Full wwPDB X-ray Structure Validation Report (i)

May 17, 2020 – 09:16 pm BST

PDB ID	:	3U9P
Title	:	Crystal Structure of Murine Siderocalin in Complex with an Fab Fragment
Authors	:	Correnti, C.; Strong, R.K.
Deposited on	:	2011-10-19
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 (i) symbol.

The following versions of software and data (see references (i)) 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 (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	Percentile Ranks	Value
Rfree		0.292
Clashscore		7
Ramachandran outliers		0.4%
Sidechain outliers		5.0%
RSRZ outliers		0.4%

Worse ← → *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
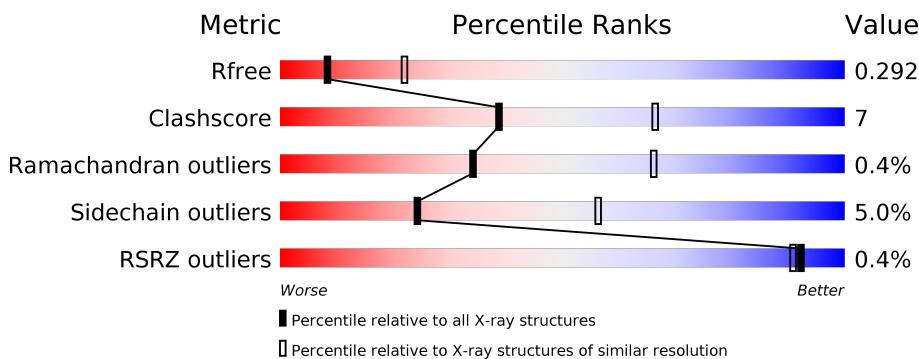
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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 <=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	C	182	79% · 13% · 7%
1	D	182	75% · 15% · 9%
2	H	216	2% 70% · 14% · 15%
2	K	216	72% · 19% · 7%
3	L	212	83% · 16% ·
3	M	212	88% · 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8339 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 Neutrophil gelatinase-associated lipocalin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	169	Total 1266	C 826	N 209	O 226	S 5	0	0	0
1	D	166	Total 1229	C 801	N 206	O 217	S 5	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	GLY	-	EXPRESSION TAG	UNP P11672
C	-6	SER	-	EXPRESSION TAG	UNP P11672
D	-7	GLY	-	EXPRESSION TAG	UNP P11672
D	-6	SER	-	EXPRESSION TAG	UNP P11672

- Molecule 2 is a protein called Monoclonal Fab Fragment Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	184	Total 1229	C 780	N 209	O 233	S 7	0	0	0
2	K	200	Total 1414	C 902	N 237	O 268	S 7	0	0	0

- Molecule 3 is a protein called Monoclonal Fab Fragment Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	212	Total 1561	C 986	N 254	O 314	S 7	0	0	0
3	M	211	Total 1579	C 997	N 257	O 318	S 7	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	4	Total 4	O 4	0	0
4	D	5	Total 5	O 5	0	0
4	H	5	Total 5	O 5	0	0
4	K	15	Total 15	O 15	0	0
4	L	18	Total 18	O 18	0	0
4	M	14	Total 14	O 14	0	0

3 Residue-property plots ⓘ

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: Neutrophil gelatinase-associated lipocalin
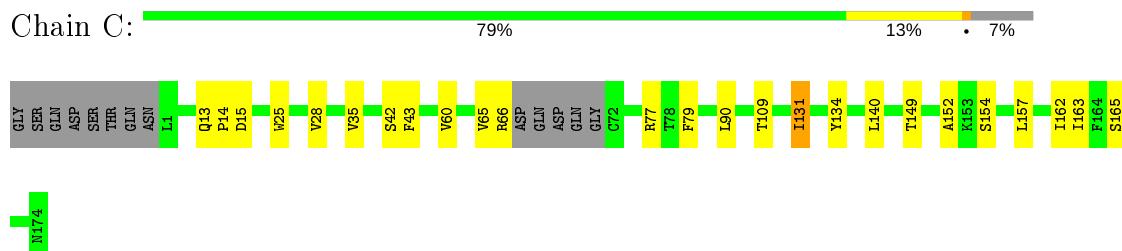
Chain C:

- Molecule 1: Neutrophil gelatinase-associated lipocalin

Chain D:

- Molecule 2: Monoclonal Fab Fragment Heavy Chain

Chain H:

- Molecule 2: Monoclonal Fab Fragment Heavy Chain

Chain K:

V155 T156 V157 L164 SER ASP V168 F171 L182 S188 W191 PRO SER GLN THR V196 T197 C198 H202 S205 S206 T207 K208 V209 D210 L213 E214 R215

• Molecule 3: Monoclonal Fab Fragment Light Chain

Chain L:

83%   16%   .

D1 S10 L11 S12 D17 K18 V19 T22 C23 I28 W35 G68 F73 V78 C88 L94 M97 E105 L106 K107 R108 P120 L125 G129 V132 F139 R142 D143 I144 S145 S162 V163 D170 T178 Y186 E187 Y192

V197 V206 N212

• Molecule 3: Monoclonal Fab Fragment Light Chain

Chain M:

88%   11%

D1 P8 L11 S12 L15 G16 D17 K18 V19 T22 W35 S56 V78 C88 L89 Q90 L104 V115 F118 L125 V133 V163 T164 D165 M175 S176 E195 V206 K207 R211 ASN
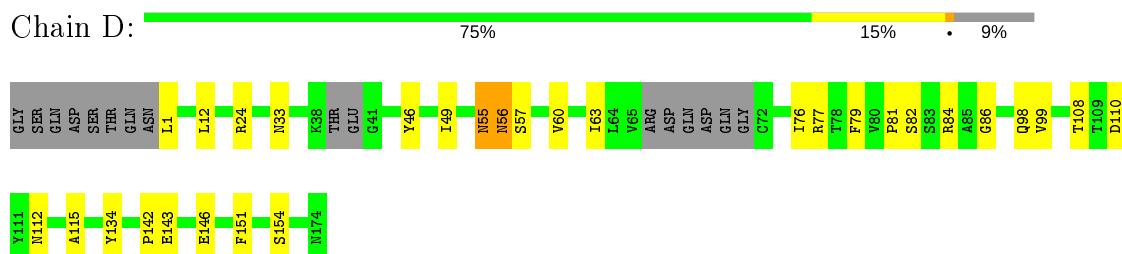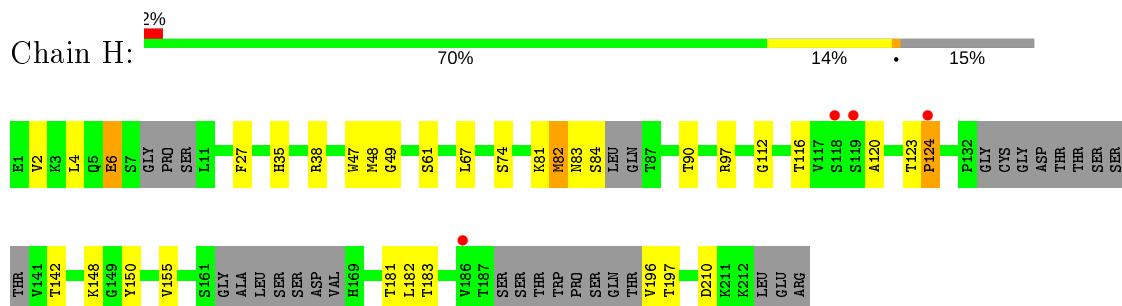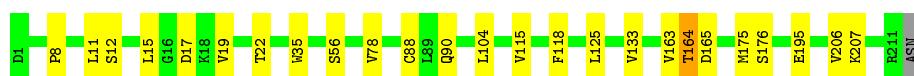
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	82.13Å 124.09Å 147.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.51 – 2.80 49.51 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.1 (49.51-2.80) 93.1 (49.51-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	4.12 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.219 , 0.292 0.222 , 0.292	Depositor DCC
R_{free} test set	1758 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	46.6	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 61.6	EDS
L-test for twinning[2]	$<|L|> = 0.50, <L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8339	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	C	0.48	0/1299	0.62	0/1771
1	D	0.44	0/1261	0.60	0/1720
2	H	0.46	0/1255	0.61	0/1726
2	K	0.54	0/1447	0.69	0/1989
3	L	0.49	0/1596	0.61	0/2178
3	M	0.53	0/1614	0.67	0/2200
All	All	0.50	0/8472	0.64	0/11584

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	C	1266	0	1135	17	0
1	D	1229	0	1078	15	1
2	H	1229	0	992	22	1
2	K	1414	0	1269	32	1
3	L	1561	0	1405	23	0
3	M	1579	0	1460	17	0
4	C	4	0	0	0	0
4	D	5	0	0	0	0
4	H	5	0	0	0	0
4	K	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	18	0	0	1	0
4	M	14	0	0	0	0
All	All	8339	0	7339	117	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 7.

All (117) 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:123:THR:HG22	2:H:124:PRO:CD	2.04	0.86
2:K:143:LEU:HB3	2:K:213:LEU:HD11	1.62	0.80
2:K:130:LEU:CD2	3:M:118:PHE:CG	2.68	0.77
2:K:66:ARG:NH2	2:K:82:MET:HE2	2.03	0.73
2:H:90:THR:HG23	2:H:116:THR:HA	1.73	0.71
3:L:17:ASP:O	3:L:78:VAL:HG23	1.93	0.69
2:H:6:GLU:OE1	2:H:112:GLY:N	2.27	0.68
1:D:115:ALA:HB3	1:D:134:TYR:HB2	1.75	0.68
2:H:123:THR:HG22	2:H:124:PRO:HD2	1.76	0.66
2:H:67:LEU:HD13	2:H:82:MET:HG3	1.76	0.65
1:C:77:ARG:HG3	1:C:90:LEU:HD11	1.78	0.65
2:K:130:LEU:HD23	3:M:118:PHE:CD2	2.31	0.65
2:K:130:LEU:HD23	3:M:118:PHE:CG	2.31	0.65
2:K:6:GLU:HG3	2:K:95:CYS:HB2	1.79	0.65
2:H:123:THR:HG22	2:H:124:PRO:HD3	1.79	0.64
1:C:60:VAL:HG21	1:C:79:PHE:CD1	2.31	0.64
3:M:164:THR:HG23	3:M:165:ASP:O	1.97	0.64
3:L:12:SER:HA	3:L:105:GLU:O	1.99	0.63
3:L:23:CYS:HG	3:L:88:CYS:HG	1.46	0.62
3:L:142:ARG:NH2	3:L:163:VAL:HG21	2.15	0.61
2:K:66:ARG:NH2	2:K:82:MET:CE	2.64	0.60
2:H:182:LEU:O	2:H:183:THR:HG23	2.01	0.59
2:K:90:THR:HG23	2:K:116:THR:HA	1.83	0.59
3:L:125:LEU:HD23	3:L:129:GLY:O	2.03	0.59
1:C:149:THR:HG23	1:C:162:ILE:CD1	2.34	0.58
3:L:206:VAL:O	3:L:206:VAL:HG22	2.02	0.58
3:L:142:ARG:CZ	3:L:163:VAL:HG21	2.34	0.57
2:H:155:VAL:HG22	2:H:182:LEU:HD13	1.87	0.56
1:C:43:PHE:CE2	1:C:163:ILE:HG22	2.40	0.56
3:L:206:VAL:CG2	3:L:206:VAL:O	2.54	0.56
3:M:8:PRO:HG3	3:M:11:LEU:HD13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:206:VAL:O	3:M:206:VAL:HG23	2.08	0.54
1:C:43:PHE:HE2	1:C:163:ILE:HG22	1.72	0.54
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.42	0.53
3:L:142:ARG:NE	3:L:163:VAL:HG11	2.24	0.53
1:D:84:ARG:HD3	3:L:94:LEU:HD12	1.90	0.53
3:L:108:ARG:NH1	3:L:170:ASP:O	2.40	0.52
3:M:35:TRP:CZ3	3:M:88:CYS:HB3	2.44	0.52
1:D:55:ASN:O	1:D:56:ASN:CB	2.56	0.52
2:H:155:VAL:CG2	2:H:182:LEU:HD13	2.40	0.52
2:H:38:ARG:HB3	2:H:48:MET:HE2	1.92	0.52
2:H:83:ASN:O	2:H:84:SER:CB	2.58	0.52
1:C:25:TRP:CE3	1:C:134:TYR:HB3	2.45	0.51
1:D:76:ILE:O	1:D:77:ARG:HD2	2.10	0.51
2:K:168:VAL:N	4:K:218:HOH:O	2.44	0.51
3:L:23:CYS:SG	3:L:88:CYS:SG	3.01	0.51
3:L:1:ASP:HB3	3:L:97:MET:CE	2.42	0.51
2:K:130:LEU:CD2	3:M:118:PHE:CB	2.88	0.51
2:K:80:LEU:HD23	2:K:80:LEU:C	2.32	0.50
2:H:150:TYR:CZ	2:H:155:VAL:HG13	2.47	0.50
2:K:124:PRO:HG3	2:K:205:SER:HB2	1.94	0.49
2:K:130:LEU:CD2	3:M:118:PHE:CD2	2.93	0.49
1:C:28:VAL:HG21	1:C:140:LEU:HD12	1.94	0.49
1:C:152:ALA:HB1	1:C:157:LEU:HD12	1.94	0.49
1:C:77:ARG:CG	1:C:90:LEU:HD11	2.43	0.49
1:D:46:TYR:HB2	1:D:63:ILE:O	2.13	0.49
1:D:151:PHE:O	1:D:154:SER:CB	2.61	0.48
3:M:115:VAL:O	3:M:207:LYS:HE2	2.12	0.48
3:L:145:SER:HB3	3:L:197:VAL:HG23	1.95	0.48
1:D:60:VAL:HG21	1:D:79:PHE:CD1	2.48	0.48
3:L:120:PRO:HD3	3:L:132:VAL:HG22	1.95	0.48
2:K:130:LEU:HD23	3:M:118:PHE:CB	2.43	0.48
2:K:124:PRO:HG3	2:K:205:SER:CB	2.44	0.47
2:K:157:VAL:HG21	2:K:182:LEU:HD21	1.95	0.47
3:M:195:GLU:CG	3:M:206:VAL:HG12	2.45	0.47
2:H:123:THR:CG2	2:H:124:PRO:HD3	2.44	0.47
2:H:4:LEU:N	2:H:4:LEU:HD12	2.29	0.47
2:K:130:LEU:HD11	3:M:133:VAL:HG21	1.96	0.47
2:K:150:TYR:CE2	2:K:155:VAL:HG13	2.50	0.47
2:K:67:LEU:HD11	2:K:80:LEU:HG	1.97	0.47
3:L:35:TRP:CE2	3:L:73:PHE:HB2	2.49	0.47
2:H:196:VAL:O	2:H:196:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:PHE:CZ	1:C:165:SER:HB3	2.50	0.47
1:D:142:PRO:O	1:D:146:GLU:N	2.48	0.47
1:D:1:LEU:HD22	1:D:33:ASN:ND2	2.30	0.47
3:L:139:PHE:CD2	3:L:144:ILE:HD12	2.50	0.47
2:K:202:HIS:HB3	2:K:207:THR:HB	1.95	0.46
2:H:148:LYS:HA	2:H:181:THR:HG23	1.98	0.46
2:K:141:VAL:N	2:K:188:SER:O	2.49	0.46
3:L:22:THR:HG22	4:L:228:HOH:O	2.16	0.46
2:H:123:THR:CG2	2:H:124:PRO:CD	2.88	0.45
2:K:209:VAL:CG1	2:K:210:ASP:N	2.79	0.45
2:K:80:LEU:HD23	2:K:81:LYS:N	2.32	0.45
2:H:150:TYR:CE2	2:H:155:VAL:HG13	2.51	0.45
3:L:19:VAL:HG13	3:L:78:VAL:HG22	1.98	0.44
1:C:149:THR:HG23	1:C:162:ILE:HD12	1.99	0.44
2:H:67:LEU:HD12	2:H:81:LYS:O	2.18	0.44
1:C:35:VAL:HG13	1:C:163:ILE:HD12	2.00	0.44
2:K:4:LEU:HD23	2:K:95:CYS:SG	2.57	0.44
1:D:12:LEU:HD11	1:D:86:GLY:HA3	1.99	0.44
1:C:28:VAL:HG21	1:C:140:LEU:CD1	2.48	0.43
1:D:60:VAL:HG21	1:D:79:PHE:CG	2.54	0.43
3:L:11:LEU:HD12	3:L:12:SER:H	1.83	0.43
1:C:13:GLN:HG2	1:C:109:THR:HG22	2.00	0.43
2:K:85:LEU:HD13	2:K:117:VAL:HG21	2.00	0.43
1:D:24:ARG:HA	1:D:49:ILE:HA	1.99	0.43
2:K:125:LYS:CB	2:K:147:VAL:HG13	2.49	0.42
3:L:28:ILE:HG23	3:L:68:GLY:HA2	2.01	0.42
3:M:163:VAL:HG22	3:M:175:MET:HG3	2.01	0.42
2:H:35:HIS:CD2	2:H:47:TRP:HE1	2.37	0.42
2:K:35:HIS:ND1	2:K:50:GLY:HA3	2.35	0.42
2:K:51:ILE:O	2:K:51:ILE:HG23	2.20	0.42
3:M:17:ASP:O	3:M:78:VAL:HG23	2.20	0.42
2:K:198:CYS:O	2:K:210:ASP:HA	2.19	0.42
3:L:186:TYR:O	3:L:192:TYR:OH	2.37	0.42
1:C:65:VAL:O	1:C:66:ARG:CB	2.68	0.42
1:C:14:PRO:O	1:C:15:ASP:C	2.59	0.41
3:L:1:ASP:HB3	3:L:97:MET:HE1	2.02	0.41
2:K:131:ALA:HB1	2:K:132:PRO:HD2	2.03	0.41
1:D:110:ASP:O	1:D:112:ASN:N	2.42	0.41
2:K:143:LEU:HD13	2:K:213:LEU:HD11	2.03	0.41
1:D:57:SER:HA	1:D:81:PRO:HD3	2.02	0.41
3:M:11:LEU:HB3	3:M:104:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:GLN:HG2	1:D:99:VAL:HG23	2.03	0.41
2:H:2:VAL:HG13	2:H:27:PHE:CD2	2.56	0.41
2:K:171:PHE:CD1	3:M:176:SER:HB2	2.56	0.41
1:C:131:ILE:HD11	1:C:152:ALA:HB2	2.03	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:D:143:GLU:OE1	2:H:210:ASP:O[3_455]	2.02	0.18
2:K:1:GLU:N	2:K:119:SER:OG[4_446]	2.18	0.02

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	C	165/182 (91%)	155 (94%)	9 (6%)	1 (1%)	25	56
1	D	160/182 (88%)	149 (93%)	10 (6%)	1 (1%)	25	56
2	H	172/216 (80%)	162 (94%)	8 (5%)	2 (1%)	13	39
2	K	192/216 (89%)	183 (95%)	9 (5%)	0	100	100
3	L	210/212 (99%)	203 (97%)	7 (3%)	0	100	100
3	M	209/212 (99%)	203 (97%)	6 (3%)	0	100	100
All	All	1108/1220 (91%)	1055 (95%)	49 (4%)	4 (0%)	34	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	124	PRO
1	D	56	ASN
2	H	120	ALA

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Mol	Chain	Res	Type
1	C	42	SER

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	C	116/165 (70%)	114 (98%)	2 (2%)	60	87
1	D	107/165 (65%)	104 (97%)	3 (3%)	43	77
2	H	98/190 (52%)	91 (93%)	7 (7%)	14	39
2	K	135/190 (71%)	124 (92%)	11 (8%)	11	33
3	L	157/189 (83%)	149 (95%)	8 (5%)	24	55
3	M	165/189 (87%)	157 (95%)	8 (5%)	25	58
All	All	778/1088 (72%)	739 (95%)	39 (5%)	24	56

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	131	ILE
1	C	154	SER
1	D	55	ASN
1	D	82	SER
1	D	108	THR
2	H	6	GLU
2	H	61	SER
2	H	74	SER
2	H	82	MET
2	H	97	ARG
2	H	142	THR
2	H	197	THR
2	K	15	SER
2	K	84	SER
2	K	96	THR
2	K	97	ARG
2	K	119	SER

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Mol	Chain	Res	Type
2	K	123	THR
2	K	130	LEU
2	K	145	CYS
2	K	182	LEU
2	K	210	ASP
2	K	213	LEU
3	L	10	SER
3	L	19	VAL
3	L	22	THR
3	L	106	LEU
3	L	108	ARG
3	L	162	SER
3	L	178	THR
3	L	187	GLU
3	M	12	SER
3	M	15	LEU
3	M	19	VAL
3	M	22	THR
3	M	56	SER
3	M	90	GLN
3	M	125	LEU
3	M	164	THR

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

Mol	Chain	Res	Type
2	H	32	ASN
2	K	13	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 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 (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(Å²)	Q<0.9
1	C	169/182 (92%)	-0.41	0	100	100	24, 44, 65, 74	0
1	D	166/182 (91%)	-0.21	0	100	100	34, 57, 92, 99	0
2	H	184/216 (85%)	0.20	4 (2%)	62	52	35, 67, 100, 114	0
2	K	200/216 (92%)	-0.27	0	100	100	21, 35, 62, 76	0
3	L	212/212 (100%)	-0.23	0	100	100	22, 38, 74, 101	0
3	M	211/212 (99%)	-0.30	0	100	100	19, 37, 54, 64	0
All	All	1142/1220 (93%)	-0.21	4 (0%)	92	91	19, 45, 86, 114	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	186	VAL	3.6
2	H	124	PRO	2.6
2	H	119	SER	2.4
2	H	118	SER	2.3

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.