Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 10:41 AM EDT

PDB ID	:	4HCR
Title	:	Crystal structure of human MAdCAM-1 D1D2 complexed with Fab PF-547659
Authors	:	Springer, T.; Yu, Y.; Zhu, J.
Deposited on	:	2012-10-01
Resolution	:	2.30 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 (i) 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 (1)) were used in the production of this report:

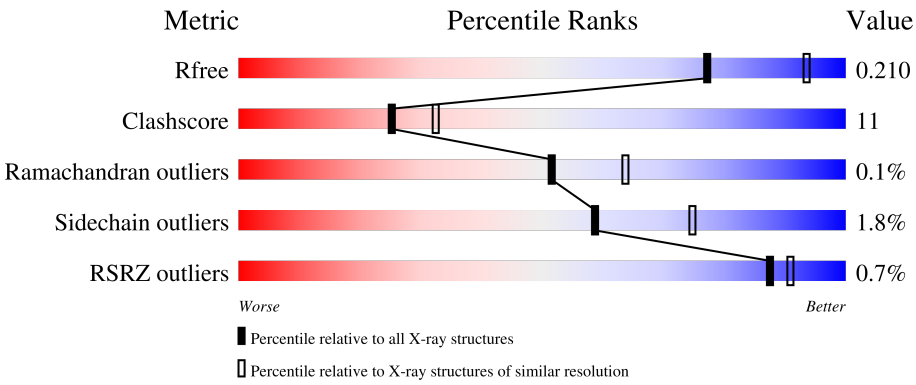
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	H	229	76% 17% • 5%
1	M	229	% 76% 19% 5%
2	L	219	84% 15%
2	N	219	80% 20%
3	A	209	% 72% 19% • 7%

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Mol	Chain	Length	Quality of chain
3	B	209	2% 62% 29% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 19974 atoms, of which 9382 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 PF-547659 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	H	217	3201	1022	1568	272	330	9	0	2	0
1	M	217	3176	1016	1554	268	329	9	0	0	0

- Molecule 2 is a protein called PF-547659 light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	L	218	3379	1079	1668	281	344	7	0	5	0
2	N	218	3379	1079	1668	281	344	7	0	5	0

- Molecule 3 is a protein called Mucosal addressin cell adhesion molecule 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	A	194	2898	907	1454	259	271	7	0	2	0
3	B	194	2925	913	1470	264	271	7	0	4	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	ASN	ASP	engineered mutation	UNP Q13477
A	204	HIS	-	expression tag	UNP Q13477
A	205	HIS	-	expression tag	UNP Q13477
A	206	HIS	-	expression tag	UNP Q13477
A	207	HIS	-	expression tag	UNP Q13477
A	208	HIS	-	expression tag	UNP Q13477
A	209	HIS	-	expression tag	UNP Q13477
B	94	ASN	ASP	engineered mutation	UNP Q13477

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Chain	Residue	Modelled	Actual	Comment	Reference
B	204	HIS	-	expression tag	UNP Q13477
B	205	HIS	-	expression tag	UNP Q13477
B	206	HIS	-	expression tag	UNP Q13477
B	207	HIS	-	expression tag	UNP Q13477
B	208	HIS	-	expression tag	UNP Q13477
B	209	HIS	-	expression tag	UNP Q13477

- Molecule 4 is water.

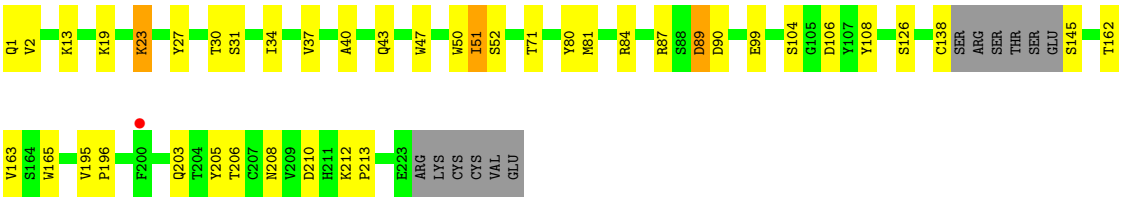
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	H	194	194	194	0	0
			Total	O		
4	L	183	183	183	0	0
			Total	O		
4	A	129	129	129	0	0
			Total	O		
4	M	194	194	194	0	0
			Total	O		
4	N	187	187	187	0	0
			Total	O		
4	B	129	129	129	0	0

3 Residue-property plots (i)

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.

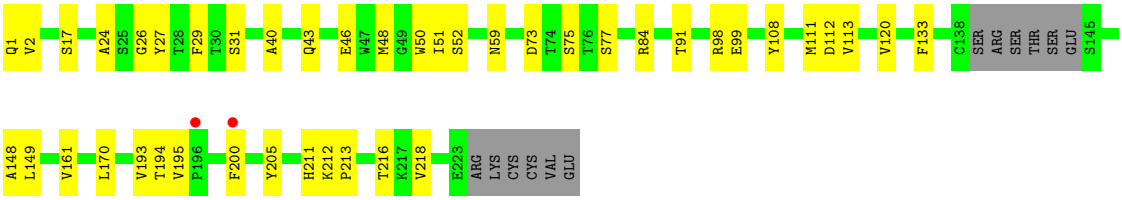
• Molecule 1: PF-547659 heavy chain

Chain H:



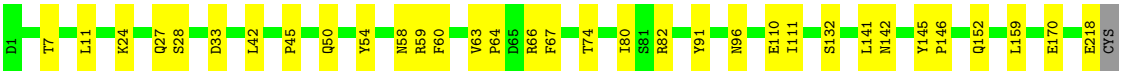
• Molecule 1: PF-547659 heavy chain

Chain M:



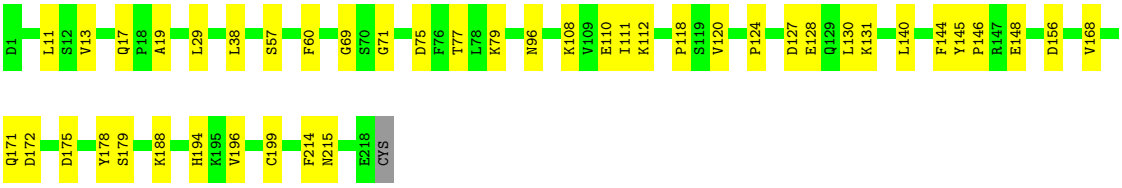
• Molecule 2: PF-547659 light chain

Chain L:



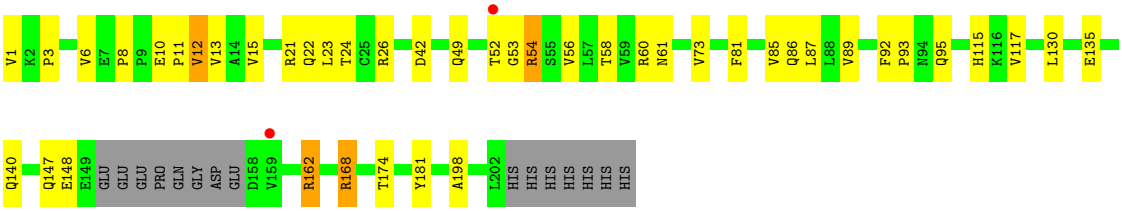
• Molecule 2: PF-547659 light chain

Chain N:



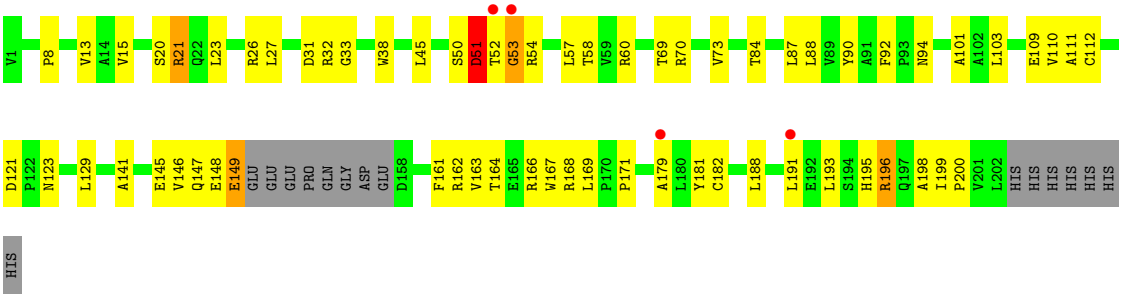
• Molecule 3: Mucosal addressin cell adhesion molecule 1

Chain A:



• Molecule 3: Mucosal addressin cell adhesion molecule 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	39.94Å 112.26Å 157.92Å 90.00° 89.95° 90.00°	Depositor
Resolution (Å)	47.66 – 2.30 47.66 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.1 (47.66-2.30) 95.9 (47.66-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.76 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.153 , 0.208 0.156 , 0.210	Depositor DCC
R_{free} test set	1010 reflections (1.70%)	wwPDB-VP
Wilson B-factor (Å^2)	20.6	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 37.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.468 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19974	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

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	H	0.49	0/1677	0.76	1/2287 (0.0%)
1	M	0.47	0/1660	0.71	0/2265
2	L	0.43	0/1768	0.72	0/2405
2	N	0.46	0/1768	0.71	1/2405 (0.0%)
3	A	0.54	0/1480	0.87	1/2027 (0.0%)
3	B	0.56	0/1498	0.85	1/2050 (0.0%)
All	All	0.49	0/9851	0.77	4/13439 (0.0%)

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	N	0	1
3	B	0	3
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	12	VAL	CA-CB-CG2	-6.62	100.98	110.90
2	N	11	LEU	CB-CG-CD2	6.35	121.79	111.00
1	H	89	ASP	CB-CA-C	-5.18	100.03	110.40
3	B	193	LEU	CB-CG-CD2	-5.16	102.23	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	147	GLN	Mainchain

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Mol	Chain	Res	Type	Group
3	B	149	GLU	Sidechain
3	B	51	ASP	Peptide
2	N	148	GLU	Sidechain

5.2 Too-close contacts (i)

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	H	1633	1568	1564	34	2
1	M	1622	1554	1556	26	0
2	L	1711	1668	1666	23	2
2	N	1711	1668	1666	26	0
3	A	1444	1454	1451	44	0
3	B	1455	1470	1462	53	0
4	A	129	0	0	2	0
4	B	129	0	0	6	0
4	H	194	0	0	8	0
4	L	183	0	0	3	0
4	M	194	0	0	2	0
4	N	187	0	0	3	0
All	All	10592	9382	9365	203	2

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 11.

All (203) 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:A:12:VAL:HG22	3:A:86:GLN:HB3	1.21	1.15
3:A:12:VAL:CG2	3:A:86:GLN:HB3	1.90	1.00
3:B:8:PRO:HD2	3:B:23:LEU:HD23	1.52	0.91
2:N:108:LYS:NZ	4:N:474:HOH:O	2.03	0.90
3:A:12:VAL:HG22	3:A:86:GLN:CB	2.05	0.87
1:H:89:ASP:OD1	1:H:89:ASP:C	2.16	0.82
3:B:103:LEU:HD11	3:B:110:VAL:HG21	1.66	0.76
1:H:84[B]:ARG:NH1	4:H:440:HOH:O	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:162:THR:OG1	1:H:210:ASP:HB3	1.90	0.71
1:H:89:ASP:OD1	1:H:90:ASP:N	2.24	0.71
3:B:8:PRO:HD2	3:B:23:LEU:CD2	2.24	0.68
3:B:110:VAL:HG23	3:B:169:LEU:HD11	1.77	0.66
3:A:148:GLU:H	3:A:148:GLU:CD	1.98	0.66
1:H:1:GLN:N	4:H:389:HOH:O	2.27	0.66
3:A:147:GLN:OE1	4:A:317:HOH:O	2.14	0.65
1:H:99:GLU:HG2	1:H:108:TYR:OH	1.98	0.64
2:N:108:LYS:HE2	4:N:470:HOH:O	1.97	0.64
1:H:145:SER:O	1:H:196:PRO:HA	1.98	0.64
3:B:112:CYS:O	3:B:164:THR:HA	1.98	0.63
3:A:147:GLN:HB2	3:A:162:ARG:HG2	1.80	0.63
1:H:2:VAL:HG13	1:H:27:TYR:CD1	2.34	0.63
3:B:148:GLU:O	3:B:149:GLU:HG2	1.98	0.63
3:B:13:VAL:HG13	3:B:21:ARG:HH11	1.64	0.62
1:H:87:ARG:NE	1:H:89:ASP:OD2	2.29	0.62
3:A:54:ARG:NE	3:A:54:ARG:HA	2.14	0.61
3:A:52:THR:HG23	3:A:56:VAL:HG21	1.83	0.61
3:B:103:LEU:HD11	3:B:110:VAL:CG2	2.30	0.61
2:L:110:GLU:HG2	2:L:111:ILE:N	2.15	0.60
3:B:23:LEU:HD12	3:B:57:LEU:HD23	1.83	0.60
1:M:195:VAL:HG11	1:M:205:TYR:CE2	2.37	0.60
2:L:42:LEU:O	2:L:50:GLN:HG2	2.00	0.60
3:A:13:VAL:CG1	3:A:21:ARG:HE	2.15	0.60
1:H:51:ILE:HD13	1:H:71:THR:HA	1.83	0.60
3:B:92:PHE:O	3:B:195:HIS:HE1	1.84	0.60
3:A:22:GLN:HG3	3:A:58:THR:OG1	2.02	0.59
1:M:216:THR:HG22	1:M:218:VAL:HG23	1.84	0.59
1:M:2:VAL:HG11	1:M:113:VAL:HG21	1.84	0.59
1:H:138:CYS:O	4:H:397:HOH:O	2.17	0.59
3:A:130:LEU:HD23	3:A:135:GLU:HA	1.84	0.58
3:A:148:GLU:N	3:A:148:GLU:OE2	2.37	0.58
1:M:149:LEU:HD22	1:M:200:PHE:CE1	2.39	0.57
3:A:147:GLN:HB2	3:A:162:ARG:CG	2.35	0.57
3:A:23:LEU:HD13	3:A:85:VAL:HG11	1.87	0.57
3:A:147:GLN:CB	3:A:162:ARG:HD3	2.36	0.55
1:H:84[A]:ARG:NH1	4:H:368:HOH:O	2.40	0.55
1:M:98:ARG:O	1:M:111:MET:HA	2.07	0.55
2:N:77:THR:HG21	2:N:79:LYS:HE3	1.88	0.54
3:A:12:VAL:HG13	3:A:86:GLN:O	2.08	0.54
1:M:1:GLN:O	1:M:26:GLY:HA3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:147:GLN:HB2	3:A:162:ARG:HD3	1.89	0.54
3:A:13:VAL:HG13	3:A:21:ARG:HE	1.72	0.54
1:H:104:SER:OG	1:H:106:ASP:HB2	2.08	0.54
3:B:148:GLU:C	3:B:149:GLU:HG2	2.29	0.53
3:A:49:GLN:HA	3:A:49:GLN:OE1	2.09	0.52
1:H:1:GLN:N	1:H:1:GLN:OE1	2.39	0.52
2:N:127:ASP:O	2:N:131:LYS:HG3	2.10	0.52
2:N:156:ASP:OD2	2:N:194:HIS:HB3	2.10	0.52
3:A:162:ARG:HG2	3:A:162:ARG:O	2.10	0.51
3:B:188:LEU:HB2	3:B:191:LEU:HB3	1.92	0.51
1:M:50:TRP:CH2	1:M:52:SER:HB2	2.45	0.51
2:N:110:GLU:HG2	2:N:111:ILE:N	2.25	0.51
3:B:146:VAL:HG22	3:B:163:VAL:HG22	1.92	0.51
3:B:181:TYR:CE1	3:B:198:ALA:HB2	2.45	0.51
2:L:45:PRO:HB3	2:L:170:GLU:CD	2.31	0.51
1:H:87:ARG:NH2	1:H:89:ASP:OD2	2.43	0.51
2:L:59:ARG:HD3	2:L:67:PHE:O	2.11	0.51
2:L:152:GLN:CG	2:L:159:LEU:HD22	2.41	0.51
3:B:88:LEU:HD23	4:B:335:HOH:O	2.11	0.51
2:L:145:TYR:CG	2:L:146:PRO:HA	2.45	0.51
2:N:110:GLU:HG3	2:N:178:TYR:OH	2.10	0.51
1:H:87:ARG:HB2	1:H:89:ASP:OD1	2.11	0.50
3:A:60:ARG:O	3:A:61:ASN:C	2.49	0.50
1:M:2:VAL:HG12	1:M:113:VAL:HG11	1.93	0.50
2:N:196:VAL:HG12	2:N:215:ASN:OD1	2.12	0.50
3:B:121:ASP:OD1	3:B:123:ASN:HB2	2.12	0.49
3:A:148:GLU:CD	3:A:148:GLU:N	2.66	0.49
3:A:148:GLU:O	3:A:162:ARG:NH1	2.46	0.49
3:B:94:ASN:OD1	3:B:195:HIS:HB3	2.13	0.49
2:L:145:TYR:CD2	2:L:146:PRO:HA	2.48	0.49
3:A:148:GLU:O	3:A:162:ARG:HD2	2.13	0.48
2:L:33:ASP:HB2	3:A:1:VAL:O	2.13	0.48
1:M:161:VAL:HG12	1:M:211:HIS:CD2	2.48	0.48
1:H:126:SER:OG	4:H:437:HOH:O	2.10	0.48
3:B:145:GLU:O	3:B:145:GLU:HG3	2.12	0.48
1:M:170:LEU:HD21	1:M:193:VAL:HG21	1.95	0.48
1:H:81:MET:SD	4:H:346:HOH:O	2.60	0.48
2:L:7[B]:THR:HG22	4:L:322:HOH:O	2.14	0.48
3:A:52:THR:O	3:A:53:GLY:C	2.50	0.48
3:A:92:PHE:HA	3:A:117:VAL:HG12	1.96	0.48
1:M:2:VAL:CG1	1:M:113:VAL:HG21	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:27:GLN:C	2:L:74:THR:HG22	2.35	0.47
3:B:21:ARG:NE	4:B:357:HOH:O	2.47	0.47
1:M:99:GLU:HG2	1:M:108:TYR:OH	2.15	0.47
3:B:182:CYS:O	3:B:196[B]:ARG:HA	2.15	0.47
2:N:120:VAL:HA	2:N:140:LEU:O	2.13	0.47
1:M:212:LYS:N	1:M:213:PRO:CD	2.77	0.47
3:B:53:GLY:N	4:B:385:HOH:O	2.47	0.47
1:H:50:TRP:CH2	1:H:52:SER:HB2	2.49	0.47
3:B:53:GLY:HA2	3:B:54:ARG:HA	1.47	0.47
2:L:28:SER:N	2:L:74:THR:HG22	2.30	0.47
1:M:170:LEU:O	4:M:416:HOH:O	2.21	0.47
1:H:40:ALA:O	1:H:43:GLN:HB2	2.14	0.46
2:N:112:LYS:HA	2:N:145:TYR:OH	2.15	0.46
3:B:148:GLU:HA	3:B:161:PHE:CD1	2.50	0.46
3:B:52:THR:O	3:B:53:GLY:C	2.53	0.46
3:B:110:VAL:HG12	3:B:111:ALA:N	2.31	0.46
1:H:34:ILE:HB	1:H:51:ILE:HG23	1.97	0.46
3:B:171:PRO:HA	4:B:330:HOH:O	2.16	0.46
3:B:27:LEU:HB3	3:B:54:ARG:HH21	1.81	0.46
3:B:31:ASP:OD1	3:B:32:ARG:HG2	2.16	0.46
3:A:93:PRO:HD2	3:A:117:VAL:HG12	1.97	0.45
2:N:17:GLN:O	4:N:329:HOH:O	2.21	0.45
1:M:112:ASP:HB2	2:N:60:PHE:CZ	2.52	0.45
2:L:7[A]:THR:HG22	4:L:437:HOH:O	2.16	0.45
1:M:31:SER:HA	3:B:73:VAL:HG21	1.99	0.45
3:B:103:LEU:HD21	3:B:110:VAL:HG22	1.99	0.45
2:L:80:ILE:HG22	2:L:82:ARG:O	2.16	0.45
2:L:218:GLU:N	2:L:218:GLU:OE1	2.50	0.45
3:B:38:TRP:HB3	3:B:45:LEU:HD11	1.99	0.45
3:B:182:CYS:O	3:B:196[A]:ARG:HA	2.16	0.45
1:M:17:SER:CB	1:M:84:ARG:HD3	2.47	0.45
2:N:171:GLN:HB2	2:N:178:TYR:CE1	2.52	0.45
2:N:13:VAL:HG21	2:N:19:ALA:HB2	1.98	0.45
2:N:156:ASP:HA	2:N:196:VAL:HG22	1.98	0.45
1:H:203:GLN:HB3	1:H:205:TYR:CE2	2.52	0.44
3:A:181:TYR:CD1	3:A:198:ALA:HA	2.53	0.44
3:A:6:VAL:HA	3:A:24:THR:O	2.18	0.44
2:L:24:LYS:HA	2:L:74:THR:O	2.17	0.44
3:A:15:VAL:HG12	3:A:87:LEU:HD11	2.00	0.44
3:B:31:ASP:C	3:B:32:ARG:HG2	2.37	0.44
2:L:142:ASN:ND2	4:L:331:HOH:O	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:8:PRO:HB2	3:A:10:GLU:OE1	2.17	0.44
1:M:29:PHE:CD2	1:M:77:SER:HA	2.52	0.44
3:A:3:PRO:HG2	3:A:81:PHE:CE2	2.52	0.44
3:B:69:THR:CG2	3:B:84:THR:CG2	2.96	0.44
1:H:195:VAL:HG11	1:H:205:TYR:CE1	2.52	0.44
3:A:11:PRO:C	3:A:12:VAL:HG23	2.37	0.44
1:M:24:ALA:HB1	1:M:27:TYR:CE1	2.52	0.44
3:B:148:GLU:O	3:B:149:GLU:CG	2.65	0.44
1:M:40:ALA:O	1:M:43:GLN:HB2	2.17	0.44
2:N:168:VAL:HG13	2:N:179:SER:O	2.17	0.44
1:H:37:VAL:HG22	1:H:47:TRP:HA	2.00	0.43
3:B:90:TYR:CE2	3:B:191:LEU:HD22	2.53	0.43
1:H:212:LYS:N	1:H:213:PRO:CD	2.81	0.43
2:L:141:LEU:HD12	2:L:141:LEU:N	2.33	0.43
3:A:13:VAL:HG13	3:A:21:ARG:HH21	1.83	0.43
2:N:71:GLY:HA3	2:N:75:ASP:O	2.19	0.43
3:A:174:THR:O	3:A:174:THR:CG2	2.66	0.43
3:B:145:GLU:CD	3:B:166:ARG:HH12	2.20	0.43
3:A:147:GLN:HB2	3:A:162:ARG:CD	2.49	0.43
3:A:174:THR:O	3:A:174:THR:HG23	2.18	0.43
1:H:19:LYS:HE2	1:H:80:TYR:CD2	2.54	0.43
2:N:130:LEU:O	2:N:188:LYS:HD2	2.18	0.43
2:L:60:PHE:O	2:L:63:VAL:HG23	2.19	0.43
3:A:11:PRO:O	3:A:12:VAL:HG23	2.19	0.43
3:B:101:ALA:O	3:B:200:PRO:HD2	2.18	0.43
2:L:66:ARG:HD3	2:L:82:ARG:NH2	2.34	0.43
3:B:69:THR:CG2	3:B:84:THR:HG23	2.49	0.43
2:L:64:PRO:HB2	2:L:66:ARG:HG2	2.01	0.42
3:A:147:GLN:HB3	3:A:162:ARG:HD3	2.01	0.42
3:B:51:ASP:OD1	3:B:51:ASP:C	2.57	0.42
3:B:141:ALA:HA	3:B:166:ARG:O	2.19	0.42
1:M:73:ASP:OD1	1:M:75:SER:OG	2.29	0.42
2:N:128[A]:GLU:O	2:N:131:LYS:HB2	2.19	0.42
2:L:42:LEU:HD13	2:L:91:TYR:CZ	2.54	0.42
2:N:145:TYR:CG	2:N:146:PRO:HA	2.54	0.42
1:H:30:THR:HG23	4:A:398:HOH:O	2.19	0.42
1:M:46:GLU:HG2	1:M:48:MET:CE	2.50	0.42
3:B:168:ARG:HD2	3:B:168:ARG:HA	1.83	0.42
1:H:23:LYS:HD2	1:H:23:LYS:C	2.40	0.42
1:H:163:VAL:HA	1:H:208:ASN:O	2.19	0.41
3:B:58:THR:HG21	3:B:60:ARG:NH1	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:110:VAL:HG11	3:B:199:ILE:HD13	2.02	0.41
3:A:95:GLN:O	3:A:115:HIS:HD2	2.04	0.41
2:L:54:TYR:CZ	2:L:58:ASN:HB3	2.56	0.41
2:N:57:SER:HB3	2:N:69:GLY:O	2.20	0.41
2:N:118:PRO:HB3	2:N:144:PHE:CD2	2.55	0.41
3:B:51:ASP:HA	3:B:52:THR:HA	1.84	0.41
3:A:140:GLN:HB3	3:A:168:ARG:HB3	2.03	0.41
3:B:20:SER:OG	3:B:60:ARG:HG2	2.20	0.41
3:B:109:GLU:HB2	3:B:167:TRP:O	2.21	0.41
3:B:179:ALA:HB2	3:B:200:PRO:HA	2.02	0.41
3:A:15:VAL:CG1	3:A:89:VAL:HG22	2.50	0.41
3:B:32:ARG:HB2	3:B:33:GLY:H	1.67	0.41
1:H:31:SER:HA	3:A:73:VAL:HG21	2.02	0.41
1:H:84[A]:ARG:NH2	4:H:409:HOH:O	2.45	0.41
1:H:99:GLU:CG	1:H:108:TYR:OH	2.67	0.41
1:M:91:THR:HA	1:M:120:VAL:O	2.21	0.41
1:M:148:ALA:HB2	1:M:194:THR:HG22	2.03	0.41
2:N:124:PRO:HB3	2:N:214:PHE:CE2	2.56	0.41
3:B:57:LEU:HD21	3:B:70:ARG:HD3	2.03	0.41
2:N:29:LEU:CD1	2:N:38:LEU:HD23	2.51	0.41
2:N:172:ASP:HB3	2:N:175:ASP:OD1	2.20	0.41
3:B:15:VAL:CG1	3:B:87:LEU:HD11	2.51	0.41
3:B:26:ARG:HG2	4:B:328:HOH:O	2.20	0.40
3:B:31:ASP:C	3:B:32:ARG:CG	2.89	0.40
1:H:43:GLN:N	4:H:405:HOH:O	2.54	0.40
1:H:165:TRP:HA	1:H:206:THR:O	2.22	0.40
1:M:59:ASN:ND2	4:M:387:HOH:O	2.51	0.40
2:N:156:ASP:HA	2:N:196:VAL:CG2	2.51	0.40

All (2) 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:1:GLN:HE22	2:L:28:SER:HG[1_655]	1.34	0.26
1:H:1:GLN:NE2	2:L:28:SER:HG[1_655]	1.59	0.01

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	H	215/229 (94%)	210 (98%)	5 (2%)	0	100	100
1	M	213/229 (93%)	208 (98%)	5 (2%)	0	100	100
2	L	221/219 (101%)	216 (98%)	5 (2%)	0	100	100
2	N	221/219 (101%)	216 (98%)	5 (2%)	0	100	100
3	A	192/209 (92%)	184 (96%)	8 (4%)	0	100	100
3	B	194/209 (93%)	185 (95%)	8 (4%)	1 (0%)	29	35
All	All	1256/1314 (96%)	1219 (97%)	36 (3%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	53	GLY

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	H	184/194 (95%)	181 (98%)	3 (2%)	62	78
1	M	182/194 (94%)	181 (100%)	1 (0%)	88	95
2	L	200/196 (102%)	198 (99%)	2 (1%)	76	87
2	N	200/196 (102%)	197 (98%)	3 (2%)	65	79
3	A	159/171 (93%)	154 (97%)	5 (3%)	40	55
3	B	160/171 (94%)	153 (96%)	7 (4%)	28	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1085/1122 (97%)	1064 (98%)	21 (2%)	59 73

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	13	LYS
1	H	23	LYS
1	H	51	ILE
2	L	11	LEU
2	L	96	ASN
3	A	26	ARG
3	A	42	ASP
3	A	54	ARG
3	A	162	ARG
3	A	168	ARG
1	M	51	ILE
2	N	96	ASN
2	N	199[A]	CYS
2	N	199[B]	CYS
3	B	21	ARG
3	B	50	SER
3	B	51	ASP
3	B	129	LEU
3	B	162	ARG
3	B	196[A]	ARG
3	B	196[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	57	ASN
3	B	195	HIS

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 (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 (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	H	217/229 (94%)	-0.41	1 (0%)	91	94	11, 22, 45, 64	0
1	M	217/229 (94%)	-0.36	2 (0%)	84	88	11, 23, 49, 68	0
2	L	218/219 (99%)	-0.49	0	100	100	12, 24, 37, 45	0
2	N	218/219 (99%)	-0.49	0	100	100	10, 22, 38, 55	0
3	A	194/209 (92%)	-0.08	2 (1%)	82	86	13, 31, 59, 72	1 (0%)
3	B	194/209 (92%)	-0.10	4 (2%)	63	70	13, 34, 52, 72	1 (0%)
All	All	1258/1314 (95%)	-0.33	9 (0%)	87	91	10, 26, 50, 72	2 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	200	PHE	4.4
3	B	52	THR	3.7
3	A	52	THR	3.6
3	B	191	LEU	3.1
3	B	179	ALA	3.1
1	M	196	PRO	2.6
3	A	159	VAL	2.5
3	B	53	GLY	2.2
1	H	200	PHE	2.1

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.