Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 01:54 AM EDT

PDB ID	:	8DMP
Title	:	Crystal structure of Legionella pneumophila macrodomain effector MavL
Authors	:	Zhang, Z.; Das, C.
Deposited on	:	2022-07-08
Resolution	:	2.17 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:

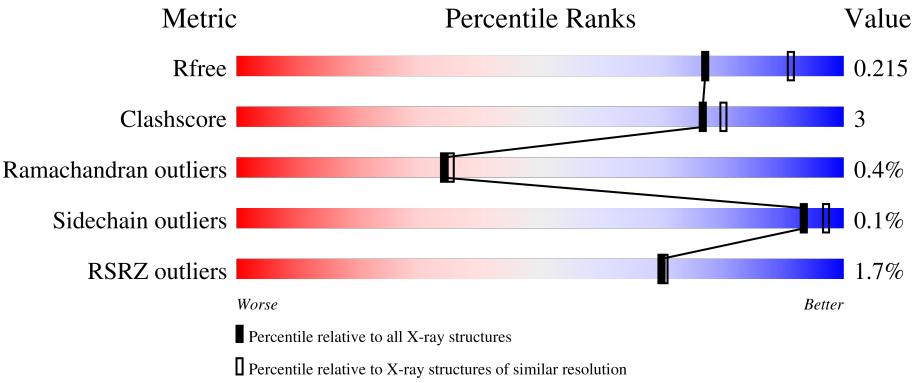
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.17 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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	399	3% 86% 8% 7%
1	B	399	% 87% 6% 8%
1	C	399	% 88% 5% 7%
1	D	399	2% 85% 8% 7%
1	E	399	% 83% 10% 7%

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Mol	Chain	Length	Quality of chain
1	F	399	2% 84% 8% 8%
1	G	399	% 82% 11% 8%
1	H	399	2% 85% 7% 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 24110 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 MavL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2857	1814	477	557	9			
1	B	369	Total	C	N	O	S	2	1	0
			2844	1804	474	556	10			
1	C	370	Total	C	N	O	S	2	1	0
			2850	1810	476	555	9			
1	D	373	Total	C	N	O	S	0	1	0
			2884	1828	483	564	9			
1	E	371	Total	C	N	O	S	5	1	0
			2872	1821	484	557	10			
1	F	369	Total	C	N	O	S	5	1	0
			2856	1812	481	553	10			
1	G	369	Total	C	N	O	S	0	1	0
			2854	1811	479	554	10			
1	H	369	Total	C	N	O	S	2	0	0
			2821	1791	472	549	9			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	GLY	-	expression tag	UNP Q5ZSJ1
A	38	PRO	-	expression tag	UNP Q5ZSJ1
A	39	LEU	-	expression tag	UNP Q5ZSJ1
A	40	GLY	-	expression tag	UNP Q5ZSJ1
A	41	SER	-	expression tag	UNP Q5ZSJ1
B	37	GLY	-	expression tag	UNP Q5ZSJ1
B	38	PRO	-	expression tag	UNP Q5ZSJ1
B	39	LEU	-	expression tag	UNP Q5ZSJ1
B	40	GLY	-	expression tag	UNP Q5ZSJ1
B	41	SER	-	expression tag	UNP Q5ZSJ1
C	37	GLY	-	expression tag	UNP Q5ZSJ1
C	38	PRO	-	expression tag	UNP Q5ZSJ1
C	39	LEU	-	expression tag	UNP Q5ZSJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	40	GLY	-	expression tag	UNP Q5ZSJ1
C	41	SER	-	expression tag	UNP Q5ZSJ1
D	37	GLY	-	expression tag	UNP Q5ZSJ1
D	38	PRO	-	expression tag	UNP Q5ZSJ1
D	39	LEU	-	expression tag	UNP Q5ZSJ1
D	40	GLY	-	expression tag	UNP Q5ZSJ1
D	41	SER	-	expression tag	UNP Q5ZSJ1
E	37	GLY	-	expression tag	UNP Q5ZSJ1
E	38	PRO	-	expression tag	UNP Q5ZSJ1
E	39	LEU	-	expression tag	UNP Q5ZSJ1
E	40	GLY	-	expression tag	UNP Q5ZSJ1
E	41	SER	-	expression tag	UNP Q5ZSJ1
F	37	GLY	-	expression tag	UNP Q5ZSJ1
F	38	PRO	-	expression tag	UNP Q5ZSJ1
F	39	LEU	-	expression tag	UNP Q5ZSJ1
F	40	GLY	-	expression tag	UNP Q5ZSJ1
F	41	SER	-	expression tag	UNP Q5ZSJ1
G	37	GLY	-	expression tag	UNP Q5ZSJ1
G	38	PRO	-	expression tag	UNP Q5ZSJ1
G	39	LEU	-	expression tag	UNP Q5ZSJ1
G	40	GLY	-	expression tag	UNP Q5ZSJ1
G	41	SER	-	expression tag	UNP Q5ZSJ1
H	37	GLY	-	expression tag	UNP Q5ZSJ1
H	38	PRO	-	expression tag	UNP Q5ZSJ1
H	39	LEU	-	expression tag	UNP Q5ZSJ1
H	40	GLY	-	expression tag	UNP Q5ZSJ1
H	41	SER	-	expression tag	UNP Q5ZSJ1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	191	Total O 191 191	0	0
2	B	178	Total O 178 178	0	0
2	C	180	Total O 180 180	0	0
2	D	159	Total O 159 159	0	0
2	E	190	Total O 190 190	0	0
2	F	132	Total O 132 132	0	0

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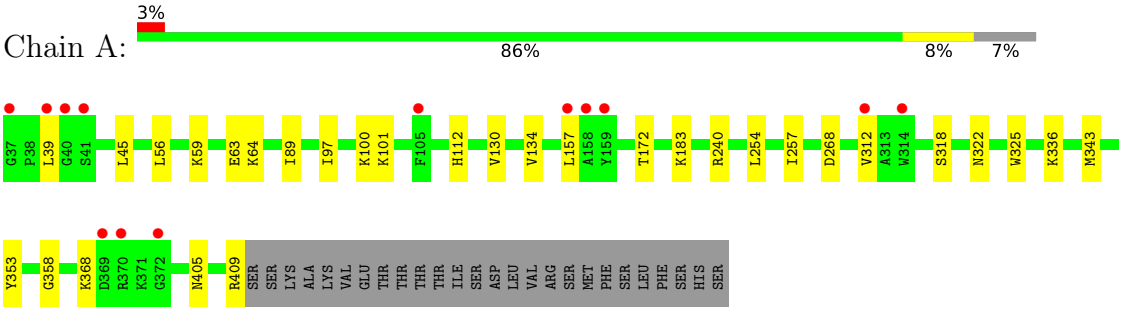
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	114	Total O 114 114	0	0
2	H	128	Total O 128 128	0	0

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.

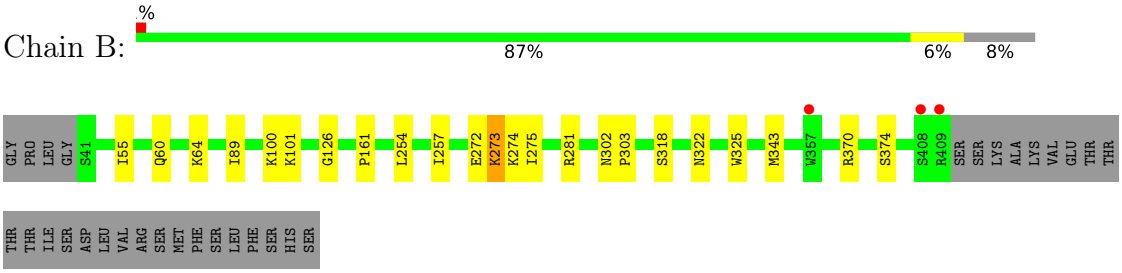
• Molecule 1: MavL

Chain A:



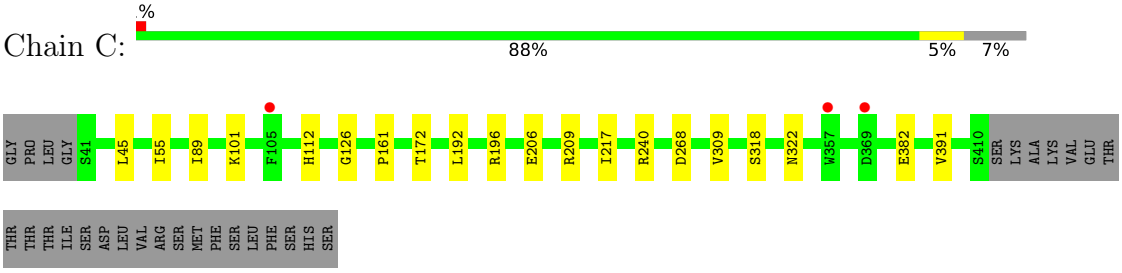
• Molecule 1: MavL

Chain B:



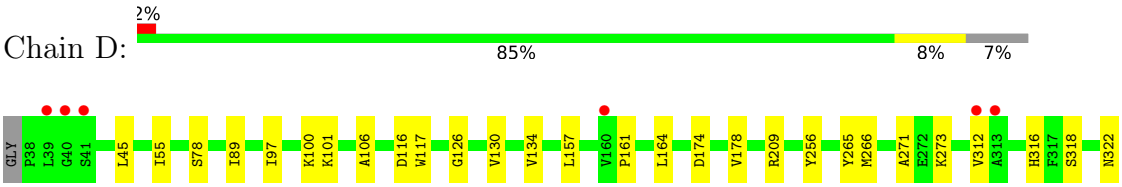
• Molecule 1: MavL

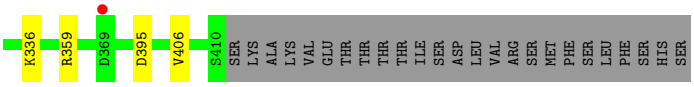
Chain C:



• Molecule 1: MavL

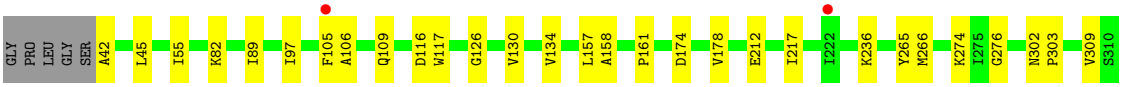
Chain D:

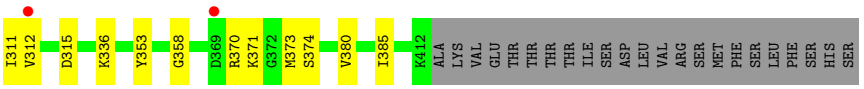




• Molecule 1: MavL

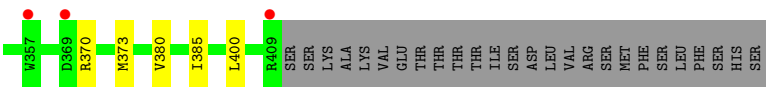
Chain E:





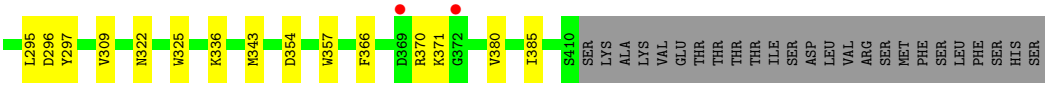
• Molecule 1: MavL

Chain F:



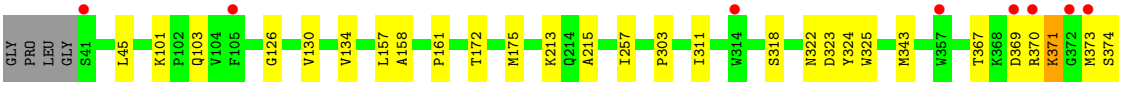
• Molecule 1: MavL

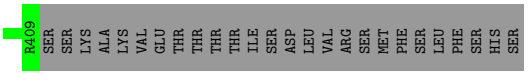
Chain G:



• Molecule 1: MavL

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.23Å 157.24Å 117.62Å 90.00° 96.20° 90.00°	Depositor
Resolution (Å)	39.31 – 2.17 38.98 – 2.17	Depositor EDS
% Data completeness (in resolution range)	98.2 (39.31-2.17) 89.5 (38.98-2.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.187 , 0.214 0.188 , 0.215	Depositor DCC
R_{free} test set	1954 reflections (1.12%)	wwPDB-VP
Wilson B-factor (Å^2)	33.8	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 31.0	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	0.96	EDS
Total number of atoms	24110	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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

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	0.26	0/2928	0.47	0/3982
1	B	0.26	0/2914	0.49	0/3962
1	C	0.26	0/2923	0.46	0/3973
1	D	0.26	0/2955	0.47	0/4014
1	E	0.26	0/2942	0.47	0/3995
1	F	0.26	0/2926	0.48	0/3975
1	G	0.26	0/2924	0.47	0/3972
1	H	0.27	0/2891	0.48	0/3935
All	All	0.26	0/23403	0.48	0/31808

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

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	2857	0	2730	17	0
1	B	2844	0	2720	12	0
1	C	2850	0	2734	11	0
1	D	2884	0	2769	18	0
1	E	2872	0	2769	26	0
1	F	2856	0	2748	18	0
1	G	2854	0	2749	22	0
1	H	2821	0	2679	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	191	0	0	0	0
2	B	178	0	0	0	0
2	C	180	0	0	1	0
2	D	159	0	0	1	0
2	E	190	0	0	3	0
2	F	132	0	0	0	0
2	G	114	0	0	0	0
2	H	128	0	0	0	0
All	All	24110	0	21898	135	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 3.

All (135) 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)
1:G:136:MET:HB2	1:G:153:ILE:HB	1.78	0.65
1:H:213:LYS:NZ	1:H:303:PRO:O	2.31	0.63
1:F:45:LEU:HD13	1:F:97:ILE:HD13	1.82	0.62
1:D:126:GLY:O	1:D:161:PRO:HG2	2.01	0.61
1:C:217:ILE:HG12	1:C:309:VAL:CG1	2.32	0.60
1:E:370:ARG:HB2	1:E:374:SER:HB3	1.83	0.59
1:A:254:LEU:HB3	1:A:257:ILE:HD12	1.86	0.58
1:F:126:GLY:O	1:F:161:PRO:HG2	2.04	0.58
1:C:126:GLY:O	1:C:161:PRO:HG2	2.04	0.57
1:C:206:GLU:OE2	1:C:209:ARG:NH2	2.37	0.57
1:G:126:GLY:O	1:G:161:PRO:HG2	2.05	0.57
1:B:126:GLY:O	1:B:161:PRO:HG2	2.05	0.57
1:C:55:ILE:HG22	1:C:89:ILE:HD11	1.87	0.56
1:E:45:LEU:HD13	1:E:97:ILE:HD13	1.87	0.56
1:G:45:LEU:HD23	1:G:130:VAL:HB	1.86	0.56
1:E:274:LYS:HE3	1:E:276:GLY:O	2.06	0.56
1:G:209:ARG:HG3	1:G:256:TYR:CZ	2.40	0.56
1:H:126:GLY:O	1:H:161:PRO:HG2	2.06	0.56
1:E:126:GLY:O	1:E:161:PRO:HG2	2.06	0.56
1:E:105:PHE:HB2	1:E:109:GLN:HG3	1.86	0.55
1:E:370:ARG:HD2	1:E:373:MET:HE2	1.88	0.55
1:F:45:LEU:HD23	1:F:130:VAL:HB	1.88	0.55
1:A:45:LEU:HD13	1:A:97:ILE:HD13	1.89	0.55
1:F:254:LEU:HB3	1:F:257:ILE:HD12	1.90	0.54
1:E:55:ILE:HG22	1:E:89:ILE:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:ALA:N	2:E:511:HOH:O	2.41	0.54
1:H:103:GLN:HG3	1:H:323:ASP:HA	1.90	0.54
1:H:172:THR:OG1	1:H:175:MET:HG3	2.09	0.53
1:F:248:GLU:OE1	1:F:251:LYS:NZ	2.42	0.53
1:H:367:THR:O	1:H:371:LYS:HA	2.10	0.52
1:E:106:ALA:HB2	1:E:315:ASP:OD1	2.08	0.52
1:F:312:VAL:HG22	1:F:336:LYS:HD3	1.92	0.52
1:D:265:TYR:CD2	1:D:266:MET:HG3	2.44	0.52
1:G:366:PHE:O	1:G:370:ARG:HG3	2.09	0.52
1:G:112:HIS:CE1	1:G:172:THR:HG22	2.45	0.51
1:A:45:LEU:HD23	1:A:130:VAL:HB	1.93	0.50
1:D:45:LEU:HD13	1:D:97:ILE:HD13	1.93	0.50
1:A:183:LYS:HG2	1:D:78:SER:O	2.11	0.50
1:D:106:ALA:O	2:D:501:HOH:O	2.20	0.50
1:D:134:VAL:HG21	1:D:157:LEU:HG	1.93	0.50
1:E:217:ILE:HG12	1:E:309:VAL:CG1	2.42	0.49
1:B:273:LYS:HG2	1:B:275:ILE:HG13	1.94	0.49
1:E:370:ARG:HD2	1:E:373:MET:CE	2.41	0.49
1:E:82:LYS:NZ	2:E:503:HOH:O	2.31	0.49
1:E:134:VAL:HG21	1:E:157:LEU:HG	1.95	0.49
1:A:101:LYS:O	1:A:318:SER:HA	2.13	0.48
1:G:295:LEU:HD21	1:G:336:LYS:HG2	1.95	0.48
1:B:370:ARG:O	1:B:374:SER:HB3	2.13	0.48
1:G:50:GLU:H	1:G:50:GLU:CD	2.18	0.48
1:F:46:LEU:HD22	1:F:400:LEU:HD22	1.95	0.47
1:E:45:LEU:HD23	1:E:130:VAL:HB	1.95	0.47
1:H:215:ALA:HB3	1:H:257:ILE:HD13	1.96	0.47
1:D:45:LEU:HD23	1:D:130:VAL:HB	1.96	0.47
1:A:134:VAL:HG21	1:A:157:LEU:HG	1.97	0.47
1:G:380:VAL:HG13	1:G:385:ILE:HB	1.97	0.47
1:B:254:LEU:HB3	1:B:257:ILE:HD12	1.97	0.46
1:G:265:TYR:CD2	1:G:266:MET:HG3	2.50	0.46
1:H:45:LEU:HD23	1:H:130:VAL:HB	1.95	0.46
1:G:296:ASP:OD1	1:G:297:TYR:N	2.48	0.46
1:C:382:GLU:O	1:E:236:LYS:HE3	2.15	0.46
1:H:158:ALA:HB3	1:H:311:ILE:HD13	1.97	0.46
1:F:68:THR:HG21	1:G:68:THR:HG23	1.98	0.46
1:D:209:ARG:HG3	1:D:256:TYR:CZ	2.52	0.45
1:E:116:ASP:OD1	1:E:117:TRP:N	2.47	0.45
1:G:217:ILE:HG12	1:G:309:VAL:CG1	2.47	0.45
1:D:55:ILE:HG22	1:D:89:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LEU:HD23	1:A:89:ILE:HD13	1.98	0.45
1:A:325:TRP:CZ2	1:A:343:MET:SD	3.09	0.45
1:E:265:TYR:CD2	1:E:266:MET:HG3	2.52	0.45
1:A:405:ASN:O	1:A:409:ARG:HG3	2.17	0.45
1:C:101:LYS:O	1:C:318:SER:HA	2.17	0.45
1:B:325:TRP:CE2	1:B:343:MET:SD	3.11	0.44
1:E:302:ASN:HB2	1:E:303:PRO:HD2	1.99	0.44
1:E:370:ARG:HB3	1:E:373:MET:HG3	1.97	0.44
1:F:103:GLN:HG2	1:F:323:ASP:HA	1.97	0.44
1:A:59:LYS:O	1:A:63:GLU:HG3	2.17	0.44
1:G:325:TRP:CE2	1:G:343:MET:SD	3.11	0.44
1:C:45:LEU:HB2	1:C:391:VAL:HG22	2.00	0.44
1:C:112:HIS:CE1	1:C:172:THR:HG22	2.52	0.44
1:H:101:LYS:O	1:H:318:SER:HA	2.17	0.44
1:D:116:ASP:OD1	1:D:117:TRP:N	2.48	0.44
1:F:380:VAL:HG13	1:F:385:ILE:HB	2.00	0.44
1:A:112:HIS:CE1	1:A:172:THR:HG22	2.52	0.43
1:F:370:ARG:HB3	1:F:373:MET:HG3	2.00	0.43
1:F:100:LYS:HE3	1:F:318:SER:O	2.18	0.43
1:F:172:THR:O	1:F:176:LYS:HG3	2.19	0.43
1:A:240:ARG:HE	1:A:268:ASP:CG	2.22	0.43
1:C:192:LEU:O	1:C:196:ARG:HG3	2.18	0.43
1:C:217:ILE:HG12	1:C:309:VAL:HG13	2.00	0.43
1:D:359:ARG:HE	1:D:359:ARG:HB2	1.60	0.43
1:D:101:LYS:O	1:D:318:SER:HA	2.18	0.43
1:H:369:ASP:C	1:H:371:LYS:H	2.22	0.43
1:B:273:LYS:HB2	1:B:273:LYS:HE3	1.70	0.42
1:D:312:VAL:HG22	1:D:336:LYS:HD3	2.01	0.42
1:H:134:VAL:HG21	1:H:157:LEU:HG	2.01	0.42
1:B:272:GLU:HG2	1:B:281:ARG:HG2	2.01	0.42
1:H:324:TYR:HD2	1:H:343:MET:HE2	1.84	0.42
1:A:64:LYS:HD3	2:C:540:HOH:O	2.17	0.42
1:G:354:ASP:OD2	1:G:357:TRP:HD1	2.03	0.42
1:E:353:TYR:OH	1:E:358:GLY:HA2	2.20	0.42
1:A:312:VAL:HG22	1:A:336:LYS:HD3	2.01	0.42
1:D:271:ALA:HB1	1:D:273:LYS:HE3	2.01	0.42
1:F:370:ARG:O	1:F:373:MET:HG3	2.20	0.42
1:G:240:ARG:HB3	1:G:262:TYR:CE2	2.55	0.42
1:H:325:TRP:CE2	1:H:343:MET:SD	3.13	0.42
1:F:263:ASP:OD2	1:F:285:SER:HB2	2.20	0.42
1:G:180:ASP:OD1	1:G:188:LYS:NZ	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:192:LEU:O	1:G:196:ARG:HG3	2.19	0.42
1:B:60:GLN:O	1:B:64:LYS:HG3	2.20	0.42
1:D:100:LYS:HE3	1:D:318:SER:O	2.19	0.42
1:A:100:LYS:HE3	1:A:318:SER:O	2.20	0.41
1:E:312:VAL:HG22	1:E:336:LYS:HD3	2.00	0.41
1:B:302:ASN:HB2	1:B:303:PRO:HD2	2.02	0.41
1:F:325:TRP:CE2	1:F:343:MET:SD	3.13	0.41
1:D:395:ASP:HB3	1:D:406:VAL:HG22	2.02	0.41
1:E:370:ARG:CB	1:E:374:SER:HB3	2.47	0.41
1:G:254:LEU:HB3	1:G:257:ILE:HD12	2.02	0.41
1:B:55:ILE:HG22	1:B:89:ILE:HD11	2.01	0.41
1:B:100:LYS:HE3	1:B:318:SER:O	2.20	0.41
1:C:240:ARG:HD3	1:C:268:ASP:OD2	2.21	0.41
1:F:101:LYS:O	1:F:318:SER:HA	2.21	0.41
1:F:217:ILE:HG12	1:F:309:VAL:CG1	2.50	0.41
1:G:45:LEU:HD13	1:G:97:ILE:HD13	2.01	0.41
1:A:325:TRP:CE2	1:A:343:MET:SD	3.13	0.41
1:A:353:TYR:OH	1:A:358:GLY:HA2	2.21	0.41
1:B:101:LYS:O	1:B:318:SER:HA	2.20	0.41
1:D:164:LEU:HB2	1:D:316:HIS:CE1	2.55	0.41
1:D:174:ASP:O	1:D:178:VAL:HG22	2.21	0.41
1:E:174:ASP:O	1:E:178:VAL:HG22	2.21	0.41
1:E:380:VAL:HG13	1:E:385:ILE:HB	2.02	0.41
1:G:134:VAL:HG21	1:G:157:LEU:HG	2.02	0.41
1:E:158:ALA:HB3	1:E:311:ILE:HD13	2.02	0.41
1:H:370:ARG:O	1:H:374:SER:HB3	2.20	0.40
1:E:212:GLU:OE1	2:E:501:HOH:O	2.22	0.40
1:G:325:TRP:CZ2	1:G:343:MET:SD	3.15	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	371/399 (93%)	354 (95%)	14 (4%)	3 (1%)	19	17
1	B	368/399 (92%)	352 (96%)	15 (4%)	1 (0%)	41	43
1	C	369/399 (92%)	353 (96%)	15 (4%)	1 (0%)	41	43
1	D	372/399 (93%)	354 (95%)	17 (5%)	1 (0%)	41	43
1	E	370/399 (93%)	350 (95%)	19 (5%)	1 (0%)	41	43
1	F	368/399 (92%)	352 (96%)	15 (4%)	1 (0%)	41	43
1	G	368/399 (92%)	351 (95%)	15 (4%)	2 (0%)	29	28
1	H	367/399 (92%)	347 (95%)	17 (5%)	3 (1%)	19	17
All	All	2953/3192 (92%)	2813 (95%)	127 (4%)	13 (0%)	34	35

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	322	ASN
1	A	368	LYS
1	C	322	ASN
1	H	322	ASN
1	H	373	MET
1	B	322	ASN
1	G	322	ASN
1	G	371	LYS
1	D	322	ASN
1	H	371	LYS
1	E	371	LYS
1	F	322	ASN

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	302/341 (89%)	302 (100%)	0	100	100
1	B	303/341 (89%)	301 (99%)	2 (1%)	84	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	303/341 (89%)	303 (100%)	0	100 100
1	D	308/341 (90%)	308 (100%)	0	100 100
1	E	307/341 (90%)	307 (100%)	0	100 100
1	F	304/341 (89%)	304 (100%)	0	100 100
1	G	305/341 (89%)	304 (100%)	1 (0%)	92 96
1	H	296/341 (87%)	296 (100%)	0	100 100
All	All	2428/2728 (89%)	2425 (100%)	3 (0%)	93 97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	273	LYS
1	B	274	LYS
1	G	206	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	44	GLN
1	E	210	GLN
1	H	330	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	373/399 (93%)	-0.03	13 (3%)	44	44	33, 42, 58, 114	0
1	B	369/399 (92%)	-0.16	3 (0%)	86	86	32, 41, 56, 86	1 (0%)
1	C	370/399 (92%)	-0.21	3 (0%)	86	86	34, 42, 57, 91	1 (0%)
1	D	373/399 (93%)	-0.05	7 (1%)	66	67	33, 43, 61, 111	0
1	E	371/399 (92%)	-0.11	4 (1%)	80	80	32, 41, 54, 114	2 (0%)
1	F	369/399 (92%)	-0.06	8 (2%)	62	62	37, 44, 59, 86	2 (0%)
1	G	369/399 (92%)	-0.10	3 (0%)	86	86	37, 46, 67, 92	0
1	H	369/399 (92%)	-0.03	8 (2%)	62	62	37, 46, 62, 129	1 (0%)
All	All	2963/3192 (92%)	-0.09	49 (1%)	70	70	32, 43, 60, 129	7 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	LEU	7.8
1	D	40	GLY	5.0
1	H	369	ASP	4.6
1	G	372[A]	GLY	4.0
1	C	105	PHE	4.0
1	F	369	ASP	3.8
1	D	41	SER	3.6
1	H	373	MET	3.6
1	H	370	ARG	3.6
1	A	369	ASP	3.3
1	A	370	ARG	3.3
1	E	105	PHE	3.1
1	B	357	TRP	3.1
1	A	41	SER	3.0
1	B	409	ARG	3.0
1	F	409	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	37	GLY	2.9
1	D	39	LEU	2.8
1	A	314	TRP	2.8
1	A	157	LEU	2.7
1	C	369	ASP	2.6
1	D	312	VAL	2.6
1	A	312	VAL	2.5
1	F	159	TYR	2.5
1	H	372	GLY	2.5
1	F	357	TRP	2.5
1	F	161	PRO	2.4
1	F	160	VAL	2.4
1	E	312	VAL	2.4
1	D	369	ASP	2.4
1	G	105	PHE	2.3
1	D	313	ALA	2.3
1	B	408	SER	2.3
1	H	314	TRP	2.3
1	A	159	TYR	2.2
1	H	41	SER	2.2
1	E	222	ILE	2.2
1	A	40	GLY	2.2
1	E	369	ASP	2.2
1	A	105	PHE	2.2
1	H	357	TRP	2.2
1	F	312	VAL	2.2
1	C	357	TRP	2.1
1	G	369	ASP	2.1
1	H	105	PHE	2.1
1	A	372	GLY	2.0
1	D	160	VAL	2.0
1	F	128	VAL	2.0
1	A	158	ALA	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.