HH11	1.95	0.74
1:A:414:GLU:CG	1:A:415:MSE:HE3	2.18	0.74
1:A:666:THR:CG2	1:A:682:GLY:H	1.97	0.74
1:B:131:LEU:HB2	1:B:218:ILE:HD11	1.70	0.73
1:A:68:ALA:HA	1:A:140:LEU:HG	1.71	0.73
1:B:144:GLU:HG3	1:B:151:LEU:HB2	1.70	0.73
1:B:456:LEU:HB2	4:B:3468:HOH:O	1.88	0.72
1:B:757:PHE:C	1:B:758:ARG:HD2	2.16	0.69
1:B:557:MSE:HA	1:B:557:MSE:HE2	1.73	0.69
1:A:678:ILE:O	1:A:683:ARG:HG2	1.93	0.69
1:A:578:LYS:HA	1:A:581:ARG:HH12	1.58	0.68
1:B:345:ARG:HG2	1:B:415:MSE:HE1	1.76	0.68
1:B:486:LEU:HG	1:B:488:ILE:HD11	1.75	0.68
1:A:231:LEU:HD13	1:A:237:VAL:HA	1.76	0.67
1:B:327:LYS:CD	1:B:744:TRP:HB2	2.25	0.67
1:B:258:SER:HA	1:B:261:ARG:HH12	1.59	0.67
1:A:192:GLU:HG3	4:A:2525:HOH:O	1.94	0.67
1:A:460:LYS:HD2	1:A:464:LYS:O	1.93	0.67
1:B:258:SER:HA	1:B:261:ARG:NH1	2.09	0.67
1:A:327:LYS:CD	1:A:744:TRP:HB2	2.25	0.67
1:B:167:ILE:N	1:B:167:ILE:HD12	2.09	0.67
1:A:258:SER:HA	1:A:261:ARG:NH1	2.09	0.66
1:A:144:GLU:HG3	1:A:151:LEU:HB2	1.77	0.66
1:B:64:ILE:C	1:B:64:ILE:HD13	2.20	0.66
1:B:601:GLN:HB3	1:B:647:ALA:HB1	1.78	0.65
1:A:414:GLU:HG2	1:A:415:MSE:CE	2.25	0.65
1:A:128:ASN:HD21	1:A:129:LYS:NZ	1.95	0.65
1:A:320:THR:HB	1:A:370:ILE:HD11	1.79	0.65
1:A:673:ALA:HB1	1:A:681:ARG:NH1	2.12	0.65
1:B:557:MSE:HE3	4:B:3872:HOH:O	1.96	0.65
1:B:683:ARG:HE	1:B:729:TYR:C	2.04	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:LYS:HA	1:A:581:ARG:NH1	2.11	0.64
1:B:666:THR:HG22	1:B:683:ARG:O	1.95	0.64
1:A:131:LEU:HB2	1:A:218:ILE:HD11	1.79	0.64
1:B:68:ALA:HA	1:B:140:LEU:HG	1.78	0.64
1:A:415:MSE:HE2	1:A:415:MSE:HA	1.78	0.64
1:A:677:ASP:HA	1:A:683:ARG:HD3	1.81	0.63
1:A:460:LYS:HE2	1:A:462:GLY:O	1.98	0.63
1:B:327:LYS:HD3	1:B:744:TRP:HB2	1.79	0.63
1:B:460:LYS:HE2	1:B:462:GLY:O	1.99	0.63
1:B:607:ARG:NH1	1:B:622:ILE:HD12	2.14	0.62
1:A:218:ILE:HD12	1:A:218:ILE:O	2.00	0.62
1:B:471:LEU:HD22	1:B:533:GLU:HG2	1.81	0.62
1:B:231:LEU:HD13	1:B:237:VAL:HA	1.81	0.61
1:A:407:GLN:HG2	4:A:2862:HOH:O	1.99	0.61
1:A:548:GLN:CA	1:A:608:ILE:HD13	2.30	0.61
1:A:125:ILE:HD12	1:A:125:ILE:N	2.16	0.60
1:B:250:ARG:HD3	4:B:3237:HOH:O	2.00	0.60
1:B:23:TYR:CZ	1:B:147:GLU:HG3	2.36	0.60
1:A:123:THR:HG22	1:A:125:ILE:CD1	2.30	0.60
1:B:458:THR:OG1	1:B:467:THR:HG22	2.02	0.60
1:B:677:ASP:HA	1:B:683:ARG:HD3	1.84	0.59
1:B:224:LEU:HD12	4:B:3001:HOH:O	2.02	0.59
1:A:104:ASP:HB3	1:A:128:ASN:OD1	2.02	0.59
1:B:84:ASP:HB2	4:B:3767:HOH:O	2.03	0.59
1:B:174:LEU:HD23	1:B:197:VAL:HB	1.84	0.59
1:A:327:LYS:HD3	1:A:744:TRP:HB2	1.84	0.59
1:A:548:GLN:N	1:A:608:ILE:HD13	2.17	0.59
1:A:696:MSE:HG2	1:A:701:TYR:CB	2.32	0.59
1:B:488:ILE:HD12	1:B:488:ILE:N	2.17	0.59
1:B:250:ARG:HB3	1:B:253:PHE:CD2	2.37	0.59
1:B:339:ILE:N	1:B:339:ILE:HD12	2.18	0.59
1:B:139:LEU:HD11	1:B:167:ILE:HD11	1.83	0.59
1:B:218:ILE:O	1:B:218:ILE:HD12	2.02	0.59
1:A:180:LYS:HE3	1:A:182:ARG:HE	1.66	0.59
1:A:602:PHE:CE2	1:A:631:GLY:HA3	2.38	0.59
1:B:582:GLN:O	1:B:586:GLN:HG3	2.04	0.58
1:A:458:THR:OG1	1:A:467:THR:HG22	2.04	0.58
1:B:253:PHE:HB3	4:B:3862:HOH:O	2.02	0.57
1:A:128:ASN:HD21	1:A:129:LYS:HZ1	1.52	0.57
1:A:757:PHE:C	1:A:758:ARG:HD2	2.29	0.57
1:B:696:MSE:HG2	1:B:701:TYR:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ILE:HD12	1:A:370:ILE:C	2.31	0.56
1:A:592:ASN:HD22	1:A:644:ASN:HD22	1.53	0.56
1:B:681:ARG:NE	4:B:3130:HOH:O	2.38	0.55
1:B:204:GLN:O	1:B:214:SER:HA	2.07	0.55
1:A:325:THR:HG22	1:A:344:ILE:HD13	1.89	0.55
1:B:550:SER:HA	1:B:605:ASP:CG	2.32	0.55
1:B:512:GLU:CD	1:B:512:GLU:H	2.15	0.55
1:A:550:SER:HA	1:A:605:ASP:CG	2.32	0.55
1:A:582:GLN:O	1:A:586:GLN:HG3	2.07	0.54
1:A:683:ARG:HE	1:A:729:TYR:C	2.15	0.54
1:A:751:MSE:HG2	4:A:2849:HOH:O	2.07	0.54
1:A:370:ILE:HD12	1:A:370:ILE:O	2.07	0.54
1:B:581:ARG:O	1:B:585:GLN:HG3	2.07	0.54
1:A:172:ASP:OD2	1:A:198:HIS:HD2	1.91	0.54
1:B:218:ILE:HD12	1:B:218:ILE:C	2.33	0.54
1:A:256:THR:O	1:A:260:GLN:HG3	2.07	0.54
1:B:460:LYS:HD2	1:B:464:LYS:O	2.08	0.53
1:B:49:THR:HA	1:B:70:ASN:HD21	1.73	0.53
1:A:20:ASP:OD1	1:A:28:ARG:HD3	2.09	0.53
1:B:78:GLN:HG2	4:B:3635:HOH:O	2.08	0.53
1:B:98:GLN:HG3	1:B:109:MSE:HE3	1.90	0.53
1:A:471:LEU:HD22	1:A:533:GLU:HG2	1.91	0.53
1:B:143:LEU:HA	1:B:156:ILE:CD1	2.39	0.53
1:A:123:THR:HB	1:A:224:LEU:HG	1.91	0.53
1:A:37:ALA:HA	1:A:116:PRO:O	2.09	0.52
1:B:139:LEU:CD1	1:B:167:ILE:HD11	2.40	0.52
1:A:2:ALA:N	4:A:2749:HOH:O	2.42	0.52
1:B:174:LEU:HD23	1:B:174:LEU:N	2.25	0.52
1:A:460:LYS:CD	1:A:465:GLU:HG2	2.34	0.52
1:B:678:ILE:O	1:B:683:ARG:HG2	2.09	0.52
1:B:172:ASP:OD2	1:B:198:HIS:HD2	1.93	0.51
1:A:62:GLU:HA	1:A:317:GLY:HA3	1.92	0.51
1:B:196:GLN:OE1	1:B:198:HIS:HE1	1.94	0.51
1:B:438:PRO:HG2	1:B:557:MSE:SE	2.61	0.51
1:A:232:LEU:HD12	1:A:232:LEU:N	2.26	0.51
1:A:218:ILE:HD12	1:A:218:ILE:C	2.35	0.50
1:A:461:LYS:HD3	1:A:483:TYR:HA	1.92	0.50
1:B:683:ARG:HH22	1:B:737:GLN:HB2	1.76	0.50
1:B:602:PHE:CE2	1:B:631:GLY:HA3	2.46	0.50
1:B:675:GLY:HA3	1:B:678:ILE:HG12	1.94	0.50
1:B:62:GLU:HA	1:B:317:GLY:HA3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:TRP:O	1:B:230:HIS:HD2	1.95	0.49
1:B:683:ARG:HH12	1:B:737:GLN:CD	2.20	0.49
1:A:276:THR:OG1	1:A:279:GLN:HG3	2.13	0.49
1:B:472:ASN:HB2	4:B:3637:HOH:O	2.13	0.49
1:B:143:LEU:HA	1:B:156:ILE:HD11	1.95	0.49
1:B:232:LEU:N	1:B:232:LEU:HD12	2.28	0.48
1:B:411:TRP:HZ3	1:B:415:MSE:HE3	1.71	0.48
1:B:86:THR:HG23	4:B:3497:HOH:O	2.11	0.48
1:B:696:MSE:HG2	1:B:701:TYR:CB	2.44	0.48
1:B:204:GLN:HG2	4:B:3868:HOH:O	2.13	0.48
1:B:666:THR:HG21	1:B:680:TRP:HA	1.95	0.48
1:A:460:LYS:HG2	4:A:2431:HOH:O	2.14	0.48
1:B:689:PHE:O	1:B:693:LEU:HD13	2.14	0.48
1:B:334:HIS:HE1	1:B:401:GLU:OE2	1.96	0.48
1:B:132:ASP:OD1	1:B:217:HIS:HD2	1.96	0.47
1:A:510:ASP:HB3	4:A:2619:HOH:O	2.15	0.47
1:B:73:ARG:HD2	4:B:3286:HOH:O	2.13	0.47
1:A:601:GLN:HB3	1:A:647:ALA:HB1	1.96	0.47
1:B:757:PHE:N	1:B:758:ARG:HH11	2.12	0.47
1:A:683:ARG:HH22	1:A:737:GLN:HB2	1.80	0.46
1:A:334:HIS:HE1	1:A:401:GLU:OE2	1.98	0.46
1:A:49:THR:HG22	1:A:70:ASN:HD21	1.80	0.46
1:A:368:ASP:OD1	1:A:391:LYS:HE2	2.14	0.46
1:B:42:LEU:HD12	1:B:55:GLY:HA3	1.98	0.46
1:A:512:GLU:CD	1:A:512:GLU:H	2.22	0.46
1:B:601:GLN:NE2	4:B:3484:HOH:O	2.47	0.46
3:B:2001:GOL:H12	4:B:3687:HOH:O	2.16	0.46
1:B:64:ILE:HD13	1:B:65:ASN:N	2.30	0.46
1:B:414:GLU:CG	1:B:415:MSE:HE2	2.46	0.46
1:A:208:ASN:ND2	4:A:2207:HOH:O	2.46	0.46
1:A:744:TRP:CD1	1:A:744:TRP:C	2.93	0.46
1:A:196:GLN:OE1	1:A:198:HIS:HE1	1.99	0.45
1:B:64:ILE:C	1:B:64:ILE:CD1	2.89	0.45
1:B:123:THR:HB	1:B:224:LEU:HG	1.98	0.45
1:A:455:MSE:O	1:A:469:SER:HA	2.17	0.45
1:A:472:ASN:HB2	4:A:2779:HOH:O	2.16	0.45
1:A:414:GLU:CD	1:A:415:MSE:HE3	2.41	0.45
1:B:123:THR:HB	1:B:224:LEU:CD1	2.46	0.45
1:B:167:ILE:N	1:B:167:ILE:CD1	2.78	0.45
1:B:207:ILE:HD13	1:B:212:PHE:HB2	1.98	0.45
1:A:38:TRP:O	1:A:230:HIS:HD2	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:TYR:OH	1:B:185:TRP:HA	2.15	0.45
1:B:192:GLU:HG3	4:B:3645:HOH:O	2.16	0.45
1:A:598:PRO:HD2	4:A:2432:HOH:O	2.17	0.45
1:A:678:ILE:C	1:A:683:ARG:HG2	2.41	0.45
1:B:36:GLY:HA2	1:B:294:TRP:O	2.16	0.45
1:B:339:ILE:N	1:B:339:ILE:CD1	2.79	0.45
1:B:23:TYR:CE2	1:B:147:GLU:HG3	2.52	0.44
1:A:102:ALA:HB3	1:A:105:VAL:O	2.18	0.44
1:B:706:LEU:CD2	1:B:758:ARG:HD3	2.41	0.44
1:A:31:PRO:HB2	1:A:33:PHE:CE2	2.52	0.44
1:A:502:ASP:HB3	4:A:2756:HOH:O	2.17	0.44
1:A:36:GLY:HA2	1:A:294:TRP:O	2.17	0.44
1:B:278:GLU:HG2	4:B:3526:HOH:O	2.17	0.44
1:B:607:ARG:HG3	1:B:622:ILE:HD12	1.96	0.44
1:B:744:TRP:CD1	1:B:744:TRP:C	2.96	0.44
1:B:182:ARG:NH1	4:B:3028:HOH:O	2.50	0.44
1:B:217:HIS:HE1	4:B:3234:HOH:O	2.00	0.44
1:B:392:PRO:HD3	1:B:497:GLU:O	2.18	0.44
1:A:324:ASP:O	1:A:328:GLN:HG3	2.18	0.44
1:A:409:LYS:HE3	4:A:2886:HOH:O	2.17	0.44
1:A:592:ASN:HD21	1:A:640:ALA:HA	1.83	0.44
1:A:633:SER:N	1:A:634:PRO:CD	2.80	0.44
1:B:264:GLU:HG3	4:B:3775:HOH:O	2.17	0.44
1:B:174:LEU:N	1:B:174:LEU:CD2	2.81	0.43
1:B:756:PHE:O	1:B:758:ARG:HD2	2.18	0.43
1:B:37:ALA:HA	1:B:116:PRO:O	2.18	0.43
1:B:510:ASP:OD1	1:B:513:GLN:HG3	2.19	0.43
1:A:320:THR:HB	1:A:370:ILE:CD1	2.47	0.43
1:A:683:ARG:CZ	4:A:2532:HOH:O	2.66	0.43
3:A:2001:GOL:H12	4:A:2598:HOH:O	2.18	0.43
1:B:230:HIS:HE1	4:B:3070:HOH:O	2.01	0.42
1:A:510:ASP:OD1	1:A:513:GLN:HG3	2.18	0.42
1:A:376:PRO:HA	1:A:380:GLY:O	2.19	0.42
1:A:384:ASN:O	1:A:385:TRP:C	2.62	0.42
1:B:166:LYS:C	1:B:167:ILE:HD12	2.45	0.42
1:B:633:SER:N	1:B:634:PRO:CD	2.82	0.42
1:B:681:ARG:CZ	4:B:3130:HOH:O	2.67	0.42
1:A:201:LEU:CD2	1:A:224:LEU:HD13	2.49	0.42
1:A:123:THR:CG2	1:A:125:ILE:HD11	2.39	0.42
1:A:500:ARG:NH2	4:A:2117:HOH:O	2.52	0.42
1:A:39:HIS:HA	1:A:57:ALA:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:MSE:HE3	1:A:696:MSE:HB2	1.91	0.42
1:A:247:ILE:HA	1:A:254:TYR:CE2	2.55	0.42
1:B:384:ASN:O	1:B:385:TRP:C	2.63	0.42
1:B:21:TYR:HB3	1:B:25:ASP:HA	2.02	0.42
1:B:285:LYS:HD2	1:B:725:ILE:HD11	2.01	0.42
1:A:180:LYS:HE3	1:A:182:ARG:NE	2.34	0.41
1:A:581:ARG:HG2	1:A:585:GLN:HE21	1.85	0.41
1:A:714:ARG:HD3	4:A:2624:HOH:O	2.19	0.41
1:A:414:GLU:C	1:A:415:MSE:HE2	2.44	0.41
1:B:239:LYS:HE2	1:B:239:LYS:HB3	1.90	0.41
1:A:390:THR:HG23	1:A:391:LYS:N	2.36	0.41
1:B:235:GLN:CD	1:B:235:GLN:N	2.78	0.41
1:B:592:ASN:HD21	1:B:640:ALA:HA	1.86	0.41
1:A:109:MSE:HA	1:A:122:GLU:O	2.21	0.41
1:A:199:LYS:HG2	1:A:226:THR:HG23	2.03	0.41
1:A:261:ARG:HH11	1:A:261:ARG:CB	2.34	0.41
1:A:278:GLU:H	1:A:278:GLU:CD	2.29	0.41
1:A:325:THR:HG23	1:A:343:ASN:CG	2.46	0.41
1:B:323:TRP:HA	1:B:323:TRP:CE3	2.56	0.41
1:B:683:ARG:CZ	4:B:3392:HOH:O	2.68	0.41
1:B:714:ARG:HD3	4:B:3989:HOH:O	2.20	0.41
1:A:182:ARG:NH1	4:A:2094:HOH:O	2.53	0.41
1:B:665:GLY:HA2	1:B:684:VAL:HG22	2.03	0.41
1:B:281:ARG:HD3	4:B:3102:HOH:O	2.20	0.41
1:A:203:VAL:HG12	1:A:216:ALA:HB2	2.02	0.41
1:A:151:LEU:HD23	4:A:2512:HOH:O	2.20	0.40
1:A:239:LYS:HE2	1:A:239:LYS:HB3	1.90	0.40
1:A:334:HIS:CE1	1:A:401:GLU:OE2	2.73	0.40
1:B:48:ASN:O	1:B:73:ARG:NH1	2.53	0.40
1:A:73:ARG:O	1:A:135:TRP:HA	2.22	0.40
1:A:131:LEU:CB	1:A:218:ILE:HD11	2.49	0.40
1:B:98:GLN:CG	1:B:109:MSE:HE3	2.50	0.40
1:B:390:THR:HG23	1:B:391:LYS:N	2.37	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	756/761 (99%)	728 (96%)	28 (4%)	0	100	100
1	B	756/761 (99%)	729 (96%)	27 (4%)	0	100	100
All	All	1512/1522 (99%)	1457 (96%)	55 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	631/619 (102%)	626 (99%)	5 (1%)	73	63
1	B	631/619 (102%)	623 (99%)	8 (1%)	61	46
All	All	1262/1238 (102%)	1249 (99%)	13 (1%)	68	55

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	224	LEU
1	A	294	TRP
1	A	744	TRP
1	A	754	ASN
1	B	64	ILE
1	B	78	GLN
1	B	167	ILE

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Mol	Chain	Res	Type
1	B	174	LEU
1	B	294	TRP
1	B	323	TRP
1	B	744	TRP
1	B	758	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	48	ASN
1	A	70	ASN
1	A	78	GLN
1	A	128	ASN
1	A	198	HIS
1	A	208	ASN
1	A	217	HIS
1	A	219	ASN
1	A	230	HIS
1	A	241	GLN
1	A	319	GLN
1	A	328	GLN
1	A	334	HIS
1	A	343	ASN
1	A	384	ASN
1	A	449	ASN
1	A	473	ASN
1	A	482	GLN
1	A	491	GLN
1	A	520	ASN
1	A	585	GLN
1	A	592	ASN
1	A	637	ASN
1	A	736	GLN
1	A	754	ASN
1	B	48	ASN
1	B	70	ASN
1	B	78	GLN
1	B	198	HIS
1	B	204	GLN
1	B	217	HIS
1	B	219	ASN

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Mol	Chain	Res	Type
1	B	230	HIS
1	B	241	GLN
1	B	319	GLN
1	B	334	HIS
1	B	384	ASN
1	B	449	ASN
1	B	491	GLN
1	B	586	GLN
1	B	592	ASN
1	B	601	GLN
1	B	737	GLN
1	B	748	HIS
1	B	754	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 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	$\# Z > 2$
3	GOL	B	2001	-	5,5,5	0.19	0	5,5,5	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	A	2001	-	5,5,5	0.19	0	5,5,5	0.32	0
3	GOL	A	2002	-	5,5,5	0.27	0	5,5,5	0.30	0
3	GOL	B	2002	-	5,5,5	0.29	0	5,5,5	0.29	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	B	2001	-	-	0/4/4/4	-
3	GOL	A	2001	-	-	0/4/4/4	-
3	GOL	A	2002	-	-	0/4/4/4	-
3	GOL	B	2002	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2001	GOL	1	0
3	A	2001	GOL	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	743/761 (97%)	-0.12	14 (1%) 66 74	6, 11, 28, 41	0
1	B	743/761 (97%)	0.01	33 (4%) 39 44	6, 12, 28, 43	0
All	All	1486/1522 (97%)	-0.06	47 (3%) 50 57	6, 11, 28, 43	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	253	PHE	5.8
1	B	23	TYR	5.6
1	B	204	GLN	4.5
1	B	579	ARG	3.7
1	B	758	ARG	3.7
1	B	128	ASN	3.6
1	B	502	ASP	3.5
1	B	246	ASP	3.3
1	B	479	GLU	3.2
1	A	218	ILE	3.1
1	B	462	GLY	3.1
1	B	512	GLU	3.0
1	B	666	THR	3.0
1	B	250	ARG	2.9
1	B	524	ARG	2.7
1	B	78	GLN	2.7
1	B	585	GLN	2.7
1	A	524	ARG	2.6
1	B	79	ASP	2.6
1	B	537	GLN	2.6
1	A	472	ASN	2.6
1	B	147	GLU	2.6
1	A	537	GLN	2.6
1	B	465	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	103	LYS	2.5
1	B	192	GLU	2.5
1	B	164	GLN	2.4
1	A	467	THR	2.4
1	A	78	GLN	2.4
1	B	538	ASP	2.4
1	B	182	ARG	2.4
1	A	464	LYS	2.3
1	B	482	GLN	2.3
1	B	463	ASP	2.3
1	A	151	LEU	2.3
1	A	201	LEU	2.3
1	B	224	LEU	2.3
1	B	520	ASN	2.3
1	B	601	GLN	2.2
1	B	472	ASN	2.2
1	A	486	LEU	2.2
1	A	182	ARG	2.1
1	B	84	ASP	2.1
1	A	481	GLY	2.1
1	A	192	GLU	2.1
1	A	512	GLU	2.0
1	B	478	VAL	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 oligosaccharides 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	2001	6/6	0.67	0.29	34,35,38,38	0
3	GOL	A	2001	6/6	0.72	0.28	33,34,36,36	0
3	GOL	A	2002	6/6	0.81	0.17	30,33,35,38	0
3	GOL	B	2002	6/6	0.82	0.17	21,27,31,35	0
2	CA	B	1001	1/1	0.99	0.02	11,11,11,11	0
2	CA	A	1001	1/1	1.00	0.01	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.