



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 08:36 PM GMT

PDB ID : 2IF7  
Title : Crystal Structure of NTB-A  
Authors : Cao, E.; Ramagopal, U.A.; Fedorov, A.A.; Fedorov, E.V.; Nathenson, S.G.;  
Almo, S.C.  
Deposited on : 2006-09-20  
Resolution : 3.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

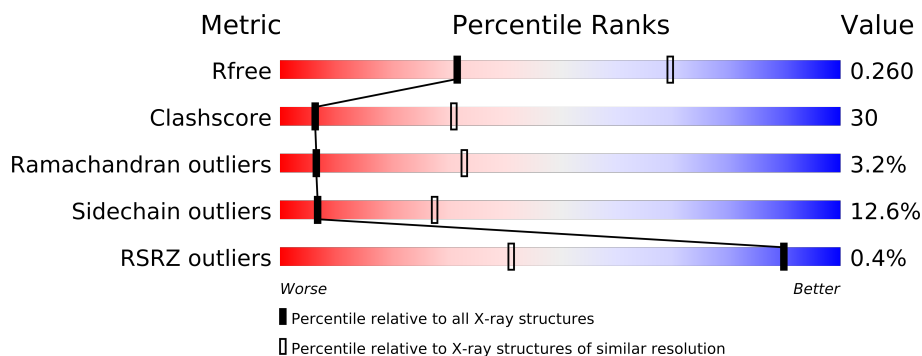
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	193	
1	B	193	
1	C	193	
1	D	193	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	CL	D	201	-	X
3	CA	A	205	-	X
3	CA	D	204	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5966 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called SLAM family member 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	0	0
			1478	925	252	294	7			
1	B	191	Total	C	N	O	S	0	0	0
			1507	945	256	299	7			
1	C	186	Total	C	N	O	S	0	0	0
			1462	914	249	292	7			
1	D	192	Total	C	N	O	S	0	0	0
			1513	948	257	301	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP Q96DU3
B	1	MET	-	INITIATING METHIONINE	UNP Q96DU3
C	1	MET	-	INITIATING METHIONINE	UNP Q96DU3
D	1	MET	-	INITIATING METHIONINE	UNP Q96DU3

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Cl	0	0
			1	1		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		

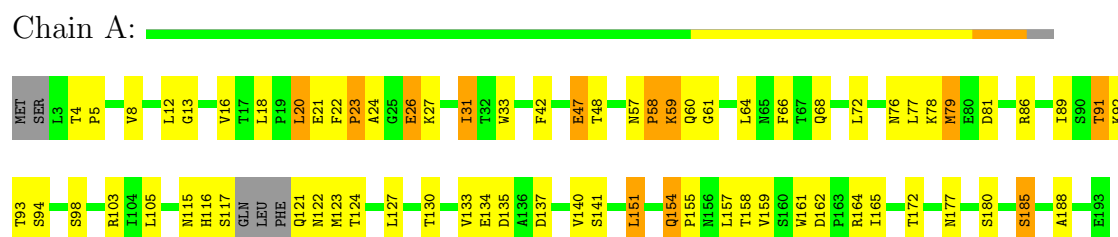
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	3	Total	O	0	0
			3	3		

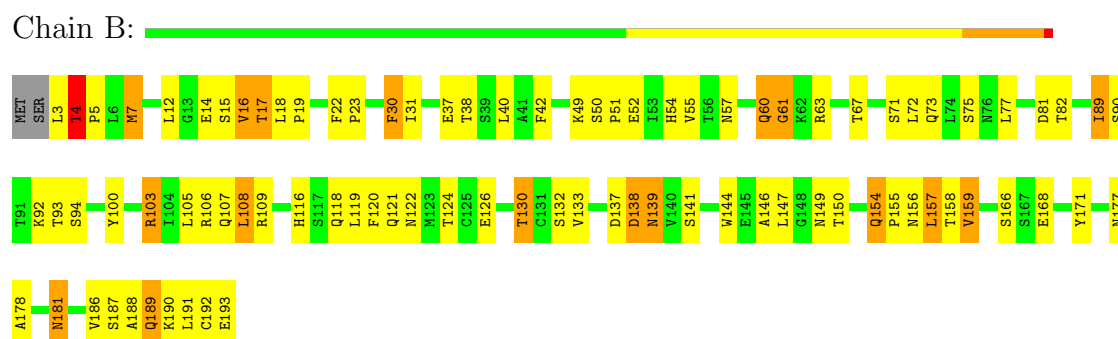
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

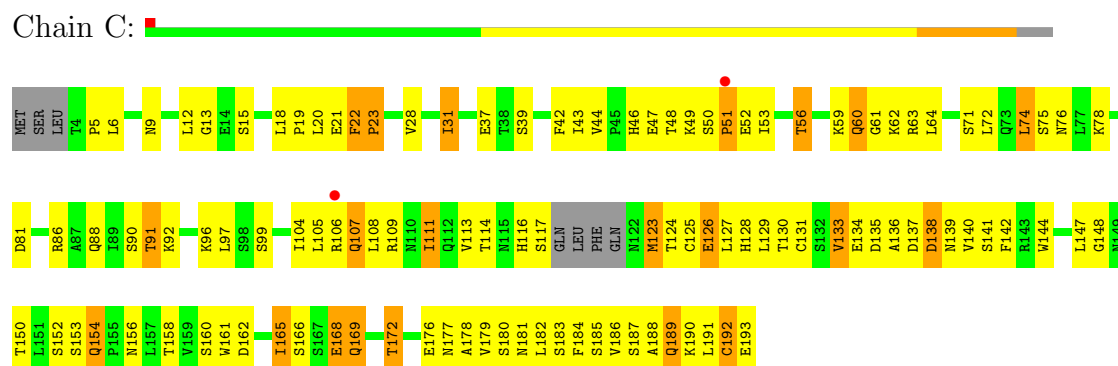
#### • Molecule 1: SLAM family member 6



#### • Molecule 1: SLAM family member 6

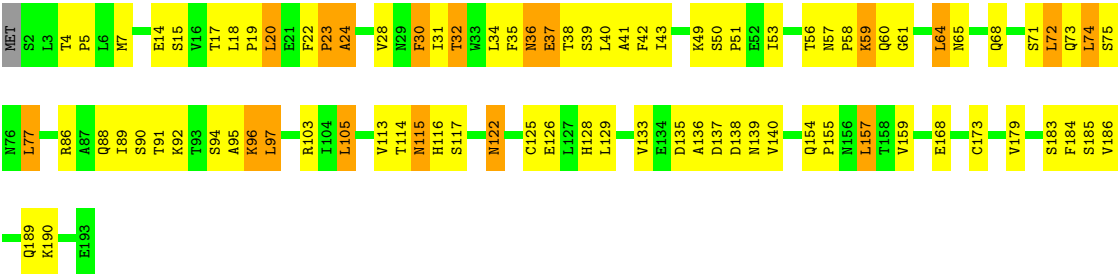


#### • Molecule 1: SLAM family member 6



#### • Molecule 1: SLAM family member 6





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.20Å 148.45Å 86.57Å 90.00° 112.86° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 39.89 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.00-3.00) 99.7 (39.89-3.00)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.12 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.213 , 0.266 0.210 , 0.260	Depositor DCC
$R_{free}$ test set	1413 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	75.2	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 101.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 28151 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5966	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.41	0/1505	0.59	0/2045
1	B	0.40	0/1536	0.57	0/2087
1	C	0.30	0/1489	0.48	0/2022
1	D	0.43	0/1542	0.57	0/2095
All	All	0.39	0/6072	0.56	0/8249

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1478	0	1452	69	0
1	B	1507	0	1481	89	0
1	C	1462	0	1433	128	0
1	D	1513	0	1486	86	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	D	3	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5966	0	5852	359	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 30.

All (359) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:125:CYS:HA	1:C:126:GLU:CB	1.56	1.25
1:A:47:GLU:OE1	1:A:48:THR:HG22	1.32	1.24
1:C:133:VAL:CG1	1:C:134:GLU:H	1.47	1.21
1:C:22:PHE:HB3	1:C:23:PRO:CD	1.73	1.15
1:C:133:VAL:HG12	1:C:134:GLU:H	1.00	1.14
1:C:133:VAL:HG12	1:C:134:GLU:N	1.56	1.11
1:C:108:LEU:O	1:C:109:ARG:HG3	1.51	1.11
1:A:91:THR:HG23	1:A:92:LYS:H	1.18	1.07
1:D:64:LEU:HD12	1:D:65:ASN:N	1.68	1.07
1:B:49:LYS:HG2	1:B:50:SER:N	1.69	1.06
1:B:49:LYS:HG2	1:B:50:SER:H	0.90	1.05
1:B:16:VAL:HG13	1:B:77:LEU:HD11	1.36	1.04
1:C:125:CYS:HA	1:C:126:GLU:HB3	1.06	1.04
1:A:91:THR:HG23	1:A:92:LYS:N	1.72	1.02
1:A:20:LEU:HD23	1:A:21:GLU:N	1.78	0.99
1:B:49:LYS:CG	1:B:50:SER:H	1.74	0.99
1:B:16:VAL:CG1	1:B:77:LEU:HD11	1.94	0.98
1:C:39:SER:O	1:C:56:THR:HB	1.65	0.96
1:C:31:ILE:HG23	1:C:43:ILE:HG13	1.45	0.96
1:C:125:CYS:CA	1:C:126:GLU:HB3	1.94	0.94
1:B:22:PHE:HB2	1:B:23:PRO:HA	1.47	0.94
1:C:125:CYS:CA	1:C:126:GLU:CB	2.44	0.94
1:B:103:ARG:HH11	1:B:103:ARG:HB2	1.34	0.92
1:C:125:CYS:HA	1:C:126:GLU:HB2	1.51	0.92
1:C:107:GLN:HB3	1:C:109:ARG:HH12	1.35	0.91
1:B:154:GLN:NE2	1:B:156:ASN:H	1.67	0.91
1:C:22:PHE:HB3	1:C:23:PRO:HD2	1.52	0.89
1:C:107:GLN:HA	1:C:107:GLN:HE21	1.38	0.89
1:C:169:GLN:HG3	1:C:189:GLN:OE1	1.73	0.88
1:C:133:VAL:CG1	1:C:134:GLU:N	2.16	0.88
1:C:22:PHE:HB3	1:C:23:PRO:HD3	1.52	0.88
1:B:60:GLN:HE21	1:B:60:GLN:H	1.21	0.88
1:A:22:PHE:HB3	1:A:23:PRO:C	1.93	0.88
1:B:60:GLN:HE21	1:B:60:GLN:N	1.75	0.84
1:C:59:LYS:O	1:C:60:GLN:HB2	1.76	0.84

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:37:GLU:H	1:D:86:ARG:HH22	1.23	0.83
1:D:36:ASN:O	1:D:37:GLU:HB2	1.78	0.83
1:C:96:LYS:HA	1:C:96:LYS:HE2	1.60	0.82
1:D:64:LEU:HD12	1:D:65:ASN:H	1.43	0.82
1:B:116:HIS:CE1	1:B:130:THR:HG21	2.14	0.82
1:C:108:LEU:HD23	1:C:180:SER:OG	1.79	0.82
1:D:168:GLU:HG2	1:D:189:GLN:NE2	1.95	0.82
1:A:91:THR:CG2	1:A:92:LYS:N	2.43	0.81
1:D:31:ILE:HG13	1:D:43:ILE:HG23	1.62	0.81
1:C:133:VAL:HG13	1:C:134:GLU:H	1.46	0.80
1:B:103:ARG:CB	1:B:103:ARG:HH11	1.93	0.80
1:B:154:GLN:HB2	1:B:155:PRO:HD2	1.64	0.79
1:A:154:GLN:HB2	1:A:155:PRO:HD2	1.63	0.79
1:C:74:LEU:HD13	1:C:75:SER:H	1.48	0.79
1:B:159:VAL:HG13	1:C:183:SER:HB2	1.64	0.78
1:B:60:GLN:HG3	1:B:63:ARG:HH12	1.49	0.78
1:C:63:ARG:HD2	1:C:75:SER:HB2	1.66	0.76
1:A:78:LYS:O	1:A:81:ASP:HB2	1.85	0.76
1:A:59:LYS:HE3	1:A:59:LYS:HA	1.69	0.75
1:C:125:CYS:O	1:C:161:TRP:N	2.17	0.74
1:C:74:LEU:CD1	1:C:75:SER:H	2.00	0.74
1:C:44:VAL:HG13	1:C:52:GLU:HB2	1.70	0.74
1:D:37:GLU:H	1:D:86:ARG:NH2	1.85	0.73
1:A:4:THR:HB	1:A:5:PRO:CD	2.18	0.73
1:B:4:THR:OG1	1:B:5:PRO:HA	1.89	0.73
1:B:166:SER:HB3	1:C:185:SER:O	1.88	0.73
1:D:137:ASP:O	1:D:140:VAL:HG12	1.90	0.72
1:B:19:PRO:O	1:B:100:TYR:OH	2.08	0.72
1:C:147:LEU:HG	1:C:168:GLU:HG2	1.72	0.72
1:D:72:LEU:HD12	1:D:73:GLN:N	2.02	0.72
1:D:157:LEU:HD22	1:D:159:VAL:HG13	1.73	0.71
1:C:18:LEU:O	1:C:71:SER:HB3	1.91	0.71
1:A:47:GLU:CD	1:A:47:GLU:H	1.89	0.70
1:B:181:ASN:C	1:B:181:ASN:HD22	1.94	0.70
1:B:17:THR:O	1:B:18:LEU:HD23	1.91	0.69
1:D:154:GLN:HB2	1:D:155:PRO:CD	2.22	0.69
1:D:43:ILE:HB	1:D:53:ILE:HG22	1.74	0.69
1:C:107:GLN:NE2	1:C:107:GLN:HA	2.09	0.68
1:A:58:PRO:HG2	1:B:94:SER:HA	1.74	0.68
1:B:63:ARG:NH2	1:B:81:ASP:OD2	2.27	0.68
1:D:64:LEU:O	1:D:65:ASN:OD1	2.11	0.68
1:C:64:LEU:O	1:C:64:LEU:HD12	1.93	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:122:ASN:ND2	1:A:123:MET:SD	2.68	0.67
1:C:162:ASP:HB3	1:C:165:ILE:HG22	1.76	0.67
1:A:20:LEU:HD23	1:A:20:LEU:C	2.13	0.67
1:D:20:LEU:HD12	1:D:20:LEU:N	2.10	0.67
1:C:47:GLU:OE1	1:C:48:THR:HG22	1.93	0.67
1:B:103:ARG:CB	1:B:103:ARG:NH1	2.58	0.67
1:D:4:THR:HG23	1:D:5:PRO:HD2	1.77	0.67
1:A:140:VAL:HG12	1:A:141:SER:N	2.08	0.67
1:B:189:GLN:H	1:B:189:GLN:CD	1.98	0.66
1:B:186:VAL:HB	1:B:191:LEU:HD11	1.77	0.66
1:D:137:ASP:OD1	1:D:138:ASP:N	2.27	0.66
1:D:91:THR:HG23	1:D:94:SER:H	1.61	0.66
1:C:172:THR:OG1	1:C:185:SER:HB3	1.95	0.66
1:C:162:ASP:H	1:C:166:SER:HB2	1.60	0.66
1:C:135:ASP:O	1:C:137:ASP:N	2.28	0.66
1:C:22:PHE:CB	1:C:23:PRO:HD2	2.23	0.65
1:D:72:LEU:C	1:D:72:LEU:HD12	2.17	0.65
1:D:105:LEU:HD23	1:D:139:ASN:ND2	2.12	0.64
1:C:131:CYS:O	1:C:142:PHE:HE2	1.80	0.64
1:B:154:GLN:HE22	1:B:156:ASN:H	1.45	0.64
1:D:17:THR:HG22	1:D:73:GLN:HG3	1.80	0.64
1:D:14:GLU:O	1:D:77:LEU:HD13	1.97	0.64
1:A:58:PRO:CG	1:B:94:SER:HA	2.27	0.64
1:A:22:PHE:CD2	1:A:24:ALA:HB2	2.33	0.64
1:C:22:PHE:CB	1:C:23:PRO:CD	2.58	0.63
1:A:26:GLU:HG2	1:A:91:THR:OG1	1.98	0.63
1:B:14:GLU:O	1:B:77:LEU:HG	1.99	0.63
1:C:169:GLN:CG	1:C:189:GLN:OE1	2.46	0.63
1:A:140:VAL:CG1	1:A:141:SER:N	2.61	0.63
1:A:91:THR:HG22	1:A:94:SER:H	1.64	0.63
1:A:47:GLU:CD	1:A:47:GLU:N	2.51	0.63
1:B:22:PHE:CB	1:B:23:PRO:HA	2.25	0.62
1:A:172:THR:OG1	1:A:185:SER:HB2	1.99	0.62
1:C:134:GLU:HA	1:C:134:GLU:OE1	1.99	0.62
1:C:9:ASN:ND2	1:C:178:ALA:HB1	2.15	0.61
1:C:181:ASN:O	1:C:182:LEU:HD23	2.00	0.61
1:C:131:CYS:O	1:C:142:PHE:CE2	2.53	0.61
1:D:40:LEU:HD11	1:D:60:GLN:OE1	2.00	0.61
1:D:86:ARG:HB2	1:D:97:LEU:HD21	1.82	0.61
1:C:12:LEU:HD22	1:C:106:ARG:HA	1.82	0.61
1:A:20:LEU:CD2	1:A:20:LEU:C	2.67	0.61
1:C:59:LYS:O	1:C:60:GLN:CB	2.48	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:15:SER:HB3	1:C:75:SER:HA	1.82	0.60
1:D:168:GLU:CG	1:D:189:GLN:NE2	2.65	0.60
1:C:107:GLN:HB3	1:C:109:ARG:NH1	2.12	0.60
1:A:20:LEU:HD11	1:A:31:ILE:HD12	1.83	0.60
1:A:4:THR:HB	1:A:5:PRO:HD3	1.84	0.60
1:C:13:GLY:N	1:C:76:ASN:O	2.35	0.60
1:C:44:VAL:CG1	1:C:52:GLU:HB2	2.31	0.59
1:A:26:GLU:CG	1:A:91:THR:OG1	2.50	0.59
1:A:20:LEU:CD1	1:A:31:ILE:HD12	2.32	0.59
1:B:15:SER:O	1:B:16:VAL:HG12	2.02	0.59
1:C:105:LEU:HD21	1:C:139:ASN:HD22	1.68	0.59
1:B:171:TYR:CE2	1:B:188:ALA:HB2	2.37	0.59
1:B:138:ASP:OD1	1:B:138:ASP:N	2.34	0.59
1:B:116:HIS:HE1	1:B:130:THR:HG21	1.63	0.59
1:B:154:GLN:HB2	1:B:155:PRO:CD	2.33	0.59
1:C:144:TRP:HB2	1:C:152:SER:HB3	1.84	0.59
1:C:108:LEU:O	1:C:109:ARG:CG	2.40	0.59
1:C:191:LEU:O	1:C:193:GLU:HG3	2.03	0.59
1:B:154:GLN:NE2	1:B:156:ASN:N	2.47	0.58
1:A:47:GLU:N	1:A:47:GLU:OE2	2.36	0.58
1:A:21:GLU:CG	1:A:22:PHE:H	2.16	0.58
1:D:128:HIS:O	1:D:129:LEU:HD23	2.02	0.58
1:B:72:LEU:C	1:B:72:LEU:HD23	2.24	0.58
1:B:19:PRO:HA	1:B:71:SER:OG	2.04	0.58
1:B:168:GLU:OE1	1:B:189:GLN:HG2	2.03	0.58
1:D:128:HIS:C	1:D:129:LEU:HD23	2.24	0.58
1:C:116:HIS:O	1:C:117:SER:CB	2.53	0.57
1:B:121:GLN:HA	1:B:121:GLN:OE1	2.04	0.57
1:B:192:CYS:O	1:B:193:GLU:HG3	2.05	0.56
1:D:36:ASN:O	1:D:37:GLU:CB	2.53	0.56
1:A:21:GLU:HG2	1:A:22:PHE:H	1.70	0.56
1:C:63:ARG:HE	1:C:74:LEU:HD11	1.71	0.56
1:B:189:GLN:N	1:B:189:GLN:OE1	2.32	0.55
1:B:108:LEU:HD13	1:B:177:ASN:ND2	2.22	0.55
1:D:168:GLU:CG	1:D:189:GLN:HE22	2.19	0.55
1:C:140:VAL:HG12	1:C:141:SER:N	2.22	0.55
1:A:133:VAL:HG13	1:A:134:GLU:N	2.21	0.55
1:B:116:HIS:CE1	1:B:130:THR:CG2	2.89	0.55
1:B:118:GLN:HE21	1:B:126:GLU:HG3	1.72	0.55
1:C:176:GLU:HA	1:C:181:ASN:HB3	1.88	0.55
1:A:116:HIS:O	1:A:117:SER:HB2	2.07	0.55
1:D:105:LEU:HD23	1:D:139:ASN:HD22	1.72	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:5:PRO:C	1:C:6:LEU:HD22	2.28	0.54
1:A:134:GLU:O	1:A:135:ASP:HB2	2.07	0.54
1:A:177:ASN:OD1	1:A:180:SER:HB2	2.07	0.54
1:A:47:GLU:CD	1:A:48:THR:H	2.10	0.54
1:D:168:GLU:HG2	1:D:189:GLN:HE21	1.69	0.54
1:B:92:LYS:HG3	1:B:93:THR:HG23	1.89	0.54
1:C:63:ARG:HH12	1:C:78:LYS:HD3	1.72	0.54
1:D:58:PRO:O	1:D:60:GLN:N	2.41	0.53
1:D:64:LEU:HD12	1:D:64:LEU:C	2.23	0.53
1:B:15:SER:C	1:B:16:VAL:CG1	2.77	0.53
1:B:186:VAL:HB	1:B:191:LEU:CD1	2.38	0.53
1:B:137:ASP:HB3	1:B:139:ASN:ND2	2.23	0.53
1:A:91:THR:CG2	1:A:93:THR:H	2.21	0.53
1:B:52:GLU:HG2	1:B:54:HIS:CE1	2.42	0.53
1:D:168:GLU:CD	1:D:189:GLN:HE22	2.11	0.53
1:D:37:GLU:N	1:D:86:ARG:HH22	2.02	0.53
1:C:125:CYS:CA	1:C:126:GLU:HB2	2.28	0.53
1:B:149:ASN:OD1	1:C:148:GLY:N	2.35	0.53
1:B:120:PHE:CD1	1:B:120:PHE:C	2.82	0.53
1:B:154:GLN:HE21	1:B:155:PRO:N	2.07	0.52
1:D:154:GLN:HB2	1:D:155:PRO:HD2	1.89	0.52
1:D:17:THR:O	1:D:18:LEU:HD23	2.08	0.52
1:C:179:VAL:O	1:C:180:SER:HB3	2.09	0.52
1:C:31:ILE:HG23	1:C:43:ILE:CG1	2.30	0.52
1:B:16:VAL:CG2	1:B:16:VAL:O	2.58	0.52
1:C:191:LEU:O	1:C:193:GLU:N	2.38	0.52
1:C:188:ALA:O	1:C:190:LYS:N	2.43	0.52
1:C:13:GLY:CA	1:C:76:ASN:O	2.58	0.52
1:C:61:GLY:C	1:C:63:ARG:H	2.14	0.51
1:D:31:ILE:HG13	1:D:43:ILE:CG2	2.39	0.51
1:C:125:CYS:O	1:C:160:SER:HA	2.11	0.51
1:A:157:LEU:CD1	1:A:159:VAL:HG13	2.41	0.51
1:A:20:LEU:HD23	1:A:21:GLU:H	1.68	0.51
1:A:26:GLU:HG3	1:A:27:LYS:N	2.26	0.51
1:C:46:HIS:HB3	1:C:49:LYS:HE3	1.92	0.51
1:A:123:MET:HG2	1:A:124:THR:N	2.26	0.51
1:A:20:LEU:HD21	1:A:89:ILE:HD11	1.93	0.50
1:C:123:MET:SD	1:C:124:THR:HG22	2.51	0.50
1:B:159:VAL:CG1	1:C:183:SER:HB2	2.39	0.50
1:C:37:GLU:HB3	1:D:97:LEU:HD11	1.93	0.50
1:D:4:THR:CG2	1:D:5:PRO:HD2	2.42	0.50
1:C:188:ALA:C	1:C:190:LYS:H	2.13	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:15:SER:HB2	1:C:74:LEU:O	2.11	0.50
1:A:157:LEU:HD11	1:A:159:VAL:HG13	1.94	0.50
1:C:187:SER:HB3	1:C:190:LYS:HB2	1.94	0.50
1:A:79:MET:C	1:A:81:ASP:H	2.15	0.50
1:D:23:PRO:O	1:D:24:ALA:HB2	2.11	0.50
1:C:140:VAL:CG1	1:C:141:SER:N	2.75	0.49
1:D:15:SER:CB	1:D:75:SER:HA	2.42	0.49
1:A:137:ASP:H	1:A:140:VAL:HG23	1.77	0.49
1:B:60:GLN:HG3	1:B:63:ARG:NH1	2.23	0.49
1:B:186:VAL:CB	1:B:191:LEU:HD11	2.42	0.49
1:D:105:LEU:HD13	1:D:179:VAL:HG13	1.94	0.49
1:B:40:LEU:HD23	1:B:57:ASN:HB3	1.95	0.49
1:C:5:PRO:O	1:C:6:LEU:HD13	2.13	0.49
1:A:21:GLU:HG2	1:A:22:PHE:O	2.13	0.49
1:D:157:LEU:CD2	1:D:159:VAL:HG13	2.42	0.49
1:D:122:ASN:H	1:D:122:ASN:ND2	2.09	0.49
1:C:81:ASP:HB2	1:C:104:ILE:HD11	1.95	0.49
1:C:123:MET:SD	1:C:124:THR:N	2.84	0.49
1:C:177:ASN:OD1	1:C:177:ASN:C	2.51	0.48
1:A:21:GLU:CG	1:A:22:PHE:N	2.76	0.48
1:D:58:PRO:O	1:D:61:GLY:N	2.40	0.48
1:A:115:ASN:ND2	1:A:116:HIS:H	2.10	0.48
1:D:115:ASN:ND2	1:D:117:SER:H	2.11	0.48
1:B:30:PHE:CD1	1:B:90:SER:HB2	2.48	0.48
1:B:103:ARG:HB3	1:B:103:ARG:NH1	2.27	0.48
1:A:21:GLU:HG2	1:A:22:PHE:N	2.28	0.48
1:D:32:THR:HG23	1:D:88:GLN:HB3	1.96	0.48
1:B:61:GLY:C	1:B:63:ARG:H	2.16	0.48
1:D:28:VAL:HG11	1:D:89:ILE:CG2	2.43	0.48
1:B:171:TYR:HE2	1:B:188:ALA:HB2	1.78	0.48
1:D:15:SER:HB3	1:D:75:SER:HA	1.96	0.48
1:C:91:THR:OG1	1:C:92:LYS:N	2.46	0.47
1:B:105:LEU:HD13	1:B:178:ALA:HB3	1.96	0.47
1:B:60:GLN:NE2	1:B:60:GLN:N	2.54	0.47
1:B:67:THR:OG1	1:B:71:SER:HB2	2.14	0.47
1:A:133:VAL:CG1	1:A:134:GLU:N	2.76	0.47
1:C:47:GLU:HA	1:C:48:THR:HA	1.47	0.47
1:C:42:PHE:CE2	1:D:42:PHE:CD2	3.02	0.47
1:B:31:ILE:HG12	1:B:89:ILE:HG22	1.97	0.47
1:B:4:THR:CB	1:B:5:PRO:CA	2.92	0.47
1:A:20:LEU:HB2	1:A:33:TRP:HZ2	1.80	0.47
1:C:5:PRO:HA	1:C:99:SER:HB2	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:92:LYS:HG2	1:D:92:LYS:O	2.14	0.47
1:A:68:GLN:HA	1:A:68:GLN:OE1	2.15	0.47
1:C:191:LEU:C	1:C:193:GLU:N	2.69	0.47
1:D:89:ILE:O	1:D:95:ALA:HA	2.15	0.46
1:C:111:ILE:CG2	1:C:184:PHE:HB2	2.45	0.46
1:C:137:ASP:O	1:C:140:VAL:HG23	2.14	0.46
1:A:86:ARG:HA	1:A:98:SER:O	2.15	0.46
1:A:157:LEU:HD11	1:A:159:VAL:CG1	2.45	0.46
1:D:173:CYS:O	1:D:183:SER:HA	2.16	0.46
1:A:59:LYS:O	1:A:60:GLN:C	2.54	0.46
1:B:3:LEU:HD23	1:B:4:THR:N	2.31	0.46
1:C:137:ASP:O	1:C:139:ASN:N	2.49	0.46
1:A:151:LEU:N	1:A:151:LEU:CD1	2.78	0.46
1:C:64:LEU:HB3	1:C:74:LEU:HD22	1.97	0.45
1:B:4:THR:HB	1:B:5:PRO:O	2.16	0.45
1:C:188:ALA:C	1:C:190:LYS:N	2.70	0.45
1:D:58:PRO:O	1:D:59:LYS:C	2.55	0.45
1:C:127:LEU:HD22	1:C:192:CYS:SG	2.56	0.45
1:B:116:HIS:ND1	1:B:130:THR:HG21	2.31	0.45
1:D:18:LEU:HA	1:D:19:PRO:HD3	1.80	0.45
1:C:107:GLN:CA	1:C:107:GLN:HE21	2.17	0.45
1:D:64:LEU:C	1:D:65:ASN:OD1	2.54	0.45
1:D:189:GLN:HB2	1:D:189:GLN:HE21	1.62	0.45
1:C:116:HIS:O	1:C:117:SER:HB3	2.15	0.45
1:C:126:GLU:HG3	1:C:126:GLU:O	2.16	0.45
1:B:4:THR:OG1	1:B:5:PRO:CA	2.61	0.45
1:B:15:SER:CB	1:B:75:SER:HA	2.46	0.45
1:C:154:GLN:O	1:C:156:ASN:N	2.50	0.45
1:A:91:THR:HG23	1:A:93:THR:H	1.81	0.45
1:D:89:ILE:HB	1:D:96:LYS:HB3	1.99	0.45
1:B:30:PHE:HD1	1:B:90:SER:HB2	1.82	0.45
1:C:113:VAL:HA	1:C:130:THR:O	2.17	0.45
1:B:72:LEU:HD23	1:B:73:GLN:N	2.31	0.45
1:C:42:PHE:CD2	1:D:42:PHE:CD2	3.04	0.45
1:C:111:ILE:HG23	1:C:184:PHE:HB2	1.99	0.45
1:D:41:ALA:HA	1:D:56:THR:H	1.82	0.44
1:C:63:ARG:HH12	1:C:78:LYS:CD	2.31	0.44
1:A:121:GLN:HA	1:A:122:ASN:HA	1.73	0.44
1:C:105:LEU:HD12	1:C:178:ALA:HB3	1.99	0.44
1:A:18:LEU:HD12	1:A:72:LEU:HD23	1.99	0.44
1:D:68:GLN:HA	1:D:68:GLN:OE1	2.18	0.44
1:D:36:ASN:H	1:D:86:ARG:HH12	1.65	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:86:ARG:HB2	1:D:97:LEU:CD2	2.47	0.44
1:D:7:MET:SD	1:D:103:ARG:HG3	2.57	0.44
1:C:63:ARG:NH1	1:C:76:ASN:OD1	2.51	0.44
1:D:115:ASN:HD22	1:D:116:HIS:N	2.15	0.44
1:C:105:LEU:HD21	1:C:139:ASN:HB2	1.99	0.43
1:A:26:GLU:HG3	1:A:91:THR:OG1	2.18	0.43
1:B:116:HIS:ND1	1:B:130:THR:CG2	2.82	0.43
1:A:162:ASP:OD1	1:A:164:ARG:HG2	2.19	0.43
1:C:153:SER:C	1:C:154:GLN:HG2	2.38	0.43
1:C:108:LEU:N	1:C:108:LEU:HD22	2.33	0.43
1:B:154:GLN:HE21	1:B:156:ASN:H	1.60	0.43
1:D:57:ASN:HA	1:D:58:PRO:HD2	1.83	0.43
1:D:31:ILE:HG22	1:D:89:ILE:HA	2.00	0.43
1:C:74:LEU:CD1	1:C:75:SER:N	2.76	0.43
1:B:144:TRP:CE3	1:B:157:LEU:HD12	2.54	0.43
1:A:4:THR:HB	1:A:5:PRO:HD2	1.99	0.43
1:C:18:LEU:HD12	1:C:72:LEU:HD23	2.00	0.43
1:D:23:PRO:CG	1:D:24:ALA:H	2.32	0.43
1:C:50:SER:HA	1:C:51:PRO:HA	1.79	0.43
1:A:31:ILE:HD11	1:A:33:TRP:NE1	2.33	0.42
1:A:13:GLY:O	1:A:76:ASN:HA	2.19	0.42
1:C:12:LEU:CD2	1:C:106:ARG:HA	2.47	0.42
1:B:122:ASN:ND2	1:B:124:THR:HG23	2.34	0.42
1:A:64:LEU:HD21	1:A:66:PHE:CZ	2.55	0.42
1:D:35:PHE:CD1	1:D:36:ASN:HB2	2.55	0.42
1:C:96:LYS:HA	1:C:96:LYS:CE	2.40	0.42
1:A:16:VAL:HB	1:A:77:LEU:HD11	2.00	0.42
1:B:157:LEU:HD22	1:B:159:VAL:HG22	2.00	0.42
1:D:20:LEU:CD1	1:D:20:LEU:N	2.81	0.42
1:D:115:ASN:HD21	1:D:117:SER:CB	2.33	0.42
1:B:146:ALA:O	1:B:147:LEU:C	2.57	0.42
1:C:128:HIS:ND1	1:C:158:THR:HB	2.35	0.42
1:C:43:ILE:HG22	1:C:53:ILE:HB	2.02	0.42
1:D:53:ILE:O	1:D:53:ILE:HD12	2.19	0.42
1:C:108:LEU:N	1:C:108:LEU:CD2	2.83	0.41
1:C:39:SER:N	1:D:88:GLN:OE1	2.52	0.41
1:A:22:PHE:HB3	1:A:23:PRO:O	2.17	0.41
1:B:22:PHE:CB	1:B:23:PRO:CA	2.97	0.41
1:B:61:GLY:C	1:B:63:ARG:N	2.73	0.41
1:D:122:ASN:HD22	1:D:122:ASN:H	1.68	0.41
1:C:81:ASP:HB2	1:C:104:ILE:CD1	2.50	0.41
1:C:114:THR:O	1:C:129:LEU:HD23	2.19	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:97:LEU:HD11	1:D:38:THR:HG22	2.01	0.41
1:A:115:ASN:CG	1:A:116:HIS:N	2.73	0.41
1:A:42:PHE:CD2	1:B:42:PHE:CD2	3.09	0.41
1:B:15:SER:O	1:B:16:VAL:CG1	2.69	0.41
1:C:88:GLN:OE1	1:D:39:SER:HB3	2.20	0.41
1:D:115:ASN:HD22	1:D:116:HIS:H	1.69	0.41
1:B:7:MET:SD	1:B:7:MET:N	2.86	0.41
1:D:15:SER:HB2	1:D:74:LEU:O	2.20	0.41
1:D:113:VAL:HG23	1:D:184:PHE:CD1	2.56	0.41
1:D:50:SER:HA	1:D:51:PRO:HD3	1.90	0.41
1:D:133:VAL:HG23	1:D:136:ALA:H	1.84	0.41
1:C:74:LEU:HD13	1:C:75:SER:N	2.27	0.41
1:C:131:CYS:HB2	1:C:144:TRP:HZ2	1.86	0.41
1:D:34:LEU:N	1:D:34:LEU:HD22	2.35	0.41
1:B:181:ASN:C	1:B:181:ASN:ND2	2.66	0.41
1:B:89:ILE:H	1:B:89:ILE:HG12	1.63	0.41
1:C:150:THR:HG23	1:C:150:THR:O	2.20	0.41
1:C:21:GLU:HG3	1:C:22:PHE:N	2.36	0.40
1:D:19:PRO:HA	1:D:71:SER:OG	2.21	0.40
1:C:18:LEU:HA	1:C:19:PRO:HD3	1.77	0.40
1:D:154:GLN:HB2	1:D:155:PRO:HD3	2.00	0.40
1:A:161:TRP:CD2	1:A:188:ALA:HB1	2.56	0.40
1:B:16:VAL:CG1	1:B:77:LEU:CD1	2.83	0.40
1:C:44:VAL:CG1	1:C:52:GLU:CB	2.98	0.40
1:C:137:ASP:C	1:C:139:ASN:N	2.73	0.40
1:B:50:SER:HB2	1:B:51:PRO:CD	2.51	0.40
1:B:15:SER:C	1:B:16:VAL:HG13	2.42	0.40
1:C:137:ASP:O	1:C:138:ASP:C	2.59	0.40
1:D:113:VAL:CG2	1:D:184:PHE:CD1	3.05	0.40
1:D:30:PHE:O	1:D:90:SER:HB3	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	184/193 (95%)	159 (86%)	20 (11%)	5 (3%)	8	38
1	B	189/193 (98%)	170 (90%)	17 (9%)	2 (1%)	21	67
1	C	182/193 (94%)	141 (78%)	28 (15%)	13 (7%)	2	9
1	D	190/193 (98%)	169 (89%)	17 (9%)	4 (2%)	11	47
All	All	745/772 (96%)	639 (86%)	82 (11%)	24 (3%)	6	33

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	PRO
1	A	59	LYS
1	B	4	THR
1	C	22	PHE
1	C	60	GLN
1	C	126	GLU
1	C	136	ALA
1	D	23	PRO
1	D	24	ALA
1	D	59	LYS
1	C	189	GLN
1	C	192	CYS
1	C	62	LYS
1	C	91	THR
1	C	138	ASP
1	C	51	PRO
1	A	58	PRO
1	A	61	GLY
1	D	22	PHE
1	C	133	VAL
1	A	165	ILE
1	B	61	GLY
1	C	23	PRO
1	C	165	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	173/178 (97%)	156 (90%)	17 (10%)	12	41
1	B	176/178 (99%)	143 (81%)	33 (19%)	2	12
1	C	171/178 (96%)	156 (91%)	15 (9%)	14	48
1	D	177/178 (99%)	154 (87%)	23 (13%)	6	26
All	All	697/712 (98%)	609 (87%)	88 (13%)	7	27

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	12	LEU
1	A	20	LEU
1	A	26	GLU
1	A	31	ILE
1	A	47	GLU
1	A	57	ASN
1	A	79	MET
1	A	91	THR
1	A	103	ARG
1	A	105	LEU
1	A	127	LEU
1	A	130	THR
1	A	151	LEU
1	A	154	GLN
1	A	158	THR
1	A	185	SER
1	B	4	THR
1	B	7	MET
1	B	12	LEU
1	B	16	VAL
1	B	17	THR
1	B	30	PHE
1	B	37	GLU
1	B	38	THR
1	B	55	VAL
1	B	60	GLN
1	B	82	THR
1	B	89	ILE
1	B	103	ARG
1	B	106	ARG
1	B	107	GLN
1	B	108	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	109	ARG
1	B	119	LEU
1	B	130	THR
1	B	132	SER
1	B	133	VAL
1	B	138	ASP
1	B	139	ASN
1	B	141	SER
1	B	150	THR
1	B	154	GLN
1	B	157	LEU
1	B	158	THR
1	B	159	VAL
1	B	181	ASN
1	B	187	SER
1	B	189	GLN
1	B	190	LYS
1	C	20	LEU
1	C	28	VAL
1	C	31	ILE
1	C	56	THR
1	C	74	LEU
1	C	86	ARG
1	C	90	SER
1	C	107	GLN
1	C	111	ILE
1	C	123	MET
1	C	154	GLN
1	C	168	GLU
1	C	169	GLN
1	C	172	THR
1	C	186	VAL
1	D	20	LEU
1	D	30	PHE
1	D	32	THR
1	D	36	ASN
1	D	37	GLU
1	D	49	LYS
1	D	64	LEU
1	D	72	LEU
1	D	74	LEU
1	D	77	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	96	LYS
1	D	97	LEU
1	D	105	LEU
1	D	114	THR
1	D	115	ASN
1	D	122	ASN
1	D	125	CYS
1	D	126	GLU
1	D	135	ASP
1	D	157	LEU
1	D	185	SER
1	D	186	VAL
1	D	190	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	107	GLN
1	A	115	ASN
1	A	116	HIS
1	A	128	HIS
1	A	169	GLN
1	A	181	ASN
1	B	9	ASN
1	B	54	HIS
1	B	60	GLN
1	B	107	GLN
1	B	112	GLN
1	B	118	GLN
1	B	139	ASN
1	B	154	GLN
1	B	181	ASN
1	C	36	ASN
1	C	65	ASN
1	C	73	GLN
1	C	107	GLN
1	C	122	ASN
1	C	139	ASN
1	C	169	GLN
1	D	9	ASN
1	D	115	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	122	ASN
1	D	149	ASN
1	D	189	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	188/193 (97%)	-0.24	0	100	100	61, 84, 102, 108	0
1	B	191/193 (98%)	-0.24	0	100	100	61, 83, 101, 109	0
1	C	186/193 (96%)	0.00	2 (1%)	77	21	57, 82, 104, 121	0
1	D	192/193 (99%)	-0.21	0	100	100	61, 82, 100, 123	0
All	All	757/772 (98%)	-0.17	2 (0%)	90	48	57, 83, 102, 123	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	51	PRO	2.4
1	C	106	ARG	2.2

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

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

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	A	205	1/1	0.50	9.98	74,74,74,74	0
3	CA	D	204	1/1	0.23	4.90	62,62,62,62	0
2	CL	D	201	1/1	0.41	4.23	107,107,107,107	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.