Full wwPDB X-ray Structure Validation Report (i)

Jan 15, 2018 – 06:45 PM EST

PDB ID	:	5YK4
Title	:	Mismatch Repair Protein
Authors	:	Nirwal, S.; Nair, D.T.
Deposited on	:	2017-10-12
Resolution	:	2.97 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736
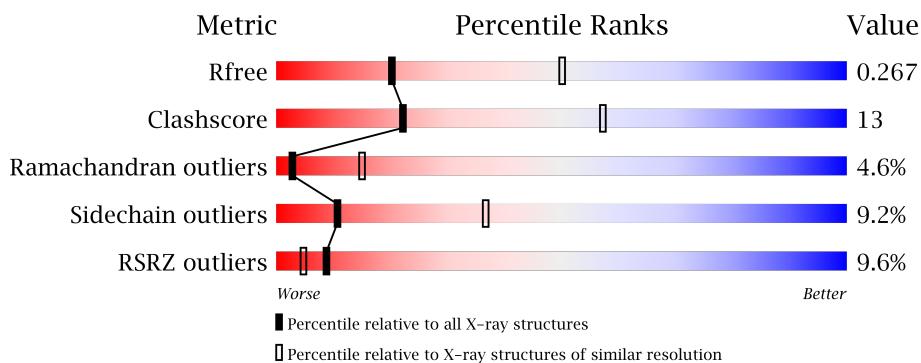
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
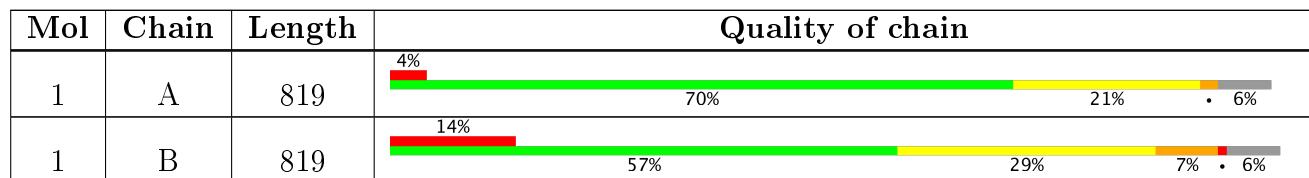
The reported resolution of this entry is 2.97 Å.

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	Percentile Ranks	Value
Rfree		0.267
Clashscore		13
Ramachandran outliers		4.6%
Sidechain outliers		9.2%
RSRZ outliers		9.6%

Worse　　　　　　　　　　　　　　　　　　　　　　Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2168 (3.00-2.96)
Clashscore	112137	2535 (3.00-2.96)
Ramachandran outliers	110173	2451 (3.00-2.96)
Sidechain outliers	110143	2454 (3.00-2.96)
RSRZ outliers	101464	2192 (3.00-2.96)

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 <=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	819	4% 70% 21% • 6%
1	B	819	14% 57% 29% 7% • 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11983 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.
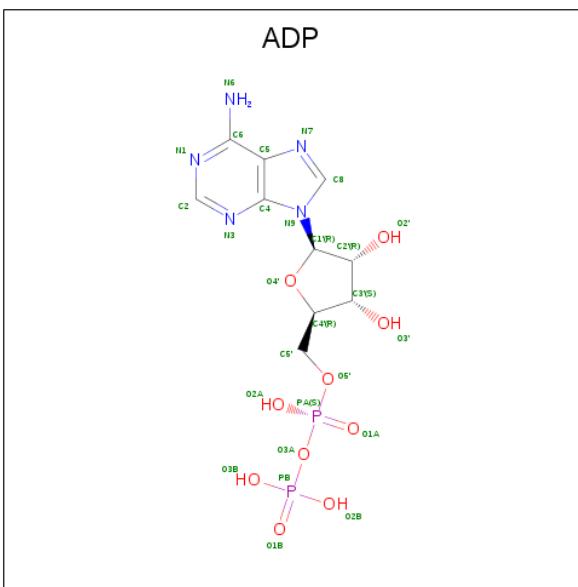
- Molecule 1 is a protein called DNA mismatch repair protein MutS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	771	Total 5906	C 3733	N 1046	O 1107	S 20	0	0	0
1	B	767	Total 5904	C 3735	N 1044	O 1106	S 19	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q5F5J4
A	-3	PRO	-	expression tag	UNP Q5F5J4
A	-2	LEU	-	expression tag	UNP Q5F5J4
A	-1	GLY	-	expression tag	UNP Q5F5J4
A	0	SER	-	expression tag	UNP Q5F5J4
B	-4	GLY	-	expression tag	UNP Q5F5J4
B	-3	PRO	-	expression tag	UNP Q5F5J4
B	-2	LEU	-	expression tag	UNP Q5F5J4
B	-1	GLY	-	expression tag	UNP Q5F5J4
B	0	SER	-	expression tag	UNP Q5F5J4

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

ADP

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
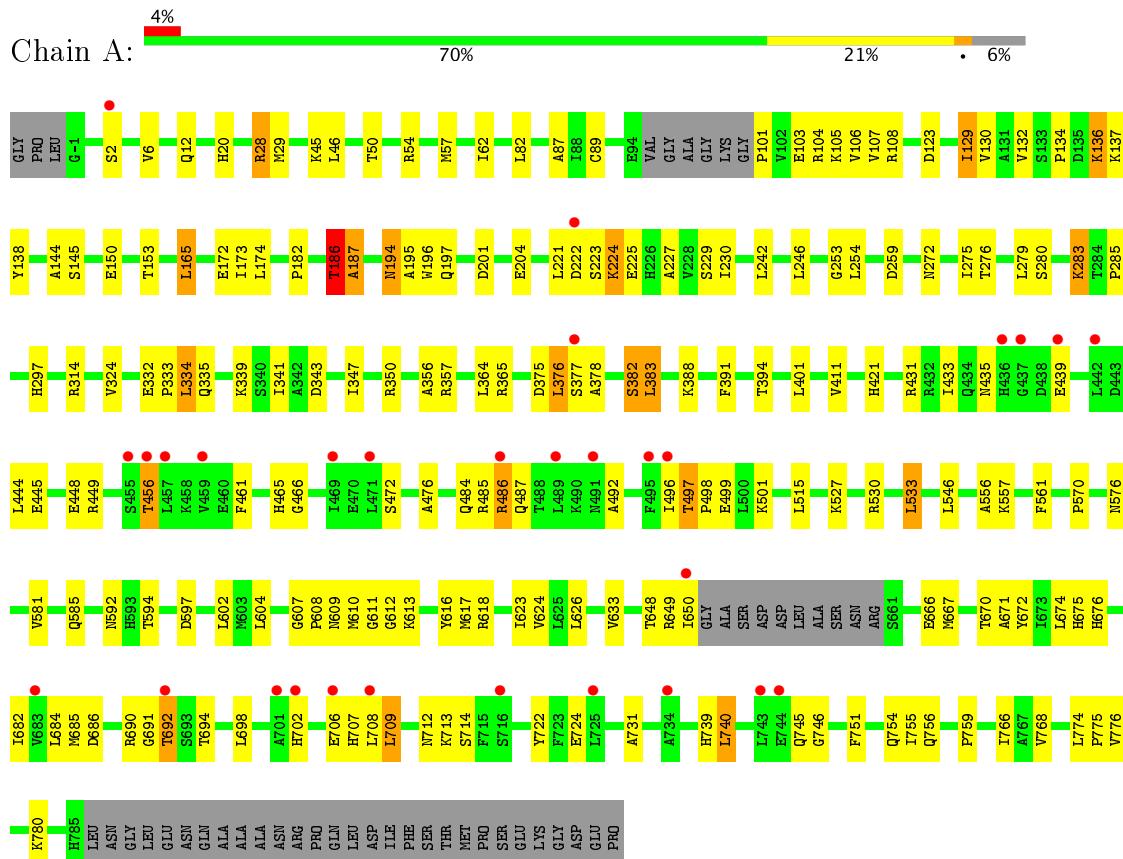
• Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	89	Total	O	0	0
			89	89		
3	B	30	Total	O	0	0
			30	30		
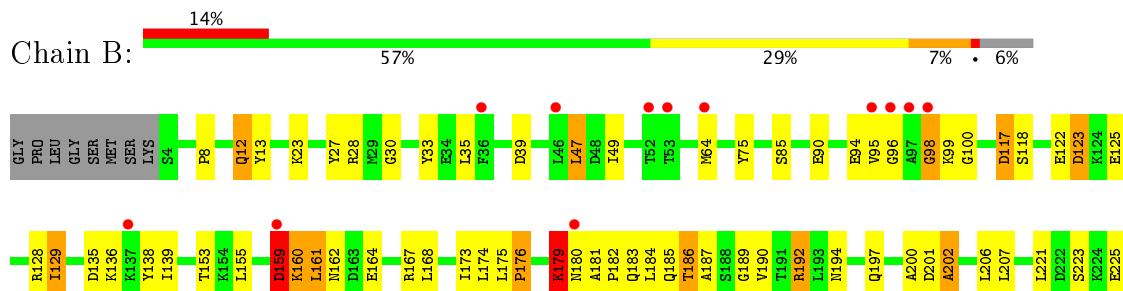
3 Residue-property plots ⓘ

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

- Molecule 1: DNA mismatch repair protein MutS

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	89.94Å 102.40Å 236.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.97 58.65 – 2.97	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.97) 99.4 (58.65-2.97)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.40 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.246 , 0.269 0.246 , 0.267	Depositor DCC
R_{free} test set	2301 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	78.6	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 62.2	EDS
L-test for twinning[2]	$<|L|> = 0.50, <L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11983	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.98% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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:
ADP

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	0.37	0/6015	0.50	2/8154 (0.0%)
1	B	0.30	0/6014	0.51	1/8154 (0.0%)
All	All	0.34	0/12029	0.51	3/16308 (0.0%)

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

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	674	LEU	CA-CB-CG	5.79	128.62	115.30
1	A	186	THR	C-N-CA	5.43	135.29	121.70
1	A	775	PRO	N-CA-CB	5.22	109.56	103.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	159	ASP	Peptide
1	B	669	GLU	Peptide

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	5906	0	5863	115	0
1	B	5904	0	5915	201	0
2	A	27	0	12	0	0
2	B	27	0	12	1	0
3	A	89	0	0	9	0
3	B	30	0	0	3	0
All	All	11983	0	11802	312	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 (312) 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:441:LEU:O	1:B:445:GLU:HB3	1.52	1.09
1:A:332:GLU:HG2	1:A:333:PRO:HD3	1.50	0.93
1:B:395:LEU:HB2	1:B:396:PRO:HD2	1.49	0.92
1:B:180:ASN:HB3	1:B:181:ALA:HA	1.50	0.92
1:B:762:LYS:HG2	1:B:763:SER:HA	1.60	0.82
1:B:395:LEU:HD22	1:B:397:VAL:HG12	1.65	0.78
1:B:221:LEU:HD23	1:B:230:ILE:HG22	1.64	0.78
1:B:49:ILE:HD11	1:B:75:TYR:HE2	1.46	0.77
1:B:487:GLN:HB3	1:B:488:THR:HA	1.66	0.76
1:A:607:GLY:HA3	3:A:1004:HOH:O	1.86	0.75
1:B:162:ASN:HD21	1:B:186:THR:HG21	1.51	0.74
1:B:318:ARG:HA	1:B:321:GLN:HB2	1.69	0.74
1:B:395:LEU:HB2	1:B:396:PRO:CD	2.18	0.73
1:A:527:LYS:HE3	1:A:530:ARG:HH22	1.54	0.73
1:A:435:ASN:O	1:A:439:GLU:HB3	1.88	0.72
1:A:376:LEU:O	1:A:378:ALA:N	2.23	0.71
1:B:527:LYS:O	1:B:529:LEU:N	2.23	0.71
1:B:712:ASN:HB3	1:B:713:LYS:HE2	1.71	0.71
1:B:284:THR:HB	1:B:285:PRO:HD2	1.72	0.71
1:B:487:GLN:NE2	1:B:489:LEU:O	2.22	0.71
1:A:649:ARG:HH22	1:A:670:THR:HG23	1.55	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:VAL:HG12	1:A:57:MET:HG3	1.71	0.70
1:A:28:ARG:O	1:A:104:ARG:NH2	2.24	0.69
1:B:760:ALA:HB1	1:B:761:GLY:HA3	1.73	0.69
1:B:378:ALA:HB1	1:B:388:LYS:HD2	1.74	0.69
1:B:762:LYS:H	1:B:762:LYS:HD3	1.57	0.68
1:A:674:LEU:O	1:A:712:ASN:ND2	2.26	0.68
1:A:365:ARG:HB2	1:A:401:LEU:HB3	1.76	0.68
1:A:649:ARG:NH2	1:A:666:GLU:O	2.27	0.68
1:B:561:PHE:HB3	1:B:632:PHE:HB2	1.76	0.67
1:B:321:GLN:HE21	1:B:564:PRO:HD2	1.59	0.67
1:B:122:GLU:HB2	1:B:125:GLU:HG3	1.75	0.67
1:B:265:MET:O	1:B:270:ARG:NH1	2.27	0.67
1:B:762:LYS:CG	1:B:763:SER:HA	2.24	0.66
1:B:270:ARG:HE	1:B:308:HIS:HD2	1.44	0.66
1:B:467:PHE:HD2	1:B:504:GLU:HB3	1.61	0.66
1:B:396:PRO:O	1:B:400:THR:OG1	2.10	0.66
1:B:457:LEU:HD21	1:B:469:ILE:HD11	1.77	0.65
1:B:167:ARG:NH2	1:B:257:GLU:OE1	2.29	0.65
1:B:395:LEU:H	1:B:395:LEU:HD13	1.61	0.65
1:B:446:ALA:HA	1:B:449:ARG:HB2	1.79	0.65
1:A:134:PRO:HG3	1:A:182:PRO:HD3	1.78	0.65
1:B:522:PHE:O	1:B:526:LEU:HB2	1.96	0.65
1:B:668:SER:OG	3:B:1001:HOH:O	2.15	0.64
1:B:468:TYR:OH	1:B:495:PHE:N	2.30	0.64
1:B:175:LEU:HD23	1:B:176:PRO:HD2	1.79	0.64
1:A:283:LYS:O	3:A:1001:HOH:O	2.15	0.64
1:A:498:PRO:HA	1:A:501:LYS:HB2	1.80	0.64
1:A:674:LEU:N	3:A:1003:HOH:O	2.31	0.64
1:B:431:ARG:O	1:B:433:ILE:N	2.28	0.64
1:B:485:ARG:NH1	1:B:496:ILE:O	2.31	0.63
1:B:577:GLY:N	1:B:592:ASN:O	2.31	0.63
1:A:712:ASN:O	1:A:714:SER:N	2.31	0.63
1:B:556:ALA:HA	1:B:561:PHE:HB2	1.80	0.62
1:A:106:VAL:O	1:A:108:ARG:N	2.28	0.62
1:B:155:LEU:HD21	1:B:226:HIS:HA	1.80	0.62
1:A:456:THR:O	1:A:456:THR:OG1	2.18	0.61
1:A:556:ALA:HA	1:A:561:PHE:HB2	1.80	0.61
1:B:396:PRO:HA	1:B:399:GLU:HB2	1.80	0.61
1:B:317:ILE:O	1:B:319:ALA:N	2.29	0.61
1:B:487:GLN:NE2	1:B:493:GLU:OE1	2.34	0.61
1:B:123:ASP:N	1:B:123:ASP:OD1	2.26	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:ARG:NH1	1:A:486:ARG:HB2	2.16	0.60
1:A:617:MET:HB3	1:A:684:LEU:HD23	1.82	0.60
1:B:164:GLU:OE1	1:B:167:ARG:NH1	2.34	0.60
1:B:439:GLU:O	1:B:441:LEU:N	2.34	0.60
1:A:497:THR:OG1	1:A:499:GLU:OE2	2.13	0.60
1:B:765:GLY:H	1:B:766:ILE:HB	1.65	0.60
1:B:298:MET:HE2	1:B:345:GLU:H	1.67	0.59
1:B:117:ASP:HA	1:B:350:ARG:HE	1.68	0.59
1:B:776:VAL:HA	1:B:779:LEU:HB3	1.84	0.59
1:B:28:ARG:NH1	1:B:30:GLY:O	2.36	0.59
1:B:270:ARG:NH2	1:B:308:HIS:O	2.36	0.58
1:B:510:ALA:HA	1:B:513:GLN:HE21	1.67	0.58
1:B:365:ARG:HB2	1:B:401:LEU:HB3	1.84	0.58
1:B:601:ARG:HH22	1:B:709:LEU:HA	1.68	0.58
1:B:244:GLN:HB3	1:B:353:VAL:HG23	1.85	0.58
1:B:475:GLN:HE22	1:B:478:GLN:HG3	1.69	0.58
1:B:362:ALA:HB1	1:B:365:ARG:HH21	1.70	0.57
1:B:763:SER:N	1:B:764:TYR:HA	2.19	0.57
1:B:574:ILE:HD11	1:B:635:ALA:HB2	1.88	0.56
1:A:624:VAL:HG11	1:A:682:ILE:HD12	1.88	0.56
1:A:12:GLN:NE2	3:A:1006:HOH:O	2.30	0.56
1:B:33:TYR:OH	1:B:90:GLU:OE2	2.19	0.56
1:B:129:ILE:HD11	1:B:174:LEU:HG	1.88	0.56
1:B:427:LEU:O	1:B:431:ARG:HG3	2.05	0.55
1:B:528:ASN:O	3:B:1002:HOH:O	2.18	0.55
1:B:586:VAL:HG23	1:B:588:HIS:H	1.71	0.55
1:B:128:ARG:NH1	1:B:168:LEU:O	2.39	0.55
1:B:311:LEU:HD12	1:B:317:ILE:HG12	1.88	0.55
1:B:264:GLY:HA3	1:B:645:GLN:HG2	1.87	0.55
1:B:49:ILE:HD11	1:B:75:TYR:CE2	2.35	0.55
1:A:611:GLY:O	1:A:613:LYS:N	2.40	0.54
1:B:383:LEU:HD23	1:B:384:LEU:N	2.23	0.54
1:B:439:GLU:HG3	1:B:440:PHE:H	1.72	0.54
1:B:467:PHE:CD2	1:B:504:GLU:HB3	2.42	0.54
1:A:186:THR:HA	1:A:187:ALA:HB3	1.88	0.54
1:A:137:LYS:HG3	1:A:138:TYR:H	1.71	0.54
1:B:387:LEU:O	1:B:390:VAL:HG12	2.08	0.54
1:A:484:GLN:HB3	1:A:486:ARG:NH2	2.22	0.54
1:B:406:MET:HG2	1:B:420:ASN:HA	1.88	0.54
1:B:729:PRO:HG3	1:B:737:ASN:HB3	1.89	0.54
1:A:435:ASN:O	1:A:439:GLU:CB	2.56	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:SER:HA	1:A:492:ALA:HA	1.89	0.54
1:B:98:GLY:O	1:B:100:GLY:N	2.40	0.54
1:B:452:THR:OG1	1:B:478:GLN:HB3	2.08	0.54
1:B:579:HIS:CE1	1:B:581:VAL:HG22	2.43	0.53
1:B:419:ILE:HD13	1:B:518:GLU:HG3	1.90	0.53
1:A:272:ASN:O	1:A:618:ARG:NH1	2.37	0.53
1:B:472:SER:OG	1:B:473:LYS:N	2.40	0.53
1:B:765:GLY:N	1:B:766:ILE:HB	2.22	0.53
1:A:347:ILE:HD13	1:A:350:ARG:HH21	1.74	0.53
1:A:592:ASN:HD21	1:A:754:GLN:HA	1.73	0.53
1:B:493:GLU:OE1	1:B:493:GLU:HA	2.08	0.53
1:B:487:GLN:CB	1:B:488:THR:HA	2.39	0.53
1:A:667:MET:O	1:A:671:ALA:HB2	2.09	0.53
1:B:12:GLN:OE1	1:B:27:TYR:OH	2.21	0.52
1:A:224:LYS:HG2	1:A:225:GLU:H	1.74	0.52
1:B:454:LEU:HB3	1:B:455:SER:HB3	1.90	0.52
1:A:186:THR:HA	1:A:187:ALA:CB	2.39	0.52
1:A:89:CYS:SG	1:A:104:ARG:HG3	2.49	0.52
1:A:46:LEU:HD22	1:A:82:LEU:HD13	1.91	0.52
1:B:118:SER:OG	1:B:350:ARG:NH1	2.43	0.52
1:B:578:ARG:NE	1:B:583:GLU:OE2	2.40	0.52
1:A:103:GLU:OE2	1:A:105:LYS:NZ	2.39	0.51
1:A:221:LEU:HD23	1:A:230:ILE:HG12	1.93	0.51
1:B:390:VAL:O	1:B:392:PRO:HD3	2.11	0.51
1:B:613:LYS:HG2	2:B:901:ADP:O1B	2.11	0.51
1:B:117:ASP:OD1	1:B:117:ASP:N	2.44	0.51
1:A:486:ARG:NH2	1:A:496:ILE:HG13	2.26	0.51
1:B:226:HIS:O	1:B:230:ILE:HG23	2.10	0.51
1:A:690:ARG:HH11	1:B:690:ARG:HH11	1.57	0.51
1:B:609:ASN:O	1:B:611:GLY:N	2.43	0.50
1:B:471:LEU:HB3	1:B:493:GLU:O	2.12	0.50
1:A:496:ILE:HD13	1:A:501:LYS:HG2	1.94	0.50
1:A:445:GLU:O	1:A:449:ARG:HG2	2.12	0.50
1:B:347:ILE:HG21	1:B:364:LEU:HB2	1.93	0.50
1:B:765:GLY:HA2	1:B:766:ILE:O	2.12	0.50
1:B:760:ALA:HB1	1:B:761:GLY:CA	2.38	0.50
1:A:129:ILE:HD12	1:A:172:GLU:HB3	1.93	0.49
1:A:570:PRO:HD3	3:A:1014:HOH:O	2.11	0.49
1:B:643:VAL:HB	1:B:681:SER:HB2	1.93	0.49
1:B:605:LEU:HD13	1:B:613:LYS:HB2	1.94	0.49
1:B:468:TYR:CE1	1:B:496:ILE:HA	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:601:ARG:NH2	1:B:709:LEU:HA	2.27	0.49
1:B:318:ARG:HB3	1:B:318:ARG:NH1	2.27	0.49
1:A:314:ARG:NH1	3:A:1018:HOH:O	2.45	0.49
1:A:272:ASN:HA	1:A:279:LEU:HD21	1.94	0.49
1:A:465:HIS:CE1	1:A:487:GLN:HE21	2.31	0.49
1:A:378:ALA:O	1:A:388:LYS:NZ	2.38	0.49
1:A:776:VAL:O	1:A:780:LYS:N	2.46	0.49
1:B:783:GLN:O	1:B:785:HIS:N	2.45	0.49
1:A:391:PHE:O	1:A:394:THR:HG22	2.12	0.49
1:B:192:ARG:HH22	1:B:194:ASN:HA	1.78	0.49
1:B:609:ASN:C	1:B:611:GLY:H	2.15	0.48
1:B:207:LEU:HD23	1:B:237:LEU:HD22	1.93	0.48
1:B:35:LEU:HB3	1:B:39:ASP:HB3	1.96	0.48
1:B:670:THR:O	1:B:673:ILE:HB	2.14	0.48
1:A:137:LYS:HG3	1:A:138:TYR:N	2.27	0.48
1:A:671:ALA:O	1:A:675:HIS:NE2	2.46	0.48
1:B:183:GLN:O	1:B:185:GLN:N	2.47	0.48
1:A:690:ARG:NH1	1:B:690:ARG:HH11	2.12	0.48
1:B:200:ALA:C	1:B:202:ALA:H	2.16	0.48
1:B:384:LEU:H	1:B:384:LEU:HD23	1.79	0.48
1:B:47:LEU:HB2	1:B:49:ILE:HD13	1.95	0.48
1:A:89:CYS:HA	1:A:105:LYS:O	2.14	0.48
1:B:258:THR:H	1:B:261:GLN:HE21	1.61	0.48
1:B:468:TYR:CG	1:B:469:ILE:N	2.82	0.48
1:B:764:TYR:CB	1:B:765:GLY:HA3	2.44	0.48
1:A:123:ASP:HB3	1:A:297:HIS:CD2	2.48	0.48
1:A:707:HIS:N	3:A:1019:HOH:O	2.47	0.48
1:B:666:GLU:O	1:B:668:SER:N	2.47	0.48
1:A:594:THR:HG1	1:A:616:TYR:HH	1.62	0.47
1:B:270:ARG:HE	1:B:308:HIS:CD2	2.28	0.47
1:B:173:ILE:HD13	1:B:187:ALA:HB1	1.96	0.47
1:B:579:HIS:HE1	1:B:581:VAL:HG22	1.80	0.47
1:B:263:ILE:HD11	1:B:643:VAL:HG22	1.96	0.47
1:B:320:ARG:O	1:B:324:VAL:HG12	2.15	0.47
1:B:390:VAL:HG11	1:B:542:ALA:CB	2.45	0.47
1:B:670:THR:HG21	1:B:704:ILE:HD13	1.97	0.47
1:B:287:LEU:HD22	1:B:622:LEU:HD22	1.96	0.47
1:B:601:ARG:HH22	1:B:710:GLN:H	1.62	0.47
1:A:706:GLU:OE2	1:B:776:VAL:HG11	2.14	0.47
1:A:608:PRO:O	1:A:613:LYS:NZ	2.48	0.47
1:B:173:ILE:HB	1:B:190:VAL:HG22	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:ARG:HH11	1:B:496:ILE:HG13	1.80	0.47
1:B:529:LEU:HA	3:B:1002:HOH:O	2.15	0.47
1:A:472:SER:O	1:A:476:ALA:N	2.47	0.47
1:A:54:ARG:O	1:A:62:ILE:HB	2.14	0.46
1:B:487:GLN:HB3	1:B:488:THR:CA	2.41	0.46
1:A:130:VAL:O	1:A:173:ILE:HA	2.15	0.46
1:A:486:ARG:NH1	1:A:496:ILE:HG23	2.30	0.46
1:B:382:SER:OG	1:B:383:LEU:N	2.47	0.46
1:A:334:LEU:HD11	1:A:546:LEU:HD21	1.98	0.46
1:B:323:ALA:HA	1:B:384:LEU:HD22	1.96	0.46
1:A:222:ASP:HB3	1:A:224:LYS:HZ2	1.80	0.46
1:A:650:ILE:HA	1:A:686:ASP:HB3	1.97	0.46
1:B:180:ASN:HB3	1:B:181:ALA:CA	2.36	0.46
1:A:444:LEU:O	1:A:448:GLU:HG2	2.16	0.46
1:A:602:LEU:HD13	1:A:709:LEU:HG	1.97	0.46
1:B:766:ILE:HG13	1:B:769:ALA:CB	2.46	0.46
1:B:138:TYR:HB2	1:B:155:LEU:HD12	1.98	0.45
1:B:206:LEU:HG	1:B:237:LEU:HD23	1.97	0.45
1:B:450:GLU:OE2	1:B:454:LEU:HA	2.16	0.45
1:B:139:ILE:HD11	1:B:161:LEU:HB2	1.99	0.45
1:A:87:ALA:HB1	1:A:106:VAL:HG13	1.99	0.45
1:B:298:MET:HG3	1:B:544:ALA:HB2	1.98	0.45
1:B:23:LYS:HB2	1:B:85:SER:HB2	1.97	0.45
1:A:275:ILE:HG22	1:A:276:THR:HG23	1.99	0.45
1:A:461:PHE:HA	1:A:466:GLY:O	2.16	0.45
1:B:752:LEU:HD23	1:B:754:GLN:HE22	1.81	0.45
1:B:153:THR:HG21	1:B:221:LEU:HD21	1.98	0.45
1:A:153:THR:OG1	1:A:229:SER:HB2	2.16	0.45
1:B:192:ARG:NH2	1:B:194:ASN:HA	2.31	0.44
1:B:424:HIS:CE1	1:B:426:GLU:HB3	2.53	0.44
1:A:356:ALA:N	3:A:1010:HOH:O	2.31	0.44
1:A:382:SER:OG	1:A:383:LEU:N	2.50	0.44
1:A:694:THR:OG1	1:B:724:GLU:OE1	2.35	0.44
1:B:94:GLU:O	1:B:96:GLY:N	2.51	0.44
1:A:201:ASP:OD1	1:A:201:ASP:N	2.49	0.44
1:B:431:ARG:HB2	1:B:431:ARG:HE	1.46	0.44
1:B:559:ARG:HH12	1:B:587:ARG:HH12	1.65	0.44
1:B:762:LYS:HD3	1:B:762:LYS:N	2.29	0.44
1:A:335:GLN:O	1:A:339:LYS:HB2	2.18	0.44
1:B:239:TYR:O	1:B:243:THR:OG1	2.31	0.44
1:B:311:LEU:HG	1:B:311:LEU:H	1.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:THR:HB	1:A:650:ILE:HD12	2.00	0.44
1:B:223:SER:O	1:B:227:ALA:HB2	2.18	0.44
1:B:349:ALA:O	1:B:353:VAL:HG12	2.18	0.44
1:B:728:LEU:N	1:B:729:PRO:HD2	2.32	0.44
1:B:458:LYS:HD2	1:B:458:LYS:HA	1.81	0.43
1:B:752:LEU:HB3	1:B:754:GLN:OE1	2.18	0.43
1:A:144:ALA:HA	1:A:150:GLU:O	2.18	0.43
1:A:766:ILE:C	1:A:768:VAL:H	2.21	0.43
1:B:317:ILE:C	1:B:319:ALA:N	2.72	0.43
1:B:450:GLU:OE2	1:B:453:GLY:HA2	2.18	0.43
1:A:123:ASP:HB3	1:A:297:HIS:CG	2.53	0.43
1:B:509:THR:HA	1:B:512:ASP:HB2	2.01	0.43
1:A:204:GLU:OE1	1:A:223:SER:OG	2.36	0.43
1:A:702:HIS:O	1:A:706:GLU:HG2	2.19	0.43
1:B:335:GLN:C	1:B:337:HIS:H	2.22	0.43
1:A:465:HIS:CE1	1:A:487:GLN:HB2	2.54	0.43
1:A:57:MET:HB2	1:A:62:ILE:HD11	2.00	0.43
1:B:587:ARG:HD3	1:B:587:ARG:HA	1.81	0.43
1:A:581:VAL:HG12	1:A:585:GLN:HE22	1.83	0.43
1:A:698:LEU:HD23	1:A:722:TYR:HB3	2.00	0.43
1:B:428:ASP:OD1	1:B:431:ARG:NH1	2.52	0.43
1:A:223:SER:O	1:A:227:ALA:HB2	2.19	0.42
1:B:494:ARG:HD3	1:B:494:ARG:HA	1.91	0.42
1:B:323:ALA:HB2	1:B:383:LEU:HD22	2.01	0.42
1:B:347:ILE:O	1:B:351:ILE:HG12	2.19	0.42
1:B:392:PRO:C	1:B:394:THR:H	2.22	0.42
1:B:468:TYR:HE1	1:B:496:ILE:HA	1.83	0.42
1:B:473:LYS:HD2	1:B:492:ALA:HB2	2.02	0.42
1:B:8:PRO:O	1:B:12:GLN:HG3	2.19	0.42
1:B:159:ASP:O	1:B:160:LYS:HB3	2.18	0.42
1:B:601:ARG:HG2	1:B:601:ARG:H	1.59	0.42
1:A:666:GLU:O	1:A:670:THR:OG1	2.32	0.42
1:A:165:LEU:HA	1:A:165:LEU:HD12	1.86	0.42
1:A:691:GLY:C	1:A:692:THR:HG1	2.22	0.42
1:B:624:VAL:HG11	1:B:682:ILE:HD13	2.01	0.42
1:A:357:ARG:HH12	1:A:411:VAL:HG13	1.85	0.42
1:B:12:GLN:OE1	1:B:13:TYR:N	2.53	0.42
1:B:179:LYS:HD2	1:B:180:ASN:O	2.20	0.42
1:A:20:HIS:HE2	1:A:106:VAL:HG21	1.85	0.42
1:A:145:SER:HB3	1:A:150:GLU:HB3	2.02	0.42
1:A:343:ASP:O	1:A:347:ILE:HG12	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:ARG:HH11	1:A:486:ARG:HB2	1.82	0.42
1:B:447:LYS:HB3	1:B:447:LYS:HE2	1.85	0.42
1:B:462:ASN:OD1	1:B:463:ARG:N	2.53	0.42
1:A:347:ILE:HG21	1:A:364:LEU:HB2	2.01	0.41
1:A:706:GLU:HB3	3:A:1016:HOH:O	2.20	0.41
1:B:270:ARG:NE	1:B:308:HIS:HD2	2.14	0.41
1:B:335:GLN:HE21	1:B:335:GLN:HB3	1.55	0.41
1:B:739:HIS:CE1	1:B:756:GLN:HB2	2.55	0.41
1:A:581:VAL:HG12	1:A:585:GLN:NE2	2.35	0.41
1:A:610:MET:HB2	1:A:751:PHE:CE2	2.55	0.41
1:B:290:ILE:HG12	1:B:581:VAL:HG12	2.02	0.41
1:B:533:LEU:HD12	1:B:533:LEU:HA	1.85	0.41
1:B:578:ARG:HE	1:B:583:GLU:CD	2.22	0.41
1:B:175:LEU:HD12	1:B:190:VAL:HG11	2.03	0.41
1:B:225:GLU:C	1:B:227:ALA:H	2.23	0.41
1:A:613:LYS:HG2	1:A:740:LEU:HD13	2.02	0.41
1:A:755:ILE:HG13	1:A:755:ILE:H	1.50	0.41
1:B:707:HIS:HA	1:B:711:LYS:HB3	2.02	0.41
1:A:486:ARG:HB3	1:A:487:GLN:H	1.66	0.41
1:B:254:LEU:HD12	1:B:254:LEU:HA	1.85	0.41
1:A:136:LYS:HA	1:A:136:LYS:HD2	1.86	0.41
1:B:424:HIS:HA	1:B:425:PRO:HD3	1.95	0.41
1:B:602:LEU:HD13	1:B:709:LEU:HD23	2.02	0.41
1:B:625:LEU:O	1:B:629:THR:HG23	2.21	0.41
1:B:616:TYR:O	1:B:619:GLN:HB3	2.20	0.41
1:B:723:PHE:O	1:B:725:LEU:N	2.47	0.41
1:A:421:HIS:CD2	1:A:431:ARG:HH11	2.39	0.41
1:A:623:ILE:HG23	1:A:633:VAL:HB	2.02	0.41
1:A:672:TYR:O	1:A:676:HIS:HB2	2.22	0.40
1:B:559:ARG:HB3	1:B:561:PHE:CE1	2.56	0.40
1:B:670:THR:HA	1:B:673:ILE:HD13	2.03	0.40
1:B:766:ILE:HG13	1:B:769:ALA:HB3	2.03	0.40
1:B:284:THR:CB	1:B:285:PRO:HD2	2.47	0.40
1:A:739:HIS:CE1	1:A:756:GLN:HB2	2.55	0.40
1:B:314:ARG:HA	1:B:318:ARG:NH2	2.36	0.40
1:B:433:ILE:HD13	1:B:510:ALA:HB1	2.04	0.40
1:B:533:LEU:HB3	1:B:534:PRO:HD3	2.03	0.40
1:B:574:ILE:HD12	1:B:623:ILE:HG21	2.03	0.40
1:A:123:ASP:HB3	1:A:297:HIS:CE1	2.57	0.40
1:A:129:ILE:HD11	1:A:174:LEU:HG	2.02	0.40
1:A:194:ASN:HB3	1:A:197:GLN:HE21	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:631:CYS:SG	1:B:632:PHE:N	2.95	0.40
1:A:45:LYS:HB3	1:A:45:LYS:HE3	1.95	0.40
1:A:533:LEU:HA	1:A:533:LEU:HD12	1.88	0.40
1:B:763:SER:O	1:B:763:SER:OG	2.24	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	765/819 (93%)	688 (90%)	55 (7%)	22 (3%)	5	26
1	B	763/819 (93%)	631 (83%)	83 (11%)	49 (6%)	1	7
All	All	1528/1638 (93%)	1319 (86%)	138 (9%)	71 (5%)	3	15

All (71) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	ALA
1	A	285	PRO
1	A	377	SER
1	A	713	LYS
1	A	774	LEU
1	B	285	PRO
1	B	395	LEU
1	B	432	ARG
1	B	484	GLN
1	B	528	ASN
1	B	667	MET
1	B	669	GLU
1	B	674	LEU
1	B	768	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	784	LYS
1	A	2	SER
1	A	107	VAL
1	A	136	LYS
1	A	195	ALA
1	A	253	GLY
1	A	376	LEU
1	A	576	ASN
1	A	612	GLY
1	B	99	LYS
1	B	136	LYS
1	B	160	LYS
1	B	182	PRO
1	B	184	LEU
1	B	201	ASP
1	B	318	ARG
1	B	394	THR
1	B	609	ASN
1	B	610	MET
1	B	692	THR
1	A	194	ASN
1	A	254	LEU
1	A	731	ALA
1	A	759	PRO
1	B	95	VAL
1	B	159	ASP
1	B	179	LYS
1	B	189	GLY
1	B	337	HIS
1	B	375	ASP
1	B	382	SER
1	B	396	PRO
1	B	440	PHE
1	B	492	ALA
1	B	677	ALA
1	B	712	ASN
1	B	725	LEU
1	A	382	SER
1	A	433	ILE
1	A	692	THR
1	B	98	GLY
1	B	135	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	202	ALA
1	B	379	THR
1	B	483	TYR
1	B	485	ARG
1	B	715	PHE
1	B	176	PRO
1	B	260	SER
1	B	760	ALA
1	B	766	ILE
1	A	485	ARG
1	B	462	ASN
1	B	480	PRO
1	B	759	PRO
1	A	746	GLY
1	B	464	VAL

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	608/669 (91%)	572 (94%)	36 (6%)	23	59
1	B	615/669 (92%)	539 (88%)	76 (12%)	5	22
All	All	1223/1338 (91%)	1111 (91%)	112 (9%)	11	37

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	29	MET
1	A	50	THR
1	A	101	PRO
1	A	129	ILE
1	A	132	VAL
1	A	165	LEU
1	A	186	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	196	TRP
1	A	224	LYS
1	A	242	LEU
1	A	246	LEU
1	A	259	ASP
1	A	280	SER
1	A	283	LYS
1	A	324	VAL
1	A	334	LEU
1	A	341	ILE
1	A	375	ASP
1	A	383	LEU
1	A	456	THR
1	A	486	ARG
1	A	497	THR
1	A	515	LEU
1	A	533	LEU
1	A	557	LYS
1	A	597	ASP
1	A	604	LEU
1	A	609	ASN
1	A	626	LEU
1	A	685	MET
1	A	708	LEU
1	A	709	LEU
1	A	724	GLU
1	A	740	LEU
1	A	745	GLN
1	B	12	GLN
1	B	47	LEU
1	B	64	MET
1	B	117	ASP
1	B	123	ASP
1	B	129	ILE
1	B	161	LEU
1	B	179	LYS
1	B	186	THR
1	B	192	ARG
1	B	197	GLN
1	B	236	LEU
1	B	243	THR
1	B	250	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	263	ILE
1	B	280	SER
1	B	284	THR
1	B	305	LEU
1	B	311	LEU
1	B	314	ARG
1	B	317	ILE
1	B	318	ARG
1	B	335	GLN
1	B	337	HIS
1	B	353	VAL
1	B	369	PHE
1	B	371	LEU
1	B	383	LEU
1	B	388	LYS
1	B	391	PHE
1	B	395	LEU
1	B	397	VAL
1	B	401	LEU
1	B	438	ASP
1	B	443	ASP
1	B	445	GLU
1	B	454	LEU
1	B	459	VAL
1	B	461	PHE
1	B	470	GLU
1	B	471	LEU
1	B	475	GLN
1	B	478	GLN
1	B	485	ARG
1	B	486	ARG
1	B	488	THR
1	B	489	LEU
1	B	490	LYS
1	B	493	GLU
1	B	495	PHE
1	B	497	THR
1	B	500	LEU
1	B	521	LEU
1	B	536	LEU
1	B	563	ARG
1	B	571	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	584	GLN
1	B	593	HIS
1	B	595	ASP
1	B	601	ARG
1	B	666	GLU
1	B	676	HIS
1	B	685	MET
1	B	688	VAL
1	B	690	ARG
1	B	707	HIS
1	B	709	LEU
1	B	710	GLN
1	B	713	LYS
1	B	737	ASN
1	B	740	LEU
1	B	743	LEU
1	B	744	GLU
1	B	748	ASP
1	B	752	LEU
1	B	762	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	GLN
1	A	249	GLN
1	A	272	ASN
1	A	321	GLN
1	A	355	ASN
1	A	421	HIS
1	A	436	HIS
1	A	465	HIS
1	A	487	GLN
1	A	511	GLN
1	A	592	ASN
1	A	732	HIS
1	A	753	HIS
1	B	20	HIS
1	B	162	ASN
1	B	197	GLN
1	B	250	HIS
1	B	261	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	308	HIS
1	B	330	GLN
1	B	335	GLN
1	B	478	GLN
1	B	513	GLN
1	B	520	GLN
1	B	573	HIS
1	B	576	ASN
1	B	585	GLN
1	B	645	GLN
1	B	707	HIS
1	B	721	HIS
1	B	737	ASN
1	B	745	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 carbohydrates in this entry.

5.6   Ligand geometry (i)

2 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	ADP	A	901	-	25,29,29	1.11	1 (4%)	24,45,45	1.55	3 (12%)
2	ADP	B	901	-	25,29,29	1.12	1 (4%)	24,45,45	1.64	2 (8%)

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	ADP	A	901	-	-	0/12/32/32	0/3/3/3
2	ADP	B	901	-	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	ADP	C5-C4	3.39	1.48	1.40
2	B	901	ADP	C5-C4	3.40	1.48	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	901	ADP	N3-C2-N1	-6.10	123.55	128.86
2	A	901	ADP	N3-C2-N1	-5.37	124.18	128.86
2	A	901	ADP	C4-C5-N7	-2.77	106.74	109.41
2	B	901	ADP	C4-C5-N7	-2.47	107.03	109.41
2	A	901	ADP	C2'-C3'-C4'	2.01	106.53	102.62

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
2	B	901	ADP	1	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 (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	771/819 (94%)	0.45	30 (3%)	40	23	42, 74, 133, 184	0
1	B	767/819 (93%)	0.94	117 (15%)	2	1	60, 113, 191, 254	0
All	All	1538/1638 (93%)	0.70	147 (9%)	9	5	42, 93, 169, 254	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	452	THR	11.7
1	B	681	SER	8.3
1	B	531	THR	7.8
1	B	459	VAL	7.7
1	B	470	GLU	7.1
1	B	457	LEU	6.9
1	B	454	LEU	6.8
1	B	677	ALA	6.5
1	B	456	THR	6.5
1	B	676	HIS	6.2
1	B	96	GLY	6.0
1	B	633	VAL	5.6
1	B	602	LEU	5.3
1	B	443	ASP	5.2
1	B	137	LYS	5.2
1	B	453	GLY	4.9
1	B	710	GLN	4.9
1	A	436	HIS	4.8
1	B	471	LEU	4.7
1	B	444	LEU	4.6
1	B	743	LEU	4.5
1	B	467	PHE	4.4
1	A	456	THR	4.4
1	B	461	PHE	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	692	THR	4.3
1	B	632	PHE	4.2
1	B	637	ALA	4.2
1	B	36	PHE	4.2
1	B	377	SER	4.0
1	B	438	ASP	4.0
1	B	480	PRO	4.0
1	B	455	SER	3.9
1	B	555	LEU	3.9
1	B	485	ARG	3.9
1	B	448	GLU	3.9
1	A	491	ASN	3.9
1	A	469	ILE	3.9
1	B	469	ILE	3.9
1	B	436	HIS	3.8
1	B	706	GLU	3.8
1	B	484	GLN	3.5
1	B	488	THR	3.4
1	B	762	LYS	3.3
1	A	744	GLU	3.3
1	B	341	ILE	3.3
1	B	601	ARG	3.2
1	B	735	ALA	3.2
1	B	605	LEU	3.2
1	B	474	THR	3.2
1	B	468	TYR	3.2
1	B	548	VAL	3.2
1	B	180	ASN	3.2
1	B	717	LEU	3.1
1	B	502	ALA	3.1
1	A	455	SER	3.1
1	B	347	ILE	3.0
1	B	466	GLY	3.0
1	B	483	TYR	3.0
1	B	497	THR	3.0
1	B	708	LEU	3.0
1	B	95	VAL	3.0
1	B	745	GLN	3.0
1	B	736	VAL	3.0
1	A	471	LEU	2.9
1	B	546	LEU	2.9
1	A	2	SER	2.8

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	254	LEU	2.8
1	B	716	SER	2.8
1	B	364	LEU	2.8
1	B	489	LEU	2.8
1	B	491	ASN	2.7
1	B	698	LEU	2.7
1	A	495	PHE	2.7
1	A	457	LEU	2.7
1	B	324	VAL	2.6
1	A	459	VAL	2.6
1	B	638	ALA	2.6
1	B	496	ILE	2.6
1	B	561	PHE	2.6
1	B	376	LEU	2.6
1	A	496	ILE	2.6
1	B	415	ASP	2.5
1	B	486	ARG	2.5
1	B	616	TYR	2.5
1	B	636	ASP	2.5
1	B	419	ILE	2.5
1	B	53	THR	2.5
1	A	222	ASP	2.4
1	A	437	GLY	2.4
1	B	692	THR	2.4
1	B	97	ALA	2.4
1	B	465	HIS	2.4
1	B	458	LYS	2.4
1	B	734	ALA	2.4
1	B	374	ILE	2.3
1	A	701	ALA	2.3
1	A	489	LEU	2.3
1	B	695	PHE	2.3
1	B	451	ARG	2.3
1	B	595	ASP	2.3
1	A	725	LEU	2.3
1	B	52	THR	2.3
1	B	581	VAL	2.3
1	B	46	LEU	2.3
1	B	387	LEU	2.3
1	A	442	LEU	2.3
1	A	377	SER	2.3
1	A	486	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	743	LEU	2.3
1	B	700	LEU	2.3
1	B	517	LEU	2.3
1	B	634	PRO	2.2
1	B	494	ARG	2.2
1	B	557	LYS	2.2
1	B	291	LEU	2.2
1	B	441	LEU	2.2
1	B	446	ALA	2.2
1	B	330	GLN	2.2
1	B	487	GLN	2.2
1	B	413	LEU	2.2
1	A	650	ILE	2.2
1	B	64	MET	2.2
1	B	299	GLY	2.2
1	B	285	PRO	2.2
1	B	519	LYS	2.2
1	B	623	ILE	2.1
1	B	682	ILE	2.1
1	B	785	HIS	2.1
1	B	622	LEU	2.1
1	A	706	GLU	2.1
1	B	159	ASP	2.1
1	A	702	HIS	2.1
1	A	734	ALA	2.1
1	B	510	ALA	2.1
1	B	287	LEU	2.1
1	B	98	GLY	2.1
1	A	683	VAL	2.1
1	B	418	VAL	2.1
1	B	412	TRP	2.0
1	B	405	VAL	2.0
1	B	508	LEU	2.0
1	B	731	ALA	2.0
1	A	439	GLU	2.0
1	A	716	SER	2.0
1	B	503	PHE	2.0
1	A	708	LEU	2.0
1	B	385	GLU	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. 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	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
2	ADP	A	901	27/27	0.94	0.25	0.06	59,64,70,73	0
2	ADP	B	901	27/27	0.93	0.20	-0.54	79,88,102,106	0

6.5 Other polymers (i)

There are no such residues in this entry.