



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:32 AM UTC

PDB ID : 8XK8 / pdb_00008xk8
Title : N1D10 Fab bound to SFTSV glycoprotein-Gn
Authors : Zhao, H.; Deng, Z.
Deposited on : 2023-12-22
Resolution : 3.53 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

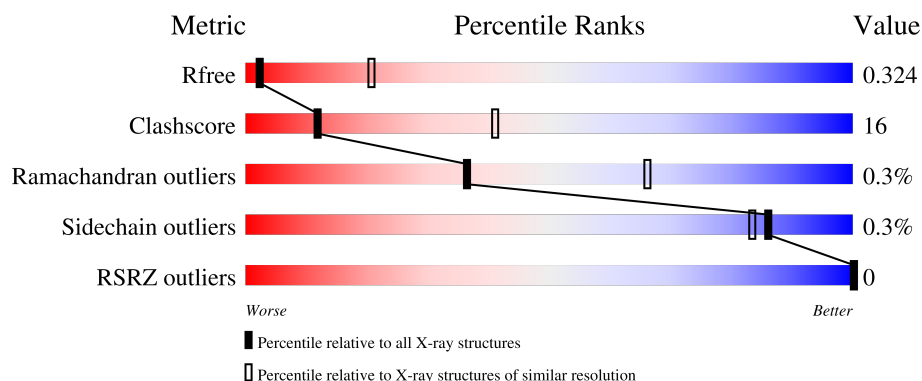
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.53 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	1008 (3.58-3.50)
Clashscore	190562	1062 (3.58-3.50)
Ramachandran outliers	187476	1033 (3.58-3.50)
Sidechain outliers	187428	1034 (3.58-3.50)
RSRZ outliers	180081	1007 (3.58-3.50)

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	357	
1	B	357	
2	C	247	
2	H	247	
3	D	238	

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Mol	Chain	Length	Quality of chain
3	L	238	58% 34% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11394 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 Envelopment polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2398	1503	415	454	26			
1	B	313	Total	C	N	O	S	0	0	0
			2402	1506	416	454	26			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	LEU	PHE	conflict	UNP R4V2Q5
A	18	GLY	SER	conflict	UNP R4V2Q5
A	21	THR	SER	conflict	UNP R4V2Q5
A	161	ARG	GLY	conflict	UNP R4V2Q5
A	340	SER	-	expression tag	UNP R4V2Q5
A	341	GLY	-	expression tag	UNP R4V2Q5
A	342	SER	-	expression tag	UNP R4V2Q5
A	343	THR	-	expression tag	UNP R4V2Q5
A	344	LEU	-	expression tag	UNP R4V2Q5
A	345	GLU	-	expression tag	UNP R4V2Q5
A	346	VAL	-	expression tag	UNP R4V2Q5
A	347	LEU	-	expression tag	UNP R4V2Q5
A	348	PHE	-	expression tag	UNP R4V2Q5
A	349	GLN	-	expression tag	UNP R4V2Q5
A	350	GLY	-	expression tag	UNP R4V2Q5
A	351	PRO	-	expression tag	UNP R4V2Q5
A	352	HIS	-	expression tag	UNP R4V2Q5
A	353	HIS	-	expression tag	UNP R4V2Q5
A	354	HIS	-	expression tag	UNP R4V2Q5
A	355	HIS	-	expression tag	UNP R4V2Q5
A	356	HIS	-	expression tag	UNP R4V2Q5
A	357	HIS	-	expression tag	UNP R4V2Q5
B	13	LEU	PHE	conflict	UNP R4V2Q5
B	18	GLY	SER	conflict	UNP R4V2Q5
B	21	THR	SER	conflict	UNP R4V2Q5

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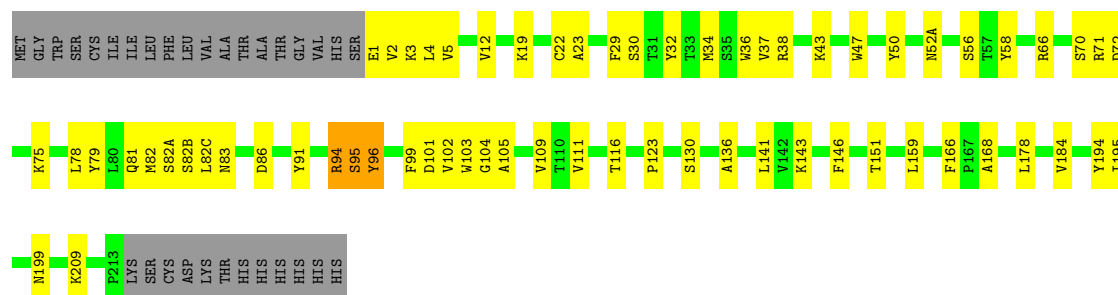
Chain	Residue	Modelled	Actual	Comment	Reference
B	161	ARG	GLY	conflict	UNP R4V2Q5
B	340	SER	-	expression tag	UNP R4V2Q5
B	341	GLY	-	expression tag	UNP R4V2Q5
B	342	SER	-	expression tag	UNP R4V2Q5
B	343	THR	-	expression tag	UNP R4V2Q5
B	344	LEU	-	expression tag	UNP R4V2Q5
B	345	GLU	-	expression tag	UNP R4V2Q5
B	346	VAL	-	expression tag	UNP R4V2Q5
B	347	LEU	-	expression tag	UNP R4V2Q5
B	348	PHE	-	expression tag	UNP R4V2Q5
B	349	GLN	-	expression tag	UNP R4V2Q5
B	350	GLY	-	expression tag	UNP R4V2Q5
B	351	PRO	-	expression tag	UNP R4V2Q5
B	352	HIS	-	expression tag	UNP R4V2Q5
B	353	HIS	-	expression tag	UNP R4V2Q5
B	354	HIS	-	expression tag	UNP R4V2Q5
B	355	HIS	-	expression tag	UNP R4V2Q5
B	356	HIS	-	expression tag	UNP R4V2Q5
B	357	HIS	-	expression tag	UNP R4V2Q5

- Molecule 2 is a protein called mAb N1D10 Fab heavy chain.

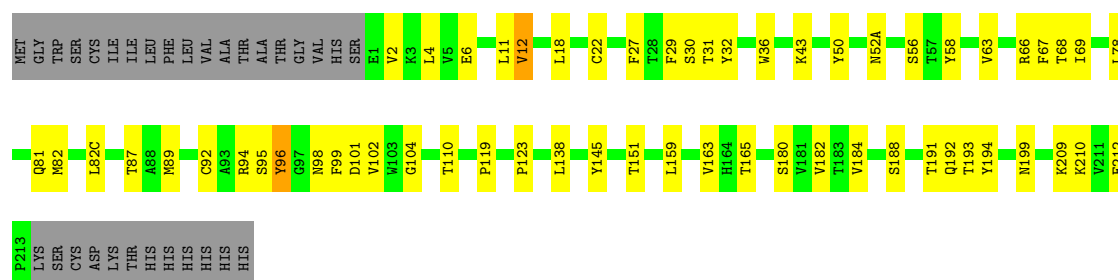
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	0	0
			1608	1014	265	322	7			
2	C	216	Total	C	N	O	S	0	0	0
			1608	1014	265	322	7			

- Molecule 3 is a protein called mAb N1D10 Fab light chain.

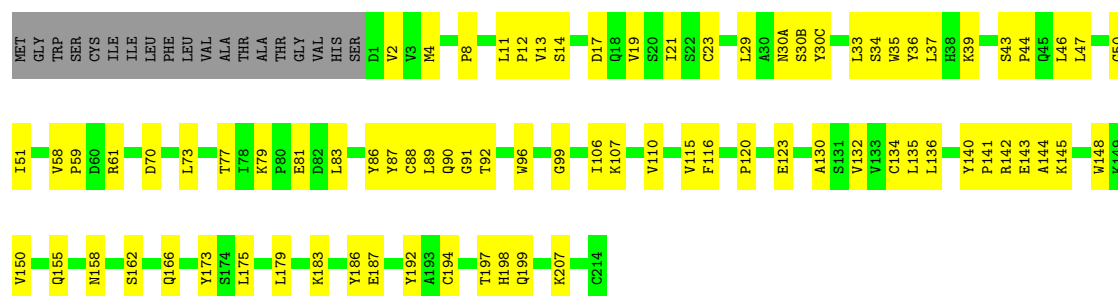
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	219	Total	C	N	O	S	0	0	0
			1689	1064	282	336	7			
3	D	219	Total	C	N	O	S	0	0	0
			1689	1064	282	336	7			



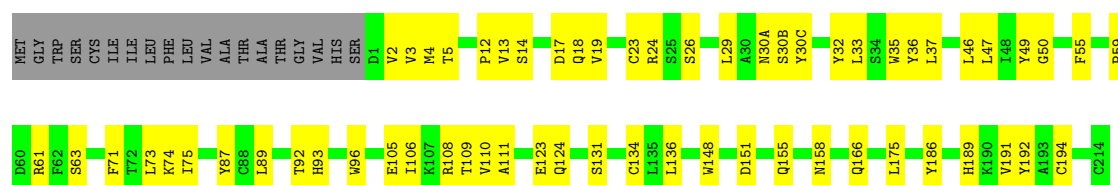
• Molecule 2: mAb N1D10 Fab heavy chain



• Molecule 3: mAb N1D10 Fab light chain



• Molecule 3: mAb N1D10 Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	84.12Å 111.91Å 87.86Å 90.00° 94.33° 90.00°	Depositor
Resolution (Å)	20.69 – 3.53 20.69 – 3.53	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.69-3.53) 87.7 (20.69-3.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 3.57Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.250 , 0.324 0.250 , 0.324	Depositor DCC
R_{free} test set	1089 reflections (5.42%)	wwPDB-VP
Wilson B-factor (Å ²)	-5.0	Xtriage
Anisotropy	-19.391	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.055 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11394	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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

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	0.19	0/2458	0.44	0/3317
1	B	0.19	0/2462	0.48	0/3321
2	C	0.19	0/1647	0.47	0/2245
2	H	0.20	0/1647	0.49	2/2245 (0.1%)
3	D	0.18	0/1729	0.42	0/2346
3	L	0.21	0/1729	0.44	0/2346
All	All	0.19	0/11672	0.46	2/15820 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
2	H	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	95	SER	CA-C-N	6.46	133.87	121.54
2	H	95	SER	C-N-CA	6.46	133.87	121.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	95	SER	Peptide
2	H	94	ARG	Peptide

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	2398	0	2296	118	0
1	B	2402	0	2307	74	0
2	C	1608	0	1571	42	0
2	H	1608	0	1571	54	0
3	D	1689	0	1645	41	1
3	L	1689	0	1645	65	1
All	All	11394	0	11035	354	1

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 16.

All (354) 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:83:TYR:OH	2:C:56:SER:OG	2.02	0.78
1:B:201:GLU:O	1:B:241:ARG:NH2	2.17	0.77
2:H:66:ARG:NH1	2:H:82(B):SER:O	2.19	0.75
3:D:108:ARG:HH21	3:D:111:ALA:HB2	1.52	0.73
3:D:13:VAL:HG12	3:D:19:VAL:HG11	1.71	0.72
2:C:22:CYS:HB3	2:C:78:LEU:HB3	1.72	0.71
2:H:82:MET:HE1	2:H:109:VAL:HG11	1.72	0.71
1:A:72:GLY:HA2	1:A:169:SER:HB3	1.72	0.71
3:L:106:ILE:O	3:L:166:GLN:NE2	2.24	0.70
1:A:83:TYR:OH	2:H:56:SER:OG	2.10	0.69
1:A:135:PHE:HD2	1:A:211:ILE:HB	1.57	0.69
1:A:201:GLU:O	1:A:241:ARG:NH2	2.26	0.69
2:H:22:CYS:HB3	2:H:78:LEU:HB3	1.78	0.66
1:B:207:LYS:HE2	1:B:219:GLU:OE1	1.95	0.66
2:H:50:TYR:HD2	2:H:58:TYR:HD2	1.44	0.65
1:A:64:HIS:HB3	1:A:111:LYS:HD3	1.78	0.65
1:B:221:LEU:HD13	3:D:32:TYR:HA	1.78	0.65
2:C:159:LEU:HD21	2:C:182:VAL:HG21	1.79	0.65
1:A:201:GLU:OE1	1:A:318:TYR:OH	2.07	0.65
3:L:136:LEU:HD22	3:L:175:LEU:HD22	1.78	0.65
3:L:47:LEU:HA	3:L:58:VAL:HG21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:LEU:HD21	1:B:129:PHE:HB2	1.80	0.64
1:A:248:VAL:O	1:A:312:GLY:HA3	1.98	0.64
1:B:72:GLY:HA2	1:B:169:SER:OG	1.98	0.64
1:A:25:ILE:HA	1:B:288:LYS:NZ	2.13	0.64
2:H:5:VAL:HG23	2:H:23:ALA:HB3	1.81	0.63
2:C:123:PRO:HD3	2:C:209:LYS:HE2	1.80	0.63
1:A:338:GLU:HG2	1:A:340:SER:H	1.64	0.62
3:L:83:LEU:HD11	3:L:106:ILE:HD11	1.82	0.61
2:H:50:TYR:CD2	2:H:58:TYR:HD2	2.19	0.61
1:A:117:MET:HA	3:L:30(C):TYR:CZ	2.36	0.61
1:A:244:LYS:HB2	1:A:317:SER:HB3	1.81	0.61
1:B:125:LYS:HD3	1:B:151:GLU:HB3	1.83	0.60
1:A:132:ARG:HH22	1:A:209:ASP:CG	2.10	0.60
3:L:12:PRO:HB3	3:L:140:TYR:OH	2.01	0.60
3:D:108:ARG:HG3	3:D:109:THR:H	1.67	0.60
3:D:136:LEU:HB2	3:D:175:LEU:HB3	1.83	0.59
3:L:144:ALA:HB2	3:L:198:HIS:HD2	1.68	0.59
1:A:119:VAL:HG22	1:A:132:ARG:HD2	1.84	0.59
1:A:283:ASP:HB3	1:B:284:MET:HE1	1.83	0.58
2:C:209:LYS:NZ	3:D:123:GLU:OE1	2.26	0.58
2:H:82:MET:HB3	2:H:82(C):LEU:HD21	1.85	0.58
1:A:230:MET:HG3	1:A:325:PRO:HB3	1.85	0.58
2:H:130:SER:HA	3:L:116:PHE:HD1	1.68	0.58
1:A:79:GLN:HB2	1:A:169:SER:OG	2.03	0.58
1:A:226:ASP:O	2:H:52(A):ASN:ND2	2.37	0.58
2:H:94:ARG:O	2:H:99:PHE:HA	2.04	0.58
1:A:227:VAL:HG21	1:A:239:ILE:HB	1.86	0.58
1:B:232:VAL:HG12	1:B:323:VAL:HG11	1.86	0.58
1:A:101:ALA:HB1	1:A:106:MET:HB2	1.86	0.57
2:C:11:LEU:HD23	2:C:18:LEU:HD12	1.85	0.57
1:A:184:THR:HG23	1:A:324:ARG:HD2	1.85	0.57
1:A:253:SER:O	1:A:275:LYS:NZ	2.32	0.57
2:H:209:LYS:NZ	3:L:123:GLU:OE1	2.23	0.57
1:B:229:TRP:HE1	1:B:331:SER:HB3	1.68	0.56
1:A:25:ILE:HA	1:B:288:LYS:HZ3	1.70	0.56
1:A:205:ILE:O	1:A:214:ASN:HB2	2.06	0.56
1:B:48:ILE:HD13	1:B:51:ILE:HD12	1.87	0.56
1:B:229:TRP:HE1	1:B:331:SER:CB	2.19	0.56
2:H:71:ARG:HB3	2:H:78:LEU:HD12	1.86	0.56
3:L:36:TYR:HE2	3:L:89:LEU:HB3	1.71	0.56
3:L:39:LYS:NZ	3:L:81:GLU:HA	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:HIS:NE2	1:B:100:ASP:OD1	2.39	0.55
1:A:285:GLN:OE1	1:A:307:LEU:HD22	2.06	0.55
1:B:205:ILE:O	1:B:214:ASN:HB2	2.06	0.55
3:L:21:ILE:HD12	3:L:73:LEU:HD23	1.89	0.55
1:A:168:PRO:HG2	1:A:171:ARG:HG2	1.89	0.55
2:H:38:ARG:NH1	2:H:86:ASP:OD1	2.31	0.55
3:L:33:LEU:HD23	3:L:34:SER:N	2.22	0.55
1:A:73:GLN:HG3	1:A:166:LEU:HB3	1.90	0.54
1:A:48:ILE:HD11	1:A:104:LEU:HD11	1.89	0.54
1:A:122:PRO:HB3	1:A:173:LEU:HD21	1.89	0.54
2:H:43:LYS:O	3:L:87:TYR:OH	2.26	0.54
2:C:11:LEU:HB3	2:C:18:LEU:HD13	1.90	0.54
1:B:154:GLU:HG2	3:D:30(B):SER:HB2	1.90	0.53
3:L:35:TRP:CD2	3:L:73:LEU:HB2	2.42	0.53
3:L:107:LYS:HA	3:L:140:TYR:OH	2.09	0.53
2:C:2:VAL:HG11	2:C:102:VAL:HG21	1.89	0.53
1:A:107:LEU:HD13	1:A:138:TYR:CD1	2.44	0.53
1:B:261:GLU:OE2	1:B:281:ARG:NH1	2.36	0.53
1:A:261:GLU:OE2	1:A:304:ARG:HD3	2.08	0.53
2:H:32:TYR:CD2	2:H:94:ARG:HD2	2.43	0.53
3:L:61:ARG:HD2	3:L:77:THR:O	2.09	0.52
2:C:210:LYS:HE2	2:C:212:GLU:HG3	1.91	0.52
2:C:119:PRO:HB3	2:C:145:TYR:HB3	1.91	0.52
3:L:14:SER:O	3:L:17:ASP:HB2	2.09	0.52
1:A:257:VAL:HG13	1:A:308:VAL:HG22	1.91	0.52
1:B:118:ILE:HG13	3:D:30(C):TYR:OH	2.10	0.52
1:B:183:MET:HE1	1:B:233:GLY:HA3	1.92	0.52
3:D:3:VAL:HB	3:D:26:SER:HB3	1.91	0.52
1:A:191:PHE:HA	1:A:194:LEU:HD12	1.90	0.52
2:H:103:TRP:CD2	3:L:44:PRO:HB2	2.45	0.52
2:C:2:VAL:HG12	2:C:102:VAL:HG11	1.92	0.52
2:H:12:VAL:HG11	2:H:82(C):LEU:HD13	1.91	0.51
3:L:4:MET:HE3	3:L:23:CYS:SG	2.50	0.51
3:D:59:PRO:HB2	3:D:61:ARG:HG2	1.92	0.51
1:B:226:ASP:HB3	1:B:330:PHE:CE1	2.45	0.51
3:L:88:CYS:O	3:L:99:GLY:N	2.43	0.51
2:H:2:VAL:HG11	2:H:102:VAL:HG21	1.91	0.51
1:A:248:VAL:HG22	1:A:313:GLU:HB2	1.93	0.51
1:A:314:VAL:O	1:A:325:PRO:HD2	2.11	0.51
1:A:314:VAL:HG21	1:A:328:TYR:CD2	2.46	0.51
3:D:155:GLN:OE1	3:D:158:ASN:ND2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:CYS:SG	1:B:53:ARG:NH1	2.83	0.51
1:B:218:GLY:O	1:B:339:VAL:N	2.44	0.51
1:B:260:LYS:HD3	1:B:302:LYS:O	2.11	0.51
1:A:62:ARG:HG2	1:A:67:PHE:O	2.12	0.50
1:A:229:TRP:HE1	1:A:331:SER:CB	2.24	0.50
2:C:188:SER:O	2:C:192:GLN:N	2.39	0.50
1:A:193:GLU:HB3	1:A:321:MET:HE1	1.94	0.50
2:H:116:THR:HA	2:H:146:PHE:O	2.11	0.50
1:B:256:PHE:O	1:B:275:LYS:NZ	2.33	0.50
3:L:4:MET:HE1	3:L:29:LEU:HD11	1.93	0.50
2:H:29:PHE:O	2:H:71:ARG:NH2	2.42	0.50
1:A:30:ILE:HG23	1:A:74:ARG:HE	1.76	0.50
1:B:241:ARG:HH12	2:C:31:THR:CG2	2.24	0.50
1:B:119:VAL:HB	1:B:332:ARG:HG2	1.94	0.50
1:B:147:LYS:HB3	1:B:156:CYS:HB3	1.93	0.50
3:L:37:LEU:HB2	3:L:47:LEU:HD11	1.94	0.49
3:L:186:TYR:HA	3:L:192:TYR:OH	2.12	0.49
1:B:184:THR:HG23	1:B:324:ARG:HD2	1.94	0.49
1:A:128:VAL:HG21	1:A:167:LEU:HD13	1.92	0.49
2:H:96:TYR:HA	3:L:96:TRP:CH2	2.47	0.49
3:D:23:CYS:HB2	3:D:35:TRP:CH2	2.48	0.49
1:B:220:SER:HB2	2:C:98:ASN:ND2	2.28	0.49
1:A:92:TRP:CD2	1:A:311:PRO:HD3	2.48	0.49
1:A:106:MET:O	1:A:326:LYS:HD2	2.13	0.49
2:C:165:THR:HA	2:C:180:SER:HA	1.94	0.49
1:A:205:ILE:HA	1:A:337:LEU:HD22	1.95	0.49
2:C:12:VAL:HG11	2:C:82(C):LEU:HD13	1.94	0.49
2:C:138:LEU:HD21	2:C:194:TYR:CD2	2.48	0.49
1:A:261:GLU:OE1	1:B:287:CYS:HB3	2.12	0.49
1:A:284:MET:HG2	1:A:288:LYS:HD3	1.95	0.49
1:B:228:ALA:O	1:B:240:MET:N	2.41	0.49
2:H:72:ASP:OD2	2:H:75:LYS:HE3	2.13	0.49
3:L:120:PRO:HG3	3:L:130:ALA:HB1	1.93	0.49
1:B:202:PHE:CE1	1:B:239:ILE:HG13	2.48	0.48
1:A:132:ARG:HG2	1:A:141:TRP:CZ3	2.48	0.48
1:B:37:ASP:HA	1:B:62:ARG:HH12	1.78	0.48
2:C:30:SER:O	2:C:52(A):ASN:HB2	2.13	0.48
2:C:43:LYS:O	3:D:87:TYR:OH	2.21	0.48
3:L:29:LEU:HD12	3:L:33:LEU:HD12	1.95	0.48
1:A:154:GLU:HG2	3:L:30(B):SER:HB2	1.96	0.48
1:A:336:THR:C	1:A:337:LEU:HD23	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:59:PRO:HB2	3:L:61:ARG:HG2	1.94	0.48
1:B:80:VAL:HG21	1:B:174:TRP:CE3	2.49	0.48
1:B:207:LYS:HG2	1:B:212:VAL:HA	1.95	0.48
1:A:130:PHE:HE2	1:A:149:ARG:HD2	1.79	0.48
1:B:269:SER:HA	1:B:272:LYS:HE2	1.95	0.48
1:B:83:TYR:CG	1:B:122:PRO:HG3	2.49	0.48
2:C:2:VAL:HG13	2:C:27:PHE:CD1	2.49	0.48
1:A:253:SER:HB3	1:A:275:LYS:HD2	1.95	0.47
2:C:50:TYR:CD2	2:C:58:TYR:HD2	2.32	0.47
1:A:127:LYS:HE2	1:A:173:LEU:HB2	1.97	0.47
3:D:106:ILE:O	3:D:166:GLN:NE2	2.39	0.47
3:L:50:GLY:O	3:L:51:ILE:HB	2.13	0.47
1:A:77:ARG:O	1:A:80:VAL:HG22	2.15	0.47
1:A:240:MET:HG2	1:A:318:TYR:CZ	2.49	0.47
1:A:255:ASP:O	1:A:308:VAL:HG23	2.14	0.47
2:H:30:SER:O	2:H:52(A):ASN:HB2	2.14	0.47
1:B:231:ASP:O	1:B:326:LYS:N	2.46	0.47
2:H:123:PRO:HD3	2:H:209:LYS:HE2	1.95	0.47
2:H:184:VAL:HG11	2:H:194:TYR:CE1	2.50	0.47
1:A:29:PRO:HD3	1:A:53:ARG:HA	1.97	0.47
1:A:260:LYS:HB2	1:A:260:LYS:HE2	1.67	0.47
1:B:183:MET:SD	1:B:233:GLY:HA3	2.55	0.47
2:C:63:VAL:HG12	2:C:66:ARG:NH2	2.30	0.47
1:A:229:TRP:CZ3	1:A:237:LYS:HE2	2.50	0.47
1:A:259:TYR:CE2	1:B:288:LYS:HE2	2.50	0.47
1:B:204:ASP:OD1	1:B:204:ASP:N	2.43	0.47
3:L:61:ARG:CZ	3:L:79:LYS:HG3	2.45	0.47
3:L:35:TRP:CZ3	3:L:88:CYS:HB3	2.50	0.47
3:L:37:LEU:HD13	3:L:86:TYR:CZ	2.50	0.47
3:L:110:VAL:HG21	3:L:199:GLN:NE2	2.30	0.47
1:B:31:HIS:HB2	1:B:166:LEU:HD22	1.97	0.46
2:C:184:VAL:HG11	2:C:194:TYR:CE1	2.50	0.46
1:A:135:PHE:CD2	1:A:211:ILE:HB	2.45	0.46
1:B:127:LYS:HE2	1:B:173:LEU:HB2	1.97	0.46
3:D:29:LEU:HD12	3:D:71:PHE:CE1	2.50	0.46
1:A:280:CYS:O	1:A:292:CYS:HA	2.14	0.46
1:B:241:ARG:HH12	2:C:31:THR:HG23	1.80	0.46
3:L:140:TYR:CG	3:L:141:PRO:HA	2.51	0.46
3:D:151:ASP:HA	3:D:191:VAL:HB	1.97	0.46
1:A:136:ASP:HB3	1:A:211:ILE:HG13	1.96	0.46
1:A:262:GLY:HA2	1:B:289:VAL:C	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:GLN:O	1:A:289:VAL:HG22	2.15	0.46
3:L:11:LEU:O	3:L:13:VAL:HG13	2.15	0.46
1:A:88:SER:HA	1:A:91:ARG:HH11	1.79	0.46
1:B:56:HIS:HB3	1:B:103:TRP:CG	2.50	0.46
1:B:120:PRO:CG	1:B:224:PRO:HG3	2.46	0.46
3:L:145:LYS:HB3	3:L:197:THR:HB	1.96	0.46
2:C:27:PHE:CE2	2:C:29:PHE:HA	2.51	0.46
3:D:18:GLN:HA	3:D:75:ILE:O	2.15	0.46
3:D:134:CYS:HB2	3:D:148:TRP:CH2	2.51	0.46
1:A:102:ASP:HA	1:A:107:LEU:O	2.16	0.46
2:C:36:TRP:HD1	2:C:69:ILE:HD12	1.81	0.46
1:A:77:ARG:C	1:A:79:GLN:H	2.23	0.46
1:B:122:PRO:HB3	1:B:173:LEU:HD21	1.98	0.46
3:L:142:ARG:HH11	3:L:143:GLU:HG3	1.81	0.46
1:A:92:TRP:CG	1:A:311:PRO:HD3	2.50	0.45
1:A:94:GLY:HA3	1:A:308:VAL:HG12	1.98	0.45
1:A:255:ASP:O	1:A:307:LEU:HD12	2.17	0.45
2:H:83:ASN:OD1	2:H:83:ASN:N	2.47	0.45
1:A:58:SER:O	1:A:62:ARG:HG3	2.16	0.45
2:C:151:THR:OG1	2:C:199:ASN:HB3	2.15	0.45
1:B:77:ARG:NE	1:B:100:ASP:OD2	2.47	0.45
2:H:52(A):ASN:OD1	2:H:52(A):ASN:N	2.44	0.45
3:L:91:GLY:HA2	3:L:96:TRP:CD1	2.51	0.45
3:D:37:LEU:HB2	3:D:47:LEU:HD11	1.97	0.45
1:A:223:GLN:NE2	2:H:95:SER:O	2.49	0.45
1:A:79:GLN:OE1	1:B:248:VAL:HG12	2.17	0.45
1:B:229:TRP:CE3	1:B:237:LYS:HD3	2.51	0.45
3:D:5:THR:O	3:D:23:CYS:HA	2.17	0.45
1:A:83:TYR:CG	1:A:122:PRO:HG3	2.52	0.45
1:A:183:MET:HE2	1:A:183:MET:HB3	1.92	0.45
1:A:283:ASP:CB	1:B:284:MET:HE1	2.47	0.45
3:L:132:VAL:HB	3:L:179:LEU:HB3	1.97	0.45
1:A:128:VAL:HG23	1:A:171:ARG:HB3	1.98	0.45
1:A:337:LEU:HD12	2:H:32:TYR:CE2	2.51	0.45
1:B:101:ALA:HB1	1:B:106:MET:HB2	1.99	0.45
2:H:168:ALA:HA	2:H:178:LEU:HB3	1.98	0.45
1:A:136:ASP:OD2	1:A:211:ILE:HD11	2.17	0.45
2:C:87:THR:HG23	2:C:110:THR:HA	1.97	0.45
3:D:186:TYR:HA	3:D:192:TYR:OH	2.16	0.45
1:A:132:ARG:NH2	1:A:209:ASP:OD2	2.50	0.45
1:B:339:VAL:HG21	3:D:49:TYR:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:105:ALA:HA	3:L:43:SER:OG	2.16	0.45
1:A:50:GLN:HB3	1:A:55:ILE:HB	1.99	0.44
3:L:89:LEU:HG	3:L:90:GLN:O	2.17	0.44
3:D:30(A):ASN:HB3	3:D:92:THR:HG23	1.99	0.44
3:D:148:TRP:HB2	3:D:155:GLN:HB2	1.99	0.44
1:A:186:ILE:HG21	1:A:323:VAL:HG12	1.99	0.44
2:H:52(A):ASN:HA	2:H:71:ARG:NH1	2.33	0.44
3:L:8:PRO:HG2	3:L:11:LEU:HB2	1.99	0.44
3:L:115:VAL:HA	3:L:135:LEU:O	2.17	0.44
3:D:124:GLN:HE22	3:D:131:SER:CB	2.30	0.44
1:A:38:ILE:HG23	1:A:62:ARG:NH1	2.33	0.44
1:A:201:GLU:HG2	1:A:241:ARG:NH2	2.32	0.44
3:D:4:MET:HE1	3:D:29:LEU:HD11	2.00	0.44
2:H:75:LYS:HE2	2:H:75:LYS:HB3	1.87	0.44
1:A:218:GLY:C	1:A:339:VAL:HG22	2.43	0.44
3:L:13:VAL:CG1	3:L:19:VAL:HG11	2.48	0.44
3:D:12:PRO:HA	3:D:105:GLU:O	2.18	0.44
2:C:99:PHE:N	3:D:36:TYR:OH	2.42	0.44
2:C:193:THR:HA	2:C:212:GLU:OE2	2.17	0.44
1:A:130:PHE:HA	1:A:173:LEU:O	2.18	0.43
1:A:118:ILE:N	3:L:30(C):TYR:OH	2.43	0.43
2:C:96:TYR:HA	3:D:96:TRP:CH2	2.53	0.43
3:D:189:HIS:HB2	3:D:192:TYR:OH	2.18	0.43
1:A:226:ASP:HB3	1:A:330:PHE:CE1	2.54	0.43
1:B:77:ARG:C	1:B:79:GLN:H	2.26	0.43
1:B:128:VAL:HG21	1:B:167:LEU:HD13	2.00	0.43
2:H:37:VAL:O	2:H:91:TYR:N	2.34	0.43
2:H:99:PHE:O	2:H:103:TRP:NE1	2.51	0.43
2:H:166:PHE:HB3	3:L:162:SER:OG	2.19	0.43
3:D:46:LEU:HD23	3:D:55:PHE:CD1	2.54	0.43
1:A:229:TRP:HE1	1:A:331:SER:HB2	1.82	0.43
1:A:275:LYS:HG2	1:A:286:PHE:HZ	1.82	0.43
2:H:4:LEU:HD12	2:H:102:VAL:HG12	2.00	0.43
2:H:141:LEU:HD21	2:H:143:LYS:HD2	2.01	0.43
3:L:110:VAL:HG22	3:L:141:PRO:HD3	2.00	0.43
2:C:89:MET:HE3	2:C:89:MET:HB2	1.93	0.43
1:A:195:LYS:HE3	1:A:236:HIS:CE1	2.54	0.43
1:A:275:LYS:HG2	1:A:286:PHE:CZ	2.53	0.43
2:H:70:SER:O	2:H:79:TYR:N	2.48	0.43
3:L:158:ASN:O	3:L:179:LEU:HD12	2.19	0.43
1:A:56:HIS:CD2	1:A:57:VAL:HG23	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LYS:HE3	1:A:170:ASP:O	2.19	0.43
1:B:120:PRO:HG2	1:B:224:PRO:HG3	2.00	0.43
2:H:47:TRP:HZ2	2:H:50:TYR:HB3	1.83	0.43
3:L:36:TYR:CE1	3:L:46:LEU:HD13	2.54	0.43
1:B:248:VAL:O	1:B:312:GLY:HA3	2.18	0.43
2:H:1:GLU:CG	2:H:3:LYS:HD2	2.48	0.43
2:H:159:LEU:HD12	2:H:159:LEU:HA	1.93	0.43
3:L:2:VAL:HB	3:L:90:GLN:NE2	2.34	0.43
1:B:219:GLU:O	1:B:219:GLU:HG2	2.18	0.42
1:B:261:GLU:H	1:B:261:GLU:CD	2.27	0.42
1:B:154:GLU:HG2	3:D:30(B):SER:CB	2.47	0.42
1:B:248:VAL:HG22	1:B:313:GLU:HB2	2.01	0.42
3:D:35:TRP:CD2	3:D:73:LEU:HB2	2.54	0.42
1:A:154:GLU:HG2	3:L:30(B):SER:CB	2.49	0.42
3:D:63:SER:OG	3:D:74:LYS:HB3	2.19	0.42
1:A:132:ARG:HH21	1:A:333:MET:HA	1.84	0.42
3:L:116:PHE:HB2	3:L:135:LEU:HB3	2.00	0.42
1:B:149:ARG:HA	1:B:155:LEU:O	2.20	0.42
2:C:94:ARG:NH2	2:C:101:ASP:OD2	2.29	0.42
3:L:148:TRP:HB2	3:L:155:GLN:HB2	2.02	0.42
1:A:96:LEU:HD22	1:A:100:ASP:HB3	2.00	0.42
1:A:117:MET:O	1:A:132:ARG:NH1	2.53	0.42
1:A:248:VAL:CG2	1:A:313:GLU:HB2	2.49	0.42
3:L:30(A):ASN:HB3	3:L:92:THR:HG22	2.01	0.42
1:B:229:TRP:CD1	1:B:333:MET:HE3	2.53	0.42
3:L:183:LYS:HE3	3:L:187:GLU:OE1	2.19	0.42
2:C:6:GLU:OE2	2:C:104:GLY:HA3	2.19	0.42
3:D:4:MET:HE3	3:D:23:CYS:SG	2.58	0.42
3:D:14:SER:O	3:D:17:ASP:HB2	2.20	0.42
3:D:136:LEU:HD13	3:D:175:LEU:HD22	2.02	0.42
1:A:51:ILE:HA	1:A:56:HIS:ND1	2.35	0.42
2:H:66:ARG:O	2:H:82(A):SER:OG	2.23	0.42
1:A:89:TYR:CD2	1:A:179:ALA:HB2	2.55	0.42
1:A:102:ASP:HB2	1:A:109:VAL:HG23	2.02	0.42
1:A:195:LYS:HE3	1:A:236:HIS:NE2	2.35	0.42
1:B:226:ASP:O	2:C:52(A):ASN:ND2	2.53	0.42
1:B:256:PHE:HB2	1:B:275:LYS:HE2	2.01	0.42
2:H:101:ASP:OD1	2:H:101:ASP:N	2.43	0.42
1:A:221:LEU:HD11	3:L:50:GLY:CA	2.49	0.41
1:A:224:PRO:HD3	2:H:96:TYR:CE2	2.55	0.41
1:A:307:LEU:HD12	1:A:307:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:VAL:HG11	1:A:328:TYR:HB3	2.02	0.41
3:D:151:ASP:N	3:D:191:VAL:O	2.29	0.41
3:D:36:TYR:HE1	3:D:89:LEU:HB3	1.85	0.41
1:A:199:GLN:HG2	1:A:213:PHE:O	2.20	0.41
1:B:130:PHE:HE1	1:B:149:ARG:HD2	1.85	0.41
2:H:4:LEU:O	2:H:104:GLY:HA2	2.19	0.41
3:L:158:ASN:HB3	3:L:179:LEU:HD12	2.03	0.41
3:L:173:TYR:CD1	3:L:173:TYR:N	2.88	0.41
1:A:98:PRO:HA	1:A:107:LEU:HD21	2.02	0.41
1:A:135:PHE:CZ	1:A:213:PHE:HD2	2.39	0.41
1:B:102:ASP:HA	1:B:107:LEU:O	2.20	0.41
2:H:29:PHE:HE1	2:H:34:MET:HE2	1.85	0.41
2:H:36:TRP:HE1	2:H:78:LEU:HG	1.85	0.41
2:H:130:SER:O	2:H:136:ALA:HA	2.21	0.41
1:A:189:GLU:O	1:A:193:GLU:HB2	2.19	0.41
1:A:225:PHE:CZ	1:A:227:VAL:HB	2.55	0.41
1:A:229:TRP:HE1	1:A:331:SER:HB3	1.86	0.41
2:H:195:ILE:HA	2:H:209:LYS:O	2.21	0.41
1:A:220:SER:O	1:A:336:THR:HB	2.20	0.41
1:B:54:LEU:HD23	1:B:56:HIS:HE1	1.85	0.41
3:L:140:TYR:CD2	3:L:141:PRO:HA	2.55	0.41
1:A:73:GLN:C	1:A:75:GLY:H	2.28	0.41
3:L:140:TYR:CD2	3:L:173:TYR:HE1	2.39	0.41
3:L:207:LYS:HA	3:L:207:LYS:HD2	1.78	0.41
2:C:4:LEU:HB3	2:C:92:CYS:SG	2.61	0.41
2:C:163:VAL:HG22	2:C:182:VAL:HB	2.03	0.41
2:C:188:SER:HA	2:C:191:THR:OG1	2.20	0.41
3:D:33:LEU:O	3:D:50:GLY:N	2.53	0.41
1:A:110:LYS:O	1:A:139:VAL:HA	2.21	0.40
1:A:244:LYS:HD2	1:A:244:LYS:N	2.36	0.40
1:B:73:GLN:C	1:B:75:GLY:H	2.28	0.40
2:H:12:VAL:CG1	2:H:111:VAL:HG22	2.52	0.40
3:L:8:PRO:HG3	3:L:11:LEU:HD13	2.02	0.40
3:L:150:VAL:HG22	3:L:192:TYR:CD2	2.56	0.40
3:D:2:VAL:HG21	3:D:93:HIS:HB2	2.03	0.40
2:H:151:THR:OG1	2:H:199:ASN:HB3	2.21	0.40
1:A:254:LYS:HA	1:A:254:LYS:HD3	1.67	0.40
1:B:337:LEU:HD13	2:C:32:TYR:CE2	2.56	0.40
3:L:23:CYS:HB2	3:L:35:TRP:CH2	2.57	0.40
1:A:249:GLN:NE2	1:A:307:LEU:HD21	2.35	0.40
2:H:19:LYS:HG3	2:H:81:GLN:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:67:PHE:CE2	2:C:82:MET:HG2	2.57	0.40
2:C:68:THR:HB	2:C:81:GLN:HB3	2.03	0.40
1:B:205:ILE:HD11	1:B:225:PHE:CZ	2.56	0.40
1:B:252:SER:N	1:B:255:ASP:OD2	2.52	0.40
2:C:2:VAL:HG13	2:C:27:PHE:HD1	1.87	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:70:ASP:O	3:D:24:ARG:NH2[1_455]	2.15	0.05

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	309/357 (87%)	286 (93%)	23 (7%)	0	100	100
1	B	309/357 (87%)	285 (92%)	24 (8%)	0	100	100
2	C	214/247 (87%)	202 (94%)	10 (5%)	2 (1%)	14	47
2	H	214/247 (87%)	205 (96%)	8 (4%)	1 (0%)	24	58
3	D	217/238 (91%)	209 (96%)	7 (3%)	1 (0%)	24	58
3	L	217/238 (91%)	208 (96%)	9 (4%)	0	100	100
All	All	1480/1684 (88%)	1395 (94%)	81 (6%)	4 (0%)	36	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	96	TYR
2	C	96	TYR
2	C	12	VAL

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Mol	Chain	Res	Type
3	D	110	VAL

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	267/309 (86%)	266 (100%)	1 (0%)	84	81
1	B	268/309 (87%)	268 (100%)	0	100	100
2	C	182/209 (87%)	182 (100%)	0	100	100
2	H	182/209 (87%)	182 (100%)	0	100	100
3	D	194/209 (93%)	193 (100%)	1 (0%)	81	81
3	L	194/209 (93%)	192 (99%)	2 (1%)	68	75
All	All	1287/1454 (88%)	1283 (100%)	4 (0%)	86	83

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	292	CYS
3	L	134	CYS
3	L	194	CYS
3	D	194	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	66	GLN
1	A	234	HIS
1	B	64	HIS
1	B	68	GLN
2	H	39	GLN
2	H	204	ASN
3	L	18	GLN

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Mol	Chain	Res	Type
3	L	38	HIS
3	L	90	GLN
3	L	199	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](#)

There are no ligands in this entry.

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	313/357 (87%)	-1.28	0 100 100	9, 31, 69, 85	0
1	B	313/357 (87%)	-1.28	0 100 100	15, 35, 93, 135	0
2	C	216/247 (87%)	-1.25	0 100 100	12, 39, 72, 84	0
2	H	216/247 (87%)	-1.35	0 100 100	9, 26, 53, 88	0
3	D	219/238 (92%)	-1.33	0 100 100	12, 31, 64, 90	0
3	L	219/238 (92%)	-1.38	0 100 100	9, 28, 50, 67	0
All	All	1496/1684 (88%)	-1.31	0 100 100	9, 31, 69, 135	0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.