



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:14 AM UTC

PDB ID : 5WBS / pdb_00005wbs
Title : Crystal structure of Frizzled-7 CRD with an inhibitor peptide Fz7-21
Authors : Nile, A.H.; Mukund, S.; Hannoush, R.N.; Wang, W.
Deposited on : 2017-06-29
Resolution : 2.88 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

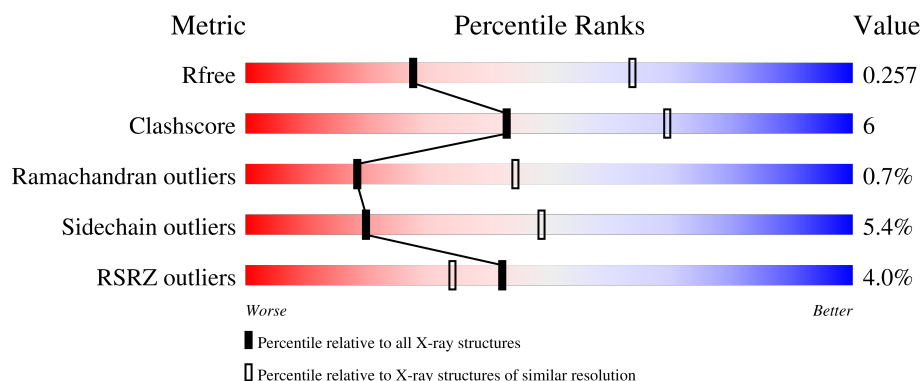
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	190	 4% 58% 14% 28%
1	B	190	 3% 58% 11% 31%
1	C	190	 3% 53% 14% 31%
1	D	190	 5% 55% 12% 32%
1	E	190	 2% 58% 9% 32%

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Mol	Chain	Length	Quality of chain
1	F	190	% 52%16%29%
1	G	190	2% 57%14%29%
1	H	190	3% 54%13%32%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8360 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 Frizzled-7,inhibitor peptide Fz7-21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	137	Total	C	N	O	S	0	0	0
			1077	683	184	196	14			
1	B	132	Total	C	N	O	S	0	0	0
			1044	665	178	187	14			
1	C	131	Total	C	N	O	S	0	0	0
			1034	659	175	186	14			
1	D	129	Total	C	N	O	S	0	0	0
			1020	647	174	185	14			
1	E	130	Total	C	N	O	S	0	0	0
			1031	656	175	186	14			
1	F	134	Total	C	N	O	S	0	0	0
			1060	672	181	193	14			
1	G	135	Total	C	N	O	S	0	0	0
			1066	676	182	194	14			
1	H	129	Total	C	N	O	S	0	0	0
			1027	654	174	185	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	ALA	conflict	UNP O75084
B	2	SER	ALA	conflict	UNP O75084
C	2	SER	ALA	conflict	UNP O75084
D	2	SER	ALA	conflict	UNP O75084
E	2	SER	ALA	conflict	UNP O75084
F	2	SER	ALA	conflict	UNP O75084
G	2	SER	ALA	conflict	UNP O75084
H	2	SER	ALA	conflict	UNP O75084

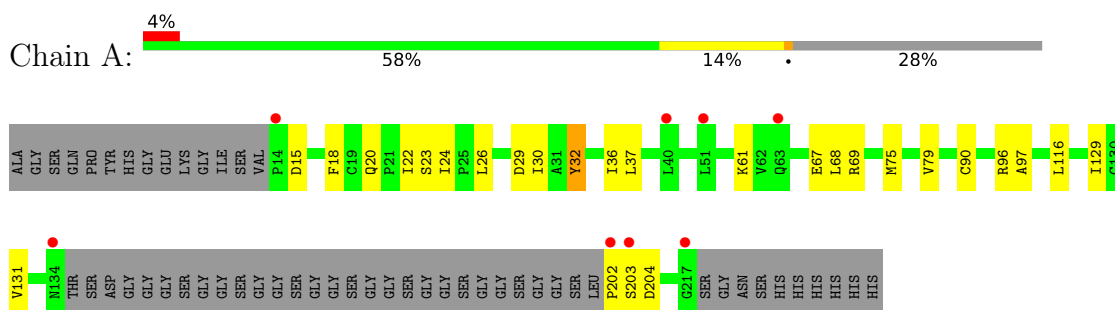
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	O	0	0
			1	1		

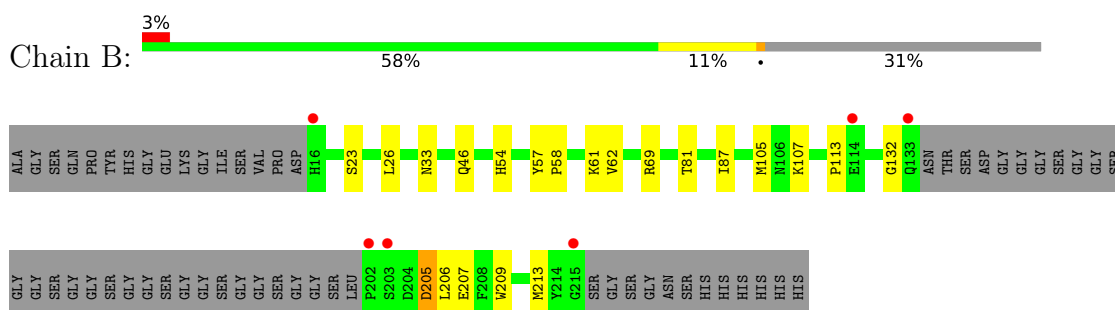
3 Residue-property plots [i](#)

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.

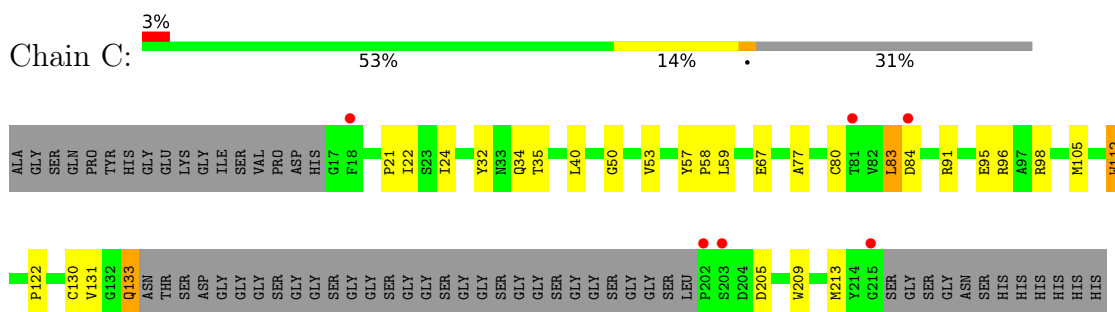
- Molecule 1: Frizzled-7,inhibitor peptide Fz7-21



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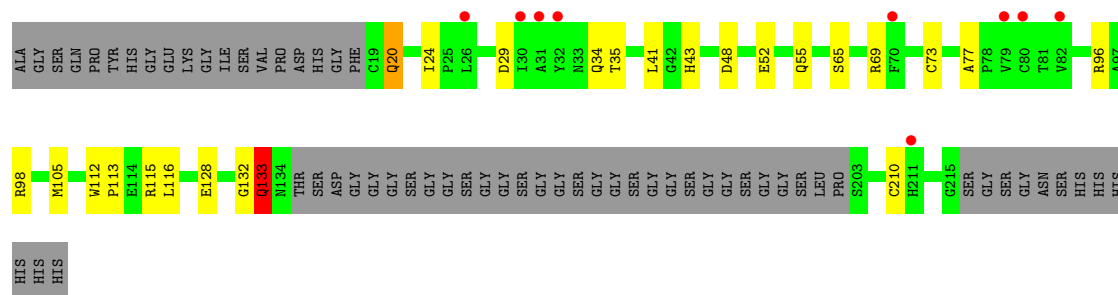


- Molecule 1: Frizzled-7,inhibitor peptide Fz7-21

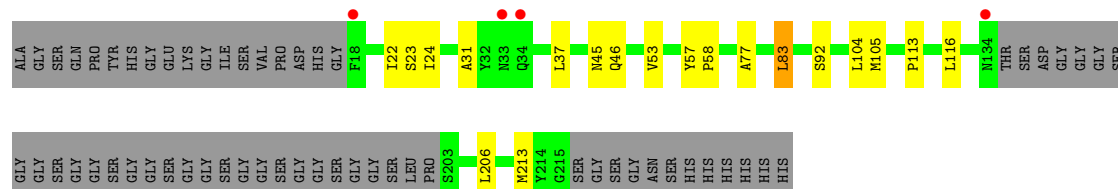


- Molecule 1: Frizzled-7,inhibitor peptide Fz7-21

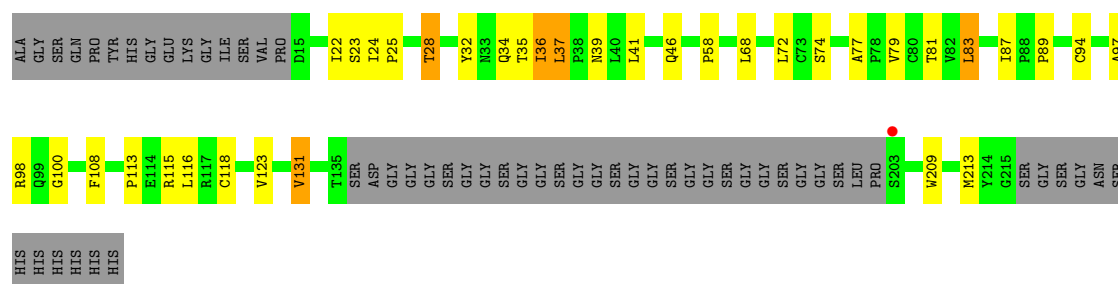




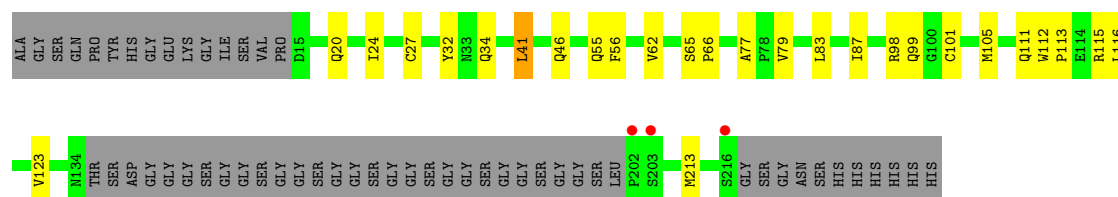
- Molecule 1: Frizzled-7,inhibitor peptide Fz7-21



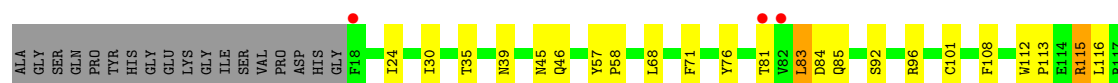
- Molecule 1: Frizzled-7,inhibitor peptide Fz7-21

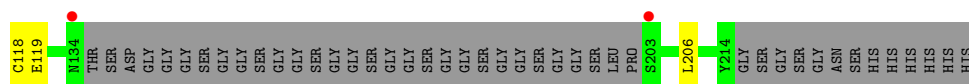


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- Molecule 1: Frizzled-7,inhibitor peptide Fz7-21





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.61Å 164.65Å 97.77Å 90.00° 108.31° 90.00°	Depositor
Resolution (Å)	38.72 – 2.88 38.72 – 2.88	Depositor EDS
% Data completeness (in resolution range)	91.1 (38.72-2.88) 99.5 (38.72-2.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.199 , 0.244 0.211 , 0.257	Depositor DCC
R_{free} test set	2128 reflections (4.38%)	wwPDB-VP
Wilson B-factor (Å ²)	81.6	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 65.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.158 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8360	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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](#)

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	0.50	0/1108	0.87	2/1505 (0.1%)
1	B	0.42	0/1074	0.82	2/1459 (0.1%)
1	C	0.44	0/1063	0.82	3/1444 (0.2%)
1	D	0.43	0/1047	0.88	4/1423 (0.3%)
1	E	0.40	0/1059	0.82	1/1439 (0.1%)
1	F	0.39	0/1089	0.79	0/1480
1	G	0.45	0/1096	0.82	0/1489
1	H	0.34	0/1055	0.79	0/1434
All	All	0.42	0/8591	0.83	12/11673 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	GLN	CA-C-N	-6.34	113.42	120.14
1	A	20	GLN	C-N-CA	-6.34	113.42	120.14
1	B	87	ILE	CA-C-N	6.00	123.98	119.66
1	B	87	ILE	C-N-CA	6.00	123.98	119.66
1	E	83	LEU	N-CA-C	-5.85	101.75	110.23
1	D	20	GLN	CA-C-N	5.49	125.49	119.89
1	D	20	GLN	C-N-CA	5.49	125.49	119.89
1	D	24	ILE	CA-C-N	5.29	125.35	119.32
1	D	24	ILE	C-N-CA	5.29	125.35	119.32
1	C	83	LEU	N-CA-C	-5.09	103.32	110.50
1	C	112	TRP	CA-C-N	5.05	125.04	119.89
1	C	112	TRP	C-N-CA	5.05	125.04	119.89

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1077	0	1012	12	0
1	B	1044	0	986	11	0
1	C	1034	0	979	18	0
1	D	1020	0	965	11	0
1	E	1031	0	974	8	0
1	F	1060	0	997	21	0
1	G	1066	0	1001	11	0
1	H	1027	0	973	14	0
2	G	1	0	0	0	0
All	All	8360	0	7887	101	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 6.

All (101) 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:F:81:THR:HG22	1:F:83:LEU:H	1.37	0.88
1:E:113:PRO:HB2	1:E:116:LEU:HB2	1.76	0.67
1:D:105:MET:HE1	1:D:113:PRO:HD3	1.78	0.64
1:H:83:LEU:O	1:H:85:GLN:N	2.29	0.62
1:E:206:LEU:HD21	1:F:108:PHE:HD1	1.66	0.61
1:E:22:ILE:HA	1:E:46:GLN:HE22	1.66	0.60
1:C:96:ARG:HH22	1:C:133:GLN:HB2	1.66	0.60
1:F:22:ILE:HG12	1:F:35:THR:HG23	1.84	0.59
1:H:83:LEU:HD12	1:H:83:LEU:H	1.68	0.59
1:C:95:GLU:OE2	1:C:98:ARG:NH2	2.36	0.58
1:D:96:ARG:HH22	1:D:133:GLN:HA	1.67	0.58
1:C:96:ARG:HH12	1:C:133:GLN:HG3	1.69	0.58
1:F:35:THR:HG21	1:F:77:ALA:HB1	1.87	0.57
1:G:24:ILE:HD12	1:G:77:ALA:HB2	1.85	0.57
1:C:24:ILE:HD12	1:C:77:ALA:HB2	1.87	0.55
1:D:35:THR:HG21	1:D:77:ALA:HB1	1.88	0.55
1:F:113:PRO:HB2	1:F:116:LEU:HD13	1.89	0.54
1:C:67:GLU:HG3	1:C:96:ARG:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:MET:HE1	1:E:113:PRO:HD3	1.90	0.54
1:G:62:VAL:HG23	1:H:108:PHE:HZ	1.73	0.53
1:G:41:LEU:HD12	1:G:115:ARG:HE	1.74	0.53
1:A:22:ILE:HD11	1:A:32:TYR:CE1	2.43	0.52
1:F:41:LEU:HD12	1:F:115:ARG:HE	1.74	0.52
1:C:57:TYR:CZ	1:C:205:ASP:HB3	2.45	0.51
1:H:68:LEU:HD22	1:H:101:CYS:SG	2.50	0.51
1:A:26:LEU:O	1:A:69:ARG:NH2	2.40	0.50
1:C:58:PRO:HD3	1:C:209:TRP:CD1	2.47	0.49
1:H:115:ARG:HH11	1:H:115:ARG:HB3	1.77	0.49
1:H:39:ASN:HD22	1:H:76:TYR:HA	1.78	0.48
1:G:98:ARG:HG3	1:G:112:TRP:CD2	2.48	0.48
1:C:96:ARG:HH22	1:C:133:GLN:CB	2.25	0.48
1:D:41:LEU:HD12	1:D:115:ARG:HE	1.78	0.48
1:H:92:SER:O	1:H:96:ARG:NH1	2.47	0.48
1:F:94:CYS:SG	1:F:118:CYS:HA	2.55	0.47
1:D:29:ASP:HB3	1:D:69:ARG:HH12	1.79	0.47
1:A:29:ASP:HB3	1:A:69:ARG:HH12	1.80	0.47
1:C:22:ILE:HG12	1:C:35:THR:OG1	2.15	0.47
1:B:58:PRO:HD3	1:B:209:TRP:CD1	2.51	0.46
1:F:32:TYR:CE2	1:F:79:VAL:HB	2.51	0.46
1:F:23:SER:O	1:F:23:SER:OG	2.33	0.45
1:A:36:ILE:O	1:A:37:LEU:HD23	2.17	0.45
1:B:23:SER:N	1:B:46:GLN:OE1	2.44	0.45
1:H:24:ILE:HG13	1:H:46:GLN:HB3	1.99	0.45
1:B:105:MET:HE1	1:B:113:PRO:HD3	1.98	0.45
1:F:58:PRO:HD3	1:F:209:TRP:CD1	2.51	0.45
1:G:56:PHE:HZ	1:G:113:PRO:HG2	1.81	0.44
1:F:39:ASN:C	1:F:41:LEU:H	2.25	0.44
1:C:59:LEU:HD11	1:C:105:MET:CG	2.47	0.44
1:H:45:ASN:OD1	1:H:45:ASN:N	2.50	0.44
1:D:52:GLU:O	1:D:55:GLN:HG3	2.18	0.44
1:A:202:PRO:O	1:A:204:ASP:N	2.46	0.44
1:C:122:PRO:HG2	1:C:130:CYS:HB3	2.00	0.44
1:E:37:LEU:HD13	1:E:45:ASN:HA	2.00	0.44
1:A:90:CYS:N	1:A:131:VAL:O	2.40	0.43
1:C:59:LEU:HD11	1:C:105:MET:HG2	1.99	0.43
1:F:89:PRO:HA	1:F:131:VAL:HG13	2.00	0.43
1:B:61:LYS:HA	1:B:61:LYS:HD2	1.87	0.43
1:A:61:LYS:HE3	1:B:107:LYS:O	2.18	0.43
1:B:26:LEU:HD11	1:B:69:ARG:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:TRP:CE2	1:C:213:MET:HG3	2.53	0.43
1:D:43:HIS:HD2	1:D:48:ASP:HB3	1.84	0.43
1:D:133:GLN:HE21	1:D:133:GLN:HB3	1.53	0.43
1:F:36:ILE:HG13	1:F:37:LEU:N	2.34	0.43
1:G:20:GLN:HG3	1:G:46:GLN:HE21	1.84	0.43
1:A:18:PHE:CE1	1:A:37:LEU:HD12	2.54	0.43
1:D:20:GLN:C	1:D:34:GLN:HG3	2.44	0.43
1:G:55:GLN:HG2	1:G:213:MET:SD	2.59	0.43
1:F:68:LEU:HD12	1:F:97:ALA:HB1	2.02	0.42
1:F:98:ARG:C	1:F:100:GLY:H	2.27	0.42
1:B:57:TYR:CZ	1:B:205:ASP:HB2	2.54	0.42
1:B:207:GLU:CD	1:C:91:ARG:HH12	2.27	0.42
1:F:209:TRP:CE2	1:F:213:MET:HG3	2.53	0.42
1:B:209:TRP:CE2	1:B:213:MET:HG3	2.55	0.42
1:G:62:VAL:HG23	1:H:108:PHE:CZ	2.54	0.42
1:E:24:ILE:HD12	1:E:77:ALA:HB2	2.02	0.42
1:A:75:MET:HE3	1:A:75:MET:HB3	1.84	0.42
1:E:213:MET:HE3	1:E:213:MET:HB2	1.77	0.42
1:D:132:GLY:O	1:D:133:GLN:HB2	2.20	0.41
1:C:50:GLY:HA2	1:C:53:VAL:HG12	2.01	0.41
1:F:25:PRO:O	1:F:28:THR:OG1	2.32	0.41
1:B:206:LEU:HA	1:B:206:LEU:HD12	1.82	0.41
1:H:206:LEU:HD12	1:H:206:LEU:HA	1.89	0.41
1:H:71:PHE:CZ	1:H:116:LEU:HD12	2.55	0.41
1:E:57:TYR:HB3	1:E:58:PRO:HD3	2.01	0.41
1:G:32:TYR:CG	1:G:79:VAL:HG23	2.56	0.41
1:F:22:ILE:HA	1:F:46:GLN:OE1	2.20	0.41
1:F:72:LEU:HD23	1:F:72:LEU:HA	1.88	0.41
1:A:68:LEU:HA	1:A:97:ALA:HB1	2.02	0.41
1:C:21:PRO:HA	1:C:34:GLN:HA	2.03	0.41
1:H:57:TYR:HB3	1:H:58:PRO:HD3	2.03	0.41
1:A:67:GLU:CD	1:A:96:ARG:HE	2.27	0.41
1:C:98:ARG:HG3	1:C:112:TRP:CD2	2.56	0.41
1:C:22:ILE:HD11	1:C:32:TYR:CD1	2.57	0.40
1:G:65:SER:HA	1:G:66:PRO:HD3	1.96	0.40
1:A:32:TYR:CD1	1:A:79:VAL:HG23	2.57	0.40
1:B:54:HIS:HE1	1:B:205:ASP:O	2.04	0.40
1:F:81:THR:HG21	1:F:87:ILE:HD11	2.04	0.40
1:H:112:TRP:HA	1:H:113:PRO:HD3	1.94	0.40
1:D:98:ARG:HG3	1:D:112:TRP:CD2	2.57	0.40
1:F:24:ILE:O	1:F:28:THR:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:101:CYS:O	1:G:105:MET:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	133/190 (70%)	125 (94%)	6 (4%)	2 (2%)	8	26
1	B	128/190 (67%)	120 (94%)	7 (6%)	1 (1%)	16	41
1	C	127/190 (67%)	123 (97%)	4 (3%)	0	100	100
1	D	125/190 (66%)	121 (97%)	3 (2%)	1 (1%)	16	41
1	E	126/190 (66%)	121 (96%)	4 (3%)	1 (1%)	16	41
1	F	130/190 (68%)	119 (92%)	11 (8%)	0	100	100
1	G	131/190 (69%)	123 (94%)	7 (5%)	1 (1%)	16	41
1	H	125/190 (66%)	118 (94%)	6 (5%)	1 (1%)	16	41
All	All	1025/1520 (67%)	970 (95%)	48 (5%)	7 (1%)	18	44

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	133	GLN
1	A	15	ASP
1	E	31	ALA
1	H	84	ASP
1	A	203	SER
1	B	132	GLY
1	G	99	GLN

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	120/151 (80%)	114 (95%)	6 (5%)	22	51
1	B	116/151 (77%)	112 (97%)	4 (3%)	32	64
1	C	115/151 (76%)	109 (95%)	6 (5%)	21	50
1	D	114/151 (76%)	108 (95%)	6 (5%)	20	49
1	E	115/151 (76%)	110 (96%)	5 (4%)	26	57
1	F	118/151 (78%)	110 (93%)	8 (7%)	14	39
1	G	119/151 (79%)	111 (93%)	8 (7%)	15	39
1	H	115/151 (76%)	108 (94%)	7 (6%)	17	43
All	All	932/1208 (77%)	882 (95%)	50 (5%)	20	49

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	SER
1	A	24	ILE
1	A	30	ILE
1	A	32	TYR
1	A	116	LEU
1	A	129	ILE
1	B	33	ASN
1	B	62	VAL
1	B	81	THR
1	B	205	ASP
1	C	40	LEU
1	C	80	CYS
1	C	83	LEU
1	C	84	ASP
1	C	131	VAL
1	C	133	GLN
1	D	65	SER
1	D	73	CYS
1	D	116	LEU

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Mol	Chain	Res	Type
1	D	128	GLU
1	D	133	GLN
1	D	210	CYS
1	E	23	SER
1	E	53	VAL
1	E	83	LEU
1	E	92	SER
1	E	104	LEU
1	F	28	THR
1	F	34	GLN
1	F	36	ILE
1	F	37	LEU
1	F	74	SER
1	F	83	LEU
1	F	123	VAL
1	F	131	VAL
1	G	27	CYS
1	G	34	GLN
1	G	41	LEU
1	G	83	LEU
1	G	87	ILE
1	G	111	GLN
1	G	116	LEU
1	G	123	VAL
1	H	30	ILE
1	H	35	THR
1	H	81	THR
1	H	83	LEU
1	H	115	ARG
1	H	118	CYS
1	H	119	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	B	20	GLN
1	B	106	ASN
1	F	20	GLN
1	G	111	GLN
1	H	54	HIS

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

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	137/190 (72%)	0.02	8 (5%)	29	22	45, 61, 114, 154	0
1	B	132/190 (69%)	0.00	6 (4%)	38	30	47, 77, 128, 177	0
1	C	131/190 (68%)	0.06	6 (4%)	37	29	43, 76, 122, 171	0
1	D	129/190 (67%)	0.24	9 (6%)	22	18	59, 97, 160, 220	0
1	E	130/190 (68%)	0.13	4 (3%)	51	42	57, 89, 130, 159	0
1	F	134/190 (70%)	0.13	1 (0%)	84	80	61, 96, 131, 154	0
1	G	135/190 (71%)	-0.12	3 (2%)	62	53	47, 65, 113, 181	0
1	H	129/190 (67%)	0.37	5 (3%)	43	35	74, 116, 147, 175	0
All	All	1057/1520 (69%)	0.10	42 (3%)	42	34	43, 84, 140, 220	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	134	ASN	4.7
1	B	133	GLN	4.5
1	C	18	PHE	4.4
1	D	79	VAL	4.0
1	B	16	HIS	3.7
1	D	32	TYR	3.4
1	B	215	GLY	3.4
1	A	202	PRO	3.2
1	G	203	SER	3.1
1	G	216	SER	3.0
1	D	80	CYS	2.9
1	A	217	GLY	2.9
1	C	203	SER	2.9
1	C	202	PRO	2.7
1	C	215	GLY	2.7
1	A	14	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	18	PHE	2.6
1	B	114	GLU	2.6
1	A	203	SER	2.5
1	C	81	THR	2.5
1	F	203	SER	2.5
1	C	84	ASP	2.4
1	G	202	PRO	2.4
1	E	33	ASN	2.4
1	D	82	VAL	2.4
1	D	31	ALA	2.4
1	H	81	THR	2.4
1	B	203	SER	2.3
1	B	202	PRO	2.3
1	H	203	SER	2.2
1	A	134	ASN	2.2
1	A	51	LEU	2.2
1	A	63	GLN	2.2
1	E	34	GLN	2.2
1	D	26	LEU	2.2
1	D	30	ILE	2.1
1	D	211	HIS	2.1
1	H	134	ASN	2.1
1	H	82	VAL	2.1
1	A	40	LEU	2.1
1	D	70	PHE	2.0
1	E	18	PHE	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.