



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 03:27 am BST

PDB ID : 4N3S
Title : Crystal structure of eukaryotic translation initiation factor eIF5B (399-852) from *Saccharomyces cerevisiae*, apo form
Authors : Kuhle, B.; Ficner, R.
Deposited on : 2013-10-07
Resolution : 1.83 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

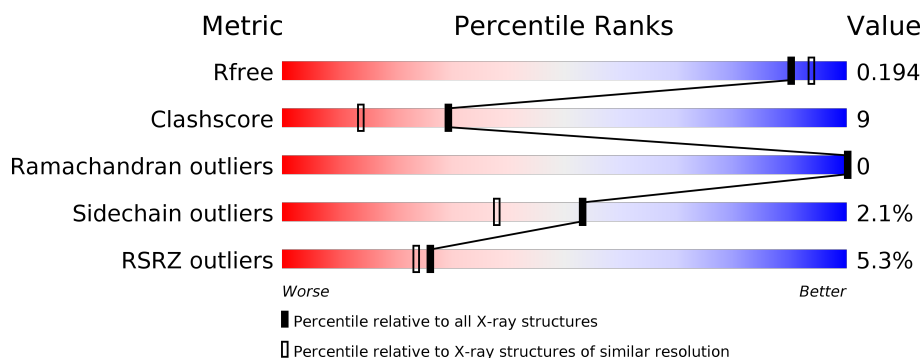
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	457	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>• •</div> </div> </div>
1	B	457	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>• •</div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7780 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.

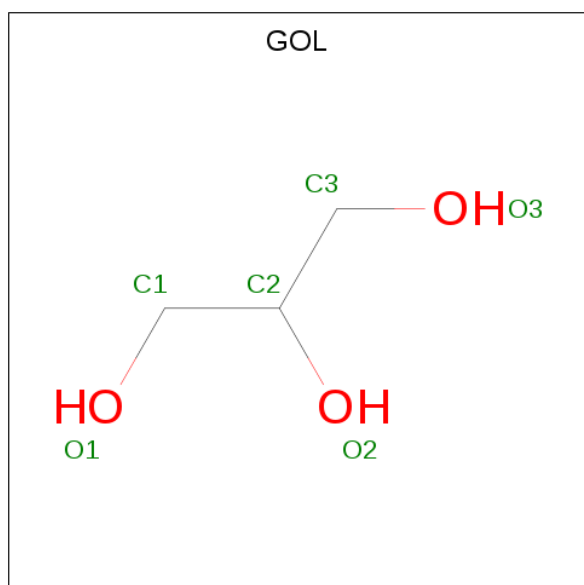
- Molecule 1 is a protein called Eukaryotic translation initiation factor 5B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	3	3	0
			3475	2213	579	665	18			
1	B	442	Total	C	N	O	S	0	3	0
			3485	2219	582	666	18			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	396	SER	-	EXPRESSION TAG	UNP P39730
A	397	HIS	-	EXPRESSION TAG	UNP P39730
A	398	MET	-	EXPRESSION TAG	UNP P39730
B	396	SER	-	EXPRESSION TAG	UNP P39730
B	397	HIS	-	EXPRESSION TAG	UNP P39730
B	398	MET	-	EXPRESSION TAG	UNP P39730

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

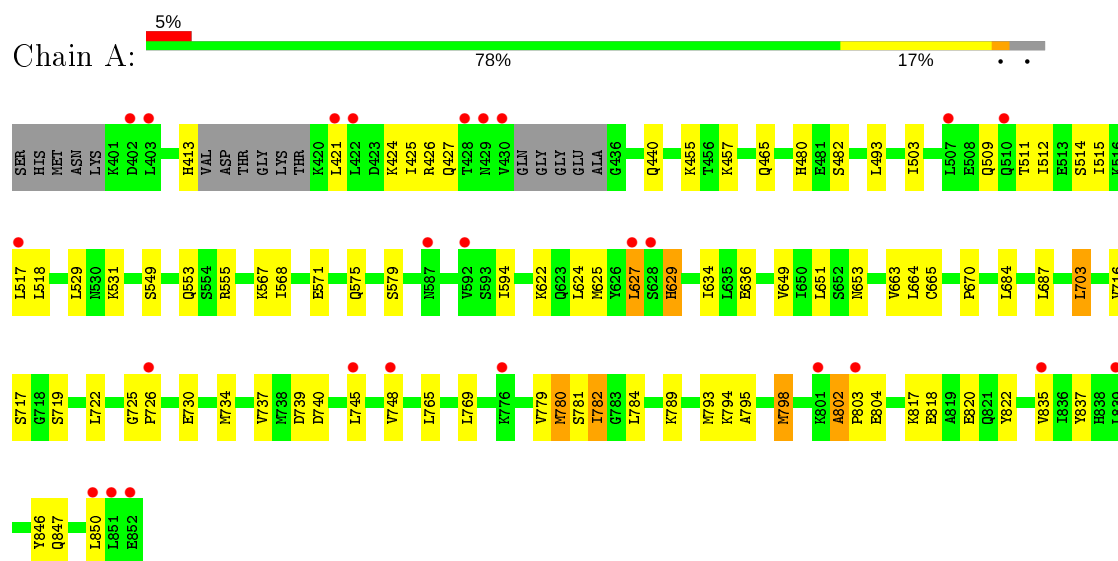
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	395	Total	O	0	5
			399	399		
4	B	380	Total	O	0	18
			397	397		

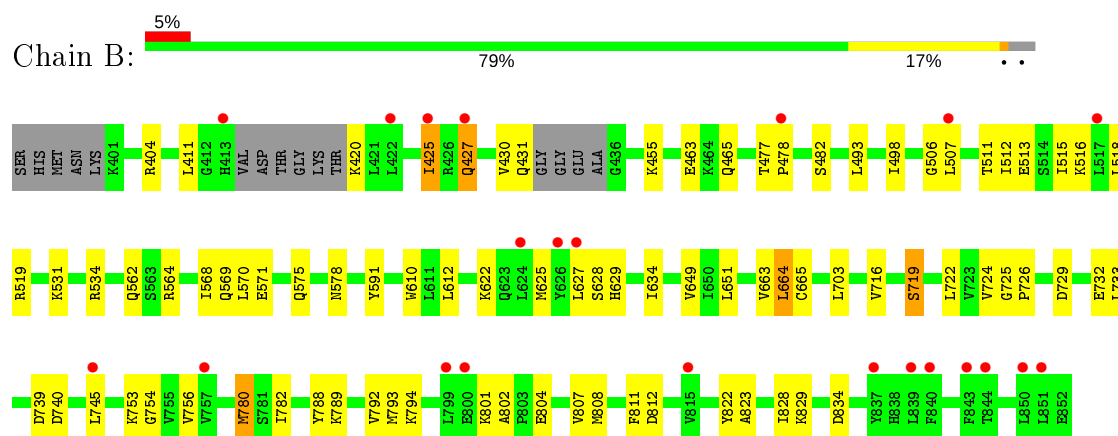
3 Residue-property plots [i](#)

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: Eukaryotic translation initiation factor 5B



- Molecule 1: Eukaryotic translation initiation factor 5B



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	118.01Å 118.01Å 77.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.95 – 1.83 46.95 – 1.83	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.95-1.83) 99.8 (46.95-1.83)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 1.83Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.168 , 0.194 0.182 , 0.194	Depositor DCC
R_{free} test set	4669 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.159 for h,-k,-l	Xtriage
Reported twinning fraction	0.200 for h,-k,-l	Depositor
Outliers	0 of 93326 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7780	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, EDO

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	0.44	2/3526 (0.1%)	0.56	2/4762 (0.0%)
1	B	0.42	1/3537 (0.0%)	0.56	2/4777 (0.0%)
All	All	0.43	3/7063 (0.0%)	0.56	4/9539 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	726	PRO	N-CD	5.25	1.55	1.47
1	A	803	PRO	N-CD	5.24	1.55	1.47
1	A	726	PRO	N-CD	5.22	1.55	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	628	SER	O-C-N	-5.75	113.49	122.70
1	A	725	GLY	C-N-CD	5.65	140.26	128.40
1	A	802	ALA	C-N-CD	5.62	140.19	128.40
1	B	725	GLY	C-N-CD	5.56	140.07	128.40

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	3475	0	3550	73	0
1	B	3485	0	3554	61	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
3	A	12	0	18	3	0
4	A	399	0	0	10	0
4	B	397	0	0	11	0
All	All	7780	0	7138	134	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 9.

All (134) 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:745:LEU:HD23	1:B:782:ILE:HD11	1.47	0.96
1:A:730:GLU:O	1:A:734:MET:HG3	1.74	0.87
1:B:622:LYS:O	1:B:625:MET:HG2	1.76	0.85
1:A:622:LYS:HD3	1:A:625:MET:SD	2.15	0.85
1:A:629:HIS:HD2	4:A:1373:HOH:O	1.61	0.84
1:A:804:GLU:OE1	1:A:804:GLU:N	2.13	0.81
1:A:802:ALA:HB1	1:A:804:GLU:CD	2.01	0.80
1:A:555:ARG:HD3	4:A:1326:HOH:O	1.82	0.79
1:A:846:TYR:CZ	1:A:850:LEU:HD11	2.22	0.75
1:B:516:LYS:CD	1:B:519:ARG:HH22	2.00	0.73
1:A:789:LYS:HG2	1:A:793:MET:HE2	1.72	0.71
1:A:780:MET:CE	1:A:794:LYS:O	2.38	0.71
1:A:804:GLU:HB2	1:A:847:GLN:OE1	1.91	0.70
1:B:562:GLN:NE2	4:B:1122:HOH:O	2.26	0.69
1:B:753:LYS:HB3	1:B:801:LYS:HE2	1.75	0.69
1:B:664:LEU:N	1:B:664:LEU:HD23	2.09	0.67
1:B:516:LYS:HD3	1:B:519:ARG:HH22	1.59	0.66
1:A:651:LEU:HB3	1:A:703:LEU:HD23	1.77	0.66
1:B:634:ILE:HA	1:B:649:VAL:HG12	1.78	0.66
1:A:482:SER:O	1:A:493:LEU:HD23	1.96	0.66
1:A:795:ALA:O	1:A:798:MET:HB2	1.95	0.65
1:A:529:LEU:HD11	1:A:568:ILE:HD13	1.77	0.65
1:A:509:GLN:HA	1:A:512:ILE:HD12	1.79	0.65
1:B:465:GLN:NE2	4:B:1334:HOH:O	2.28	0.64
1:B:724:VAL:HG22	1:B:733:LEU:HD12	1.80	0.64
1:A:780:MET:HE1	1:A:794:LYS:O	1.97	0.64
1:B:425:ILE:HG13	1:B:455:LYS:HG3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:754:GLY:O	1:B:780:MET:HG2	2.00	0.62
1:A:480:HIS:ND1	4:A:1287:HOH:O	2.31	0.61
1:B:404:ARG:NH1	4:B:1127:HOH:O	2.32	0.61
1:A:802:ALA:HB1	1:A:804:GLU:OE2	2.00	0.60
1:A:629:HIS:CD2	4:A:1373:HOH:O	2.42	0.60
1:B:420:LYS:NZ	4:B:1362:HOH:O	2.33	0.60
1:A:622:LYS:CD	1:A:625:MET:SD	2.89	0.60
1:A:627:LEU:HB3	1:A:653:ASN:ND2	2.18	0.59
1:A:663[A]:VAL:HG22	1:A:722:LEU:HB2	1.84	0.59
1:A:503:ILE:HA	1:A:568:ILE:HD11	1.84	0.58
1:B:482:SER:CB	4:B:1301[B]:HOH:O	2.51	0.58
1:B:663:VAL:CG2	1:B:722:LEU:HB2	2.34	0.57
1:A:517:LEU:HD11	3:A:904:EDO:H12	1.86	0.57
1:A:511:THR:O	1:A:515:ILE:HG13	2.04	0.56
1:B:482:SER:O	1:B:493:LEU:HD23	2.05	0.56
1:A:780:MET:HE3	1:A:794:LYS:O	2.04	0.56
1:A:424:LYS:NZ	4:A:1295:HOH:O	2.39	0.55
1:A:579:SER:HB2	1:A:594:ILE:HD11	1.90	0.54
1:A:835:VAL:HG11	1:A:837:TYR:CE1	2.42	0.54
1:A:531:LYS:HD3	4:A:1352:HOH:O	2.07	0.54
1:A:465:GLN:NE2	4:A:1188:HOH:O	2.35	0.54
1:A:512:ILE:HG23	1:A:575:GLN:OE1	2.08	0.53
1:B:807:VAL:HG12	1:B:829:LYS:HB2	1.90	0.53
1:A:748:VAL:HG11	1:A:782:ILE:HD13	1.92	0.52
1:B:512:ILE:HG23	1:B:575:GLN:OE1	2.09	0.52
1:B:664:LEU:CD2	1:B:664:LEU:N	2.73	0.52
1:A:780:MET:HG3	1:A:781:SER:N	2.25	0.52
1:B:788:TYR:O	1:B:792:VAL:HG23	2.11	0.51
1:A:426:ARG:NH1	1:A:440:GLN:OE1	2.44	0.51
1:B:516:LYS:CD	1:B:519:ARG:NH2	2.73	0.51
1:A:779:VAL:O	1:A:779:VAL:HG23	2.11	0.51
1:A:629:HIS:CE1	4:A:1164:HOH:O	2.64	0.50
1:B:802:ALA:HB1	1:B:804:GLU:CD	2.32	0.50
1:A:802:ALA:HB1	1:A:804:GLU:OE1	2.11	0.50
1:B:739:ASP:OD1	1:B:740:ASP:N	2.46	0.49
1:A:789:LYS:HB2	1:A:818:GLU:HG2	1.93	0.49
1:B:511:THR:O	1:B:515:ILE:HG13	2.12	0.49
1:B:663:VAL:HG22	1:B:722:LEU:HB2	1.95	0.49
1:A:798:MET:CE	1:A:798:MET:HA	2.41	0.49
1:A:781:SER:O	1:A:782:ILE:HD12	2.13	0.48
1:A:427:GLN:O	1:A:455:LYS:NZ	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:651:LEU:HB3	1:B:703[A]:LEU:HD23	1.95	0.48
1:B:651:LEU:HB3	1:B:703[B]:LEU:HD23	1.95	0.48
1:B:724:VAL:HG22	1:B:733:LEU:CD1	2.43	0.48
1:A:413:HIS:ND1	1:A:413:HIS:O	2.46	0.48
1:A:670:PRO:HB2	1:A:734:MET:HE3	1.96	0.48
1:B:578:ASN:HB3	1:B:591:TYR:CD1	2.49	0.48
1:A:789:LYS:O	1:A:793:MET:HG3	2.14	0.48
1:A:734:MET:O	1:A:737:VAL:HG12	2.13	0.47
1:A:765:LEU:O	1:A:769:LEU:HG	2.14	0.47
1:A:804:GLU:O	1:A:846:TYR:HE2	1.96	0.47
1:B:629[A]:HIS:O	1:B:629[A]:HIS:HD2	1.98	0.47
1:B:756:VAL:HG11	1:B:794:LYS:HE3	1.96	0.47
1:B:516:LYS:HD3	1:B:519:ARG:NH2	2.28	0.47
1:A:413:HIS:CD2	4:A:1299:HOH:O	2.68	0.47
1:A:457:LYS:HE2	1:A:457:LYS:HB2	1.67	0.47
1:B:789:LYS:O	1:B:793:MET:HG3	2.16	0.46
1:B:811:PHE:HE1	1:B:834:ASP:C	2.19	0.46
1:B:754:GLY:C	1:B:780:MET:HG2	2.36	0.46
1:A:684:LEU:HD12	1:A:687:LEU:HD12	1.98	0.46
1:A:634:ILE:HA	1:A:649[A]:VAL:HG12	1.98	0.46
1:B:519:ARG:HB2	4:B:1156:HOH:O	2.16	0.46
1:B:498:ILE:HD11	1:B:612:LEU:HD11	1.97	0.46
1:A:529:LEU:CD1	1:A:568:ILE:HD13	2.44	0.45
1:B:564:ARG:O	1:B:568:ILE:HG12	2.15	0.45
1:B:411:LEU:HD11	1:B:518:LEU:HD21	1.97	0.45
1:B:430:VAL:HG12	1:B:431:GLN:N	2.32	0.45
1:A:739:ASP:OD1	1:A:740:ASP:N	2.50	0.45
1:B:482:SER:HB2	4:B:1301[B]:HOH:O	2.15	0.45
1:B:716:VAL:O	1:B:719:SER:HB3	2.16	0.45
1:B:629[A]:HIS:CD2	1:B:629[A]:HIS:O	2.70	0.45
1:A:665:CYS:HB3	1:A:719:SER:HB2	1.98	0.44
1:B:506:GLY:HA2	1:B:568:ILE:CD1	2.46	0.44
1:A:514:SER:O	1:A:518:LEU:HG	2.17	0.44
1:B:569:GLN:NE2	4:B:1327:HOH:O	2.51	0.44
1:B:507:LEU:HD13	1:B:571:GLU:CB	2.47	0.44
1:A:636:GLU:HG3	4:A:1057:HOH:O	2.18	0.43
1:B:665:CYS:HB3	1:B:719:SER:HB2	1.99	0.43
1:A:503:ILE:HA	1:A:568:ILE:CD1	2.48	0.43
1:B:430:VAL:CG1	1:B:431:GLN:N	2.82	0.43
1:B:477:THR:HA	1:B:478:PRO:HD3	1.74	0.43
1:A:663[A]:VAL:CG2	1:A:722:LEU:HB2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:HIS:CG	1:A:413:HIS:O	2.70	0.43
1:B:482:SER:OG	4:B:1301[B]:HOH:O	2.20	0.43
1:A:670:PRO:HG2	1:A:734:MET:HE2	2.01	0.42
1:B:789:LYS:HE3	1:B:822:TYR:CD1	2.54	0.42
1:A:622:LYS:CE	1:A:625:MET:SD	3.07	0.42
1:B:729:ASP:OD2	1:B:732:GLU:HG3	2.20	0.42
1:A:634:ILE:HD11	1:A:664:LEU:HD23	2.02	0.42
1:B:427:GLN:NE2	4:B:1337:HOH:O	2.52	0.42
1:B:627:LEU:HD13	1:B:629[A]:HIS:NE2	2.35	0.42
1:A:517:LEU:CD1	3:A:904:EDO:H12	2.49	0.42
1:B:507:LEU:HD13	1:B:571:GLU:HB3	2.02	0.42
1:A:793:MET:HG2	1:A:822:TYR:CZ	2.54	0.41
1:B:531:LYS:HE3	1:B:534:ARG:HG3	2.02	0.41
1:A:745:LEU:HD23	1:A:782:ILE:HG21	2.02	0.41
1:A:717:SER:OG	3:A:903:EDO:H22	2.20	0.41
1:B:792:VAL:HA	1:B:808:MET:SD	2.60	0.41
1:A:567:LYS:O	1:A:571:GLU:HG3	2.20	0.41
1:A:716:VAL:HG13	1:A:784:LEU:HD13	2.03	0.41
1:B:823:ALA:HB1	1:B:828:ILE:O	2.21	0.41
1:B:570:LEU:HD13	4:B:1192:HOH:O	2.21	0.41
1:A:670:PRO:HB2	1:A:734:MET:CE	2.50	0.41
1:A:421:LEU:O	1:A:425:ILE:HG13	2.21	0.41
1:A:622:LYS:HA	1:A:622:LYS:HD3	1.84	0.40
1:A:549:SER:O	1:A:553:GLN:HG2	2.21	0.40
1:B:463:GLU:HB3	1:B:610:TRP:CZ2	2.57	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	438/457 (96%)	434 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	439/457 (96%)	435 (99%)	4 (1%)	0	100	100
All	All	877/914 (96%)	869 (99%)	8 (1%)	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	388/398 (98%)	379 (98%)	9 (2%)	50	34
1	B	388/398 (98%)	381 (98%)	7 (2%)	59	44
All	All	776/796 (98%)	760 (98%)	16 (2%)	53	38

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	624	LEU
1	A	627	LEU
1	A	629	HIS
1	A	703	LEU
1	A	780	MET
1	A	782	ILE
1	A	798	MET
1	A	817	LYS
1	A	820	GLU
1	B	425	ILE
1	B	427	GLN
1	B	513	GLU
1	B	664	LEU
1	B	719	SER
1	B	780	MET
1	B	812	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	838	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

5 ligands are 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	901	-	5,5,5	0.37	0	5,5,5	0.24	0
2	GOL	B	901	-	5,5,5	0.24	0	5,5,5	0.27	0
3	EDO	A	903	-	3,3,3	0.50	0	2,2,2	0.15	0
3	EDO	A	904	-	3,3,3	0.50	0	2,2,2	0.13	0
3	EDO	A	902	-	3,3,3	0.47	0	2,2,2	0.38	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	901	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	901	-	-	4/4/4/4	-
3	EDO	A	903	-	-	1/1/1/1	-
3	EDO	A	904	-	-	0/1/1/1	-
3	EDO	A	902	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	GOL	O1-C1-C2-C3
2	B	901	GOL	O1-C1-C2-C3
2	B	901	GOL	C1-C2-C3-O3
2	A	901	GOL	O1-C1-C2-O2
2	B	901	GOL	O2-C2-C3-O3
3	A	903	EDO	O1-C1-C2-O2
2	B	901	GOL	O1-C1-C2-O2
3	A	902	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	903	EDO	1	0
3	A	904	EDO	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	441/457 (96%)	0.25	25 (5%) 23 21	20, 42, 92, 155	0
1	B	442/457 (96%)	0.20	22 (4%) 28 26	20, 38, 96, 156	0
All	All	883/914 (96%)	0.23	47 (5%) 26 24	20, 41, 95, 156	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	430	VAL	8.1
1	A	850	LEU	6.2
1	B	799	LEU	6.1
1	B	839	LEU	5.7
1	B	850	LEU	4.1
1	B	843	PHE	4.1
1	B	745	LEU	4.0
1	A	745	LEU	3.9
1	A	803	PRO	3.9
1	A	851	LEU	3.9
1	A	422	LEU	3.8
1	A	801	LYS	3.8
1	A	429	ASN	3.6
1	A	839	LEU	3.6
1	A	403	LEU	3.5
1	B	815	VAL	3.4
1	A	517	LEU	3.4
1	B	425	ILE	3.3
1	A	507	LEU	3.3
1	A	592	VAL	3.3
1	B	627	LEU	3.2
1	B	507	LEU	3.2
1	B	422	LEU	3.1
1	A	726	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	402	ASP	3.0
1	A	852	GLU	2.9
1	B	840	PHE	2.9
1	A	776	LYS	2.7
1	A	748	VAL	2.7
1	B	624	LEU	2.6
1	A	510	GLN	2.6
1	A	428	THR	2.5
1	B	844	THR	2.5
1	A	628	SER	2.4
1	B	851	LEU	2.4
1	B	837	TYR	2.4
1	B	427	GLN	2.3
1	A	627	LEU	2.3
1	B	413	HIS	2.2
1	B	626	TYR	2.2
1	A	835	VAL	2.1
1	B	517	LEU	2.1
1	B	800	GLU	2.0
1	A	587	ASN	2.0
1	B	478	PRO	2.0
1	B	757	VAL	2.0
1	A	421	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	A	903	4/4	0.46	0.24	65,66,67,67	0
2	GOL	B	901	6/6	0.71	0.32	58,64,65,66	0
2	GOL	A	901	6/6	0.76	0.23	43,47,52,53	6
3	EDO	A	904	4/4	0.78	0.21	71,72,73,73	0
3	EDO	A	902	4/4	0.90	0.13	30,37,45,50	0

6.5 Other polymers

There are no such residues in this entry.