Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 05:39 pm BST

PDB ID	:	2B98
Title	:	Crystal Structure of an archaeal pentameric riboflavin synthase
Authors	:	Ramsperger, A.; Augustin, M.; Schott, A.K.; Gerhardt, S.; Krojer, T.; Eisenreich, W.; Illarionov, B.; Cushman, M.; Bacher, A.; Huber, R.; Fischer, M.
Deposited on	:	2005-10-11
Resolution	:	2.30 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 following versions of software and data (see references ⓘ) were used in the production of this report:

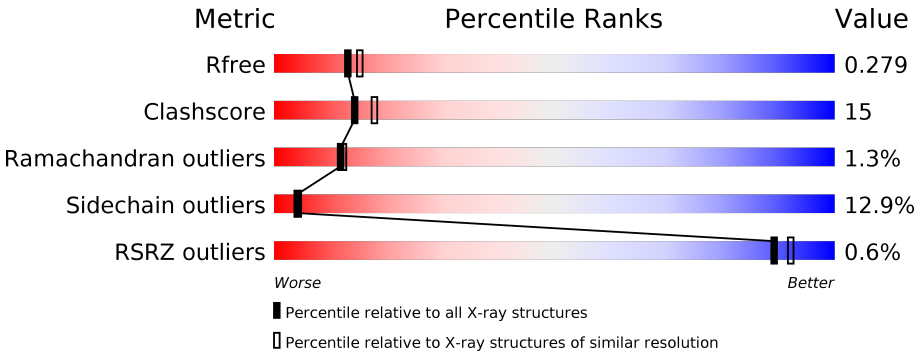
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	156	% 53% 28% 8% • 10%
1	B	156	% 49% 32% 6% • 10%
1	C	156	63% 28% 6% •
1	D	156	% 53% 32% • • 10%
1	E	156	56% 34% 6% • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5989 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 Riboflavin synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	63	0	0
			1106	707	188	202	9			
1	B	141	Total	C	N	O	S	94	0	0
			1109	709	188	203	9			
1	C	152	Total	C	N	O	S	72	0	0
			1189	758	203	219	9			
1	D	140	Total	C	N	O	S	66	0	0
			1102	705	187	201	9			
1	E	152	Total	C	N	O	S	57	0	0
			1189	758	203	219	9			

- Molecule 2 is water.

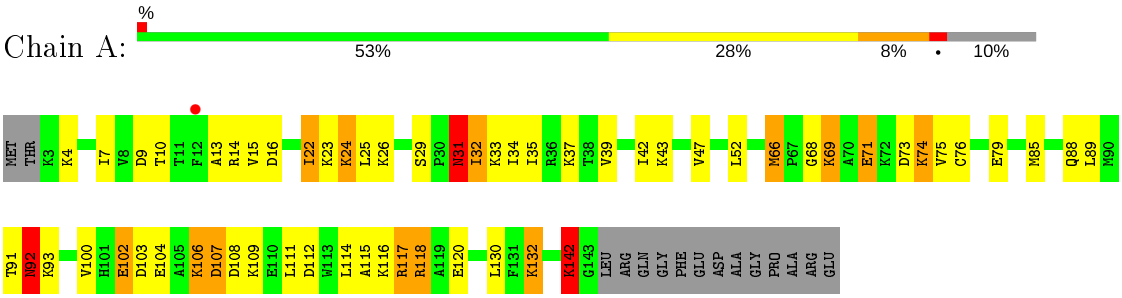
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	64	Total	O	0	0
			64	64		
2	B	62	Total	O	0	0
			62	62		
2	C	61	Total	O	0	0
			61	61		
2	D	52	Total	O	0	0
			52	52		
2	E	55	Total	O	0	0
			55	55		

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 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.

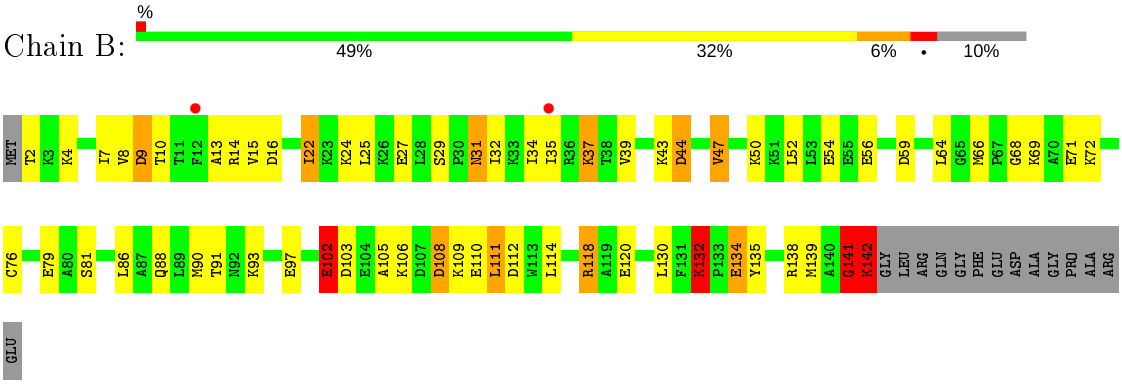
- Molecule 1: Riboflavin synthase

Chain A:



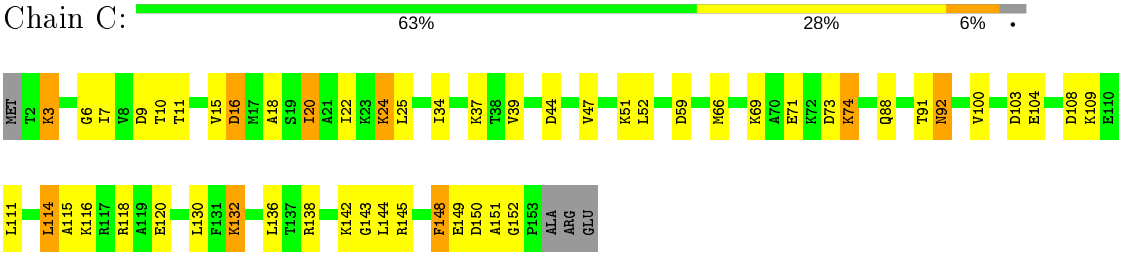
- Molecule 1: Riboflavin synthase

Chain B:



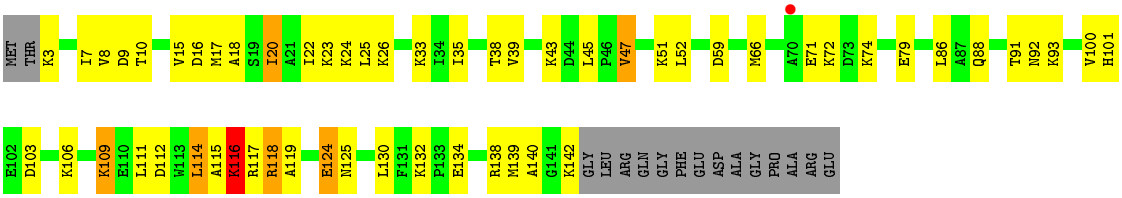
- Molecule 1: Riboflavin synthase

Chain C:



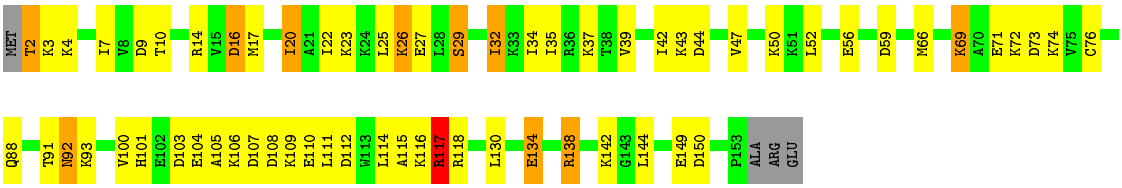
- Molecule 1: Riboflavin synthase

Chain D:



- Molecule 1: Riboflavin synthase

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	41.77Å 72.69Å 72.70Å 68.48° 74.61° 74.90°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.30) 94.7 (20.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.24 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.208 , 0.276 0.212 , 0.279	Depositor DCC
R_{free} test set	1677 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å^2)	28.5	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 34.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.095 for h,h-k,h-l 0.257 for -h,-l,-k 0.089 for -h,-h+l,-h+k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5989	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% 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	2.50	11/1122 (1.0%)	1.64	23/1504 (1.5%)
1	B	5.55	17/1125 (1.5%)	2.54	34/1509 (2.3%)
1	C	1.94	8/1207 (0.7%)	1.37	21/1619 (1.3%)
1	D	1.90	13/1118 (1.2%)	1.56	23/1499 (1.5%)
1	E	1.84	14/1207 (1.2%)	1.33	22/1619 (1.4%)
All	All	3.07	63/5779 (1.1%)	1.74	123/7750 (1.6%)

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	2
1	B	0	3
1	C	0	1
1	D	0	1
All	All	0	7

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	134	GLU	CD-OE1	161.56	3.03	1.25
1	B	134	GLU	CD-OE2	70.17	2.02	1.25
1	D	124	GLU	CG-CD	50.00	2.27	1.51
1	A	71	GLU	CG-CD	48.47	2.24	1.51
1	E	74	LYS	CD-CE	41.81	2.55	1.51
1	C	109	LYS	CG-CD	40.77	2.91	1.52
1	C	144	LEU	CG-CD2	39.12	2.96	1.51
1	A	132	LYS	CG-CD	37.81	2.81	1.52
1	A	109	LYS	CD-CE	-30.48	0.75	1.51
1	E	117	ARG	CG-CD	-29.06	0.79	1.51
1	A	26	LYS	CD-CE	28.06	2.21	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	135	TYR	CB-CG	26.68	1.91	1.51
1	C	148	PHE	CB-CG	24.59	1.93	1.51
1	A	117	ARG	CG-CD	22.39	2.08	1.51
1	B	14	ARG	CB-CG	20.80	2.08	1.52
1	B	2	THR	CA-CB	20.36	2.06	1.53
1	B	142	LYS	CG-CD	17.55	2.12	1.52
1	E	2	THR	CB-CG2	17.54	2.10	1.52
1	B	102	GLU	CG-CD	17.07	1.77	1.51
1	D	26	LYS	CD-CE	16.89	1.93	1.51
1	B	141	GLY	CA-C	16.21	1.77	1.51
1	A	74	LYS	CD-CE	16.13	1.91	1.51
1	D	116	LYS	CE-NZ	14.55	1.85	1.49
1	A	112	ASP	CB-CG	14.37	1.81	1.51
1	C	37	LYS	CB-CG	-14.17	1.14	1.52
1	B	27	GLU	CB-CG	-14.09	1.25	1.52
1	B	139	MET	CA-CB	12.63	1.81	1.53
1	A	69	LYS	CG-CD	12.33	1.94	1.52
1	B	141	GLY	C-N	12.16	1.62	1.34
1	E	73	ASP	CB-CG	-12.05	1.26	1.51
1	D	142	LYS	CG-CD	-11.74	1.12	1.52
1	E	14	ARG	CA-CB	-11.41	1.28	1.53
1	E	138	ARG	CG-CD	11.33	1.80	1.51
1	D	118	ARG	CG-CD	11.30	1.80	1.51
1	B	69	LYS	CB-CG	11.19	1.82	1.52
1	E	37	LYS	CG-CD	10.56	1.88	1.52
1	E	72	LYS	CA-CB	-10.14	1.31	1.53
1	B	132	LYS	CD-CE	-9.86	1.26	1.51
1	E	134	GLU	CB-CG	9.80	1.70	1.52
1	C	144	LEU	CB-CG	9.69	1.80	1.52
1	D	138	ARG	CB-CG	9.40	1.77	1.52
1	D	117	ARG	CD-NE	9.13	1.61	1.46
1	D	74	LYS	CB-CG	-8.96	1.28	1.52
1	D	72	LYS	CB-CG	-8.77	1.28	1.52
1	E	149	GLU	CB-CG	8.61	1.68	1.52
1	B	79	GLU	CA-CB	-8.57	1.35	1.53
1	B	71	GLU	CB-CG	-8.46	1.36	1.52
1	D	109	LYS	CB-CG	8.46	1.75	1.52
1	A	23	LYS	CA-CB	-7.93	1.36	1.53
1	D	33	LYS	CG-CD	7.79	1.78	1.52
1	E	26	LYS	CD-CE	-7.49	1.32	1.51
1	E	69	LYS	CG-CD	-7.38	1.27	1.52
1	B	72	LYS	CB-CG	7.38	1.72	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	142	LYS	CG-CD	-7.23	1.27	1.52
1	C	138	ARG	CG-CD	-7.10	1.34	1.51
1	B	138	ARG	CB-CG	-6.79	1.34	1.52
1	C	142	LYS	CE-NZ	6.00	1.64	1.49
1	A	111	LEU	CA-CB	5.80	1.67	1.53
1	D	112	ASP	CB-CG	5.55	1.63	1.51
1	E	109	LYS	CB-CG	-5.43	1.37	1.52
1	D	23	LYS	CB-CG	-5.11	1.38	1.52
1	E	23	LYS	CB-CG	-5.11	1.38	1.52
1	C	111	LEU	CA-CB	5.00	1.65	1.53

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	134	GLU	OE1-CD-OE2	-64.04	46.45	123.30
1	B	141	GLY	O-C-N	-42.17	55.23	122.70
1	D	124	GLU	CG-CD-OE2	-28.90	60.49	118.30
1	A	71	GLU	CG-CD-OE2	-24.92	68.45	118.30
1	C	148	PHE	CB-CG-CD1	-23.05	104.67	120.80
1	B	142	LYS	CB-CG-CD	21.89	168.51	111.60
1	D	124	GLU	CG-CD-OE1	21.19	160.68	118.30
1	E	2	THR	OG1-CB-CG2	-19.50	65.15	110.00
1	C	109	LYS	CB-CG-CD	-19.18	61.74	111.60
1	B	108	ASP	CB-CG-OD2	18.78	135.21	118.30
1	B	108	ASP	CB-CG-OD1	-18.61	101.55	118.30
1	C	148	PHE	CB-CG-CD2	17.76	133.23	120.80
1	A	71	GLU	CB-CG-CD	-17.33	67.41	114.20
1	D	142	LYS	CB-CG-CD	16.61	154.78	111.60
1	A	132	LYS	CB-CG-CD	-16.44	68.85	111.60
1	A	109	LYS	CD-CE-NZ	15.35	147.00	111.70
1	E	117	ARG	CG-CD-NE	15.27	143.86	111.80
1	A	69	LYS	CG-CD-CE	-14.64	67.99	111.90
1	B	141	GLY	C-N-CA	-14.58	85.24	121.70
1	A	71	GLU	CG-CD-OE1	14.55	147.40	118.30
1	C	3	LYS	CD-CE-NZ	14.31	144.61	111.70
1	A	109	LYS	CG-CD-CE	14.24	154.63	111.90
1	D	124	GLU	CB-CG-CD	-14.14	76.01	114.20
1	E	117	ARG	CB-CG-CD	13.95	147.87	111.60
1	B	2	THR	N-CA-CB	13.41	135.78	110.30
1	B	132	LYS	CD-CE-NZ	12.96	141.50	111.70
1	D	116	LYS	CD-CE-NZ	12.86	141.27	111.70
1	A	26	LYS	CD-CE-NZ	12.84	141.22	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	117	ARG	CB-CG-CD	-12.59	78.88	111.60
1	C	109	LYS	CG-CD-CE	-12.16	75.43	111.90
1	E	73	ASP	CB-CG-OD1	12.01	129.11	118.30
1	E	73	ASP	CB-CG-OD2	-11.47	107.97	118.30
1	D	118	ARG	CB-CG-CD	-11.39	82.00	111.60
1	E	26	LYS	CD-CE-NZ	11.13	137.30	111.70
1	D	118	ARG	CG-CD-NE	10.95	134.80	111.80
1	E	138	ARG	CG-CD-NE	10.64	134.14	111.80
1	A	142	LYS	CB-CG-CD	-10.33	84.75	111.60
1	B	102	GLU	CB-CG-CD	10.20	141.73	114.20
1	B	102	GLU	CG-CD-OE2	-9.53	99.24	118.30
1	E	37	LYS	CB-CG-CD	-9.37	87.23	111.60
1	C	148	PHE	CA-CB-CG	-9.11	92.03	113.90
1	A	26	LYS	CG-CD-CE	-9.08	84.67	111.90
1	E	69	LYS	CG-CD-CE	8.95	138.76	111.90
1	B	118	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	D	71	GLU	N-CA-CB	8.77	126.39	110.60
1	A	37	LYS	CB-CG-CD	-8.67	89.06	111.60
1	B	118	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	D	117	ARG	CG-CD-NE	-8.54	93.86	111.80
1	A	108	ASP	CB-CG-OD1	-8.52	110.64	118.30
1	E	138	ARG	CB-CG-CD	-8.39	89.79	111.60
1	B	135	TYR	CB-CG-CD1	-8.31	116.02	121.00
1	A	108	ASP	CB-CG-OD2	8.15	125.64	118.30
1	C	142	LYS	CD-CE-NZ	-8.01	93.27	111.70
1	B	139	MET	N-CA-CB	-7.96	96.27	110.60
1	A	132	LYS	CG-CD-CE	7.96	135.77	111.90
1	B	135	TYR	CB-CG-CD2	7.83	125.70	121.00
1	E	9	ASP	CB-CG-OD2	7.77	125.30	118.30
1	A	108	ASP	CA-CB-CG	7.70	130.34	113.40
1	B	14	ARG	NE-CZ-NH2	-7.59	116.51	120.30
1	B	135	TYR	CA-CB-CG	-7.53	99.08	113.40
1	D	112	ASP	CB-CG-OD1	7.51	125.06	118.30
1	E	16	ASP	CB-CG-OD2	7.42	124.98	118.30
1	A	16	ASP	CB-CG-OD2	7.32	124.88	118.30
1	B	27	GLU	CA-CB-CG	7.22	129.29	113.40
1	D	112	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	B	118	ARG	CG-CD-NE	-7.08	96.92	111.80
1	B	14	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	A	111	LEU	CB-CA-C	-6.77	97.34	110.20
1	D	16	ASP	CB-CG-OD2	6.74	124.37	118.30
1	C	69	LYS	CA-CB-CG	-6.56	98.96	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	111	LEU	CA-CB-CG	6.51	130.28	115.30
1	C	71	GLU	N-CA-CB	6.45	122.22	110.60
1	C	16	ASP	CB-CG-OD2	6.37	124.03	118.30
1	B	16	ASP	CB-CG-OD2	6.29	123.97	118.30
1	D	109	LYS	CB-CG-CD	6.24	127.81	111.60
1	C	9	ASP	CB-CG-OD2	6.19	123.87	118.30
1	D	103	ASP	CB-CG-OD2	6.16	123.85	118.30
1	C	73	ASP	CB-CA-C	-6.15	98.09	110.40
1	E	109	LYS	CB-CG-CD	6.12	127.52	111.60
1	C	108	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	31	ASN	CB-CG-ND2	-6.08	102.10	116.70
1	B	142	LYS	CG-CD-CE	6.08	130.14	111.90
1	C	74	LYS	CG-CD-CE	6.05	130.05	111.90
1	C	59	ASP	CB-CG-OD2	6.05	123.74	118.30
1	B	31	ASN	CB-CG-ND2	-6.02	102.25	116.70
1	E	150	ASP	CB-CG-OD2	5.99	123.69	118.30
1	D	106	LYS	CA-CB-CG	5.96	126.51	113.40
1	B	71	GLU	CB-CG-CD	-5.95	98.14	114.20
1	D	9	ASP	CB-CG-OD2	5.92	123.63	118.30
1	D	117	ARG	CD-NE-CZ	-5.84	115.43	123.60
1	D	112	ASP	CA-CB-CG	-5.81	100.62	113.40
1	B	59	ASP	CB-CG-OD2	5.78	123.51	118.30
1	A	9	ASP	CB-CG-OD2	5.76	123.48	118.30
1	D	59	ASP	CB-CG-OD2	5.74	123.46	118.30
1	E	103	ASP	CB-CG-OD2	5.69	123.42	118.30
1	D	71	GLU	CA-CB-CG	-5.68	100.91	113.40
1	D	33	LYS	CB-CG-CD	-5.65	96.90	111.60
1	C	37	LYS	CA-CB-CG	5.64	125.82	113.40
1	C	103	ASP	CB-CG-OD2	5.64	123.38	118.30
1	E	112	ASP	CB-CG-OD2	5.62	123.36	118.30
1	C	3	LYS	CG-CD-CE	5.61	128.74	111.90
1	B	112	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	9	ASP	CB-CG-OD2	5.56	123.30	118.30
1	B	44	ASP	CB-CG-OD2	5.43	123.19	118.30
1	E	44	ASP	CB-CG-OD2	5.40	123.16	118.30
1	C	73	ASP	N-CA-CB	-5.40	100.88	110.60
1	E	14	ARG	NE-CZ-NH1	-5.39	117.60	120.30
1	A	103	ASP	CB-CG-OD2	5.37	123.14	118.30
1	B	141	GLY	N-CA-C	-5.37	99.66	113.10
1	C	150	ASP	CB-CG-OD2	5.37	123.14	118.30
1	C	44	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	71	GLU	CA-CB-CG	-5.31	101.71	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	37	LYS	CB-CG-CD	-5.31	97.79	111.60
1	A	73	ASP	CB-CG-OD2	5.24	123.02	118.30
1	B	31	ASN	CB-CG-OD1	5.21	132.01	121.60
1	E	59	ASP	CB-CG-OD2	5.19	122.97	118.30
1	D	114	LEU	CA-CB-CG	5.18	127.22	115.30
1	E	26	LYS	CG-CD-CE	5.15	127.36	111.90
1	D	134	GLU	CA-CB-CG	-5.15	102.06	113.40
1	B	141	GLY	CA-C-N	5.13	128.50	117.20
1	E	109	LYS	CA-CB-CG	5.13	124.68	113.40
1	E	142	LYS	CD-CE-NZ	-5.08	100.02	111.70
1	A	31	ASN	CA-CB-CG	5.05	124.51	113.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	31	ASN	Sidechain
1	A	71	GLU	Sidechain
1	B	102	GLU	Sidechain
1	B	134	GLU	Sidechain
1	B	141	GLY	Mainchain
1	C	148	PHE	Sidechain
1	D	124	GLU	Sidechain

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	1106	0	1162	43	0
1	B	1109	0	1166	33	0
1	C	1189	0	1238	40	0
1	D	1102	0	1159	30	0
1	E	1189	0	1238	42	0
2	A	64	0	0	3	0
2	B	62	0	0	2	0
2	C	61	0	0	5	0
2	D	52	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	55	0	0	8	0
All	All	5989	0	5963	166	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 (166) 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:C:47:VAL:HG21	1:E:88:GLN:HB3	1.24	1.11
1:A:88:GLN:HB3	1:E:47:VAL:HG21	1.25	1.09
1:E:7:ILE:HG22	2:E:196:HOH:O	1.60	1.02
1:A:47:VAL:HG21	1:B:88:GLN:HB3	1.35	1.02
1:E:20:ILE:HD13	1:E:20:ILE:H	1.25	1.00
1:B:88:GLN:O	1:B:91:THR:O	1.82	0.97
1:D:20:ILE:HB	2:D:169:HOH:O	1.66	0.95
1:A:88:GLN:HB3	1:E:47:VAL:CG2	1.98	0.92
1:B:13:ALA:HB1	1:B:66:MET:HE3	1.53	0.90
1:A:7:ILE:HG12	1:A:22:ILE:HD11	1.54	0.90
1:C:20:ILE:HD13	1:C:20:ILE:H	1.38	0.89
1:C:88:GLN:O	1:C:91:THR:O	1.88	0.88
1:E:20:ILE:HD13	1:E:20:ILE:N	1.88	0.86
1:A:13:ALA:HB1	1:A:66:MET:HE3	1.58	0.85
1:C:47:VAL:HG21	1:E:88:GLN:CB	2.06	0.83
1:D:43:LYS:HE2	1:D:79:GLU:OE1	1.78	0.82
1:A:47:VAL:CG2	1:B:88:GLN:HB3	2.08	0.82
1:E:29:SER:O	1:E:32:ILE:HG13	1.79	0.81
1:B:13:ALA:HB1	1:B:66:MET:CE	2.10	0.81
1:E:91:THR:O	1:E:93:LYS:N	2.13	0.81
1:C:47:VAL:CG2	1:E:88:GLN:HB3	2.09	0.80
1:A:13:ALA:HB1	1:A:66:MET:CE	2.11	0.80
1:C:104:GLU:HB2	2:C:201:HOH:O	1.82	0.79
1:E:91:THR:O	1:E:91:THR:OG1	1.95	0.76
1:A:88:GLN:CB	1:E:47:VAL:HG21	2.10	0.75
1:B:29:SER:O	1:B:32:ILE:HG13	1.87	0.75
1:C:18:ALA:O	1:C:22:ILE:HG12	1.85	0.74
1:D:88:GLN:O	1:D:91:THR:O	2.06	0.74
1:C:149:GLU:CD	1:C:149:GLU:H	1.92	0.72
1:E:4:LYS:HE3	1:E:35:ILE:HG13	1.70	0.71
1:E:47:VAL:HG23	2:E:157:HOH:O	1.89	0.71
1:D:15:VAL:HB	1:D:66:MET:CE	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:SER:O	1:A:32:ILE:HG13	1.92	0.70
1:A:91:THR:O	1:A:93:LYS:N	2.25	0.69
1:C:66:MET:HG2	1:C:100:VAL:O	1.93	0.69
1:A:43:LYS:CE	1:A:76:CYS:SG	2.81	0.68
1:A:7:ILE:HD13	1:A:34:ILE:HG23	1.75	0.68
1:C:20:ILE:N	1:C:20:ILE:HD13	2.08	0.68
1:B:7:ILE:HD13	1:B:34:ILE:HG23	1.77	0.67
1:D:18:ALA:O	1:D:22:ILE:HG12	1.95	0.66
1:C:116:LYS:HD2	2:C:180:HOH:O	1.95	0.66
1:E:117:ARG:HG3	2:E:188:HOH:O	1.94	0.66
1:A:92:ASN:HD21	1:E:50:LYS:CE	2.09	0.66
1:D:91:THR:O	1:D:93:LYS:N	2.29	0.65
1:E:20:ILE:N	1:E:20:ILE:CD1	2.59	0.65
1:A:7:ILE:HG12	1:A:22:ILE:CD1	2.26	0.64
1:A:92:ASN:HD21	1:E:50:LYS:HE3	1.61	0.64
1:A:47:VAL:HG21	1:B:88:GLN:CB	2.22	0.64
1:E:4:LYS:HE2	1:E:56:GLU:O	1.98	0.64
1:D:20:ILE:HG13	1:D:116:LYS:HG2	1.80	0.64
1:B:105:ALA:HB1	1:B:110:GLU:HB3	1.80	0.62
1:A:43:LYS:HE3	1:A:76:CYS:SG	2.40	0.62
1:C:15:VAL:HB	1:C:66:MET:HE1	1.81	0.62
1:D:66:MET:SD	2:D:207:HOH:O	2.56	0.61
1:E:92:ASN:N	2:E:173:HOH:O	2.33	0.61
1:B:68:GLY:HA2	1:B:102:GLU:HG3	1.83	0.61
1:E:7:ILE:HD13	1:E:22:ILE:HG13	1.82	0.61
1:A:7:ILE:CG1	1:A:22:ILE:HD11	2.31	0.60
1:E:10:THR:HA	1:E:39:VAL:O	2.01	0.60
1:E:100:VAL:HG21	1:E:115:ALA:HA	1.83	0.60
1:C:20:ILE:CD1	1:C:20:ILE:H	2.04	0.59
1:B:43:LYS:HE2	1:B:76:CYS:SG	2.43	0.58
1:D:15:VAL:HB	1:D:66:MET:HE2	1.83	0.58
1:C:143:GLY:HA3	1:C:152:GLY:H	1.68	0.57
1:B:132:LYS:HD3	2:B:174:HOH:O	2.05	0.56
1:A:10:THR:HA	1:A:39:VAL:O	2.05	0.56
1:C:143:GLY:HA3	1:C:152:GLY:CA	2.35	0.56
1:C:7:ILE:HD13	1:C:22:ILE:CD1	2.35	0.56
1:C:143:GLY:HA3	1:C:152:GLY:N	2.21	0.56
1:E:4:LYS:HE3	1:E:35:ILE:CG1	2.35	0.56
1:C:100:VAL:HG21	1:C:115:ALA:HA	1.86	0.56
1:A:34:ILE:O	1:A:35:ILE:HD13	2.07	0.55
1:C:66:MET:HB3	2:C:182:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101:HIS:HB2	1:E:104:GLU:HG3	1.88	0.54
1:A:29:SER:O	1:A:32:ILE:CG1	2.54	0.54
1:A:88:GLN:CB	1:E:47:VAL:CG2	2.76	0.54
1:A:47:VAL:HG23	2:B:157:HOH:O	2.08	0.54
1:D:66:MET:HG2	1:D:100:VAL:O	2.08	0.54
1:D:10:THR:HA	1:D:39:VAL:O	2.06	0.54
1:A:24:LYS:HD2	1:A:120:GLU:HG2	1.89	0.53
1:D:47:VAL:HG23	2:D:157:HOH:O	2.08	0.53
1:D:125:ASN:ND2	2:D:167:HOH:O	2.41	0.53
1:C:10:THR:HA	1:C:39:VAL:O	2.08	0.53
1:A:14:ARG:HA	1:B:142:LYS:H	1.73	0.52
1:A:85:MET:HB3	2:A:187:HOH:O	2.09	0.51
1:C:16:ASP:O	1:C:20:ILE:HD11	2.11	0.51
1:C:51:LYS:HG2	1:E:92:ASN:HB3	1.94	0.50
1:A:4:LYS:HE2	1:A:35:ILE:HG13	1.94	0.50
1:B:9:ASP:HB3	1:B:64:LEU:HD12	1.93	0.50
1:A:88:GLN:O	1:A:91:THR:O	2.30	0.50
1:C:88:GLN:HB3	1:D:47:VAL:CG2	2.42	0.50
1:D:3:LYS:HA	2:D:172:HOH:O	2.12	0.50
1:D:15:VAL:HB	1:D:66:MET:HE1	1.94	0.50
1:B:24:LYS:HD3	1:B:120:GLU:HG2	1.93	0.49
1:A:91:THR:O	1:A:91:THR:OG1	2.23	0.49
1:B:86:LEU:HB3	1:B:90:MET:CE	2.43	0.49
1:A:7:ILE:N	1:A:7:ILE:HD12	2.28	0.49
1:D:101:HIS:HE1	2:D:161:HOH:O	1.96	0.49
1:D:7:ILE:HD13	1:D:22:ILE:HD13	1.94	0.48
1:B:8:VAL:HA	1:B:37:LYS:O	2.14	0.48
1:E:88:GLN:NE2	2:E:160:HOH:O	2.47	0.48
1:C:47:VAL:CG2	1:E:88:GLN:CB	2.81	0.48
1:E:43:LYS:HE2	1:E:76:CYS:SG	2.53	0.48
1:B:91:THR:O	1:B:93:LYS:N	2.42	0.47
1:C:15:VAL:HB	1:C:66:MET:CE	2.43	0.47
1:E:22:ILE:HG12	1:E:34:ILE:HG21	1.95	0.47
1:E:91:THR:C	2:E:173:HOH:O	2.53	0.47
1:A:13:ALA:HA	2:A:197:HOH:O	2.14	0.47
1:B:50:LYS:HE2	1:B:54:GLU:OE2	2.15	0.47
1:B:13:ALA:HB1	1:B:66:MET:HE2	1.95	0.47
1:D:20:ILE:HD13	2:D:206:HOH:O	2.14	0.46
1:D:47:VAL:CG2	2:D:157:HOH:O	2.64	0.46
1:A:68:GLY:HA2	1:A:102:GLU:HG3	1.98	0.46
1:C:92:ASN:N	2:C:179:HOH:O	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ARG:HG2	2:A:205:HOH:O	2.15	0.46
1:B:4:LYS:HE3	1:B:35:ILE:HG13	1.97	0.46
1:D:15:VAL:N	1:D:66:MET:HE1	2.31	0.46
1:E:22:ILE:O	1:E:26:LYS:HG3	2.16	0.46
1:C:6:GLY:HA3	1:C:52:LEU:HD23	1.97	0.45
1:C:15:VAL:H	1:C:66:MET:HE1	1.81	0.45
1:B:47:VAL:HG21	1:D:88:GLN:HE21	1.81	0.45
1:B:81:SER:OG	1:B:97:GLU:OE1	2.33	0.45
1:E:26:LYS:HG2	1:E:32:ILE:HD11	1.98	0.45
1:A:43:LYS:HE2	1:A:76:CYS:SG	2.56	0.45
1:E:16:ASP:O	1:E:20:ILE:HD11	2.17	0.45
1:B:32:ILE:HG13	1:B:32:ILE:H	1.61	0.45
1:A:89:LEU:O	1:E:50:LYS:HE2	2.17	0.45
1:D:15:VAL:H	1:D:66:MET:HE1	1.82	0.44
1:B:7:ILE:HG12	1:B:22:ILE:HD11	1.97	0.44
1:C:24:LYS:HD3	1:C:120:GLU:HG2	1.98	0.44
1:D:100:VAL:HG21	1:D:115:ALA:HA	1.99	0.44
1:B:29:SER:O	1:B:32:ILE:CG1	2.62	0.44
1:E:7:ILE:HD12	1:E:34:ILE:HG23	2.00	0.44
1:B:10:THR:HA	1:B:39:VAL:O	2.18	0.44
1:E:101:HIS:HE1	2:E:167:HOH:O	1.99	0.43
1:E:17:MET:O	1:E:20:ILE:HG12	2.18	0.43
1:E:105:ALA:HB1	1:E:110:GLU:HB3	1.99	0.43
1:A:104:GLU:OE1	1:A:118:ARG:NH2	2.48	0.43
1:C:88:GLN:HB3	1:D:47:VAL:HG22	2.01	0.43
1:B:39:VAL:HB	1:B:44:ASP:HB2	2.00	0.43
1:C:143:GLY:O	1:C:151:ALA:N	2.51	0.43
1:E:20:ILE:HG13	1:E:116:LYS:HG2	2.01	0.43
1:B:15:VAL:H	1:B:66:MET:HE3	1.84	0.42
1:B:43:LYS:CE	1:B:76:CYS:SG	3.07	0.42
1:A:75:VAL:O	1:A:79:GLU:HG3	2.19	0.42
1:C:92:ASN:O	1:D:51:LYS:HE2	2.19	0.42
1:C:11:THR:HB	1:E:144:LEU:HD22	2.01	0.42
1:C:132:LYS:HA	1:C:132:LYS:HD2	1.74	0.42
1:B:4:LYS:HE2	1:B:56:GLU:O	2.20	0.42
1:C:136:LEU:O	1:D:38:THR:HG21	2.20	0.42
1:D:20:ILE:H	1:D:20:ILE:HG12	1.46	0.42
1:A:69:LYS:HG3	1:A:102:GLU:HB2	2.02	0.42
1:A:22:ILE:N	1:A:22:ILE:HD13	2.35	0.42
1:A:15:VAL:HB	1:A:66:MET:SD	2.60	0.42
1:B:86:LEU:HB3	1:B:90:MET:HE3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:VAL:HG21	1:A:115:ALA:HA	2.01	0.41
1:C:22:ILE:HD12	1:C:34:ILE:HG21	2.02	0.41
1:C:47:VAL:HG23	2:E:159:HOH:O	2.20	0.41
1:C:143:GLY:HA3	1:C:152:GLY:HA2	2.01	0.41
1:C:92:ASN:HD22	1:C:92:ASN:HA	1.55	0.41
1:C:114:LEU:HD12	2:C:201:HOH:O	2.21	0.41
1:A:4:LYS:HE2	1:A:35:ILE:CG1	2.51	0.41
1:A:106:LYS:O	1:A:107:ASP:O	2.39	0.40
1:D:8:VAL:HG12	1:D:45:LEU:CD2	2.50	0.40
1:B:106:LYS:HD3	1:B:106:LYS:HA	1.87	0.40
1:D:17:MET:HB3	1:D:119:ALA:HB2	2.04	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	139/156 (89%)	132 (95%)	4 (3%)	3 (2%)	6 5
1	B	139/156 (89%)	136 (98%)	2 (1%)	1 (1%)	22 26
1	C	150/156 (96%)	144 (96%)	6 (4%)	0	100 100
1	D	138/156 (88%)	131 (95%)	5 (4%)	2 (1%)	11 11
1	E	150/156 (96%)	143 (95%)	4 (3%)	3 (2%)	7 6
All	All	716/780 (92%)	686 (96%)	21 (3%)	9 (1%)	12 12

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	ASP
1	E	92	ASN
1	D	140	ALA

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Mol	Chain	Res	Type
1	A	92	ASN
1	A	142	LYS
1	D	92	ASN
1	E	3	LYS
1	E	107	ASP
1	B	141	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	119/130 (92%)	100 (84%)	19 (16%)	2 2
1	B	120/130 (92%)	106 (88%)	14 (12%)	5 6
1	C	127/130 (98%)	116 (91%)	11 (9%)	10 12
1	D	119/130 (92%)	104 (87%)	15 (13%)	4 4
1	E	127/130 (98%)	107 (84%)	20 (16%)	2 2
All	All	612/650 (94%)	533 (87%)	79 (13%)	4 4

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ILE
1	A	24	LYS
1	A	25	LEU
1	A	31	ASN
1	A	32	ILE
1	A	33	LYS
1	A	42	ILE
1	A	52	LEU
1	A	66	MET
1	A	74	LYS
1	A	92	ASN
1	A	102	GLU
1	A	106	LYS

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Mol	Chain	Res	Type
1	A	114	LEU
1	A	116	LYS
1	A	118	ARG
1	A	130	LEU
1	A	132	LYS
1	A	142	LYS
1	B	22	ILE
1	B	25	LEU
1	B	31	ASN
1	B	47	VAL
1	B	52	LEU
1	B	103	ASP
1	B	108	ASP
1	B	109	LYS
1	B	111	LEU
1	B	114	LEU
1	B	118	ARG
1	B	130	LEU
1	B	132	LYS
1	B	142	LYS
1	C	3	LYS
1	C	20	ILE
1	C	24	LYS
1	C	25	LEU
1	C	74	LYS
1	C	92	ASN
1	C	114	LEU
1	C	118	ARG
1	C	130	LEU
1	C	132	LYS
1	C	145	ARG
1	D	20	ILE
1	D	24	LYS
1	D	25	LEU
1	D	35	ILE
1	D	47	VAL
1	D	52	LEU
1	D	86	LEU
1	D	109	LYS
1	D	111	LEU
1	D	114	LEU
1	D	116	LYS

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Mol	Chain	Res	Type
1	D	118	ARG
1	D	130	LEU
1	D	132	LYS
1	D	139	MET
1	E	2	THR
1	E	20	ILE
1	E	25	LEU
1	E	27	GLU
1	E	29	SER
1	E	32	ILE
1	E	42	ILE
1	E	52	LEU
1	E	66	MET
1	E	69	LYS
1	E	71	GLU
1	E	106	LYS
1	E	108	ASP
1	E	111	LEU
1	E	114	LEU
1	E	117	ARG
1	E	118	ARG
1	E	130	LEU
1	E	134	GLU
1	E	138	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	92	ASN
1	A	122	HIS
1	A	125	ASN
1	B	88	GLN
1	B	92	ASN
1	B	122	HIS
1	B	125	ASN
1	C	88	GLN
1	C	92	ASN
1	C	125	ASN
1	D	88	GLN
1	D	92	ASN
1	D	125	ASN

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Mol	Chain	Res	Type
1	E	88	GLN
1	E	92	ASN
1	E	101	HIS
1	E	125	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 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	141:GLY	C	142:LYS	N	1.62

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	141/156 (90%)	-0.43	1 (0%) 87 91	25, 34, 43, 46	18 (12%)
1	B	141/156 (90%)	-0.40	2 (1%) 75 80	24, 34, 41, 60	25 (17%)
1	C	152/156 (97%)	-0.44	0 100 100	25, 33, 44, 48	21 (13%)
1	D	140/156 (89%)	-0.50	1 (0%) 87 91	24, 33, 42, 69	18 (12%)
1	E	152/156 (97%)	-0.48	0 100 100	25, 34, 41, 46	16 (10%)
All	All	726/780 (93%)	-0.45	4 (0%) 89 92	24, 34, 42, 69	98 (13%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	70	ALA	2.9
1	A	12	PHE	2.7
1	B	35	ILE	2.6
1	B	12	PHE	2.5

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 carbohydrates 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.