



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 07:54 PM UTC

PDB ID : 4WJU / pdb_00004wju
Title : Crystal structure of Rsa4 from *Saccharomyces cerevisiae*
Authors : Holdermann, I.; Bassler, J.; Hurt, E.; Sinning, I.
Deposited on : 2014-10-01
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

<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

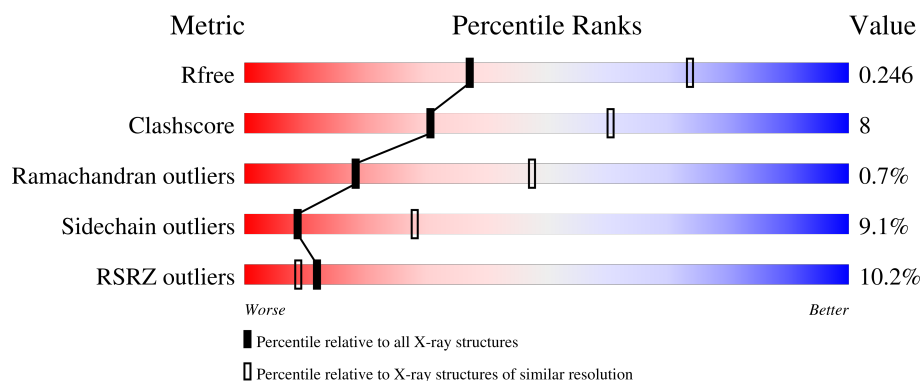
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 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	515	8% 68% 16% • 11%
1	B	515	10% 65% 18% • 13%

2 Entry composition [i](#)

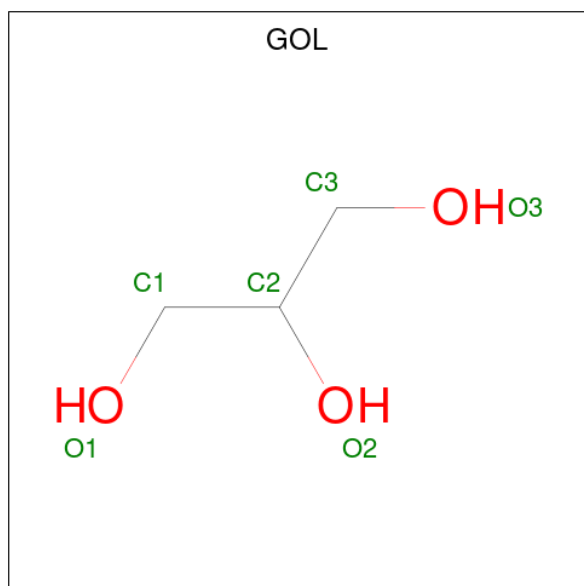
There are 2 unique types of molecules in this entry. The entry contains 7061 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ribosome assembly protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	0	0
			3562	2239	634	668	21			
1	B	446	Total	C	N	O	S	0	0	0
			3493	2200	623	650	20			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).

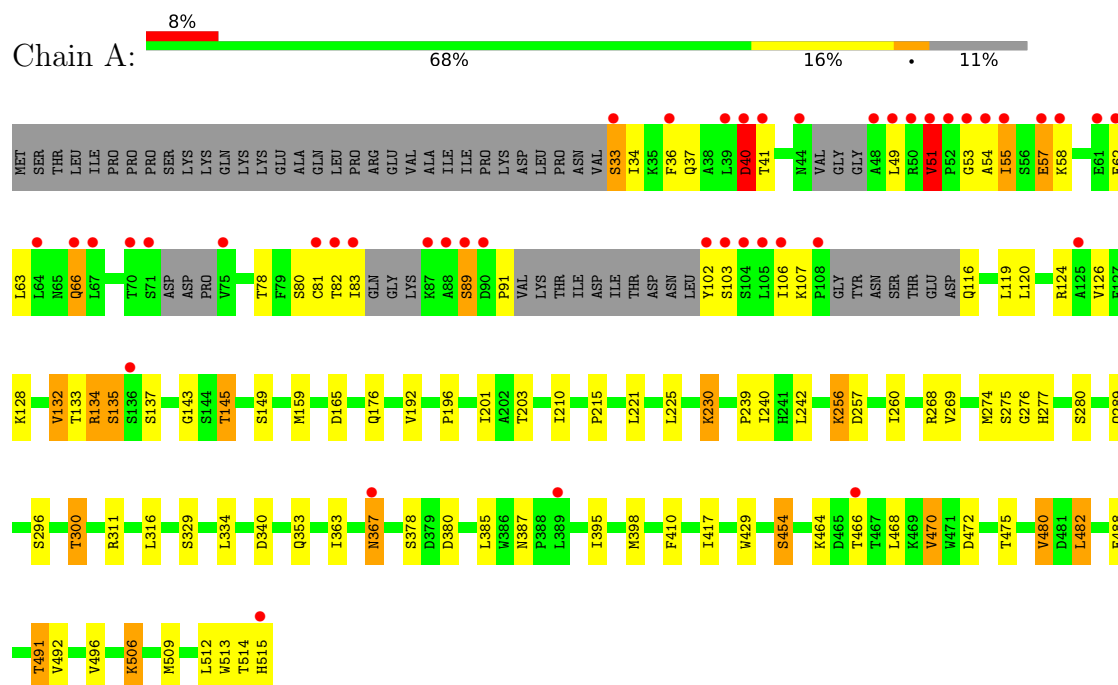


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		

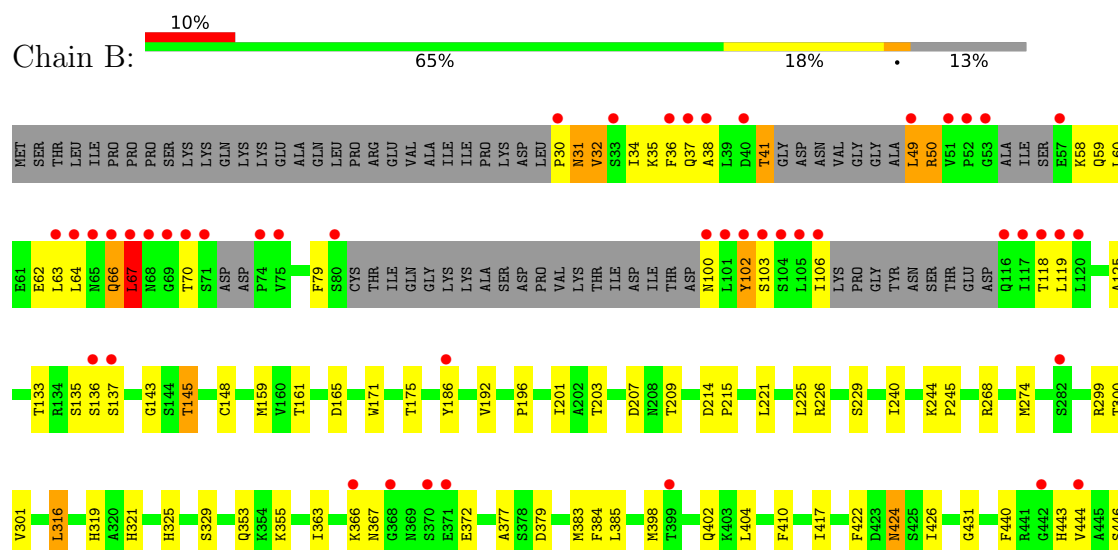
3 Residue-property plots [i](#)

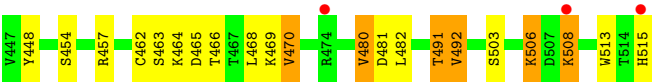
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Ribosome assembly protein 4



• Molecule 1: Ribosome assembly protein 4





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	96.87Å 108.47Å 261.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.61 – 2.80 43.61 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.2 (43.61-2.80) 89.4 (43.61-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.203 , 0.246 0.206 , 0.246	Depositor DCC
R_{free} test set	2000 reflections (5.80%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.738	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7061	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: 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	0/3646	0.74	4/4941 (0.1%)
1	B	0.40	0/3577	0.76	2/4846 (0.0%)
All	All	0.37	0/7223	0.75	6/9787 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	32	VAL	N-CA-C	5.47	115.98	107.28
1	B	67	LEU	CA-CB-CG	5.29	134.82	116.30
1	A	51	VAL	CA-C-N	-5.13	114.67	119.85
1	A	51	VAL	C-N-CA	-5.13	114.67	119.85
1	A	387	ASN	CA-C-N	5.07	125.35	119.47
1	A	387	ASN	C-N-CA	5.07	125.35	119.47

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	49	LEU	Peptide
1	B	66	GLN	Peptide

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	3562	0	3510	55	0
1	B	3493	0	3446	62	0
2	A	6	0	8	3	0
All	All	7061	0	6964	117	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 8.

All (117) 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:B:469:LYS:NZ	1:B:481:ASP:OD1	2.05	0.88
1:B:31:ASN:HB3	1:B:50:ARG:HD3	1.54	0.87
1:B:59:GLN:O	1:B:63:LEU:N	2.08	0.84
1:B:64:LEU:HA	1:B:67:LEU:HD21	1.63	0.81
1:A:311:ARG:HB2	2:A:601:GOL:H32	1.64	0.80
1:A:311:ARG:NH1	2:A:601:GOL:H12	1.96	0.79
1:A:134:ARG:NH1	1:A:515:HIS:O	2.17	0.77
1:A:221:LEU:O	1:A:268:ARG:NH2	2.20	0.75
1:A:311:ARG:HH11	2:A:601:GOL:H12	1.50	0.73
1:A:80:SER:HB2	1:A:120:LEU:HB2	1.73	0.70
1:B:143:GLY:N	1:B:165:ASP:OD2	2.22	0.70
1:A:33:SER:HA	1:A:51:VAL:HA	1.74	0.69
1:B:38:ALA:HB3	1:B:41:THR:HG22	1.74	0.69
1:A:126:VAL:O	1:A:128:LYS:NZ	2.25	0.68
1:A:143:GLY:N	1:A:165:ASP:OD2	2.24	0.67
1:B:62:GLU:O	1:B:63:LEU:C	2.38	0.66
1:B:221:LEU:O	1:B:268:ARG:NH2	2.30	0.65
1:B:192:VAL:HG12	1:B:203:THR:HG22	1.80	0.62
1:B:462:CYS:HB3	1:B:492:VAL:HG13	1.82	0.61
1:B:34:ILE:H	1:B:49:LEU:HD23	1.66	0.60
1:A:192:VAL:HG12	1:A:203:THR:HG22	1.84	0.58
1:B:214:ASP:HB2	1:B:221:LEU:HD21	1.85	0.57
1:A:57:GLU:OE2	1:A:58:LYS:HG3	2.04	0.57
1:B:60:LEU:O	1:B:64:LEU:N	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:VAL:HG13	1:B:480:VAL:HG13	1.85	0.57
1:A:239:PRO:HG2	1:A:242:LEU:HD12	1.85	0.56
1:A:239:PRO:HB3	1:A:334:LEU:HD22	1.86	0.56
1:A:277:HIS:CE1	1:A:300:THR:HG22	2.41	0.55
1:A:367:ASN:OD1	1:A:367:ASN:N	2.39	0.55
1:A:470:VAL:HG13	1:A:480:VAL:HG13	1.89	0.54
1:B:508:LYS:HB2	1:B:508:LYS:NZ	2.23	0.54
1:B:133:THR:HG22	1:B:515:HIS:HA	1.89	0.54
1:B:145:THR:HB	1:B:506:LYS:HA	1.91	0.53
1:A:83:ILE:HG12	1:A:89:SER:HA	1.91	0.53
1:A:472:ASP:HB3	1:A:475:THR:HG22	1.92	0.52
1:B:32:VAL:N	1:B:50:ARG:HG2	2.24	0.52
1:A:176:GLN:HG3	1:A:512:LEU:HD12	1.91	0.52
1:B:186:TYR:CE1	1:B:207:ASP:HB2	2.44	0.52
1:B:417:ILE:HG13	1:B:431:GLY:HA2	1.92	0.52
1:A:385:LEU:HB2	1:A:398:MET:CE	2.40	0.51
1:A:57:GLU:OE2	1:A:58:LYS:N	2.41	0.50
1:B:79:PHE:HB3	1:B:119:LEU:HD21	1.93	0.50
1:A:134:ARG:HD2	1:A:514:THR:HG23	1.93	0.50
1:A:378:SER:OG	1:A:380:ASP:OD1	2.21	0.50
1:A:40:ASP:N	1:A:40:ASP:OD1	2.43	0.50
1:A:132:VAL:HA	1:A:515:HIS:HA	1.94	0.49
1:B:221:LEU:HB2	1:B:268:ARG:HH22	1.77	0.49
1:A:277:HIS:ND1	1:A:296:SER:HB3	2.27	0.49
1:A:468:LEU:HB2	1:A:482:LEU:HD12	1.93	0.49
1:B:59:GLN:HA	1:B:62:GLU:HB2	1.94	0.49
1:B:63:LEU:HG	1:B:67:LEU:HD11	1.95	0.49
1:A:149:SER:N	1:A:491:THR:HG21	2.28	0.48
1:B:426:ILE:HB	1:B:440:PHE:HB2	1.95	0.48
1:B:35:LYS:HB3	1:B:118:THR:HA	1.94	0.48
1:B:301:VAL:HB	1:B:316:LEU:HB2	1.94	0.48
1:B:58:LYS:O	1:B:62:GLU:N	2.43	0.47
1:B:383:MET:HB2	1:B:398:MET:HG3	1.96	0.47
1:A:201:ILE:HG13	1:A:215:PRO:HG3	1.96	0.47
1:A:135:SER:HB3	1:A:513:TRP:CZ3	2.49	0.47
1:B:325:HIS:HB2	1:B:377:ALA:HB3	1.96	0.46
1:B:209:THR:HG22	1:B:226:ARG:HG2	1.97	0.46
1:A:145:THR:HB	1:A:506:LYS:HA	1.97	0.46
1:B:196:PRO:HB2	1:B:240:ILE:HG12	1.97	0.46
1:A:385:LEU:HB2	1:A:398:MET:HE3	1.97	0.46
1:B:424:ASN:HD22	1:B:424:ASN:N	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ILE:HB	1:A:274:MET:HB2	1.98	0.45
1:A:53:GLY:O	1:A:55:ILE:HG12	2.16	0.45
1:B:161:THR:CG2	1:B:171:TRP:HE1	2.30	0.45
1:B:367:ASN:OD1	1:B:367:ASN:N	2.44	0.45
1:A:54:ALA:HB1	1:A:102:TYR:HD2	1.82	0.45
1:B:299:ARG:HG2	1:B:321:HIS:C	2.42	0.45
1:B:103:SER:HA	1:B:106:ILE:HG12	1.99	0.45
1:A:81:CYS:O	1:A:82:THR:OG1	2.31	0.44
1:B:36:PHE:HE1	1:B:119:LEU:HD22	1.82	0.44
1:B:125:ALA:O	1:B:457:ARG:NH2	2.51	0.44
1:B:424:ASN:N	1:B:424:ASN:ND2	2.66	0.44
1:A:37:GLN:O	1:A:120:LEU:HA	2.16	0.44
1:A:62:GLU:O	1:A:66:GLN:HB3	2.18	0.44
1:A:210:ILE:HB	1:A:225:LEU:HB2	1.99	0.44
1:B:385:LEU:HB2	1:B:398:MET:HE1	1.99	0.44
1:B:30:PRO:HG2	1:B:102:TYR:OH	2.18	0.44
1:B:59:GLN:O	1:B:63:LEU:HB2	2.18	0.44
1:B:446:SER:O	1:B:463:SER:OG	2.27	0.43
1:A:149:SER:H	1:A:491:THR:HG21	1.83	0.43
1:B:201:ILE:HG13	1:B:215:PRO:HG3	2.01	0.43
1:B:468:LEU:HD11	1:B:503:SER:HB3	2.01	0.43
1:B:148:CYS:HA	1:B:491:THR:HG21	2.00	0.43
1:A:36:PHE:HE1	1:A:119:LEU:HD23	1.82	0.43
1:A:80:SER:N	1:A:120:LEU:O	2.51	0.43
1:A:417:ILE:HB	1:A:429:TRP:HB2	1.99	0.43
1:B:30:PRO:C	1:B:31:ASN:HD22	2.23	0.43
1:B:319:HIS:CE1	1:B:384:PHE:HD2	2.37	0.42
1:B:468:LEU:HB2	1:B:482:LEU:HB2	2.01	0.42
1:B:355:LYS:HE3	1:B:355:LYS:HB2	1.78	0.42
1:A:464:LYS:HG3	1:A:488:GLU:HG2	2.00	0.42
1:B:67:LEU:HD22	1:B:67:LEU:N	2.34	0.42
1:B:448:TYR:HE2	1:B:464:LYS:HB2	1.85	0.42
1:B:443:HIS:ND1	1:B:465:ASP:OD2	2.51	0.42
1:B:329:SER:HA	1:B:410:PHE:CG	2.55	0.41
1:B:63:LEU:HD12	1:B:63:LEU:HA	1.90	0.41
1:A:159:MET:HE3	1:A:159:MET:HB3	1.91	0.41
1:A:196:PRO:HB2	1:A:240:ILE:HG12	2.03	0.41
1:A:81:CYS:H	1:A:91:PRO:HG3	1.85	0.41
1:A:256:LYS:NZ	1:A:280:SER:OG	2.53	0.41
1:B:135:SER:HB2	1:B:513:TRP:CZ3	2.55	0.41
1:A:80:SER:HA	1:A:91:PRO:CG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ILE:H	1:B:49:LEU:CD2	2.32	0.41
1:A:329:SER:HA	1:A:410:PHE:CG	2.55	0.41
1:B:422:PHE:HA	1:B:446:SER:HB3	2.02	0.41
1:A:454:SER:OG	1:A:496:VAL:O	2.30	0.41
1:B:64:LEU:CA	1:B:67:LEU:HD21	2.41	0.40
1:B:136:SER:OG	1:B:137:SER:N	2.55	0.40
1:A:33:SER:HB3	1:A:116:GLN:HB2	2.02	0.40
1:A:230:LYS:HB2	1:A:257:ASP:HB3	2.03	0.40
1:A:103:SER:O	1:A:107:LYS:HG2	2.21	0.40
1:A:196:PRO:HG2	1:A:240:ILE:HD11	2.04	0.40
1:B:244:LYS:HA	1:B:245:PRO:HD3	1.98	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	445/515 (86%)	421 (95%)	20 (4%)	4 (1%)	14	41
1	B	434/515 (84%)	414 (95%)	18 (4%)	2 (0%)	24	55
All	All	879/1030 (85%)	835 (95%)	38 (4%)	6 (1%)	18	47

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	B	50	ARG
1	B	67	LEU
1	A	40	ASP
1	A	276	GLY
1	A	51	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	398/451 (88%)	359 (90%)	39 (10%)	7	25
1	B	391/451 (87%)	358 (92%)	33 (8%)	10	32
All	All	789/902 (88%)	717 (91%)	72 (9%)	9	28

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	SER
1	A	34	ILE
1	A	40	ASP
1	A	49	LEU
1	A	55	ILE
1	A	57	GLU
1	A	63	LEU
1	A	66	GLN
1	A	78	THR
1	A	89	SER
1	A	106	ILE
1	A	124	ARG
1	A	132	VAL
1	A	133	THR
1	A	134	ARG
1	A	135	SER
1	A	137	SER
1	A	145	THR
1	A	230	LYS
1	A	256	LYS
1	A	269	VAL
1	A	275	SER
1	A	289	GLN
1	A	300	THR
1	A	316	LEU
1	A	340	ASP
1	A	353	GLN

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Mol	Chain	Res	Type
1	A	363	ILE
1	A	367	ASN
1	A	395	ILE
1	A	454	SER
1	A	466	THR
1	A	470	VAL
1	A	480	VAL
1	A	482	LEU
1	A	491	THR
1	A	492	VAL
1	A	506	LYS
1	A	509	MET
1	B	31	ASN
1	B	37	GLN
1	B	41	THR
1	B	66	GLN
1	B	67	LEU
1	B	70	THR
1	B	100	ASN
1	B	102	TYR
1	B	145	THR
1	B	159	MET
1	B	175	THR
1	B	225	LEU
1	B	229	SER
1	B	274	MET
1	B	300	THR
1	B	316	LEU
1	B	353	GLN
1	B	363	ILE
1	B	366	LYS
1	B	372	GLU
1	B	379	ASP
1	B	402	GLN
1	B	404	LEU
1	B	424	ASN
1	B	444	VAL
1	B	454	SER
1	B	466	THR
1	B	470	VAL
1	B	480	VAL
1	B	491	THR

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Mol	Chain	Res	Type
1	B	492	VAL
1	B	506	LYS
1	B	508	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	321	HIS
1	A	369	ASN
1	A	406	ASN
1	B	68	ASN
1	B	341	HIS
1	B	424	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](#)

1 ligand is modelled in this entry.

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	GOL	A	601	-	5,5,5	0.36	0	5,5,5	0.56	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
2	GOL	A	601	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GOL	O1-C1-C2-C3
2	A	601	GOL	O1-C1-C2-O2
2	A	601	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	GOL	3	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	457/515 (88%)	0.27	43 (9%)	14 10	16, 37, 119, 160	0
1	B	446/515 (86%)	0.62	49 (10%)	10 8	19, 52, 116, 168	0
All	All	903/1030 (87%)	0.44	92 (10%)	12 9	16, 44, 118, 168	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	48	ALA	6.7
1	B	104	SER	5.8
1	B	101	LEU	5.5
1	A	50	ARG	5.4
1	B	71	SER	5.2
1	B	53	GLY	5.2
1	B	102	TYR	5.1
1	A	49	LEU	4.9
1	B	49	LEU	4.8
1	B	371	GLU	4.8
1	A	102	TYR	4.8
1	B	64	LEU	4.6
1	B	106	ILE	4.5
1	A	81	CYS	4.5
1	B	67	LEU	4.5
1	A	44	ASN	4.4
1	A	51	VAL	4.1
1	B	74	PRO	4.0
1	A	87	LYS	3.9
1	A	66	GLN	3.8
1	B	30	PRO	3.7
1	B	51	VAL	3.7
1	A	52	PRO	3.6
1	A	83	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	366	LYS	3.5
1	B	33	SER	3.5
1	B	80	SER	3.5
1	B	105	LEU	3.5
1	A	108	PRO	3.4
1	A	82	THR	3.4
1	A	54	ALA	3.4
1	A	40	ASP	3.4
1	A	106	ILE	3.3
1	A	67	LEU	3.3
1	B	69	GLY	3.3
1	A	53	GLY	3.3
1	B	117	ILE	3.2
1	B	444	VAL	3.1
1	B	136	SER	3.1
1	A	90	ASP	3.1
1	A	389	LEU	3.1
1	B	63	LEU	3.1
1	B	515	HIS	3.0
1	B	57	GLU	3.0
1	B	100	ASN	2.9
1	A	71	SER	2.8
1	A	70	THR	2.7
1	A	39	LEU	2.7
1	B	119	LEU	2.7
1	B	137	SER	2.7
1	A	75	VAL	2.7
1	B	474	ARG	2.7
1	A	33	SER	2.7
1	B	37	GLN	2.6
1	B	116	GLN	2.6
1	A	36	PHE	2.6
1	A	89	SER	2.6
1	B	103	SER	2.6
1	B	70	THR	2.6
1	A	515	HIS	2.5
1	A	367	ASN	2.5
1	A	62	GLU	2.5
1	A	41	THR	2.5
1	A	105	LEU	2.5
1	B	66	GLN	2.5
1	B	508	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	370	SER	2.4
1	B	36	PHE	2.3
1	A	55	ILE	2.3
1	B	65	ASN	2.3
1	B	52	PRO	2.3
1	B	368	GLY	2.3
1	B	68	ASN	2.2
1	B	40	ASP	2.2
1	B	282	SER	2.2
1	B	399	THR	2.2
1	A	61	GLU	2.2
1	A	466	THR	2.2
1	B	186	TYR	2.2
1	A	103	SER	2.2
1	A	88	ALA	2.1
1	A	58	LYS	2.1
1	B	120	LEU	2.1
1	A	104	SER	2.1
1	A	64	LEU	2.1
1	A	125	ALA	2.1
1	A	57	GLU	2.1
1	B	442	GLY	2.1
1	B	118	THR	2.1
1	A	136	SER	2.0
1	B	38	ALA	2.0
1	B	75	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	A	601	6/6	0.86	0.21	34,54,61,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.