Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2023 – 06:21 PM EDT

PDB ID	:	3EOA
Title	:	Crystal structure the Fab fragment of Efalizumab in complex with LFA-1 I domain, Form I
Authors	:	Li, S.; Ding, J.
Deposited on	:	2008-09-26
Resolution	:	2.80 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:

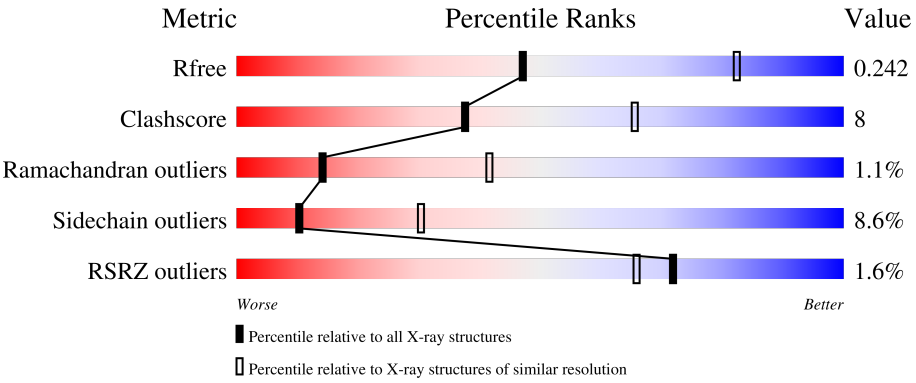
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	214	72% 25%
1	L	214	3% 71% 23% 6%
2	B	220	81% 15%
2	H	220	78% 18%
3	I	181	75% 20%

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Mol	Chain	Length	Quality of chain
3	J	181	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9804 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 Efalizumab Fab fragment, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1646	1030	276	334	6			
1	A	214	Total	C	N	O	S	0	0	0
			1646	1030	276	334	6			

- Molecule 2 is a protein called Efalizumab Fab fragment, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	215	Total	C	N	O	S	0	0	0
			1640	1043	273	317	7			
2	B	215	Total	C	N	O	S	0	0	0
			1640	1043	273	317	7			

- Molecule 3 is a protein called Integrin alpha-L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	179	Total	C	N	O	S	0	0	0
			1438	929	231	274	4			
3	J	179	Total	C	N	O	S	0	0	0
			1438	929	231	274	4			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	36	Total	O	0	0
			36	36		
4	A	80	Total	O	0	0
			80	80		
4	H	66	Total	O	0	0
			66	66		
4	B	64	Total	O	0	0
			64	64		

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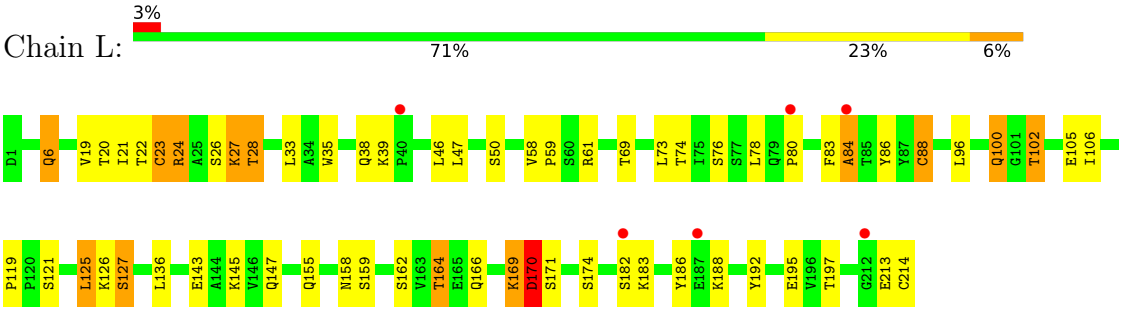
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	60	Total O 60 60	0	0
4	J	50	Total O 50 50	0	0

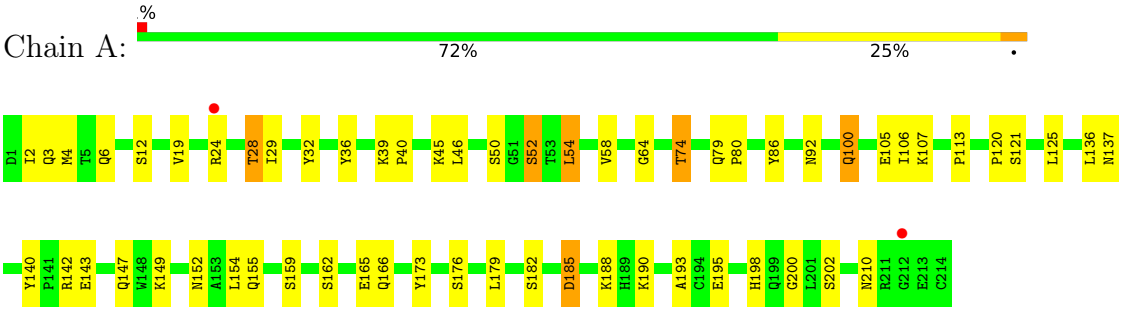
3 Residue-property plots

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.

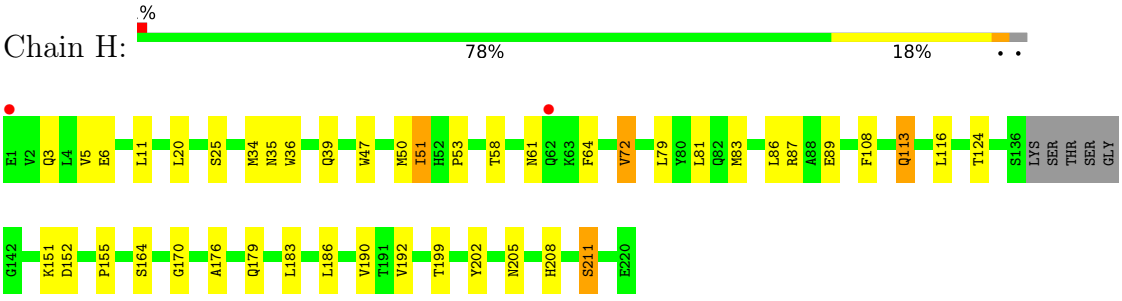
• Molecule 1: Efalizumab Fab fragment, light chain



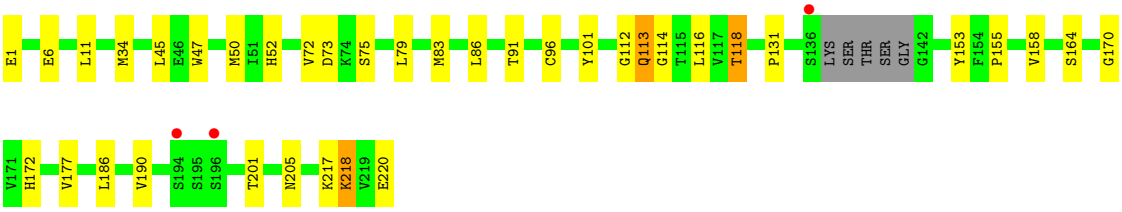
• Molecule 1: Efalizumab Fab fragment, light chain



• Molecule 2: Efalizumab Fab fragment, heavy chain

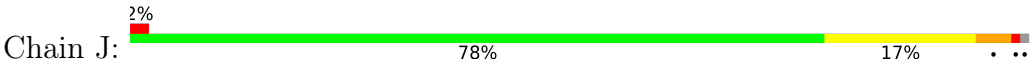


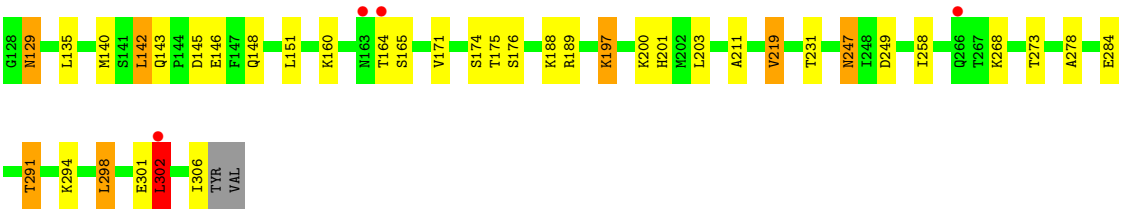
• Molecule 2: Efalizumab Fab fragment, heavy chain



• Molecule 3: Integrin alpha-L

• Molecule 3: Integrin alpha-L





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.72Å 81.70Å 281.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 49.93 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.00-2.80) 98.1 (49.93-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	3.09 (at 2.81Å)	Xtriage
Refinement program	CNS, REFMAC 5.2.0019	Depositor
R, R_{free}	0.225 , 0.264 0.233 , 0.242	Depositor DCC
R_{free} test set	1856 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	36.6	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 47.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9804	wwPDB-VP
Average B, all atoms (Å^2)	31.0	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 24.04 % 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 4.1410e-03. 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, 0.333 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	0.39	1/1681 (0.1%)	0.52	0/2280
1	L	0.54	3/1681 (0.2%)	0.56	1/2280 (0.0%)
2	B	0.37	0/1683	0.54	0/2291
2	H	0.37	0/1683	0.53	0/2291
3	I	0.46	0/1465	0.57	1/1970 (0.1%)
3	J	0.52	1/1465 (0.1%)	0.58	1/1970 (0.1%)
All	All	0.45	5/9658 (0.1%)	0.55	3/13082 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	302	LEU	N-CA	9.21	1.64	1.46
1	L	121	SER	CB-OG	7.37	1.51	1.42
1	L	50	SER	CB-OG	5.34	1.49	1.42
1	L	169	LYS	CE-NZ	5.15	1.61	1.49
1	A	143	GLU	CG-CD	5.04	1.59	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	262	GLY	N-CA-C	6.38	129.04	113.10
3	J	302	LEU	N-CA-C	5.34	125.41	111.00
1	L	171	SER	N-CA-C	5.26	125.19	111.00

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	1646	0	1608	32	0
1	L	1646	0	1608	32	0
2	B	1640	0	1591	20	0
2	H	1640	0	1591	29	0
3	I	1438	0	1449	19	0
3	J	1438	0	1449	21	0
4	A	80	0	0	0	0
4	B	64	0	0	0	0
4	H	66	0	0	0	0
4	I	60	0	0	3	0
4	J	50	0	0	0	0
4	L	36	0	0	0	0
All	All	9804	0	9296	145	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 8.

All (145) 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:J:129:ASN:HB3	3:J:165:SER:HB2	1.53	0.89
2:B:164:SER:H	2:B:205:ASN:HD21	1.23	0.87
2:H:83:MET:HB3	2:H:86:LEU:HD21	1.57	0.85
1:A:2:ILE:HG22	1:A:4:MET:HE3	1.58	0.85
3:I:287:LYS:HE3	4:I:366:HOH:O	1.75	0.85
1:L:38:GLN:HE22	2:H:39:GLN:HE22	1.26	0.80
1:L:80:PRO:HA	1:L:106:ILE:HD13	1.64	0.78
2:H:164:SER:H	2:H:205:ASN:HD21	1.31	0.78
1:L:106:ILE:H	1:L:166:GLN:HE22	1.33	0.77
3:I:287:LYS:CE	4:I:366:HOH:O	2.29	0.77
2:H:51:ILE:HD12	2:H:58:THR:HG23	1.74	0.70
1:A:6:GLN:H	1:A:100:GLN:HE22	1.42	0.67
1:L:106:ILE:N	1:L:166:GLN:HE22	1.94	0.64
2:B:83:MET:HB3	2:B:86:LEU:HD21	1.79	0.64
2:B:91:THR:HG23	2:B:118:THR:HA	1.79	0.63
3:J:140:MET:HA	3:J:203:LEU:HD22	1.81	0.63
3:J:291:THR:HG23	3:J:294:LYS:HG3	1.81	0.62
1:L:147:GLN:HB3	1:L:195:GLU:HB3	1.81	0.62
3:I:164:THR:HG23	3:I:166:TYR:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:208:HIS:ND1	2:H:211:SER:HB3	2.15	0.61
2:H:113:GLN:H	2:H:113:GLN:HE21	1.48	0.60
1:A:2:ILE:HG22	1:A:4:MET:CE	2.29	0.59
3:J:129:ASN:CB	3:J:165:SER:HB2	2.31	0.59
1:A:12:SER:HA	1:A:105:GLU:O	2.02	0.59
1:A:80:PRO:HA	1:A:106:ILE:HD13	1.84	0.59
1:A:190:LYS:HD3	1:A:210:ASN:HD22	1.68	0.57
3:I:129:ASN:HB3	3:I:165:SER:HB2	1.87	0.57
3:I:287:LYS:HE2	4:I:366:HOH:O	2.01	0.57
2:H:51:ILE:HG21	2:H:79:LEU:CD1	2.35	0.57
3:J:142:LEU:HD12	3:J:146:GLU:HG3	1.86	0.57
1:L:6:GLN:H	1:L:100:GLN:HE22	1.53	0.56
1:L:26:SER:O	1:L:27:LYS:HD2	2.04	0.56
1:A:106:ILE:H	1:A:166:GLN:HE22	1.53	0.56
2:H:113:GLN:H	2:H:113:GLN:NE2	2.03	0.56
1:L:145:LYS:HB3	1:L:197:THR:HB	1.87	0.56
3:I:247:ASN:HD22	3:I:249:ASP:H	1.52	0.56
3:J:247:ASN:HD22	3:J:249:ASP:H	1.53	0.56
1:L:83:PHE:O	1:L:84:ALA:HB2	2.05	0.56
1:L:106:ILE:H	1:L:166:GLN:NE2	2.01	0.55
1:L:6:GLN:NE2	1:L:86:TYR:O	2.38	0.55
2:B:52:HIS:CE1	3:J:197:LYS:HB2	2.42	0.55
1:A:155:GLN:HG2	1:A:179:LEU:HD11	1.89	0.55
3:J:258:ILE:HG22	3:J:278:ALA:HB2	1.87	0.55
1:L:164:THR:HG22	1:L:174:SER:H	1.73	0.54
1:A:79:GLN:HG3	1:A:80:PRO:HD2	1.90	0.54
1:A:113:PRO:HD3	1:A:198:HIS:CD2	2.43	0.53
2:H:179:GLN:HG2	2:H:183:LEU:O	2.09	0.53
3:I:258:ILE:HG22	3:I:278:ALA:HB2	1.90	0.53
1:L:125:LEU:O	1:L:183:LYS:HE2	2.10	0.52
3:I:137:ASP:HB2	3:I:238:THR:HA	1.92	0.52
1:L:20:THR:HG22	1:L:74:THR:HG23	1.91	0.52
2:H:170:GLY:O	2:H:190:VAL:HA	2.10	0.52
1:A:6:GLN:NE2	1:A:86:TYR:O	2.36	0.52
2:B:131:PRO:HD3	2:B:217:LYS:HE3	1.91	0.52
1:L:155:GLN:HE21	1:L:158:ASN:HD21	1.57	0.52
2:H:5:VAL:HA	2:H:113:GLN:HE22	1.75	0.51
2:B:164:SER:H	2:B:205:ASN:ND2	2.02	0.51
1:L:125:LEU:C	1:L:127:SER:H	2.14	0.51
1:L:19:VAL:HG21	1:L:78:LEU:HD13	1.92	0.51
2:H:87:ARG:HD2	2:H:89:GLU:OE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:129:ASN:ND2	3:J:129:ASN:H	2.09	0.50
1:L:47:LEU:HA	1:L:58:VAL:HG21	1.94	0.50
1:A:2:ILE:CG2	1:A:4:MET:HE3	2.36	0.50
3:J:164:THR:HG22	3:J:165:SER:H	1.76	0.49
1:L:35:TRP:CE2	1:L:73:LEU:HB2	2.48	0.49
1:A:121:SER:O	1:A:125:LEU:HD12	2.12	0.49
2:H:51:ILE:HD12	2:H:58:THR:CG2	2.41	0.49
2:H:11:LEU:HB2	2:H:155:PRO:HG3	1.94	0.49
3:J:171:VAL:HG21	3:J:219:VAL:HG11	1.95	0.49
2:H:6:GLU:H	2:H:113:GLN:HE22	1.60	0.49
2:B:73:ASP:OD2	2:B:75:SER:HB3	2.13	0.48
1:L:96:LEU:HD12	2:H:108:PHE:HZ	1.78	0.48
1:A:142:ARG:HG3	1:A:173:TYR:CD2	2.48	0.48
2:H:34:MET:HB3	2:H:79:LEU:HD22	1.95	0.48
3:I:289:LEU:HD21	3:I:298:LEU:HD12	1.94	0.48
3:J:143:GLN:HB2	3:J:146:GLU:HG2	1.94	0.48
2:H:20:LEU:HD12	2:H:81:LEU:HD23	1.96	0.48
3:J:201:HIS:CE1	3:J:203:LEU:HD23	2.49	0.48
2:B:201:THR:HG23	2:B:218:LYS:HE2	1.96	0.48
2:B:158:VAL:CG2	2:B:186:LEU:HD21	2.44	0.48
1:A:39:LYS:HB3	1:A:40:PRO:HD2	1.95	0.48
1:A:198:HIS:CD2	1:A:200:GLY:H	2.32	0.48
2:H:164:SER:H	2:H:205:ASN:ND2	2.06	0.48
2:B:158:VAL:HG22	2:B:186:LEU:HD21	1.96	0.47
2:H:61:ASN:HB3	2:H:64:PHE:HD1	1.79	0.47
1:A:147:GLN:HB3	1:A:195:GLU:HB3	1.96	0.47
1:A:40:PRO:HB3	1:A:165:GLU:HG3	1.95	0.46
2:B:101:TYR:O	3:J:200:LYS:HD3	2.14	0.46
1:L:21:ILE:HG23	1:L:102:THR:HG21	1.97	0.46
1:L:24:ARG:HA	1:L:69:THR:O	2.14	0.46
1:A:52:SER:HB3	1:A:64:GLY:O	2.16	0.46
1:L:186:TYR:HA	1:L:192:TYR:OH	2.16	0.46
2:H:47:TRP:HZ2	2:H:50:MET:HG2	1.81	0.46
3:I:171:VAL:HG21	3:I:219:VAL:HG21	1.98	0.46
1:A:19:VAL:O	1:A:74:THR:HA	2.17	0.45
1:L:38:GLN:HE22	2:H:39:GLN:NE2	2.06	0.45
2:B:47:TRP:HZ2	2:B:50:MET:HG2	1.81	0.45
2:H:36:TRP:CE2	2:H:81:LEU:HB2	2.52	0.45
1:L:39:LYS:HD3	1:L:84:ALA:HB2	1.99	0.45
1:L:169:LYS:HB2	1:L:170:ASP:H	1.53	0.45
3:I:296:LYS:O	3:I:300:THR:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:148:GLN:HA	3:J:151:LEU:HD12	1.98	0.44
2:B:170:GLY:O	2:B:190:VAL:HA	2.18	0.44
1:L:119:PRO:HG2	1:L:214:CYS:HB3	2.00	0.44
2:H:176:ALA:HA	2:H:186:LEU:HB3	1.98	0.44
1:A:106:ILE:N	1:A:166:GLN:HE22	2.16	0.43
2:B:112:GLY:O	2:B:114:GLY:N	2.51	0.43
2:B:11:LEU:HB2	2:B:155:PRO:HG3	2.00	0.43
1:L:59:PRO:HB2	1:L:61:ARG:HG2	2.01	0.43
3:J:174:SER:HB3	3:J:175:THR:H	1.68	0.43
1:L:23:CYS:HB2	1:L:35:TRP:CH2	2.53	0.43
3:I:151:LEU:O	3:I:155:LYS:HG3	2.19	0.43
2:H:152:ASP:HB3	2:H:183:LEU:HD13	2.01	0.43
2:H:192:VAL:HG11	2:H:202:TYR:CE2	2.54	0.43
1:A:36:TYR:HA	1:A:45:LYS:O	2.19	0.42
1:A:107:LYS:HA	1:A:140:TYR:OH	2.20	0.42
3:J:164:THR:HG22	3:J:165:SER:N	2.34	0.42
1:A:190:LYS:HD3	1:A:210:ASN:ND2	2.33	0.42
2:B:34:MET:HB3	2:B:79:LEU:HD22	2.01	0.42
3:I:265:PHE:HA	3:I:270:SER:OG	2.19	0.42
3:I:227:ARG:HA	3:I:228:PRO:HD3	1.83	0.42
1:A:182:SER:OG	1:A:185:ASP:HB2	2.20	0.42
2:B:153:TYR:OH	2:B:186:LEU:HD23	2.20	0.42
1:A:28:THR:OG1	3:I:249:ASP:HB3	2.20	0.41
1:A:32:TYR:HD1	1:A:92:ASN:HD22	1.68	0.41
3:J:298:LEU:O	3:J:302:LEU:HG	2.20	0.41
3:J:135:LEU:HD11	3:J:211:ALA:HB1	2.01	0.41
1:A:125:LEU:HD12	1:A:125:LEU:H	1.85	0.41
3:J:284:GLU:HG3	3:J:284:GLU:O	2.21	0.41
1:L:100:GLN:HE21	1:L:100:GLN:N	2.19	0.41
2:B:45:LEU:N	2:B:45:LEU:HD12	2.35	0.41
3:I:288:ILE:O	3:I:288:ILE:HG13	2.20	0.41
3:J:188:LYS:HE3	3:J:188:LYS:HB2	1.86	0.41
1:A:54:LEU:HD22	1:A:58:VAL:HB	2.03	0.41
3:I:189:ARG:O	3:I:190:LYS:HB2	2.20	0.41
1:L:96:LEU:HD12	2:H:108:PHE:CZ	2.56	0.41
3:I:298:LEU:O	3:I:301:GLU:HB2	2.21	0.41
2:B:6:GLU:OE2	2:B:96:CYS:SG	2.79	0.41
3:I:220:PHE:CE1	3:I:232:LYS:HG3	2.55	0.41
1:A:137:ASN:HD21	2:B:172:HIS:CD2	2.38	0.40
2:H:53:PRO:HA	2:H:72:VAL:HG11	2.03	0.40
1:A:2:ILE:HD13	1:A:29:ILE:HG22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:LYS:HB2	1:A:193:ALA:HB3	2.04	0.40
2:H:35:ASN:OD1	2:H:50:MET:HB3	2.21	0.40
1:L:33:LEU:HD11	1:L:88:CYS:SG	2.61	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	212/214 (99%)	201 (95%)	10 (5%)	1 (0%)	29 61
1	L	212/214 (99%)	195 (92%)	12 (6%)	5 (2%)	6 20
2	B	211/220 (96%)	201 (95%)	9 (4%)	1 (0%)	29 61
2	H	211/220 (96%)	204 (97%)	7 (3%)	0	100 100
3	I	177/181 (98%)	165 (93%)	8 (4%)	4 (2%)	6 21
3	J	177/181 (98%)	163 (92%)	12 (7%)	2 (1%)	14 41
All	All	1200/1230 (98%)	1129 (94%)	58 (5%)	13 (1%)	14 41

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	84	ALA
1	L	170	ASP
1	L	213	GLU
2	B	113	GLN
3	I	262	GLY
3	J	302	LEU
3	I	263	LYS
1	L	126	LYS
3	I	174	SER

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Mol	Chain	Res	Type
3	I	283	SER
3	J	301	GLU
1	L	28	THR
1	A	120	PRO

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	189/189 (100%)	171 (90%)	18 (10%)	8 25
1	L	189/189 (100%)	167 (88%)	22 (12%)	5 17
2	B	182/186 (98%)	174 (96%)	8 (4%)	28 61
2	H	182/186 (98%)	172 (94%)	10 (6%)	21 52
3	I	159/161 (99%)	141 (89%)	18 (11%)	6 18
3	J	159/161 (99%)	144 (91%)	15 (9%)	8 26
All	All	1060/1072 (99%)	969 (91%)	91 (9%)	10 30

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	6	GLN
1	L	22	THR
1	L	23	CYS
1	L	24	ARG
1	L	27	LYS
1	L	28	THR
1	L	46	LEU
1	L	76	SER
1	L	88	CYS
1	L	100	GLN
1	L	102	THR
1	L	105	GLU
1	L	125	LEU
1	L	127	SER

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Mol	Chain	Res	Type
1	L	136	LEU
1	L	143	GLU
1	L	159	SER
1	L	162	SER
1	L	164	THR
1	L	170	ASP
1	L	182	SER
1	L	188	LYS
1	A	3	GLN
1	A	24	ARG
1	A	28	THR
1	A	46	LEU
1	A	50	SER
1	A	52	SER
1	A	54	LEU
1	A	74	THR
1	A	100	GLN
1	A	136	LEU
1	A	152	ASN
1	A	154	LEU
1	A	159	SER
1	A	162	SER
1	A	176	SER
1	A	185	ASP
1	A	188	LYS
1	A	202	SER
2	H	3	GLN
2	H	25	SER
2	H	51	ILE
2	H	72	VAL
2	H	113	GLN
2	H	116	LEU
2	H	124	THR
2	H	151	LYS
2	H	199	THR
2	H	211	SER
2	B	1	GLU
2	B	72	VAL
2	B	113	GLN
2	B	116	LEU
2	B	118	THR
2	B	177	VAL

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Mol	Chain	Res	Type
2	B	218	LYS
2	B	220	GLU
3	I	129	ASN
3	I	142	LEU
3	I	143	GLN
3	I	160	LYS
3	I	164	THR
3	I	177	TYR
3	I	189	ARG
3	I	231	THR
3	I	232	LYS
3	I	243	THR
3	I	247	ASN
3	I	252	LYS
3	I	263	LYS
3	I	266	GLN
3	I	267	THR
3	I	272	GLU
3	I	288	ILE
3	I	304	LYS
3	J	129	ASN
3	J	142	LEU
3	J	145	ASP
3	J	160	LYS
3	J	176	SER
3	J	189	ARG
3	J	197	LYS
3	J	219	VAL
3	J	231	THR
3	J	247	ASN
3	J	268	LYS
3	J	273	THR
3	J	291	THR
3	J	298	LEU
3	J	306	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	92	ASN
1	L	100	GLN
1	L	124	GLN

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Mol	Chain	Res	Type
1	L	152	ASN
1	L	155	GLN
1	L	166	GLN
1	L	199	GLN
1	A	92	ASN
1	A	100	GLN
1	A	137	ASN
1	A	166	GLN
1	A	198	HIS
2	H	3	GLN
2	H	39	GLN
2	H	113	GLN
2	H	179	GLN
2	H	200	GLN
2	H	205	ASN
2	B	84	ASN
2	B	113	GLN
2	B	205	ASN
3	I	129	ASN
3	I	247	ASN
3	I	264	HIS
3	J	129	ASN
3	J	247	ASN
3	J	266	GLN
3	J	271	GLN

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 monosaccharides 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	214/214 (100%)	-0.12	2 (0%)	84	80	14, 29, 43, 66	0
1	L	214/214 (100%)	0.38	6 (2%)	53	43	22, 38, 53, 69	0
2	B	215/220 (97%)	-0.01	3 (1%)	75	70	13, 26, 52, 66	0
2	H	215/220 (97%)	0.27	2 (0%)	84	80	20, 31, 45, 61	0
3	I	179/181 (98%)	-0.03	2 (1%)	80	75	13, 27, 45, 53	0
3	J	179/181 (98%)	0.07	4 (2%)	62	52	11, 27, 51, 61	0
All	All	1216/1230 (98%)	0.10	19 (1%)	72	66	11, 31, 48, 69	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	136	SER	3.2
1	L	212	GLY	3.1
1	A	212	GLY	2.8
3	I	163	ASN	2.5
3	J	163	ASN	2.5
2	B	194	SER	2.5
3	I	302	LEU	2.4
1	L	40	PRO	2.3
2	B	196	SER	2.3
1	L	80	PRO	2.2
3	J	302	LEU	2.2
1	L	182	SER	2.1
1	L	84	ALA	2.1
1	L	187	GLU	2.1
2	H	1	GLU	2.1
1	A	24	ARG	2.1
3	J	164	THR	2.0
3	J	266	GLN	2.0
2	H	62	GLN	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 monosaccharides 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.