



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:20 PM UTC

PDB ID : 1JFZ / pdb_00001jtz
Title : Crystal Structure of MN(II)-Complex of RNase III Endonuclease Domain from Aquifex Aeolicus at 2.10 Angstrom Resolution
Authors : Blaszczyk, J.; Ji, X.
Deposited on : 2001-06-22
Resolution : 2.10 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
Xtriage (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

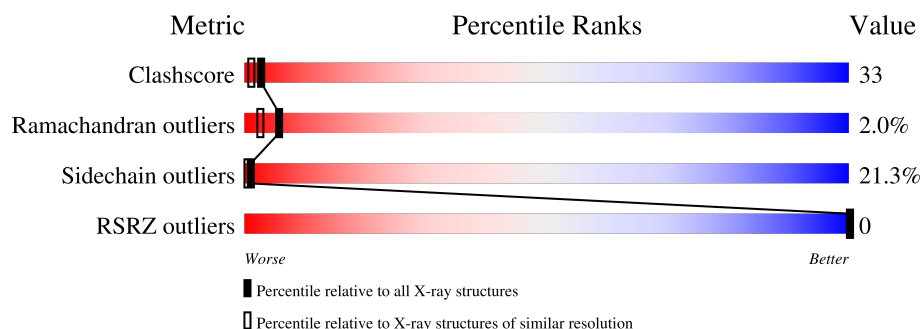
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	154	
1	B	154	
1	C	154	
1	D	154	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5664 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 RIBONUCLEASE III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	148	Total	C	N	O	S	0	2	0
			1233	809	199	223	2			
1	B	149	Total	C	N	O	S	0	3	0
			1247	818	202	225	2			
1	C	149	Total	C	N	O	S	0	2	0
			1243	816	202	223	2			
1	D	148	Total	C	N	O	S	0	0	0
			1225	805	198	220	2			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	SEE REMARK 999	UNP O67082
A	148	HIS	-	expression tag	UNP O67082
A	149	HIS	-	expression tag	UNP O67082
A	150	HIS	-	expression tag	UNP O67082
A	151	HIS	-	expression tag	UNP O67082
A	152	HIS	-	expression tag	UNP O67082
A	153	HIS	-	expression tag	UNP O67082
B	200	GLY	-	SEE REMARK 999	UNP O67082
B	348	HIS	-	expression tag	UNP O67082
B	349	HIS	-	expression tag	UNP O67082
B	350	HIS	-	expression tag	UNP O67082
B	351	HIS	-	expression tag	UNP O67082
B	352	HIS	-	expression tag	UNP O67082
B	353	HIS	-	expression tag	UNP O67082
C	400	GLY	-	SEE REMARK 999	UNP O67082
C	548	HIS	-	expression tag	UNP O67082
C	549	HIS	-	expression tag	UNP O67082
C	550	HIS	-	expression tag	UNP O67082
C	551	HIS	-	expression tag	UNP O67082
C	552	HIS	-	expression tag	UNP O67082
C	553	HIS	-	expression tag	UNP O67082

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	600	GLY	-	SEE REMARK 999	UNP O67082
D	748	HIS	-	expression tag	UNP O67082
D	749	HIS	-	expression tag	UNP O67082
D	750	HIS	-	expression tag	UNP O67082
D	751	HIS	-	expression tag	UNP O67082
D	752	HIS	-	expression tag	UNP O67082
D	753	HIS	-	expression tag	UNP O67082

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mn 1	0	0
2	B	1	Total 1	Mn 1	0	0
2	C	1	Total 1	Mn 1	0	0
2	D	1	Total 1	Mn 1	0	0

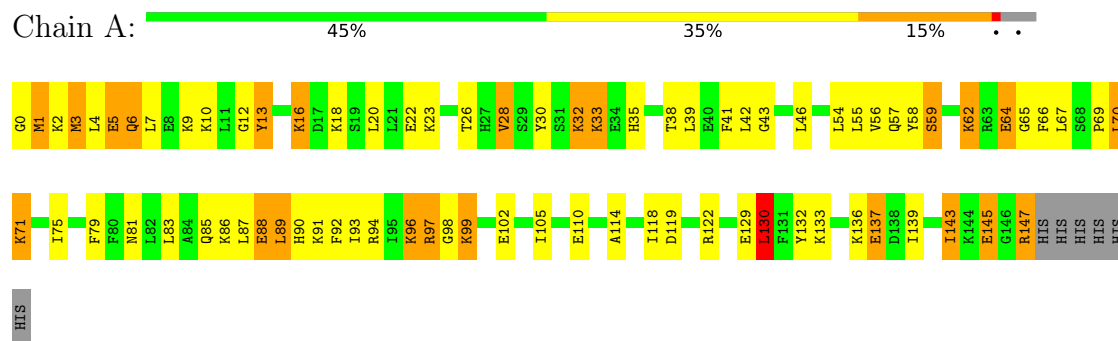
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	201	Total 201	O 201	0	0
3	B	166	Total 166	O 166	0	0
3	C	175	Total 175	O 175	0	0
3	D	170	Total 170	O 170	0	0

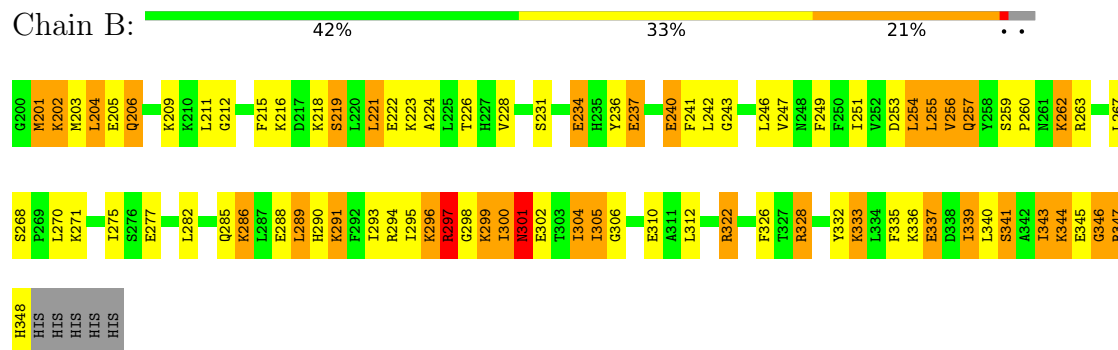
3 Residue-property plots

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.

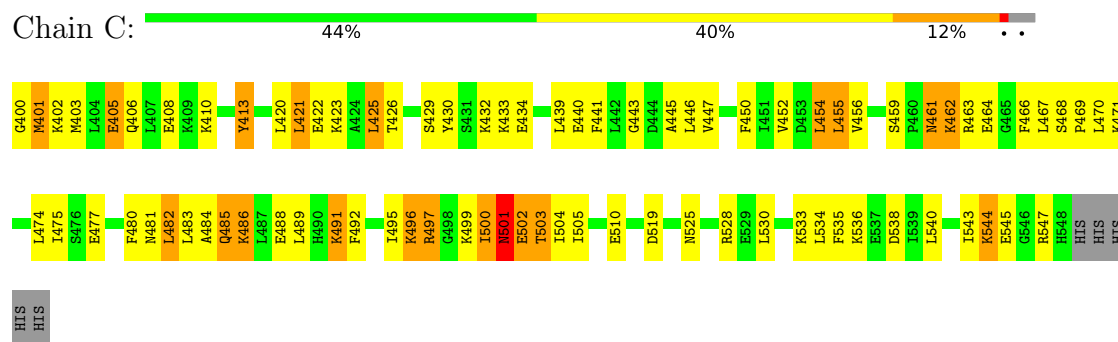
• Molecule 1: RIBONUCLEASE III



• Molecule 1: RIBONUCLEASE III



• Molecule 1: RIBONUCLEASE III



• Molecule 1: RIBONUCLEASE III



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.74Å 140.55Å 49.76Å 90.00° 117.42° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	89.2 (30.00-2.10) 82.8 (30.00-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.81 (at 2.10Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.195 , 0.286 0.188 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.530	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.064 for -h-l,k,h 0.064 for l,k,-h-l 0.072 for h,-k,-h-l 0.076 for -h-l,-k,l 0.430 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5664	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.35% 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: MN

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	0.42	0/1268	1.27	7/1699 (0.4%)
1	B	0.43	0/1288	1.27	5/1725 (0.3%)
1	C	0.37	0/1279	1.19	8/1713 (0.5%)
1	D	0.43	0/1250	1.24	8/1675 (0.5%)
All	All	0.41	0/5085	1.24	28/6812 (0.4%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	301	ASN	CA-CB-CG	9.05	121.65	112.60
1	B	336	LYS	CA-C-N	6.59	129.96	120.79
1	B	336	LYS	C-N-CA	6.59	129.96	120.79
1	A	130	LEU	CA-C-N	6.10	128.46	120.28
1	A	130	LEU	C-N-CA	6.10	128.46	120.28
1	D	666	PHE	CA-CB-CG	6.07	119.87	113.80
1	B	326	PHE	CA-CB-CG	5.98	119.78	113.80
1	B	249	PHE	CA-CB-CG	5.63	119.43	113.80
1	C	454	LEU	CA-C-N	5.53	127.95	120.65
1	C	454	LEU	C-N-CA	5.53	127.95	120.65
1	D	700	ILE	CA-CB-CG1	5.50	119.75	110.40
1	A	12	GLY	N-CA-C	-5.49	107.20	115.32
1	A	13	TYR	CA-C-N	5.47	130.27	122.72
1	A	13	TYR	C-N-CA	5.47	130.27	122.72
1	D	728	ARG	CA-C-O	5.47	126.33	120.70
1	C	484	ALA	CA-C-N	5.43	127.87	120.54
1	C	484	ALA	C-N-CA	5.43	127.87	120.54
1	C	413	TYR	CA-C-N	5.42	130.64	123.05
1	C	413	TYR	C-N-CA	5.42	130.64	123.05
1	D	700	ILE	O-C-N	-5.35	115.88	122.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	ILE	CA-C-N	5.29	125.82	120.00
1	A	105	ILE	C-N-CA	5.29	125.82	120.00
1	D	698	GLY	N-CA-C	5.25	121.75	114.92
1	D	700	ILE	N-CA-C	5.25	120.25	109.34
1	C	501	ASN	CA-C-N	5.04	127.54	120.28
1	C	501	ASN	C-N-CA	5.04	127.54	120.28
1	D	699	LYS	CA-C-N	-5.01	112.96	121.97
1	D	699	LYS	C-N-CA	-5.01	112.96	121.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1233	0	1263	84	0
1	B	1247	0	1274	91	0
1	C	1243	0	1272	69	0
1	D	1225	0	1254	96	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	201	0	0	16	0
3	B	166	0	0	15	0
3	C	175	0	0	16	0
3	D	170	0	0	16	0
All	All	5664	0	5063	333	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 33.

All (333) 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:205[B]:GLU:HG2	1:B:206:GLN:H	1.07	1.12
1:C:430:TYR:HA	1:C:496:LYS:HD3	1.41	1.01
1:A:96:LYS:HG2	1:A:97:ARG:HD2	1.55	0.89
1:B:205[B]:GLU:HG2	1:B:206:GLN:N	1.83	0.86
1:A:71:LYS:HE2	1:A:75:ILE:HD13	1.56	0.85
1:C:461:ASN:HD22	1:C:461:ASN:H	1.26	0.82
1:D:661:ASN:HD22	1:D:666:PHE:HB3	1.44	0.82
1:B:205[B]:GLU:CG	1:B:206:GLN:H	1.93	0.81
1:A:145:GLU:HA	3:A:1552:HOH:O	1.80	0.80
1:D:633:LYS:HG2	1:D:634:GLU:HG2	1.62	0.80
1:D:686:LYS:HE2	1:D:738:ASP:OD2	1.83	0.79
3:A:1657:HOH:O	1:B:322:ARG:HD3	1.83	0.79
1:A:1:MET:HE2	1:A:3:MET:HB2	1.65	0.78
1:A:1:MET:HE2	1:A:3:MET:CB	2.14	0.77
1:B:301:ASN:HA	3:B:1666:HOH:O	1.83	0.77
1:A:33:LYS:HB2	3:A:1172:HOH:O	1.86	0.76
1:C:502:GLU:HG2	3:C:1097:HOH:O	1.84	0.76
1:D:700:ILE:O	1:D:701:ASN:HB2	1.84	0.76
1:B:270:LEU:HD11	1:B:346:GLY:HA2	1.65	0.76
1:D:661:ASN:OD1	1:D:663:ARG:HG3	1.86	0.75
1:B:341:SER:HA	1:B:344:LYS:HD2	1.69	0.75
1:A:129:GLU:HG3	3:A:1444:HOH:O	1.86	0.74
1:B:223:LYS:HE2	3:B:1240:HOH:O	1.88	0.73
1:A:66:PHE:O	1:A:69:PRO:HD2	1.89	0.72
1:B:206:GLN:HG2	1:B:209:LYS:HE2	1.72	0.71
1:C:540:LEU:O	1:C:544:LYS:HG2	1.91	0.71
1:D:616:LYS:HG2	1:D:719:ASP:OD2	1.90	0.71
1:C:505:ILE:HG23	3:C:1388:HOH:O	1.91	0.71
1:B:300:ILE:HG23	1:B:301:ASN:H	1.55	0.70
1:B:301:ASN:ND2	1:B:304:ILE:H	1.89	0.70
1:D:661:ASN:ND2	1:D:663:ARG:H	1.89	0.70
1:B:295:ILE:HD12	1:B:304:ILE:HD12	1.74	0.69
1:D:670:LEU:HG	1:D:746:GLY:HA3	1.73	0.69
1:B:294:ARG:HD3	3:B:1215:HOH:O	1.91	0.69
1:D:681:ASN:O	1:D:685:GLN:HG2	1.92	0.69
1:A:13:TYR:HB2	1:A:130:LEU:HD11	1.74	0.69
1:B:203:MET:HG3	1:B:204:LEU:H	1.58	0.68
1:D:747:ARG:HG2	3:D:1149:HOH:O	1.93	0.68
1:B:219:SER:HA	1:B:222:GLU:HG3	1.75	0.67
1:D:693:ILE:HG22	1:D:695:ILE:HG22	1.77	0.67
1:C:405:GLU:HB3	3:C:1382:HOH:O	1.93	0.67
1:A:3:MET:HE3	1:A:6[A]:GLN:HE22	1.60	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HG2	1:A:4:LEU:H	1.59	0.67
3:A:1068:HOH:O	1:D:696:LYS:HD3	1.95	0.66
1:C:441:PHE:HB2	1:D:664:GLU:OE1	1.95	0.66
1:B:205[B]:GLU:CG	1:B:206:GLN:N	2.52	0.66
1:A:1:MET:CG	1:A:4:LEU:H	2.09	0.66
1:C:466:PHE:O	1:C:469:PRO:HD2	1.96	0.65
1:C:429:SER:O	1:C:496:LYS:HE2	1.96	0.65
1:C:445:ALA:HB2	1:D:652:VAL:HG21	1.77	0.65
1:D:676:SER:HB2	3:D:1407:HOH:O	1.96	0.65
1:D:734:LEU:HD23	3:D:1353:HOH:O	1.97	0.65
1:D:686:LYS:HG3	3:D:1330:HOH:O	1.97	0.65
1:B:253:ASP:O	1:B:257:GLN:HG3	1.96	0.65
1:D:610:LYS:HE2	1:D:687:LEU:O	1.97	0.65
1:C:455:LEU:HD22	1:C:474:LEU:HD12	1.79	0.64
1:B:256:VAL:O	1:B:262:LYS:HE2	1.98	0.64
1:D:671:LYS:HD3	3:D:1234:HOH:O	1.98	0.64
1:B:237:GLU:HB3	3:B:1232:HOH:O	1.97	0.64
1:B:212:GLY:HA2	3:B:1350:HOH:O	1.98	0.63
1:A:97:ARG:HD2	1:A:97:ARG:H	1.62	0.63
1:B:215:PHE:CZ	1:B:221:LEU:HG	2.34	0.63
1:C:533[A]:LYS:HE2	3:C:1273:HOH:O	1.98	0.62
1:D:700:ILE:O	1:D:701:ASN:CB	2.46	0.62
1:A:59:SER:O	1:A:62:LYS:HE3	1.99	0.62
1:C:456:VAL:O	1:C:462:LYS:HE3	2.00	0.62
1:A:81:ASN:O	1:A:85:GLN:HG3	2.00	0.62
1:D:647:VAL:O	1:D:651:ILE:HD13	2.00	0.61
1:A:1:MET:HG3	1:A:3:MET:N	2.16	0.61
1:D:670:LEU:HD21	1:D:743:ILE:O	1.99	0.61
1:A:0:GLY:O	1:A:4:LEU:HB2	2.01	0.61
1:A:88:GLU:HG3	1:A:91:LYS:HE3	1.82	0.61
1:A:3:MET:HE3	1:A:6[A]:GLN:NE2	2.15	0.60
1:D:632:LYS:HG2	3:D:1206:HOH:O	2.00	0.60
1:D:689:LEU:O	1:D:693:ILE:HG12	2.01	0.60
1:A:139:ILE:O	1:A:143:ILE:HG12	2.00	0.60
1:D:661:ASN:HD21	1:D:663:ARG:HB2	1.66	0.60
1:D:615:PHE:CD1	1:D:621:LEU:HD12	2.37	0.60
1:D:606:GLN:HA	3:D:1372:HOH:O	2.00	0.60
1:D:668:SER:O	1:D:671:LYS:HB3	2.02	0.60
1:A:20:LEU:HD23	1:A:119:ASP:HB2	1.83	0.60
1:A:41:PHE:CD2	1:B:267:LEU:HD13	2.37	0.60
1:C:475:ILE:HA	1:C:480:PHE:CE1	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:734:LEU:HG	3:D:1366:HOH:O	2.01	0.59
1:B:218:LYS:O	1:B:222:GLU:HG3	2.02	0.59
1:D:681:ASN:OD1	1:D:702:GLU:HG2	2.01	0.59
1:D:628:VAL:HG13	1:D:635:HIS:CE1	2.37	0.59
1:D:658:TYR:O	1:D:743:ILE:HG21	2.03	0.59
1:C:443:GLY:O	1:C:447:VAL:HG23	2.03	0.59
1:D:736:LYS:HE2	3:D:1248:HOH:O	2.02	0.59
1:B:240:GLU:HG3	1:B:241:PHE:N	2.17	0.58
1:A:4:LEU:HD11	1:A:22:GLU:HG2	1.86	0.58
1:D:737:GLU:HA	1:D:737:GLU:OE1	2.02	0.58
1:A:71:LYS:HD2	3:A:1380:HOH:O	2.04	0.58
1:A:0:GLY:N	1:A:18:LYS:HE3	2.19	0.57
1:C:464:GLU:HA	1:C:467:LEU:HD12	1.86	0.57
1:C:489:LEU:HB3	3:C:1388:HOH:O	2.03	0.57
1:B:223:LYS:HG3	1:B:234:GLU:HB3	1.85	0.57
1:D:689:LEU:HD13	1:D:708:VAL:HG12	1.86	0.57
1:B:282:LEU:HG	3:B:1175:HOH:O	2.02	0.57
1:D:733:LYS:HG2	3:D:1473:HOH:O	2.04	0.57
1:B:277:GLU:OE2	1:B:302:GLU:HB3	2.06	0.56
1:C:406:GLN:HG2	1:C:492:PHE:CZ	2.40	0.56
1:B:259:SER:O	1:B:262:LYS:HE3	2.05	0.56
1:B:301:ASN:HD22	1:B:304:ILE:HG22	1.71	0.56
1:C:421:LEU:HD22	1:C:425:LEU:CD2	2.35	0.56
1:D:605:GLU:O	1:D:608:GLU:HG3	2.05	0.56
1:D:661:ASN:ND2	1:D:666:PHE:HB3	2.18	0.56
1:C:489:LEU:HD23	3:C:1388:HOH:O	2.06	0.56
1:D:733:LYS:HG3	3:D:1353:HOH:O	2.05	0.56
1:C:443:GLY:HA3	1:C:510:GLU:O	2.05	0.56
1:B:205[A]:GLU:OE2	1:B:221:LEU:HD13	2.06	0.56
1:D:628:VAL:HG22	3:D:1128:HOH:O	2.06	0.56
1:A:23:LYS:HD2	1:A:39:LEU:HD11	1.87	0.56
1:B:341:SER:O	1:B:344:LYS:HG2	2.06	0.56
1:A:71:LYS:O	1:A:75:ILE:HG12	2.06	0.55
1:D:735:PHE:O	1:D:739:ILE:HG13	2.05	0.55
1:C:406:GLN:HG2	1:C:492:PHE:HZ	1.71	0.55
1:D:661:ASN:HD21	1:D:663:ARG:CB	2.17	0.55
1:A:1:MET:HE2	1:A:3:MET:HB3	1.88	0.55
1:B:224:ALA:O	1:B:236:TYR:HB3	2.06	0.55
1:D:661:ASN:O	1:D:667:LEU:HD21	2.06	0.55
1:D:693:ILE:HD11	1:D:708:VAL:HG11	1.89	0.55
1:C:405:GLU:HG3	3:C:1142:HOH:O	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:VAL:O	1:B:251:ILE:HD13	2.07	0.54
1:A:30:TYR:CE1	1:A:94:ARG:HD2	2.43	0.54
1:C:433:LYS:O	1:C:434:GLU:HG3	2.06	0.54
1:D:693:ILE:CD1	1:D:708:VAL:HG11	2.37	0.54
1:B:296:LYS:O	1:B:297:ARG:HB2	2.06	0.54
1:B:204:LEU:O	1:B:205[A]:GLU:HG3	2.08	0.54
1:B:255:LEU:HD22	1:B:267:LEU:CD2	2.37	0.54
1:B:335:PHE:O	1:B:339:ILE:HD12	2.08	0.54
1:C:466:PHE:C	1:C:469:PRO:HD2	2.33	0.54
1:B:299[B]:LYS:NZ	3:B:1666:HOH:O	2.40	0.53
1:A:64:GLU:HG3	1:A:65:GLY:N	2.22	0.53
1:C:454:LEU:HD21	1:C:536:LYS:HG3	1.89	0.53
1:D:646:LEU:HD11	1:D:717:TYR:HB2	1.90	0.53
1:B:201:MET:O	1:B:202:LYS:HB2	2.06	0.53
1:D:602:LYS:HB3	1:D:606:GLN:HG2	1.90	0.53
1:C:481:ASN:CG	1:C:502:GLU:HG3	2.34	0.53
1:C:403:MET:HE3	1:C:492:PHE:CD2	2.43	0.53
1:C:401:MET:SD	1:C:403:MET:HB2	2.48	0.53
1:C:421:LEU:HD22	1:C:425:LEU:HD22	1.89	0.52
1:A:7:LEU:HB2	1:A:92:PHE:CE2	2.45	0.52
1:C:471:LYS:HD3	3:C:1194:HOH:O	2.09	0.52
1:A:26:THR:HA	1:A:94:ARG:HB2	1.92	0.52
1:C:501:ASN:HD22	1:C:503:THR:H	1.57	0.52
1:A:43:GLY:HA3	1:A:110:GLU:O	2.10	0.52
1:A:55:LEU:HD11	1:A:70:LEU:CD2	2.40	0.52
1:D:701:ASN:O	1:D:705:ILE:HG13	2.10	0.52
1:A:122:ARG:NH2	1:B:257:GLN:HG2	2.24	0.52
1:A:0:GLY:H3	1:A:18:LYS:HE3	1.75	0.52
1:D:616:LYS:HG2	1:D:719:ASP:CG	2.34	0.52
1:A:0:GLY:O	1:A:1:MET:HG2	2.10	0.51
1:B:240:GLU:HG3	3:B:1291:HOH:O	2.08	0.51
1:D:640:GLU:HG3	1:D:641:PHE:N	2.24	0.51
1:B:241:PHE:HA	3:B:1291:HOH:O	2.10	0.51
1:D:603:MET:HG2	1:D:604:LEU:HD23	1.92	0.51
1:D:747:ARG:HA	3:D:1149:HOH:O	2.10	0.51
1:C:421:LEU:O	1:C:425:LEU:HD22	2.11	0.51
1:B:211:LEU:HD11	1:B:312:LEU:HD11	1.93	0.51
1:B:215:PHE:CE1	1:B:221:LEU:HG	2.46	0.51
1:A:1:MET:HG3	1:A:3:MET:H	1.76	0.51
1:A:90:HIS:HA	1:A:93:ILE:HD12	1.93	0.51
1:B:300:ILE:O	1:B:301:ASN:ND2	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:634:GLU:HA	1:D:634:GLU:OE1	2.11	0.51
1:C:477:GLU:OE1	1:C:503:THR:HG22	2.11	0.50
1:A:136:LYS:HB3	3:A:1376:HOH:O	2.10	0.50
1:B:344:LYS:HG2	1:B:345:GLU:N	2.26	0.50
1:C:488:GLU:O	1:C:488:GLU:HG3	2.12	0.50
1:A:22:GLU:HB3	1:A:94:ARG:NH2	2.26	0.50
1:A:55:LEU:HD11	1:A:70:LEU:HD23	1.93	0.50
1:A:67:LEU:HA	1:A:70:LEU:HD21	1.93	0.50
1:C:440:GLU:HG3	1:C:510:GLU:OE1	2.11	0.50
1:D:625:LEU:HD13	1:D:692:PHE:O	2.12	0.50
1:A:35:HIS:HD2	3:A:1150:HOH:O	1.95	0.49
1:C:470:LEU:O	1:C:474:LEU:HG	2.13	0.49
1:D:666:PHE:O	1:D:669:PRO:HG2	2.12	0.49
1:B:226:THR:HG21	1:B:231:SER:HB3	1.94	0.49
1:C:410:LYS:HE3	1:C:488:GLU:CD	2.38	0.49
1:C:413:TYR:HB2	1:C:530:LEU:HD21	1.93	0.49
1:D:607:LEU:O	1:D:611:LEU:HB2	2.13	0.49
1:D:626:THR:O	1:D:636:TYR:HD2	1.95	0.49
1:A:54:LEU:HD21	1:A:136:LYS:HD2	1.95	0.49
1:C:525:ASN:HB3	3:C:1151:HOH:O	2.13	0.48
1:D:746:GLY:O	1:D:747:ARG:O	2.30	0.48
1:C:501:ASN:ND2	1:C:504:ILE:H	2.11	0.48
1:C:401:MET:HB2	1:C:402:LYS:H	1.46	0.48
1:A:79:PHE:CE2	1:A:83:LEU:HD21	2.49	0.48
1:A:10:LYS:HG3	3:A:1305:HOH:O	2.12	0.48
1:A:70:LEU:HD13	1:A:70:LEU:H	1.79	0.48
1:A:66:PHE:C	1:A:69:PRO:HD2	2.39	0.47
1:C:463:ARG:NH1	3:C:1679:HOH:O	2.46	0.47
1:B:206:GLN:HG2	1:B:209:LYS:CE	2.44	0.47
1:B:259:SER:OG	1:B:260:PRO:HD2	2.14	0.47
1:B:300:ILE:HG12	1:B:304:ILE:HG21	1.96	0.47
1:D:635:HIS:HD2	1:D:637:GLU:H	1.60	0.47
1:D:689:LEU:CD1	1:D:708:VAL:HG12	2.44	0.47
1:A:32:LYS:HE2	3:A:1443:HOH:O	2.15	0.47
1:A:96:LYS:HG2	1:A:97:ARG:CD	2.37	0.47
1:B:337:GLU:OE1	1:B:337:GLU:HA	2.15	0.47
1:D:674:LEU:HD22	1:D:739:ILE:HG23	1.97	0.47
1:B:254:LEU:HD13	1:B:332:TYR:CZ	2.50	0.46
1:D:603:MET:HG2	1:D:604:LEU:CD2	2.45	0.46
1:C:400:GLY:HA2	1:C:422:GLU:OE2	2.15	0.46
1:C:400:GLY:N	3:C:1463:HOH:O	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:TYR:OH	1:B:304:ILE:HG12	2.15	0.46
1:C:461:ASN:HD22	1:C:461:ASN:N	1.98	0.46
1:A:147:ARG:HA	1:A:147:ARG:HD3	1.60	0.46
1:D:690:HIS:HA	1:D:693:ILE:HG12	1.97	0.46
1:B:302:GLU:HB2	3:B:1531:HOH:O	2.14	0.46
1:A:38:THR:HG21	1:B:262:LYS:HG3	1.97	0.46
1:C:488:GLU:OE2	1:C:491:LYS:HE2	2.16	0.46
1:D:744:LYS:HA	1:D:744:LYS:HD3	1.61	0.45
1:A:16:LYS:HE3	1:A:119:ASP:O	2.16	0.45
1:A:71:LYS:HE2	1:A:75:ILE:CD1	2.40	0.45
1:B:243:GLY:HA3	1:B:310:GLU:O	2.16	0.45
1:C:534:LEU:HD21	3:C:1430:HOH:O	2.16	0.45
1:D:639:LEU:HG	3:D:1038:HOH:O	2.15	0.45
1:B:295:ILE:HD12	1:B:304:ILE:CD1	2.45	0.45
1:D:656:VAL:O	1:D:662:LYS:NZ	2.49	0.45
1:D:712:LEU:O	1:D:715:ALA:N	2.50	0.45
1:A:96:LYS:O	1:A:98:GLY:N	2.50	0.45
1:B:295:ILE:CD1	1:B:304:ILE:HD12	2.45	0.45
1:D:744:LYS:O	1:D:745:GLU:HB2	2.17	0.45
1:C:452:VAL:O	1:C:456:VAL:HG12	2.17	0.45
1:B:300:ILE:HG12	1:B:304:ILE:CG2	2.47	0.45
1:A:18:LYS:HB2	3:A:1542:HOH:O	2.16	0.45
1:A:122:ARG:O	1:B:328:ARG:NH2	2.49	0.45
1:D:675:ILE:O	1:D:675:ILE:HG13	2.16	0.45
1:D:601:MET:O	1:D:602:LYS:CB	2.65	0.44
1:D:623:LYS:HD2	3:D:1218:HOH:O	2.17	0.44
1:C:528:ARG:NH2	3:C:1151:HOH:O	2.50	0.44
1:D:615:PHE:O	1:D:618:LYS:HE2	2.17	0.44
1:A:56:VAL:HG21	1:B:242:LEU:HB2	1.98	0.44
1:B:286:LYS:NZ	3:B:1207:HOH:O	2.50	0.44
1:C:420:LEU:HD23	1:C:519:ASP:HB2	1.99	0.44
1:C:475:ILE:HD12	3:C:1358:HOH:O	2.16	0.44
1:A:0:GLY:O	1:A:5:GLU:HG2	2.17	0.44
1:B:297:ARG:HB3	1:B:298:GLY:H	1.61	0.44
1:B:253:ASP:C	1:B:257:GLN:HE21	2.23	0.44
1:A:32:LYS:H	1:A:32:LYS:HG3	1.49	0.44
1:A:67:LEU:O	1:A:71:LYS:HB2	2.18	0.44
1:A:114:ALA:O	1:A:118:ILE:HG13	2.18	0.44
1:B:226:THR:CG2	1:B:231:SER:HB3	2.47	0.44
1:C:422:GLU:O	1:C:426:THR:OG1	2.30	0.44
1:C:459:SER:O	1:C:462:LYS:NZ	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:684:ALA:O	1:D:687:LEU:N	2.50	0.44
1:A:137:GLU:N	3:A:1376:HOH:O	2.50	0.44
1:B:203:MET:HG3	1:B:204:LEU:N	2.29	0.44
1:C:461:ASN:OD1	1:C:463:ARG:NH1	2.50	0.44
1:D:602:LYS:CB	1:D:606:GLN:HG2	2.47	0.44
1:B:247:VAL:HG13	1:B:251:ILE:HD13	2.00	0.43
1:A:32:LYS:HD3	3:A:1221:HOH:O	2.17	0.43
1:B:301:ASN:ND2	1:B:304:ILE:HG22	2.33	0.43
1:B:344:LYS:HE3	1:B:344:LYS:HB3	1.75	0.43
1:B:347:ARG:NH2	3:B:1493:HOH:O	2.50	0.43
1:D:669:PRO:HG2	3:D:1348:HOH:O	2.18	0.43
1:B:340:LEU:O	1:B:343:ILE:HB	2.18	0.43
1:C:482:LEU:O	1:C:485:GLN:HB2	2.18	0.43
1:D:658:TYR:CD2	1:D:740:LEU:HD11	2.53	0.43
1:C:470:LEU:HD23	1:C:470:LEU:HA	1.92	0.43
1:A:88:GLU:HG2	3:A:1305:HOH:O	2.18	0.43
1:B:288:GLU:HA	1:B:290:HIS:CE1	2.53	0.43
1:D:661:ASN:CG	1:D:663:ARG:HG3	2.44	0.43
1:B:305:ILE:HG22	1:B:306:GLY:N	2.32	0.43
1:B:285:GLN:HB3	3:B:1197:HOH:O	2.18	0.43
1:A:133:LYS:HD3	3:A:1544:HOH:O	2.18	0.43
1:B:257:GLN:HG3	1:B:257:GLN:H	1.65	0.43
1:D:601:MET:HB3	1:D:601:MET:HE2	1.73	0.43
1:D:648:ASN:O	1:D:652:VAL:HG23	2.19	0.43
1:A:147:ARG:NH2	3:A:1351:HOH:O	2.51	0.42
1:D:668:SER:N	1:D:669:PRO:HD2	2.33	0.42
1:C:483:LEU:HD22	1:C:535:PHE:CD1	2.54	0.42
1:D:725:ASN:O	1:D:729:GLU:HG2	2.19	0.42
1:D:706:GLY:O	1:D:709:PHE:HB3	2.20	0.42
1:A:28:VAL:HB	1:A:35:HIS:CD2	2.55	0.42
1:D:654:LEU:HD22	1:D:732:TYR:CE1	2.55	0.42
1:D:659:SER:OG	1:D:666:PHE:HE1	2.02	0.42
1:D:688:GLU:OE1	1:D:691:LYS:NZ	2.51	0.42
1:A:54:LEU:HG	1:A:132:TYR:CZ	2.54	0.42
1:B:347:ARG:O	1:B:348:HIS:HB2	2.19	0.42
1:A:89:LEU:O	1:A:93:ILE:HG13	2.19	0.42
1:B:263:ARG:NH2	3:B:1277:HOH:O	2.52	0.42
1:C:450:PHE:CD1	1:C:528:ARG:HG3	2.54	0.42
1:A:56:VAL:O	1:A:62:LYS:HE2	2.19	0.42
1:B:341:SER:CA	1:B:344:LYS:HD2	2.46	0.42
1:C:423:LYS:HE3	3:C:1462:HOH:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:ARG:HH11	1:B:263:ARG:HG3	1.84	0.42
1:D:681:ASN:ND2	1:D:702:GLU:O	2.52	0.42
1:A:143:ILE:HG12	1:A:143:ILE:H	1.60	0.42
1:B:254:LEU:HD22	1:B:332:TYR:CE1	2.55	0.42
1:D:685:GLN:HG2	1:D:685:GLN:H	1.58	0.42
1:D:717:TYR:CZ	1:D:722:ARG:HB3	2.55	0.41
1:A:70:LEU:N	1:A:70:LEU:HD22	2.34	0.41
1:B:293:ILE:HG21	1:B:304:ILE:CD1	2.50	0.41
1:A:1:MET:HG3	1:A:2:LYS:N	2.35	0.41
1:A:10:LYS:HG2	1:A:10:LYS:H	1.72	0.41
1:A:99:LYS:HD2	1:A:99:LYS:H	1.86	0.41
1:C:496:LYS:HB3	1:C:496:LYS:HE3	1.85	0.41
1:A:130:LEU:HD23	1:A:130:LEU:HA	1.86	0.41
1:B:291:LYS:HB2	1:B:291:LYS:HE3	1.52	0.41
1:B:297:ARG:NH1	1:B:297:ARG:HG3	2.35	0.41
1:B:256:VAL:HG12	1:B:257:GLN:N	2.35	0.41
1:C:501:ASN:HD22	1:C:503:THR:N	2.19	0.41
1:D:658:TYR:CG	1:D:740:LEU:HD11	2.55	0.41
1:D:700:ILE:HD12	1:D:700:ILE:HG21	1.92	0.41
1:B:289:LEU:HD23	1:B:289:LEU:HA	1.84	0.41
1:B:300:ILE:CG2	1:B:301:ASN:H	2.28	0.41
1:D:661:ASN:HB3	1:D:666:PHE:CG	2.55	0.41
1:A:58:TYR:O	1:A:59:SER:O	2.39	0.41
1:D:601:MET:O	1:D:602:LYS:HB2	2.20	0.41
1:D:654:LEU:HD12	1:D:654:LEU:HA	1.85	0.41
1:A:58:TYR:O	1:A:59:SER:HB3	2.20	0.40
1:B:297:ARG:HG3	1:B:297:ARG:HH11	1.86	0.40
1:A:1:MET:CE	1:A:3:MET:HB3	2.51	0.40
1:C:495:ILE:HG21	1:C:500:ILE:HD12	2.03	0.40
1:B:300:ILE:HG23	1:B:301:ASN:N	2.30	0.40
1:A:102:GLU:CD	1:A:102:GLU:H	2.27	0.40
1:B:333:LYS:HE3	3:B:1266:HOH:O	2.21	0.40
1:C:481:ASN:ND2	1:C:502:GLU:HG3	2.37	0.40
1:C:486:LYS:HD3	1:C:538:ASP:OD2	2.22	0.40
1:C:497:ARG:NH2	3:C:1187:HOH:O	2.54	0.40
1:C:540:LEU:HA	1:C:543:ILE:HD12	2.03	0.40
1:D:620:LEU:HD23	1:D:620:LEU:HA	1.95	0.40
1:D:628:VAL:HG13	1:D:635:HIS:ND1	2.36	0.40
1:A:79:PHE:CZ	1:A:83:LEU:HD21	2.56	0.40
1:C:405:GLU:HA	1:C:408:GLU:OE1	2.22	0.40
1:C:423:LYS:CD	1:C:439:LEU:HD11	2.52	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:682:LEU:HD12	1:D:682:LEU:HA	1.91	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	148/154 (96%)	134 (90%)	10 (7%)	4 (3%)	4	1
1	B	150/154 (97%)	136 (91%)	10 (7%)	4 (3%)	4	1
1	C	149/154 (97%)	143 (96%)	6 (4%)	0	100	100
1	D	146/154 (95%)	129 (88%)	13 (9%)	4 (3%)	4	1
All	All	593/616 (96%)	542 (91%)	39 (7%)	12 (2%)	6	2

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	ARG
1	B	206	GLN
1	D	602	LYS
1	D	700	ILE
1	D	701	ASN
1	D	745	GLU
1	B	301	ASN
1	B	346	GLY
1	B	297	ARG
1	A	1	MET
1	A	3	MET
1	A	59	SER

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	133/137 (97%)	107 (80%)	26 (20%)	1	1
1	B	135/137 (98%)	96 (71%)	39 (29%)	0	0
1	C	134/137 (98%)	110 (82%)	24 (18%)	2	1
1	D	131/137 (96%)	106 (81%)	25 (19%)	1	1
All	All	533/548 (97%)	419 (79%)	114 (21%)	1	0

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	6[A]	GLN
1	A	6[B]	GLN
1	A	9	LYS
1	A	16	LYS
1	A	28	VAL
1	A	32	LYS
1	A	33	LYS
1	A	42	LEU
1	A	46	LEU
1	A	57	GLN
1	A	62	LYS
1	A	64	GLU
1	A	70	LEU
1	A	71	LYS
1	A	86	LYS
1	A	87	LEU
1	A	88	GLU
1	A	89	LEU
1	A	96	LYS
1	A	99	LYS
1	A	130	LEU
1	A	137	GLU
1	A	143	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	145	GLU
1	A	147	ARG
1	B	201	MET
1	B	202	LYS
1	B	204	LEU
1	B	216	LYS
1	B	219	SER
1	B	221	LEU
1	B	228	VAL
1	B	234	GLU
1	B	237	GLU
1	B	240	GLU
1	B	246	LEU
1	B	254	LEU
1	B	255	LEU
1	B	256	VAL
1	B	257	GLN
1	B	262	LYS
1	B	268	SER
1	B	271	LYS
1	B	275	ILE
1	B	286	LYS
1	B	289	LEU
1	B	291	LYS
1	B	296	LYS
1	B	297	ARG
1	B	299[A]	LYS
1	B	299[B]	LYS
1	B	300	ILE
1	B	301	ASN
1	B	304	ILE
1	B	305	ILE
1	B	322	ARG
1	B	328	ARG
1	B	333	LYS
1	B	337	GLU
1	B	339	ILE
1	B	341	SER
1	B	343	ILE
1	B	344	LYS
1	B	347	ARG
1	C	401	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	405	GLU
1	C	421	LEU
1	C	425	LEU
1	C	432	LYS
1	C	446	LEU
1	C	455	LEU
1	C	461	ASN
1	C	462	LYS
1	C	468	SER
1	C	482	LEU
1	C	485	GLN
1	C	486	LYS
1	C	491	LYS
1	C	496	LYS
1	C	497	ARG
1	C	499	LYS
1	C	500	ILE
1	C	501	ASN
1	C	502	GLU
1	C	503	THR
1	C	544	LYS
1	C	545	GLU
1	C	547	ARG
1	D	601	MET
1	D	603	MET
1	D	604	LEU
1	D	606	GLN
1	D	616	LYS
1	D	618	LYS
1	D	628	VAL
1	D	633	LYS
1	D	640	GLU
1	D	642	LEU
1	D	646	LEU
1	D	654	LEU
1	D	655	LEU
1	D	662	LYS
1	D	664	GLU
1	D	670	LEU
1	D	685	GLN
1	D	689	LEU
1	D	700	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	704	ILE
1	D	737	GLU
1	D	739	ILE
1	D	740	LEU
1	D	743	ILE
1	D	744	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	57	GLN
1	A	85	GLN
1	B	206	GLN
1	B	227	HIS
1	B	235	HIS
1	B	301	ASN
1	C	435	HIS
1	C	485	GLN
1	C	501	ASN
1	D	635	HIS
1	D	661	ASN

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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	148/154 (96%)	-1.65	0 100 100	8, 23, 51, 86	2 (1%)
1	B	149/154 (96%)	-1.58	0 100 100	12, 30, 61, 106	3 (2%)
1	C	149/154 (96%)	-1.66	0 100 100	8, 23, 60, 93	2 (1%)
1	D	148/154 (96%)	-1.58	0 100 100	13, 30, 61, 84	0
All	All	594/616 (96%)	-1.62	0 100 100	8, 27, 61, 106	7 (1%)

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
2	MN	A	761	1/1	1.00	0.01	24,24,24,24	0
2	MN	B	762	1/1	1.00	0.02	46,46,46,46	0
2	MN	C	763	1/1	1.00	0.01	29,29,29,29	0
2	MN	D	764	1/1	1.00	0.01	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.