Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:50 PM GMT

PDB ID	:	3V3K
Title	:	Human caspase 9 in complex with bacterial effector protein
Authors	:	Moertl, M.; Maskos, K.; Steuber, H.
Deposited on	:	2011-12-13
Resolution	:	3.49 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

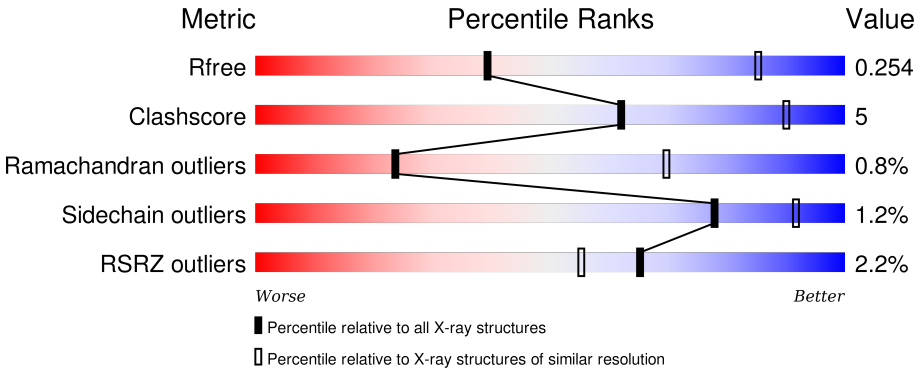
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	276	79% 9% 11%
1	C	276	75% 11% 14%
1	E	276	75% 13% 12%
1	G	276	75% 10% 15%
1	I	276	76% 12% 12%

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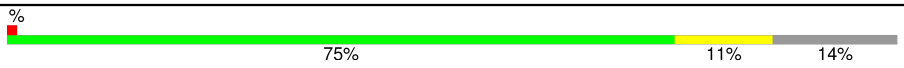
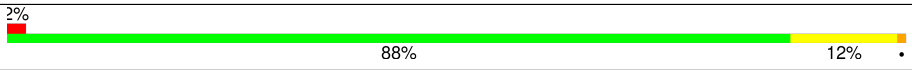
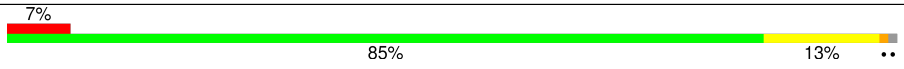
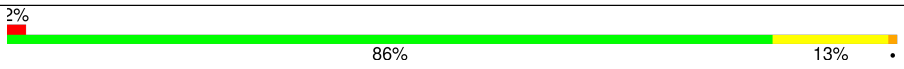
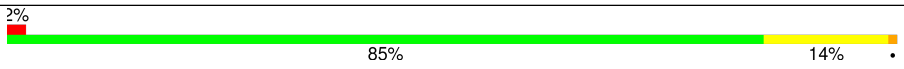
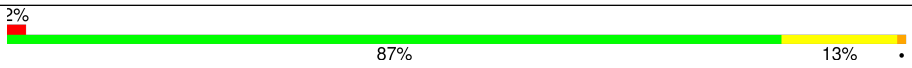
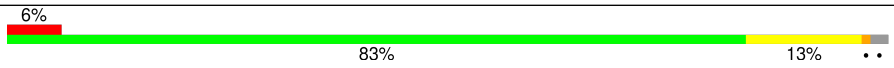
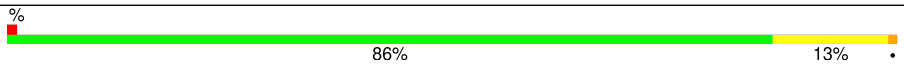
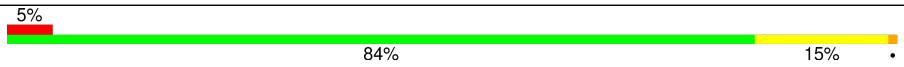
Mol	Chain	Length	Quality of chain
1	K	276	
1	M	276	
1	O	276	
2	B	165	
2	D	165	
2	F	165	
2	H	165	
2	J	165	
2	L	165	
2	N	165	
2	P	165	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25428 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 Caspase-9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	29	0	0
			1898	1209	326	348	15			
1	C	237	Total	C	N	O	S	34	0	0
			1839	1172	315	337	15			
1	E	243	Total	C	N	O	S	43	0	0
			1885	1200	324	346	15			
1	G	235	Total	C	N	O	S	26	0	0
			1828	1166	313	334	15			
1	I	244	Total	C	N	O	S	44	0	0
			1890	1203	325	347	15			
1	K	237	Total	C	N	O	S	16	0	0
			1839	1172	315	337	15			
1	M	245	Total	C	N	O	S	37	0	0
			1898	1209	326	348	15			
1	O	237	Total	C	N	O	S	34	0	0
			1839	1172	315	337	15			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	220	ARG	GLN	SEE REMARK 999	UNP P55211
C	220	ARG	GLN	SEE REMARK 999	UNP P55211
E	220	ARG	GLN	SEE REMARK 999	UNP P55211
G	220	ARG	GLN	SEE REMARK 999	UNP P55211
I	220	ARG	GLN	SEE REMARK 999	UNP P55211
K	220	ARG	GLN	SEE REMARK 999	UNP P55211
M	220	ARG	GLN	SEE REMARK 999	UNP P55211
O	220	ARG	GLN	SEE REMARK 999	UNP P55211

- Molecule 2 is a protein called Putative uncharacterized protein ECs1815.

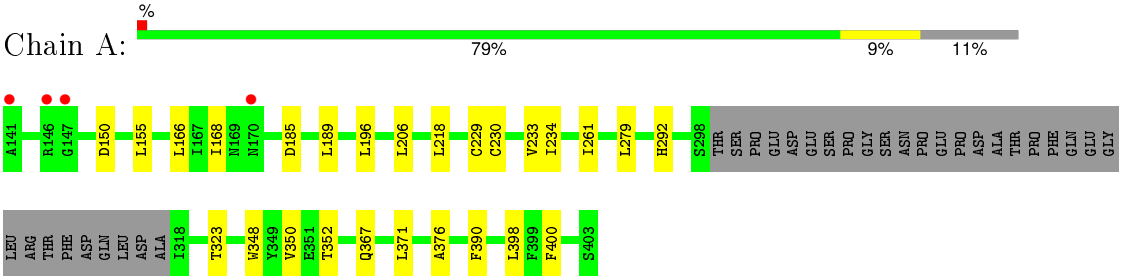
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	165	Total	C	N	O	S	54	0	0
			1319	819	226	264	10			
2	D	164	Total	C	N	O	S	114	0	0
			1312	815	225	262	10			
2	F	165	Total	C	N	O	S	56	0	0
			1319	819	226	264	10			
2	H	165	Total	C	N	O	S	58	0	0
			1319	819	226	264	10			
2	J	165	Total	C	N	O	S	78	0	0
			1319	819	226	264	10			
2	L	161	Total	C	N	O	S	112	0	0
			1286	799	222	255	10			
2	N	165	Total	C	N	O	S	95	0	0
			1319	819	226	264	10			
2	P	165	Total	C	N	O	S	112	0	0
			1319	819	226	264	10			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

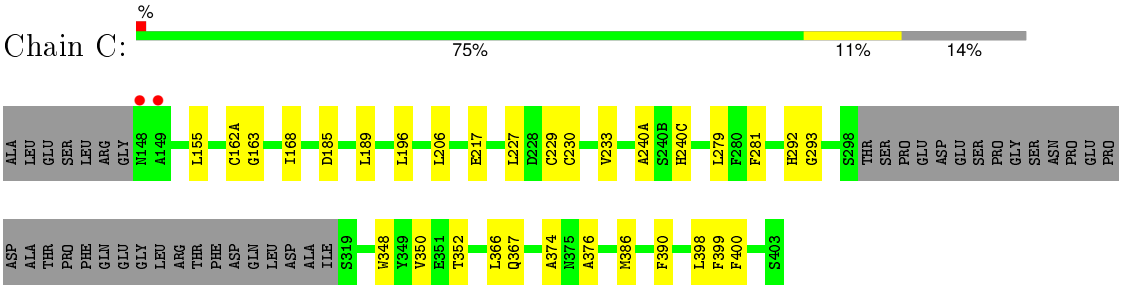
- Molecule 1: Caspase-9

Chain A:



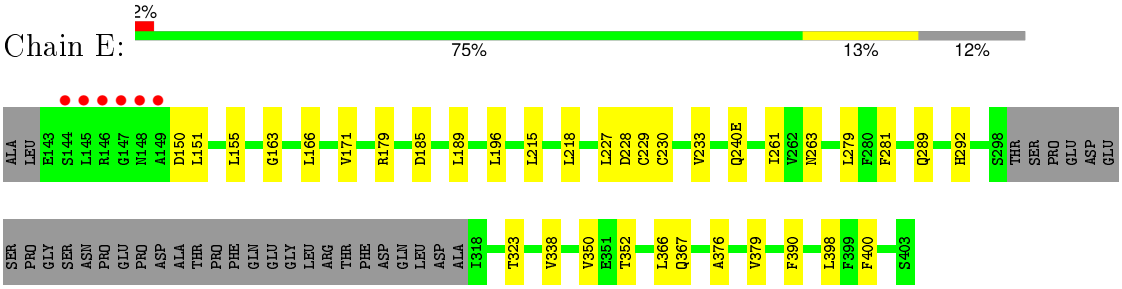
- Molecule 1: Caspase-9

Chain C:



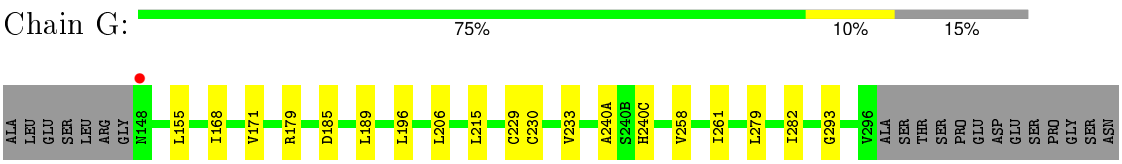
- Molecule 1: Caspase-9

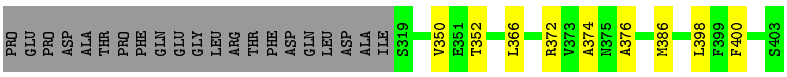
Chain E:



- Molecule 1: Caspase-9

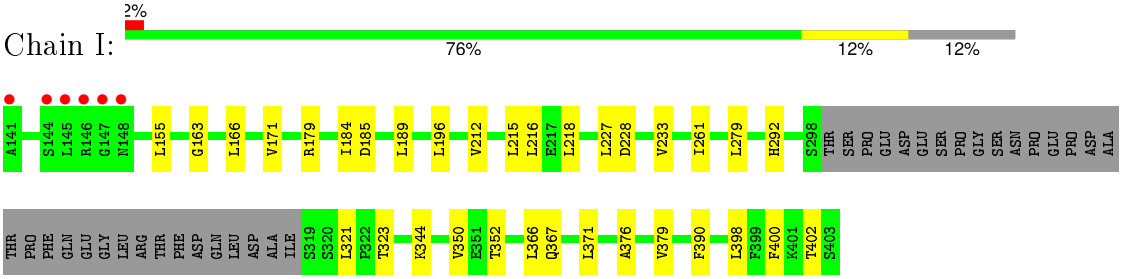
Chain G:





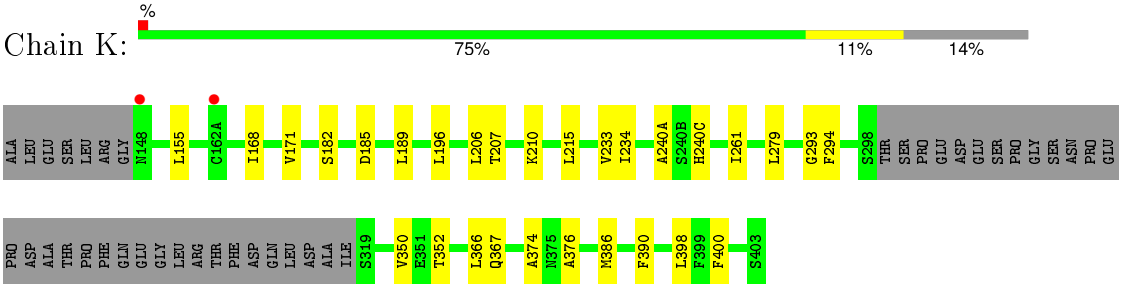
• Molecule 1: Caspase-9

Chain I:



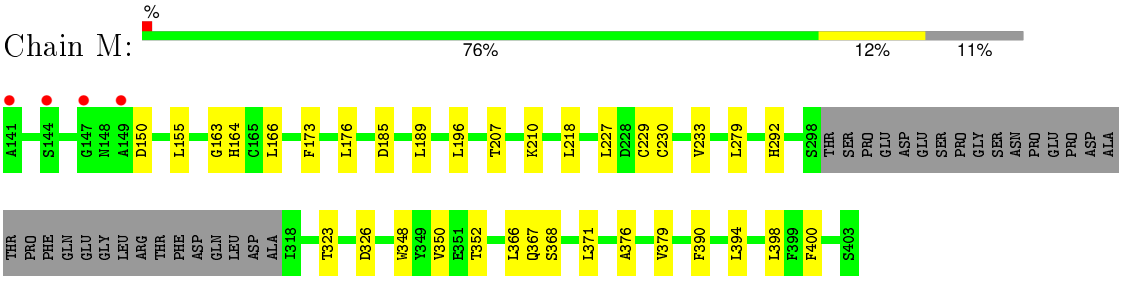
• Molecule 1: Caspase-9

Chain K:



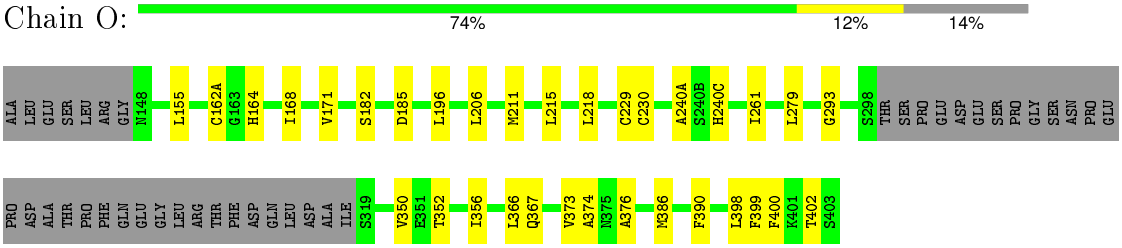
• Molecule 1: Caspase-9

Chain M:



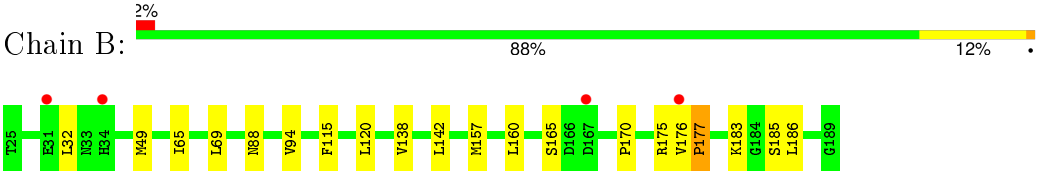
• Molecule 1: Caspase-9

Chain O:



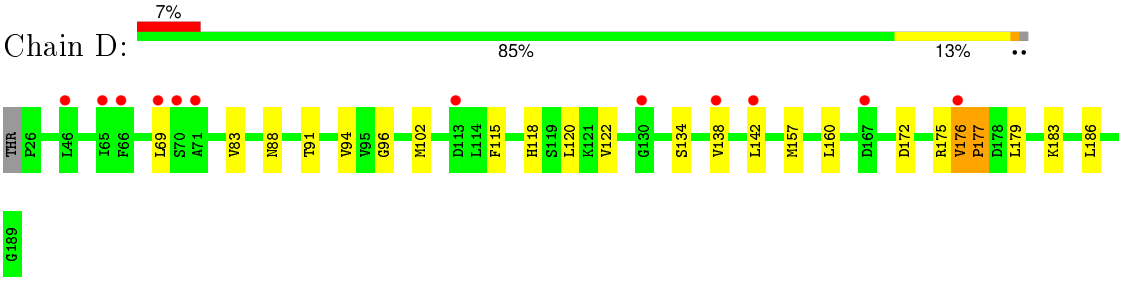
• Molecule 2: Putative uncharacterized protein ECs1815

Chain B:



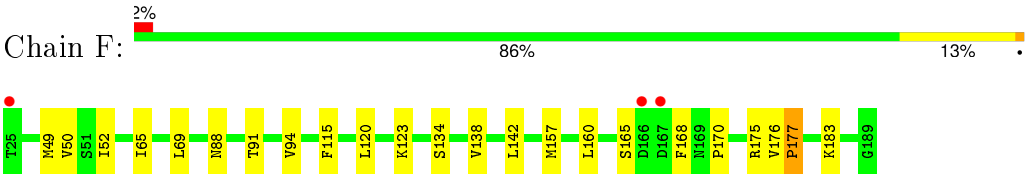
• Molecule 2: Putative uncharacterized protein ECs1815

Chain D:



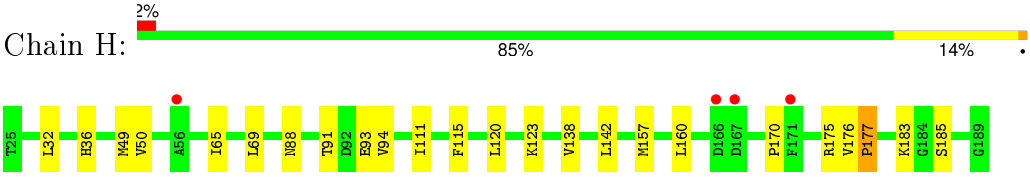
• Molecule 2: Putative uncharacterized protein ECs1815

Chain F:



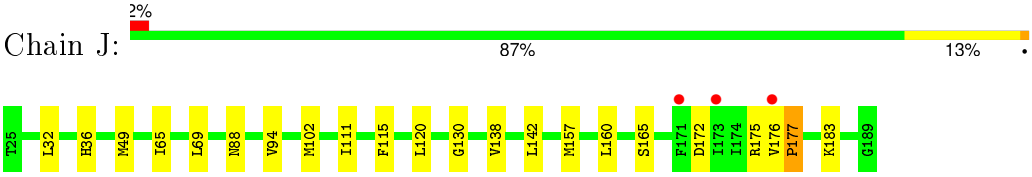
• Molecule 2: Putative uncharacterized protein ECs1815

Chain H:



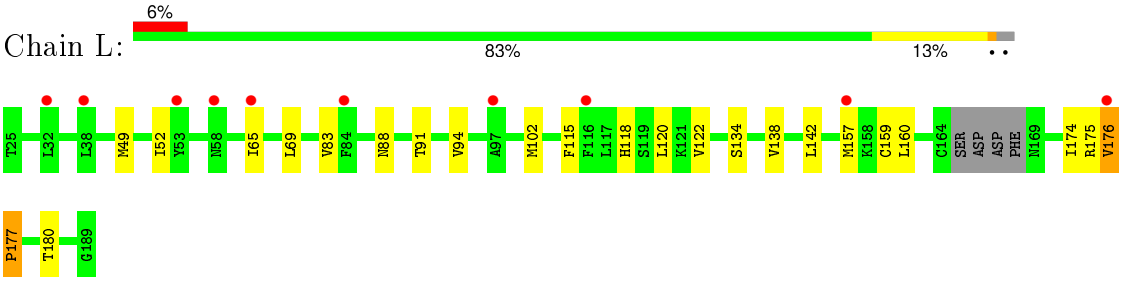
• Molecule 2: Putative uncharacterized protein ECs1815

Chain J:



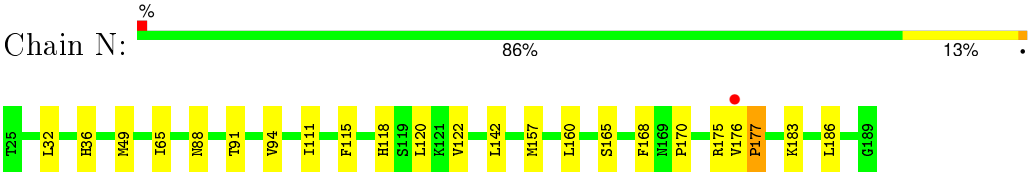
• Molecule 2: Putative uncharacterized protein ECs1815

Chain L:



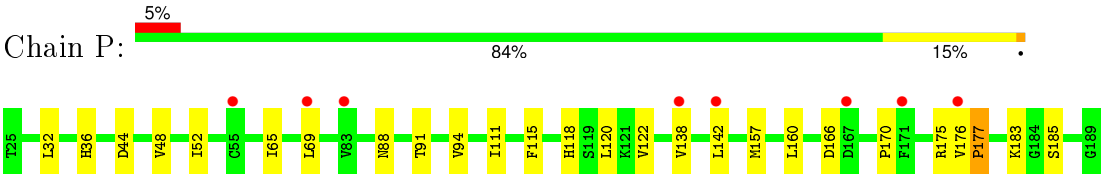
• Molecule 2: Putative uncharacterized protein ECs1815

Chain N:



• Molecule 2: Putative uncharacterized protein ECs1815

Chain P:


5%
84%
15%
T25
L32
H36
D44
V48
I52
C55
I65
L69
V83
N88
T91
V94
I111
F115
H118
S119
L120
K121
V122
V138
L142
M157
L160
D166
D167
P170
F171
R175
V176
P177
K183
G184
S185
G189

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	100.70Å 209.91Å 317.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	174.08 – 3.49 48.39 – 3.49	Depositor EDS
% Data completeness (in resolution range)	98.4 (174.08-3.49) 98.5 (48.39-3.49)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.239 , 0.259 0.236 , 0.254	Depositor DCC
R_{free} test set	1689 reflections (2.03%)	DCC
Wilson B-factor (Å^2)	91.1	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 25.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Outliers	0 of 84730 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	25428	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.39	0/1940	0.52	0/2619
1	C	0.40	1/1881 (0.1%)	0.52	0/2540
1	E	0.40	0/1927	0.52	0/2601
1	G	0.42	0/1870	0.54	0/2525
1	I	0.41	0/1932	0.52	0/2608
1	K	0.40	0/1881	0.52	0/2540
1	M	0.40	0/1940	0.52	0/2619
1	O	0.43	0/1881	0.53	0/2540
2	B	0.45	0/1341	0.52	0/1805
2	D	0.43	0/1334	0.51	0/1794
2	F	0.43	0/1341	0.52	0/1805
2	H	0.45	1/1341 (0.1%)	0.52	0/1805
2	J	0.42	0/1341	0.52	0/1805
2	L	0.43	0/1306	0.50	0/1756
2	N	0.45	0/1341	0.50	0/1805
2	P	0.46	0/1341	0.53	0/1805
All	All	0.42	2/25938 (0.0%)	0.52	0/34972

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	217	GLU	CG-CD	-5.48	1.43	1.51
2	H	93	GLU	CD-OE1	-5.41	1.19	1.25

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	1898	0	1883	17	0
1	C	1839	0	1818	18	0
1	E	1885	0	1867	19	0
1	G	1828	0	1808	18	0
1	I	1890	0	1872	20	0
1	K	1839	0	1818	18	0
1	M	1898	0	1883	21	0
1	O	1839	0	1818	21	0
2	B	1319	0	1272	16	0
2	D	1312	0	1266	14	0
2	F	1319	0	1272	15	0
2	H	1319	0	1272	15	0
2	J	1319	0	1272	14	0
2	L	1286	0	1249	15	0
2	N	1319	0	1272	16	0
2	P	1319	0	1272	15	0
All	All	25428	0	24914	259	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 5.

All (259) 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:O:366:LEU:HD22	1:O:398:LEU:HD23	1.62	0.82
2:H:120:LEU:HD22	2:H:142:LEU:HD11	1.67	0.75
2:D:120:LEU:HD22	2:D:142:LEU:HD11	1.70	0.73
1:K:366:LEU:HD22	1:K:398:LEU:HD23	1.72	0.70
2:L:176:VAL:HG12	2:L:177:PRO:HD3	1.77	0.66
2:H:176:VAL:HG12	2:H:177:PRO:HD3	1.78	0.66
2:F:120:LEU:HD22	2:F:142:LEU:HD11	1.78	0.65
1:C:168:ILE:HG23	1:C:206:LEU:HD12	1.77	0.65
2:H:91:THR:O	2:H:94:VAL:HG23	1.97	0.63
1:K:215:LEU:HD13	1:K:261:ILE:HG23	1.80	0.62
2:L:120:LEU:HD22	2:L:142:LEU:HD11	1.81	0.62
1:I:215:LEU:HD13	1:I:261:ILE:HG23	1.82	0.62
1:I:366:LEU:HD22	1:I:398:LEU:HD23	1.80	0.62
1:G:366:LEU:HD22	1:G:398:LEU:HD23	1.83	0.61
2:P:120:LEU:HD22	2:P:142:LEU:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:176:VAL:HG12	2:P:177:PRO:HD3	1.83	0.61
1:G:215:LEU:HD13	1:G:261:ILE:HG23	1.81	0.61
2:J:120:LEU:HD22	2:J:142:LEU:HD11	1.84	0.60
1:K:185:ASP:HB3	1:K:350:VAL:HG11	1.83	0.60
2:N:176:VAL:HG12	2:N:177:PRO:HD3	1.84	0.60
2:P:115:PHE:CD2	2:P:157:MET:HE1	2.37	0.60
2:D:176:VAL:HG12	2:D:177:PRO:HD3	1.83	0.59
2:D:91:THR:O	2:D:94:VAL:HG23	2.02	0.59
2:N:49:MET:HG2	2:N:65:ILE:HD12	1.84	0.58
2:B:120:LEU:HD22	2:B:142:LEU:HD11	1.85	0.58
2:L:52:ILE:HG21	2:L:65:ILE:HD11	1.85	0.58
1:O:374:ALA:HB1	1:O:386:MET:HE1	1.86	0.58
1:A:189:LEU:HD13	1:A:233:VAL:HG11	1.84	0.58
2:F:176:VAL:HG12	2:F:177:PRO:HD3	1.86	0.58
2:N:160:LEU:HD12	2:N:176:VAL:HG23	1.85	0.57
2:F:160:LEU:HD12	2:F:176:VAL:HG23	1.86	0.57
1:C:366:LEU:HD22	1:C:398:LEU:HD23	1.85	0.57
2:B:176:VAL:HG12	2:B:177:PRO:HD3	1.85	0.57
2:H:160:LEU:HD12	2:H:176:VAL:HG23	1.85	0.57
2:P:69:LEU:HD12	2:P:138:VAL:HG13	1.85	0.57
2:D:69:LEU:HD12	2:D:138:VAL:HG13	1.87	0.57
2:L:69:LEU:HD12	2:L:138:VAL:HG13	1.86	0.57
2:L:83:VAL:HG22	2:L:102:MET:HE2	1.86	0.57
2:H:69:LEU:HD12	2:H:138:VAL:HG13	1.87	0.56
2:L:120:LEU:CD2	2:L:142:LEU:HD11	2.36	0.56
2:J:176:VAL:HG12	2:J:177:PRO:HD3	1.87	0.56
1:E:166:LEU:HB2	1:E:218:LEU:HD22	1.85	0.56
2:D:83:VAL:HG22	2:D:102:MET:HE2	1.88	0.56
1:K:196:LEU:HD22	1:K:400:PHE:HB3	1.87	0.56
2:J:94:VAL:HG21	2:J:183:LYS:O	2.06	0.56
1:C:196:LEU:HD22	1:C:400:PHE:HB3	1.88	0.55
1:E:215:LEU:HD13	1:E:261:ILE:HG23	1.88	0.55
2:H:115:PHE:CD2	2:H:157:MET:HE1	2.41	0.55
2:J:120:LEU:CD2	2:J:142:LEU:HD11	2.37	0.55
2:H:88:ASN:O	2:H:94:VAL:HG22	2.06	0.55
1:M:279:LEU:HD11	1:M:398:LEU:HD21	1.89	0.55
2:L:91:THR:O	2:L:94:VAL:HG23	2.07	0.55
2:P:91:THR:O	2:P:94:VAL:HG23	2.07	0.54
1:K:155:LEU:HD11	1:K:398:LEU:HD11	1.89	0.54
1:I:279:LEU:HD11	1:I:398:LEU:HD21	1.89	0.54
1:A:279:LEU:HD11	1:A:398:LEU:HD21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:166:LEU:HB2	1:I:218:LEU:HD22	1.90	0.54
2:F:94:VAL:HG21	2:F:183:LYS:O	2.08	0.54
2:B:120:LEU:CD2	2:B:142:LEU:HD11	2.38	0.53
1:I:196:LEU:HD22	1:I:400:PHE:HB3	1.90	0.53
2:L:115:PHE:CD2	2:L:157:MET:HE1	2.43	0.53
1:G:240(A):ALA:HB3	1:G:240(C):HIS:NE2	2.23	0.53
1:M:352:THR:HG21	1:M:376:ALA:HB3	1.88	0.53
1:I:352:THR:HG21	1:I:376:ALA:HB3	1.91	0.53
2:P:160:LEU:HD12	2:P:176:VAL:HG23	1.91	0.53
2:B:160:LEU:HD12	2:B:176:VAL:HG23	1.91	0.53
2:J:160:LEU:HD12	2:J:176:VAL:HG23	1.91	0.53
1:I:189:LEU:HD13	1:I:233:VAL:HG11	1.91	0.53
1:K:168:ILE:HG23	1:K:206:LEU:HD12	1.90	0.53
2:N:88:ASN:O	2:N:94:VAL:HG22	2.09	0.53
2:B:94:VAL:HG21	2:B:183:LYS:O	2.08	0.52
2:J:115:PHE:CD2	2:J:157:MET:HE1	2.44	0.52
2:J:69:LEU:HD12	2:J:138:VAL:HG13	1.91	0.52
1:C:185:ASP:HB3	1:C:350:VAL:HG11	1.92	0.52
2:J:176:VAL:CG1	2:J:177:PRO:HD3	2.39	0.52
1:E:323:THR:HG23	1:G:293:GLY:HA2	1.92	0.52
2:B:49:MET:HG2	2:B:65:ILE:HD12	1.90	0.52
1:G:185:ASP:HB3	1:G:350:VAL:HG11	1.91	0.52
1:G:155:LEU:HD11	1:G:398:LEU:HD11	1.92	0.52
2:F:88:ASN:O	2:F:94:VAL:HG22	2.09	0.52
1:A:371:LEU:HD11	1:C:367:GLN:NE2	2.25	0.52
1:A:168:ILE:HG23	1:A:206:LEU:HD12	1.92	0.52
1:O:196:LEU:HD22	1:O:400:PHE:HB3	1.91	0.52
1:G:352:THR:HG21	1:G:376:ALA:HB3	1.91	0.52
1:M:189:LEU:HD13	1:M:233:VAL:HG11	1.91	0.51
1:M:371:LEU:HD11	1:O:367:GLN:NE2	2.25	0.51
2:F:176:VAL:CG1	2:F:177:PRO:HD3	2.40	0.51
1:A:196:LEU:HD22	1:A:400:PHE:HB3	1.93	0.51
1:E:366:LEU:HD22	1:E:398:LEU:HD23	1.93	0.51
2:H:94:VAL:HG21	2:H:183:LYS:O	2.10	0.51
1:A:323:THR:HG23	1:C:293:GLY:HA2	1.92	0.51
2:N:94:VAL:HG21	2:N:183:LYS:O	2.11	0.51
2:F:52:ILE:HG21	2:F:65:ILE:HD11	1.92	0.51
2:B:115:PHE:HA	2:B:157:MET:HE2	1.92	0.50
2:F:120:LEU:CD2	2:F:142:LEU:HD11	2.40	0.50
1:M:229:CYS:SG	1:M:230:CYS:N	2.85	0.50
2:N:115:PHE:CD2	2:N:157:MET:HE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:120:LEU:CD2	2:N:142:LEU:HD11	2.42	0.50
1:E:185:ASP:HB3	1:E:350:VAL:HG11	1.93	0.50
1:I:323:THR:HG23	1:K:293:GLY:HA2	1.92	0.50
2:B:69:LEU:HD12	2:B:138:VAL:HG13	1.94	0.49
1:O:215:LEU:HD13	1:O:261:ILE:HG23	1.95	0.49
1:O:168:ILE:HG23	1:O:206:LEU:HD12	1.94	0.49
1:G:168:ILE:HG23	1:G:206:LEU:HD12	1.94	0.49
1:E:155:LEU:HD23	1:E:228:ASP:HB3	1.95	0.49
2:J:49:MET:HG2	2:J:65:ILE:HD12	1.94	0.48
1:M:196:LEU:HD22	1:M:400:PHE:HB3	1.94	0.48
1:K:279:LEU:HD11	1:K:398:LEU:HD21	1.95	0.48
1:G:374:ALA:HB1	1:G:386:MET:HE1	1.96	0.48
1:I:279:LEU:HD11	1:I:398:LEU:CD2	2.44	0.48
1:C:279:LEU:HD11	1:C:398:LEU:CD2	2.43	0.48
2:F:69:LEU:HD12	2:F:138:VAL:HG13	1.95	0.48
2:F:115:PHE:CD2	2:F:157:MET:HE1	2.49	0.48
1:M:166:LEU:HB2	1:M:218:LEU:HD22	1.96	0.48
1:A:229:CYS:SG	1:A:230:CYS:N	2.86	0.48
1:A:352:THR:HG21	1:A:376:ALA:HB3	1.96	0.47
1:A:185:ASP:HB3	1:A:350:VAL:HG11	1.96	0.47
2:N:32:LEU:HD21	2:N:176:VAL:HG21	1.95	0.47
1:K:240(A):ALA:HB3	1:K:240(C):HIS:NE2	2.30	0.47
2:P:52:ILE:HG21	2:P:65:ILE:HD11	1.96	0.47
2:B:176:VAL:CG1	2:B:177:PRO:HD3	2.45	0.47
2:P:94:VAL:HG21	2:P:183:LYS:O	2.15	0.47
1:A:348:TRP:HZ2	2:B:186:LEU:HD21	1.80	0.47
2:H:32:LEU:HD21	2:H:176:VAL:HG21	1.96	0.47
1:E:279:LEU:HD11	1:E:398:LEU:HD21	1.96	0.47
1:C:229:CYS:SG	1:C:230:CYS:N	2.88	0.47
1:M:173:PHE:CD2	1:M:176:LEU:HD12	2.49	0.47
2:H:120:LEU:CD2	2:H:142:LEU:HD11	2.39	0.47
2:J:88:ASN:O	2:J:94:VAL:HG22	2.14	0.47
1:C:155:LEU:HD22	1:C:162(A):CYS:SG	2.54	0.47
1:M:155:LEU:HD11	1:M:398:LEU:HD11	1.96	0.47
2:N:115:PHE:HA	2:N:157:MET:HE2	1.97	0.47
2:J:49:MET:HG2	2:J:65:ILE:HG23	1.97	0.47
1:K:374:ALA:HB1	1:K:386:MET:HE1	1.96	0.47
1:K:155:LEU:HD11	1:K:398:LEU:CD1	2.45	0.47
2:N:49:MET:HG2	2:N:65:ILE:HG23	1.97	0.46
1:E:196:LEU:HD22	1:E:400:PHE:HB3	1.97	0.46
1:I:155:LEU:HD23	1:I:228:ASP:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:94:VAL:HG12	2:L:180:THR:HG22	1.98	0.46
1:E:376:ALA:O	1:E:379:VAL:HG22	2.15	0.46
2:N:176:VAL:CG1	2:N:177:PRO:HD3	2.45	0.46
1:O:155:LEU:HD22	1:O:162(A):CYS:SG	2.55	0.46
1:O:196:LEU:HD23	1:O:402:THR:HG22	1.98	0.46
1:O:168:ILE:HD13	1:O:211:MET:HG2	1.98	0.46
1:E:163:GLY:HA2	1:E:227:LEU:HD22	1.98	0.46
2:H:176:VAL:CG1	2:H:177:PRO:HD3	2.45	0.45
1:M:366:LEU:HD22	1:M:398:LEU:HD23	1.97	0.45
2:L:118:HIS:O	2:L:122:VAL:HG23	2.16	0.45
1:G:189:LEU:HD13	1:G:233:VAL:HG11	1.98	0.45
1:C:279:LEU:HD11	1:C:398:LEU:HD21	1.98	0.45
1:I:371:LEU:HD11	1:K:367:GLN:NE2	2.31	0.45
2:H:36:HIS:ND1	2:H:111:ILE:HG21	2.31	0.45
1:G:229:CYS:SG	1:G:230:CYS:N	2.90	0.45
2:D:94:VAL:HG21	2:D:183:LYS:O	2.17	0.45
2:D:88:ASN:O	2:D:94:VAL:HG22	2.16	0.45
1:C:240(A):ALA:HB3	1:C:240(C):HIS:NE2	2.31	0.45
1:E:151:LEU:HD21	1:G:372:ARG:CZ	2.47	0.45
1:A:348:TRP:CZ2	2:B:186:LEU:HD21	2.52	0.45
1:C:348:TRP:CZ2	2:D:186:LEU:HD21	2.51	0.45
1:G:155:LEU:HD11	1:G:398:LEU:CD1	2.46	0.44
1:O:352:THR:HG21	1:O:376:ALA:HB3	1.99	0.44
2:F:50:VAL:HG21	2:F:123:LYS:HD2	1.98	0.44
1:M:207:THR:HG22	1:M:210:LYS:CD	2.47	0.44
2:P:36:HIS:ND1	2:P:111:ILE:HG21	2.33	0.44
1:E:189:LEU:HD13	1:E:233:VAL:HG11	2.00	0.44
1:G:279:LEU:HD11	1:G:398:LEU:HD21	1.99	0.44
2:L:83:VAL:HG22	2:L:102:MET:CE	2.47	0.44
2:P:44:ASP:O	2:P:48:VAL:HG23	2.18	0.44
1:M:279:LEU:HD11	1:M:398:LEU:CD2	2.46	0.44
1:M:348:TRP:HZ2	2:N:186:LEU:HD21	1.82	0.44
2:D:83:VAL:HG22	2:D:102:MET:CE	2.47	0.44
1:I:212:VAL:HG12	1:I:216:LEU:HD12	2.00	0.44
2:D:160:LEU:HD12	2:D:176:VAL:HG23	2.00	0.44
1:C:374:ALA:HB1	1:C:386:MET:HE1	2.00	0.44
2:L:159:CYS:HB3	2:L:174:ILE:HD13	2.00	0.43
1:O:229:CYS:SG	1:O:230:CYS:N	2.91	0.43
1:I:155:LEU:HD11	1:I:398:LEU:HD11	2.00	0.43
1:O:374:ALA:HB1	1:O:386:MET:CE	2.47	0.43
2:B:32:LEU:HD21	2:B:176:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:LEU:HD13	1:C:233:VAL:HG11	1.99	0.43
2:J:36:HIS:ND1	2:J:111:ILE:HG21	2.32	0.43
1:O:279:LEU:HD11	1:O:398:LEU:HD21	1.99	0.43
2:H:160:LEU:HD12	2:H:176:VAL:CG2	2.49	0.43
1:K:189:LEU:HD13	1:K:233:VAL:HG11	2.00	0.43
1:G:258:VAL:HG22	1:G:282:ILE:HD13	2.01	0.43
1:E:229:CYS:SG	1:E:230:CYS:N	2.91	0.43
1:I:321:LEU:HD23	1:K:294:PHE:CE1	2.53	0.43
2:F:91:THR:O	2:F:94:VAL:HG23	2.18	0.43
1:E:289:GLN:O	1:E:338:VAL:HG23	2.19	0.43
2:J:115:PHE:HA	2:J:157:MET:HE2	2.00	0.43
1:K:352:THR:HG21	1:K:376:ALA:HB3	1.99	0.43
1:G:196:LEU:HD22	1:G:400:PHE:HB3	2.00	0.43
1:K:234:ILE:CD1	1:K:261:ILE:HD13	2.48	0.43
2:F:49:MET:HG2	2:F:65:ILE:HD12	2.01	0.43
1:O:185:ASP:HB3	1:O:350:VAL:HG11	2.00	0.43
1:I:171:VAL:HG13	1:I:179:ARG:O	2.18	0.43
1:O:171:VAL:HG22	1:O:182:SER:HB3	2.01	0.43
2:D:118:HIS:O	2:D:122:VAL:HG23	2.18	0.43
1:M:155:LEU:HD11	1:M:398:LEU:CD1	2.49	0.43
2:L:88:ASN:O	2:L:94:VAL:HG22	2.18	0.43
1:M:368:SER:HA	1:M:371:LEU:HD12	2.01	0.43
1:M:163:GLY:HA2	1:M:227:LEU:HD22	2.01	0.43
1:M:185:ASP:HB3	1:M:350:VAL:HG11	2.01	0.43
2:P:176:VAL:CG1	2:P:177:PRO:HD3	2.49	0.43
2:N:120:LEU:HD22	2:N:142:LEU:HD11	2.00	0.43
1:E:352:THR:HG21	1:E:376:ALA:HB3	2.01	0.43
1:E:233:VAL:HG22	1:E:281:PHE:HB2	2.00	0.43
2:N:91:THR:O	2:N:94:VAL:HG23	2.19	0.42
1:C:352:THR:HG21	1:C:376:ALA:HB3	2.01	0.42
1:O:356:ILE:HD12	1:O:373:VAL:HG22	2.01	0.42
1:A:189:LEU:CD1	1:A:233:VAL:HG11	2.50	0.42
1:A:279:LEU:HD21	1:A:398:LEU:CD2	2.49	0.42
2:D:115:PHE:CD2	2:D:157:MET:HE1	2.54	0.42
1:A:166:LEU:HB2	1:A:218:LEU:HD22	2.00	0.42
2:P:120:LEU:CD2	2:P:142:LEU:HD11	2.46	0.42
2:P:32:LEU:HD21	2:P:176:VAL:HG21	2.01	0.42
1:E:240(E):GLN:NE2	1:E:263:ASN:HD21	2.17	0.42
2:P:118:HIS:O	2:P:122:VAL:HG23	2.19	0.42
1:C:155:LEU:HD12	1:C:399:PHE:O	2.20	0.42
2:B:160:LEU:HD12	2:B:176:VAL:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:196:LEU:HD23	1:I:402:THR:HG22	2.00	0.42
1:M:326:ASP:HA	1:M:394:LEU:HD23	2.02	0.42
2:J:32:LEU:HD21	2:J:176:VAL:HG21	2.02	0.42
2:P:88:ASN:O	2:P:94:VAL:HG22	2.20	0.42
1:A:234:ILE:CD1	1:A:261:ILE:HD13	2.49	0.42
1:M:376:ALA:O	1:M:379:VAL:HG22	2.20	0.42
1:E:155:LEU:HD11	1:E:398:LEU:HD11	2.02	0.42
1:M:323:THR:HG23	1:O:293:GLY:HA2	2.02	0.41
2:L:49:MET:HG2	2:L:65:ILE:HG23	2.01	0.41
2:B:49:MET:HG2	2:B:65:ILE:HG23	2.01	0.41
2:F:49:MET:HG2	2:F:65:ILE:HG23	2.01	0.41
1:O:155:LEU:HD12	1:O:399:PHE:O	2.20	0.41
1:C:233:VAL:HG22	1:C:281:PHE:HB2	2.01	0.41
1:A:279:LEU:HD11	1:A:398:LEU:CD2	2.49	0.41
1:I:185:ASP:HB3	1:I:350:VAL:HG11	2.02	0.41
2:D:160:LEU:HD12	2:D:176:VAL:CG2	2.51	0.41
1:M:164:HIS:HB2	1:M:218:LEU:HD11	2.03	0.41
1:K:207:THR:HG23	1:K:210:LYS:H	1.86	0.41
1:G:171:VAL:HG13	1:G:179:ARG:O	2.21	0.41
1:O:240(A):ALA:HB3	1:O:240(C):HIS:NE2	2.36	0.41
2:N:36:HIS:ND1	2:N:111:ILE:HG21	2.36	0.41
1:O:196:LEU:CD2	1:O:402:THR:HG22	2.51	0.41
2:B:88:ASN:O	2:B:94:VAL:HG22	2.20	0.41
2:H:50:VAL:HG21	2:H:123:LYS:HD2	2.03	0.41
1:E:171:VAL:HG13	1:E:179:ARG:O	2.20	0.41
2:N:118:HIS:O	2:N:122:VAL:HG23	2.20	0.41
1:K:171:VAL:HG22	1:K:182:SER:HB3	2.03	0.41
1:C:163:GLY:HA2	1:C:227:LEU:HD13	2.03	0.41
1:G:279:LEU:HD11	1:G:398:LEU:CD2	2.51	0.41
2:F:115:PHE:HA	2:F:157:MET:HE2	2.03	0.41
2:H:49:MET:HG2	2:H:65:ILE:HG23	2.03	0.41
2:L:160:LEU:HD12	2:L:176:VAL:HG23	2.03	0.40
1:A:155:LEU:HD11	1:A:398:LEU:HD11	2.03	0.40
1:I:163:GLY:HA2	1:I:227:LEU:HD22	2.04	0.40
1:I:376:ALA:O	1:I:379:VAL:HG22	2.21	0.40
1:I:184:ILE:HD12	1:I:344:LYS:O	2.22	0.40
2:D:96:GLY:HA3	2:D:179:LEU:HD12	2.03	0.40
2:B:115:PHE:CD2	2:B:157:MET:HE1	2.55	0.40
1:O:164:HIS:CB	1:O:218:LEU:HD11	2.52	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	241/276 (87%)	231 (96%)	10 (4%)	0	100	100
1	C	233/276 (84%)	229 (98%)	4 (2%)	0	100	100
1	E	239/276 (87%)	230 (96%)	9 (4%)	0	100	100
1	G	231/276 (84%)	224 (97%)	7 (3%)	0	100	100
1	I	240/276 (87%)	232 (97%)	8 (3%)	0	100	100
1	K	233/276 (84%)	225 (97%)	8 (3%)	0	100	100
1	M	241/276 (87%)	231 (96%)	10 (4%)	0	100	100
1	O	233/276 (84%)	227 (97%)	6 (3%)	0	100	100
2	B	163/165 (99%)	144 (88%)	15 (9%)	4 (2%)	7	46
2	D	162/165 (98%)	147 (91%)	13 (8%)	2 (1%)	16	61
2	F	163/165 (99%)	146 (90%)	13 (8%)	4 (2%)	7	46
2	H	163/165 (99%)	148 (91%)	12 (7%)	3 (2%)	11	53
2	J	163/165 (99%)	145 (89%)	15 (9%)	3 (2%)	11	53
2	L	157/165 (95%)	146 (93%)	9 (6%)	2 (1%)	15	60
2	N	163/165 (99%)	148 (91%)	12 (7%)	3 (2%)	11	53
2	P	163/165 (99%)	148 (91%)	12 (7%)	3 (2%)	11	53
All	All	3188/3528 (90%)	3001 (94%)	163 (5%)	24 (1%)	24	70

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	177	PRO
2	F	177	PRO
2	H	177	PRO
2	P	177	PRO
2	B	177	PRO
2	F	165	SER

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Mol	Chain	Res	Type
2	J	165	SER
2	J	177	PRO
2	L	177	PRO
2	N	177	PRO
2	B	165	SER
2	F	134	SER
2	H	170	PRO
2	L	134	SER
2	N	165	SER
2	B	185	SER
2	D	134	SER
2	H	185	SER
2	P	185	SER
2	B	170	PRO
2	P	170	PRO
2	N	170	PRO
2	F	170	PRO
2	J	130	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	A	211/238 (89%)	207 (98%)	4 (2%)	65 87
1	C	205/238 (86%)	203 (99%)	2 (1%)	82 93
1	E	210/238 (88%)	206 (98%)	4 (2%)	65 87
1	G	204/238 (86%)	204 (100%)	0	100 100
1	I	210/238 (88%)	207 (99%)	3 (1%)	74 91
1	K	205/238 (86%)	204 (100%)	1 (0%)	92 97
1	M	211/238 (89%)	207 (98%)	4 (2%)	65 87
1	O	205/238 (86%)	204 (100%)	1 (0%)	92 97
2	B	152/152 (100%)	151 (99%)	1 (1%)	88 96
2	D	151/152 (99%)	148 (98%)	3 (2%)	63 87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	F	152/152 (100%)	150 (99%)	2 (1%)	76 91
2	H	152/152 (100%)	151 (99%)	1 (1%)	88 96
2	J	152/152 (100%)	149 (98%)	3 (2%)	63 87
2	L	148/152 (97%)	146 (99%)	2 (1%)	74 91
2	N	152/152 (100%)	150 (99%)	2 (1%)	76 91
2	P	152/152 (100%)	150 (99%)	2 (1%)	76 91
All	All	2872/3120 (92%)	2837 (99%)	35 (1%)	78 92

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150	ASP
1	A	292	HIS
1	A	367	GLN
1	A	390	PHE
2	B	175	ARG
1	C	292	HIS
1	C	390	PHE
2	D	172	ASP
2	D	175	ARG
2	D	176	VAL
1	E	150	ASP
1	E	292	HIS
1	E	367	GLN
1	E	390	PHE
2	F	168	PHE
2	F	175	ARG
2	H	175	ARG
1	I	292	HIS
1	I	367	GLN
1	I	390	PHE
2	J	102	MET
2	J	172	ASP
2	J	175	ARG
1	K	390	PHE
2	L	175	ARG
2	L	176	VAL
1	M	150	ASP
1	M	292	HIS
1	M	367	GLN

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Mol	Chain	Res	Type
1	M	390	PHE
2	N	168	PHE
2	N	175	ARG
1	O	390	PHE
2	P	166	ASP
2	P	175	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	385	GLN
1	C	283	GLN
1	E	240(E)	GLN
1	E	283	GLN
1	E	385	GLN
1	G	148	ASN
2	H	59	ASN
1	I	240(E)	GLN
1	I	263	ASN
1	I	283	GLN
1	I	385	GLN
1	K	367	GLN
1	M	240(E)	GLN
1	M	263	ASN
1	M	385	GLN
1	O	240(E)	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	245/276 (88%)	0.15	4 (1%)	74	65	47, 69, 102, 147	11 (4%)
1	C	237/276 (85%)	0.00	2 (0%)	87	80	51, 70, 95, 115	12 (5%)
1	E	243/276 (88%)	0.05	6 (2%)	61	50	47, 69, 102, 140	15 (6%)
1	G	235/276 (85%)	-0.07	1 (0%)	93	90	51, 71, 93, 118	9 (3%)
1	I	244/276 (88%)	0.02	6 (2%)	61	50	47, 70, 103, 151	16 (6%)
1	K	237/276 (85%)	-0.06	2 (0%)	87	80	51, 71, 95, 115	8 (3%)
1	M	245/276 (88%)	-0.01	4 (1%)	74	65	47, 69, 103, 146	14 (5%)
1	O	237/276 (85%)	-0.11	0	100	100	51, 72, 95, 116	13 (5%)
2	B	165/165 (100%)	0.08	4 (2%)	62	52	60, 90, 125, 139	16 (9%)
2	D	164/165 (99%)	0.38	12 (7%)	18	14	71, 98, 131, 137	31 (18%)
2	F	165/165 (100%)	0.21	3 (1%)	71	62	62, 90, 124, 136	17 (10%)
2	H	165/165 (100%)	0.21	4 (2%)	62	52	70, 98, 134, 140	21 (12%)
2	J	165/165 (100%)	0.13	3 (1%)	71	62	62, 90, 124, 141	24 (14%)
2	L	161/165 (97%)	0.49	10 (6%)	24	19	71, 98, 130, 137	32 (19%)
2	N	165/165 (100%)	0.07	1 (0%)	90	85	62, 90, 124, 141	27 (16%)
2	P	165/165 (100%)	0.44	8 (4%)	34	27	71, 98, 134, 139	33 (20%)
All	All	3238/3528 (91%)	0.10	70 (2%)	65	55	47, 78, 124, 151	299 (9%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	141	ALA	6.7
1	E	147	GLY	4.8
2	P	171	PHE	4.5
1	M	141	ALA	4.2
2	P	176	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
2	F	167	ASP	3.7
1	E	144	SER	3.6
2	D	142	LEU	3.5
2	J	176	VAL	3.4
2	P	69	LEU	3.4
1	M	147	GLY	3.3
2	H	166	ASP	3.3
1	I	144	SER	3.3
1	G	148	ASN	3.2
1	E	146	ARG	3.2
1	A	147	GLY	3.2
2	P	55	CYS	3.1
2	L	176	VAL	3.0
2	L	53	TYR	3.0
1	I	145	LEU	2.9
2	D	69	LEU	2.9
2	P	138	VAL	2.9
2	D	138	VAL	2.8
2	B	176	VAL	2.8
2	N	176	VAL	2.8
1	K	162(A)	CYS	2.8
1	E	149	ALA	2.7
2	L	58	ASN	2.7
1	A	141	ALA	2.7
2	H	167	ASP	2.6
1	K	148	ASN	2.5
1	I	146	ARG	2.5
2	D	176	VAL	2.5
2	P	83	VAL	2.5
2	D	113	ASP	2.5
2	F	166	ASP	2.4
1	I	147	GLY	2.4
1	C	148	ASN	2.4
2	B	34	HIS	2.4
2	B	31	GLU	2.4
1	M	149	ALA	2.4
2	P	142	LEU	2.3
2	L	157	MET	2.3
2	J	171	PHE	2.3
2	F	25	THR	2.3
2	L	116	PHE	2.3
1	E	145	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	171	PHE	2.2
1	A	146	ARG	2.2
2	D	70	SER	2.2
1	A	170	ASN	2.2
1	E	148	ASN	2.2
2	P	167	ASP	2.2
1	M	144	SER	2.2
2	L	97	ALA	2.2
2	L	32	LEU	2.2
1	I	148	ASN	2.2
2	L	84	PHE	2.2
2	J	173	ILE	2.1
2	L	38	LEU	2.1
2	D	167	ASP	2.1
2	D	65	ILE	2.1
2	D	46	LEU	2.1
2	B	167	ASP	2.1
2	D	130	GLY	2.0
2	D	66	PHE	2.0
2	D	71	ALA	2.0
2	H	56	ALA	2.0
1	C	149	ALA	2.0
2	L	65	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.