



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 07:58 am BST

PDB ID : 6HX4
Title : Fab fragment of a native monomer-selective antibody in complex with alpha-1-antitrypsin
Authors : Elliston, E.L.K.; Miranda, E.; Perez, J.; Jagger, A.M.; Lomas, D.A.; Irving, J.A.
Deposited on : 2018-10-15
Resolution : 2.95 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

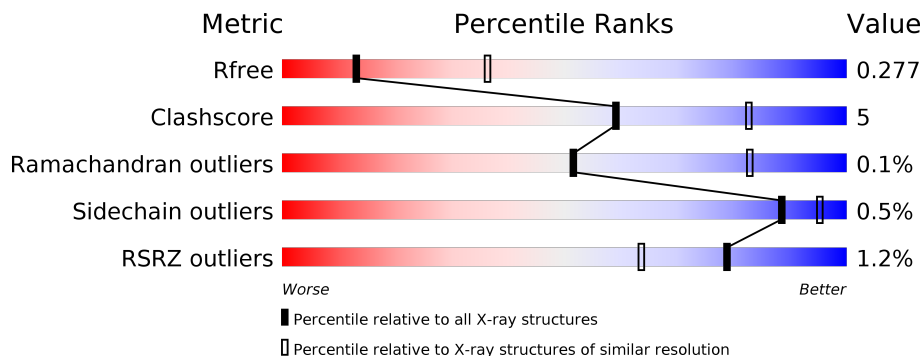
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 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	397	 2% 72% 14% 13%
1	B	397	 2% 71% 11% 18%
2	H	228	 89% 8%
2	I	228	 2% 75% 14% 11%
3	L	217	 92% 8%
3	M	217	 2% 92% 8% . . .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10921 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 Alpha-1-antitrypsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	344	Total	C	N	O	S	0	0	0
			2448	1604	388	448	8			
1	B	325	Total	C	N	O	S	0	0	0
			2294	1500	377	409	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP P01009
A	-1	ARG	-	expression tag	UNP P01009
A	0	GLY	ALA	conflict	UNP P01009
A	1	SER	GLU	conflict	UNP P01009
B	-2	MET	-	initiating methionine	UNP P01009
B	-1	ARG	-	expression tag	UNP P01009
B	0	GLY	ALA	conflict	UNP P01009
B	1	SER	GLU	conflict	UNP P01009

- Molecule 2 is a protein called Fab 1D9 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	222	Total	C	N	O	S	0	0	0
			1638	1046	261	322	9			
2	I	204	Total	C	N	O	S	0	0	0
			1425	912	228	278	7			

- Molecule 3 is a protein called Fab 1D9 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	217	Total	C	N	O	S	0	0	0
			1638	1025	271	334	8			
3	M	210	Total	C	N	O	S	0	0	0
			1473	931	240	294	8			

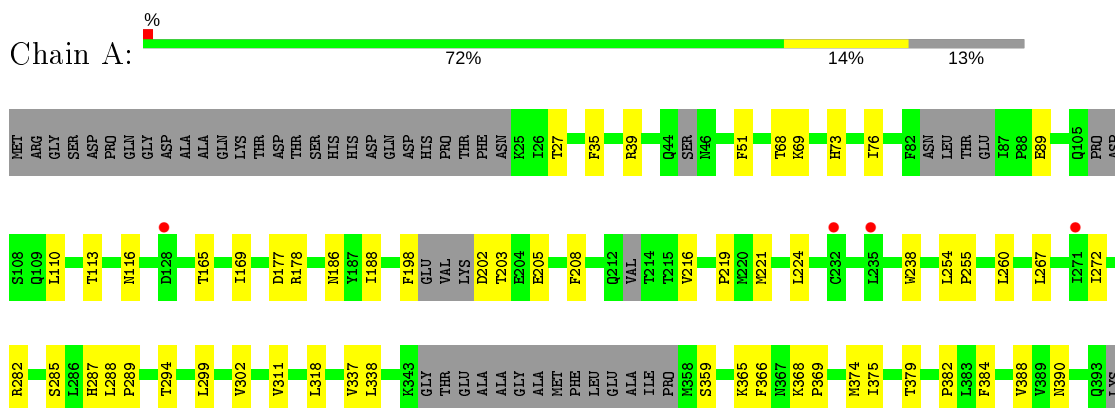
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 1 1	0	0
4	B	1	Total O 1 1	0	0
4	L	3	Total O 3 3	0	0

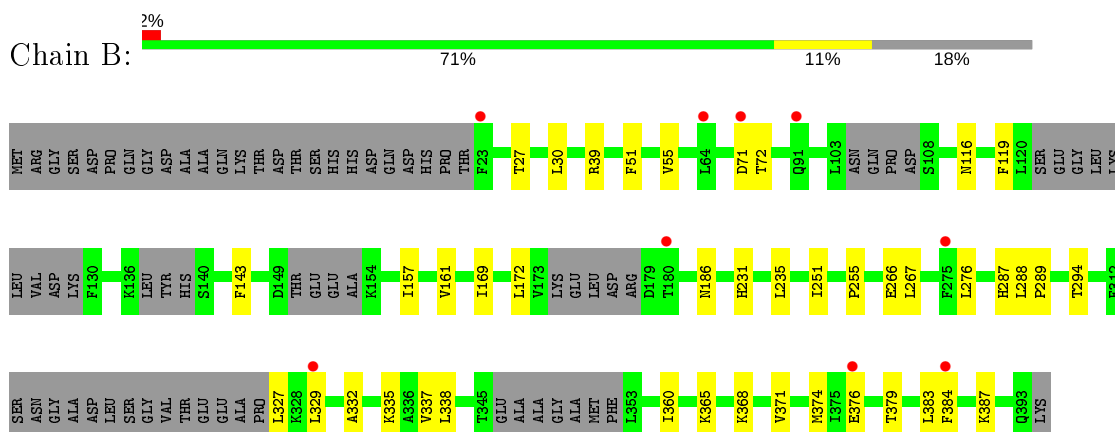
3 Residue-property plots [i](#)

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.

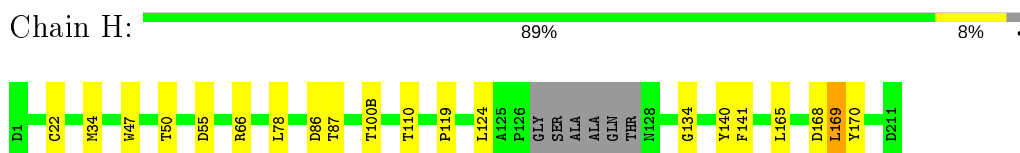
- Molecule 1: Alpha-1-antitrypsin



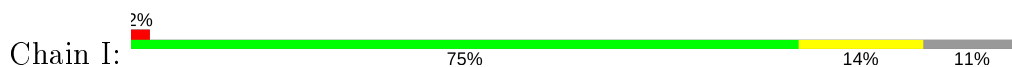
- Molecule 1: Alpha-1-antitrypsin

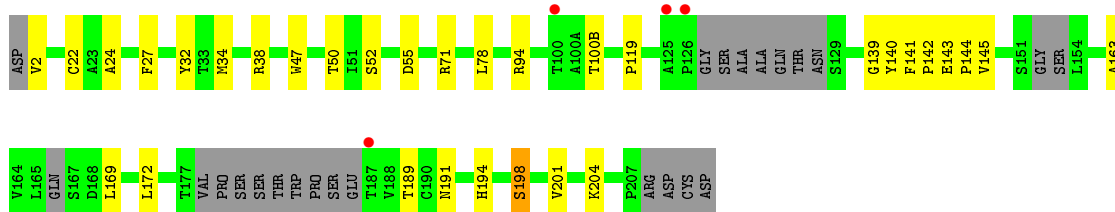


- Molecule 2: Fab 1D9 heavy chain



- Molecule 2: Fab 1D9 heavy chain

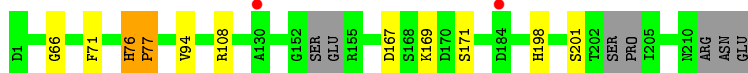
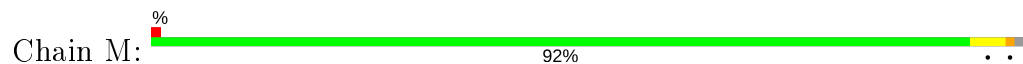




- Molecule 3: Fab 1D9 light chain



- Molecule 3: Fab 1D9 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	247.48 Å 36.75 Å 201.78 Å 90.00° 126.07° 90.00°	Depositor
Resolution (Å)	39.69 – 2.95 39.69 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.1 (39.69-2.95) 92.6 (39.69-2.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.95 Å)	Xtrriage
Refinement program	PHENIX 1.13-2998	Depositor
R, R_{free}	0.231 , 0.277 0.231 , 0.277	Depositor DCC
R_{free} test set	1503 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	66.8	Xtrriage
Anisotropy	0.023	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.005 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10921	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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	0.24	0/2496	0.43	0/3408
1	B	0.24	0/2339	0.42	0/3194
2	H	0.24	0/1681	0.46	0/2301
2	I	0.26	0/1461	0.47	0/2011
3	L	0.25	0/1677	0.43	0/2284
3	M	0.25	0/1509	0.47	0/2071
All	All	0.25	0/11163	0.44	0/15269

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	I	0	1
3	M	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	198	SER	Peptide
3	M	76	HIS	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2448	0	2205	31	0
1	B	2294	0	2069	23	0
2	H	1638	0	1565	12	0
2	I	1425	0	1262	18	0
3	L	1638	0	1508	11	0
3	M	1473	0	1250	7	0
4	A	1	0	0	0	0
4	B	1	0	0	1	0
4	L	3	0	0	0	0
All	All	10921	0	9859	98	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 5.

All (98) 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:H:47:TRP:HE1	2:H:50:THR:HG1	1.34	0.76
1:B:255:PRO:O	1:B:368:LYS:NZ	2.19	0.75
3:L:108:ARG:HD2	3:L:171:SER:HB2	1.69	0.73
3:L:61:ARG:NH2	3:L:82:ASP:OD1	2.24	0.71
1:A:39:ARG:NH2	1:A:267:LEU:O	2.23	0.70
3:M:198:HIS:H	3:M:201:SER:HB3	1.60	0.66
2:I:47:TRP:HE1	2:I:50:THR:HG1	1.44	0.65
3:L:27(B):VAL:HA	3:L:92:LYS:HD2	1.79	0.64
1:A:238:TRP:HB2	1:A:254:LEU:HB3	1.82	0.62
2:H:22:CYS:HB3	2:H:78:LEU:HB3	1.83	0.60
1:A:282:ARG:NH1	2:I:100(B):THR:O	2.34	0.60
2:I:22:CYS:HB3	2:I:78:LEU:HB3	1.83	0.60
3:L:13:VAL:HG21	3:L:19:ALA:HB2	1.84	0.58
2:I:163:ALA:HB2	2:I:172:LEU:HD23	1.87	0.57
1:A:287:HIS:HB2	1:A:365:LYS:HA	1.87	0.56
2:H:55:ASP:OD1	2:H:55:ASP:N	2.38	0.56
1:A:116:ASN:OD1	1:A:186:ASN:ND2	2.28	0.56
1:B:116:ASN:OD1	1:B:186:ASN:ND2	2.35	0.56
2:H:34:MET:HB3	2:H:78:LEU:HD22	1.88	0.55
1:B:374:MET:HB2	1:B:384:PHE:HB2	1.87	0.55
1:B:30:LEU:HD21	1:B:55:VAL:HG12	1.88	0.55
3:M:76:HIS:HB3	3:M:77:PRO:CD	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:119:PRO:HB3	2:I:140:TYR:HB3	1.87	0.55
1:A:165:THR:HG21	1:A:169:ILE:HD12	1.88	0.54
3:M:108:ARG:HD2	3:M:171:SER:HB2	1.90	0.54
3:M:76:HIS:HB3	3:M:77:PRO:HD2	1.89	0.54
1:A:224:LEU:HD12	1:A:285:SER:HB2	1.90	0.53
1:B:287:HIS:HB2	1:B:365:LYS:HA	1.90	0.53
1:A:208:PHE:N	1:A:216:VAL:O	2.35	0.52
2:I:52:SER:O	2:I:71:ARG:NH1	2.42	0.52
1:B:39:ARG:NH2	1:B:267:LEU:O	2.43	0.51
3:M:66:GLY:HA3	3:M:71:PHE:HA	1.92	0.51
1:A:255:PRO:O	1:A:368:LYS:NZ	2.28	0.51
1:B:51:PHE:CZ	1:B:338:LEU:HB2	2.46	0.51
2:I:143:GLU:HG3	2:I:144:PRO:HA	1.91	0.51
1:A:288:LEU:HD12	1:A:289:PRO:HD2	1.93	0.51
1:B:186:ASN:ND2	4:B:401:HOH:O	2.39	0.50
1:B:288:LEU:HD12	1:B:289:PRO:HD2	1.93	0.50
3:L:35:TRP:HB2	3:L:48:ILE:HB	1.94	0.50
3:L:61:ARG:HH21	3:L:82:ASP:CG	2.15	0.50
2:H:66:ARG:NH2	2:H:86:ASP:OD2	2.45	0.49
1:A:76:ILE:HD11	1:A:311:VAL:HG11	1.93	0.49
2:H:168:ASP:O	2:H:169:LEU:HG	2.12	0.49
1:B:251:ILE:HD11	1:B:276:LEU:HD21	1.95	0.49
1:A:216:VAL:HG11	1:A:390:ASN:OD1	2.13	0.49
1:B:294:THR:HG23	1:B:337:VAL:HG22	1.95	0.49
2:H:87:THR:HG23	2:H:110:THR:HA	1.96	0.48
1:B:27:THR:HG21	1:B:379:THR:O	2.14	0.48
2:H:165:LEU:HB2	2:H:170:TYR:CE1	2.48	0.48
1:B:119:PHE:HA	1:B:143:PHE:O	2.13	0.48
1:B:169:ILE:HG23	1:B:335:LYS:HD3	1.96	0.48
1:A:375:ILE:HD13	1:A:382:PRO:HA	1.96	0.48
1:B:371:VAL:HG22	1:B:387:LYS:HG3	1.96	0.48
1:A:202:ASP:OD1	1:A:202:ASP:N	2.47	0.47
2:I:189:THR:HA	2:I:204:LYS:HA	1.95	0.47
1:A:294:THR:HG22	1:A:337:VAL:HG13	1.96	0.47
2:I:55:ASP:N	2:I:55:ASP:OD1	2.44	0.47
3:L:27(C):ASP:O	3:L:92:LYS:NZ	2.48	0.47
2:I:34:MET:HB3	2:I:78:LEU:HD22	1.97	0.46
1:A:51:PHE:CZ	1:A:338:LEU:HB2	2.50	0.46
1:A:27:THR:HG21	1:A:379:THR:O	2.16	0.46
1:A:113:THR:O	1:A:188:ILE:HA	2.16	0.46
1:A:203:THR:HB	1:A:221:MET:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:MET:HB2	1:A:384:PHE:HB2	1.98	0.45
1:B:157:ILE:HD12	1:B:157:ILE:H	1.82	0.45
1:A:254:LEU:HB2	1:A:366:PHE:CE2	2.52	0.45
1:B:235:LEU:HD23	1:B:266:GLU:HB3	1.99	0.45
1:A:89:GLU:N	1:A:89:GLU:OE2	2.49	0.44
1:A:255:PRO:HG3	1:A:260:LEU:HD12	1.99	0.44
2:I:139:GLY:HA2	2:I:169:LEU:HB3	1.98	0.44
3:M:167:ASP:C	3:M:169:LYS:H	2.20	0.44
1:A:68:THR:HG22	1:A:318:LEU:HD23	1.99	0.44
1:B:360:ILE:HD12	3:L:96:TRP:CZ2	2.53	0.44
1:A:359:SER:HA	3:M:94:VAL:HG23	2.00	0.44
1:A:69:LYS:O	1:A:73:HIS:N	2.34	0.44
1:B:329:LEU:HD21	1:B:332:ALA:HB2	2.00	0.43
2:I:32:TYR:CD1	2:I:94:ARG:HD3	2.53	0.43
2:I:141:PHE:HA	2:I:142:PRO:HA	1.78	0.43
3:L:150:ILE:HD11	3:L:179:LEU:HD21	1.99	0.43
2:H:141:PHE:HB2	2:H:169:LEU:HD13	2.00	0.43
1:A:177:ASP:OD1	1:A:178:ARG:N	2.52	0.42
1:A:35:PHE:HZ	1:A:272:ILE:HD12	1.82	0.42
1:B:71:ASP:OD1	1:B:72:THR:N	2.53	0.42
1:B:161:VAL:HG21	1:B:172:LEU:HD12	2.02	0.42
2:I:2:VAL:HG22	2:I:94:ARG:HH22	1.84	0.42
3:L:119:PRO:HB3	3:L:209:PHE:CE2	2.55	0.41
2:I:24:ALA:HB1	2:I:27:PHE:CE1	2.56	0.41
3:L:136:LEU:HD13	3:L:175:MET:HE3	2.01	0.41
2:H:124:LEU:HB2	2:H:134:GLY:HA3	2.02	0.41
2:I:191:ASN:HA	2:I:201:VAL:O	2.20	0.41
1:A:369:PRO:HA	1:A:388:VAL:O	2.20	0.41
1:A:299:LEU:HA	1:A:302:VAL:HG22	2.03	0.41
1:B:231:HIS:O	2:H:100(B):THR:HA	2.20	0.41
1:B:376:GLU:HG3	1:B:383:LEU:HB2	2.03	0.41
2:H:119:PRO:HB3	2:H:140:TYR:HB3	2.01	0.41
2:I:143:GLU:CG	2:I:144:PRO:HA	2.51	0.41
2:I:194:HIS:HB3	2:I:198:SER:CB	2.51	0.41
1:A:205:GLU:HA	1:A:219:PRO:HA	2.02	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	330/397 (83%)	317 (96%)	13 (4%)	0	100	100
1	B	309/397 (78%)	295 (96%)	14 (4%)	0	100	100
2	H	218/228 (96%)	213 (98%)	4 (2%)	1 (0%)	29	64
2	I	194/228 (85%)	190 (98%)	4 (2%)	0	100	100
3	L	215/217 (99%)	208 (97%)	7 (3%)	0	100	100
3	M	204/217 (94%)	194 (95%)	9 (4%)	1 (0%)	29	64
All	All	1470/1684 (87%)	1417 (96%)	51 (4%)	2 (0%)	51	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	77	PRO
2	H	169	LEU

5.3.2 Protein sidechains [i](#)

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	220/350 (63%)	218 (99%)	2 (1%)	78	91
1	B	205/350 (59%)	204 (100%)	1 (0%)	88	95
2	H	178/196 (91%)	178 (100%)	0	100	100
2	I	139/196 (71%)	137 (99%)	2 (1%)	67	86
3	L	176/190 (93%)	176 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	M	138/190 (73%)	138 (100%)	0	100	100
All	All	1056/1472 (72%)	1051 (100%)	5 (0%)	88	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	LEU
1	A	198	PHE
1	B	327	LEU
2	I	38	ARG
2	I	145	VAL

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	A	344/397 (86%)	-0.09	4 (1%) 79 63	54, 81, 107, 119	0
1	B	325/397 (81%)	0.03	9 (2%) 53 36	40, 82, 110, 120	0
2	H	222/228 (97%)	-0.32	0 100 100	37, 49, 72, 102	0
2	I	204/228 (89%)	0.12	4 (1%) 65 48	61, 88, 107, 114	0
3	L	217/217 (100%)	-0.35	0 100 100	33, 48, 70, 80	0
3	M	210/217 (96%)	0.11	2 (0%) 82 68	63, 91, 111, 118	0
All	All	1522/1684 (90%)	-0.08	19 (1%) 79 63	33, 76, 107, 120	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	71	ASP	4.3
1	A	235	LEU	4.1
1	B	329	LEU	3.2
1	B	64	LEU	3.0
2	I	125	ALA	3.0
1	B	376	GLU	2.8
2	I	187	THR	2.7
1	A	271	ILE	2.7
1	B	91	GLN	2.6
3	M	184	ASP	2.6
2	I	126	PRO	2.6
2	I	100	THR	2.5
1	A	128	ASP	2.4
3	M	130	ALA	2.4
1	B	23	PHE	2.4
1	A	232	CYS	2.3
1	B	180	THR	2.2
1	B	275	PHE	2.1
1	B	384	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 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.