



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:02 AM UTC

PDB ID : 2IF7 / pdb_00002if7
Title : Crystal Structure of NTB-A
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Deposited on : 2006-09-20
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
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

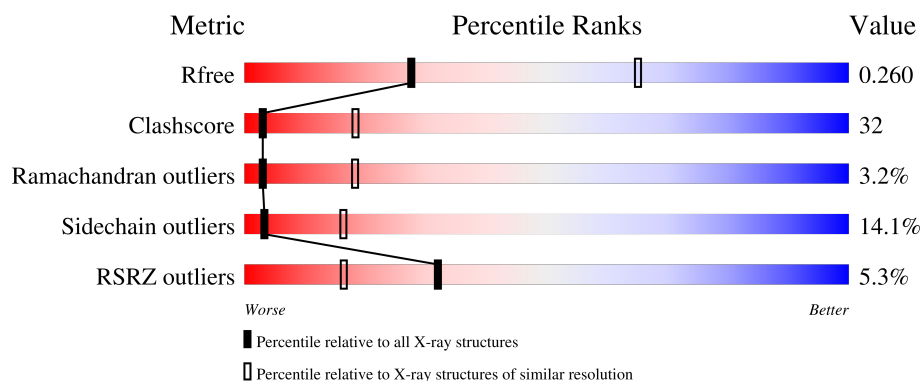
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	193	2% 59% 31% 7% ..
1	B	193	5% 51% 38% 9% ..
1	C	193	8% 34% 50% 12% ..
1	D	193	6% 52% 39% 9% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5966 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 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 CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 4 is water.

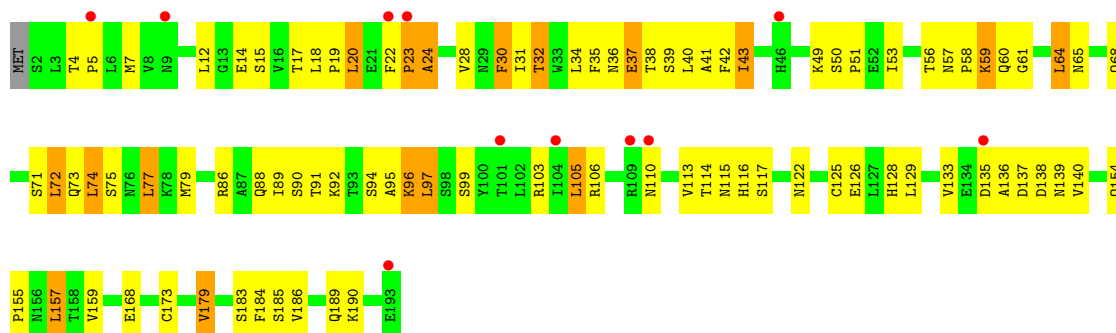
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	3	Total	O	0	0
			3	3		

- 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, α , β , γ	121.20Å 148.45Å 86.57Å 90.00° 112.86° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 40.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.00-3.00) 99.6 (40.00-3.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.213 , 0.266 0.208 , 0.260	Depositor DCC
R_{free} test set	1413 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	75.2	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 89.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5966	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.52	0/1505	0.87	4/2045 (0.2%)
1	B	0.50	0/1536	0.86	2/2087 (0.1%)
1	C	0.37	0/1489	0.75	0/2022
1	D	0.53	0/1542	0.82	0/2095
All	All	0.48	0/6072	0.82	6/8249 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	186	VAL	CB-CA-C	-6.39	104.30	111.45
1	A	57	ASN	CA-C-N	5.73	127.00	119.84
1	A	57	ASN	C-N-CA	5.73	127.00	119.84
1	A	22	PHE	CA-C-N	5.34	139.82	127.00
1	A	22	PHE	C-N-CA	5.34	139.82	127.00
1	B	185	SER	N-CA-C	5.23	117.53	107.44

There are no chirality outliers.

There are no planarity outliers.

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	1478	0	1452	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1507	0	1481	94	0
1	C	1462	0	1433	137	0
1	D	1513	0	1486	87	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
3	D	1	0	0	0	0
4	D	3	0	0	0	0
All	All	5966	0	5852	374	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 32.

All (374) 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: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: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:A:91:THR:HG23	1:A:92:LYS:N	1.72	0.94
1:B:103:ARG:HH11	1:B:103:ARG:HB2	1.34	0.92
1:A:22:PHE:HB3	1:A:23:PRO:C	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE21	1:C:107:GLN:HA	1.38	0.89
1:C:169:GLN:HG3	1:C:189:GLN:OE1	1.73	0.88
1:C:22:PHE:HB3	1:C:23:PRO:HD3	1.52	0.88
1:C:133:VAL:CG1	1:C:134:GLU:N	2.16	0.88
1:B:60:GLN:H	1:B:60:GLN:HE21	1.21	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
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:HE2	1:C:96:LYS:HA	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:HH11	1:B:103:ARG:CB	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:47:GLU:H	1:A:47:GLU:CD	1.89	0.75
1:A:59:LYS:HE3	1:A:59:LYS:HA	1.69	0.75
1:B:181:ASN:C	1:B:181:ASN:HD22	1.94	0.74
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:A:20:LEU:HD23	1:A:20:LEU:C	2.13	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:LEU:HD12	1:D:73:GLN:N	2.02	0.72
1:B:189:GLN:CD	1:B:189:GLN:H	1.98	0.71
1:C:79:MET:HE1	1:C:104:ILE:O	1.91	0.71
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:D:72:LEU:HD12	1:D:72:LEU:C	2.17	0.69
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:A:58:PRO:HG2	1:B:94:SER:HA	1.74	0.68
1:C:107:GLN:HA	1:C:107:GLN:NE2	2.09	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:A:122:ASN:ND2	1:A:123:MET:SD	2.68	0.67
1:C:64:LEU:O	1:C:64:LEU:HD12	1.93	0.67
1:C:162:ASP:HB3	1:C:165:ILE:HG22	1.76	0.67
1:C:47:GLU:OE1	1:C:48:THR:HG22	1.93	0.67
1:D:20:LEU:HD12	1:D:20:LEU:N	2.10	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:A:20:LEU:C	1:A:20:LEU:CD2	2.67	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:162:ASP:H	1:C:166:SER:HB2	1.60	0.66
1:C:172:THR:OG1	1:C:185:SER:HB3	1.95	0.66
1:C:135:ASP:O	1:C:137:ASP:N	2.28	0.66
1:A:47:GLU:CD	1:A:47:GLU:N	2.51	0.65
1:C:22:PHE:CB	1:C:23:PRO:HD2	2.23	0.65
1:C:131:CYS:O	1:C:142:PHE:HE2	1.80	0.64
1:D:105:LEU:HD23	1:D:139:ASN:ND2	2.12	0.64
1:B:154:GLN:HE22	1:B:156:ASN:H	1.45	0.64
1:D:14:GLU:O	1:D:77:LEU:HD13	1.97	0.64
1:D:17:THR:HG22	1:D:73:GLN:HG3	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:22:PHE:CB	1:B:23:PRO:HA	2.25	0.62
1:D:128:HIS:C	1:D:129:LEU:HD23	2.24	0.62
1:A:172:THR:OG1	1:A:185:SER:HB2	1.99	0.62
1:B:72:LEU:C	1:B:72:LEU:HD23	2.24	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:C:12:LEU:HD22	1:C:106:ARG:HA	1.82	0.61
1:D:86:ARG:HB2	1:D:97:LEU:HD21	1.82	0.61
1:C:59:LYS:O	1:C:60:GLN:CB	2.48	0.61
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:A:4:THR:HB	1:A:5:PRO:HD3	1.84	0.60
1:A:20:LEU:HD11	1:A:31:ILE:HD12	1.83	0.60
1:C:107:GLN:HB3	1:C:109:ARG:NH1	2.12	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:C:5:PRO:C	1:C:6:LEU:HD22	2.28	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:A:47:GLU:CD	1:A:48:THR:H	2.10	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:21:GLU:CG	1:A:22:PHE:H	2.16	0.58
1:A:47:GLU:N	1:A:47:GLU:OE2	2.36	0.58
1:D:128:HIS:O	1:D:129:LEU:HD23	2.02	0.58
1:D:64:LEU:HD12	1:D:64:LEU:C	2.23	0.58
1:B:15:SER:C	1:B:16:VAL:CG1	2.77	0.58
1:B:19:PRO:HA	1:B:71:SER:OG	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:GLU:OE1	1:B:189:GLN:HG2	2.03	0.58
1:B:120:PHE:CD1	1:B:120:PHE:C	2.82	0.57
1:D:168:GLU:CD	1:D:189:GLN:HE22	2.11	0.57
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:C:188:ALA:C	1:C:190:LYS:H	2.13	0.56
1:C:61:GLY:C	1:C:63:ARG:H	2.14	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:C:122:ASN:HD21	1:C:123:MET:HE3	1.71	0.55
1:B:108:LEU:HD13	1:B:177:ASN:ND2	2.22	0.55
1:B:189:GLN:OE1	1:B:189:GLN:N	2.32	0.55
1:A:133:VAL:HG13	1:A:134:GLU:N	2.21	0.55
1:C:140:VAL:HG12	1:C:141:SER:N	2.22	0.55
1:D:168:GLU:CG	1:D:189:GLN:HE22	2.19	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:D:105:LEU:HD23	1:D:139:ASN:HD22	1.72	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:B:92:LYS:HG3	1:B:93:THR:HG23	1.89	0.54
1:D:168:GLU:HG2	1:D:189:GLN:HE21	1.69	0.54
1:A:79:MET:C	1:A:81:ASP:H	2.15	0.54
1:C:63:ARG:HH12	1:C:78:LYS:HD3	1.72	0.54
1:A:116:HIS:O	1:A:117:SER:HB2	2.07	0.54
1:D:58:PRO:O	1:D:60:GLN:N	2.41	0.53
1:B:137:ASP:HB3	1:B:139:ASN:ND2	2.23	0.53
1:B:186:VAL:HB	1:B:191:LEU:CD1	2.38	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:C:177:ASN:OD1	1:C:177:ASN:C	2.51	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:D:79:MET:HE3	1:D:106:ARG:NH1	2.24	0.53
1:B:149:ASN:OD1	1:C:148:GLY:N	2.35	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:B:61:GLY:C	1:B:63:ARG:H	2.16	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:59:LYS:O	1:A:60:GLN:C	2.54	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:C:188:ALA:C	1:C:190:LYS:N	2.70	0.50
1:D:4:THR:CG2	1:D:5:PRO:HD2	2.42	0.50
1:D:58:PRO:O	1:D:59:LYS:C	2.55	0.50
1:A:157:LEU:HD11	1:A:159:VAL:HG13	1.94	0.50
1:C:15:SER:HB2	1:C:74:LEU:O	2.11	0.50
1:D:64:LEU:C	1:D:65:ASN:OD1	2.54	0.50
1:B:16:VAL:O	1:B:16:VAL:CG2	2.58	0.50
1:C:187:SER:HB3	1:C:190:LYS:HB2	1.94	0.50
1:C:191:LEU:C	1:C:193:GLU:N	2.69	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:40:LEU:HD23	1:B:57:ASN:HB3	1.95	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: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:C:81:ASP:HB2	1:C:104:ILE:HD11	1.95	0.49
1:D:122:ASN:ND2	1:D:122:ASN:H	2.09	0.49
1:D:157:LEU:CD2	1:D:159:VAL:HG13	2.42	0.49
1:C:123:MET:SD	1:C:124:THR:N	2.84	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:30:PHE:CD1	1:B:90:SER:HB2	2.48	0.48
1:D:115:ASN:ND2	1:D:117:SER:H	2.11	0.48
1:B:103:ARG:NH1	1:B:103:ARG:HB3	2.27	0.48
1:A:21:GLU:HG2	1:A:22:PHE:N	2.28	0.48
1:D:28:VAL:HG11	1:D:89:ILE:CG2	2.43	0.48
1:D:32:THR:HG23	1:D:88:GLN:HB3	1.96	0.48
1:B:171:TYR:HE2	1:B:188:ALA:HB2	1.78	0.48
1:C:153:SER:C	1:C:154:GLN:HG2	2.38	0.48
1:D:15:SER:HB3	1:D:75:SER:HA	1.96	0.48
1:B:105:LEU:HD13	1:B:178:ALA:HB3	1.96	0.47
1:C:91:THR:OG1	1:C:92:LYS:N	2.46	0.47
1:B:60:GLN:N	1:B:60:GLN:NE2	2.54	0.47
1:B:67:THR:OG1	1:B:71:SER:HB2	2.14	0.47
1:B:31:ILE:HG12	1:B:89:ILE:HG22	1.97	0.47
1:C:42:PHE:CE2	1:D:42:PHE:CD2	3.02	0.47
1:C:47:GLU:HA	1:C:48:THR:HA	1.47	0.47
1:A:133:VAL:CG1	1:A:134:GLU:N	2.76	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:A:68:GLN:HA	1:A:68:GLN:OE1	2.15	0.47
1:C:5:PRO:HA	1:C:99:SER:HB2	1.96	0.47
1:D:92:LYS:O	1:D:92:LYS:HG2	2.14	0.47
1:B:146:ALA:O	1:B:147:LEU:C	2.57	0.47
1:C:111:ILE:CG2	1:C:184:PHE:HB2	2.45	0.46
1:D:89:ILE:O	1:D:95:ALA:HA	2.15	0.46
1:A:86:ARG:HA	1:A:98:SER:O	2.15	0.46
1:C:137:ASP:O	1:C:140:VAL:HG23	2.14	0.46
1:B:61:GLY:C	1:B:63:ARG:N	2.73	0.46
1:A:115:ASN:CG	1:A:116:HIS:N	2.73	0.46
1:A:157:LEU:HD11	1:A:159:VAL:CG1	2.45	0.46
1:C:122:ASN:ND2	1:C:123:MET:HE3	2.30	0.46
1:D:173:CYS:O	1:D:183:SER:HA	2.16	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:CD1	1:A:151:LEU:N	2.78	0.46
1:B:4:THR:HB	1:B:5:PRO:O	2.16	0.45
1:C:64:LEU:HB3	1:C:74:LEU:HD22	1.97	0.45
1:C:127:LEU:HD22	1:C:192:CYS:SG	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE21	1:C:107:GLN:CA	2.17	0.45
1:D:189:GLN:HE21	1:D:189:GLN:HB2	1.62	0.45
1:C:116:HIS:O	1:C:117:SER:HB3	2.15	0.45
1:B:4:THR:OG1	1:B:5:PRO:CA	2.61	0.45
1:C:126:GLU:O	1:C:126:GLU:HG3	2.16	0.45
1:B:15:SER:CB	1:B:75:SER:HA	2.46	0.45
1:C:137:ASP:C	1:C:139:ASN:N	2.73	0.45
1:C:137:ASP:O	1:C:138:ASP:C	2.59	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: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:D:89:ILE:HB	1:D:96:LYS:HB3	1.99	0.45
1:B:181:ASN:C	1:B:181:ASN:ND2	2.66	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:B:15:SER:C	1:B:16:VAL:HG13	2.42	0.44
1:D:41:ALA:HA	1:D:56:THR:H	1.82	0.44
1:A:121:GLN:HA	1:A:122:ASN:HA	1.73	0.44
1:C:63:ARG:HH12	1:C:78:LYS:CD	2.31	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:OE1	1:D:68:GLN:HA	2.18	0.44
1:D:7:MET:SD	1:D:103:ARG:HG3	2.57	0.44
1:D:36:ASN:H	1:D:86:ARG:HH12	1.65	0.44
1:D:86:ARG:HB2	1:D:97:LEU:CD2	2.47	0.44
1:C:48:THR:C	1:C:50:SER:H	2.25	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:B:72:LEU:HD23	1:B:73:GLN:N	2.31	0.43
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:A:162:ASP:OD1	1:A:164:ARG:HG2	2.19	0.43
1:B:116:HIS:ND1	1:B:130:THR:CG2	2.82	0.43
1:B:154:GLN:HE21	1:B:156:ASN:H	1.60	0.43
1:C:108:LEU:HD22	1:C:108:LEU:N	2.33	0.43
1:D:57:ASN:HA	1:D:58:PRO:HD2	1.83	0.43
1:A:4:THR:HB	1:A:5:PRO:HD2	1.99	0.43
1:B:144:TRP:CE3	1:B:157:LEU:HD12	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:LEU:CD1	1:C:75:SER:N	2.76	0.43
1:D:31:ILE:HG22	1:D:89:ILE:HA	2.00	0.43
1:B:4:THR:HB	1:B:5:PRO:C	2.43	0.43
1:C:18:LEU:HD12	1:C:72:LEU:HD23	2.00	0.43
1:C:50:SER:HA	1:C:51:PRO:HA	1.79	0.43
1:D:23:PRO:CG	1:D:24:ALA:H	2.32	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:B:72:LEU:C	1:B:72:LEU:CD2	2.92	0.42
1:B:122:ASN:ND2	1:B:124:THR:HG23	2.34	0.42
1:C:12:LEU:CD2	1:C:106:ARG:HA	2.47	0.42
1:A:64:LEU:HD21	1:A:66:PHE:CZ	2.55	0.42
1:B:75:SER:O	1:B:76:ASN:C	2.62	0.42
1:C:20:LEU:C	1:C:20:LEU:HD12	2.43	0.42
1:A:16:VAL:HB	1:A:77:LEU:HD11	2.00	0.42
1:C:96:LYS:HA	1:C:96:LYS:CE	2.40	0.42
1:D:35:PHE:CD1	1:D:36:ASN:HB2	2.55	0.42
1:B:63:ARG:HH22	1:B:81:ASP:CG	2.28	0.42
1:B:157:LEU:HD22	1:B:159:VAL:HG22	2.00	0.42
1:D:20:LEU:N	1:D:20:LEU:CD1	2.81	0.42
1:D:115:ASN:HD21	1:D:117:SER:CB	2.33	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:HD12	1:D:53:ILE:O	2.19	0.42
1:C:39:SER:N	1:D:88:GLN:OE1	2.52	0.41
1:C:68:GLN:N	1:C:68:GLN:CD	2.78	0.41
1:C:108:LEU:N	1:C:108:LEU:CD2	2.83	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:C:81:ASP:HB2	1:C:104:ILE:CD1	2.50	0.41
1:C:97:LEU:HD11	1:D:38:THR:HG22	2.01	0.41
1:C:114:THR:O	1:C:129:LEU:HD23	2.19	0.41
1:D:122:ASN:H	1:D:122:ASN:HD22	1.68	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:B:7:MET:SD	1:B:7:MET:N	2.86	0.41
1:D:115:ASN:HD22	1:D:116:HIS:H	1.69	0.41
1:C:23:PRO:C	1:C:25:GLY:H	2.29	0.41
1:D:15:SER:HB2	1:D:74:LEU:O	2.20	0.41
1:D:50:SER:HA	1:D:51:PRO:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:VAL:HG23	1:D:184:PHE:CD1	2.56	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:89:ILE:H	1:B:89:ILE:HG12	1.63	0.41
1:B:177:ASN:O	1:B:178:ALA:C	2.63	0.41
1:C:150:THR:O	1:C:150:THR:HG23	2.20	0.41
1:C:18:LEU:HA	1:C:19:PRO:HD3	1.77	0.40
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:A:161:TRP:CD2	1:A:188:ALA:HB1	2.56	0.40
1:C:154:GLN:C	1:C:156:ASN:N	2.79	0.40
1:D:154:GLN:HB2	1:D:155:PRO:HD3	2.00	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:B:50:SER:HB2	1:B:51:PRO:CD	2.51	0.40
1:C:57:ASN:O	1:C:58:PRO:C	2.62	0.40
1:D:30:PHE:O	1:D:90:SER:HB3	2.22	0.40
1:D:113:VAL:CG2	1:D:184:PHE:CD1	3.05	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%)	4	22
1	B	189/193 (98%)	170 (90%)	17 (9%)	2 (1%)	11	43
1	C	182/193 (94%)	141 (78%)	28 (15%)	13 (7%)	1	4
1	D	190/193 (98%)	169 (89%)	17 (9%)	4 (2%)	5	27
All	All	745/772 (96%)	639 (86%)	82 (11%)	24 (3%)	3	18

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%)	153 (88%)	20 (12%)	5	23
1	B	176/178 (99%)	141 (80%)	35 (20%)	1	7
1	C	171/178 (96%)	153 (90%)	18 (10%)	6	27
1	D	177/178 (99%)	152 (86%)	25 (14%)	3	16
All	All	697/712 (98%)	599 (86%)	98 (14%)	3	16

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	8	VAL
1	A	12	LEU
1	A	20	LEU
1	A	26	GLU
1	A	31	ILE
1	A	37	GLU
1	A	47	GLU
1	A	59	LYS
1	A	79	MET
1	A	91	THR
1	A	105	LEU
1	A	107	GLN
1	A	127	LEU
1	A	130	THR
1	A	133	VAL
1	A	151	LEU
1	A	154	GLN
1	A	157	LEU
1	A	158	THR
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	47	GLU
1	B	55	VAL
1	B	60	GLN
1	B	82	THR
1	B	89	ILE
1	B	98	SER
1	B	103	ARG
1	B	107	GLN
1	B	108	LEU
1	B	109	ARG
1	B	119	LEU
1	B	130	THR
1	B	132	SER
1	B	133	VAL

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Mol	Chain	Res	Type
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	174	ILE
1	B	181	ASN
1	B	187	SER
1	B	189	GLN
1	B	190	LYS
1	C	6	LEU
1	C	20	LEU
1	C	28	VAL
1	C	31	ILE
1	C	56	THR
1	C	74	LEU
1	C	90	SER
1	C	107	GLN
1	C	111	ILE
1	C	123	MET
1	C	134	GLU
1	C	145	GLU
1	C	154	GLN
1	C	168	GLU
1	C	169	GLN
1	C	172	THR
1	C	186	VAL
1	C	189	GLN
1	D	12	LEU
1	D	20	LEU
1	D	30	PHE
1	D	32	THR
1	D	37	GLU
1	D	43	ILE
1	D	49	LYS
1	D	64	LEU
1	D	72	LEU
1	D	74	LEU
1	D	77	LEU

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Mol	Chain	Res	Type
1	D	96	LYS
1	D	97	LEU
1	D	99	SER
1	D	105	LEU
1	D	110	ASN
1	D	114	THR
1	D	125	CYS
1	D	126	GLU
1	D	135	ASP
1	D	157	LEU
1	D	179	VAL
1	D	185	SER
1	D	186	VAL
1	D	190	LYS

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

Mol	Chain	Res	Type
1	A	9	ASN
1	A	60	GLN
1	A	73	GLN
1	A	107	GLN
1	A	115	ASN
1	A	128	HIS
1	A	169	GLN
1	B	9	ASN
1	B	54	HIS
1	B	60	GLN
1	B	107	GLN
1	B	118	GLN
1	B	128	HIS
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	154	GLN
1	C	169	GLN

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Mol	Chain	Res	Type
1	D	110	ASN
1	D	115	ASN
1	D	116	HIS
1	D	122	ASN
1	D	149	ASN
1	D	156	ASN
1	D	169	GLN
1	D	189	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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.

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 ⓘ

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, 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	188/193 (97%)	0.47	4 (2%) 63 40	61, 84, 102, 108	0
1	B	191/193 (98%)	0.72	10 (5%) 33 17	61, 83, 101, 109	0
1	C	186/193 (96%)	0.73	15 (8%) 18 9	57, 82, 104, 121	0
1	D	192/193 (99%)	0.62	11 (5%) 29 15	61, 82, 100, 123	0
All	All	757/772 (98%)	0.63	40 (5%) 32 16	57, 83, 102, 123	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	117	SER	3.6
1	C	106	ARG	3.3
1	B	193	GLU	3.2
1	D	5	PRO	3.1
1	C	84	SER	3.0
1	C	181	ASN	3.0
1	C	105	LEU	3.0
1	C	182	LEU	2.9
1	D	9	ASN	2.9
1	A	115	ASN	2.8
1	B	106	ARG	2.8
1	C	171	TYR	2.8
1	B	132	SER	2.7
1	B	192	CYS	2.7
1	D	193	GLU	2.7
1	A	117	SER	2.7
1	C	110	ASN	2.6
1	C	111	ILE	2.6
1	A	110	ASN	2.6
1	A	22	PHE	2.5
1	C	183	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	135	ASP	2.4
1	B	4	THR	2.4
1	B	101	THR	2.4
1	C	144	TRP	2.4
1	C	192	CYS	2.4
1	D	23	PRO	2.4
1	C	5	PRO	2.3
1	D	46	HIS	2.3
1	B	107	GLN	2.3
1	D	104	ILE	2.2
1	C	12	LEU	2.2
1	B	111	ILE	2.2
1	D	22	PHE	2.1
1	B	3	LEU	2.1
1	B	109	ARG	2.1
1	D	110	ASN	2.1
1	C	107	GLN	2.1
1	D	101	THR	2.0
1	D	109	ARG	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 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
3	CL	D	201	1/1	0.91	0.12	107,107,107,107	0
2	CA	A	205	1/1	0.94	0.08	74,74,74,74	0
2	CA	D	204	1/1	0.99	0.08	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.