



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 08:12 AM GMT

PDB ID : 2WP8
Title : yeast rrp44 nuclease
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Deposited on : 2009-08-03
Resolution : 3.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

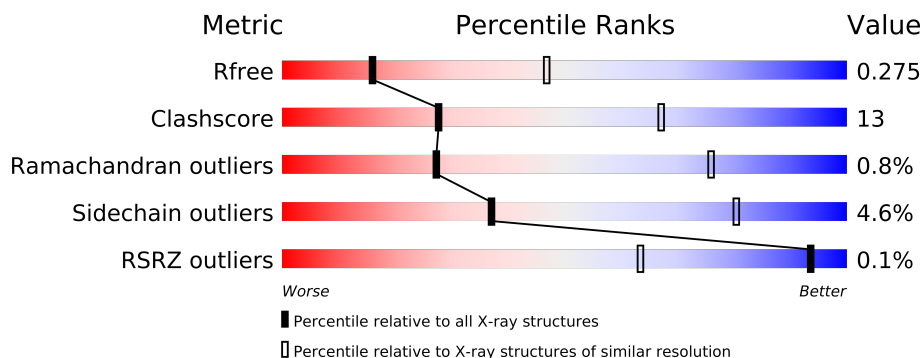
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.00 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}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	305	
2	B	246	
3	J	977	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	GOL	J	2002	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10816 atoms, of which 0 are hydrogen and 0 are deuterium.

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 EXOSOME COMPLEX COMPONENT RRP45.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			1946	1232	329	370	15			

- Molecule 2 is a protein called EXOSOME COMPLEX COMPONENT SKI6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1647	1031	285	323	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	79	ASN	THR	CONFLICT	UNP P46948

- Molecule 3 is a protein called EXOSOME COMPLEX EXONUCLEASE DIS3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	918	Total	C	N	O	S	0	0	0
			7216	4574	1250	1359	33			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	551	ASN	ASP	ENGINEERED MUTATION	UNP Q08162

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



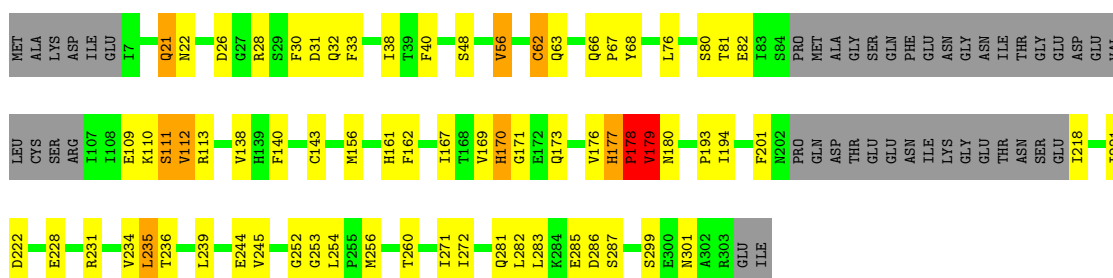
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	J	1	Total	C	O	0	0
			6	3	3		

3 Residue-property plots

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

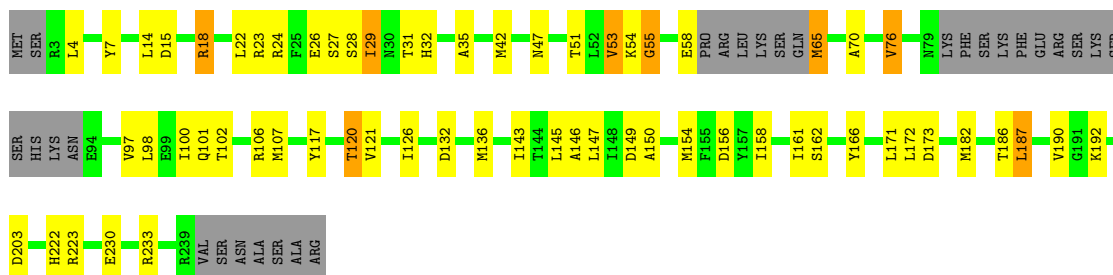
- Molecule 1: EXOSOME COMPLEX COMPONENT RRP45

Chain A: 



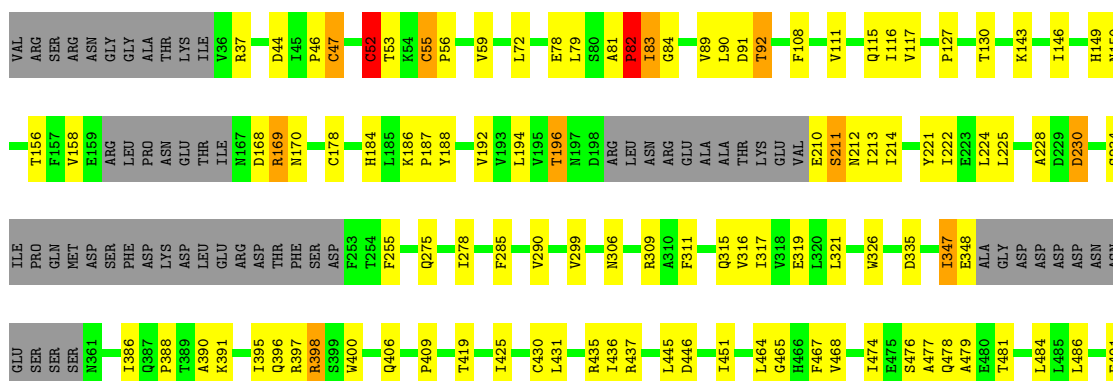
- Molecule 2: EXOSOME COMPLEX COMPONENT SKI6

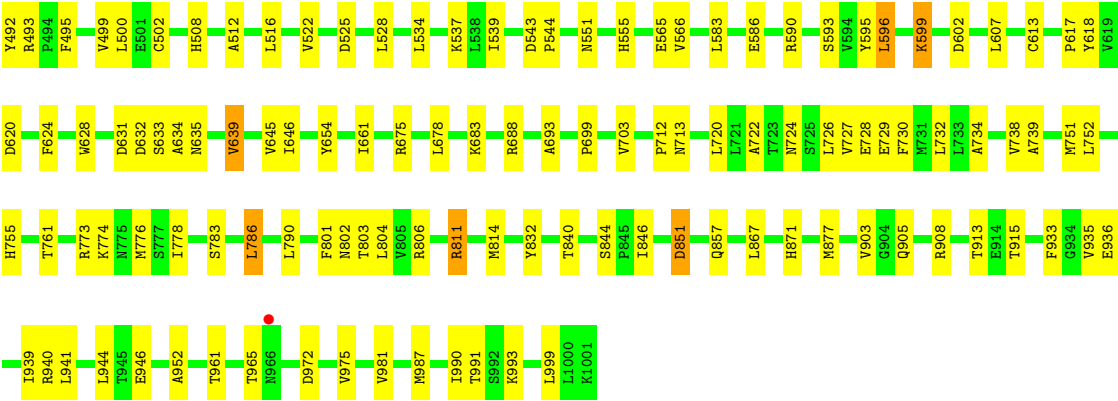
Chain B: 



- Molecule 3: EXOSOME COMPLEX EXONUCLEASE DIS3

Chain J: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.90Å 125.68Å 139.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.00 19.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-3.00) 100.0 (19.99-3.00)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.60 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.207 , 0.273 0.212 , 0.275	Depositor DCC
R_{free} test set	1185 reflections (3.09%)	DCC
Wilson B-factor (Å ²)	54.6	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , -0.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 39511 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10816	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

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

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	0.72	0/1973	0.82	3/2668 (0.1%)
2	B	0.68	0/1665	0.81	2/2254 (0.1%)
3	J	0.67	7/7362 (0.1%)	0.81	4/10007 (0.0%)
All	All	0.68	7/11000 (0.1%)	0.81	9/14929 (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	A	0	3
3	J	0	3
All	All	0	6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	82	PRO	C-N	-15.57	0.98	1.34
3	J	430	CYS	CB-SG	-7.98	1.68	1.82
3	J	52	CYS	CB-SG	7.58	1.95	1.82
3	J	55	CYS	CB-SG	7.04	1.94	1.82
3	J	502	CYS	CB-SG	-6.43	1.71	1.82
3	J	211	SER	C-N	5.41	1.46	1.34
3	J	613	CYS	CB-SG	-5.07	1.73	1.81

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	82	PRO	O-C-N	-23.90	84.46	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	82	PRO	CA-C-N	17.47	155.63	117.20
3	J	82	PRO	C-N-CA	12.62	153.25	121.70
2	B	18	ARG	NE-CZ-NH2	-6.36	117.12	120.30
2	B	18	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	A	170	HIS	N-CA-C	-5.38	96.48	111.00
1	A	177	HIS	C-N-CD	-5.23	109.09	120.60
1	A	253	GLY	N-CA-C	-5.03	100.52	113.10
3	J	169	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	PRO	Peptide
1	A	21	GLN	Peptide
1	A	252	GLY	Peptide
3	J	168	ASP	Peptide
3	J	82	PRO	Mainchain,Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1946	0	1883	56	0
2	B	1647	0	1616	59	0
3	J	7216	0	7084	164	0
4	B	1	0	0	0	0
5	J	6	0	8	1	0
All	All	10816	0	10591	274	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (274) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:66:GLN:O	1:A:67:PRO:N	1.76	1.19
3:J:210:GLU:CB	3:J:211:SER:HA	1.76	1.15
3:J:210:GLU:CB	3:J:211:SER:CA	2.29	1.10
3:J:52:CYS:SG	3:J:184:HIS:NE2	2.24	1.09
2:B:31:THR:HG22	2:B:32:HIS:CD2	1.90	1.06
1:A:178:PRO:HB2	1:A:179:VAL:CG2	1.87	1.03
1:A:169:VAL:HG12	1:A:169:VAL:O	1.55	1.02
1:A:178:PRO:CB	1:A:179:VAL:HG22	1.91	1.01
1:A:33:PHE:HB2	1:A:271:ILE:HD13	1.49	0.94
1:A:178:PRO:HB2	1:A:179:VAL:HG22	0.96	0.94
3:J:210:GLU:CB	3:J:211:SER:C	2.37	0.93
3:J:751:MET:H	3:J:857:GLN:HE22	1.14	0.92
2:B:47:ASN:HD21	2:B:132:ASP:H	1.18	0.91
3:J:778:ILE:CG2	3:J:786:LEU:HD13	2.02	0.89
1:A:31:ASP:HA	1:A:221:ILE:HD12	1.56	0.87
3:J:406:GLN:OE1	3:J:993:LYS:NZ	2.07	0.86
3:J:275:GLN:HE21	3:J:396:GLN:HE22	1.16	0.86
3:J:55:CYS:SG	3:J:184:HIS:NE2	2.53	0.82
2:B:161:ILE:HD11	2:B:172:LEU:HD11	1.62	0.82
3:J:628:TRP:CD1	3:J:639:VAL:HG13	2.16	0.80
3:J:47:CYS:CB	3:J:52:CYS:SG	2.70	0.79
3:J:210:GLU:CB	3:J:211:SER:O	2.30	0.79
1:A:167:ILE:HG22	1:A:177:HIS:HB3	1.62	0.79
3:J:275:GLN:HE21	3:J:396:GLN:NE2	1.81	0.79
2:B:47:ASN:ND2	2:B:132:ASP:H	1.81	0.78
1:A:169:VAL:O	1:A:169:VAL:CG1	2.30	0.77
3:J:150:ASN:HB2	3:J:156:THR:HG21	1.71	0.73
3:J:981:VAL:HG23	3:J:999:LEU:O	1.90	0.72
1:A:66:GLN:O	1:A:66:GLN:CA	2.37	0.72
3:J:703:VAL:HG22	3:J:713:ASN:ND2	2.05	0.71
2:B:31:THR:HG22	2:B:32:HIS:NE2	2.07	0.70
1:A:167:ILE:HG22	1:A:177:HIS:CB	2.22	0.69
3:J:678:LEU:HD11	3:J:722:ALA:HB1	1.75	0.69
3:J:946:GLU:HG3	3:J:965:THR:HG23	1.73	0.69
1:A:112:VAL:HG23	1:A:113:ARG:H	1.57	0.69
1:A:178:PRO:HA	1:A:179:VAL:HG13	1.74	0.69
1:A:301:ASN:ND2	3:J:602:ASP:OD2	2.27	0.68
2:B:161:ILE:CD1	2:B:172:LEU:HD11	2.23	0.68
3:J:275:GLN:NE2	3:J:396:GLN:HE22	1.91	0.68
2:B:161:ILE:HD11	2:B:172:LEU:CD1	2.23	0.68
2:B:76:VAL:HG12	2:B:101:GLN:HG3	1.75	0.67
2:B:172:LEU:O	2:B:172:LEU:HG	1.94	0.67
3:J:436:ILE:HG22	3:J:465:GLY:C	2.15	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:J:221:TYR:HD2	3:J:222:ILE:HD13	1.60	0.66
3:J:92:THR:HA	3:J:117:VAL:HG13	1.77	0.66
3:J:255:PHE:CG	3:J:309:ARG:HD2	2.31	0.65
3:J:491:GLU:OE1	3:J:493:ARG:HG3	1.96	0.65
3:J:481:THR:HG23	3:J:596:LEU:HD23	1.77	0.65
1:A:228:GLU:HG3	1:A:231:ARG:NH2	2.12	0.64
2:B:23:ARG:NH1	2:B:173:ASP:OD2	2.31	0.63
1:A:235:LEU:HD13	1:A:256:MET:SD	2.39	0.63
3:J:255:PHE:CD1	3:J:309:ARG:HD2	2.32	0.63
1:A:171:GLY:O	1:A:173:GLN:N	2.30	0.62
3:J:778:ILE:HG21	3:J:786:LEU:HD13	1.82	0.61
1:A:112:VAL:HG23	1:A:113:ARG:N	2.14	0.61
3:J:79:LEU:HD12	3:J:83:ILE:HG21	1.82	0.61
3:J:508:HIS:CE1	3:J:607:LEU:HD23	2.36	0.61
3:J:321:LEU:HD21	3:J:391:LYS:HB3	1.82	0.61
2:B:70:ALA:HB2	2:B:117:TYR:O	2.01	0.61
3:J:91:ASP:HB2	3:J:196:THR:HG23	1.82	0.60
3:J:476:SER:O	3:J:477:ALA:HB3	2.01	0.60
2:B:98:LEU:O	2:B:102:THR:HG23	2.01	0.60
2:B:172:LEU:CG	2:B:172:LEU:O	2.49	0.60
3:J:566:VAL:HG11	3:J:730:PHE:CE2	2.36	0.60
3:J:871:HIS:HA	3:J:877:MET:CE	2.31	0.60
2:B:117:TYR:O	2:B:120:THR:HG22	2.01	0.60
3:J:941:LEU:HA	3:J:944:LEU:HD12	1.84	0.59
1:A:26:ASP:OD1	1:A:28:ARG:HG2	2.01	0.59
3:J:981:VAL:CG2	3:J:999:LEU:O	2.49	0.59
2:B:14:LEU:HD13	3:J:37:ARG:HD2	1.84	0.59
2:B:107:MET:HE1	2:B:158:ILE:HG21	1.84	0.59
2:B:23:ARG:HG2	2:B:173:ASP:OD1	2.03	0.59
1:A:236:THR:HG23	1:A:236:THR:O	2.03	0.59
2:B:171:LEU:HD12	2:B:182:MET:CE	2.33	0.58
1:A:178:PRO:CA	1:A:179:VAL:HG13	2.32	0.58
3:J:311:PHE:CD2	3:J:431:LEU:HD22	2.39	0.58
3:J:47:CYS:CB	3:J:55:CYS:SG	2.92	0.58
1:A:66:GLN:O	1:A:67:PRO:CA	2.52	0.58
3:J:317:ILE:HD11	3:J:396:GLN:NE2	2.19	0.57
3:J:72:LEU:HD11	3:J:146:ILE:HG12	1.85	0.57
2:B:147:LEU:HD13	2:B:154:MET:HE3	1.85	0.57
1:A:228:GLU:O	1:A:231:ARG:HG2	2.05	0.57
3:J:435:ARG:NH2	3:J:464:LEU:HB2	2.19	0.57
1:A:28:ARG:NH2	1:A:222:ASP:O	2.36	0.57
3:J:551:ASN:HD22	3:J:844:SER:HA	1.70	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:J:633:SER:O	3:J:634:ALA:HB3	2.04	0.57
3:J:734:ALA:O	3:J:738:VAL:HG23	2.06	0.56
1:A:167:ILE:HD12	1:A:169:VAL:CG2	2.35	0.56
3:J:755:HIS:HE1	3:J:814:MET:O	1.87	0.56
2:B:31:THR:CG2	2:B:32:HIS:CD2	2.79	0.56
3:J:783:SER:HB3	3:J:832:TYR:CZ	2.41	0.56
2:B:28:SER:O	2:B:29:ILE:HD13	2.05	0.56
1:A:239:LEU:HB2	1:A:272:ILE:CD1	2.36	0.56
1:A:299:SER:OG	3:J:590:ARG:NH1	2.39	0.55
2:B:156:ASP:HB3	2:B:190:VAL:HG13	1.88	0.55
3:J:871:HIS:HA	3:J:877:MET:HE3	1.87	0.55
3:J:278:ILE:O	3:J:278:ILE:HG23	2.06	0.55
3:J:952:ALA:HB3	3:J:961:THR:HB	1.89	0.55
2:B:24:ARG:NH1	2:B:26:GLU:OE1	2.39	0.55
3:J:802:ASN:OD1	3:J:806:ARG:NH2	2.40	0.54
3:J:285:PHE:O	5:J:2002:GOL:O2	2.25	0.54
3:J:315:GLN:HB2	3:J:397:ARG:HB3	1.88	0.54
2:B:187:LEU:N	2:B:187:LEU:HD23	2.23	0.54
3:J:425:ILE:HD12	3:J:425:ILE:N	2.23	0.54
2:B:100:ILE:HD13	2:B:136:MET:HE1	1.89	0.54
3:J:52:CYS:SG	3:J:184:HIS:CE1	3.00	0.54
2:B:22:LEU:HD12	2:B:223:ARG:HG2	1.89	0.54
2:B:172:LEU:HD12	2:B:172:LEU:O	2.07	0.54
3:J:961:THR:HG23	3:J:972:ASP:OD1	2.08	0.53
3:J:481:THR:HG21	3:J:599:LYS:HD2	1.91	0.53
3:J:783:SER:HB3	3:J:832:TYR:CE1	2.44	0.53
1:A:178:PRO:CB	1:A:179:VAL:HG13	2.39	0.53
2:B:23:ARG:HH11	2:B:173:ASP:CG	2.13	0.53
2:B:51:THR:HG23	2:B:126:ILE:HG12	1.90	0.52
3:J:81:ALA:HB1	3:J:82:PRO:HA	1.91	0.52
3:J:186:LYS:HB3	3:J:187:PRO:HD3	1.91	0.52
2:B:29:ILE:HD11	2:B:145:LEU:HB3	1.91	0.52
3:J:451:ILE:HG22	3:J:467:PHE:HA	1.91	0.52
3:J:728:GLU:HG2	3:J:732:LEU:HD23	1.91	0.52
3:J:991:THR:HG22	3:J:993:LYS:H	1.74	0.52
2:B:100:ILE:HD13	2:B:136:MET:CE	2.40	0.52
3:J:53:THR:HG22	3:J:188:TYR:OH	2.10	0.52
3:J:476:SER:HB3	3:J:479:ALA:HB3	1.91	0.51
3:J:720:LEU:HD22	3:J:724:ASN:ND2	2.25	0.51
1:A:193:PRO:O	1:A:194:ILE:HD13	2.11	0.51
3:J:724:ASN:O	3:J:727:VAL:HG12	2.10	0.51
3:J:127:PRO:O	3:J:130:THR:HB	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:J:537:LYS:NZ	3:J:565:GLU:OE2	2.34	0.51
3:J:446:ASP:O	3:J:474:ILE:HG23	2.10	0.51
2:B:32:HIS:HB3	2:B:35:ALA:HB3	1.92	0.51
3:J:156:THR:O	3:J:156:THR:HG22	2.10	0.51
3:J:751:MET:O	3:J:752:LEU:HD23	2.10	0.50
1:A:56:VAL:HG22	1:A:140:PHE:CE1	2.46	0.50
1:A:22:ASN:CG	1:A:22:ASN:O	2.49	0.50
3:J:551:ASN:OD1	3:J:846:ILE:HD12	2.12	0.50
1:A:38:ILE:HB	1:A:282:LEU:HD13	1.93	0.50
3:J:508:HIS:ND1	3:J:607:LEU:HD23	2.27	0.50
1:A:218:ILE:HG23	1:A:218:ILE:O	2.12	0.50
2:B:18:ARG:HD2	3:J:44:ASP:OD2	2.12	0.50
3:J:534:LEU:HB2	3:J:646:ILE:HG22	1.93	0.49
3:J:78:GLU:HA	3:J:84:GLY:O	2.13	0.49
3:J:525:ASP:OD1	3:J:525:ASP:C	2.50	0.49
3:J:661:ILE:HG23	3:J:675:ARG:HG2	1.93	0.49
1:A:112:VAL:HG12	1:A:156:MET:HE3	1.93	0.49
3:J:55:CYS:SG	3:J:184:HIS:CE1	3.05	0.49
2:B:47:ASN:ND2	2:B:132:ASP:N	2.56	0.49
3:J:92:THR:CA	3:J:117:VAL:HG13	2.42	0.49
3:J:116:ILE:HD11	3:J:170:ASN:OD1	2.12	0.49
3:J:116:ILE:HD12	3:J:169:ARG:NH2	2.28	0.49
3:J:91:ASP:CB	3:J:196:THR:HG23	2.42	0.48
3:J:595:TYR:CG	3:J:712:PRO:HB3	2.48	0.48
1:A:40:PHE:CZ	1:A:283:LEU:HD23	2.47	0.48
3:J:89:VAL:O	3:J:194:LEU:HD12	2.12	0.48
3:J:347:ILE:HD12	3:J:437:ARG:HB2	1.94	0.48
1:A:201:PHE:O	1:A:254:LEU:HD11	2.13	0.48
3:J:688:ARG:O	3:J:693:ALA:CB	2.61	0.48
2:B:172:LEU:O	2:B:172:LEU:CD1	2.62	0.48
2:B:161:ILE:CD1	2:B:172:LEU:CD1	2.88	0.48
1:A:239:LEU:CD2	1:A:245:VAL:HG22	2.44	0.48
2:B:186:THR:C	2:B:187:LEU:HD23	2.33	0.48
1:A:177:HIS:O	1:A:177:HIS:CG	2.67	0.48
2:B:230:GLU:HA	2:B:233:ARG:NH2	2.28	0.48
3:J:409:PRO:HA	3:J:445:LEU:HD11	1.96	0.47
1:A:281:GLN:HE21	1:A:285:GLU:HG3	1.78	0.47
3:J:211:SER:O	3:J:213:ILE:N	2.47	0.47
3:J:778:ILE:HG23	3:J:786:LEU:HD13	1.91	0.47
3:J:990:ILE:N	3:J:990:ILE:HD12	2.28	0.47
3:J:778:ILE:CG2	3:J:786:LEU:CD1	2.84	0.47
3:J:688:ARG:O	3:J:693:ALA:HB2	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:J:543:ASP:HB3	3:J:544:PRO:HD2	1.96	0.47
2:B:192:LYS:HA	2:B:222:HIS:CD2	2.50	0.47
3:J:811:ARG:NH2	3:J:936:GLU:OE2	2.47	0.47
1:A:239:LEU:HD23	1:A:245:VAL:HA	1.96	0.47
2:B:107:MET:CE	2:B:158:ILE:HG21	2.44	0.47
3:J:905:GLN:HE22	3:J:908:ARG:NH1	2.13	0.47
1:A:161:HIS:HE1	1:A:286:ASP:OD1	1.97	0.47
2:B:51:THR:HG21	2:B:143:ILE:HA	1.97	0.47
1:A:167:ILE:HA	1:A:176:VAL:O	2.14	0.47
3:J:512:ALA:HB3	3:J:620:ASP:HB2	1.96	0.47
1:A:167:ILE:HD12	1:A:169:VAL:HG23	1.96	0.46
3:J:903:VAL:HG22	3:J:933:PHE:CD2	2.51	0.46
3:J:811:ARG:NH1	3:J:936:GLU:OE2	2.48	0.46
2:B:161:ILE:HG12	2:B:162:SER:N	2.31	0.46
3:J:435:ARG:O	3:J:464:LEU:HD12	2.15	0.46
2:B:53:VAL:CG2	2:B:150:ALA:HB2	2.44	0.46
3:J:451:ILE:HA	3:J:468:VAL:HG23	1.96	0.46
3:J:617:PRO:HB2	3:J:618:TYR:CD1	2.51	0.46
3:J:46:PRO:HG3	3:J:59:VAL:HG22	1.98	0.46
3:J:654:TYR:OH	3:J:727:VAL:HG11	2.15	0.46
1:A:299:SER:CB	3:J:590:ARG:HH12	2.28	0.46
3:J:586:GLU:O	3:J:590:ARG:HG3	2.15	0.46
3:J:90:LEU:HD11	3:J:111:VAL:HG11	1.98	0.46
1:A:179:VAL:HG23	1:A:180:ASN:H	1.81	0.45
3:J:46:PRO:HG3	3:J:59:VAL:CG2	2.46	0.45
3:J:211:SER:C	3:J:213:ILE:H	2.19	0.45
3:J:512:ALA:HB3	3:J:620:ASP:CB	2.46	0.45
2:B:54:LYS:O	2:B:55:GLY:O	2.35	0.45
3:J:499:VAL:HG13	3:J:583:LEU:HD13	1.97	0.45
3:J:83:ILE:HG12	3:J:214:ILE:HD13	1.98	0.45
2:B:14:LEU:HD12	2:B:15:ASP:N	2.31	0.45
1:A:22:ASN:HB2	1:A:30:PHE:CZ	2.50	0.45
3:J:335:ASP:OD2	3:J:940:ARG:NH2	2.49	0.45
1:A:28:ARG:HB2	1:A:32:GLN:CD	2.37	0.45
3:J:299:VAL:HG23	3:J:388:PRO:O	2.17	0.45
3:J:720:LEU:HD22	3:J:724:ASN:HD22	1.81	0.45
1:A:156:MET:HB2	1:A:156:MET:HE2	1.57	0.44
2:B:100:ILE:HA	2:B:136:MET:HE1	1.99	0.44
3:J:857:GLN:HA	3:J:867:LEU:HD13	2.00	0.44
1:A:21:GLN:H	1:A:22:ASN:HA	1.83	0.44
1:A:169:VAL:C	1:A:170:HIS:O	2.49	0.44
2:B:117:TYR:O	2:B:120:THR:CG2	2.64	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:58:GLU:HA	2:B:58:GLU:OE1	2.18	0.44
3:J:774:LYS:O	3:J:776:MET:HG3	2.18	0.44
3:J:871:HIS:HA	3:J:877:MET:HE1	1.98	0.44
2:B:53:VAL:HG13	2:B:146:ALA:HB1	1.99	0.44
3:J:939:ILE:HG22	3:J:944:LEU:HG	1.99	0.44
1:A:81:THR:HG22	1:A:138:VAL:HB	1.99	0.44
3:J:631:ASP:OD1	3:J:635:ASN:N	2.42	0.43
2:B:117:TYR:HB3	2:B:120:THR:HG21	2.00	0.43
3:J:688:ARG:NH2	3:J:729:GLU:OE2	2.51	0.43
3:J:484:LEU:HA	3:J:484:LEU:HD23	1.76	0.43
3:J:108:PHE:O	3:J:143:LYS:NZ	2.33	0.43
3:J:632:ASP:O	3:J:683:LYS:NZ	2.44	0.43
3:J:230:ASP:N	3:J:230:ASP:OD1	2.51	0.43
3:J:516:LEU:HD11	3:J:645:VAL:HG21	1.99	0.43
2:B:7:TYR:HB3	2:B:166:TYR:CE2	2.53	0.43
3:J:306:ASN:ND2	3:J:321:LEU:HD11	2.33	0.43
3:J:991:THR:HG22	3:J:993:LYS:HB2	2.00	0.43
3:J:851:ASP:N	3:J:851:ASP:OD1	2.52	0.43
3:J:395:ILE:HG21	3:J:398:ARG:HD3	2.00	0.43
2:B:70:ALA:CB	2:B:120:THR:CG2	2.97	0.43
1:A:68:TYR:CE2	1:A:76:LEU:HD22	2.54	0.43
1:A:239:LEU:HB2	1:A:272:ILE:HD12	1.99	0.43
3:J:678:LEU:HB2	3:J:726:LEU:HD12	2.01	0.42
2:B:70:ALA:CB	2:B:120:THR:HG22	2.49	0.42
1:A:239:LEU:HB2	1:A:272:ILE:HD13	2.00	0.42
3:J:946:GLU:CG	3:J:965:THR:HG23	2.46	0.42
3:J:319:GLU:O	3:J:390:ALA:HB1	2.19	0.42
3:J:89:VAL:HG11	3:J:178:CYS:SG	2.60	0.42
2:B:29:ILE:HG23	2:B:149:ASP:OD1	2.18	0.42
3:J:278:ILE:O	3:J:278:ILE:CG2	2.66	0.42
3:J:79:LEU:HD22	3:J:224:LEU:O	2.20	0.42
3:J:81:ALA:HA	3:J:82:PRO:C	2.39	0.42
3:J:290:VAL:HG12	3:J:290:VAL:O	2.20	0.42
3:J:115:GLN:HB2	3:J:149:HIS:HA	2.02	0.42
3:J:186:LYS:HB3	3:J:187:PRO:CD	2.50	0.42
3:J:221:TYR:CE2	3:J:225:LEU:HD21	2.55	0.41
3:J:89:VAL:HG23	3:J:192:VAL:HG13	2.01	0.41
1:A:62:CYS:HB3	1:A:162:PHE:HZ	1.85	0.41
3:J:79:LEU:O	3:J:84:GLY:HA2	2.19	0.41
3:J:633:SER:O	3:J:634:ALA:CB	2.68	0.41
3:J:347:ILE:O	3:J:348:GLU:CB	2.68	0.41
3:J:398:ARG:HG3	3:J:400:TRP:CD2	2.55	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:29:ILE:HD13	2:B:29:ILE:HA	1.68	0.41
3:J:699:PRO:HB3	3:J:720:LEU:HD21	2.02	0.41
3:J:778:ILE:HG23	3:J:786:LEU:CD1	2.51	0.41
3:J:225:LEU:O	3:J:228:ALA:HB2	2.21	0.41
3:J:499:VAL:O	3:J:500:LEU:C	2.59	0.41
3:J:739:ALA:HB2	3:J:840:THR:HG22	2.02	0.41
2:B:97:VAL:CG1	2:B:98:LEU:N	2.84	0.41
3:J:90:LEU:CD1	3:J:111:VAL:HG11	2.51	0.41
3:J:801:PHE:O	3:J:804:LEU:HB3	2.21	0.41
3:J:55:CYS:N	3:J:56:PRO:CD	2.84	0.40
1:A:112:VAL:CG2	1:A:113:ARG:N	2.84	0.40
2:B:29:ILE:HG23	2:B:149:ASP:CG	2.41	0.40
3:J:495:PHE:CD2	3:J:586:GLU:HG2	2.56	0.40
3:J:486:LEU:CD1	3:J:492:TYR:OH	2.69	0.40
3:J:326:TRP:HB3	3:J:386:ILE:CG2	2.51	0.40
2:B:65:MET:O	2:B:65:MET:CG	2.70	0.40
3:J:726:LEU:C	3:J:726:LEU:HD23	2.42	0.40
3:J:877:MET:HE2	3:J:877:MET:CA	2.51	0.40
3:J:877:MET:HA	3:J:877:MET:HE2	2.02	0.40
2:B:4:LEU:HA	2:B:4:LEU:HD23	1.82	0.40
3:J:539:ILE:HG12	3:J:555:HIS:HB3	2.04	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	252/305 (83%)	231 (92%)	15 (6%)	6 (2%)	9	42
2	B	211/246 (86%)	195 (92%)	15 (7%)	1 (0%)	38	84
3	J	908/977 (93%)	862 (95%)	42 (5%)	4 (0%)	43	87
All	All	1371/1528 (90%)	1288 (94%)	72 (5%)	11 (1%)	27	76

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	SER
1	A	178	PRO
1	A	179	VAL
3	J	212	ASN
2	B	55	GLY
1	A	110	LYS
3	J	47	CYS
1	A	109	GLU
3	J	347	ILE
1	A	112	VAL
3	J	83	ILE

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	204/266 (77%)	190 (93%)	14 (7%)	22	62
2	B	175/218 (80%)	164 (94%)	11 (6%)	25	66
3	J	789/881 (90%)	760 (96%)	29 (4%)	45	86
All	All	1168/1365 (86%)	1114 (95%)	54 (5%)	37	80

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	SER
1	A	56	VAL
1	A	62	CYS
1	A	63	GLN
1	A	80	SER
1	A	82	GLU
1	A	111	SER
1	A	143	CYS
1	A	179	VAL
1	A	234	VAL
1	A	235	LEU
1	A	244	GLU
1	A	260	THR

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Mol	Chain	Res	Type
1	A	287	SER
2	B	27	SER
2	B	29	ILE
2	B	42	MET
2	B	53	VAL
2	B	65	MET
2	B	76	VAL
2	B	106	ARG
2	B	120	THR
2	B	121	VAL
2	B	187	LEU
2	B	203	ASP
3	J	52	CYS
3	J	92	THR
3	J	158	VAL
3	J	196	THR
3	J	230	ASP
3	J	234	SER
3	J	316	VAL
3	J	398	ARG
3	J	419	THR
3	J	478	GLN
3	J	522	VAL
3	J	528	LEU
3	J	593	SER
3	J	596	LEU
3	J	599	LYS
3	J	624	PHE
3	J	639	VAL
3	J	761	THR
3	J	773	ARG
3	J	786	LEU
3	J	790	LEU
3	J	803	THR
3	J	811	ARG
3	J	851	ASP
3	J	913	THR
3	J	915	THR
3	J	935	VAL
3	J	975	VAL
3	J	987	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	HIS
1	A	180	ASN
1	A	281	GLN
2	B	32	HIS
2	B	47	ASN
2	B	180	ASN
3	J	275	GLN
3	J	315	GLN
3	J	396	GLN
3	J	551	ASN
3	J	569	HIS
3	J	667	ASN
3	J	713	ASN
3	J	755	HIS
3	J	857	GLN
3	J	890	ASN
3	J	905	GLN
3	J	910	ASN
3	J	923	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z > 2$
5	GOL	J	2002	-	5,5,5	0.49	0	5,5,5	0.86	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
5	GOL	J	2002	-	-	0/4/4/4	0/0/0/0

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	260/305 (85%)	-0.23	0	100	100	18, 29, 49, 55	0
2	B	217/246 (88%)	-0.25	0	100	100	17, 25, 43, 66	0
3	J	918/977 (93%)	-0.24	1 (0%)	93	63	14, 29, 45, 61	0
All	All	1395/1528 (91%)	-0.24	1 (0%)	93	63	14, 28, 45, 66	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	966	ASN	2.4

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	GOL	J	2002	6/6	0.35	3.37	33,36,38,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CL	B	1240	1/1	0.10	-2.04	44,44,44,44	0

6.5 Other polymers ⓘ

There are no such residues in this entry.