



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:30 PM UTC

PDB ID : 2WP8 / pdb_00002wp8
Title : yeast rrp44 nuclease
Authors : Basquin, J.; Bonneau, F.; Ebert, J.; Lorentzen, E.; Conti, E.
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 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)
Xtrriage (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

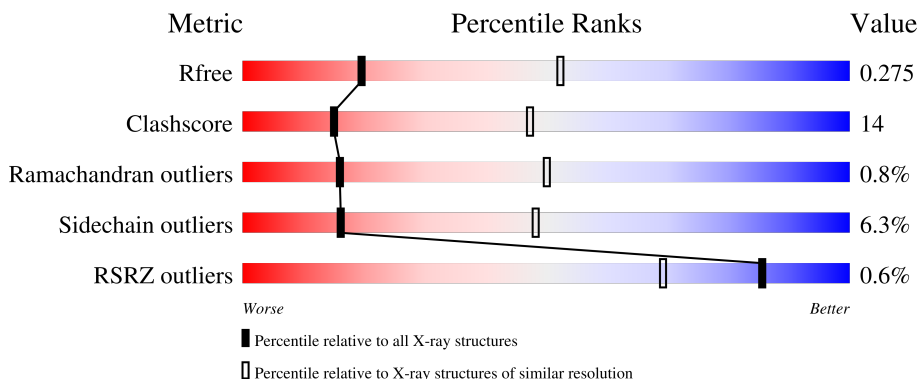
1 Overall quality at a glance i

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 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	305	 60% 22% 15% 1% 1%
2	B	246	 59% 24% 12% 5%
3	J	977	 69% 22% 6% 3%

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
			Total	C	N	O	S			
1	A	260	1946	1232	329	370	15	0	0	0

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

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

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
			Total	C	N	O	S			
3	J	918	7216	4574	1250	1359	33	0	0	0

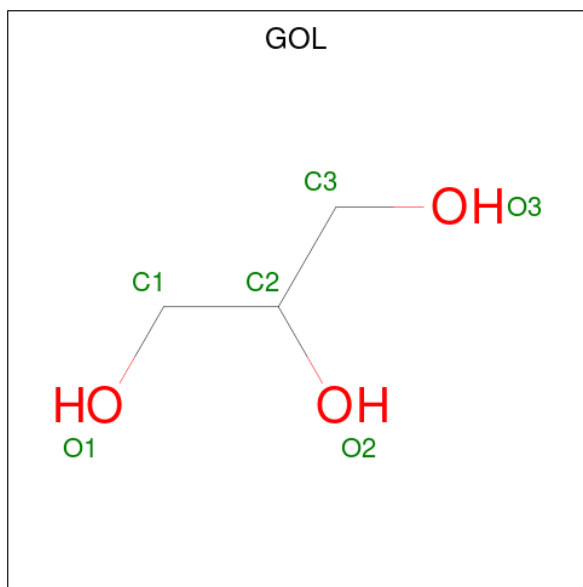
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	551	ASN	ASP	engineered mutation	UNP Q08162

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



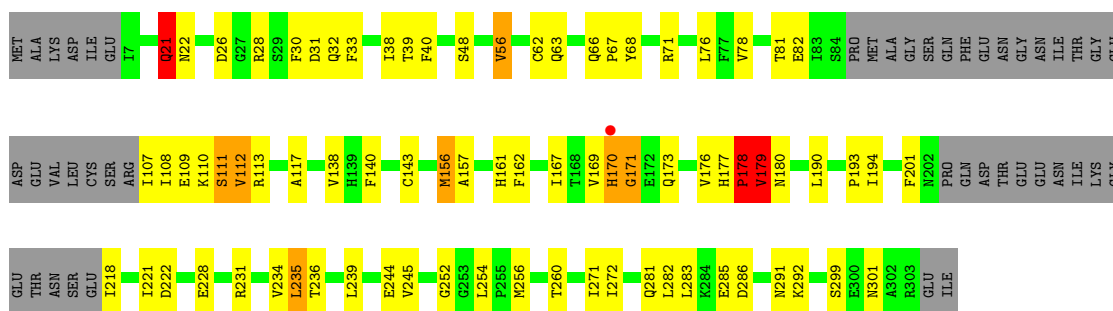
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	J	1	Total	C	O	0	0
			6	3	3		

3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

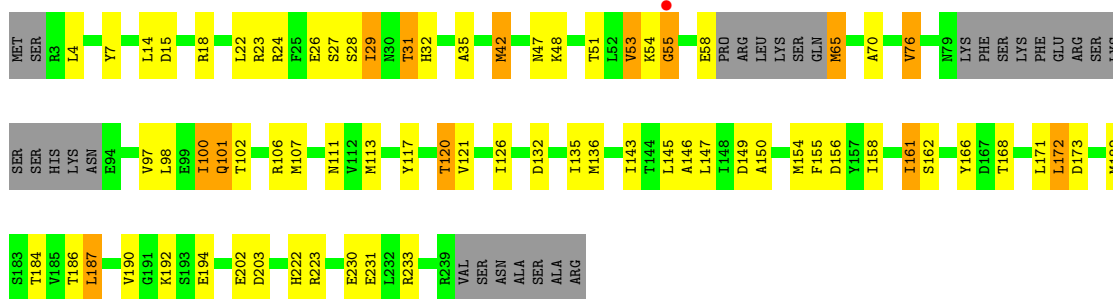
• Molecule 1: EXOSOME COMPLEX COMPONENT RRP45

Chain A: 



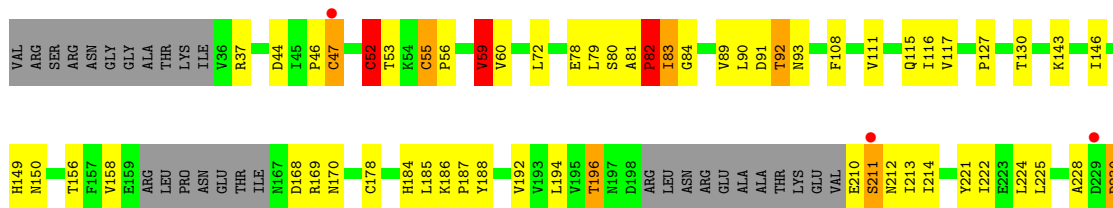
• Molecule 2: EXOSOME COMPLEX COMPONENT SKI6

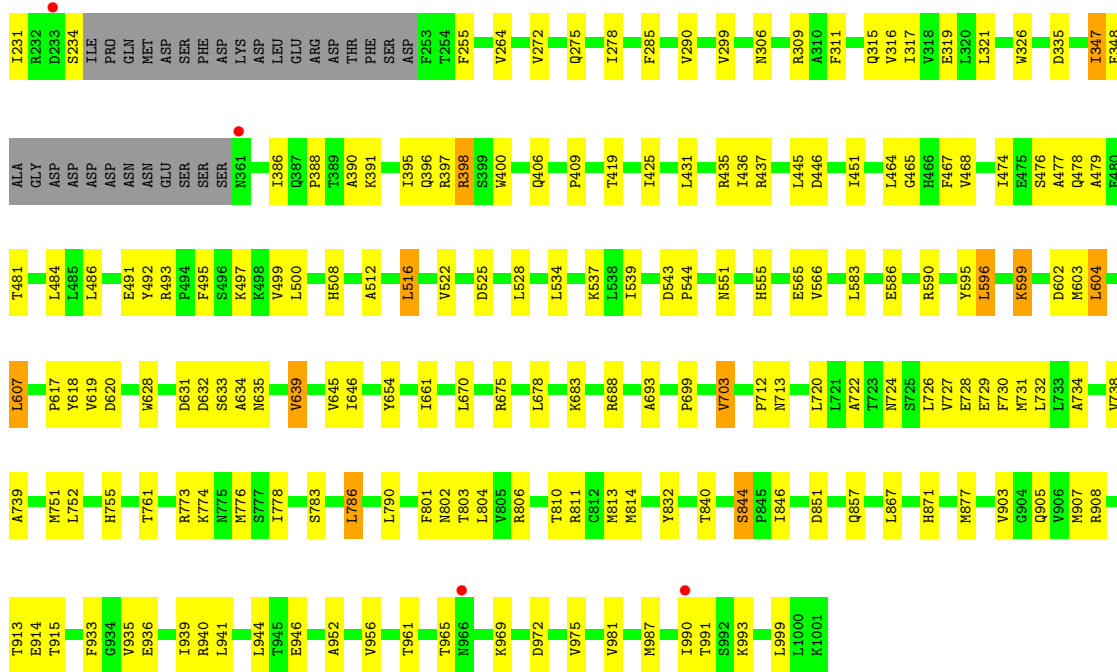
Chain B: 



• 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) 99.6 (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)	Xtrriage
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	Xtrriage
Anisotropy	0.094	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10816	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage'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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CL, 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	0.93	0/1973	1.06	5/2668 (0.2%)
2	B	0.88	0/1665	1.04	4/2254 (0.2%)
3	J	0.87	6/7362 (0.1%)	1.02	7/10007 (0.1%)
All	All	0.88	6/11000 (0.1%)	1.03	16/14929 (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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	82	PRO	C-N	-26.03	0.98	1.33
3	J	211	SER	C-N	9.14	1.46	1.33
3	J	80	SER	C-N	-7.24	1.22	1.33
3	J	60	VAL	CA-CB	5.32	1.61	1.54
3	J	264	VAL	CA-CB	5.14	1.60	1.54
3	J	55	CYS	CA-C	5.08	1.59	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	82	PRO	O-C-N	-19.28	84.46	121.10
3	J	82	PRO	CA-C-N	17.38	153.25	121.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	82	PRO	C-N-CA	17.38	153.25	121.97
1	A	170	HIS	N-CA-C	-10.65	96.48	110.43
1	A	21	GLN	N-CA-C	7.31	122.64	113.43
2	B	135	ILE	N-CA-CB	6.61	118.28	110.55
3	J	59	VAL	N-CA-C	6.46	118.00	109.21
1	A	171	GLY	N-CA-C	-6.38	106.52	115.32
1	A	157	ALA	N-CA-C	-6.03	104.63	111.14
3	J	231	ILE	N-CA-C	5.77	114.66	106.53
2	B	172	LEU	CA-C-N	-5.53	113.02	121.26
2	B	172	LEU	C-N-CA	-5.53	113.02	121.26
3	J	844	SER	N-CA-C	5.43	117.39	109.30
1	A	117	ALA	N-CA-C	-5.28	105.44	111.14
3	J	52	CYS	N-CA-C	-5.26	102.06	109.96
2	B	161	ILE	CB-CA-C	-5.11	106.94	111.74

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	Peptide,Mainchain

5.2 Too-close contacts [i](#)

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	59	0
2	B	1647	0	1616	66	0
3	J	7216	0	7084	173	0
4	B	1	0	0	0	0
5	J	6	0	8	1	0
All	All	10816	0	10591	293	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 14.

All (293) 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
3:J:210:GLU:CB	3:J:211:SER:C	2.37	0.98
2:B:171:LEU:HD12	2:B:182:MET:HE1	1.44	0.97
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: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
1:A:112:VAL:HG12	1:A:156:MET:HE1	1.56	0.85
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:903:VAL:HG13	3:J:907:MET:HE3	1.66	0.76
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
3:J:436:ILE:HG22	3:J:465:GLY:C	2.15	0.71
2:B:100:ILE:HD13	2:B:136:MET:HE2	1.72	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG	2:B:172:LEU:O	1.94	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
3:J:810:THR:HA	3:J:813:MET:HE2	1.80	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
3:J:903:VAL:CG1	3:J:907:MET:HE3	2.29	0.62
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: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
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:O	2:B:172:LEU:CG	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
2:B:171:LEU:CD1	2:B:182:MET:HE1	2.27	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:23:ARG:HG2	2:B:173:ASP:OD1	2.03	0.59
1:A:178:PRO:CA	1:A:179:VAL:HG13	2.32	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:311:PHE:CD2	3:J:431:LEU:HD22	2.39	0.58
2:B:113:MET:HE3	2:B:155:PHE:CE1	2.38	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
1:A:236:THR:HG23	1:A:236:THR:O	2.03	0.57
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:23:ARG:HH11	2:B:173:ASP:CG	2.13	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
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
3:J:871:HIS:HA	3:J:877:MET:HE3	1.86	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
1:A:22:ASN:CG	1:A:22:ASN:O	2.49	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
3:J:525:ASP:OD1	3:J:525:ASP:C	2.50	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:O	2:B:172:LEU:HD12	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:100:ILE:HA	2:B:136:MET:HE1	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:THR:C	2:B:187:LEU:HD23	2.33	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
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:HG22	3:J:156:THR:O	2.10	0.51
3:J:211:SER:C	3:J:213:ILE:H	2.19	0.51
3:J:731:MET:N	3:J:731:MET:HE2	2.26	0.51
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
1:A:156:MET:HE2	1:A:156:MET:N	2.27	0.49
3:J:78:GLU:HA	3:J:84:GLY:O	2.13	0.49
3:J:661:ILE:HG23	3:J:675:ARG:HG2	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
1:A:28:ARG:HB2	1:A:32:GLN:CD	2.37	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:107:MET:HE1	2:B:158:ILE:HG21	1.95	0.48
3:J:688:ARG:O	3:J:693:ALA:CB	2.61	0.48
2:B:172:LEU:CD1	2:B:172:LEU:O	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
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
2:B:111:ASN:OD1	2:B:154:MET:HE2	2.15	0.47
3:J:778:ILE:HG23	3:J:786:LEU:HD13	1.91	0.47
3:J:990:ILE:HD12	3:J:990:ILE:N	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
3:J:81:ALA:HA	3:J:82:PRO:C	2.39	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
1:A:169:VAL:C	1:A:170:HIS:O	2.49	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:46:PRO:HG3	3:J:59:VAL:HG22	1.98	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:90:LEU:HD11	3:J:111:VAL:HG11	1.98	0.46
3:J:499:VAL:O	3:J:500:LEU:C	2.59	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:29:ILE:HG23	2:B:149:ASP:CG	2.41	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:512:ALA:HB3	3:J:620:ASP:CB	2.46	0.45
3:J:537:LYS:NZ	3:J:565:GLU:OE2	2.34	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:726:LEU:C	3:J:726:LEU:HD23	2.42	0.45
3:J:335:ASP:OD2	3:J:940:ARG:NH2	2.49	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
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
3:J:46:PRO:O	3:J:47:CYS:C	2.61	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
3:J:907:MET:HE2	3:J:914:GLU:HG3	1.99	0.44
2:B:53:VAL:HG13	2:B:146:ALA:HB1	1.99	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
1:A:156:MET:HE2	1:A:156:MET:CA	2.48	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
2:B:42:MET:HE2	2:B:42:MET:HB2	1.54	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
2:B:14:LEU:HD12	2:B:14:LEU:C	2.44	0.43
2:B:147:LEU:CD1	2:B:154:MET:HE1	2.49	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:851:ASP:OD1	3:J:851:ASP:N	2.52	0.43
3:J:991:THR:HG22	3:J:993:LYS:HB2	2.00	0.43
1:A:291:ASN:O	1:A:292:LYS:C	2.60	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:91:ASP:CG	3:J:92:THR:N	2.77	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:185:LEU:O	3:J:186:LYS:C	2.62	0.42
3:J:319:GLU:O	3:J:390:ALA:HB1	2.19	0.42
3:J:871:HIS:HA	3:J:877:MET:HE1	1.99	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: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:89:VAL:HG23	3:J:192:VAL:HG13	2.01	0.41
3:J:221:TYR:CE2	3:J:225:LEU:HD21	2.55	0.41
3:J:603:MET:HE3	3:J:604:LEU:HD13	2.02	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: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
3:J:877:MET:CA	3:J:877:MET:HE2	2.50	0.41
2:B:97:VAL:CG1	2:B:98:LEU:N	2.84	0.41
2:B:23:ARG:NH1	2:B:173:ASP:CG	2.76	0.41
3:J:90:LEU:CD1	3:J:111:VAL:HG11	2.51	0.41
3:J:603:MET:HE3	3:J:604:LEU:CD1	2.51	0.41
3:J:801:PHE:O	3:J:804:LEU:HB3	2.21	0.41
2:B:107:MET:HB3	2:B:107:MET:HE2	1.84	0.41
1:A:112:VAL:CG2	1:A:113:ARG:N	2.84	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:877:MET:HE2	3:J:877:MET:HA	2.02	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
1:A:107:ILE:O	1:A:108:ILE:C	2.64	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 [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%)	4	24
2	B	211/246 (86%)	195 (92%)	15 (7%)	1 (0%)	24	60
3	J	908/977 (93%)	862 (95%)	42 (5%)	4 (0%)	30	65
All	All	1371/1528 (90%)	1288 (94%)	72 (5%)	11 (1%)	16	50

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	J	347	ILE
1	A	112	VAL
3	J	83	ILE

5.3.2 Protein sidechains [i](#)

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%)	188 (92%)	16 (8%)	11	39
2	B	175/218 (80%)	155 (89%)	20 (11%)	5	24
3	J	789/881 (90%)	751 (95%)	38 (5%)	23	57
All	All	1168/1365 (86%)	1094 (94%)	74 (6%)	16	48

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	THR
1	A	48	SER
1	A	56	VAL
1	A	63	GLN
1	A	71	ARG
1	A	78	VAL
1	A	82	GLU
1	A	111	SER
1	A	143	CYS
1	A	156	MET
1	A	179	VAL
1	A	190	LEU
1	A	234	VAL
1	A	235	LEU
1	A	244	GLU
1	A	260	THR
2	B	27	SER
2	B	29	ILE
2	B	31	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	42	MET
2	B	48	LYS
2	B	53	VAL
2	B	65	MET
2	B	76	VAL
2	B	100	ILE
2	B	101	GLN
2	B	106	ARG
2	B	120	THR
2	B	121	VAL
2	B	168	THR
2	B	184	THR
2	B	187	LEU
2	B	194	GLU
2	B	202	GLU
2	B	203	ASP
2	B	231	GLU
3	J	52	CYS
3	J	59	VAL
3	J	92	THR
3	J	93	ASN
3	J	158	VAL
3	J	196	THR
3	J	230	ASP
3	J	234	SER
3	J	272	VAL
3	J	290	VAL
3	J	316	VAL
3	J	398	ARG
3	J	419	THR
3	J	478	GLN
3	J	497	LYS
3	J	516	LEU
3	J	522	VAL
3	J	528	LEU
3	J	596	LEU
3	J	599	LYS
3	J	604	LEU
3	J	607	LEU
3	J	619	VAL
3	J	639	VAL
3	J	670	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	J	703	VAL
3	J	761	THR
3	J	773	ARG
3	J	786	LEU
3	J	790	LEU
3	J	803	THR
3	J	913	THR
3	J	915	THR
3	J	935	VAL
3	J	956	VAL
3	J	969	LYS
3	J	975	VAL
3	J	987	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) 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	73	ASN
2	B	79	ASN
2	B	115	ASN
2	B	180	ASN
2	B	235	HIS
3	J	275	GLN
3	J	315	GLN
3	J	396	GLN
3	J	569	HIS
3	J	640	ASN
3	J	656	GLN
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	949	ASN
3	J	982	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	0.58	0	5,5,5	0.92	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	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	J	2002	GOL	O1-C1-C2-C3
5	J	2002	GOL	O1-C1-C2-O2

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%)	-0.36	1 (0%) 88 76	18, 29, 49, 55	0
2	B	217/246 (88%)	-0.29	1 (0%) 87 72	17, 25, 43, 66	0
3	J	918/977 (93%)	-0.32	7 (0%) 82 64	14, 29, 45, 61	0
All	All	1395/1528 (91%)	-0.32	9 (0%) 85 69	14, 28, 45, 66	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	966	ASN	5.3
1	A	170	HIS	3.1
3	J	47	CYS	3.1
3	J	211	SER	2.9
3	J	229	ASP	2.9
2	B	55	GLY	2.6
3	J	233	ASP	2.5
3	J	990	ILE	2.2
3	J	361	ASN	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 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(\AA^2)	Q<0.9
5	GOL	J	2002	6/6	0.89	0.14	33,36,38,39	0
4	CL	B	1240	1/1	0.95	0.12	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.