Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:42 PM GMT

PDB ID	:	1LK3
Title	:	ENGINEERED HUMAN INTERLEUKIN-10 MONOMER COMPLEXED TO 9D7 FAB FRAGMENT
Authors	:	Josephson, K.; Jones, B.C.; Walter, L.J.; DiGiacomo, R.; Indelicato, S.R.; Walter, M.R.
Deposited on	:	2002-04-23
Resolution	:	1.91 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

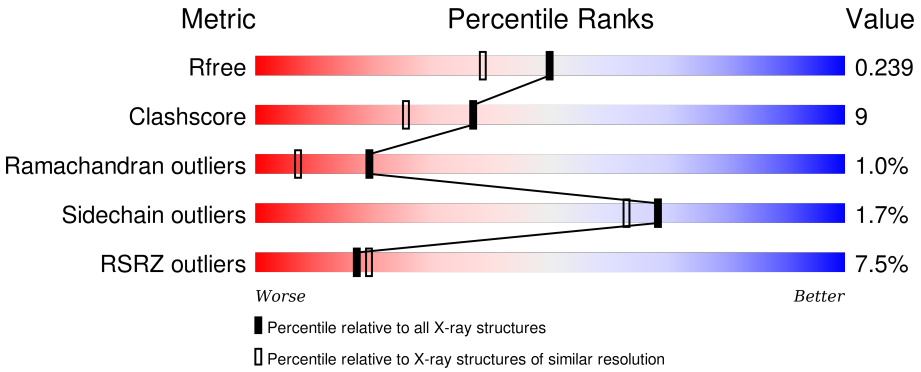
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.91 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}	91344	5832 (1.94-1.90)
Clashscore	102246	6540 (1.94-1.90)
Ramachandran outliers	100387	6464 (1.94-1.90)
Sidechain outliers	100360	6465 (1.94-1.90)
RSRZ outliers	91569	5846 (1.94-1.90)

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 <=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	160	16% 63% 21% • 15%
1	B	160	26% 51% 32% •• 15%
2	L	210	92% 8%
2	M	210	% 88% 12%
3	H	219	4% 87% 11% •

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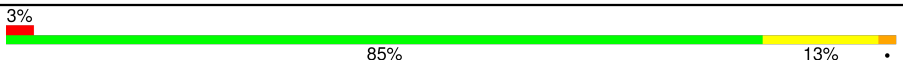
Mol	Chain	Length	Quality of chain
3	I	219	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9973 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 Interleukin-10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	136	Total	C	N	O	S	0	0	0
			1127	718	193	206	10			
1	B	136	Total	C	N	O	S	0	0	0
			1127	718	193	206	10			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	INITIATING METHIONINE	UNP P22301
A	116A	GLY	-	INSERTION	UNP P22301
A	116B	GLY	-	INSERTION	UNP P22301
A	116C	GLY	-	INSERTION	UNP P22301
A	116D	SER	-	INSERTION	UNP P22301
A	116E	GLY	-	INSERTION	UNP P22301
A	116F	GLY	-	INSERTION	UNP P22301
B	7	MET	-	INITIATING METHIONINE	UNP P22301
B	116A	GLY	-	INSERTION	UNP P22301
B	116B	GLY	-	INSERTION	UNP P22301
B	116C	GLY	-	INSERTION	UNP P22301
B	116D	SER	-	INSERTION	UNP P22301
B	116E	GLY	-	INSERTION	UNP P22301
B	116F	GLY	-	INSERTION	UNP P22301

- Molecule 2 is a protein called 9D7 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	210	Total	C	N	O	S	0	0	0
			1600	1000	268	325	7			
2	M	210	Total	C	N	O	S	0	0	0
			1600	1000	268	325	7			

- Molecule 3 is a protein called 9D7 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	219	Total	C	N	O	S	0	0	0
			1658	1055	274	323	6			
3	I	219	Total	C	N	O	S	0	0	0
			1658	1055	274	323	6			

- Molecule 4 is water.

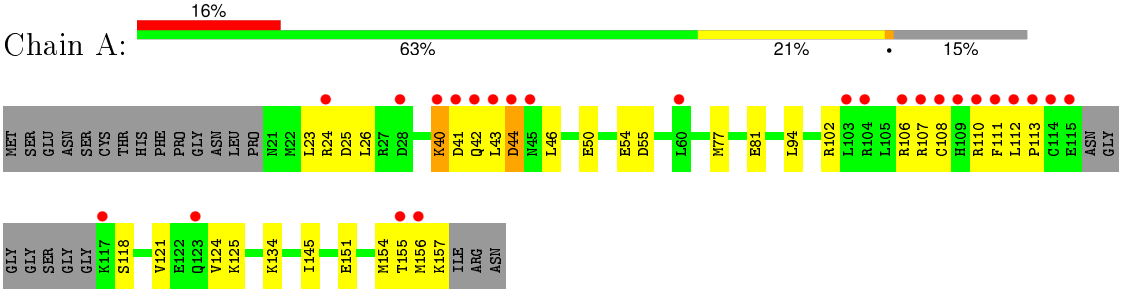
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	72	Total	O	0	0
			72	72		
4	B	36	Total	O	0	0
			36	36		
4	H	296	Total	O	0	0
			296	296		
4	I	262	Total	O	0	0
			262	262		
4	L	288	Total	O	0	0
			288	288		
4	M	249	Total	O	0	0
			249	249		

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 errors 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.

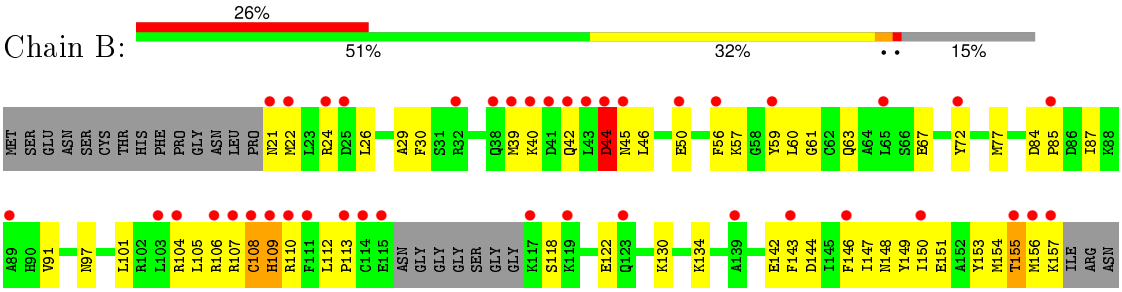
- Molecule 1: Interleukin-10

Chain A:



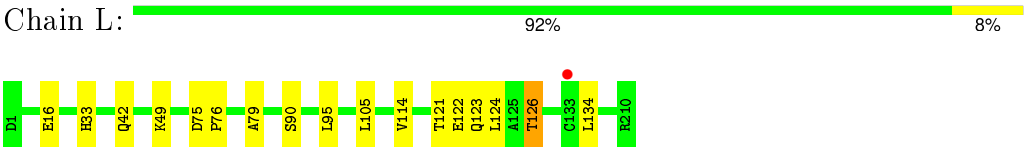
- Molecule 1: Interleukin-10

Chain B:



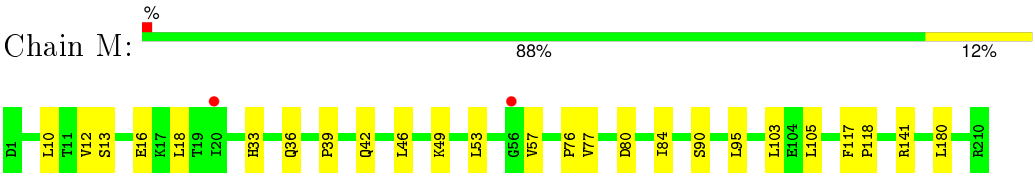
- Molecule 2: 9D7 Light Chain

Chain L:



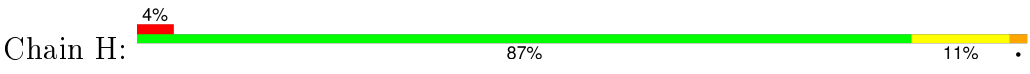
- Molecule 2: 9D7 Light Chain

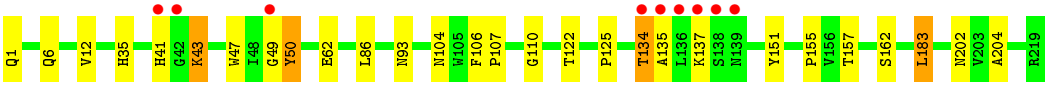
Chain M:



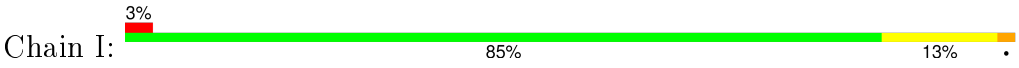
- Molecule 3: 9D7 Heavy Chain

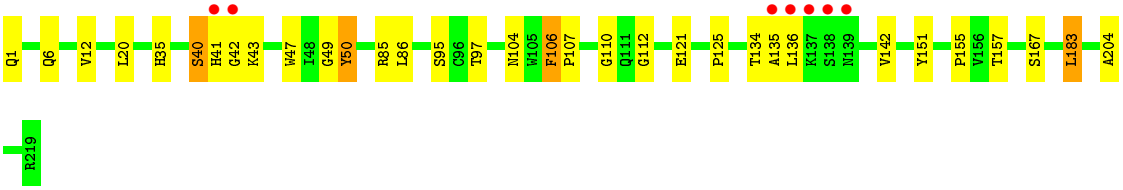
Chain H:





- Molecule 3: 9D7 Heavy Chain





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.55Å 75.62Å 111.97Å 90.00° 96.85° 90.00°	Depositor
Resolution (Å)	50.00 – 1.91 22.39 – 1.91	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-1.91) 90.8 (22.39-1.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 1.90Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.187 , 0.240 0.187 , 0.239	Depositor DCC
R_{free} test set	1397 reflections (1.44%)	DCC
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 56.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 96708 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9973	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.14 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.3162e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.48	0/1144	0.61	0/1527
1	B	0.44	0/1144	0.62	0/1527
2	L	0.54	0/1635	0.75	0/2224
2	M	0.55	0/1635	0.76	0/2224
3	H	0.54	0/1704	0.80	1/2331 (0.0%)
3	I	0.52	0/1704	0.80	2/2331 (0.1%)
All	All	0.52	0/8966	0.74	3/12164 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	43	LYS	N-CA-C	6.14	127.57	111.00
3	I	106	PHE	N-CA-C	5.61	126.15	111.00
3	I	183	LEU	CA-CB-CG	5.22	127.31	115.30

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	1127	0	1136	31	0
1	B	1127	0	1136	49	0
2	L	1600	0	1564	15	0
2	M	1600	0	1564	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1658	0	1629	24	0
3	I	1658	0	1629	27	0
4	A	72	0	0	2	0
4	B	36	0	0	0	0
4	H	296	0	0	4	1
4	I	262	0	0	5	0
4	L	288	0	0	3	1
4	M	249	0	0	4	0
All	All	9973	0	8658	163	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 9.

All (163) 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)
3:I:85:ARG:HG3	4:I:391:HOH:O	1.59	1.00
2:M:84:ILE:HD13	3:I:43:LYS:HD2	1.42	0.99
3:H:162:SER:H	3:H:202:ASN:HD21	1.13	0.93
3:I:35:HIS:HD2	3:I:47:TRP:HE1	1.21	0.88
3:H:35:HIS:HD2	3:H:47:TRP:HE1	1.17	0.87
2:M:13:SER:HB2	2:M:16:GLU:OE1	1.75	0.85
1:A:111:PHE:HA	1:A:157:LYS:HE2	1.63	0.79
1:B:42:GLN:NE2	1:B:134:LYS:HE3	1.96	0.79
2:M:12:VAL:HG12	2:M:103:LEU:HD11	1.67	0.77
2:M:33:HIS:HD2	2:M:49:LYS:H	1.32	0.76
3:H:35:HIS:CD2	3:H:47:TRP:HE1	2.02	0.75
2:M:33:HIS:CD2	2:M:49:LYS:H	2.05	0.74
2:L:33:HIS:HD2	2:L:49:LYS:H	1.35	0.74
3:I:42:GLY:O	3:I:43:LYS:HG2	1.89	0.73
2:L:33:HIS:CD2	2:L:49:LYS:H	2.08	0.72
2:M:39:PRO:HG2	4:M:397:HOH:O	1.89	0.72
3:I:35:HIS:CD2	3:I:47:TRP:HE1	2.08	0.70
3:H:35:HIS:HD2	3:H:47:TRP:NE1	1.92	0.68
2:L:16:GLU:HG3	4:L:483:HOH:O	1.95	0.67
1:B:21:ASN:CG	1:B:22:MET:H	1.99	0.66
1:A:112:LEU:N	1:A:113:PRO:HD3	2.11	0.66
1:A:50:GLU:O	1:A:54:GLU:HG3	1.96	0.66
1:B:112:LEU:N	1:B:113:PRO:HD3	2.11	0.65
3:H:12:VAL:HG21	3:H:86:LEU:HD13	1.78	0.65
1:B:21:ASN:O	1:B:24:ARG:HG2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:1:GLN:HB3	4:H:254:HOH:O	1.97	0.63
1:B:21:ASN:CG	1:B:22:MET:N	2.50	0.63
1:A:24:ARG:HG3	1:A:25:ASP:N	2.13	0.63
1:A:156:MET:O	1:A:157:LYS:HG3	1.99	0.62
1:B:56:PHE:CE2	1:B:149:TYR:HB3	2.34	0.61
1:A:40:LYS:O	1:A:42:GLN:N	2.33	0.61
2:L:123:GLN:O	2:L:126:THR:HB	2.00	0.61
2:M:53:LEU:HD21	2:M:57:VAL:O	2.01	0.61
1:B:118:SER:O	1:B:122:GLU:HG2	2.00	0.61
3:H:162:SER:H	3:H:202:ASN:ND2	1.94	0.61
1:B:154:MET:C	1:B:156:MET:H	2.05	0.60
3:I:35:HIS:HD2	3:I:47:TRP:NE1	1.97	0.60
1:B:155:THR:HG22	1:B:155:THR:O	2.01	0.59
2:M:33:HIS:HE1	2:M:90:SER:OG	1.84	0.59
3:H:6:GLN:HE21	3:H:110:GLY:HA3	1.68	0.59
2:M:10:LEU:HD13	2:M:18:LEU:HD11	1.84	0.59
2:L:33:HIS:HE1	2:L:90:SER:OG	1.86	0.58
1:B:105:LEU:HD21	1:B:154:MET:CE	2.33	0.58
1:B:57:LYS:HG2	1:B:156:MET:HE3	1.85	0.58
1:B:110:ARG:HD2	1:B:157:LYS:HB3	1.84	0.57
2:M:95:LEU:HD11	3:I:104:ASN:HB3	1.87	0.57
3:I:12:VAL:HG21	3:I:86:LEU:HD12	1.87	0.57
2:L:42:GLN:HA	2:L:42:GLN:HE21	1.68	0.57
2:M:77:VAL:HG22	2:M:105:LEU:HD11	1.86	0.56
3:I:42:GLY:HA3	4:I:459:HOH:O	2.05	0.56
1:B:146:PHE:O	1:B:150:ILE:HD13	2.06	0.56
1:B:56:PHE:HE2	1:B:149:TYR:HB3	1.71	0.56
3:H:1:GLN:OE1	3:H:1:GLN:HA	2.06	0.55
2:M:12:VAL:CG1	2:M:103:LEU:HD11	2.36	0.55
1:B:30:PHE:CE1	1:B:143:PHE:HB3	2.42	0.54
1:B:22:MET:HG3	1:B:104:ARG:HG3	1.88	0.54
3:I:35:HIS:HB2	3:I:97:THR:OG1	2.08	0.54
1:A:102:ARG:HD2	4:A:220:HOH:O	2.07	0.54
1:B:21:ASN:ND2	1:B:22:MET:H	2.05	0.54
1:B:130:LYS:HE3	4:M:286:HOH:O	2.08	0.54
3:I:134:THR:HG22	3:I:135:ALA:N	2.22	0.54
1:A:154:MET:C	1:A:156:MET:H	2.10	0.53
2:M:42:GLN:HE21	2:M:42:GLN:HA	1.73	0.53
1:B:87:ILE:O	1:B:91:VAL:HG23	2.08	0.53
1:A:156:MET:O	1:A:156:MET:HG2	2.09	0.53
1:A:42:GLN:C	1:A:44:ASP:H	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:43:LYS:HE2	4:H:396:HOH:O	2.07	0.53
1:A:23:LEU:HD11	1:A:154:MET:HE3	1.91	0.53
1:B:40:LYS:C	1:B:42:GLN:H	2.13	0.52
1:A:77:MET:O	1:A:81:GLU:HG3	2.10	0.51
3:I:134:THR:CG2	3:I:135:ALA:N	2.74	0.51
1:B:56:PHE:O	1:B:61:GLY:HA3	2.11	0.51
3:I:6:GLN:NE2	3:I:112:GLY:H	2.08	0.51
2:M:16:GLU:OE1	4:M:302:HOH:O	2.19	0.50
1:A:102:ARG:HD3	1:A:106:ARG:HH11	1.75	0.50
2:M:36:GLN:HB2	2:M:46:LEU:HD11	1.93	0.50
1:A:111:PHE:CD2	1:A:157:LYS:HE3	2.46	0.50
1:B:63:GLN:O	1:B:67:GLU:HG3	2.11	0.50
1:B:57:LYS:HB3	1:B:156:MET:HE1	1.94	0.49
1:A:155:THR:O	1:A:155:THR:HG22	2.11	0.49
1:B:110:ARG:HG3	1:B:157:LYS:HB3	1.94	0.49
3:H:162:SER:N	3:H:202:ASN:HD21	1.95	0.49
3:I:6:GLN:HE22	3:I:95:SER:HA	1.78	0.49
1:B:29:ALA:HB2	1:B:97:ASN:ND2	2.28	0.49
3:H:47:TRP:CZ2	3:H:49:GLY:HA2	2.48	0.49
3:I:47:TRP:CZ2	3:I:49:GLY:HA2	2.48	0.48
1:A:23:LEU:HD11	1:A:154:MET:CE	2.43	0.48
1:A:151:GLU:HA	1:A:154:MET:HE2	1.95	0.48
2:L:122:GLU:HB2	4:L:482:HOH:O	2.13	0.48
2:L:42:GLN:NE2	2:L:42:GLN:HA	2.28	0.48
3:I:42:GLY:O	3:I:43:LYS:CG	2.59	0.48
3:H:41:HIS:HA	3:H:43:LYS:NZ	2.28	0.48
3:H:134:THR:HG23	3:H:135:ALA:N	2.28	0.48
1:B:39:MET:CE	1:B:42:GLN:HE22	2.26	0.48
2:M:80:ASP:HB2	4:M:303:HOH:O	2.14	0.48
3:I:50:TYR:CD1	3:I:50:TYR:C	2.87	0.47
3:I:6:GLN:HE21	3:I:110:GLY:HA3	1.79	0.47
2:M:18:LEU:HD22	2:M:103:LEU:HD13	1.96	0.47
2:L:122:GLU:HG2	4:L:498:HOH:O	2.15	0.47
1:A:107:ARG:O	1:A:107:ARG:HG2	2.15	0.47
1:B:144:ASP:OD1	1:B:144:ASP:N	2.47	0.47
1:A:110:ARG:O	1:A:113:PRO:HD3	2.14	0.47
1:B:42:GLN:O	1:B:44:ASP:N	2.43	0.47
2:L:121:THR:HG21	1:B:59:TYR:CD2	2.50	0.47
2:L:95:LEU:HD11	3:H:104:ASN:HB3	1.98	0.46
1:B:105:LEU:HD21	1:B:154:MET:HE3	1.98	0.46
1:B:148:ASN:O	1:B:151:GLU:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:LEU:HD21	1:B:154:MET:HE2	1.98	0.45
1:A:118:SER:HB3	1:A:121:VAL:HB	1.99	0.45
1:B:110:ARG:CG	1:B:157:LYS:HB3	2.46	0.45
2:M:53:LEU:HD11	2:M:57:VAL:HG12	1.98	0.45
1:A:42:GLN:O	1:A:44:ASP:N	2.38	0.45
1:B:153:TYR:O	1:B:156:MET:HB3	2.16	0.45
1:A:46:LEU:HD11	1:A:145:ILE:HD13	1.98	0.45
1:B:30:PHE:CD1	1:B:143:PHE:HB3	2.52	0.45
1:B:60:LEU:HD22	1:B:63:GLN:NE2	2.32	0.45
3:H:183:LEU:HD12	3:H:183:LEU:C	2.37	0.45
2:L:79:ALA:HA	2:L:105:LEU:HG	1.98	0.44
3:I:85:ARG:N	4:I:391:HOH:O	2.49	0.44
3:H:125:PRO:HB3	3:H:151:TYR:HB3	1.98	0.44
3:I:125:PRO:HB3	3:I:151:TYR:HB3	2.00	0.44
1:B:72:TYR:O	1:B:77:MET:HG3	2.17	0.44
1:B:154:MET:C	1:B:156:MET:N	2.70	0.44
3:I:157:THR:OG1	3:I:204:ALA:HB3	2.18	0.43
2:L:75:ASP:HA	2:L:76:PRO:HA	1.90	0.43
3:I:106:PHE:HA	3:I:107:PRO:HD2	1.95	0.43
2:L:124:LEU:C	2:L:126:THR:H	2.21	0.43
1:B:60:LEU:HD22	1:B:63:GLN:HE22	1.83	0.43
3:I:20:LEU:HB3	4:I:353:HOH:O	2.18	0.43
1:A:42:GLN:OE1	1:A:134:LYS:HE3	2.19	0.43
1:B:107:ARG:O	1:B:108:CYS:HB2	2.19	0.43
3:H:157:THR:OG1	3:H:204:ALA:HB3	2.18	0.42
3:H:122:THR:HG23	4:H:414:HOH:O	2.18	0.42
1:A:121:VAL:HG12	1:A:125:LYS:HE3	2.01	0.42
1:B:110:ARG:CD	1:B:157:LYS:HB3	2.49	0.42
3:I:40:SER:O	3:I:41:HIS:C	2.58	0.42
1:A:154:MET:C	1:A:156:MET:N	2.73	0.42
3:H:12:VAL:CG2	3:H:86:LEU:HD13	2.48	0.42
1:A:77:MET:HE1	1:A:94:LEU:HG	2.02	0.42
1:B:26:LEU:HD22	1:B:101:LEU:HD22	2.01	0.42
1:A:106:ARG:N	1:A:112:LEU:HD12	2.34	0.42
2:M:180:LEU:N	2:M:180:LEU:HD23	2.35	0.42
1:B:46:LEU:HA	1:B:142:GLU:OE1	2.20	0.41
2:L:114:VAL:HA	2:L:134:LEU:O	2.20	0.41
3:H:1:GLN:N	4:H:437:HOH:O	2.44	0.41
3:I:136:LEU:HD11	3:I:142:VAL:HB	2.02	0.41
3:H:50:TYR:CD1	3:H:50:TYR:C	2.93	0.41
2:M:141:ARG:HG2	2:M:141:ARG:HH11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:PHE:CD2	1:B:149:TYR:HB3	2.56	0.41
1:B:147:ILE:O	1:B:150:ILE:HB	2.20	0.41
1:B:150:ILE:O	1:B:154:MET:HG3	2.20	0.41
1:A:26:LEU:HD12	1:A:94:LEU:HD12	2.03	0.41
1:A:124:VAL:HG23	4:A:194:HOH:O	2.20	0.41
3:H:106:PHE:HA	3:H:107:PRO:HD2	1.93	0.41
3:I:1:GLN:HA	3:I:1:GLN:OE1	2.20	0.41
1:B:109:HIS:HB3	1:B:110:ARG:H	1.73	0.40
2:M:117:PHE:HA	2:M:118:PRO:HD3	1.93	0.40
3:H:134:THR:O	3:H:135:ALA:HB3	2.22	0.40
1:B:50:GLU:HG3	1:B:50:GLU:H	1.61	0.40
3:I:35:HIS:HE1	4:I:378:HOH:O	2.03	0.40
1:A:110:ARG:O	1:A:157:LYS:HE2	2.20	0.40
1:A:23:LEU:HD21	1:A:154:MET:HE1	2.04	0.40
1:B:84:ASP:HA	1:B:85:PRO:HD3	1.96	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)
4:L:441:HOH:O	4:H:233:HOH:O[2_655]	2.10	0.10

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	132/160 (82%)	121 (92%)	6 (4%)	5 (4%)	4 0
1	B	132/160 (82%)	118 (89%)	9 (7%)	5 (4%)	4 0
2	L	208/210 (99%)	203 (98%)	5 (2%)	0	100 100
2	M	208/210 (99%)	201 (97%)	7 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	H	217/219 (99%)	213 (98%)	3 (1%)	1 (0%)	34 20
3	I	217/219 (99%)	212 (98%)	5 (2%)	0	100 100
All	All	1114/1178 (95%)	1068 (96%)	35 (3%)	11 (1%)	19 7

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ASP
1	B	106	ARG
1	B	109	HIS
1	A	108	CYS
1	B	44	ASP
1	B	108	CYS
1	A	40	LYS
1	A	43	LEU
1	A	44	ASP
1	B	155	THR
3	H	137	LYS

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	124/142 (87%)	123 (99%)	1 (1%)	86 85
1	B	124/142 (87%)	122 (98%)	2 (2%)	70 65
2	L	183/183 (100%)	182 (100%)	1 (0%)	92 92
2	M	183/183 (100%)	182 (100%)	1 (0%)	92 92
3	H	188/188 (100%)	182 (97%)	6 (3%)	46 35
3	I	188/188 (100%)	182 (97%)	6 (3%)	46 35
All	All	990/1026 (96%)	973 (98%)	17 (2%)	68 63

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ASP
2	L	126	THR
3	H	50	TYR
3	H	62	GLU
3	H	93	ASN
3	H	134	THR
3	H	155	PRO
3	H	183	LEU
1	B	44	ASP
1	B	45	ASN
2	M	76	PRO
3	I	40	SER
3	I	50	TYR
3	I	121	GLU
3	I	155	PRO
3	I	167	SER
3	I	183	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	82	ASN
2	L	33	HIS
2	L	41	GLN
2	L	42	GLN
2	L	136	ASN
2	L	137	ASN
3	H	3	ASN
3	H	6	GLN
3	H	35	HIS
3	H	202	ASN
1	B	21	ASN
1	B	42	GLN
1	B	63	GLN
1	B	82	ASN
1	B	97	ASN
1	B	109	HIS
1	B	129	ASN
2	M	33	HIS
2	M	42	GLN
2	M	209	ASN
3	I	6	GLN

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Mol	Chain	Res	Type
3	I	35	HIS
3	I	54	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 carbohydrates 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

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^{th} 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	136/160 (85%)	0.86	25 (18%) 2 2	20, 35, 84, 104	0
1	B	136/160 (85%)	1.72	41 (30%) 1 0	24, 50, 89, 104	0
2	L	210/210 (100%)	-0.28	1 (0%) 91 92	16, 23, 34, 42	0
2	M	210/210 (100%)	-0.27	2 (0%) 84 86	16, 24, 37, 52	0
3	H	219/219 (100%)	-0.15	9 (4%) 41 45	16, 24, 40, 76	0
3	I	219/219 (100%)	-0.15	7 (3%) 51 55	15, 27, 44, 78	0
All	All	1130/1178 (95%)	0.15	85 (7%) 17 19	15, 26, 64, 104	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	43	LEU	18.1
1	A	108	CYS	12.1
1	A	43	LEU	10.6
3	H	136	LEU	10.4
1	B	107	ARG	10.3
3	I	136	LEU	9.7
1	B	115	GLU	9.2
1	B	42	GLN	8.7
1	B	111	PHE	8.4
1	A	107	ARG	8.2
1	B	41	ASP	7.8
1	B	59	TYR	7.5
3	H	137	LYS	7.3
1	A	111	PHE	7.2
1	A	41	ASP	7.1
3	I	137	LYS	6.9
1	B	114	CYS	6.8
3	I	42	GLY	6.7
1	A	109	HIS	6.5

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Mol	Chain	Res	Type	RSRZ
3	H	138	SER	6.2
1	B	156	MET	6.0
3	H	135	ALA	5.9
1	B	44	ASP	5.8
1	A	115	GLU	5.6
1	B	40	LYS	5.6
1	B	110	ARG	5.6
1	B	108	CYS	5.5
1	B	113	PRO	5.5
3	I	41	HIS	5.4
1	A	42	GLN	5.2
1	B	106	ARG	5.1
1	B	22	MET	5.0
1	A	110	ARG	4.7
1	B	39	MET	4.5
1	B	104	ARG	4.4
1	A	106	ARG	4.4
1	A	117	LYS	4.1
1	A	60	LEU	4.1
1	A	114	CYS	4.0
1	B	146	PHE	4.0
1	A	104	ARG	3.9
1	B	24	ARG	3.9
1	B	109	HIS	3.7
1	A	155	THR	3.6
1	A	103	LEU	3.5
1	B	45	ASN	3.5
3	I	138	SER	3.5
3	I	135	ALA	3.5
1	B	103	LEU	3.3
1	B	38	GLN	3.2
1	A	45	ASN	3.2
3	H	41	HIS	3.1
1	B	119	LYS	3.1
1	B	50	GLU	3.1
3	H	134	THR	3.0
3	I	139	ASN	3.0
1	B	155	THR	2.9
1	A	113	PRO	2.9
1	A	156	MET	2.7
1	B	139	ALA	2.7
1	A	112	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	89	ALA	2.6
1	B	72	TYR	2.6
1	A	24	ARG	2.5
1	B	157	LYS	2.5
1	B	25	ASP	2.5
1	B	56	PHE	2.4
1	A	44	ASP	2.4
3	H	139	ASN	2.3
1	B	143	PHE	2.3
2	M	56	GLY	2.3
3	H	49	GLY	2.3
3	H	42	GLY	2.2
1	B	150	ILE	2.2
2	M	20	ILE	2.2
1	A	123	GLN	2.2
1	B	85	PRO	2.2
1	A	28	ASP	2.1
2	L	133	CYS	2.1
1	A	40	LYS	2.1
1	B	65	LEU	2.1
1	B	21	ASN	2.1
1	B	32	ARG	2.0
1	B	123	GLN	2.0
1	B	117	LYS	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.