



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:42 PM UTC

PDB ID : 2B98 / pdb_00002b98
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 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

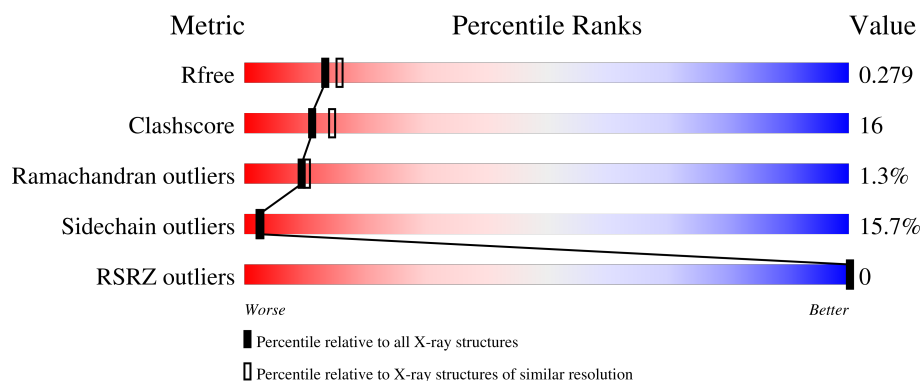
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

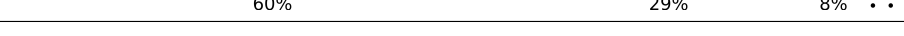
The reported resolution of this entry is 2.30 Å.

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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 $\leq 5\%$. 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	156	
1	B	156	
1	C	156	
1	D	156	
1	E	156	

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			

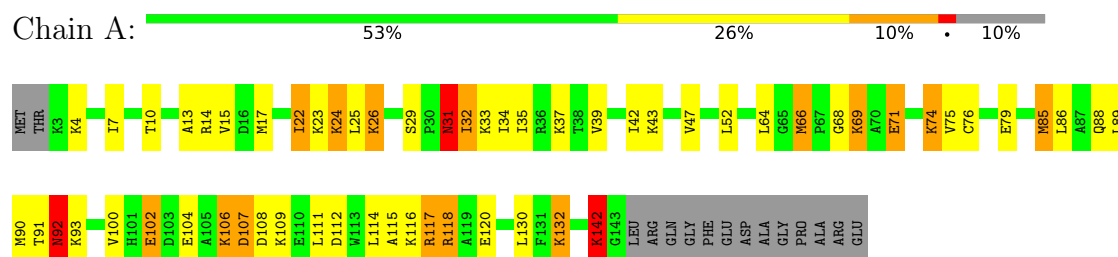
- Molecule 2 is water.

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		

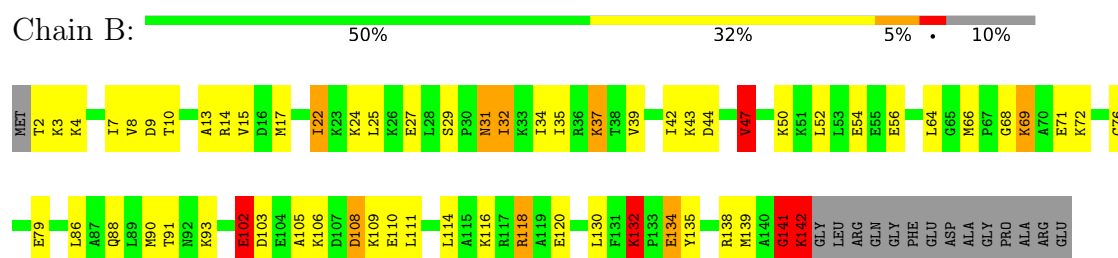
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

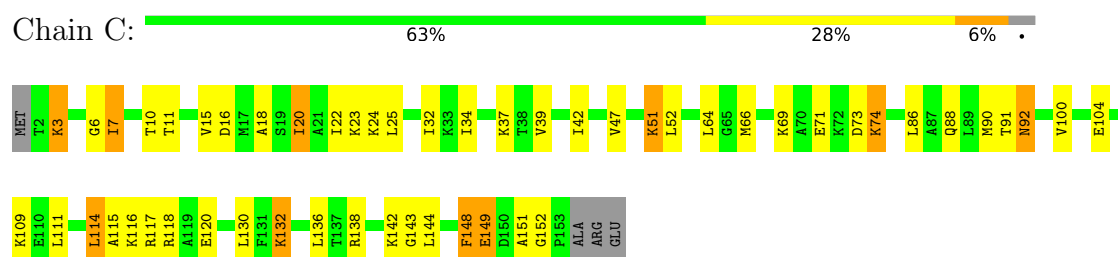
• Molecule 1: Riboflavin synthase



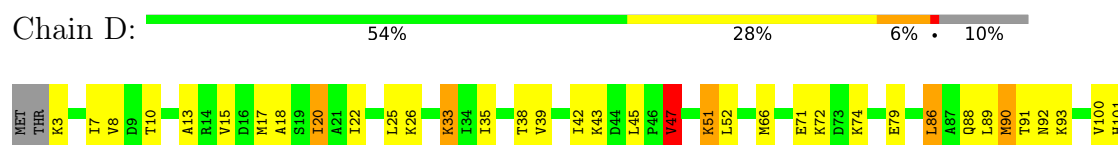
• Molecule 1: Riboflavin synthase

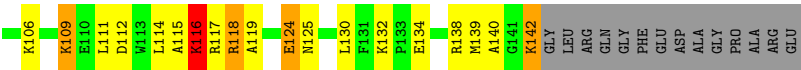


• Molecule 1: Riboflavin synthase

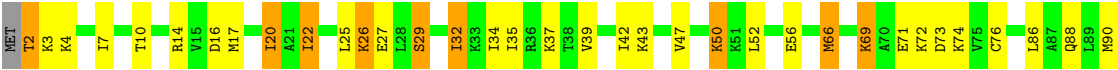


• Molecule 1: Riboflavin synthase





● Molecule 1: Riboflavin synthase



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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)	0.35 , 32.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	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	0.97	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	2.20	11/1122 (1.0%)	1.94	21/1504 (1.4%)
1	B	3.54	18/1125 (1.6%)	2.36	28/1509 (1.9%)
1	C	2.11	9/1207 (0.7%)	1.46	17/1619 (1.1%)
1	D	1.48	13/1118 (1.2%)	1.69	19/1499 (1.3%)
1	E	1.69	12/1207 (1.0%)	1.46	14/1619 (0.9%)
All	All	2.31	63/5779 (1.1%)	1.80	99/7750 (1.3%)

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	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	93.69	3.03	1.25
1	C	109	LYS	CG-CD	46.21	2.91	1.52
1	C	144	LEU	CG-CD2	43.65	2.96	1.52
1	A	132	LYS	CG-CD	42.85	2.81	1.52
1	B	134	GLU	CD-OE2	40.78	2.02	1.25
1	E	74	LYS	CD-CE	34.45	2.55	1.52
1	D	124	GLU	CG-CD	29.96	2.27	1.52
1	A	71	GLU	CG-CD	29.04	2.24	1.52
1	A	109	LYS	CD-CE	-25.80	0.75	1.52
1	E	117	ARG	CG-CD	-24.39	0.79	1.52
1	A	26	LYS	CD-CE	22.99	2.21	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	141	GLY	C-N	20.48	1.62	1.33
1	B	142	LYS	CG-CD	19.89	2.12	1.52
1	B	139	MET	CA-CB	19.45	1.81	1.53
1	B	2	THR	CA-CB	19.20	2.06	1.54
1	B	14	ARG	CB-CG	18.75	2.08	1.52
1	A	117	ARG	CG-CD	18.49	2.08	1.52
1	C	148	PHE	CB-CG	18.48	1.93	1.50
1	B	141	GLY	CA-C	18.37	1.77	1.51
1	B	135	TYR	CB-CG	18.19	1.91	1.51
1	E	2	THR	CB-CG2	17.48	2.10	1.52
1	A	69	LYS	CG-CD	13.97	1.94	1.52
1	E	14	ARG	CA-CB	-13.88	1.28	1.53
1	D	26	LYS	CD-CE	13.67	1.93	1.52
1	E	72	LYS	CA-CB	-13.61	1.31	1.53
1	C	144	LEU	CB-CG	13.60	1.80	1.53
1	D	142	LYS	CG-CD	-13.31	1.12	1.52
1	A	74	LYS	CD-CE	13.04	1.91	1.52
1	C	37	LYS	CB-CG	-12.72	1.14	1.52
1	D	116	LYS	CE-NZ	12.03	1.85	1.49
1	E	37	LYS	CG-CD	11.97	1.88	1.52
1	A	112	ASP	CB-CG	11.95	1.81	1.52
1	B	79	GLU	CA-CB	-11.78	1.35	1.53
1	D	117	ARG	CD-NE	11.23	1.61	1.46
1	A	23	LYS	CA-CB	-10.87	1.36	1.53
1	E	73	ASP	CB-CG	-10.24	1.26	1.52
1	B	102	GLU	CG-CD	10.20	1.77	1.52
1	B	69	LYS	CB-CG	10.11	1.82	1.52
1	E	138	ARG	CG-CD	9.27	1.80	1.52
1	D	118	ARG	CG-CD	9.25	1.80	1.52
1	B	27	GLU	CB-CG	-9.02	1.25	1.52
1	A	111	LEU	CA-CB	8.86	1.67	1.53
1	D	33	LYS	CG-CD	8.83	1.78	1.52
1	B	132	LYS	CD-CE	-8.62	1.26	1.52
1	D	138	ARG	CB-CG	8.49	1.77	1.52
1	E	69	LYS	CG-CD	-8.36	1.27	1.52
1	A	142	LYS	CG-CD	-8.20	1.27	1.52
1	D	74	LYS	CB-CG	-8.03	1.28	1.52
1	D	72	LYS	CB-CG	-7.86	1.28	1.52
1	D	109	LYS	CB-CG	7.64	1.75	1.52
1	C	111	LEU	CA-CB	7.53	1.65	1.53
1	B	72	LYS	CB-CG	6.67	1.72	1.52
1	E	26	LYS	CD-CE	-6.64	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	73	ASP	CA-CB	6.23	1.63	1.53
1	E	134	GLU	CB-CG	6.11	1.70	1.52
1	C	138	ARG	CG-CD	-6.08	1.34	1.52
1	B	138	ARG	CB-CG	-6.07	1.34	1.52
1	D	71	GLU	CA-CB	-5.88	1.44	1.53
1	B	71	GLU	CB-CG	-5.46	1.36	1.52
1	B	3	LYS	CG-CD	-5.39	1.36	1.52
1	E	149	GLU	CB-CG	5.35	1.68	1.52
1	C	32	ILE	CA-CB	5.34	1.59	1.54
1	D	90	MET	SD-CE	-5.07	1.66	1.79

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	141	GLY	O-C-N	-51.90	55.23	122.70
1	B	134	GLU	OE1-CD-OE2	-31.85	46.45	122.90
1	A	71	GLU	CB-CG-CD	-26.58	67.41	112.60
1	D	124	GLU	CG-CD-OE2	-25.18	60.49	118.40
1	B	142	LYS	CB-CG-CD	24.87	168.51	111.30
1	E	2	THR	OG1-CB-CG2	-22.07	65.15	109.30
1	C	148	PHE	CA-CB-CG	-21.77	92.03	113.80
1	A	71	GLU	CG-CD-OE2	-21.72	68.45	118.40
1	C	109	LYS	CB-CG-CD	-21.55	61.74	111.30
1	D	124	GLU	CB-CG-CD	-21.52	76.01	112.60
1	B	141	GLY	CA-C-N	-20.26	85.24	121.70
1	B	141	GLY	C-N-CA	-20.26	85.24	121.70
1	D	142	LYS	CB-CG-CD	18.91	154.78	111.30
1	A	109	LYS	CG-CD-CE	18.84	154.63	111.30
1	A	69	LYS	CG-CD-CE	-18.83	67.99	111.30
1	A	132	LYS	CB-CG-CD	-18.46	68.85	111.30
1	D	124	GLU	CG-CD-OE1	18.38	160.68	118.40
1	A	108	ASP	CA-CB-CG	17.74	130.34	112.60
1	B	102	GLU	CB-CG-CD	17.14	141.73	112.60
1	E	117	ARG	CB-CG-CD	15.90	147.87	111.30
1	C	109	LYS	CG-CD-CE	-15.60	75.43	111.30
1	E	117	ARG	CG-CD-NE	14.48	143.86	112.00
1	B	2	THR	N-CA-CB	14.28	135.78	111.50
1	A	117	ARG	CB-CG-CD	-14.10	78.88	111.30
1	D	118	ARG	CB-CG-CD	-12.74	82.00	111.30
1	A	71	GLU	CG-CD-OE1	12.61	147.40	118.40
1	D	112	ASP	CA-CB-CG	-11.98	100.62	112.60
1	E	69	LYS	CG-CD-CE	11.94	138.76	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ASN	CA-CB-CG	11.91	124.51	112.60
1	A	26	LYS	CG-CD-CE	-11.58	84.67	111.30
1	A	142	LYS	CB-CG-CD	-11.54	84.75	111.30
1	A	109	LYS	CD-CE-NZ	10.97	147.00	111.90
1	D	71	GLU	N-CA-CB	10.97	126.39	110.16
1	E	73	ASP	CA-CB-CG	10.82	123.42	112.60
1	A	132	LYS	CG-CD-CE	10.64	135.77	111.30
1	E	37	LYS	CB-CG-CD	-10.46	87.23	111.30
1	D	118	ARG	CG-CD-NE	10.37	134.80	112.00
1	C	3	LYS	CD-CE-NZ	10.22	144.61	111.90
1	E	138	ARG	CG-CD-NE	10.06	134.14	112.00
1	B	139	MET	N-CA-CB	-9.69	96.27	110.70
1	A	37	LYS	CB-CG-CD	-9.67	89.06	111.30
1	B	31	ASN	CA-CB-CG	9.61	122.21	112.60
1	A	31	ASN	CB-CG-ND2	-9.53	102.10	116.40
1	B	31	ASN	CB-CG-ND2	-9.44	102.25	116.40
1	C	148	PHE	CB-CG-CD1	-9.43	104.67	120.70
1	E	138	ARG	CB-CG-CD	-9.35	89.79	111.30
1	B	132	LYS	CD-CE-NZ	9.25	141.50	111.90
1	D	116	LYS	CD-CE-NZ	9.18	141.27	111.90
1	A	26	LYS	CD-CE-NZ	9.16	141.22	111.90
1	A	111	LEU	CB-CA-C	-8.62	97.34	110.88
1	B	71	GLU	CB-CG-CD	-8.51	98.14	112.60
1	B	102	GLU	CG-CD-OE2	-8.33	99.24	118.40
1	D	117	ARG	CG-CD-NE	-8.25	93.86	112.00
1	B	135	TYR	CA-CB-CG	-8.23	99.08	113.90
1	B	142	LYS	CG-CD-CE	8.19	130.14	111.30
1	C	74	LYS	CG-CD-CE	8.15	130.05	111.30
1	E	26	LYS	CD-CE-NZ	7.94	137.30	111.90
1	B	27	GLU	CA-CB-CG	7.60	129.29	114.10
1	C	3	LYS	CG-CD-CE	7.58	128.74	111.30
1	C	69	LYS	CA-CB-CG	-7.57	98.96	114.10
1	C	148	PHE	CB-CG-CD2	7.37	133.23	120.70
1	B	108	ASP	CB-CG-OD1	-7.33	101.55	118.40
1	B	108	ASP	CB-CG-OD2	7.31	135.21	118.40
1	B	108	ASP	CA-CB-CG	7.21	119.81	112.60
1	D	109	LYS	CB-CG-CD	7.18	127.81	111.30
1	A	112	ASP	CA-CB-CG	-7.16	105.44	112.60
1	E	109	LYS	CB-CG-CD	7.05	127.52	111.30
1	E	26	LYS	CG-CD-CE	6.98	127.36	111.30
1	B	118	ARG	CG-CD-NE	-6.85	96.92	112.00
1	C	71	GLU	N-CA-CB	6.70	122.22	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	91	THR	CB-CA-C	-6.67	102.61	111.82
1	D	71	GLU	CA-CB-CG	-6.60	100.91	114.10
1	C	73	ASP	CB-CA-C	-6.55	98.09	110.67
1	D	47	VAL	CB-CA-C	-6.43	103.34	112.22
1	D	117	ARG	CD-NE-CZ	-6.41	115.43	124.40
1	B	27	GLU	CB-CG-CD	6.36	123.42	112.60
1	D	134	GLU	CB-CG-CD	-6.35	101.80	112.60
1	D	33	LYS	CB-CG-CD	-6.26	96.90	111.30
1	D	106	LYS	CA-CB-CG	6.20	126.51	114.10
1	B	71	GLU	CA-CB-CG	-6.20	101.71	114.10
1	C	73	ASP	N-CA-CB	-6.07	100.88	110.28
1	D	134	GLU	CA-CB-CG	-6.02	102.06	114.10
1	E	134	GLU	CB-CG-CD	5.88	122.59	112.60
1	B	37	LYS	CB-CG-CD	-5.88	97.79	111.30
1	C	37	LYS	CA-CB-CG	5.86	125.82	114.10
1	C	142	LYS	CD-CE-NZ	-5.82	93.27	111.90
1	C	73	ASP	CA-CB-CG	-5.71	106.89	112.60
1	B	141	GLY	N-CA-C	-5.70	99.66	113.18
1	A	23	LYS	CB-CA-C	5.63	119.72	110.88
1	B	31	ASN	CB-CG-OD1	5.61	132.01	120.80
1	D	26	LYS	CG-CD-CE	-5.54	98.56	111.30
1	B	47	VAL	CB-CA-C	-5.49	104.73	112.14
1	C	3	LYS	N-CA-C	5.39	117.23	111.36
1	A	74	LYS	CG-CD-CE	5.39	123.69	111.30
1	B	139	MET	CB-CA-C	-5.39	102.05	110.94
1	A	111	LEU	N-CA-CB	5.30	117.70	110.01
1	E	109	LYS	CA-CB-CG	5.29	124.68	114.10
1	B	132	LYS	CG-CD-CE	-5.28	99.15	111.30
1	C	23	LYS	CB-CG-CD	-5.21	99.32	111.30

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 ⓘ

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	47	0
1	B	1109	0	1166	34	0
1	C	1189	0	1238	41	0
1	D	1102	0	1159	32	0
1	E	1189	0	1238	44	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
2	E	55	0	0	8	0
All	All	5989	0	5963	175	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 16.

All (175) 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:13:ALA:HB1	1:B:66:MET:HE3	1.26	1.13
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:D:15:VAL:HB	1:D:66:MET:HE1	1.35	1.04
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:B:17:MET:HE2	1:B:66:MET:HE2	1.51	0.93
1:A:88:GLN:HB3	1:E:47:VAL:CG2	1.98	0.92
1:A:7:ILE:HG12	1:A:22:ILE:HD11	1.54	0.90
1:C:20:ILE:H	1:C:20:ILE:HD13	1.38	0.89
1:C:88:GLN:O	1:C:91:THR:O	1.88	0.88
1:C:15:VAL:HB	1:C:66:MET:HE1	1.54	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	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:149:GLU:H	1:C:149:GLU:CD	1.92	0.77
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:B:13:ALA:HB1	1:B:66:MET:CE	2.10	0.74
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:B:86:LEU:HB3	1:B:90:MET:HE3	1.69	0.73
1:A:86:LEU:HB3	1:A:90:MET:HE3	1.72	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: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:HD13	1:C:20:ILE:N	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:A:92:ASN:HD21	1:E:50:LYS:CE	2.09	0.66
1:E:117:ARG:HG3	2:E:188:HOH:O	1.94	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:D:15:VAL:CB	1:D:66:MET:HE1	2.19	0.64
1:A:47:VAL:HG21	1:B:88:GLN:CB	2.22	0.64
1:D:13:ALA:HB1	1:D:66:MET:HE3	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:86:LEU:HD22	1:D:90:MET:HE2	1.82	0.60
1:E:100:VAL:HG21	1:E:115:ALA:HA	1.83	0.60
1:D:15:VAL:HB	1:D:66:MET:CE	2.21	0.59
1:C:20:ILE:H	1:C:20:ILE:CD1	2.04	0.59
1:B:43:LYS:HE2	1:B:76:CYS:SG	2.43	0.58
1:C:143:GLY:HA3	1:C:152:GLY:H	1.68	0.57
1:A:91:THR:O	1:A:91:THR:OG1	2.23	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:7:ILE:HD13	1:C:22:ILE:CD1	2.35	0.56
1:C:143:GLY:HA3	1:C:152:GLY:CA	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
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:B:15:VAL:H	1:B:66:MET:HE1	1.71	0.54
1:A:47:VAL:HG23	2:B:157:HOH:O	2.08	0.54
1:D:10:THR:HA	1:D:39:VAL:O	2.06	0.54
1:D:66:MET:HG2	1:D:100:VAL:O	2.08	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:D:17:MET:HE2	1:D:66:MET:HE2	1.92	0.52
1:E:91:THR:C	2:E:173:HOH:O	2.53	0.52
1:A:85:MET:HB3	2:A:187:HOH:O	2.09	0.51
1:C:15:VAL:CB	1:C:66:MET:HE1	2.33	0.51
1:C:16:ASP:O	1:C:20:ILE:HD11	2.11	0.51
1:C:86:LEU:HB3	1:C:90:MET:HE3	1.92	0.51
1:C:51:LYS:HG2	1:E:92:ASN:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LYS:HE2	1:A:35:ILE:HG13	1.94	0.50
1:A:17:MET:HE2	1:A:66:MET:HE2	1.93	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:B:24:LYS:HD3	1:B:120:GLU:HG2	1.93	0.49
1:A:7:ILE:HD12	1:A:7:ILE:N	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: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:E:22:ILE:HG12	1:E:34:ILE:HG21	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:17:MET:HE2	1:A:66:MET:CE	2.45	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
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:E:66:MET:HE2	1:E:100:VAL:HB	1.97	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:B:47:VAL:HG21	1:D:88:GLN:HE21	1.81	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: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:B:86:LEU:HB3	1:B:90:MET:CE	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:149:GLU:CD	1:C:149:GLU:N	2.68	0.43
1:E:86:LEU:HB3	1:E:90:MET:HE3	1.99	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: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:11:THR:HB	1:E:144:LEU:HD22	2.01	0.42
1:C:92:ASN:O	1:D:51:LYS:HE2	2.19	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:22:ILE:N	1:A:22:ILE:HD13	2.35	0.42
1:A:69:LYS:HG3	1:A:102:GLU:HB2	2.02	0.42
1:A:15:VAL:HB	1:A:66:MET:SD	2.60	0.42
1:A:100:VAL:HG21	1:A:115:ALA:HA	2.01	0.41
1:B:50:LYS:NZ	1:D:89:LEU:O	2.39	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:B:15:VAL:O	1:B:66:MET:HE1	2.20	0.41
1:C:92:ASN:HD22	1:C:92:ASN:HA	1.55	0.41
1:C:143:GLY:HA3	1:C:152:GLY:HA2	2.01	0.41
1:A:15:VAL:O	1:A:66:MET:HE1	2.21	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:HA	1:B:106:LYS:HD3	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%)	5	4
1	B	139/156 (89%)	136 (98%)	2 (1%)	1 (1%)	18	23
1	C	150/156 (96%)	144 (96%)	6 (4%)	0	100	100
1	D	138/156 (88%)	131 (95%)	5 (4%)	2 (1%)	9	9
1	E	150/156 (96%)	143 (95%)	4 (3%)	3 (2%)	6	5
All	All	716/780 (92%)	686 (96%)	21 (3%)	9 (1%)	9	10

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	ASP
1	E	92	ASN
1	D	140	ALA
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%)	97 (82%)	22 (18%)	1	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	120/130 (92%)	102 (85%)	18 (15%)	3	3
1	C	127/130 (98%)	112 (88%)	15 (12%)	5	6
1	D	119/130 (92%)	101 (85%)	18 (15%)	3	3
1	E	127/130 (98%)	104 (82%)	23 (18%)	2	2
All	All	612/650 (94%)	516 (84%)	96 (16%)	2	2

All (96) 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	26	LYS
1	A	31	ASN
1	A	32	ILE
1	A	33	LYS
1	A	42	ILE
1	A	52	LEU
1	A	64	LEU
1	A	66	MET
1	A	74	LYS
1	A	85	MET
1	A	92	ASN
1	A	102	GLU
1	A	106	LYS
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	32	ILE
1	B	42	ILE
1	B	47	VAL
1	B	52	LEU
1	B	69	LYS
1	B	103	ASP
1	B	108	ASP

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Mol	Chain	Res	Type
1	B	109	LYS
1	B	111	LEU
1	B	114	LEU
1	B	116	LYS
1	B	118	ARG
1	B	130	LEU
1	B	132	LYS
1	B	142	LYS
1	C	3	LYS
1	C	7	ILE
1	C	20	ILE
1	C	25	LEU
1	C	42	ILE
1	C	51	LYS
1	C	64	LEU
1	C	74	LYS
1	C	92	ASN
1	C	114	LEU
1	C	117	ARG
1	C	118	ARG
1	C	130	LEU
1	C	132	LYS
1	C	149	GLU
1	D	20	ILE
1	D	25	LEU
1	D	33	LYS
1	D	35	ILE
1	D	42	ILE
1	D	47	VAL
1	D	51	LYS
1	D	52	LEU
1	D	86	LEU
1	D	109	LYS
1	D	111	LEU
1	D	114	LEU
1	D	116	LYS
1	D	118	ARG
1	D	130	LEU
1	D	132	LYS
1	D	139	MET
1	D	142	LYS
1	E	2	THR

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Mol	Chain	Res	Type
1	E	20	ILE
1	E	22	ILE
1	E	25	LEU
1	E	27	GLU
1	E	29	SER
1	E	32	ILE
1	E	42	ILE
1	E	50	LYS
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	132	LYS
1	E	134	GLU
1	E	138	ARG

Sometimes 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	125	ASN
1	E	31	ASN
1	E	88	GLN
1	E	92	ASN

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Mol	Chain	Res	Type
1	E	101	HIS
1	E	125	ASN

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 oligosaccharides 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](#)

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 [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	141/156 (90%)	-1.59	0 100 100	15, 31, 42, 46	18 (12%)
1	B	141/156 (90%)	-1.58	0 100 100	14, 30, 40, 43	25 (17%)
1	C	152/156 (97%)	-1.60	0 100 100	16, 31, 42, 48	21 (13%)
1	D	140/156 (89%)	-1.60	0 100 100	15, 31, 42, 46	18 (12%)
1	E	152/156 (97%)	-1.61	0 100 100	13, 32, 40, 46	16 (10%)
All	All	726/780 (93%)	-1.60	0 100 100	13, 31, 41, 48	98 (13%)

There are no RSRZ outliers to report.

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 oligosaccharides 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.