



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:34 am GMT

PDB ID : 3C2A
Title : Antibody Fab fragment 447-52D in complex with UG1033 peptide
Authors : Dhillon, A.K.; Stanfield, R.L.; Wilson, I.A.
Deposited on : 2008-01-24
Resolution : 2.10 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

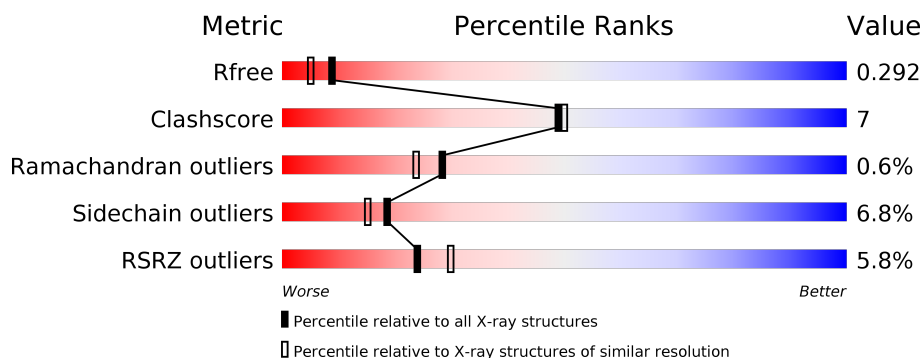
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	L	216	<div> <div>87%</div> <div>12%</div> <div>•</div> </div>
1	M	216	<div> <div>6%</div> <div>80%</div> <div>18%</div> <div>•</div> </div>
2	H	231	<div> <div>3%</div> <div>85%</div> <div>13%</div> <div>•</div> </div>
2	I	231	<div> <div>7%</div> <div>77%</div> <div>20%</div> <div>•</div> </div>
3	P	13	<div> <div>46%</div> <div>54%</div> <div>31%</div> <div>15%</div> </div>
3	Q	13	<div> <div>54%</div> <div>54%</div> <div>31%</div> <div>15%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7071 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 Lambda-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	216	Total	C	N	O	S	0	0	0
			1603	1007	266	325	5			
1	M	216	Total	C	N	O	S	0	0	0
			1603	1007	266	325	5			

- Molecule 2 is a protein called Fab 447-52D, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	231	Total	C	N	O	S	0	0	0
			1739	1095	291	345	8			
2	I	231	Total	C	N	O	S	0	0	0
			1739	1095	291	345	8			

- Molecule 3 is a protein called Envelope glycoprotein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	13	Total	C	N	O	2	0	0
			100	66	19	15			
3	Q	13	Total	C	N	O	2	0	0
			100	66	19	15			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	63	Total	O	0	0
			63	63		
4	I	33	Total	O	0	0
			33	33		
4	L	64	Total	O	0	0
			64	64		
4	M	24	Total	O	0	0
			24	24		

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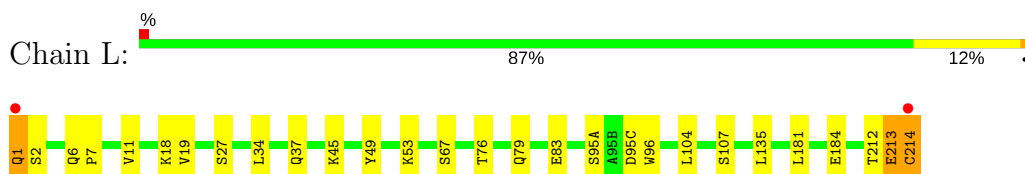
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	2	Total	O	0	0
			2	2		
4	Q	1	Total	O	0	0
			1	1		

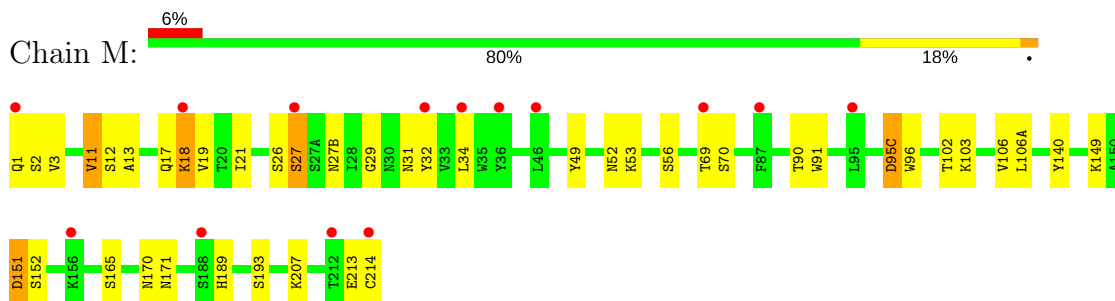
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

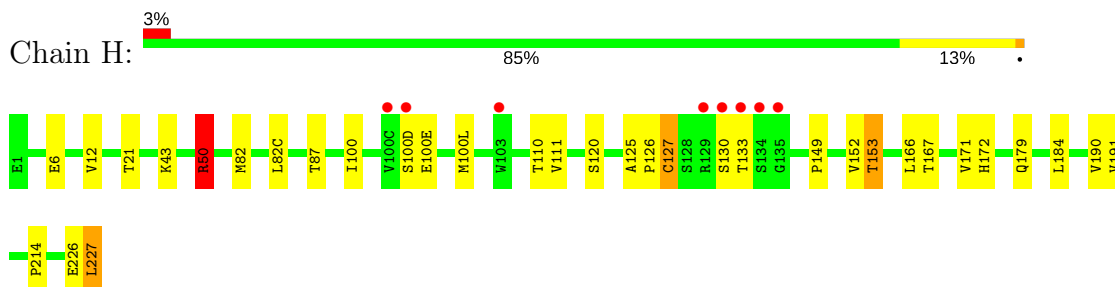
- Molecule 1: Lambda-chain



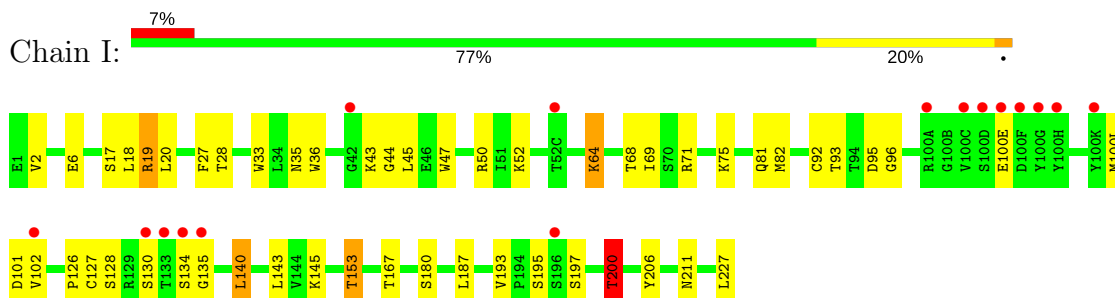
- Molecule 1: Lambda-chain



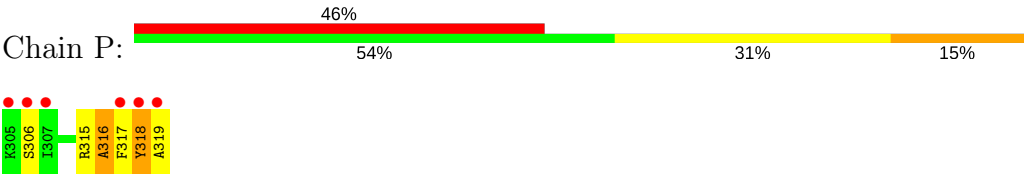
- Molecule 2: Fab 447-52D, heavy chain



- Molecule 2: Fab 447-52D, heavy chain



● Molecule 3: Envelope glycoprotein



● Molecule 3: Envelope glycoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.25Å 76.48Å 114.13Å 90.00° 101.49° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 32.92 – 2.08	Depositor EDS
% Data completeness (in resolution range)	85.7 (50.00-2.10) 85.4 (32.92-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.93 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.240 , 0.298 0.242 , 0.292	Depositor DCC
R_{free} test set	1397 reflections (2.41%)	DCC
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7071	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.90% 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	L	0.84	0/1644	0.81	1/2247 (0.0%)
1	M	0.95	8/1644 (0.5%)	0.72	0/2247
2	H	0.83	1/1778 (0.1%)	0.82	2/2421 (0.1%)
2	I	0.73	2/1778 (0.1%)	0.78	2/2421 (0.1%)
3	P	2.04	2/103 (1.9%)	1.98	2/137 (1.5%)
3	Q	1.02	1/103 (1.0%)	0.82	1/137 (0.7%)
All	All	0.87	14/7050 (0.2%)	0.81	8/9610 (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
3	P	0	2
3	Q	0	2
All	All	0	4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	318	TYR	C-O	16.57	1.54	1.23
1	M	26	SER	CB-OG	14.03	1.60	1.42
1	M	27	SER	CB-OG	12.09	1.57	1.42
1	M	152	SER	CB-OG	9.85	1.55	1.42
3	P	316	ALA	C-O	9.81	1.42	1.23
2	I	64	LYS	CD-CE	9.27	1.74	1.51
2	I	64	LYS	CE-NZ	9.24	1.72	1.49
1	M	18	LYS	CE-NZ	8.82	1.71	1.49
1	M	27(B)	ASN	CB-CG	8.74	1.71	1.51
3	Q	318	TYR	C-O	7.85	1.38	1.23
1	M	18	LYS	CD-CE	5.87	1.66	1.51
1	M	151	ASP	CG-OD2	5.28	1.37	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	27(B)	ASN	CA-CB	5.26	1.66	1.53
2	H	127	CYS	CB-SG	5.11	1.91	1.82

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	318	TYR	O-C-N	-17.48	94.73	122.70
3	P	318	TYR	CA-C-O	-11.59	95.76	120.10
2	I	64	LYS	CD-CE-NZ	-7.47	94.53	111.70
2	H	50	ARG	NE-CZ-NH2	-7.27	116.66	120.30
1	L	181	LEU	CA-CB-CG	5.83	128.70	115.30
2	H	227	LEU	CA-CB-CG	5.66	128.32	115.30
2	I	140	LEU	CA-CB-CG	5.42	127.77	115.30
3	Q	318	TYR	O-C-N	-5.06	114.60	122.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	P	316	ALA	Mainchain
3	P	318	TYR	Mainchain
3	Q	316	ALA	Mainchain
3	Q	318	TYR	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	L	1603	0	1556	17	0
1	M	1603	0	1556	27	0
2	H	1739	0	1705	20	0
2	I	1739	0	1705	35	0
3	P	100	0	100	3	0
3	Q	100	0	100	4	0
4	H	63	0	0	1	0
4	I	33	0	0	1	0
4	L	64	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	24	0	0	1	0
4	P	2	0	0	2	0
4	Q	1	0	0	1	0
All	All	7071	0	6722	93	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 7.

All (93) 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:M:18:LYS:NZ	1:M:18:LYS:CE	1.71	1.54
2:I:64:LYS:CE	2:I:64:LYS:NZ	1.72	1.48
2:I:19:ARG:HH11	2:I:19:ARG:HG2	0.88	1.02
2:I:19:ARG:HH11	2:I:19:ARG:CG	1.72	1.02
2:I:126:PRO:HG3	2:I:130:SER:HB2	1.42	1.01
2:I:19:ARG:NH1	2:I:19:ARG:HG2	1.61	0.99
1:M:90:THR:HG22	1:M:91:TRP:H	1.36	0.89
2:H:153:THR:HG22	4:H:244:HOH:O	1.78	0.81
1:L:96:TRP:CD1	2:H:100(L):MET:HE2	2.21	0.76
2:I:126:PRO:CG	2:I:130:SER:HB2	2.16	0.75
1:M:214:CYS:HB3	2:I:127:CYS:HA	1.70	0.73
2:H:126:PRO:HG3	2:H:130:SER:HB2	1.71	0.73
1:L:11:VAL:HG12	4:L:278:HOH:O	1.88	0.72
2:I:126:PRO:HG3	2:I:130:SER:CB	2.19	0.71
2:I:64:LYS:CD	2:I:64:LYS:NZ	2.54	0.70
2:H:125:ALA:HB1	2:H:227:LEU:HD22	1.75	0.68
2:I:153:THR:HG22	2:I:211:ASN:HB3	1.78	0.64
1:M:27:SER:HA	1:M:29:GLY:HA3	1.78	0.64
1:M:18:LYS:NZ	1:M:18:LYS:CD	2.60	0.63
1:L:37:GLN:OE1	1:L:45:LYS:HE2	1.97	0.63
3:Q:315:ARG:NH1	4:Q:85:HOH:O	2.23	0.63
1:M:32:TYR:O	1:M:90:THR:HG23	1.98	0.63
2:H:125:ALA:CB	2:H:227:LEU:CD2	2.78	0.62
2:H:125:ALA:HB1	2:H:227:LEU:CD2	2.29	0.61
1:L:96:TRP:CD1	2:H:100(L):MET:CE	2.84	0.61
1:L:213:GLU:C	1:L:214:CYS:SG	2.79	0.61
1:M:11:VAL:HG23	1:M:102:THR:CG2	2.31	0.61
1:M:12:SER:HB2	1:M:106(A):LEU:HD21	1.84	0.60
2:I:96:GLY:HA3	2:I:101:ASP:HB2	1.85	0.59
1:L:37:GLN:OE1	1:L:45:LYS:CE	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2:VAL:HG13	2:I:27:PHE:HD1	1.68	0.58
1:L:18:LYS:HB3	1:L:76:THR:HA	1.85	0.58
1:M:90:THR:HG22	1:M:91:TRP:N	2.13	0.57
1:L:1:GLN:O	2:H:43:LYS:HE2	2.05	0.57
1:M:11:VAL:HG23	1:M:102:THR:HG21	1.86	0.56
1:L:184:GLU:H	1:L:184:GLU:CD	2.10	0.55
2:I:153:THR:HG23	4:I:231:HOH:O	2.07	0.54
2:H:82:MET:HB3	2:H:82(C):LEU:HD21	1.87	0.54
2:I:193:VAL:HG11	2:I:206:TYR:CZ	2.43	0.53
2:H:171:VAL:HG22	2:H:191:VAL:HG22	1.90	0.53
1:L:135:LEU:CD1	2:H:190:VAL:HG11	2.38	0.53
2:I:2:VAL:HG13	2:I:27:PHE:CD1	2.45	0.52
1:L:213:GLU:HB2	1:L:214:CYS:SG	2.50	0.52
3:P:306:SER:HB2	3:P:319:ALA:HB3	1.92	0.51
1:L:6:GLN:HB3	1:L:7:PRO:HD2	1.92	0.51
2:I:33:TRP:CH2	3:Q:315:ARG:HG3	2.46	0.51
1:M:214:CYS:CB	2:I:127:CYS:HA	2.41	0.50
2:H:100(D):SER:HB3	2:H:100(E):GLU:HG2	1.94	0.49
1:M:31:ASN:HB2	1:M:90:THR:HG21	1.94	0.49
2:I:68:THR:HB	2:I:81:GLN:HB3	1.93	0.49
1:M:170:ASN:O	1:M:171:ASN:HB2	2.13	0.49
2:I:43:LYS:HD3	2:I:44:GLY:H	1.78	0.49
2:I:6:GLU:OE2	2:I:92:CYS:SG	2.72	0.48
1:L:34:LEU:HD23	1:L:49:TYR:HA	1.94	0.48
2:H:179:GLN:HG3	2:H:184:LEU:O	2.14	0.48
2:I:93:THR:HA	2:I:102:VAL:O	2.15	0.47
1:M:31:ASN:HB2	1:M:90:THR:CG2	2.44	0.47
3:P:315:ARG:NH2	4:P:130:HOH:O	2.34	0.47
2:I:143:LEU:HG	2:I:145:LYS:HG3	1.95	0.47
1:M:32:TYR:CE1	3:Q:309:LEU:HD22	2.49	0.47
2:I:36:TRP:CD1	2:I:69:ILE:HG12	2.50	0.47
1:M:149:LYS:HB2	1:M:193:SER:HB2	1.97	0.47
1:M:91:TRP:HB2	3:Q:313:PRO:HB3	1.97	0.47
2:I:20:LEU:HD21	2:I:82:MET:HE1	1.97	0.46
1:M:106(A):LEU:HA	1:M:140:TYR:OH	2.16	0.45
1:M:49:TYR:CE2	1:M:53:LYS:HD3	2.52	0.45
2:I:187:LEU:HD12	2:I:187:LEU:C	2.36	0.45
1:M:11:VAL:HG21	1:M:21:ILE:HG12	1.99	0.45
1:M:34:LEU:HD23	1:M:49:TYR:HA	1.97	0.45
3:P:315:ARG:NE	4:P:130:HOH:O	2.38	0.44
1:M:96:TRP:CD1	2:I:100(L):MET:HE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:126:PRO:CG	2:H:130:SER:HB2	2.44	0.44
2:H:152:VAL:HG12	2:H:153:THR:N	2.32	0.44
1:M:17:GLN:NE2	4:M:222:HOH:O	2.50	0.44
2:I:193:VAL:HG11	2:I:206:TYR:CE1	2.54	0.43
2:I:52:LYS:O	2:I:71:ARG:NH1	2.52	0.43
2:I:43:LYS:HD3	2:I:44:GLY:N	2.34	0.42
1:M:95(C):ASP:HA	2:I:47:TRP:CE3	2.55	0.42
2:I:18:LEU:HB3	2:I:82:MET:HE3	2.01	0.42
2:I:33:TRP:HB2	2:I:95:ASP:HB2	2.01	0.42
1:L:49:TYR:OH	2:H:100:ILE:HD11	2.20	0.41
2:I:17:SER:HA	2:I:82:MET:O	2.20	0.41
2:I:197:SER:O	2:I:200:THR:OG1	2.39	0.41
1:L:83:GLU:HG3	1:L:104:LEU:O	2.21	0.41
1:M:13:ALA:O	1:M:106:VAL:HA	2.20	0.41
2:H:12:VAL:O	2:H:111:VAL:HA	2.20	0.41
2:H:149:PRO:HD2	2:H:214:PRO:CB	2.51	0.41
2:I:35:ASN:HB2	2:I:93:THR:OG1	2.21	0.41
2:H:87:THR:HG23	2:H:110:THR:HA	2.02	0.41
1:L:18:LYS:HE2	1:L:76:THR:CG2	2.51	0.41
1:L:95(A):SER:O	2:H:50:ARG:NH2	2.54	0.41
1:M:151:ASP:OD2	1:M:189:HIS:ND1	2.45	0.41
1:M:11:VAL:CG2	1:M:102:THR:HG21	2.50	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	L	214/216 (99%)	209 (98%)	5 (2%)	0	100	100
1	M	214/216 (99%)	201 (94%)	13 (6%)	0	100	100
2	H	229/231 (99%)	220 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	229/231 (99%)	211 (92%)	15 (7%)	3 (1%)	14	8
3	P	11/13 (85%)	9 (82%)	1 (9%)	1 (9%)	1	0
3	Q	11/13 (85%)	10 (91%)	0	1 (9%)	1	0
All	All	908/920 (99%)	860 (95%)	43 (5%)	5 (1%)	28	24

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	200	THR
3	Q	317	PHE
3	P	317	PHE
2	I	134	SER
2	I	135	GLY

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	L	180/180 (100%)	168 (93%)	12 (7%)	19	15
1	M	180/180 (100%)	166 (92%)	14 (8%)	15	11
2	H	196/196 (100%)	185 (94%)	11 (6%)	25	21
2	I	196/196 (100%)	182 (93%)	14 (7%)	17	13
3	P	9/9 (100%)	9 (100%)	0	100	100
3	Q	9/9 (100%)	8 (89%)	1 (11%)	7	4
All	All	770/770 (100%)	718 (93%)	52 (7%)	18	15

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	GLN
1	L	2	SER
1	L	19	VAL

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Mol	Chain	Res	Type
1	L	27	SER
1	L	53	LYS
1	L	67	SER
1	L	79	GLN
1	L	95(C)	ASP
1	L	107	SER
1	L	212	THR
1	L	213	GLU
1	L	214	CYS
2	H	6	GLU
2	H	21	THR
2	H	50	ARG
2	H	120	SER
2	H	127	CYS
2	H	133	THR
2	H	153	THR
2	H	166	LEU
2	H	167	THR
2	H	172	HIS
2	H	226	GLU
1	M	1	GLN
1	M	2	SER
1	M	3	VAL
1	M	11	VAL
1	M	19	VAL
1	M	52	ASN
1	M	56	SER
1	M	69	THR
1	M	70	SER
1	M	95(C)	ASP
1	M	103	LYS
1	M	165	SER
1	M	207	LYS
1	M	213	GLU
2	I	19	ARG
2	I	28	THR
2	I	45	LEU
2	I	50	ARG
2	I	75	LYS
2	I	100(E)	GLU
2	I	128	SER
2	I	140	LEU

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Mol	Chain	Res	Type
2	I	153	THR
2	I	167	THR
2	I	180	SER
2	I	195	SER
2	I	200	THR
2	I	227	LEU
3	Q	317	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates 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	L	216/216 (100%)	-0.16	2 (0%) 84 86	20, 30, 42, 62	0
1	M	216/216 (100%)	0.42	14 (6%) 20 25	31, 50, 87, 103	0
2	H	231/231 (100%)	0.10	8 (3%) 44 51	18, 30, 60, 81	0
2	I	231/231 (100%)	0.40	16 (6%) 18 22	24, 41, 76, 100	0
3	P	13/13 (100%)	2.24	6 (46%) 0 0	28, 48, 81, 86	1 (7%)
3	Q	13/13 (100%)	3.12	7 (53%) 0 0	62, 71, 99, 112	1 (7%)
All	All	920/920 (100%)	0.26	53 (5%) 24 30	18, 36, 78, 112	2 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	P	318	TYR	9.6
3	Q	318	TYR	8.6
3	Q	317	PHE	7.7
3	Q	319	ALA	6.7
1	L	214	CYS	6.4
3	P	317	PHE	6.4
1	M	214	CYS	6.4
3	P	319	ALA	6.3
2	H	134	SER	5.8
2	I	133	THR	5.4
2	I	130	SER	4.9
2	I	134	SER	4.8
1	M	1	GLN	4.6
2	H	130	SER	4.1
2	H	133	THR	4.0
3	Q	307	ILE	3.7
3	Q	305	LYS	3.7
3	P	305	LYS	3.4
1	M	212	THR	3.2

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Mol	Chain	Res	Type	RSRZ
2	I	135	GLY	3.1
2	H	100(C)	VAL	3.1
2	I	100(E)	GLU	3.0
2	I	196	SER	3.0
2	H	135	GLY	2.9
1	L	1	GLN	2.8
2	I	100(G)	TYR	2.8
3	Q	306	SER	2.7
2	I	52(C)	THR	2.7
3	Q	316	ALA	2.6
1	M	69	THR	2.6
2	H	100(D)	SER	2.5
1	M	32	TYR	2.5
2	I	100(K)	TYR	2.5
1	M	46	LEU	2.4
2	I	42	GLY	2.4
3	P	306	SER	2.3
2	I	100(H)	TYR	2.3
1	M	95	LEU	2.3
1	M	36	TYR	2.3
1	M	18	LYS	2.2
1	M	188	SER	2.2
2	I	100(A)	ARG	2.1
3	P	307	ILE	2.1
1	M	34	LEU	2.1
2	H	103	TRP	2.1
2	H	129	ARG	2.1
2	I	100(F)	ASP	2.1
1	M	156	LYS	2.1
1	M	27	SER	2.0
2	I	100(C)	VAL	2.0
2	I	100(D)	SER	2.0
1	M	87	PHE	2.0
2	I	102	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.