



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 04:35 pm GMT

PDB ID : 3NR2
Title : Crystal structure of Caspase-6 zymogen
Authors : Su, X.-D.; Wang, X.-J.; Liu, X.; Mi, W.; Wang, K.-T.
Deposited on : 2010-06-30
Resolution : 2.90 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	:	trunk28620
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)	:	recalc28949

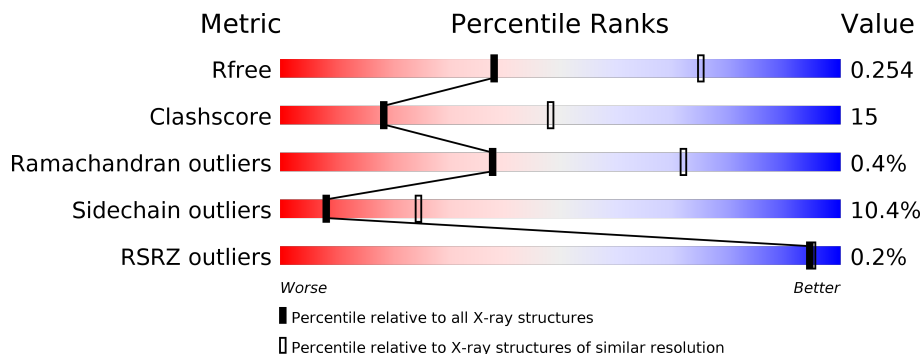
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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	294	<div> <div>54%</div> <div>21%</div> <div>•</div> <div>21%</div> </div>
1	B	294	<div> <div>54%</div> <div>21%</div> <div>•</div> <div>22%</div> </div>

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 3652 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-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	0
			1834	1176	312	334	12			
1	B	230	Total	C	N	O	S	0	0	0
			1818	1163	311	332	12			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	MET	-	EXPRESSION TAG	UNP P55212
A	9	ALA	-	EXPRESSION TAG	UNP P55212
A	10	SER	-	EXPRESSION TAG	UNP P55212
A	11	MET	-	EXPRESSION TAG	UNP P55212
A	12	THR	-	EXPRESSION TAG	UNP P55212
A	13	GLY	-	EXPRESSION TAG	UNP P55212
A	14	GLY	-	EXPRESSION TAG	UNP P55212
A	15	GLN	-	EXPRESSION TAG	UNP P55212
A	16	GLN	-	EXPRESSION TAG	UNP P55212
A	17	MET	-	EXPRESSION TAG	UNP P55212
A	18	GLY	-	EXPRESSION TAG	UNP P55212
A	19	ARG	-	EXPRESSION TAG	UNP P55212
A	20	ASP	-	EXPRESSION TAG	UNP P55212
A	21	PRO	-	EXPRESSION TAG	UNP P55212
A	22	ASN	-	EXPRESSION TAG	UNP P55212
A	23	SER	-	EXPRESSION TAG	UNP P55212
A	93	VAL	ALA	ENGINEERED MUTATION	UNP P55212
A	163	ALA	CYS	ENGINEERED MUTATION	UNP P55212
A	294	LEU	-	EXPRESSION TAG	UNP P55212
A	295	GLU	-	EXPRESSION TAG	UNP P55212
A	296	HIS	-	EXPRESSION TAG	UNP P55212
A	297	HIS	-	EXPRESSION TAG	UNP P55212
A	298	HIS	-	EXPRESSION TAG	UNP P55212
A	299	HIS	-	EXPRESSION TAG	UNP P55212
A	300	HIS	-	EXPRESSION TAG	UNP P55212

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Chain	Residue	Modelled	Actual	Comment	Reference
A	301	HIS	-	EXPRESSION TAG	UNP P55212
B	8	MET	-	EXPRESSION TAG	UNP P55212
B	9	ALA	-	EXPRESSION TAG	UNP P55212
B	10	SER	-	EXPRESSION TAG	UNP P55212
B	11	MET	-	EXPRESSION TAG	UNP P55212
B	12	THR	-	EXPRESSION TAG	UNP P55212
B	13	GLY	-	EXPRESSION TAG	UNP P55212
B	14	GLY	-	EXPRESSION TAG	UNP P55212
B	15	GLN	-	EXPRESSION TAG	UNP P55212
B	16	GLN	-	EXPRESSION TAG	UNP P55212
B	17	MET	-	EXPRESSION TAG	UNP P55212
B	18	GLY	-	EXPRESSION TAG	UNP P55212
B	19	ARG	-	EXPRESSION TAG	UNP P55212
B	20	ASP	-	EXPRESSION TAG	UNP P55212
B	21	PRO	-	EXPRESSION TAG	UNP P55212
B	22	ASN	-	EXPRESSION TAG	UNP P55212
B	23	SER	-	EXPRESSION TAG	UNP P55212
B	93	VAL	ALA	ENGINEERED MUTATION	UNP P55212
B	163	ALA	CYS	ENGINEERED MUTATION	UNP P55212
B	294	LEU	-	EXPRESSION TAG	UNP P55212
B	295	GLU	-	EXPRESSION TAG	UNP P55212
B	296	HIS	-	EXPRESSION TAG	UNP P55212
B	297	HIS	-	EXPRESSION TAG	UNP P55212
B	298	HIS	-	EXPRESSION TAG	UNP P55212
B	299	HIS	-	EXPRESSION TAG	UNP P55212
B	300	HIS	-	EXPRESSION TAG	UNP P55212
B	301	HIS	-	EXPRESSION TAG	UNP P55212

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	127.98Å 127.98Å 167.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.90 – 2.90 29.90 – 2.90	Depositor EDS
% Data completeness (in resolution range)	81.8 (29.90-2.90) 81.9 (29.90-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.179 , 0.237 0.197 , 0.254	Depositor DCC
R_{free} test set	1683 reflections (10.00%)	DCC
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3652	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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 [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	A	0.70	1/1876 (0.1%)	0.64	0/2530
1	B	0.56	0/1858	0.64	0/2506
All	All	0.63	1/3734 (0.0%)	0.64	0/5036

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	116	CYS	CB-SG	-7.54	1.69	1.82

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	A	1834	0	1766	62	0
1	B	1818	0	1762	54	0
All	All	3652	0	3528	107	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 15.

All (107) 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:B:123:GLU:HB2	1:B:164:ARG:HH21	1.06	1.08
1:B:75:THR:HB	1:B:85:VAL:HG11	1.42	1.02
1:A:44:ARG:HG3	1:A:44:ARG:HH11	1.30	0.95
1:B:123:GLU:HB2	1:B:164:ARG:NH2	1.81	0.94
1:A:125:ASN:HD22	1:A:125:ASN:H	1.10	0.91
1:A:246:THR:O	1:A:250:THR:HG22	1.72	0.89
1:B:44:ARG:HG3	1:B:44:ARG:HH11	1.36	0.89
1:A:77:ARG:HG3	1:A:77:ARG:HH21	1.42	0.84
1:A:149:HIS:O	1:A:152:VAL:HG12	1.80	0.81
1:A:44:ARG:HG3	1:A:44:ARG:NH1	1.98	0.78
1:B:201:PRO:HB2	1:B:281:MET:SD	2.27	0.74
1:B:71:ARG:O	1:B:75:THR:HG22	1.87	0.74
1:A:254:ARG:HD3	1:B:283:THR:O	1.92	0.68
1:A:44:ARG:HD2	1:A:81:LEU:O	1.95	0.66
1:A:125:ASN:N	1:A:125:ASN:HD22	1.81	0.66
1:B:44:ARG:NH1	1:B:44:ARG:HG3	2.05	0.66
1:A:251:LEU:HD21	1:B:33:PRO:HA	1.78	0.65
1:A:108:HIS:HB2	1:A:150:SER:HB2	1.77	0.65
1:A:201:PRO:HB2	1:A:281:MET:SD	2.38	0.64
1:A:149:HIS:O	1:A:152:VAL:CG1	2.45	0.64
1:A:125:ASN:ND2	1:A:125:ASN:H	1.90	0.64
1:B:144:LYS:HE2	1:B:202:ALA:O	1.99	0.63
1:B:146:ASP:CG	1:B:147:LYS:N	2.53	0.61
1:A:72:ASP:HA	1:A:75:THR:HG22	1.81	0.61
1:B:77:ARG:HD2	1:B:77:ARG:N	2.16	0.60
1:B:201:PRO:HA	1:B:208:MET:HG3	1.84	0.59
1:B:72:ASP:HA	1:B:75:THR:HG23	1.84	0.58
1:A:77:ARG:NH2	1:A:77:ARG:HG3	2.12	0.58
1:B:189:ILE:O	1:B:221:GLU:HA	2.04	0.57
1:B:137:GLN:NE2	1:B:137:GLN:H	2.03	0.57
1:A:201:PRO:HA	1:A:208:MET:HG3	1.87	0.57
1:B:200:LEU:HB2	1:B:201:PRO:HD2	1.87	0.56
1:A:120:SER:OG	1:A:121:HIS:N	2.37	0.56
1:A:60:THR:HG22	1:A:60:THR:O	2.06	0.55
1:B:74:LEU:HD22	1:B:78:PHE:HE1	1.70	0.55
1:B:201:PRO:CB	1:B:281:MET:SD	2.95	0.55
1:B:123:GLU:CB	1:B:164:ARG:HH21	1.98	0.54
1:B:135:GLU:HG3	1:B:138:THR:HG23	1.88	0.54
1:A:115:VAL:HG22	1:A:157:ILE:HB	1.90	0.53
1:A:207:LEU:HD21	1:A:249:LEU:CD1	2.38	0.53
1:A:201:PRO:HG3	1:B:277:CYS:SG	2.49	0.53
1:B:71:ARG:O	1:B:75:THR:CG2	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:ASN:ND2	1:B:67:THR:OG1	2.40	0.53
1:B:290:PRO:O	1:B:291:LYS:CB	2.56	0.53
1:A:44:ARG:CG	1:A:44:ARG:HH11	2.10	0.52
1:A:108:HIS:H	1:A:150:SER:CB	2.23	0.51
1:A:72:ASP:HA	1:A:75:THR:CG2	2.39	0.51
1:A:71:ARG:O	1:A:75:THR:HG22	2.10	0.51
1:A:33:PRO:HG3	1:B:239:TYR:CZ	2.45	0.50
1:A:33:PRO:HA	1:B:251:LEU:HD21	1.93	0.50
1:A:135:GLU:HB2	1:A:138:THR:HG23	1.93	0.50
1:A:189:ILE:O	1:A:222:THR:HG23	2.12	0.49
1:A:33:PRO:HG3	1:B:239:TYR:OH	2.12	0.48
1:B:126:HIS:HB3	1:B:133:LYS:HB2	1.96	0.48
1:A:247:GLU:OE2	1:B:285:LYS:CE	2.62	0.48
1:B:55:PHE:O	1:B:56:PHE:C	2.52	0.48
1:B:217:TYR:O	1:B:274:GLN:HB2	2.13	0.48
1:A:35:GLU:HG2	1:A:284:LYS:HG2	1.97	0.47
1:A:157:ILE:N	1:A:157:ILE:HD12	2.30	0.47
1:A:207:LEU:HD21	1:A:249:LEU:HD11	1.95	0.47
1:B:125:ASN:HB2	1:B:137:GLN:HE22	1.80	0.47
1:B:74:LEU:HD22	1:B:78:PHE:CE1	2.49	0.47
1:A:149:HIS:C	1:A:152:VAL:HG12	2.34	0.47
1:B:160:ILE:HG13	1:B:210:TYR:CE1	2.51	0.46
1:A:131:ASP:N	1:A:131:ASP:OD2	2.49	0.46
1:A:217:TYR:N	1:A:217:TYR:CD2	2.85	0.45
1:A:251:LEU:HD22	1:B:31:PHE:CZ	2.51	0.45
1:A:201:PRO:CB	1:A:281:MET:SD	3.05	0.45
1:B:137:GLN:HE21	1:B:137:GLN:H	1.65	0.45
1:B:199:THR:OG1	1:B:199:THR:O	2.33	0.45
1:B:69:ALA:O	1:B:73:ASN:HB2	2.17	0.45
1:A:141:GLY:HA2	1:A:144:LYS:HG3	1.99	0.45
1:A:57:TRP:NE1	1:A:58:HIS:CD2	2.85	0.44
1:B:32:ASP:HA	1:B:33:PRO:HD3	1.79	0.44
1:A:135:GLU:HB3	1:A:137:GLN:NE2	2.32	0.43
1:A:149:HIS:HA	1:A:152:VAL:HG12	1.99	0.43
1:A:199:THR:O	1:A:199:THR:OG1	2.34	0.43
1:A:37:TYR:CD2	1:A:155:PRO:HG3	2.53	0.43
1:B:51:ASN:O	1:B:89:ASN:HA	2.18	0.43
1:A:190:THR:HB	1:A:221:GLU:HG2	2.00	0.43
1:A:57:TRP:CD1	1:A:58:HIS:CD2	3.07	0.43
1:A:57:TRP:NE1	1:A:58:HIS:NE2	2.67	0.43
1:A:239:TYR:CZ	1:B:33:PRO:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:ASP:CG	1:B:147:LYS:H	2.21	0.43
1:B:127:ILE:HG12	1:B:127:ILE:H	1.68	0.43
1:B:212:VAL:O	1:B:212:VAL:HG13	2.17	0.43
1:A:102:GLU:O	1:A:106:VAL:HG13	2.19	0.43
1:B:97:LEU:HA	1:B:97:LEU:HD12	1.74	0.43
1:B:99:LYS:HA	1:B:99:LYS:HD3	1.64	0.43
1:A:97:LEU:HA	1:A:97:LEU:HD12	1.86	0.42
1:B:117:VAL:HG22	1:B:159:ILE:HB	2.02	0.42
1:B:151:LEU:HD23	1:B:151:LEU:HA	1.69	0.42
1:A:74:LEU:HD13	1:A:117:VAL:HG11	2.02	0.42
1:B:161:GLN:HA	1:B:211:SER:HB3	2.00	0.42
1:B:60:THR:HG22	1:B:60:THR:O	2.20	0.42
1:A:137:GLN:H	1:A:137:GLN:CD	2.23	0.41
1:A:256:VAL:C	1:A:258:GLN:H	2.23	0.41
1:A:59:LEU:HA	1:A:59:LEU:HD12	1.77	0.41
1:A:78:PHE:O	1:A:83:PHE:HB2	2.20	0.41
1:B:64:ARG:O	1:B:67:THR:HG22	2.21	0.41
1:A:199:THR:HA	1:A:210:TYR:CZ	2.56	0.41
1:A:52:HIS:CE1	1:A:129:ALA:HA	2.56	0.41
1:B:55:PHE:C	1:B:56:PHE:O	2.56	0.40
1:B:91:LEU:O	1:B:129:ALA:HB1	2.21	0.40
1:A:93:VAL:HG21	1:A:132:ALA:HB3	2.03	0.40
1:A:126:HIS:NE2	1:A:135:GLU:HG2	2.37	0.40
1:A:164:ARG:O	1:A:193:ASP:HB3	2.21	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	227/294 (77%)	207 (91%)	20 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	224/294 (76%)	206 (92%)	16 (7%)	2 (1%)	20	54
All	All	451/588 (77%)	413 (92%)	36 (8%)	2 (0%)	38	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	202	ALA
1	B	201	PRO

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	192/258 (74%)	172 (90%)	20 (10%)	8	25
1	B	193/258 (75%)	173 (90%)	20 (10%)	8	25
All	All	385/516 (75%)	345 (90%)	40 (10%)	8	25

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	54	ARG
1	A	59	LEU
1	A	65	ARG
1	A	73	ASN
1	A	77	ARG
1	A	97	LEU
1	A	98	LEU
1	A	116	CYS
1	A	125	ASN
1	A	133	LYS
1	A	149	HIS
1	A	150	SER
1	A	152	VAL

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Mol	Chain	Res	Type
1	A	190	THR
1	A	199	THR
1	A	200	LEU
1	A	242	SER
1	A	250	THR
1	A	255	LYS
1	B	35	GLU
1	B	38	LYS
1	B	44	ARG
1	B	59	LEU
1	B	61	LEU
1	B	73	ASN
1	B	75	THR
1	B	77	ARG
1	B	98	LEU
1	B	106	VAL
1	B	125	ASN
1	B	127	ILE
1	B	137	GLN
1	B	142	LEU
1	B	146	ASP
1	B	150	SER
1	B	166	ASN
1	B	191	GLU
1	B	199	THR
1	B	242	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	52	HIS
1	A	73	ASN
1	A	101	HIS
1	A	121	HIS
1	A	125	ASN
1	A	149	HIS
1	A	224	ASN
1	A	230	GLN
1	B	51	ASN
1	B	73	ASN
1	B	125	ASN

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Mol	Chain	Res	Type
1	B	137	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	233/294 (79%)	-0.63	1 (0%) 92 92	16, 29, 50, 76	1 (0%)
1	B	230/294 (78%)	-0.66	0 100 100	14, 25, 48, 65	0
All	All	463/588 (78%)	-0.65	1 (0%) 94 95	14, 27, 48, 76	1 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	292	SER	4.0

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.