



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 01:38 pm 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 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
Xtriage (Phenix)	:	1.13
EDS	:	trunk31020
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk31020

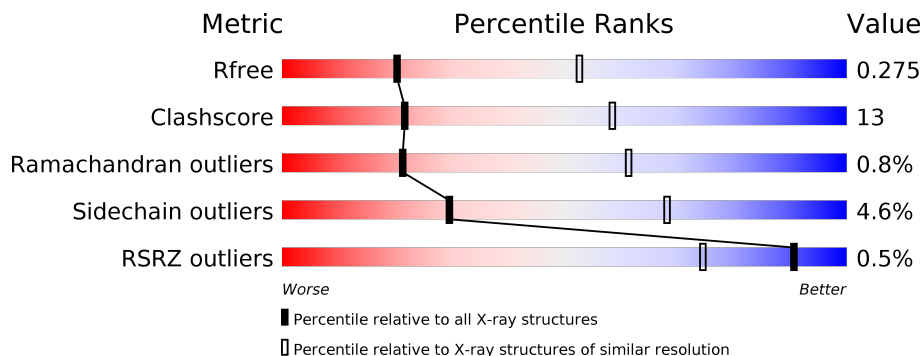
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	111664	1851 (3.00-3.00)
Clashscore	122126	2167 (3.00-3.00)
Ramachandran outliers	120053	2101 (3.00-3.00)
Sidechain outliers	120020	2104 (3.00-3.00)
RSRZ outliers	108989	1751 (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. 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	305	
2	B	246	
3	J	977	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10816 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 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		

● Molecule 1: EXOSOME COMPLEX COMPONENT RRP45





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 0.211 , 0.275	Depositor DCC
R_{free} test set	1185 reflections (3.00%)	wwPDB-VP
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 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	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.

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, 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 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	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

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 13.

All (274) 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: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
1:A:167:ILE:HG22	1:A:177:HIS:HB3	1.62	0.79
3:J:210:GLU:CB	3:J:211:SER:O	2.30	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
2:B:161:ILE:HD11	2:B:172:LEU:CD1	2.23	0.68
3:J:275:GLN:NE2	3:J:396:GLN:HE22	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:436:ILE:HG22	3:J:465:GLY:C	2.15	0.67
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:481:THR:HG23	3:J:596:LEU:HD23	1.77	0.65
3:J:491:GLU:OE1	3:J:493:ARG:HG3	1.96	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
1:A:112:VAL:HG23	1:A:113:ARG:N	2.14	0.61
3:J:778:ILE:HG21	3:J:786:LEU:HD13	1.82	0.61
3:J:508:HIS:CE1	3:J:607:LEU:HD23	2.36	0.61
3:J:79:LEU:HD12	3:J:83:ILE:HG21	1.82	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
2:B:98:LEU:O	2:B:102:THR:HG23	2.01	0.60
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: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
2:B:14:LEU:HD13	3:J:37:ARG:HD2	1.84	0.59
3:J:981:VAL:CG2	3:J:999:LEU:O	2.49	0.59
2:B:107:MET:HE1	2:B:158:ILE:HG21	1.84	0.59
1:A:236:THR:HG23	1:A:236:THR:O	2.03	0.59
2:B:23:ARG:HG2	2:B:173:ASP:OD1	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:72:LEU:HD11	3:J:146:ILE:HG12	1.85	0.57
3:J:317:ILE:HD11	3:J:396:GLN:NE2	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:28:SER:O	2:B:29:ILE:HD13	2.05	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
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:278:ILE:O	3:J:278:ILE:HG23	2.06	0.55
3:J:871:HIS:HA	3:J:877:MET:HE3	1.87	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
2:B:100:ILE:HD13	2:B:136:MET:HE1	1.89	0.54
3:J:425:ILE:HD12	3:J:425:ILE:N	2.23	0.54
2:B:22:LEU:HD12	2:B:223:ARG:HG2	1.89	0.54
3:J:52:CYS:SG	3:J:184:HIS:CE1	3.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:22:ASN:CG	1:A:22:ASN:O	2.49	0.50
1:A:56:VAL:HG22	1:A:140:PHE:CE1	2.46	0.50
3:J:751:MET:O	3:J:752:LEU:HD23	2.10	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
2:B:47:ASN:ND2	2:B:132:ASP:N	2.56	0.49
3:J:55:CYS:SG	3:J:184:HIS:CE1	3.05	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:595:TYR:CG	3:J:712:PRO:HB3	2.48	0.48
3:J:91:ASP:CB	3:J:196:THR:HG23	2.42	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
1:A:239:LEU:CD2	1:A:245:VAL:HG22	2.44	0.48
2:B:161:ILE:CD1	2:B:172:LEU:CD1	2.88	0.48
2:B:186:THR:C	2:B:187:LEU:HD23	2.33	0.48
1:A:177:HIS:CG	1:A:177:HIS:O	2.67	0.48
2:B:230:GLU:HA	2:B:233:ARG:NH2	2.28	0.48
1:A:281:GLN:HE21	1:A:285:GLU:HG3	1.78	0.47
3:J:409:PRO:HA	3:J:445:LEU:HD11	1.96	0.47
3:J:211:SER:O	3:J:213:ILE:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:192:LYS:HA	2:B:222:HIS:CD2	2.50	0.47
3:J:543:ASP:HB3	3:J:544:PRO:HD2	1.96	0.47
3:J:688:ARG:O	3:J:693:ALA:HB2	2.14	0.47
3:J:778:ILE:CG2	3:J:786:LEU:CD1	2.84	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
1:A:161:HIS:HE1	1:A:286:ASP:OD1	1.97	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
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:53:VAL:CG2	2:B:150:ALA:HB2	2.44	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
3:J:451:ILE:HA	3:J:468:VAL:HG23	1.96	0.46
3:J:46:PRO:HG3	3:J:59:VAL:HG22	1.98	0.46
3:J:617:PRO:HB2	3:J:618:TYR:CD1	2.51	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
2:B:54:LYS:O	2:B:55:GLY:O	2.35	0.45
3:J:211:SER:C	3:J:213:ILE:H	2.19	0.45
3:J:499:VAL:HG13	3:J:583:LEU:HD13	1.97	0.45
3:J:512:ALA:HB3	3:J:620:ASP:CB	2.46	0.45
1:A:22:ASN:HB2	1:A:30:PHE:CZ	2.50	0.45
2:B:14:LEU:HD12	2:B:15:ASP:N	2.31	0.45
3:J:83:ILE:HG12	3:J:214:ILE:HD13	1.98	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:HE2	1:A:156:MET:HB2	1.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:53:VAL:HG13	2:B:146:ALA:HB1	1.99	0.44
3:J:871:HIS:HA	3:J:877:MET:HE1	1.98	0.44
1:A:81:THR:HG22	1:A:138:VAL:HB	1.99	0.44
3:J:939:ILE:HG22	3:J:944:LEU:HG	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:108:PHE:O	3:J:143:LYS:NZ	2.33	0.43
3:J:484:LEU:HA	3:J:484:LEU:HD23	1.76	0.43
3:J:632:ASP:O	3:J:683:LYS:NZ	2.44	0.43
3:J:688:ARG:NH2	3:J:729:GLU:OE2	2.51	0.43
3:J:230:ASP:N	3:J:230:ASP:OD1	2.51	0.43
2:B:7:TYR:HB3	2:B:166:TYR:CE2	2.53	0.43
3:J:516:LEU:HD11	3:J:645:VAL:HG21	1.99	0.43
3:J:306:ASN:ND2	3:J:321:LEU:HD11	2.33	0.43
3:J:395:ILE:HG21	3:J:398:ARG:HD3	2.00	0.43
3:J:851:ASP:N	3:J:851:ASP:OD1	2.52	0.43
3:J:991:THR:HG22	3:J:993:LYS:HB2	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
2:B:70:ALA:CB	2:B:120:THR:HG22	2.49	0.42
3:J:678:LEU:HB2	3:J:726:LEU:HD12	2.01	0.42
1:A:239:LEU:HB2	1:A:272:ILE:HD13	2.00	0.42
3:J:319:GLU:O	3:J:390:ALA:HB1	2.19	0.42
3:J:946:GLU:CG	3:J:965:THR:HG23	2.46	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:115:GLN:HB2	3:J:149:HIS:HA	2.02	0.42
3:J:290:VAL:HG12	3:J:290:VAL:O	2.20	0.42
3:J:186:LYS:HB3	3:J:187:PRO:CD	2.50	0.42
3:J:89:VAL:HG23	3:J:192:VAL:HG13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:221:TYR:CE2	3:J:225:LEU:HD21	2.55	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: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
3:J:633:SER:O	3:J:634:ALA:CB	2.68	0.41
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: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
3:J:778:ILE:HG23	3:J:786:LEU:CD1	2.51	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
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:55:CYS:N	3:J:56:PRO:CD	2.84	0.40
3:J:495:PHE:CD2	3:J:586:GLU:HG2	2.56	0.40
3:J:326:TRP:HB3	3:J:386:ILE:CG2	2.51	0.40
3:J:486:LEU:CD1	3:J:492:TYR:OH	2.69	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
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
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

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	252/305 (83%)	231 (92%)	15 (6%)	6 (2%)	6	32
2	B	211/246 (86%)	195 (92%)	15 (7%)	1 (0%)	31	71
3	J	908/977 (93%)	862 (95%)	42 (5%)	4 (0%)	36	76
All	All	1371/1528 (90%)	1288 (94%)	72 (5%)	11 (1%)	21	61

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%)	17	51
2	B	175/218 (80%)	164 (94%)	11 (6%)	20	55
3	J	789/881 (90%)	760 (96%)	29 (4%)	37	74
All	All	1168/1365 (86%)	1114 (95%)	54 (5%)	29	68

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

Mol	Chain	Res	Type
1	A	48	SER
1	A	56	VAL

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 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](#)

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	0.55	0	5,5,5	0.87	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	2002	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	J	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	82:PRO	C	83:ILE	N	0.98

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.42	1 (0%) 92 78	18, 29, 49, 55	0
2	B	217/246 (88%)	-0.55	0 100 100	17, 25, 43, 66	0
3	J	918/977 (93%)	-0.44	6 (0%) 87 68	14, 29, 45, 61	0
All	All	1395/1528 (91%)	-0.45	7 (0%) 90 74	14, 28, 45, 66	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	966	ASN	6.9
3	J	361	ASN	4.0
3	J	362	THR	3.3
3	J	211	SER	2.6
3	J	994	ARG	2.4
3	J	229	ASP	2.3
1	A	171	GLY	2.1

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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	J	2002	6/6	0.91	0.26	33,36,38,39	0
4	CL	B	1240	1/1	0.95	0.10	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.