



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2017 – 04:30 PM EDT

PDB ID : 5IC4
Title : Crystal structure of caspase-3 DEVE peptide complex
Authors : Seaman, J.E.; Julien, O.; Lee, P.S.; Rettenmaier, T.J.; Thomsen, N.D.; Wells, J.A.
Deposited on : unknown
Resolution : 2.65 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20029824

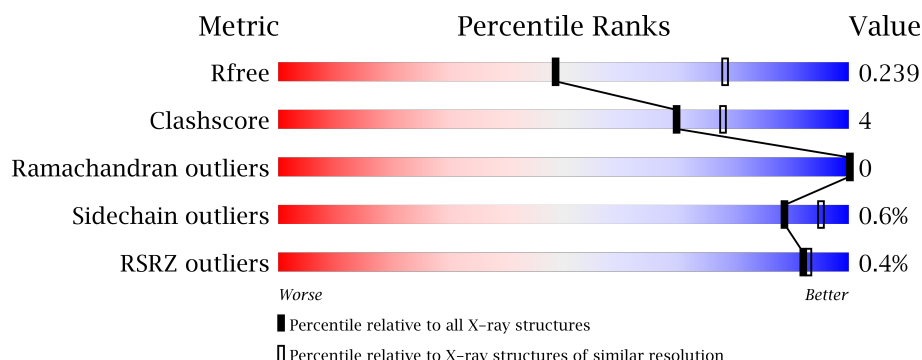
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	100719	3491 (2.70-2.62)
Clashscore	112137	1026 (2.68-2.64)
Ramachandran outliers	110173	1010 (2.68-2.64)
Sidechain outliers	110143	1010 (2.68-2.64)
RSRZ outliers	101464	3511 (2.70-2.62)

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 $\leq 5\%$. 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	175	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; text-align: center;">%</div> <div style="position: absolute; top: 0; left: 0; width: 69%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 69%; width: 11%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 80%; width: 20%; height: 10px; background-color: grey;"></div> <div style="position: absolute; top: 0; left: 69%; width: 11%; text-align: center;">69%</div> <div style="position: absolute; top: 0; left: 80%; width: 20%; text-align: center;">11% 21%</div> </div> </div>
1	C	175	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; text-align: center;">%</div> <div style="position: absolute; top: 0; left: 0; width: 67%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 67%; width: 13%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 80%; width: 20%; height: 10px; background-color: grey;"></div> <div style="position: absolute; top: 0; left: 67%; width: 13%; text-align: center;">67%</div> <div style="position: absolute; top: 0; left: 80%; width: 20%; text-align: center;">13% 21%</div> </div> </div>
1	E	175	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; text-align: center;">%</div> <div style="position: absolute; top: 0; left: 0; width: 72%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 72%; width: 7%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 79%; width: 21%; height: 10px; background-color: grey;"></div> <div style="position: absolute; top: 0; left: 72%; width: 7%; text-align: center;">72%</div> <div style="position: absolute; top: 0; left: 79%; width: 21%; text-align: center;">7% 21%</div> </div> </div>
1	G	175	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: 0; left: 0; width: 66%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 66%; width: 13%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 79%; width: 21%; height: 10px; background-color: grey;"></div> <div style="position: absolute; top: 0; left: 66%; width: 13%; text-align: center;">66%</div> <div style="position: absolute; top: 0; left: 79%; width: 21%; text-align: center;">13% • 21%</div> </div> </div>
2	B	107	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: 0; left: 0; width: 76%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 76%; width: 10%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 86%; width: 14%; height: 10px; background-color: grey;"></div> <div style="position: absolute; top: 0; left: 76%; width: 10%; text-align: center;">76%</div> <div style="position: absolute; top: 0; left: 86%; width: 14%; text-align: center;">10% 14%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	D	107	 79% 7% 15%
2	F	107	 75% 10% 15%
2	H	107	 80% 6% 14%
3	I	4	 75% 25%
3	J	4	 100%
3	K	4	 100%
3	L	4	 50% 50%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7656 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-3 subunit p17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	139	Total	C	N	O	S	0	0	0
			1105	684	200	212	9			
1	C	139	Total	C	N	O	S	0	0	0
			1105	684	200	212	9			
1	E	139	Total	C	N	O	S	0	0	0
			1105	684	200	212	9			
1	G	139	Total	C	N	O	S	0	0	0
			1104	684	199	212	9			

- Molecule 2 is a protein called Caspase-3 subunit p12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	92	Total	C	N	O	S	0	0	0
			767	505	122	135	5			
2	D	91	Total	C	N	O	S	0	0	0
			757	499	119	134	5			
2	F	91	Total	C	N	O	S	0	0	0
			757	499	119	134	5			
2	H	92	Total	C	N	O	S	0	0	0
			767	505	122	135	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	277	HIS	-	expression tag	UNP P42574
B	278	HIS	-	expression tag	UNP P42574
B	279	HIS	-	expression tag	UNP P42574
B	280	HIS	-	expression tag	UNP P42574
B	281	HIS	-	expression tag	UNP P42574
B	282	HIS	-	expression tag	UNP P42574
D	277	HIS	-	expression tag	UNP P42574
D	278	HIS	-	expression tag	UNP P42574

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Chain	Residue	Modelled	Actual	Comment	Reference
D	279	HIS	-	expression tag	UNP P42574
D	280	HIS	-	expression tag	UNP P42574
D	281	HIS	-	expression tag	UNP P42574
D	282	HIS	-	expression tag	UNP P42574
F	277	HIS	-	expression tag	UNP P42574
F	278	HIS	-	expression tag	UNP P42574
F	279	HIS	-	expression tag	UNP P42574
F	280	HIS	-	expression tag	UNP P42574
F	281	HIS	-	expression tag	UNP P42574
F	282	HIS	-	expression tag	UNP P42574
H	277	HIS	-	expression tag	UNP P42574
H	278	HIS	-	expression tag	UNP P42574
H	279	HIS	-	expression tag	UNP P42574
H	280	HIS	-	expression tag	UNP P42574
H	281	HIS	-	expression tag	UNP P42574
H	282	HIS	-	expression tag	UNP P42574

- Molecule 3 is a protein called DEVE peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	4	Total	C	N	O	0	0	0
			34	20	4	10			
3	J	4	Total	C	N	O	0	0	0
			34	20	4	10			
3	K	4	Total	C	N	O	0	0	0
			34	20	4	10			
3	L	4	Total	C	N	O	0	0	0
			34	20	4	10			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		
4	B	4	Total	O	0	0
			4	4		
4	C	9	Total	O	0	0
			9	9		
4	D	4	Total	O	0	0
			4	4		
4	E	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	4	Total 4	O 4	0	0
4	G	9	Total 9	O 9	0	0
4	H	6	Total 6	O 6	0	0
4	J	1	Total 1	O 1	0	0

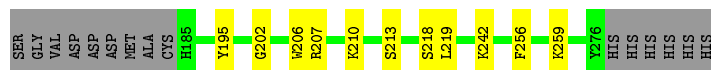
- Molecule 1: Caspase-3 subunit p17





- Molecule 2: Caspase-3 subunit p12

Chain B: 76% 10% 14%



- Molecule 2: Caspase-3 subunit p12

Chain D: 79% 7% 15%



- Molecule 2: Caspase-3 subunit p12

Chain F: 75% 10% 15%



- Molecule 2: Caspase-3 subunit p12

Chain H: 80% 6% 14%



- Molecule 3: DEVE peptide

Chain I: 75% 25%



- Molecule 3: DEVE peptide

Chain J: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: DEVE peptide

Chain K: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: DEVE peptide

Chain L:



D1	E2	V3	?4
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4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	133.82Å 177.80Å 193.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.36 – 2.65 48.36 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.36-2.65) 99.8 (48.36-2.65)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.207 , 0.239 0.199 , 0.239	Depositor DCC
R_{free} test set	1695 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.523	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7656	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: MKE

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	0.22	0/1120	0.41	0/1499
1	C	0.23	0/1120	0.44	0/1499
1	E	0.22	0/1120	0.41	0/1499
1	G	0.23	0/1119	0.42	0/1498
2	B	0.23	0/791	0.40	0/1068
2	D	0.23	0/780	0.39	0/1053
2	F	0.23	0/780	0.39	0/1053
2	H	0.23	0/791	0.40	0/1068
3	I	0.17	0/23	0.36	0/30
3	J	0.19	0/23	0.36	0/30
3	K	0.17	0/23	0.37	0/30
3	L	0.18	0/23	0.37	0/30
All	All	0.23	0/7713	0.41	0/10357

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	1105	0	1102	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1105	0	1102	12	0
1	E	1105	0	1102	8	0
1	G	1104	0	1103	16	0
2	B	767	0	747	10	0
2	D	757	0	740	5	0
2	F	757	0	740	6	0
2	H	767	0	747	7	0
3	I	34	0	28	1	0
3	J	34	0	28	0	0
3	K	34	0	28	0	0
3	L	34	0	28	2	0
4	A	9	0	0	1	0
4	B	4	0	0	0	0
4	C	9	0	0	0	0
4	D	4	0	0	0	0
4	E	7	0	0	0	0
4	F	4	0	0	0	0
4	G	9	0	0	0	0
4	H	6	0	0	0	0
4	J	1	0	0	0	0
All	All	7656	0	7495	64	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 4.

All (64) 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:A:100:MET:HG3	1:A:139:ILE:HG23	1.69	0.73
1:G:173:GLU:N	1:G:173:GLU:OE1	2.25	0.69
1:E:100:MET:HG3	1:E:139:ILE:HG23	1.75	0.68
1:A:173:GLU:OE1	1:A:173:GLU:N	2.29	0.66
1:G:100:MET:HG3	1:G:139:ILE:HG23	1.78	0.66
2:H:209:SER:OG	3:L:2:GLU:OE2	2.16	0.63
2:H:207:ARG:HA	2:H:213:SER:HA	1.81	0.61
2:B:207:ARG:HA	2:B:213:SER:HA	1.83	0.61
2:F:207:ARG:HA	2:F:213:SER:HA	1.83	0.61
1:G:159:ILE:HD13	2:H:219:LEU:HD21	1.84	0.59
1:A:137:LYS:NZ	4:A:201:HOH:O	2.37	0.58
1:C:100:MET:HG3	1:C:139:ILE:HG23	1.87	0.57
1:C:168:LEU:HD22	2:D:259:LYS:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:244:ALA:O	2:F:260:LYS:NZ	2.33	0.56
1:G:74:LEU:HD13	1:G:117:VAL:HG11	1.88	0.56
2:D:207:ARG:HA	2:D:213:SER:HA	1.89	0.55
1:E:74:LEU:HD13	1:E:117:VAL:HG11	1.89	0.53
1:A:168:LEU:HD22	2:B:259:LYS:HG3	1.92	0.52
2:B:210:LYS:N	2:B:210:LYS:HD2	2.25	0.51
1:C:159:ILE:HD13	2:D:219:LEU:HD21	1.92	0.51
1:E:119:LEU:HD23	1:E:161:GLN:HB3	1.92	0.51
1:A:119:LEU:HD23	1:A:161:GLN:HB3	1.94	0.50
1:E:159:ILE:HD13	2:F:219:LEU:HD21	1.94	0.49
1:C:74:LEU:HD13	1:C:117:VAL:HG11	1.94	0.49
2:D:238:ARG:HG2	2:D:241:ARG:NH2	2.28	0.49
1:C:119:LEU:HD23	1:C:161:GLN:HB3	1.95	0.48
2:B:206:TRP:HH2	2:B:256:PHE:HB3	1.79	0.48
1:A:74:LEU:HD13	1:A:117:VAL:HG11	1.95	0.47
1:E:120:SER:OG	1:E:121:HIS:N	2.48	0.47
1:C:42:PRO:HG2	1:C:110:LYS:HB3	1.96	0.47
1:E:52:ASN:HB2	1:E:120:SER:HB2	1.97	0.46
1:G:119:LEU:HD23	1:G:161:GLN:HB3	1.97	0.46
1:G:120:SER:OG	1:G:121:HIS:N	2.48	0.46
1:C:120:SER:OG	1:C:121:HIS:N	2.48	0.46
1:A:120:SER:OG	1:A:121:HIS:N	2.49	0.45
1:C:123:GLU:HB2	1:C:126:ILE:HB	1.98	0.45
2:H:207:ARG:HE	3:L:4:MKE:CD	2.30	0.45
1:A:123:GLU:HB2	1:A:126:ILE:HB	1.98	0.45
1:G:57:LYS:HG3	1:G:57:LYS:H	1.47	0.45
2:F:232:PHE:HA	2:F:235:ILE:HD12	1.98	0.44
1:G:113:SER:HB3	1:G:155:PRO:HG2	1.99	0.44
1:A:159:ILE:HD13	2:B:219:LEU:HD21	1.97	0.44
1:G:100:MET:HE3	1:G:143:PHE:CE2	2.53	0.44
2:F:270:THR:HB	2:H:241:ARG:HB2	1.98	0.44
1:C:38:LYS:HD3	1:C:41:TYR:CE1	2.53	0.44
1:E:37:TYR:CD1	1:E:155:PRO:HD3	2.53	0.43
1:A:167:GLU:HB2	2:B:202:GLY:O	2.18	0.43
1:C:140:THR:HG21	2:D:195:TYR:HE2	1.83	0.43
1:G:123:GLU:HB2	1:G:126:ILE:HB	2.00	0.43
1:A:52:ASN:HB2	1:A:120:SER:HB2	2.00	0.43
2:B:259:LYS:HA	2:B:259:LYS:HD3	1.77	0.43
1:G:140:THR:HG21	2:H:195:TYR:HE1	1.84	0.43
2:B:207:ARG:HE	3:I:4:MKE:CD	2.32	0.43
1:G:37:TYR:CD1	1:G:155:PRO:HD3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:145:GLY:O	1:G:152:THR:OG1	2.34	0.42
2:B:218:SER:HB3	2:B:242:LYS:HD3	2.01	0.41
1:C:56:HIS:CE1	1:C:131:ASN:HB3	2.54	0.41
1:G:76:GLU:O	1:G:80:ASN:ND2	2.53	0.41
1:G:105:LYS:HB2	1:G:105:LYS:HE2	1.77	0.41
1:E:35:ASN:HB2	2:H:241:ARG:NH1	2.35	0.41
1:C:37:TYR:CD1	1:C:155:PRO:HD3	2.56	0.41
2:F:238:ARG:HG2	2:F:241:ARG:HH11	1.86	0.41
1:G:52:ASN:HB2	1:G:120:SER:HB2	2.03	0.40
1:A:140:THR:HG21	2:B:195:TYR:HE1	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	137/175 (78%)	135 (98%)	2 (2%)	0	100	100
1	C	137/175 (78%)	136 (99%)	1 (1%)	0	100	100
1	E	137/175 (78%)	135 (98%)	2 (2%)	0	100	100
1	G	137/175 (78%)	135 (98%)	2 (2%)	0	100	100
2	B	90/107 (84%)	89 (99%)	1 (1%)	0	100	100
2	D	89/107 (83%)	88 (99%)	1 (1%)	0	100	100
2	F	89/107 (83%)	88 (99%)	1 (1%)	0	100	100
2	H	90/107 (84%)	89 (99%)	1 (1%)	0	100	100
3	I	2/4 (50%)	2 (100%)	0	0	100	100
3	J	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
3	K	2/4 (50%)	2 (100%)	0	0	100	100
3	L	2/4 (50%)	2 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	914/1144 (80%)	902 (99%)	12 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	125/159 (79%)	123 (98%)	2 (2%)	68	84
1	C	125/159 (79%)	124 (99%)	1 (1%)	85	93
1	E	125/159 (79%)	125 (100%)	0	100	100
1	G	125/159 (79%)	124 (99%)	1 (1%)	85	93
2	B	82/95 (86%)	82 (100%)	0	100	100
2	D	81/95 (85%)	81 (100%)	0	100	100
2	F	81/95 (85%)	80 (99%)	1 (1%)	75	89
2	H	82/95 (86%)	82 (100%)	0	100	100
3	I	3/3 (100%)	3 (100%)	0	100	100
3	J	3/3 (100%)	3 (100%)	0	100	100
3	K	3/3 (100%)	3 (100%)	0	100	100
3	L	3/3 (100%)	3 (100%)	0	100	100
All	All	838/1028 (82%)	833 (99%)	5 (1%)	89	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LYS
1	A	110	LYS
1	C	173	GLU
2	F	210	LYS
1	G	57	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	225	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(Å ²)	Q<0.9
1	A	139/175 (79%)	0.09	1 (0%) 87 88	30, 38, 48, 67	0
1	C	139/175 (79%)	0.20	2 (1%) 75 74	34, 43, 55, 65	0
1	E	139/175 (79%)	0.10	1 (0%) 87 88	32, 41, 49, 75	0
1	G	139/175 (79%)	0.15	0 100 100	33, 42, 54, 88	0
2	B	92/107 (85%)	-0.08	0 100 100	30, 37, 50, 54	0
2	D	91/107 (85%)	-0.10	0 100 100	30, 37, 46, 60	0
2	F	91/107 (85%)	-0.12	0 100 100	31, 38, 50, 55	0
2	H	92/107 (85%)	-0.03	0 100 100	31, 37, 47, 59	0
3	I	3/4 (75%)	-0.31	0 100 100	40, 40, 43, 48	0
3	J	3/4 (75%)	-0.35	0 100 100	36, 36, 42, 42	0
3	K	3/4 (75%)	-0.14	0 100 100	42, 42, 47, 48	0
3	L	3/4 (75%)	0.04	0 100 100	50, 50, 50, 57	0
All	All	934/1144 (81%)	0.05	4 (0%) 92 93	30, 40, 52, 88	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	40	ASP	2.3
1	E	107	ASP	2.3
1	C	173	GLU	2.1
1	C	98	GLU	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.