



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 30, 2026 – 04:04 PM EDT

PDB ID : 12NP / pdb\_000012np  
Title : Crystal structure of the CD7 ectodomain bound to K12  
Authors : Mcshan, A.C.; Miles, U.Z.  
Deposited on : 2026-04-13  
Resolution : 2.40 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](mailto: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>.

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

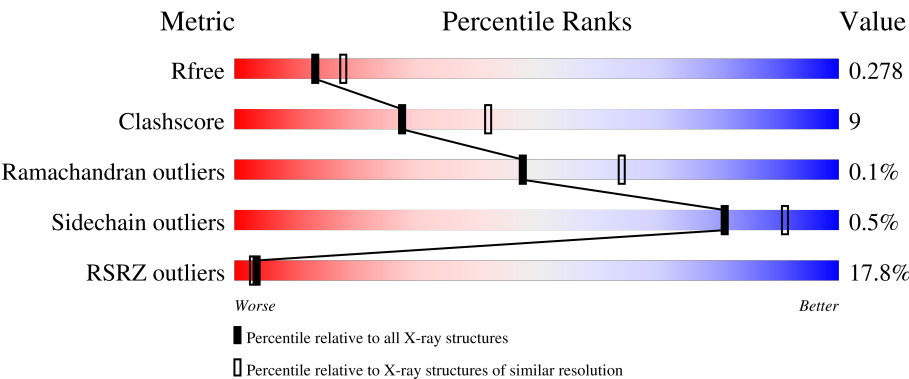
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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 <sub>free</sub>	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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  $\geq 3$ , 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	109	<div><div>17%</div><div>89%</div><div>8%</div><div>.</div></div>
1	B	109	<div><div>10%</div><div>82%</div><div>16%</div><div>.</div></div>
1	F	109	<div><div>18%</div><div>86%</div><div>11%</div><div>.</div></div>
1	H	109	<div><div>14%</div><div>84%</div><div>11%</div><div>5%</div></div>
2	C	120	<div><div>22%</div><div>77%</div><div>18%</div><div>..</div></div>

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Mol	Chain	Length	Quality of chain
2	D	120	<div><div>22%</div><div><div></div><div></div><div></div></div><div>74%</div><div>22%</div><div><div></div><div></div></div></div>
2	E	120	<div><div>18%</div><div><div></div><div></div><div></div></div><div>76%</div><div>21%</div><div><div></div><div></div></div></div>
2	G	120	<div><div>18%</div><div><div></div><div></div><div></div></div><div>77%</div><div>20%</div><div><div></div><div></div></div></div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7077 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 Secreted and transmembrane protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	106	Total	C	N	O	S	0	0	0
			819	509	152	154	4			
1	A	106	Total	C	N	O	S	0	0	0
			824	512	153	155	4			
1	F	106	Total	C	N	O	S	0	0	0
			819	509	152	154	4			
1	H	104	Total	C	N	O	S	0	0	0
			802	500	149	149	4			

- Molecule 2 is a protein called T-cell antigen CD7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	116	Total	C	N	O	S	0	0	0
			894	549	160	180	5			
2	D	117	Total	C	N	O	S	0	0	0
			903	554	162	182	5			
2	G	117	Total	C	N	O	S	0	0	0
			903	554	162	182	5			
2	E	117	Total	C	N	O	S	0	0	0
			903	554	162	182	5			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	30	Total	O	0	0
			30	30		
3	A	27	Total	O	0	0
			27	27		
3	C	28	Total	O	0	0
			28	28		
3	D	27	Total	O	0	0
			27	27		

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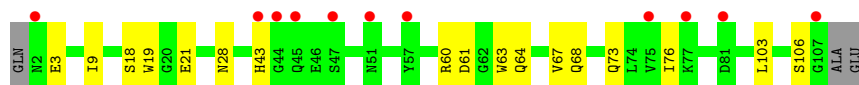
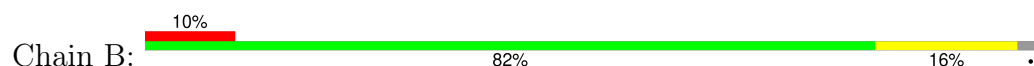
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	25	Total 25	O 25	0	0
3	G	25	Total 25	O 25	0	0
3	H	26	Total 26	O 26	0	0
3	E	22	Total 22	O 22	0	0

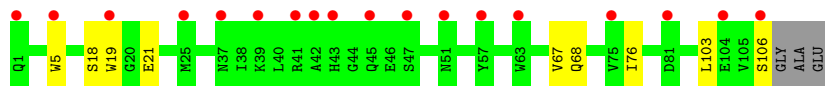
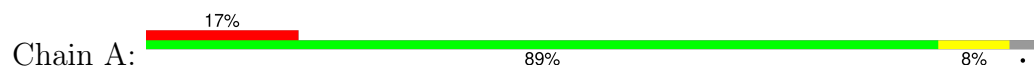
### 3 Residue-property plots [i](#)

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.

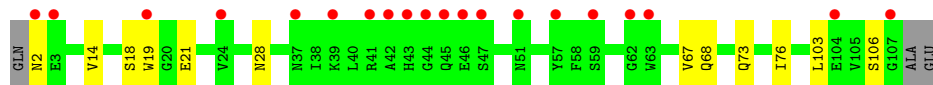
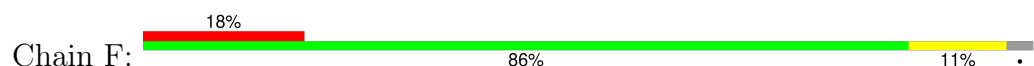
- Molecule 1: Secreted and transmembrane protein 1



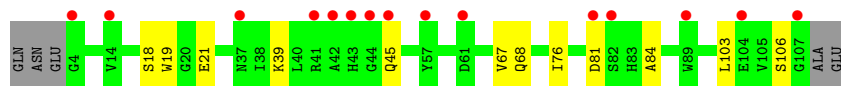
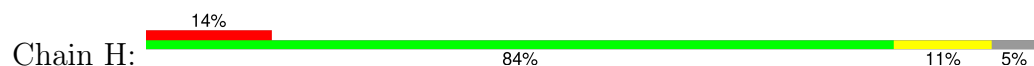
- Molecule 1: Secreted and transmembrane protein 1



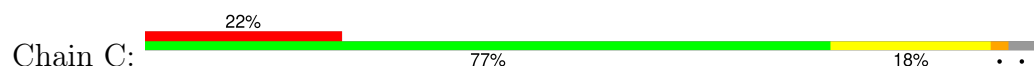
- Molecule 1: Secreted and transmembrane protein 1

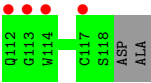


- Molecule 1: Secreted and transmembrane protein 1

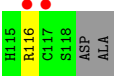
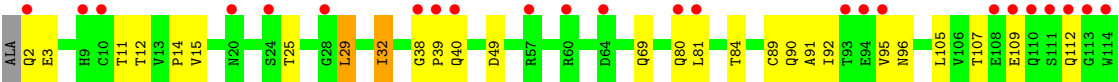


- Molecule 2: T-cell antigen CD7

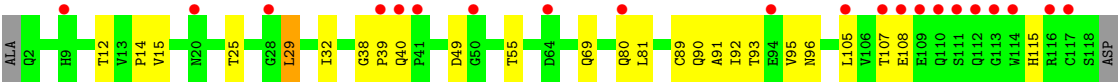
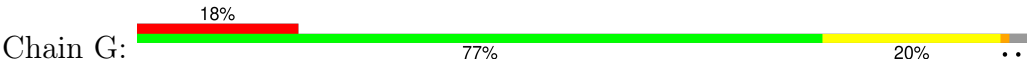




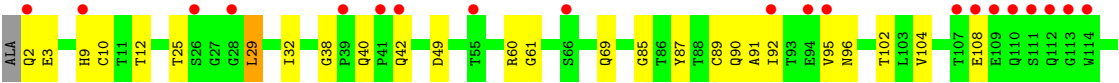
• Molecule 2: T-cell antigen CD7



• Molecule 2: T-cell antigen CD7



• Molecule 2: T-cell antigen CD7



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.68Å 121.95Å 88.87Å 90.00° 102.99° 90.00°	Depositor
Resolution (Å)	44.99 – 2.40 44.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.99-2.40) 99.7 (44.99-2.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 2.39Å)	Xtriage
Refinement program	PHENIX 2.0_5885	Depositor
R, $R_{free}$	0.241 , 0.278 0.241 , 0.278	Depositor DCC
$R_{free}$ test set	1955 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.3	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 59.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7077	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.84% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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	0.39	0/843	0.57	0/1144
1	B	0.38	0/838	0.58	0/1137
1	F	0.38	0/838	0.57	0/1137
1	H	0.38	0/821	0.58	0/1114
2	C	0.39	0/910	0.74	5/1239 (0.4%)
2	D	0.41	0/919	0.71	1/1251 (0.1%)
2	E	0.40	0/919	0.68	1/1251 (0.1%)
2	G	0.39	0/919	0.64	1/1251 (0.1%)
All	All	0.39	0/7007	0.64	8/9524 (0.1%)

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

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	C	40	GLN	CA-C-N	5.51	125.83	119.93
2	C	40	GLN	C-N-CA	5.51	125.83	119.93
2	C	107	THR	CA-C-N	5.50	130.31	122.72
2	C	107	THR	C-N-CA	5.50	130.31	122.72
2	E	29	LEU	CA-CB-CG	-5.32	97.67	116.30
2	C	29	LEU	CA-CB-CG	-5.32	97.68	116.30
2	D	29	LEU	CA-CB-CG	-5.31	97.71	116.30
2	G	29	LEU	CA-CB-CG	-5.31	97.72	116.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	107	THR	Mainchain

## 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	824	0	781	6	0
1	B	819	0	773	14	0
1	F	819	0	773	8	0
1	H	802	0	761	10	0
2	C	894	0	858	21	0
2	D	903	0	866	24	0
2	E	903	0	866	19	0
2	G	903	0	866	26	0
3	A	27	0	0	0	0
3	B	30	0	0	7	0
3	C	28	0	0	4	0
3	D	27	0	0	7	0
3	E	22	0	0	4	0
3	F	25	0	0	1	0
3	G	25	0	0	9	0
3	H	26	0	0	6	0
All	All	7077	0	6544	121	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 9.

All (121) 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)
2:D:29:LEU:HD11	2:D:91:ALA:HB1	1.61	0.82
2:E:29:LEU:HD11	2:E:91:ALA:HB1	1.61	0.82
2:C:29:LEU:HD11	2:C:91:ALA:HB1	1.61	0.82
2:G:14:PRO:HA	3:G:201:HOH:O	1.79	0.82
2:G:29:LEU:HD11	2:G:91:ALA:HB1	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ARG:HB3	3:B:201:HOH:O	1.78	0.81
2:G:80:GLN:NE2	2:G:81:LEU:H	1.81	0.78
2:G:12:THR:HG22	2:G:105:LEU:HD12	1.67	0.75
1:H:45:GLN:HG2	3:H:216:HOH:O	1.88	0.73
2:C:108:GLU:HG2	2:C:109:GLU:OE1	1.88	0.73
2:E:87:TYR:HD1	3:E:201:HOH:O	1.72	0.71
1:H:103:LEU:HB3	3:H:201:HOH:O	1.88	0.70
3:C:221:HOH:O	2:D:39:PRO:HD3	1.92	0.69
2:D:107:THR:C	3:D:203:HOH:O	2.39	0.65
2:G:39:PRO:HD2	3:G:213:HOH:O	1.95	0.64
2:G:107:THR:C	3:G:201:HOH:O	2.40	0.64
2:C:66:SER:HB2	3:C:212:HOH:O	1.98	0.63
2:D:112:GLN:O	2:D:116:ARG:HG2	2.00	0.62
2:D:14:PRO:HA	3:D:203:HOH:O	1.99	0.60
1:A:18:SER:HB2	1:A:21:GLU:HG3	1.84	0.60
1:F:18:SER:HB2	1:F:21:GLU:HG3	1.84	0.60
2:G:38:GLY:HA3	3:G:213:HOH:O	2.01	0.60
2:G:80:GLN:CD	2:G:81:LEU:H	2.09	0.60
1:B:61:ASP:N	3:B:201:HOH:O	2.34	0.60
2:E:104:VAL:HG23	3:E:201:HOH:O	2.01	0.59
1:B:43:HIS:HB2	3:B:219:HOH:O	2.03	0.59
1:A:5:TRP:CZ2	2:C:43:ASP:HB3	2.38	0.58
2:C:94:GLU:HG2	2:C:95:VAL:HG23	1.84	0.58
2:G:25:THR:HG21	2:G:29:LEU:HD13	1.86	0.58
1:H:18:SER:HB2	1:H:21:GLU:HG3	1.84	0.58
2:D:25:THR:HG21	2:D:29:LEU:HD13	1.86	0.58
1:B:18:SER:HB2	1:B:21:GLU:HG3	1.84	0.58
2:E:40:GLN:O	2:E:42:GLN:HG3	2.03	0.57
2:E:25:THR:HG21	2:E:29:LEU:HD13	1.86	0.57
2:C:25:THR:HG21	2:C:29:LEU:HD13	1.86	0.57
1:B:9:ILE:HG13	3:B:204:HOH:O	2.05	0.56
2:E:38:GLY:C	2:E:40:GLN:H	2.14	0.53
2:E:85:GLY:O	3:E:201:HOH:O	2.18	0.53
2:D:109:GLU:HA	3:D:212:HOH:O	2.09	0.53
2:D:38:GLY:C	2:D:40:GLN:H	2.16	0.52
2:E:9:HIS:ND1	2:E:10:CYS:HB3	2.25	0.52
2:D:11:THR:C	3:D:201:HOH:O	2.53	0.51
2:G:15:VAL:N	3:G:201:HOH:O	2.34	0.51
2:G:93:THR:HG21	3:G:206:HOH:O	2.10	0.51
2:G:40:GLN:HG2	2:G:40:GLN:O	2.12	0.50
2:E:60:ARG:HD3	2:E:61:GLY:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:39:PRO:HG2	3:C:211:HOH:O	2.11	0.49
2:D:105:LEU:HB2	3:D:201:HOH:O	2.11	0.49
1:H:76:ILE:HD12	1:H:103:LEU:HD22	1.95	0.49
1:F:2:ASN:HD22	1:F:2:ASN:N	2.10	0.49
1:B:76:ILE:HD12	1:B:103:LEU:HD22	1.95	0.49
2:D:32:ILE:HD11	2:D:89:CYS:HB3	1.95	0.48
1:F:76:ILE:HD12	1:F:103:LEU:HD22	1.95	0.48
1:A:76:ILE:HD12	1:A:103:LEU:HD22	1.95	0.48
2:C:5:GLN:NE2	3:C:201:HOH:O	2.44	0.47
2:D:15:VAL:N	3:D:203:HOH:O	2.36	0.47
2:D:95:VAL:HG12	2:D:96:ASN:N	2.29	0.47
2:G:95:VAL:HG12	2:G:96:ASN:N	2.29	0.47
2:D:80:GLN:CD	2:D:81:LEU:H	2.22	0.47
1:H:84:ALA:HA	3:H:201:HOH:O	2.14	0.47
2:G:32:ILE:HD11	2:G:89:CYS:HB3	1.97	0.47
2:E:95:VAL:HG12	2:E:96:ASN:N	2.29	0.47
1:B:28:ASN:HB2	1:F:73:GLN:OE1	2.14	0.47
2:C:95:VAL:HG12	2:C:96:ASN:N	2.29	0.47
2:G:108:GLU:HA	3:G:201:HOH:O	2.15	0.46
2:C:94:GLU:H	2:C:94:GLU:CD	2.22	0.46
1:A:67:VAL:C	1:A:68:GLN:HG2	2.41	0.46
2:D:90:GLN:HE21	2:D:92:ILE:CD1	2.29	0.46
2:C:32:ILE:HD11	2:C:89:CYS:HB3	1.97	0.46
1:H:67:VAL:C	1:H:68:GLN:HG2	2.41	0.46
2:E:90:GLN:HE21	2:E:92:ILE:CD1	2.29	0.46
1:B:3:GLU:HG2	2:G:55:THR:O	2.16	0.46
2:G:80:GLN:CD	2:G:81:LEU:N	2.73	0.46
1:B:67:VAL:C	1:B:68:GLN:HG2	2.41	0.45
1:H:19:TRP:HD1	3:H:208:HOH:O	1.99	0.45
2:C:90:GLN:HE21	2:C:92:ILE:CD1	2.29	0.45
2:D:49:ASP:OD1	2:D:69:GLN:HG2	2.17	0.45
2:C:49:ASP:OD1	2:C:69:GLN:HG2	2.17	0.45
1:F:67:VAL:C	1:F:68:GLN:HG2	2.41	0.45
2:E:32:ILE:HD11	2:E:89:CYS:HB3	1.97	0.45
2:E:60:ARG:HD3	2:E:60:ARG:C	2.42	0.45
2:G:90:GLN:HE21	2:G:92:ILE:CD1	2.29	0.45
2:D:80:GLN:NE2	2:D:81:LEU:H	2.15	0.44
2:C:95:VAL:HG12	2:C:96:ASN:H	1.83	0.44
2:G:49:ASP:OD1	2:G:69:GLN:HG2	2.17	0.44
2:E:49:ASP:OD1	2:E:69:GLN:HG2	2.17	0.44
1:B:64:GLN:NE2	3:B:205:HOH:O	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:TRP:HE3	3:B:201:HOH:O	1.99	0.44
2:D:95:VAL:HG12	2:D:96:ASN:H	1.83	0.44
1:F:14:VAL:CG1	3:F:201:HOH:O	2.65	0.44
2:C:84:THR:O	2:D:38:GLY:HA2	2.17	0.44
2:E:95:VAL:HG12	2:E:96:ASN:H	1.83	0.44
2:G:95:VAL:HG12	2:G:96:ASN:H	1.83	0.44
1:B:63:TRP:HB2	3:B:201:HOH:O	2.18	0.43
1:H:19:TRP:HB2	1:H:106:SER:O	2.18	0.43
1:B:19:TRP:HB2	1:B:106:SER:O	2.18	0.43
1:A:19:TRP:HB2	1:A:106:SER:O	2.18	0.43
1:F:19:TRP:HB2	1:F:106:SER:O	2.18	0.43
1:H:39:LYS:NZ	3:H:204:HOH:O	2.51	0.43
2:G:93:THR:CG2	3:G:206:HOH:O	2.67	0.43
2:G:39:PRO:HG2	2:G:40:GLN:OE1	2.18	0.43
2:D:29:LEU:HA	2:D:29:LEU:HD12	1.32	0.43
2:C:29:LEU:HD12	2:C:29:LEU:HA	1.32	0.43
2:G:29:LEU:HA	2:G:29:LEU:HD12	1.32	0.43
2:G:108:GLU:N	3:G:201:HOH:O	2.50	0.42
2:C:38:GLY:HA2	2:D:84:THR:O	2.18	0.42
2:E:90:GLN:HE21	2:E:92:ILE:HD11	1.85	0.42
2:C:40:GLN:HA	2:C:41:PRO:HD2	1.84	0.42
2:D:90:GLN:HE21	2:D:92:ILE:HD11	1.85	0.42
2:D:2:GLN:C	2:D:3:GLU:HG2	2.44	0.42
2:C:90:GLN:HE21	2:C:92:ILE:HD11	1.85	0.42
1:B:73:GLN:OE1	1:F:28:ASN:HB2	2.19	0.42
2:E:29:LEU:HD12	2:E:29:LEU:HA	1.32	0.42
2:G:90:GLN:HE21	2:G:92:ILE:HD11	1.85	0.42
2:C:29:LEU:CD1	2:C:91:ALA:HB1	2.43	0.41
2:E:2:GLN:C	2:E:3:GLU:HG2	2.45	0.41
2:G:12:THR:HG21	2:G:115:HIS:O	2.21	0.41
2:E:102:THR:O	3:E:201:HOH:O	2.22	0.41
1:H:81:ASP:CG	3:H:208:HOH:O	2.64	0.41
2:D:105:LEU:CB	3:D:201:HOH:O	2.68	0.40
1:A:5:TRP:CE2	2:C:43:ASP:HB2	2.57	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	104/109 (95%)	99 (95%)	5 (5%)	0	100	100
1	B	104/109 (95%)	99 (95%)	5 (5%)	0	100	100
1	F	104/109 (95%)	99 (95%)	5 (5%)	0	100	100
1	H	102/109 (94%)	97 (95%)	5 (5%)	0	100	100
2	C	114/120 (95%)	105 (92%)	9 (8%)	0	100	100
2	D	115/120 (96%)	106 (92%)	9 (8%)	0	100	100
2	E	115/120 (96%)	107 (93%)	7 (6%)	1 (1%)	14	22
2	G	115/120 (96%)	107 (93%)	8 (7%)	0	100	100
All	All	873/916 (95%)	819 (94%)	53 (6%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	108	GLU

### 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	88/89 (99%)	88 (100%)	0	100	100
1	B	87/89 (98%)	87 (100%)	0	100	100
1	F	87/89 (98%)	87 (100%)	0	100	100
1	H	85/89 (96%)	85 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	102/104 (98%)	101 (99%)	1 (1%)	68	84
2	D	103/104 (99%)	101 (98%)	2 (2%)	50	71
2	E	103/104 (99%)	102 (99%)	1 (1%)	68	84
2	G	103/104 (99%)	103 (100%)	0	100	100
All	All	758/772 (98%)	754 (100%)	4 (0%)	81	91

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

Mol	Chain	Res	Type
2	C	12	THR
2	D	12	THR
2	D	32	ILE
2	E	12	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	2	ASN
1	A	94	HIS
2	C	90	GLN
2	C	110	GLN
2	D	2	GLN
2	D	80	GLN
2	D	90	GLN
2	D	110	GLN
1	F	66	GLN
2	G	80	GLN
2	G	90	GLN
2	E	42	GLN
2	E	90	GLN

### 5.3.3 RNA ⓘ

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 ⓘ

### 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	106/109 (97%)	1.00	18 (16%) 4 3	39, 58, 110, 177	0
1	B	106/109 (97%)	0.94	11 (10%) 11 9	39, 58, 117, 148	0
1	F	106/109 (97%)	1.13	20 (18%) 3 2	39, 58, 126, 207	0
1	H	104/109 (95%)	0.98	15 (14%) 6 4	39, 57, 110, 228	0
2	C	116/120 (96%)	1.17	26 (22%) 2 2	41, 61, 160, 501	0
2	D	117/120 (97%)	1.06	26 (22%) 2 2	41, 61, 159, 469	0
2	E	117/120 (97%)	1.05	21 (17%) 3 3	41, 61, 139, 234	0
2	G	117/120 (97%)	0.99	21 (17%) 3 3	41, 61, 156, 346	0
All	All	889/916 (97%)	1.04	158 (17%) 4 3	39, 60, 137, 501	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	43	HIS	5.5
1	F	45	GLN	5.4
2	G	109	GLU	5.4
2	G	113	GLY	5.0
2	D	109	GLU	5.0
2	C	112	GLN	5.0
2	E	112	GLN	4.9
1	H	57	TYR	4.6
1	H	43	HIS	4.6
1	H	107	GLY	4.6
2	D	108	GLU	4.6
1	B	45	GLN	4.6
2	G	39	PRO	4.5
2	C	39	PRO	4.4
1	B	43	HIS	4.4
2	G	107	THR	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	37	ASN	4.3
1	F	44	GLY	4.2
1	F	3	GLU	4.0
1	F	107	GLY	4.0
1	H	44	GLY	4.0
2	C	114	TRP	4.0
1	A	57	TYR	4.0
2	D	39	PRO	4.0
1	A	51	ASN	3.9
2	C	28	GLY	3.9
2	E	111	SER	3.9
2	G	112	GLN	3.9
2	C	113	GLY	3.9
1	B	107	GLY	3.8
2	C	108	GLU	3.8
2	E	114	TRP	3.8
2	G	28	GLY	3.8
1	F	57	TYR	3.8
2	C	109	GLU	3.8
1	F	42	ALA	3.6
2	G	117	CYS	3.6
1	F	47	SER	3.6
2	C	111	SER	3.6
2	G	111	SER	3.6
2	D	113	GLY	3.6
2	C	40	GLN	3.5
1	A	43	HIS	3.4
2	C	9	HIS	3.4
2	C	26	SER	3.4
2	D	112	GLN	3.4
2	D	114	TRP	3.3
2	G	9	HIS	3.3
2	D	81	LEU	3.2
2	E	39	PRO	3.2
1	B	47	SER	3.1
2	G	94	GLU	3.1
1	H	4	GLY	3.1
2	E	113	GLY	3.1
2	D	110	GLN	3.0
1	H	45	GLN	3.0
1	B	2	ASN	3.0
2	E	28	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	104	GLU	3.0
2	C	107	THR	3.0
2	G	108	GLU	2.9
1	A	39	LYS	2.9
1	B	57	TYR	2.9
1	A	42	ALA	2.9
2	D	80	GLN	2.9
1	A	1	GLN	2.9
2	C	94	GLU	2.9
2	G	40	GLN	2.8
1	H	14	VAL	2.8
1	A	47	SER	2.8
1	F	2	ASN	2.8
2	D	40	GLN	2.7
2	C	117	CYS	2.7
2	G	105	LEU	2.7
2	D	60	ARG	2.7
2	E	95	VAL	2.7
1	A	104	GLU	2.6
2	C	38	GLY	2.6
2	D	28	GLY	2.6
1	F	51	ASN	2.6
2	G	80	GLN	2.6
2	D	64	ASP	2.6
1	F	37	ASN	2.6
2	D	95	VAL	2.6
2	D	57	ARG	2.6
1	A	19	TRP	2.5
1	F	19	TRP	2.5
2	E	109	GLU	2.5
1	H	42	ALA	2.5
2	C	19	VAL	2.5
2	D	111	SER	2.5
2	D	94	GLU	2.5
2	E	107	THR	2.5
1	F	104	GLU	2.5
2	E	108	GLU	2.5
2	E	66	SER	2.5
2	E	117	CYS	2.4
2	G	64	ASP	2.4
2	D	9	HIS	2.4
2	D	93	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	105	LEU	2.4
1	A	25	MET	2.4
2	D	20	ASN	2.4
1	A	81	ASP	2.4
1	H	61	ASP	2.4
2	C	42	GLN	2.4
2	G	110	GLN	2.4
2	D	24	SER	2.4
2	E	2	GLN	2.4
1	B	51	ASN	2.4
2	E	94	GLU	2.3
2	G	41	PRO	2.3
2	C	93	THR	2.3
1	A	106	SER	2.3
2	C	57	ARG	2.3
2	C	64	ASP	2.3
1	F	24	VAL	2.3
1	F	46	GLU	2.3
2	G	114	TRP	2.3
1	F	41	ARG	2.3
2	E	26	SER	2.3
2	C	110	GLN	2.2
2	E	42	GLN	2.2
2	E	92	ILE	2.2
1	A	75	VAL	2.2
1	F	39	LYS	2.2
2	D	117	CYS	2.2
1	B	44	GLY	2.2
1	F	62	GLY	2.2
1	H	82	SER	2.2
1	B	81	ASP	2.2
1	H	81	ASP	2.2
1	H	41	ARG	2.2
2	G	20	ASN	2.2
2	C	58	ARG	2.2
2	D	38	GLY	2.1
2	D	10	CYS	2.1
2	E	41	PRO	2.1
1	A	63	TRP	2.1
1	A	45	GLN	2.1
1	B	77	LYS	2.1
2	D	2	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	79	LEU	2.1
2	E	55	THR	2.1
2	G	116	ARG	2.1
1	A	5	TRP	2.1
1	A	41	ARG	2.1
2	D	116	ARG	2.1
2	G	50	GLY	2.1
1	F	59	SER	2.1
2	E	110	GLN	2.0
2	C	71	ASN	2.0
1	H	89	TRP	2.0
2	C	92	ILE	2.0
1	B	75	VAL	2.0
1	H	37	ASN	2.0
1	F	63	TRP	2.0
2	E	9	HIS	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.