Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:27 AM GMT

PDB ID	:	2H8L
Title	:	Crystal structure of the bb' fragment of ERp57
Authors	:	Kozlov, G.; Schrag, J.D.; Cygler, M.; Gehring, K.
Deposited on	:	2006-06-07
Resolution	:	2.00 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:

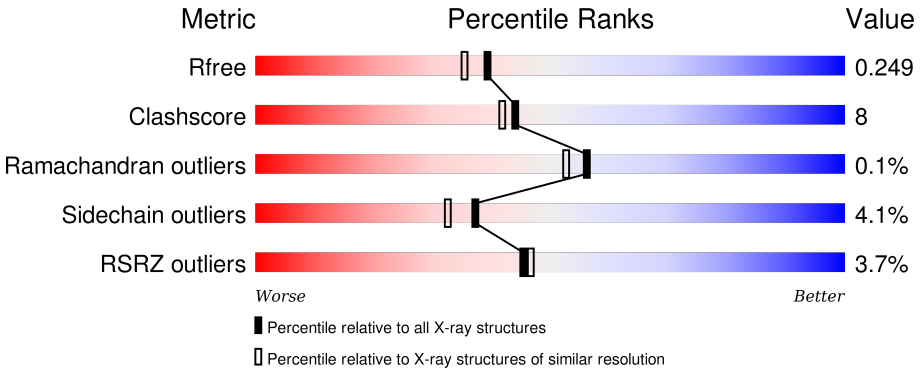
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	252	4% 76% 13% • 8%
1	B	252	6% 69% 19% • 9%
1	C	252	74% 15% • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6087 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 Protein disulfide-isomerase A3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	Se	0	0	0
			1883	1198	318	361	1	5			
1	B	230	Total	C	N	O	S	Se	0	0	0
			1868	1187	316	359	1	5			
1	C	232	Total	C	N	O	S	Se	0	0	0
			1883	1198	318	361	1	5			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	GLY	-	CLONING ARTIFACT	UNP P30101
A	130	PRO	-	CLONING ARTIFACT	UNP P30101
A	131	LEU	-	CLONING ARTIFACT	UNP P30101
A	132	GLY	-	CLONING ARTIFACT	UNP P30101
A	133	SER	-	CLONING ARTIFACT	UNP P30101
A	227	MSE	MET	MODIFIED RESIDUE	UNP P30101
A	247	MSE	MET	MODIFIED RESIDUE	UNP P30101
A	284	MSE	MET	MODIFIED RESIDUE	UNP P30101
A	285	MSE	MET	MODIFIED RESIDUE	UNP P30101
A	338	MSE	MET	MODIFIED RESIDUE	UNP P30101
A	377	ALA	-	CLONING ARTIFACT	UNP P30101
A	378	ALA	-	CLONING ARTIFACT	UNP P30101
A	379	ALA	-	CLONING ARTIFACT	UNP P30101
A	380	SER	-	CLONING ARTIFACT	UNP P30101
B	129	GLY	-	CLONING ARTIFACT	UNP P30101
B	130	PRO	-	CLONING ARTIFACT	UNP P30101
B	131	LEU	-	CLONING ARTIFACT	UNP P30101
B	132	GLY	-	CLONING ARTIFACT	UNP P30101
B	133	SER	-	CLONING ARTIFACT	UNP P30101
B	227	MSE	MET	MODIFIED RESIDUE	UNP P30101
B	247	MSE	MET	MODIFIED RESIDUE	UNP P30101
B	284	MSE	MET	MODIFIED RESIDUE	UNP P30101
B	285	MSE	MET	MODIFIED RESIDUE	UNP P30101

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Chain	Residue	Modelled	Actual	Comment	Reference
B	338	MSE	MET	MODIFIED RESIDUE	UNP P30101
B	377	ALA	-	CLONING ARTIFACT	UNP P30101
B	378	ALA	-	CLONING ARTIFACT	UNP P30101
B	379	ALA	-	CLONING ARTIFACT	UNP P30101
B	380	SER	-	CLONING ARTIFACT	UNP P30101
C	129	GLY	-	CLONING ARTIFACT	UNP P30101
C	130	PRO	-	CLONING ARTIFACT	UNP P30101
C	131	LEU	-	CLONING ARTIFACT	UNP P30101
C	132	GLY	-	CLONING ARTIFACT	UNP P30101
C	133	SER	-	CLONING ARTIFACT	UNP P30101
C	227	MSE	MET	MODIFIED RESIDUE	UNP P30101
C	247	MSE	MET	MODIFIED RESIDUE	UNP P30101
C	284	MSE	MET	MODIFIED RESIDUE	UNP P30101
C	285	MSE	MET	MODIFIED RESIDUE	UNP P30101
C	338	MSE	MET	MODIFIED RESIDUE	UNP P30101
C	377	ALA	-	CLONING ARTIFACT	UNP P30101
C	378	ALA	-	CLONING ARTIFACT	UNP P30101
C	379	ALA	-	CLONING ARTIFACT	UNP P30101
C	380	SER	-	CLONING ARTIFACT	UNP P30101

- Molecule 2 is water.

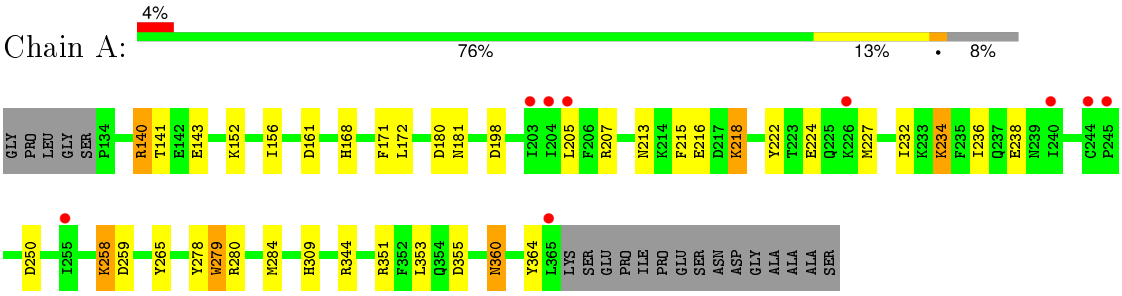
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	184	Total O 184 184	0	0
2	B	129	Total O 129 129	0	0
2	C	140	Total O 140 140	0	0

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.

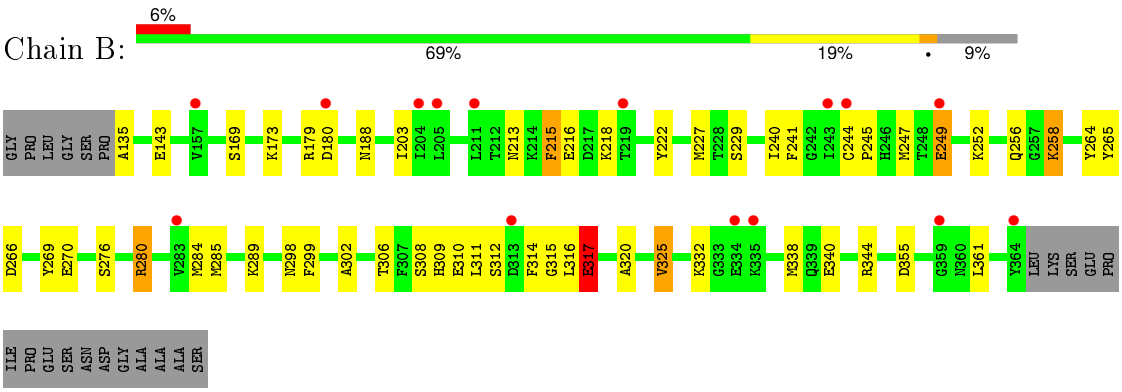
- Molecule 1: Protein disulfide-isomerase A3

Chain A:



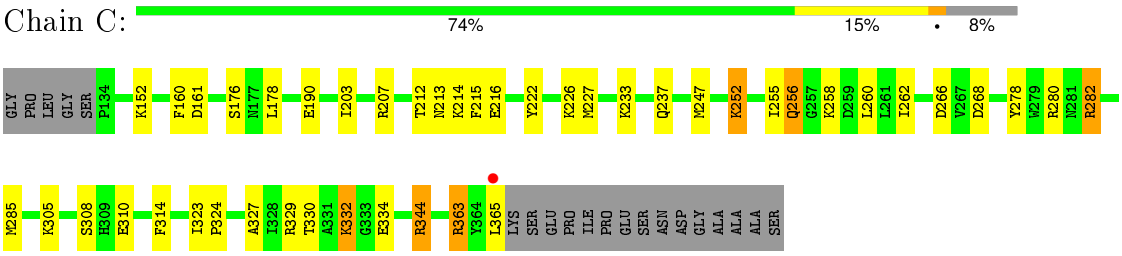
- Molecule 1: Protein disulfide-isomerase A3

Chain B:



- Molecule 1: Protein disulfide-isomerase A3

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.34Å 62.41Å 99.29Å 90.00° 98.40° 90.00°	Depositor
Resolution (Å)	32.70 – 2.00 32.74 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (32.70-2.00) 99.7 (32.74-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.85 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.194 , 0.250 0.193 , 0.249	Depositor DCC
R_{free} test set	3162 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	39.1	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 42.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 62515 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6087	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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	1.15	3/1918 (0.2%)	0.98	8/2566 (0.3%)
1	B	1.49	16/1902 (0.8%)	1.04	6/2544 (0.2%)
1	C	1.04	2/1918 (0.1%)	1.08	12/2566 (0.5%)
All	All	1.24	21/5738 (0.4%)	1.04	26/7676 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	317	GLU	CG-CD	27.32	1.93	1.51
1	B	317	GLU	CD-OE1	18.53	1.46	1.25
1	B	312	SER	CB-OG	11.18	1.56	1.42
1	B	312	SER	C-N	11.10	1.59	1.34
1	B	314	PHE	C-N	9.42	1.50	1.33
1	B	310	GLU	C-O	9.18	1.40	1.23
1	B	249	GLU	CD-OE1	8.86	1.35	1.25
1	B	317	GLU	C-O	8.00	1.38	1.23
1	C	344	ARG	CZ-NH1	7.91	1.43	1.33
1	C	365	LEU	C-O	6.90	1.36	1.23
1	A	279	TRP	CB-CG	6.82	1.62	1.50
1	A	218	LYS	CE-NZ	6.59	1.65	1.49
1	B	269	TYR	CD1-CE1	6.12	1.48	1.39
1	B	314	PHE	C-O	6.07	1.34	1.23
1	A	278	TYR	CD2-CE2	5.99	1.48	1.39
1	B	222	TYR	CD2-CE2	5.75	1.48	1.39
1	B	252	LYS	CD-CE	5.48	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	310	GLU	C-N	5.47	1.46	1.34
1	B	143	GLU	CD-OE1	5.39	1.31	1.25
1	B	215	PHE	CE2-CZ	5.23	1.47	1.37
1	B	249	GLU	CD-OE2	5.04	1.31	1.25

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	344	ARG	NE-CZ-NH2	-15.50	112.55	120.30
1	C	207	ARG	NE-CZ-NH1	13.21	126.91	120.30
1	C	207	ARG	NE-CZ-NH2	-11.97	114.31	120.30
1	C	344	ARG	NE-CZ-NH1	11.47	126.04	120.30
1	C	266	ASP	CB-CG-OD1	7.51	125.06	118.30
1	B	280	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	A	207	ARG	NE-CZ-NH1	-6.72	116.94	120.30
1	B	317	GLU	OE1-CD-OE2	6.66	131.29	123.30
1	A	344	ARG	NE-CZ-NH2	6.38	123.49	120.30
1	B	344	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	A	259	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	A	344	ARG	NE-CZ-NH1	-5.97	117.32	120.30
1	C	268	ASP	CB-CG-OD1	5.90	123.61	118.30
1	B	266	ASP	CB-CG-OD1	5.86	123.57	118.30
1	C	282	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	B	312	SER	O-C-N	5.72	131.85	122.70
1	C	266	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	B	312	SER	C-N-CA	-5.51	107.91	121.70
1	C	207	ARG	CD-NE-CZ	5.34	131.08	123.60
1	C	365	LEU	CA-CB-CG	5.32	127.55	115.30
1	A	259	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	351	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	C	280	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	353	LEU	CB-CG-CD2	-5.13	102.28	111.00
1	C	329	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	218	LYS	CD-CE-NZ	5.05	123.32	111.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	364	TYR	Peptide

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	1883	0	1829	31	1
1	B	1868	0	1810	31	1
1	C	1883	0	1829	28	2
2	A	184	0	0	9	1
2	B	129	0	0	2	0
2	C	140	0	0	4	1
All	All	6087	0	5468	89	3

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 8.

All (89) 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:317:GLU:CD	1:B:317:GLU:CG	1.92	1.37
1:A:227:MSE:HE3	1:A:232:ILE:HD11	1.40	1.03
1:A:218:LYS:HE3	2:A:418:HOH:O	1.57	1.02
1:A:140:ARG:HH11	1:A:140:ARG:HG3	1.26	1.00
1:A:258:LYS:HG3	2:A:506:HOH:O	1.65	0.96
1:A:218:LYS:CE	2:A:418:HOH:O	2.11	0.92
1:B:247:MSE:HE1	1:B:256:GLN:HG3	1.52	0.90
1:B:203:ILE:HD11	1:B:227:MSE:HE3	1.54	0.89
1:C:305:LYS:HG2	2:C:474:HOH:O	1.74	0.86
1:C:278:TYR:OH	1:C:344:ARG:HD3	1.77	0.84
1:B:169:SER:O	1:B:173:LYS:HG3	1.80	0.82
1:C:233:LYS:O	1:C:237:GLN:HG3	1.81	0.81
1:B:247:MSE:CE	1:B:256:GLN:HG3	2.14	0.76
1:A:152:LYS:HE2	2:A:532:HOH:O	1.85	0.76
1:B:247:MSE:HE1	1:B:256:GLN:CG	2.17	0.75
1:B:316:LEU:HD13	1:B:325:VAL:HG13	1.70	0.73
1:C:213:ASN:HD22	1:C:215:PHE:H	1.39	0.70
1:B:213:ASN:HD21	1:B:216:GLU:HG2	1.56	0.69
1:A:309:HIS:CD2	1:A:309:HIS:H	2.09	0.69
1:B:203:ILE:HD11	1:B:227:MSE:CE	2.22	0.68
1:C:247:MSE:HE1	1:C:260:LEU:HD21	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ARG:NH1	1:A:140:ARG:HG3	2.02	0.66
1:A:213:ASN:HD22	1:A:215:PHE:H	1.45	0.65
1:B:249:GLU:OE1	1:B:249:GLU:HA	1.97	0.65
1:A:234:LYS:HD3	1:A:238:GLU:OE2	1.98	0.63
1:B:135:ALA:HA	1:B:179:ARG:HE	1.64	0.63
1:B:355:ASP:HB3	1:B:361:LEU:HG	1.80	0.63
1:C:178:LEU:HD21	1:C:233:LYS:HG3	1.83	0.60
1:C:247:MSE:HE2	1:C:255:ILE:HG21	1.83	0.59
1:C:285:MSE:HE2	2:C:508:HOH:O	2.03	0.58
1:B:213:ASN:HD22	1:B:215:PHE:H	1.50	0.57
1:A:168:HIS:CE1	1:A:172:LEU:HD11	2.39	0.56
1:B:258:LYS:HB2	1:B:298:ASN:HD22	1.69	0.56
1:B:306:THR:O	1:B:309:HIS:CE1	2.58	0.56
1:A:280:ARG:O	1:A:284:MSE:HG3	2.05	0.56
1:C:314:PHE:CD1	1:C:327:ALA:HB1	2.40	0.55
1:C:247:MSE:HE2	1:C:255:ILE:CG2	2.38	0.53
1:C:252:LYS:O	1:C:256:GLN:HG2	2.09	0.52
1:C:203:ILE:HD11	1:C:227:MSE:HE3	1.92	0.52
1:A:227:MSE:CE	1:A:232:ILE:HD11	2.29	0.52
1:B:317:GLU:CD	1:B:317:GLU:CB	2.76	0.52
1:A:141:THR:HG23	2:A:462:HOH:O	2.10	0.52
1:A:227:MSE:HE3	1:A:232:ILE:CD1	2.27	0.51
1:A:181:ASN:ND2	2:A:479:HOH:O	2.31	0.51
1:B:258:LYS:HB2	1:B:298:ASN:ND2	2.25	0.51
1:B:306:THR:O	1:B:309:HIS:HE1	1.92	0.51
1:B:218:LYS:HE2	2:B:500:HOH:O	2.10	0.51
1:B:241:PHE:HB3	1:B:245:PRO:HB3	1.94	0.50
1:B:338:MSE:HE3	1:B:340:GLU:O	2.12	0.50
1:C:161:ASP:HB3	2:C:431:HOH:O	2.12	0.50
1:B:265:TYR:HE1	1:B:276:SER:HA	1.77	0.49
1:A:250:ASP:HB3	2:A:531:HOH:O	2.12	0.49
1:B:244:CYS:HB3	1:B:284:MSE:HG2	1.95	0.49
1:A:141:THR:HG22	1:A:143:GLU:N	2.28	0.49
1:B:280:ARG:O	1:B:284:MSE:HG3	2.13	0.48
1:A:168:HIS:HE1	1:A:172:LEU:HD11	1.76	0.48
1:A:171:PHE:HB2	1:A:227:MSE:HE1	1.95	0.48
1:A:218:LYS:NZ	2:A:418:HOH:O	2.43	0.47
1:A:213:ASN:HD21	1:A:216:GLU:HG2	1.78	0.47
1:C:213:ASN:ND2	1:C:215:PHE:H	2.09	0.47
1:B:338:MSE:CE	1:B:340:GLU:O	2.62	0.47
1:B:264:TYR:HA	1:B:302:ALA:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ILE:O	1:A:236:ILE:HG13	2.15	0.46
1:B:245:PRO:HD2	1:B:299:PHE:O	2.15	0.46
2:A:527:HOH:O	1:B:285:MSE:HE2	2.16	0.45
1:A:213:ASN:ND2	1:A:215:PHE:H	2.12	0.45
1:B:213:ASN:ND2	1:B:216:GLU:HG2	2.30	0.45
1:C:213:ASN:HD21	1:C:216:GLU:HG2	1.82	0.45
1:C:332:LYS:HE2	1:C:334:GLU:HG2	1.99	0.45
1:A:355:ASP:HA	1:A:360:ASN:HD22	1.82	0.44
1:A:140:ARG:NH1	1:A:140:ARG:CG	2.78	0.44
1:C:247:MSE:HE1	1:C:262:ILE:HD11	2.00	0.43
1:A:222:TYR:CE2	1:A:224:GLU:HB2	2.54	0.43
1:C:330:THR:OG1	1:C:332:LYS:HE2	2.19	0.43
1:C:160:PHE:CZ	1:C:227:MSE:HE1	2.54	0.43
1:A:227:MSE:HE2	1:A:227:MSE:HB3	1.91	0.42
1:C:363:ARG:H	1:C:363:ARG:NE	2.17	0.42
1:A:180:ASP:O	1:C:226:LYS:HE3	2.19	0.42
1:C:278:TYR:CE1	1:C:282:ARG:NH2	2.88	0.41
1:B:188:ASN:HB2	2:B:434:HOH:O	2.20	0.41
1:C:323:ILE:HA	1:C:324:PRO:HD3	1.90	0.41
1:A:265:TYR:CE1	1:A:279:TRP:HB2	2.56	0.41
1:C:214:LYS:NZ	2:C:508:HOH:O	2.48	0.41
1:C:314:PHE:CE1	1:C:327:ALA:HB1	2.56	0.41
1:C:222:TYR:CE2	1:C:227:MSE:HG2	2.56	0.41
1:C:160:PHE:CE1	1:C:227:MSE:HE1	2.56	0.41
1:B:311:LEU:O	1:B:315:GLY:N	2.54	0.40
1:A:156:ILE:HG12	1:A:205:LEU:HD22	2.03	0.40
1:C:256:GLN:HE21	1:C:256:GLN:HB3	1.65	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:ARG:NH1	2:A:487:HOH:O[1_455]	2.09	0.11
1:B:320:ALA:CB	2:C:516:HOH:O[1_545]	2.15	0.05
1:A:198:ASP:OD1	1:C:282:ARG:NH2[1_655]	2.18	0.02

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	230/252 (91%)	224 (97%)	6 (3%)	0	100 100
1	B	228/252 (90%)	214 (94%)	13 (6%)	1 (0%)	39 33
1	C	230/252 (91%)	220 (96%)	10 (4%)	0	100 100
All	All	688/756 (91%)	658 (96%)	29 (4%)	1 (0%)	56 53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	332	LYS

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	202/211 (96%)	197 (98%)	5 (2%)	55 55
1	B	200/211 (95%)	191 (96%)	9 (4%)	34 29
1	C	202/211 (96%)	191 (95%)	11 (5%)	27 21
All	All	604/633 (95%)	579 (96%)	25 (4%)	37 32

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	ARG
1	A	161	ASP

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Mol	Chain	Res	Type
1	A	234	LYS
1	A	258	LYS
1	A	360	ASN
1	B	180	ASP
1	B	229	SER
1	B	240	ILE
1	B	258	LYS
1	B	270	GLU
1	B	289	LYS
1	B	308	SER
1	B	317	GLU
1	B	325	VAL
1	C	152	LYS
1	C	176	SER
1	C	190	GLU
1	C	212	THR
1	C	252	LYS
1	C	256	GLN
1	C	258	LYS
1	C	308	SER
1	C	310	GLU
1	C	332	LYS
1	C	363	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	168	HIS
1	A	213	ASN
1	A	256	GLN
1	A	277	ASN
1	A	281	ASN
1	A	360	ASN
1	B	177	ASN
1	B	194	ASN
1	B	213	ASN
1	B	277	ASN
1	B	281	ASN
1	B	298	ASN
1	B	309	HIS
1	C	213	ASN
1	C	246	HIS

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Mol	Chain	Res	Type
1	C	256	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	227/252 (90%)	0.18	9 (3%) 42 44	35, 42, 51, 59	0
1	B	225/252 (89%)	0.47	15 (6%) 21 22	32, 42, 51, 54	0
1	C	227/252 (90%)	-0.04	1 (0%) 93 93	36, 42, 51, 54	0
All	All	679/756 (89%)	0.20	25 (3%) 45 47	32, 42, 51, 59	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	365	LEU	5.1
1	A	205	LEU	3.8
1	B	204	ILE	3.1
1	B	335	LYS	3.1
1	B	180	ASP	3.0
1	A	365	LEU	2.9
1	A	226	LYS	2.8
1	B	364	TYR	2.6
1	A	240	ILE	2.6
1	B	211	LEU	2.6
1	B	157	VAL	2.6
1	B	205	LEU	2.5
1	B	313	ASP	2.4
1	B	244	CYS	2.4
1	A	203	ILE	2.3
1	A	245	PRO	2.3
1	A	204	ILE	2.3
1	B	243	ILE	2.3
1	A	255	ILE	2.1
1	B	219	THR	2.1
1	B	249	GLU	2.1
1	A	244	CYS	2.0
1	B	359	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	334	GLU	2.0
1	B	283	VAL	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.