



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:20 AM UTC

PDB ID : 5B4M / pdb_00005b4m
Title : Crystal structure of an Fab against human influenza A
Authors : Yuan, Y.A.
Deposited on : 2016-04-05
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

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

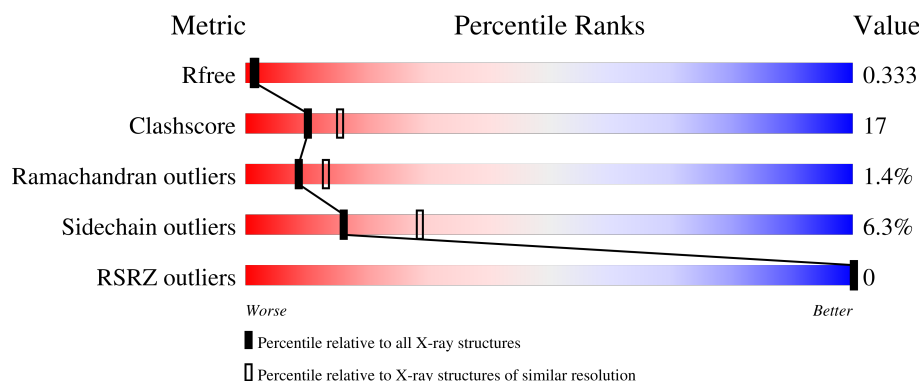
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

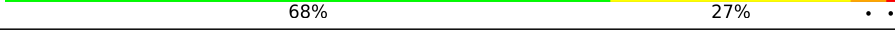
The reported resolution of this entry is 2.40 Å.

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_{free}	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 ≥ 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	C	221	
1	H	221	
2	D	218	
2	L	218	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6738 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 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	221	Total	C	N	O	S	0	0	0
			1687	1068	284	328	7			
1	C	221	Total	C	N	O	S	0	0	0
			1687	1068	284	328	7			

- Molecule 2 is a protein called Fab light chain.

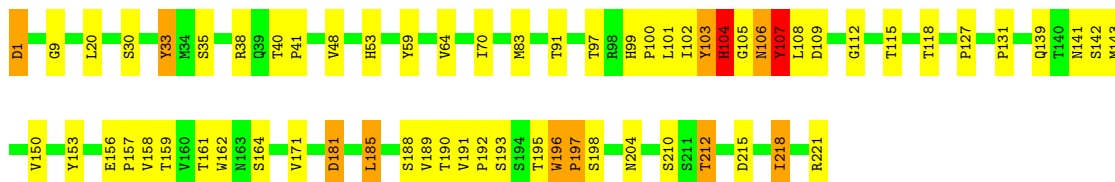
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	218	Total	C	N	O	S	0	0	0
			1682	1046	280	350	6			
2	D	218	Total	C	N	O	S	0	0	0
			1682	1046	280	350	6			

3 Residue-property plots

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.

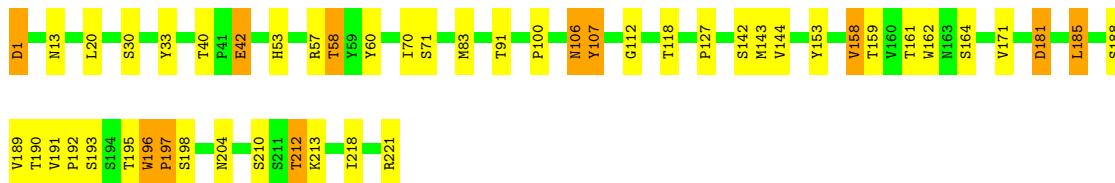
- Molecule 1: Fab heavy chain

Chain H: 



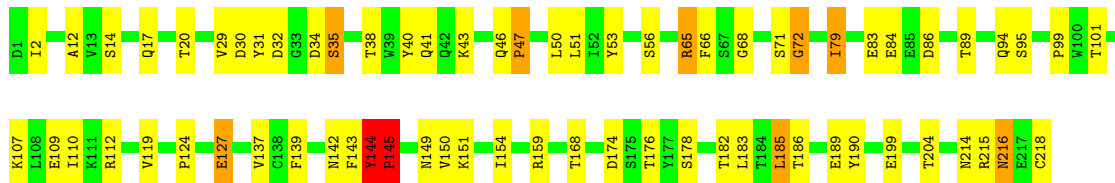
- Molecule 1: Fab heavy chain

Chain C: 



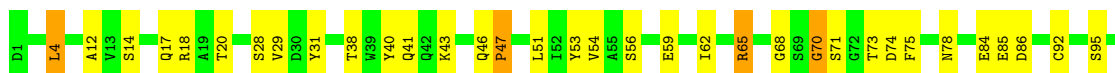
- Molecule 2: Fab light chain

Chain L: 



- Molecule 2: Fab light chain

Chain D: 



E109	I110	K111	R112	V119	P124	E127	V137	C138	F139	L140	F143	Y144	P145	N149	V150	I154	S157	E158	R159	V163	T168	D171	S172	K173	D174	S175	T176	Y177	S178	M179	T182	L183	T184	L185	T186	K187	D188	E189	Y190	T204	R215	W216	E217	C218
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.59Å 90.94Å 81.44Å 90.00° 92.21° 90.00°	Depositor
Resolution (Å)	81.38 – 2.40 81.38 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (81.38-2.40) 98.5 (81.38-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.285 , 0.338 0.282 , 0.333	Depositor DCC
R_{free} test set	1477 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.930	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 16.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.059 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6738	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.57% 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	C	0.75	1/1730 (0.1%)	0.94	3/2363 (0.1%)
1	H	0.80	1/1730 (0.1%)	0.97	7/2363 (0.3%)
2	D	0.81	1/1721 (0.1%)	0.99	6/2343 (0.3%)
2	L	0.85	1/1721 (0.1%)	1.01	3/2343 (0.1%)
All	All	0.80	4/6902 (0.1%)	0.98	19/9412 (0.2%)

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	D	0	1
2	L	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	106	ASN	CA-C	-6.62	1.44	1.52
1	H	106	ASN	CA-C	-6.09	1.45	1.52
2	D	47	PRO	CA-C	5.81	1.57	1.52
2	L	47	PRO	CA-C	5.61	1.57	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	144	TYR	CA-C-N	10.53	133.00	119.84
2	L	144	TYR	C-N-CA	10.53	133.00	119.84
2	D	144	TYR	CA-C-N	9.45	131.65	119.84
2	D	144	TYR	C-N-CA	9.45	131.65	119.84
1	H	196	TRP	CA-C-N	-7.22	110.82	119.84
1	H	196	TRP	C-N-CA	-7.22	110.82	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	31	TYR	N-CA-C	7.15	120.07	108.41
1	C	196	TRP	CA-C-N	-6.77	111.37	119.84
1	C	196	TRP	C-N-CA	-6.77	111.37	119.84
1	H	106	ASN	CB-CA-C	-5.90	99.80	109.53
2	L	145	PRO	CA-N-CD	-5.89	103.75	112.00
2	D	145	PRO	CA-N-CD	-5.87	103.78	112.00
1	H	104	HIS	N-CA-C	-5.79	102.86	110.33
1	H	109	ASP	N-CA-CB	-5.60	101.88	110.16
1	H	108	LEU	CA-C-N	5.59	128.22	120.29
1	H	108	LEU	C-N-CA	5.59	128.22	120.29
2	D	144	TYR	N-CA-C	5.52	114.65	108.25
2	D	70	GLY	N-CA-C	5.14	125.36	113.18
1	C	106	ASN	CB-CA-C	-5.01	101.03	109.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	144	TYR	Peptide
2	L	144	TYR	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	C	1687	0	1664	48	0
1	H	1687	0	1664	77	1
2	D	1682	0	1592	68	1
2	L	1682	0	1592	82	0
All	All	6738	0	6512	227	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 17.

All (227) 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:H:106:ASN:ND2	2:L:38:THR:HG23	1.74	1.02
1:C:171:VAL:HG22	1:C:189:VAL:HG22	1.48	0.94
1:H:171:VAL:HG22	1:H:189:VAL:HG22	1.48	0.94
2:L:79:ILE:HD11	2:L:86:ASP:OD2	1.68	0.93
1:H:196:TRP:HH2	1:H:218:ILE:O	1.53	0.89
2:D:186:THR:OG1	2:D:188:ASP:OD1	1.90	0.89
2:D:41:GLN:HB2	2:D:51:LEU:HD11	1.61	0.83
1:H:210:SER:OG	1:H:212:THR:OG1	1.88	0.82
1:C:106:ASN:HB2	2:D:53:TYR:HB3	1.60	0.81
2:L:30:ASP:OD2	2:L:72:GLY:N	2.12	0.81
2:L:41:GLN:HB2	2:L:51:LEU:HD11	1.60	0.81
1:H:210:SER:HG	1:H:212:THR:HG1	1.18	0.81
1:H:106:ASN:ND2	2:L:38:THR:CG2	2.45	0.79
1:H:164:SER:O	1:C:159:THR:HG21	1.81	0.79
1:H:106:ASN:OD1	1:H:107:TYR:N	2.16	0.79
2:D:154:ILE:HD12	2:D:159:ARG:HD3	1.66	0.78
1:C:20:LEU:HG	1:C:83:MET:HE2	1.67	0.77
1:C:106:ASN:ND2	2:D:38:THR:OG1	2.19	0.76
1:H:196:TRP:CH2	1:H:218:ILE:O	2.38	0.76
1:C:106:ASN:OD1	1:C:107:TYR:N	2.19	0.76
1:H:59:TYR:OH	2:L:99:PRO:HB3	1.85	0.75
2:L:66:PHE:CZ	2:L:79:ILE:HD12	2.21	0.75
1:C:143:MET:HE3	1:C:190:THR:HG22	1.69	0.74
1:C:112:GLY:O	2:D:47:PRO:HB3	1.88	0.74
1:H:20:LEU:HG	1:H:83:MET:HE2	1.70	0.73
2:D:154:ILE:HD11	2:D:183:LEU:HD21	1.71	0.72
2:L:154:ILE:HD11	2:L:183:LEU:HD21	1.71	0.71
1:H:106:ASN:HD21	2:L:38:THR:HG23	1.54	0.71
2:D:71:SER:O	2:D:75:PHE:CZ	2.44	0.71
2:L:29:VAL:CG2	2:L:94:GLN:OE1	2.39	0.70
1:H:106:ASN:HD21	2:L:38:THR:CG2	2.05	0.70
2:L:174:ASP:OD1	2:L:176:THR:HG22	1.92	0.69
1:H:102:ILE:C	1:H:104:HIS:H	2.01	0.68
1:C:112:GLY:O	2:D:47:PRO:CB	2.43	0.67
2:D:140:LEU:HD11	2:D:150:VAL:HG22	1.76	0.66
2:L:38:THR:HG21	2:L:40:TYR:CZ	2.30	0.66
2:L:29:VAL:CG1	2:L:94:GLN:OE1	2.43	0.66
1:H:171:VAL:HG22	1:H:189:VAL:CG2	2.25	0.65
1:C:210:SER:OG	1:C:212:THR:OG1	1.95	0.65
1:H:102:ILE:O	1:H:104:HIS:N	2.30	0.64
1:C:106:ASN:ND2	2:D:38:THR:HG23	2.13	0.63
1:C:171:VAL:HG22	1:C:189:VAL:CG2	2.25	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:196:TRP:CH2	1:H:218:ILE:HG22	2.33	0.63
2:D:38:THR:HG21	2:D:40:TYR:CZ	2.32	0.63
1:H:100:PRO:HD3	1:H:106:ASN:O	1.99	0.63
2:L:30:ASP:OD1	2:L:35:SER:HB2	1.99	0.63
2:L:144:TYR:CD1	2:L:145:PRO:CD	2.81	0.63
1:H:143:MET:HE3	1:H:190:THR:HG22	1.79	0.63
1:C:221:ARG:NH2	2:D:124:PRO:O	2.31	0.62
1:C:107:TYR:CD1	2:D:95:SER:OG	2.52	0.62
2:L:65:ARG:O	2:L:79:ILE:HA	1.99	0.62
2:D:144:TYR:CD1	2:D:145:PRO:CD	2.82	0.62
2:L:65:ARG:NH2	2:L:86:ASP:OD2	2.33	0.61
2:D:188:ASP:OD1	2:D:189:GLU:N	2.33	0.61
1:H:106:ASN:HD21	2:L:38:THR:CB	2.13	0.61
1:H:91:THR:HG23	1:H:118:THR:HA	1.80	0.61
1:H:131:PRO:HD3	2:L:127:GLU:OE1	2.01	0.61
1:H:106:ASN:HB2	2:L:53:TYR:HB3	1.82	0.60
1:C:91:THR:HG23	1:C:118:THR:HA	1.83	0.60
2:D:65:ARG:NH2	2:D:86:ASP:OD2	2.34	0.60
1:C:100:PRO:HD3	1:C:106:ASN:O	2.02	0.60
2:D:29:VAL:HG12	2:D:29:VAL:O	2.00	0.60
2:L:29:VAL:O	2:L:29:VAL:HG12	2.01	0.59
2:L:143:PHE:N	2:L:176:THR:OG1	2.35	0.59
1:C:162:TRP:CG	1:C:189:VAL:HG21	2.38	0.59
2:L:137:VAL:HG13	2:L:182:THR:HG22	1.85	0.58
1:C:107:TYR:HD1	2:D:95:SER:OG	1.86	0.58
1:H:162:TRP:CG	1:H:189:VAL:HG21	2.38	0.58
1:H:106:ASN:ND2	2:L:53:TYR:HB3	2.19	0.58
2:L:32:ASP:C	2:L:34:ASP:H	2.12	0.58
1:C:107:TYR:HD1	2:D:95:SER:HG	1.50	0.57
2:D:85:GLU:OE1	2:D:85:GLU:N	2.35	0.57
2:L:83:GLU:OE2	2:D:65:ARG:HD3	2.05	0.57
1:H:196:TRP:HH2	1:H:218:ILE:C	2.12	0.57
2:L:144:TYR:CD1	2:L:145:PRO:HD3	2.40	0.56
1:C:106:ASN:ND2	2:D:38:THR:CG2	2.69	0.56
1:H:141:ASN:O	1:H:193:SER:OG	2.14	0.56
2:L:29:VAL:HG21	2:L:94:GLN:OE1	2.05	0.56
1:H:106:ASN:HD22	2:L:53:TYR:HB3	1.70	0.56
1:C:106:ASN:HD21	2:D:38:THR:CB	2.18	0.56
1:C:188:SER:HB3	2:D:139:PHE:CE1	2.41	0.55
1:C:106:ASN:CB	2:D:53:TYR:HB3	2.34	0.55
1:C:106:ASN:HD22	2:D:53:TYR:HB3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:TRP:O	1:C:197:PRO:C	2.49	0.55
1:H:196:TRP:O	1:H:197:PRO:C	2.47	0.55
2:D:137:VAL:HG13	2:D:182:THR:HG22	1.89	0.55
2:D:143:PHE:O	2:D:176:THR:HG22	2.07	0.55
2:L:186:THR:OG1	2:L:189:GLU:HG2	2.07	0.54
2:D:144:TYR:CD1	2:D:145:PRO:HD3	2.42	0.54
2:D:51:LEU:O	2:D:62:ILE:HD13	2.06	0.54
1:H:215:ASP:OD2	1:C:213:LYS:NZ	2.40	0.54
1:H:40:THR:HG23	1:H:41:PRO:HD2	1.90	0.54
1:C:161:THR:HB	1:C:204:ASN:HB2	1.88	0.54
1:H:106:ASN:CB	2:L:53:TYR:HB3	2.39	0.53
2:D:174:ASP:CG	2:D:176:THR:HG1	2.17	0.53
2:L:29:VAL:HG13	2:L:94:GLN:NE2	2.24	0.52
2:L:30:ASP:OD1	2:L:35:SER:CB	2.57	0.52
1:C:106:ASN:HD22	2:D:53:TYR:CB	2.22	0.52
2:D:73:THR:HG22	2:D:74:ASP:OD1	2.09	0.52
2:L:79:ILE:CD1	2:L:86:ASP:OD2	2.52	0.52
2:D:51:LEU:O	2:D:62:ILE:CD1	2.57	0.52
1:H:9:GLY:HA3	1:H:115:THR:HG22	1.92	0.52
2:L:31:TYR:C	2:L:31:TYR:CD2	2.87	0.52
1:C:40:THR:OG1	1:C:42:GLU:OE2	2.27	0.52
2:L:2:ILE:HD13	2:L:94:GLN:NE2	2.25	0.51
2:D:190:TYR:CZ	2:D:215:ARG:HG3	2.45	0.51
1:H:40:THR:CG2	1:H:41:PRO:HD2	2.40	0.51
1:H:150:VAL:CG2	1:H:185:LEU:HG	2.40	0.51
2:L:154:ILE:HD12	2:L:159:ARG:HD2	1.92	0.51
2:D:84:GLU:O	2:D:110:ILE:CD1	2.58	0.51
1:H:159:THR:HG21	1:C:164:SER:O	2.11	0.51
2:L:84:GLU:O	2:L:110:ILE:CD1	2.59	0.51
2:D:43:LYS:O	2:D:46:GLN:HB2	2.11	0.51
2:D:186:THR:OG1	2:D:189:GLU:HG2	2.11	0.50
1:H:35:SER:OG	1:H:97:THR:OG1	2.05	0.50
1:H:102:ILE:C	1:H:104:HIS:N	2.68	0.50
2:L:29:VAL:HG11	2:L:94:GLN:OE1	2.11	0.49
2:L:119:VAL:HA	2:L:139:PHE:O	2.12	0.49
1:H:221:ARG:NH2	2:L:124:PRO:O	2.45	0.49
1:C:161:THR:HG22	1:C:162:TRP:N	2.27	0.49
2:D:154:ILE:HD12	2:D:159:ARG:CD	2.40	0.49
2:L:32:ASP:O	2:L:34:ASP:N	2.45	0.49
2:D:84:GLU:O	2:D:110:ILE:HD11	2.13	0.49
2:L:31:TYR:HD2	2:L:31:TYR:O	1.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:106:ASN:HB2	2:L:50:LEU:CD1	2.43	0.48
2:L:214:ASN:HB3	2:L:216:ASN:OD1	2.13	0.48
2:D:119:VAL:HA	2:D:139:PHE:O	2.13	0.48
1:H:1:ASP:OD2	2:D:112:ARG:NH1	2.46	0.48
1:H:150:VAL:HG23	1:H:150:VAL:O	2.13	0.48
2:L:43:LYS:O	2:L:46:GLN:HB2	2.13	0.48
1:H:162:TRP:CD2	1:H:189:VAL:HG21	2.49	0.48
2:D:12:ALA:HA	2:D:109:GLU:O	2.13	0.48
2:D:143:PHE:C	2:D:176:THR:HG22	2.39	0.47
1:H:161:THR:HG22	1:H:162:TRP:N	2.29	0.47
2:L:29:VAL:HG13	2:L:94:GLN:CD	2.39	0.47
1:H:103:TYR:C	1:H:104:HIS:O	2.50	0.47
1:C:106:ASN:ND2	2:D:53:TYR:CB	2.78	0.47
2:L:12:ALA:HA	2:L:109:GLU:O	2.14	0.47
2:L:84:GLU:O	2:L:110:ILE:HD11	2.14	0.47
1:H:106:ASN:OD1	1:H:106:ASN:C	2.57	0.47
2:L:204:THR:HG22	2:L:204:THR:O	2.14	0.47
1:H:139:GLN:NE2	1:H:141:ASN:HD22	2.12	0.47
2:L:185:LEU:HD12	2:L:185:LEU:N	2.29	0.47
1:H:107:TYR:HD1	2:L:95:SER:CB	2.28	0.47
1:H:107:TYR:HD1	2:L:95:SER:OG	1.98	0.47
2:D:188:ASP:OD1	2:D:189:GLU:HG2	2.15	0.47
2:L:29:VAL:HG22	2:L:94:GLN:OE1	2.15	0.47
1:H:139:GLN:HE21	1:H:141:ASN:HD22	1.62	0.46
2:L:190:TYR:CE2	2:L:215:ARG:HD2	2.51	0.46
2:D:59:GLU:HB3	2:D:62:ILE:HD11	1.98	0.46
2:L:32:ASP:C	2:L:34:ASP:N	2.72	0.46
2:L:56:SER:HB2	2:L:68:GLY:O	2.15	0.46
1:C:106:ASN:ND2	2:D:38:THR:CB	2.79	0.45
1:C:162:TRP:CD2	1:C:189:VAL:HG21	2.51	0.45
2:D:56:SER:HB2	2:D:68:GLY:O	2.16	0.45
1:H:106:ASN:HB2	2:L:50:LEU:HD11	1.98	0.45
1:H:106:ASN:CB	2:L:50:LEU:HD13	2.47	0.45
2:L:149:ASN:OD1	2:L:150:VAL:N	2.49	0.45
2:D:150:VAL:HG21	2:D:179:MET:CE	2.46	0.45
2:L:190:TYR:CZ	2:L:215:ARG:HG3	2.52	0.45
2:D:51:LEU:HA	2:D:62:ILE:HD13	1.99	0.45
2:D:149:ASN:OD1	2:D:150:VAL:N	2.49	0.45
1:H:185:LEU:C	1:H:185:LEU:HD12	2.42	0.45
2:L:66:PHE:CE1	2:L:79:ILE:HD12	2.53	0.44
2:L:79:ILE:HD11	2:L:86:ASP:CG	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:139:GLN:HE21	1:H:141:ASN:ND2	2.16	0.44
1:C:106:ASN:ND2	2:D:53:TYR:HB3	2.32	0.44
2:L:144:TYR:CE1	2:L:145:PRO:HD3	2.53	0.44
1:C:185:LEU:C	1:C:185:LEU:HD12	2.42	0.44
1:H:9:GLY:H	1:H:115:THR:HG21	1.82	0.44
2:D:171:ASP:OD1	2:D:173:LYS:N	2.51	0.44
1:H:33:TYR:HB3	1:H:99:HIS:CG	2.53	0.43
1:C:196:TRP:O	1:C:196:TRP:CD1	2.71	0.43
1:H:106:ASN:HB3	2:L:50:LEU:HD22	2.00	0.43
1:C:191:VAL:HG13	1:C:192:PRO:HD2	2.01	0.43
1:H:107:TYR:HD1	2:L:95:SER:HB2	1.84	0.43
2:L:142:ASN:HA	2:L:176:THR:HG21	2.01	0.43
2:D:4:LEU:HD23	2:D:92:CYS:SG	2.59	0.43
1:C:192:PRO:O	1:C:195:THR:HB	2.19	0.43
2:L:112:ARG:NH1	1:C:1:ASP:OD2	2.35	0.43
1:C:196:TRP:N	1:C:197:PRO:HD2	2.34	0.43
1:H:192:PRO:O	1:H:195:THR:HB	2.19	0.42
2:L:30:ASP:OD2	2:L:71:SER:HA	2.19	0.42
2:D:29:VAL:O	2:D:29:VAL:CG1	2.67	0.42
1:H:161:THR:HB	1:H:204:ASN:HB2	2.01	0.42
2:D:171:ASP:OD1	2:D:171:ASP:C	2.62	0.42
1:H:127:PRO:HB3	1:H:153:TYR:HB3	2.02	0.42
2:D:149:ASN:OD1	2:D:149:ASN:C	2.63	0.42
2:D:168:THR:HG21	2:D:178:SER:HB2	2.00	0.42
1:H:196:TRP:O	1:H:196:TRP:CE3	2.72	0.42
1:C:158:VAL:CG1	1:C:159:THR:N	2.83	0.42
1:H:196:TRP:N	1:H:197:PRO:HD2	2.35	0.42
1:C:127:PRO:HB3	1:C:153:TYR:HB3	2.01	0.42
1:H:106:ASN:ND2	2:L:53:TYR:CB	2.83	0.42
1:H:106:ASN:CB	2:L:50:LEU:CD1	2.97	0.42
1:H:196:TRP:CZ2	1:H:218:ILE:HG22	2.54	0.42
1:H:20:LEU:CG	1:H:83:MET:HE2	2.44	0.41
1:H:191:VAL:HG13	1:H:192:PRO:HD2	2.02	0.41
1:C:42:GLU:H	1:C:42:GLU:HG3	1.60	0.41
1:C:30:SER:O	1:C:53:HIS:HB2	2.20	0.41
1:C:196:TRP:O	1:C:197:PRO:O	2.38	0.41
2:D:185:LEU:HD12	2:D:185:LEU:N	2.35	0.41
1:H:101:LEU:HB3	1:H:102:ILE:HG13	2.02	0.41
2:L:14:SER:HB2	2:L:17:GLN:CD	2.45	0.41
2:D:70:GLY:HA3	2:D:75:PHE:CD2	2.55	0.41
2:D:119:VAL:HG13	2:D:140:LEU:CD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:150:VAL:O	2:L:150:VAL:HG23	2.21	0.41
2:L:168:THR:HG21	2:L:178:SER:HB2	2.01	0.41
1:C:144:VAL:HG23	1:C:193:SER:HA	2.02	0.41
1:H:188:SER:HB3	2:L:139:PHE:CE1	2.56	0.41
2:L:142:ASN:HA	2:L:176:THR:CG2	2.50	0.41
2:D:204:THR:O	2:D:204:THR:HG22	2.20	0.41
2:L:30:ASP:CG	2:L:35:SER:OG	2.64	0.41
1:H:30:SER:O	1:H:53:HIS:HB2	2.21	0.41
1:H:112:GLY:O	2:L:47:PRO:HB3	2.21	0.41
2:D:18:ARG:HD3	2:D:78:ASN:OD1	2.20	0.41
2:D:54:VAL:O	2:D:54:VAL:HG12	2.21	0.41
1:H:196:TRP:O	1:H:197:PRO:O	2.40	0.40
2:D:14:SER:HB2	2:D:17:GLN:CD	2.47	0.40
2:L:29:VAL:HG13	2:L:94:GLN:HE22	1.86	0.40
1:C:58:THR:HG21	1:C:60:TYR:OH	2.22	0.40
1:H:156:GLU:OE2	1:H:157:PRO:HA	2.22	0.40
1:H:38:ARG:HD3	1:H:48:VAL:HG11	2.04	0.40
1:H:107:TYR:CD1	2:L:95:SER:HB2	2.56	0.40
1:H:193:SER:C	1:H:195:THR:H	2.29	0.40
2:L:151:LYS:HB2	2:L:199:GLU:HB2	2.02	0.40
2:D:144:TYR:CG	2:D:145:PRO:N	2.89	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)
1:H:103:TYR:OH	2:D:163:VAL:O[2_645]	1.85	0.35

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	C	219/221 (99%)	202 (92%)	14 (6%)	3 (1%)	9	13
1	H	219/221 (99%)	203 (93%)	11 (5%)	5 (2%)	5	6
2	D	216/218 (99%)	203 (94%)	11 (5%)	2 (1%)	14	22
2	L	216/218 (99%)	202 (94%)	12 (6%)	2 (1%)	14	22
All	All	870/878 (99%)	810 (93%)	48 (6%)	12 (1%)	9	13

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	103	TYR
1	H	105	GLY
1	H	181	ASP
2	L	145	PRO
1	C	181	ASP
2	D	145	PRO
1	C	107	TYR
2	D	217	GLU
1	H	107	TYR
2	L	72	GLY
1	C	197	PRO
1	H	197	PRO

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	C	192/192 (100%)	177 (92%)	15 (8%)	11	20
1	H	192/192 (100%)	179 (93%)	13 (7%)	14	25
2	D	191/191 (100%)	182 (95%)	9 (5%)	23	41
2	L	191/191 (100%)	180 (94%)	11 (6%)	18	32
All	All	766/766 (100%)	718 (94%)	48 (6%)	16	29

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	1	ASP
1	H	33	TYR
1	H	64	VAL
1	H	70	ILE
1	H	104	HIS
1	H	107	TYR
1	H	142	SER
1	H	158	VAL
1	H	181	ASP
1	H	185	LEU
1	H	198	SER
1	H	212	THR
1	H	218	ILE
2	L	20	THR
2	L	35	SER
2	L	65	ARG
2	L	79	ILE
2	L	89	THR
2	L	101	THR
2	L	107	LYS
2	L	127	GLU
2	L	185	LEU
2	L	216	ASN
2	L	218	CYS
1	C	1	ASP
1	C	13	ASN
1	C	33	TYR
1	C	42	GLU
1	C	57	ARG
1	C	58	THR
1	C	70	ILE
1	C	71	SER
1	C	142	SER
1	C	158	VAL
1	C	181	ASP
1	C	185	LEU
1	C	198	SER
1	C	212	THR
1	C	218	ILE
2	D	4	LEU
2	D	20	THR
2	D	28	SER
2	D	65	ARG

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Mol	Chain	Res	Type
2	D	127	GLU
2	D	157	SER
2	D	176	THR
2	D	185	LEU
2	D	215	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	77	ASN
1	H	139	GLN
2	L	57	ASN
2	L	96	ASN
2	L	214	ASN
1	C	77	ASN
1	C	106	ASN
2	D	57	ASN
2	D	96	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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	C	221/221 (100%)	-0.93	0 100 100	32, 41, 50, 56	0
1	H	221/221 (100%)	-0.98	0 100 100	31, 38, 49, 52	0
2	D	218/218 (100%)	-0.89	0 100 100	32, 39, 55, 62	0
2	L	218/218 (100%)	-0.96	0 100 100	30, 37, 49, 69	0
All	All	878/878 (100%)	-0.94	0 100 100	30, 39, 51, 69	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.