Full wwPDB X-ray Structure Validation Report ⓘ

Oct 18, 2023 – 01:21 PM EDT

PDB ID	:	1MC8
Title	:	Crystal Structure of Flap Endonuclease-1 R42E mutant from Pyrococcus horikoshii
Authors	:	Matsui, E.; Musti, K.V.; Abe, J.; Yamazaki, K.; Matsui, I.; Harata, K.
Deposited on	:	2002-08-06
Resolution	:	3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

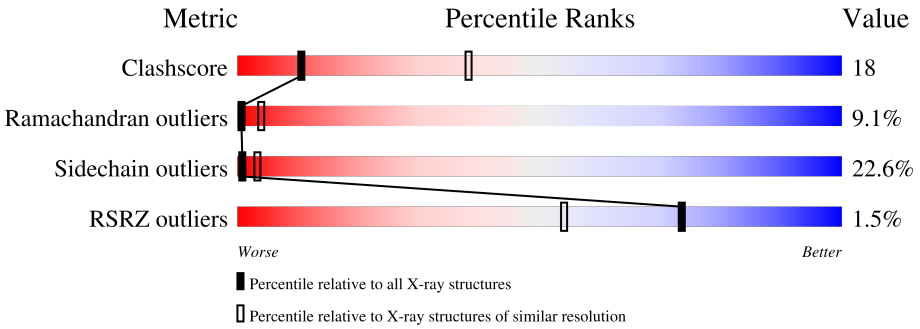
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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))
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	343	2% 40% 37% 13% 6% ·
1	B	343	% 41% 40% 11% 5% ·

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5274 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 Flap Endonuclease-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2637	1683	453	494	7			
1	B	331	Total	C	N	O	S	0	0	0
			2637	1683	453	494	7			

There are 2 discrepancies between the modelled and reference sequences:

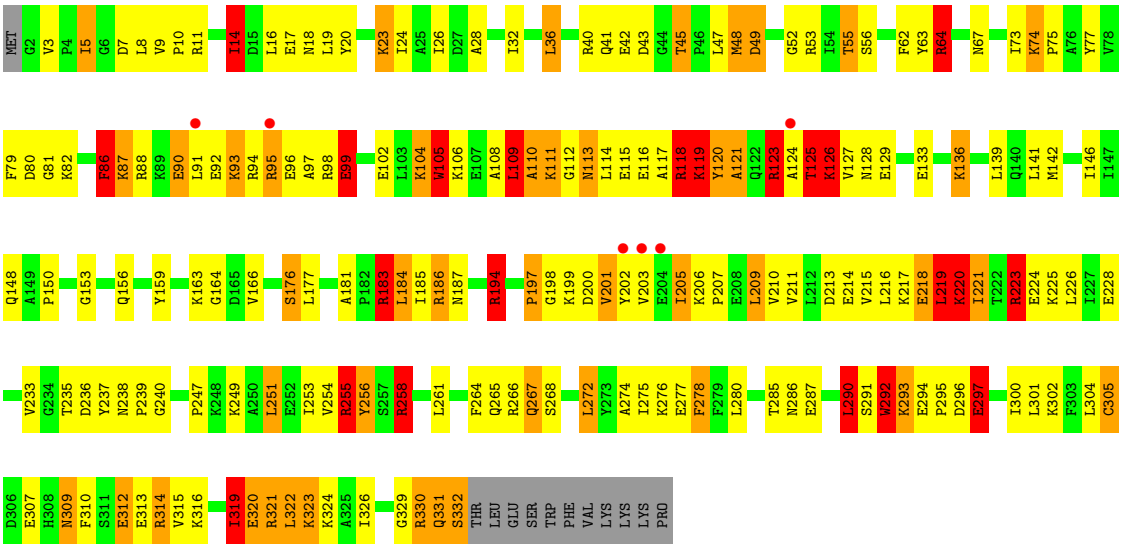
Chain	Residue	Modelled	Actual	Comment	Reference
A	42	GLU	ARG	engineered mutation	UNP O50123
B	42	GLU	ARG	engineered mutation	UNP O50123

3 Residue-property plots (i)

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

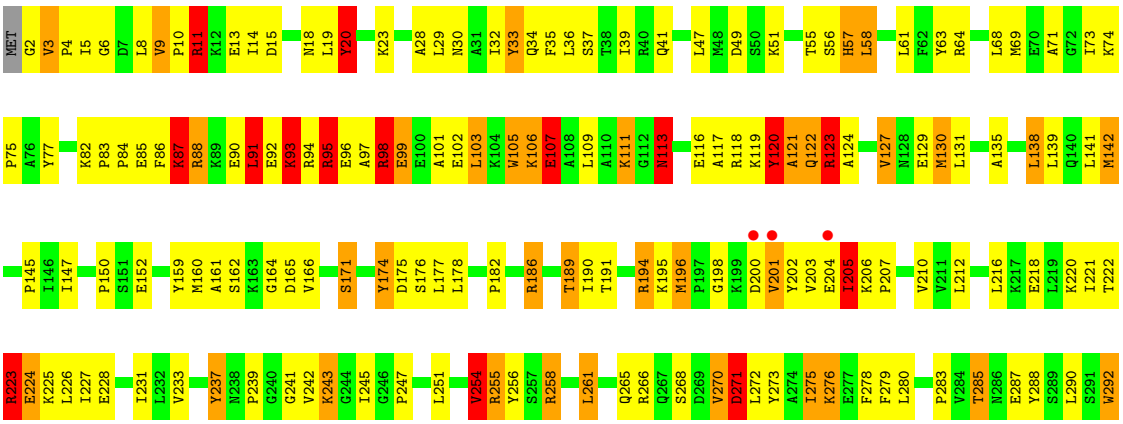
• Molecule 1: Flap Endonuclease-1

Chain A:



• Molecule 1: Flap Endonuclease-1

Chain B:




K293
E294
P295
D296
E297
E298
G299
I300
L301
K302
F303
L304
C305
D306
E307
F310
S311
E312
E313
R314
V315
K316
I319
E320
R321
I326
K327
R330
Q331
S332
THR
LEU
GLU
SER
TRP
PHE
VAL
LYS
LYS
LYS
PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	62.67Å 62.67Å 180.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 3.10 34.72 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-3.10) 100.0 (34.72-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 3.00Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.190 , 0.279 0.194 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	76.7	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l 0.469 for h,-h-k,-l 0.025 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5274	wwPDB-VP
Average B, all atoms (Å^2)	41.0	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.96	0/2682	1.98	83/3606 (2.3%)
1	B	0.93	1/2682 (0.0%)	1.91	66/3606 (1.8%)
All	All	0.95	1/5364 (0.0%)	1.94	149/7212 (2.1%)

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	B	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	105	TRP	CG-CD2	-5.06	1.35	1.43

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	321	ARG	NE-CZ-NH1	14.43	127.52	120.30
1	B	98	ARG	NE-CZ-NH1	11.34	125.97	120.30
1	B	120	TYR	CB-CG-CD2	9.98	126.99	121.00
1	A	314	ARG	NE-CZ-NH1	9.75	125.17	120.30
1	B	255	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	B	186	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	B	11	ARG	NE-CZ-NH2	-8.96	115.82	120.30
1	B	142	MET	CA-CB-CG	8.91	128.45	113.30
1	A	95	ARG	NE-CZ-NH1	8.69	124.64	120.30
1	B	271	ASP	CA-C-N	-8.61	98.26	117.20
1	A	223	ARG	NE-CZ-NH1	8.49	124.54	120.30
1	B	98	ARG	NE-CZ-NH2	-8.35	116.13	120.30
1	B	255	ARG	NE-CZ-NH2	-8.29	116.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	106	LYS	N-CA-C	-8.23	88.78	111.00
1	B	13	GLU	CA-CB-CG	8.18	131.40	113.40
1	A	127	VAL	CA-C-N	-8.15	99.27	117.20
1	A	292	TRP	CE2-CD2-CG	-8.02	100.89	107.30
1	B	258	ARG	NE-CZ-NH1	7.95	124.27	120.30
1	A	292	TRP	CD1-CG-CD2	7.88	112.60	106.30
1	A	290	LEU	CA-C-N	7.87	134.50	117.20
1	A	200	ASP	N-CA-C	-7.75	90.06	111.00
1	B	292	TRP	CE2-CD2-CG	-7.71	101.14	107.30
1	B	120	TYR	CB-CG-CD1	-7.70	116.38	121.00
1	B	105	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	A	330	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	B	77	TYR	CB-CG-CD2	-7.61	116.43	121.00
1	A	105	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	B	123	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	A	215	VAL	CG1-CB-CG2	-7.55	98.82	110.90
1	B	88	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	B	292	TRP	CD1-CG-CD2	7.54	112.33	106.30
1	B	159	TYR	CB-CG-CD1	-7.50	116.50	121.00
1	B	186	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	B	94	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	63	TYR	CB-CG-CD1	-7.44	116.54	121.00
1	A	88	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	B	270	VAL	CG1-CB-CG2	-7.22	99.35	110.90
1	B	105	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	A	105	TRP	CB-CG-CD1	-7.14	117.71	127.00
1	A	292	TRP	CG-CD2-CE3	7.14	140.32	133.90
1	B	9	VAL	N-CA-CB	-7.13	95.82	111.50
1	A	205	ILE	CA-C-N	-7.09	101.61	117.20
1	A	331	GLN	N-CA-C	-7.08	91.89	111.00
1	B	20	TYR	CA-CB-CG	7.06	126.81	113.40
1	B	95	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	A	105	TRP	CA-CB-CG	6.89	126.79	113.70
1	A	186	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	B	205	ILE	N-CA-C	6.70	129.10	111.00
1	B	11	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	105	TRP	CG-CD2-CE3	6.55	139.80	133.90
1	A	109	LEU	CA-CB-CG	6.55	130.38	115.30
1	B	84	PRO	N-CA-C	6.50	128.99	112.10
1	B	105	TRP	N-CA-C	-6.49	93.48	111.00
1	A	64	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	199	LYS	N-CA-C	-6.47	93.54	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	20	TYR	CB-CG-CD1	-6.43	117.14	121.00
1	B	194	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	A	292	TRP	CB-CG-CD1	-6.37	118.72	127.00
1	A	118	ARG	N-CA-C	-6.37	93.81	111.00
1	A	106	LYS	CA-CB-CG	-6.35	99.43	113.40
1	A	330	ARG	N-CA-C	6.25	127.87	111.00
1	A	104	LYS	N-CA-C	-6.24	94.16	111.00
1	A	223	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	319	ILE	CB-CA-C	-6.14	99.31	111.60
1	B	87	LYS	N-CA-CB	-6.12	99.58	110.60
1	A	123	ARG	CA-CB-CG	6.11	126.83	113.40
1	A	330	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	B	103	LEU	CA-CB-CG	6.06	129.24	115.30
1	B	223	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	A	105	TRP	CD1-CG-CD2	6.02	111.12	106.30
1	B	33	TYR	CA-CB-CG	-6.02	101.96	113.40
1	B	28	ALA	CB-CA-C	-5.96	101.16	110.10
1	A	42	GLU	CA-CB-CG	5.94	126.47	113.40
1	B	120	TYR	CA-CB-CG	5.94	124.68	113.40
1	A	86	PHE	N-CA-C	5.86	126.81	111.00
1	A	267	GLN	CA-C-N	-5.85	104.33	117.20
1	B	292	TRP	CB-CG-CD1	-5.77	119.50	127.00
1	B	270	VAL	CA-C-N	-5.77	104.50	117.20
1	B	271	ASP	N-CA-C	5.76	126.56	111.00
1	A	63	TYR	CB-CG-CD2	5.76	124.45	121.00
1	A	205	ILE	C-N-CA	5.76	136.09	121.70
1	A	290	LEU	O-C-N	-5.74	113.52	122.70
1	A	219	LEU	CA-CB-CG	5.73	128.47	115.30
1	B	87	LYS	N-CA-C	5.70	126.38	111.00
1	A	233	VAL	CG1-CB-CG2	-5.69	101.80	110.90
1	A	258	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	105	TRP	CA-C-N	-5.66	104.75	117.20
1	A	205	ILE	O-C-N	5.63	131.72	122.70
1	B	256	TYR	CB-CG-CD1	-5.61	117.63	121.00
1	A	90	GLU	N-CA-C	5.59	126.10	111.00
1	A	106	LYS	N-CA-CB	5.59	120.66	110.60
1	B	113	ASN	O-C-N	-5.58	113.77	122.70
1	A	278	PHE	N-CA-CB	-5.57	100.58	110.60
1	A	292	TRP	N-CA-C	5.56	126.01	111.00
1	A	300	ILE	CA-C-N	5.56	129.43	117.20
1	A	127	VAL	O-C-N	5.55	131.58	122.70
1	A	213	ASP	CA-CB-CG	5.55	125.61	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	205	ILE	CA-CB-CG2	-5.55	99.81	110.90
1	A	123	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	237	TYR	CB-CG-CD1	-5.54	117.68	121.00
1	A	80	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	268	SER	N-CA-C	5.52	125.89	111.00
1	A	120	TYR	N-CA-C	-5.49	96.17	111.00
1	A	202	TYR	CB-CG-CD1	-5.49	117.71	121.00
1	A	321	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	B	9	VAL	CB-CA-C	5.43	121.72	111.40
1	A	297	GLU	CA-CB-CG	5.42	125.33	113.40
1	B	3	VAL	CA-CB-CG2	-5.42	102.77	110.90
1	A	156	GLN	N-CA-C	-5.42	96.38	111.00
1	A	251	LEU	CB-CA-C	-5.41	99.92	110.20
1	A	99	GLU	CA-CB-CG	5.40	125.29	113.40
1	A	112	GLY	N-CA-C	-5.39	99.62	113.10
1	B	99	GLU	CA-CB-CG	5.36	125.20	113.40
1	B	107	GLU	CA-CB-CG	5.36	125.20	113.40
1	B	315	VAL	CG1-CB-CG2	-5.32	102.39	110.90
1	B	174	TYR	CB-CG-CD2	-5.31	117.81	121.00
1	B	321	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	A	110	ALA	N-CA-C	5.30	125.32	111.00
1	A	183	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	69	MET	CA-CB-CG	-5.30	104.29	113.30
1	A	194	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	332	SER	CA-CB-OG	-5.28	96.93	111.20
1	A	292	TRP	CG-CD1-NE1	-5.28	104.83	110.10
1	B	218	GLU	CA-CB-CG	-5.25	101.84	113.40
1	B	288	TYR	CB-CG-CD2	-5.24	117.85	121.00
1	A	256	TYR	CA-CB-CG	5.23	123.33	113.40
1	A	322	LEU	CA-CB-CG	5.22	127.31	115.30
1	B	290	LEU	CA-CB-CG	5.22	127.31	115.30
1	A	95	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	159	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	B	91	LEU	N-CA-C	-5.19	96.98	111.00
1	A	210	VAL	CG1-CB-CG2	-5.18	102.61	110.90
1	A	82	LYS	N-CA-C	-5.17	97.03	111.00
1	B	147	ILE	N-CA-C	-5.13	97.15	111.00
1	A	184	LEU	N-CA-C	-5.11	97.19	111.00
1	A	55	THR	N-CA-CB	-5.11	100.59	110.30
1	A	123	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	B	242	VAL	N-CA-C	-5.10	97.23	111.00
1	A	127	VAL	CA-CB-CG1	-5.08	103.27	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	202	TYR	N-CA-C	-5.08	97.29	111.00
1	A	254	VAL	CA-CB-CG2	-5.07	103.30	110.90
1	B	93	LYS	CA-C-N	-5.07	106.05	117.20
1	B	224	GLU	CA-CB-CG	5.06	124.54	113.40
1	B	141	LEU	CA-CB-CG	5.05	126.91	115.30
1	B	102	GLU	CA-C-N	-5.04	106.11	117.20
1	B	57	HIS	CA-CB-CG	5.03	122.15	113.60
1	B	233	VAL	CG1-CB-CG2	-5.02	102.87	110.90
1	A	285	THR	CA-CB-CG2	5.01	119.41	112.40
1	B	20	TYR	CA-C-N	-5.01	106.19	116.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	196	MET	Peptide
1	B	20	TYR	Sidechain
1	B	82	LYS	Peptide
1	B	83	PRO	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	2637	0	2719	102	0
1	B	2637	0	2719	99	0
All	All	5274	0	5438	198	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 18.

All (198) 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:14:ILE:HD12	1:A:209:LEU:HB2	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:GLU:HG3	1:A:326:ILE:HD13	1.58	0.84
1:A:104:LYS:HD3	1:A:126:LYS:HD2	1.69	0.75
1:A:221:ILE:HD11	1:A:255:ARG:HA	1.67	0.74
1:B:11:ARG:HB3	1:B:210:VAL:HG22	1.70	0.72
1:B:11:ARG:HB3	1:B:210:VAL:CG2	2.19	0.72
1:B:57:HIS:O	1:B:61:LEU:HB2	1.90	0.72
1:B:145:PRO:HD2	1:B:292:TRP:CD1	2.24	0.71
1:A:3:VAL:HG22	1:A:5:ILE:HG23	1.72	0.71
1:B:138:LEU:HD22	1:B:142:MET:SD	2.29	0.71
1:A:294:GLU:HG2	1:A:295:PRO:HD3	1.73	0.70
1:A:125:THR:N	1:A:126:LYS:HZ2	1.90	0.70
1:A:214:GLU:O	1:A:218:GLU:HG2	1.92	0.70
1:A:251:LEU:O	1:A:255:ARG:HB2	1.91	0.69
1:A:125:THR:H	1:A:126:LYS:HZ2	1.39	0.69
1:B:190:ILE:HD11	1:B:201:VAL:HG23	1.74	0.69
1:A:187:ASN:HB2	1:A:207:PRO:HA	1.76	0.67
1:B:191:THR:HG23	1:B:207:PRO:HD3	1.75	0.67
1:A:305:CYS:SG	1:A:312:GLU:HA	2.35	0.66
1:B:29:LEU:HD21	1:B:122:GLN:HA	1.75	0.66
1:A:315:VAL:O	1:A:319:ILE:HG13	1.96	0.65
1:B:20:TYR:HB3	1:B:71:ALA:O	1.96	0.65
1:B:227:ILE:O	1:B:231:ILE:HG12	1.97	0.64
1:A:91:LEU:HD12	1:A:94:ARG:HG2	1.81	0.63
1:A:16:LEU:HD13	1:A:207:PRO:HG3	1.78	0.63
1:A:49:ASP:HA	1:A:309:ASN:HD21	1.64	0.63
1:A:16:LEU:CD1	1:A:207:PRO:HG3	2.28	0.63
1:A:221:ILE:HG12	1:A:255:ARG:HD3	1.80	0.63
1:B:203:VAL:HG12	1:B:204:GLU:HG2	1.81	0.62
1:B:61:LEU:HD21	1:B:135:ALA:HB1	1.81	0.62
1:B:105:TRP:HE3	1:B:106:LYS:HG2	1.65	0.62
1:B:212:LEU:HD21	1:B:223:ARG:HD2	1.81	0.62
1:A:183:ARG:HG3	1:A:209:LEU:HD21	1.82	0.62
1:B:118:ARG:HG3	1:B:122:GLN:HB3	1.81	0.61
1:A:235:THR:HG22	1:A:238:ASN:OD1	2.00	0.61
1:B:64:ARG:HH22	1:B:191:THR:HB	1.66	0.61
1:B:88:ARG:HB3	1:B:93:LYS:HB3	1.82	0.60
1:A:79:PHE:HB2	1:A:148:GLN:HA	1.84	0.60
1:A:125:THR:H	1:A:126:LYS:NZ	1.99	0.60
1:A:312:GLU:O	1:A:316:LYS:HG3	2.02	0.59
1:B:119:LYS:HB2	1:B:120:TYR:CD2	2.37	0.59
1:A:8:LEU:HD11	1:A:247:PRO:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LEU:HG	1:A:251:LEU:HD21	1.85	0.59
1:A:64:ARG:HE	1:A:67:ASN:HD22	1.50	0.58
1:A:109:LEU:HD23	1:B:243:LYS:HG2	1.86	0.58
1:A:105:TRP:HA	1:A:108:ALA:HB2	1.86	0.58
1:B:311:SER:HB3	1:B:314:ARG:HG2	1.85	0.58
1:B:36:LEU:HD11	1:B:131:LEU:HD21	1.85	0.58
1:A:19:LEU:HD21	1:A:185:ILE:HD13	1.86	0.57
1:B:223:ARG:HG2	1:B:223:ARG:HH11	1.69	0.57
1:A:86:PHE:HE1	1:A:274:ALA:HB1	1.69	0.57
1:B:41:GLN:HG2	1:B:47:LEU:HD23	1.85	0.57
1:B:123:ARG:HH22	1:B:239:PRO:HB3	1.69	0.57
1:B:101:ALA:O	1:B:103:LEU:HD22	2.05	0.57
1:A:225:LYS:HA	1:A:228:GLU:OE1	2.06	0.56
1:B:295:PRO:HD3	1:B:326:ILE:HD11	1.89	0.55
1:A:121:ALA:HA	1:A:126:LYS:CG	2.36	0.55
1:A:19:LEU:HB3	1:A:73:ILE:HG12	1.88	0.55
1:A:235:THR:HG23	1:A:237:TYR:H	1.72	0.55
1:B:119:LYS:HB2	1:B:120:TYR:HD2	1.72	0.55
1:A:40:ARG:HH22	1:A:111:LYS:HG3	1.70	0.55
1:A:121:ALA:HA	1:A:126:LYS:HG3	1.88	0.55
1:B:201:VAL:HG22	1:B:202:TYR:H	1.73	0.54
1:A:48:MET:HB3	1:A:52:GLY:O	2.06	0.54
1:B:23:LYS:HA	1:B:74:LYS:O	2.08	0.54
1:A:14:ILE:CD1	1:A:209:LEU:HB2	2.36	0.54
1:B:29:LEU:CD2	1:B:122:GLN:HA	2.38	0.54
1:B:237:TYR:CZ	1:B:278:PHE:HE2	2.25	0.54
1:B:23:LYS:HD2	1:B:165:ASP:O	2.09	0.53
1:B:273:TYR:O	1:B:276:LYS:HB2	2.08	0.53
1:B:313:GLU:HA	1:B:316:LYS:HB2	1.91	0.53
1:A:249:LYS:O	1:A:253:ILE:HG12	2.08	0.53
1:A:141:LEU:O	1:A:295:PRO:HA	2.08	0.53
1:A:301:LEU:HD21	1:A:316:LYS:HG2	1.90	0.52
1:A:14:ILE:HG22	1:A:207:PRO:HG2	1.92	0.52
1:B:39:ILE:HB	1:B:56:SER:HB3	1.92	0.52
1:B:150:PRO:HD3	1:B:285:THR:HB	1.92	0.52
1:A:211:VAL:HB	1:A:214:GLU:HG3	1.91	0.52
1:A:19:LEU:HD22	1:A:24:ILE:HD11	1.92	0.51
1:A:41:GLN:HG3	1:A:45:THR:O	2.09	0.51
1:A:110:ALA:O	1:A:113:ASN:HA	2.11	0.51
1:B:206:LYS:NZ	1:B:206:LYS:HB2	2.25	0.51
1:B:123:ARG:NH2	1:B:239:PRO:HB3	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:ILE:HG22	1:B:279:PHE:CE2	2.45	0.51
1:A:216:LEU:HD21	1:A:226:LEU:HD22	1.92	0.51
1:B:225:LYS:HB3	1:B:254:VAL:HG13	1.92	0.51
1:B:6:GLY:HA2	1:B:174:TYR:CE2	2.46	0.51
1:B:99:GLU:HG3	1:B:127:VAL:HG13	1.93	0.51
1:A:126:LYS:N	1:A:126:LYS:HD3	2.27	0.50
1:A:221:ILE:HD12	1:A:225:LYS:HB3	1.93	0.50
1:A:26:ILE:O	1:A:77:TYR:HA	2.12	0.50
1:A:123:ARG:H	1:A:126:LYS:HZ1	1.60	0.50
1:B:293:LYS:O	1:B:326:ILE:HD12	2.12	0.50
1:A:55:THR:HG23	1:A:310:PHE:HE1	1.76	0.49
1:B:116:GLU:O	1:B:119:LYS:HG3	2.13	0.49
1:A:114:LEU:HD11	1:B:245:ILE:O	2.12	0.49
1:A:123:ARG:CD	1:A:126:LYS:HE3	2.42	0.49
1:A:139:LEU:O	1:A:142:MET:HB2	2.12	0.49
1:A:258:ARG:HB3	1:A:258:ARG:NH1	2.28	0.49
1:A:74:LYS:NZ	1:A:291:SER:HB3	2.27	0.49
1:B:194:ARG:HA	1:B:205:ILE:HG12	1.95	0.49
1:A:62:PHE:HD2	1:A:142:MET:SD	2.35	0.49
1:A:321:ARG:O	1:A:324:LYS:HB3	2.13	0.48
1:B:299:GLY:O	1:B:302:LYS:HB2	2.13	0.48
1:B:178:LEU:HD23	1:B:279:PHE:CE1	2.49	0.48
1:B:194:ARG:HG3	1:B:205:ILE:HD11	1.95	0.48
1:B:55:THR:HG22	1:B:58:LEU:HD22	1.96	0.48
1:A:18:ASN:O	1:A:18:ASN:ND2	2.46	0.48
1:B:231:ILE:HD12	1:B:275:ILE:HB	1.95	0.48
1:A:23:LYS:HB3	1:A:166:VAL:HG12	1.96	0.47
1:B:301:LEU:O	1:B:305:CYS:HB2	2.14	0.47
1:B:109:LEU:HB3	1:B:117:ALA:HB2	1.95	0.47
1:A:36:LEU:HB3	1:A:111:LYS:HD3	1.96	0.47
1:B:90:GLU:HG3	1:B:95:ARG:HB2	1.97	0.47
1:B:105:TRP:CE3	1:B:106:LYS:HG2	2.48	0.47
1:A:275:ILE:O	1:A:278:PHE:HB3	2.15	0.47
1:B:276:LYS:CE	1:B:280:LEU:HD11	2.44	0.47
1:B:296:ASP:O	1:B:299:GLY:N	2.48	0.47
1:A:114:LEU:HD21	1:B:245:ILE:O	2.15	0.47
1:A:225:LYS:HD3	1:A:228:GLU:OE1	2.15	0.47
1:A:136:LYS:HB2	1:A:146:ILE:HD12	1.97	0.46
1:A:261:LEU:HD12	1:A:272:LEU:HB3	1.97	0.46
1:A:186:ARG:O	1:A:187:ASN:HB2	2.15	0.46
1:B:212:LEU:CD2	1:B:223:ARG:HD2	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:VAL:HG22	1:B:202:TYR:N	2.30	0.46
1:B:314:ARG:HG3	1:B:315:VAL:N	2.31	0.46
1:B:63:TYR:HE1	1:B:310:PHE:HE2	1.65	0.45
1:A:292:TRP:O	1:A:293:LYS:HB2	2.15	0.45
1:A:93:LYS:HZ2	1:A:95:ARG:HG2	1.82	0.45
1:A:304:LEU:O	1:A:310:PHE:HB2	2.17	0.45
1:B:11:ARG:HB3	1:B:210:VAL:HG23	1.99	0.45
1:B:161:ALA:HB3	1:B:182:PRO:HD2	1.97	0.45
1:B:64:ARG:NH2	1:B:191:THR:HB	2.30	0.45
1:B:195:LYS:C	1:B:196:MET:SD	2.96	0.45
1:A:221:ILE:HG12	1:A:255:ARG:CD	2.46	0.45
1:A:276:LYS:HE3	1:A:280:LEU:HD11	1.99	0.45
1:A:118:ARG:HH11	1:A:119:LYS:HG2	1.82	0.44
1:A:217:LYS:O	1:A:220:LYS:HG3	2.18	0.44
1:B:271:ASP:O	1:B:275:ILE:HG12	2.17	0.44
1:A:62:PHE:CD2	1:A:142:MET:SD	3.11	0.44
1:B:8:LEU:HD11	1:B:247:PRO:HB2	1.99	0.44
1:B:160:MET:HB3	1:B:166:VAL:CG2	2.47	0.44
1:A:40:ARG:NH2	1:A:111:LYS:O	2.51	0.44
1:A:116:GLU:OE2	1:A:116:GLU:HA	2.18	0.44
1:B:275:ILE:HG22	1:B:279:PHE:HE2	1.81	0.44
1:A:86:PHE:N	1:A:87:LYS:NZ	2.66	0.44
1:B:2:GLY:O	1:B:3:VAL:HB	2.18	0.44
1:B:36:LEU:HD11	1:B:131:LEU:CD2	2.47	0.44
1:A:198:GLY:HA3	1:A:201:VAL:HG13	2.00	0.44
1:A:258:ARG:HB3	1:A:258:ARG:HH11	1.82	0.43
1:B:64:ARG:HA	1:B:64:ARG:HD2	1.87	0.43
1:B:225:LYS:O	1:B:228:GLU:N	2.51	0.43
1:B:265:GLN:OE1	1:B:272:LEU:N	2.52	0.43
1:B:35:PHE:CZ	1:B:189:THR:HG22	2.54	0.43
1:A:221:ILE:HD13	1:A:221:ILE:HA	1.60	0.43
1:A:176:SER:HB2	1:A:181:ALA:HB2	2.00	0.43
1:B:98:ARG:HH11	1:B:98:ARG:HG2	1.83	0.43
1:A:297:GLU:O	1:A:301:LEU:HD12	2.19	0.43
1:B:221:ILE:HG21	1:B:254:VAL:HG12	2.00	0.43
1:A:81:GLY:HA3	1:A:150:PRO:O	2.19	0.43
1:B:120:TYR:CD2	1:B:120:TYR:N	2.86	0.43
1:A:8:LEU:CD1	1:A:247:PRO:HB3	2.49	0.43
1:A:28:ALA:HA	1:A:77:TYR:HD2	1.84	0.43
1:B:216:LEU:HD23	1:B:216:LEU:HA	1.81	0.42
1:A:125:THR:HB	1:A:126:LYS:H	1.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:LEU:HA	1:A:142:MET:HB2	2.02	0.42
1:B:34:GLN:O	1:B:37:SER:HB3	2.19	0.42
1:A:117:ALA:HB1	1:A:120:TYR:CD1	2.54	0.42
1:A:9:VAL:HA	1:A:10:PRO:HD2	1.66	0.42
1:A:185:ILE:HG12	1:A:209:LEU:HD23	2.01	0.42
1:B:87:LYS:HE3	1:B:87:LYS:HB3	1.96	0.42
1:B:294:GLU:OE1	1:B:327:LYS:HG2	2.20	0.42
1:B:315:VAL:HG12	1:B:319:ILE:HD13	2.00	0.42
1:A:97:ALA:O	1:A:99:GLU:N	2.53	0.42
1:A:105:TRP:O	1:A:128:ASN:ND2	2.52	0.42
1:A:121:ALA:HA	1:A:126:LYS:HG2	2.01	0.42
1:B:61:LEU:HD21	1:B:135:ALA:CB	2.47	0.42
1:A:36:LEU:HD23	1:A:111:LYS:CD	2.50	0.42
1:A:205:ILE:HD13	1:A:205:ILE:HG21	1.84	0.42
1:A:255:ARG:HH11	1:A:255:ARG:HD2	1.72	0.42
1:B:303:PHE:CD2	1:B:304:LEU:HD12	2.55	0.41
1:A:264:PHE:O	1:A:266:ARG:N	2.54	0.41
1:B:254:VAL:HG12	1:B:255:ARG:N	2.35	0.41
1:A:320:GLU:HA	1:A:323:LYS:HD3	2.02	0.41
1:B:206:LYS:HB2	1:B:206:LYS:HZ2	1.85	0.41
1:B:196:MET:O	1:B:198:GLY:N	2.53	0.41
1:B:33:TYR:OH	1:B:121:ALA:HB3	2.20	0.41
1:B:261:LEU:O	1:B:265:GLN:N	2.53	0.41
1:B:186:ARG:HH22	1:B:202:TYR:CB	2.34	0.41
1:B:276:LYS:HE2	1:B:280:LEU:HD11	2.02	0.41
1:B:111:LYS:O	1:B:113:ASN:N	2.54	0.41
1:A:124:ALA:O	1:A:125:THR:HG23	2.21	0.40
1:B:29:LEU:HD21	1:B:121:ALA:O	2.21	0.40
1:B:9:VAL:HA	1:B:10:PRO:HD2	1.99	0.40
1:B:191:THR:CG2	1:B:207:PRO:HD3	2.49	0.40
1:B:160:MET:HB3	1:B:166:VAL:HG21	2.03	0.40
1:A:55:THR:HG23	1:A:310:PHE:CE1	2.55	0.40
1:B:138:LEU:O	1:B:142:MET:HG2	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	329/343 (96%)	228 (69%)	68 (21%)	33 (10%)	0 3
1	B	329/343 (96%)	243 (74%)	59 (18%)	27 (8%)	1 5
All	All	658/686 (96%)	471 (72%)	127 (19%)	60 (9%)	1 4

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	ILE
1	A	90	GLU
1	A	98	ARG
1	A	126	LYS
1	A	194	ARG
1	A	197	PRO
1	A	272	LEU
1	A	293	LYS
1	A	330	ARG
1	A	331	GLN
1	B	85	GLU
1	B	91	LEU
1	B	107	GLU
1	B	124	ALA
1	B	200	ASP
1	B	205	ILE
1	B	266	ARG
1	B	268	SER
1	B	270	VAL
1	B	296	ASP
1	B	297	GLU
1	A	102	GLU
1	A	119	LYS
1	A	125	THR
1	A	153	GLY

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Mol	Chain	Res	Type
1	A	164	GLY
1	A	265	GLN
1	B	96	GLU
1	B	97	ALA
1	B	121	ALA
1	B	201	VAL
1	B	271	ASP
1	A	92	GLU
1	A	96	GLU
1	A	220	LYS
1	A	223	ARG
1	B	130	MET
1	B	171	SER
1	B	283	PRO
1	A	36	LEU
1	A	121	ALA
1	A	255	ARG
1	A	309	ASN
1	A	313	GLU
1	A	163	LYS
1	A	290	LEU
1	A	292	TRP
1	B	4	PRO
1	B	106	LYS
1	A	203	VAL
1	A	239	PRO
1	A	240	GLY
1	B	164	GLY
1	A	5	ILE
1	B	5	ILE
1	B	14	ILE
1	A	329	GLY
1	B	127	VAL
1	B	241	GLY
1	B	254	VAL

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	281/293 (96%)	210 (75%)	71 (25%)	0 1
1	B	281/293 (96%)	225 (80%)	56 (20%)	1 5
All	All	562/586 (96%)	435 (77%)	127 (23%)	1 3

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	11	ARG
1	A	14	ILE
1	A	17	GLU
1	A	20	TYR
1	A	23	LYS
1	A	32	ILE
1	A	43	ASP
1	A	45	THR
1	A	47	LEU
1	A	48	MET
1	A	49	ASP
1	A	53	ARG
1	A	56	SER
1	A	64	ARG
1	A	74	LYS
1	A	75	PRO
1	A	86	PHE
1	A	87	LYS
1	A	93	LYS
1	A	99	GLU
1	A	105	TRP
1	A	109	LEU
1	A	111	LYS
1	A	113	ASN
1	A	115	GLU
1	A	118	ARG
1	A	119	LYS
1	A	123	ARG
1	A	125	THR
1	A	126	LYS
1	A	129	GLU
1	A	133	GLU
1	A	136	LYS

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Mol	Chain	Res	Type
1	A	176	SER
1	A	177	LEU
1	A	183	ARG
1	A	184	LEU
1	A	194	ARG
1	A	197	PRO
1	A	201	VAL
1	A	206	LYS
1	A	209	LEU
1	A	218	GLU
1	A	219	LEU
1	A	220	LYS
1	A	221	ILE
1	A	223	ARG
1	A	224	GLU
1	A	236	ASP
1	A	255	ARG
1	A	256	TYR
1	A	258	ARG
1	A	267	GLN
1	A	277	GLU
1	A	286	ASN
1	A	287	GLU
1	A	290	LEU
1	A	292	TRP
1	A	296	ASP
1	A	297	GLU
1	A	302	LYS
1	A	305	CYS
1	A	307	GLU
1	A	312	GLU
1	A	314	ARG
1	A	319	ILE
1	A	320	GLU
1	A	322	LEU
1	A	323	LYS
1	A	332	SER
1	B	11	ARG
1	B	15	ASP
1	B	18	ASN
1	B	19	LEU
1	B	30	ASN

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Mol	Chain	Res	Type
1	B	32	ILE
1	B	49	ASP
1	B	51	LYS
1	B	58	LEU
1	B	68	LEU
1	B	73	ILE
1	B	75	PRO
1	B	86	PHE
1	B	87	LYS
1	B	91	LEU
1	B	92	GLU
1	B	93	LYS
1	B	95	ARG
1	B	98	ARG
1	B	107	GLU
1	B	111	LYS
1	B	113	ASN
1	B	120	TYR
1	B	122	GLN
1	B	123	ARG
1	B	129	GLU
1	B	130	MET
1	B	138	LEU
1	B	139	LEU
1	B	152	GLU
1	B	162	SER
1	B	171	SER
1	B	175	ASP
1	B	176	SER
1	B	177	LEU
1	B	189	THR
1	B	220	LYS
1	B	222	THR
1	B	223	ARG
1	B	224	GLU
1	B	226	LEU
1	B	243	LYS
1	B	251	LEU
1	B	254	VAL
1	B	258	ARG
1	B	261	LEU
1	B	275	ILE

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Mol	Chain	Res	Type
1	B	276	LYS
1	B	285	THR
1	B	287	GLU
1	B	294	GLU
1	B	296	ASP
1	B	301	LEU
1	B	307	GLU
1	B	330	ARG
1	B	331	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	34	GLN
1	A	57	HIS
1	A	67	ASN
1	A	113	ASN
1	A	331	GLN
1	B	34	GLN
1	B	57	HIS
1	B	122	GLN
1	B	187	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

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

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	331/343 (96%)	-0.54	6 (1%)	68	47	13, 37, 74, 83	0
1	B	331/343 (96%)	-0.54	4 (1%)	79	61	10, 37, 70, 84	0
All	All	662/686 (96%)	-0.54	10 (1%)	73	54	10, 37, 71, 84	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	124	ALA	3.3
1	A	202	TYR	2.8
1	B	326	ILE	2.8
1	B	204	GLU	2.8
1	B	200	ASP	2.5
1	B	201	VAL	2.5
1	A	91	LEU	2.4
1	A	203	VAL	2.4
1	A	204	GLU	2.3
1	A	95	ARG	2.1

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.