



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:41 AM UTC

PDB ID : 5WRF / pdb_00005wrf
Title : Crystal structure of dodecameric type II dehydroquinase dehydratase from *Acinetobacter baumannii* with unexplained connecting electron density between free cysteine residues of molecular pairs
Authors : Iqbal, N.; Singh, P.K.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2016-12-01
Resolution : 2.51 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

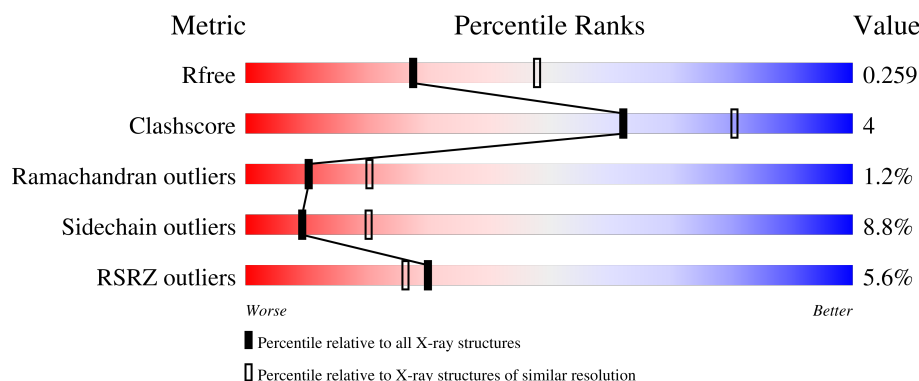
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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.



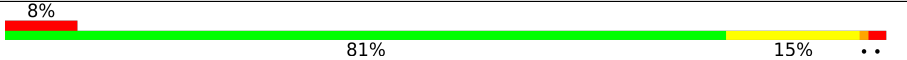
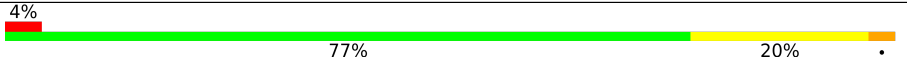
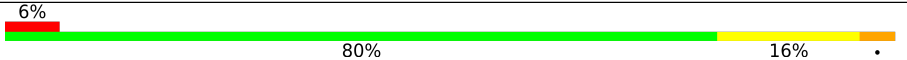
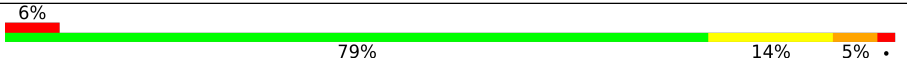
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	145	6% 86% 8% 5% .
1	B	145	6% 81% 11% 6% .
1	C	145	4% 85% 12% . .
1	D	145	9% 81% 14% . .
1	E	145	5% 79% 18% . .

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Mol	Chain	Length	Quality of chain
1	F	145	
1	G	145	
1	H	145	
1	I	145	
1	J	145	
1	K	145	
1	L	145	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13645 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 3-dehydroquinate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	B	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	C	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	D	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	E	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	F	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	G	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	H	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	I	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	J	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	K	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	L	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total	O	0	0
			34	34		
3	B	23	Total	O	0	0
			23	23		
3	C	27	Total	O	0	0
			27	27		
3	D	17	Total	O	0	0
			17	17		
3	E	16	Total	O	0	0
			16	16		
3	F	19	Total	O	0	0
			19	19		
3	G	11	Total	O	0	0
			11	11		
3	H	9	Total	O	0	0
			9	9		
3	I	6	Total	O	0	0
			6	6		
3	J	17	Total	O	0	0
			17	17		
3	K	14	Total	O	0	0
			14	14		

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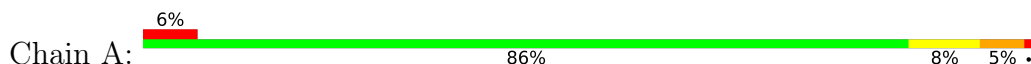
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	8	Total	O	0	0
			8	8		

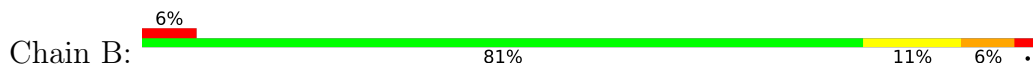
3 Residue-property plots [i](#)

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.

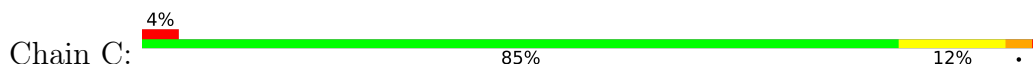
- Molecule 1: 3-dehydroquinase dehydratase



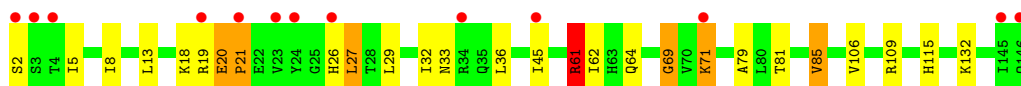
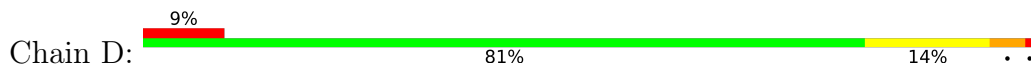
- Molecule 1: 3-dehydroquinase dehydratase



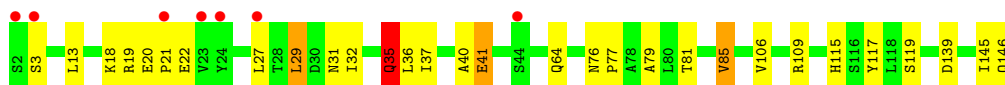
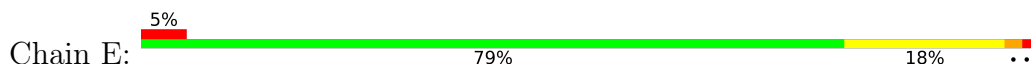
- Molecule 1: 3-dehydroquinase dehydratase



- Molecule 1: 3-dehydroquinase dehydratase

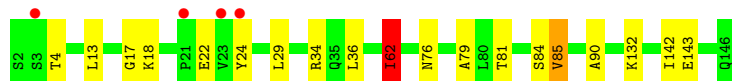


- Molecule 1: 3-dehydroquinase dehydratase



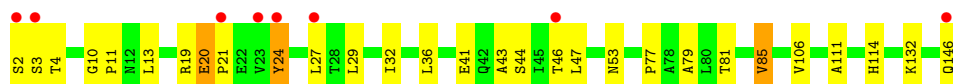
- Molecule 1: 3-dehydroquinase dehydratase

Chain F:  3% 87% 12% ..



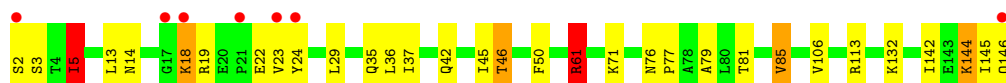
• Molecule 1: 3-dehydroquinase dehydratase

Chain G:  6% 80% 18% .



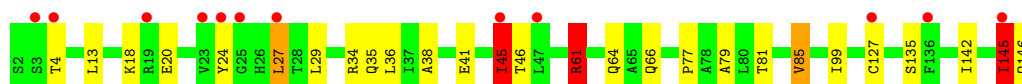
• Molecule 1: 3-dehydroquinase dehydratase

Chain H:  5% 78% 18% ..



• Molecule 1: 3-dehydroquinase dehydratase

Chain I:  8% 81% 15% ..



• Molecule 1: 3-dehydroquinase dehydratase

Chain J:  4% 77% 20% .



• Molecule 1: 3-dehydroquinase dehydratase

Chain K:  6% 80% 16% .



• Molecule 1: 3-dehydroquinase dehydratase

Chain L:  6% 79% 14% 5% .



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	97.80Å 135.75Å 142.74Å 90.00° 97.53° 90.00°	Depositor
Resolution (Å)	37.75 – 2.51 37.75 – 2.51	Depositor EDS
% Data completeness (in resolution range)	94.7 (37.75-2.51) 94.7 (37.75-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.209 , 0.256 0.213 , 0.259	Depositor DCC
R_{free} test set	1159 reflections (1.84%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13645	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO

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	1.20	0/1141	1.20	5/1551 (0.3%)
1	B	1.21	1/1141 (0.1%)	1.34	10/1551 (0.6%)
1	C	1.25	6/1141 (0.5%)	1.22	2/1551 (0.1%)
1	D	1.37	4/1141 (0.4%)	1.33	5/1551 (0.3%)
1	E	1.28	3/1141 (0.3%)	1.23	6/1551 (0.4%)
1	F	1.25	2/1141 (0.2%)	1.23	5/1551 (0.3%)
1	G	1.28	4/1141 (0.4%)	1.20	3/1551 (0.2%)
1	H	1.25	2/1141 (0.2%)	1.31	10/1551 (0.6%)
1	I	1.40	6/1141 (0.5%)	1.37	4/1551 (0.3%)
1	J	1.35	7/1141 (0.6%)	1.39	7/1551 (0.5%)
1	K	1.38	8/1141 (0.7%)	1.29	5/1551 (0.3%)
1	L	1.43	6/1141 (0.5%)	1.42	14/1551 (0.9%)
All	All	1.31	49/13692 (0.4%)	1.30	76/18612 (0.4%)

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	2
1	D	0	2
1	E	0	1
1	G	0	2
1	H	0	3
1	J	0	1
1	K	0	1
1	L	0	1
All	All	0	13

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	30	ASP	C-O	-10.07	1.12	1.24
1	I	145	ILE	CA-C	8.46	1.63	1.52
1	J	65	ALA	C-O	-8.42	1.13	1.24
1	K	25	GLY	N-CA	7.30	1.54	1.44
1	E	64	GLN	C-O	-7.12	1.15	1.24
1	G	41	GLU	C-O	-6.42	1.16	1.24
1	I	61	ARG	C-O	-6.39	1.16	1.24
1	C	4	THR	C-O	-6.24	1.16	1.24
1	H	35	GLN	C-O	-6.21	1.16	1.24
1	C	20	GLU	N-CA	6.18	1.52	1.46
1	D	45	ILE	C-O	-6.18	1.18	1.24
1	K	5	ILE	N-CA	6.15	1.53	1.46
1	K	5	ILE	C-O	-6.09	1.18	1.24
1	D	5	ILE	C-O	-6.09	1.17	1.24
1	L	16	LEU	CA-C	6.07	1.60	1.52
1	D	33	ASN	C-O	-6.03	1.17	1.24
1	C	145	ILE	CA-C	6.00	1.58	1.52
1	F	143	GLU	N-CA	5.98	1.53	1.46
1	F	24	TYR	CA-C	5.83	1.60	1.52
1	J	32	ILE	C-O	5.80	1.30	1.24
1	I	45	ILE	C-O	5.78	1.30	1.24
1	E	35	GLN	C-O	-5.71	1.17	1.24
1	E	3	SER	N-CA	5.62	1.53	1.46
1	L	137	ALA	C-O	-5.61	1.17	1.24
1	I	99	ILE	C-O	-5.60	1.18	1.24
1	H	142	ILE	C-O	-5.56	1.18	1.24
1	G	24	TYR	C-O	-5.49	1.17	1.24
1	J	142	ILE	C-O	-5.48	1.18	1.24
1	I	64	GLN	C-O	-5.42	1.17	1.24
1	K	144	LYS	C-O	-5.41	1.17	1.24
1	K	113	ARG	C-O	-5.39	1.17	1.24
1	L	59	VAL	C-O	-5.39	1.18	1.24
1	L	85	VAL	C-O	-5.37	1.17	1.24
1	D	69	GLY	C-O	-5.35	1.18	1.24
1	C	67	THR	CA-CB	5.32	1.62	1.53
1	J	45	ILE	C-O	-5.31	1.18	1.24
1	K	20	GLU	N-CA	5.30	1.51	1.46
1	I	135	SER	N-CA	5.30	1.52	1.46
1	L	4	THR	CA-C	5.29	1.59	1.52
1	C	137	ALA	C-O	-5.28	1.18	1.24
1	G	43	ALA	C-O	5.19	1.30	1.24
1	J	41	GLU	N-CA	5.19	1.52	1.46
1	G	32	ILE	C-O	-5.13	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	19	ARG	N-CA	5.13	1.52	1.46
1	C	136	PHE	C-O	-5.13	1.18	1.24
1	K	23	VAL	N-CA	5.09	1.52	1.46
1	J	29	LEU	C-O	-5.07	1.18	1.24
1	L	16	LEU	N-CA	5.05	1.52	1.46
1	J	3	SER	CA-C	5.01	1.59	1.52

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	ILE	CB-CA-C	15.29	136.36	111.29
1	B	146	GLN	N-CA-CB	14.23	134.69	110.50
1	F	62	ILE	CB-CA-C	8.96	124.24	112.14
1	J	113	ARG	CG-CD-NE	-8.89	92.44	112.00
1	B	106	VAL	O-C-N	8.28	134.47	122.04
1	L	81	THR	CB-CA-C	-8.01	97.49	110.79
1	K	109	ARG	CG-CD-NE	7.93	129.46	112.00
1	H	24	TYR	N-CA-C	-7.62	98.72	109.69
1	I	64	GLN	CB-CG-CD	7.09	124.65	112.60
1	L	142	ILE	CA-CB-CG1	7.04	122.37	110.40
1	H	3	SER	N-CA-C	6.87	120.38	108.76
1	L	109	ARG	CG-CD-NE	6.74	126.83	112.00
1	J	34	ARG	CA-CB-CG	6.65	127.40	114.10
1	H	23	VAL	N-CA-C	-6.63	105.86	111.56
1	H	145	ILE	N-CA-C	6.59	117.58	111.45
1	E	41	GLU	CA-CB-CG	6.39	126.88	114.10
1	H	61	ARG	NE-CZ-NH1	-6.37	115.14	121.50
1	L	110	GLU	CG-CD-OE1	-6.33	103.84	118.40
1	J	113	ARG	NE-CZ-NH1	-6.21	115.29	121.50
1	C	61	ARG	CG-CD-NE	6.13	125.50	112.00
1	J	65	ALA	N-CA-CB	6.11	120.82	110.49
1	L	45	ILE	CG1-CB-CG2	-6.07	92.49	110.70
1	K	109	ARG	NE-CZ-NH1	-6.07	115.43	121.50
1	F	62	ILE	N-CA-CB	6.03	118.73	110.54
1	F	142	ILE	CA-CB-CG1	5.99	120.59	110.40
1	B	106	VAL	CA-C-N	-5.98	109.34	121.18
1	B	106	VAL	C-N-CA	-5.98	109.34	121.18
1	I	66	GLN	N-CA-CB	5.95	118.87	110.12
1	L	4	THR	CA-C-O	5.92	127.41	120.96
1	I	61	ARG	CG-CD-NE	5.89	124.97	112.00
1	A	21	PRO	CB-CA-C	-5.76	102.74	111.44
1	K	109	ARG	NE-CZ-NH2	5.75	124.38	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	5	ILE	CG1-CB-CG2	-5.71	93.58	110.70
1	L	142	ILE	CA-C-O	-5.70	115.19	121.29
1	F	81	THR	CB-CA-C	-5.68	101.03	110.68
1	L	84	SER	N-CA-C	5.67	118.29	107.75
1	A	20	GLU	N-CA-C	5.65	122.29	109.81
1	B	143	GLU	CB-CG-CD	5.62	122.16	112.60
1	D	81	THR	CB-CA-C	-5.61	101.14	110.68
1	H	23	VAL	CB-CA-C	5.61	116.77	111.44
1	K	20	GLU	N-CA-C	5.59	119.85	112.35
1	E	20	GLU	N-CA-C	5.58	120.09	112.55
1	D	85	VAL	CA-CB-CG2	5.58	119.89	110.40
1	H	5	ILE	CA-CB-CG1	5.54	119.81	110.40
1	J	18	LYS	N-CA-C	5.54	119.78	111.81
1	E	29	LEU	O-C-N	5.48	127.93	122.12
1	D	61	ARG	CG-CD-NE	5.46	124.01	112.00
1	L	110	GLU	CG-CD-OE2	5.46	130.96	118.40
1	B	105	ASN	O-C-N	-5.45	116.31	123.02
1	E	64	GLN	CB-CG-CD	-5.38	103.45	112.60
1	K	81	THR	CB-CA-C	-5.34	101.93	110.79
1	L	144	LYS	CD-CE-NZ	5.33	128.96	111.90
1	B	2	SER	N-CA-CB	5.31	119.53	110.50
1	L	110	GLU	CB-CA-C	5.31	119.31	109.54
1	H	144	LYS	CD-CE-NZ	5.28	128.81	111.90
1	A	3	SER	N-CA-C	5.28	117.12	108.52
1	H	46	THR	N-CA-CB	5.24	118.26	110.29
1	L	16	LEU	CA-CB-CG	5.21	134.55	116.30
1	C	3	SER	N-CA-C	5.20	117.00	108.52
1	B	68	GLU	CB-CA-C	5.20	119.37	110.01
1	J	61	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	D	61	ARG	CA-C-O	5.20	125.97	120.10
1	I	34	ARG	CB-CG-CD	5.17	123.18	111.30
1	B	5	ILE	CB-CA-C	-5.13	103.74	110.98
1	G	10	GLY	CA-C-N	5.10	125.09	119.89
1	G	10	GLY	C-N-CA	5.10	125.09	119.89
1	E	119	SER	N-CA-C	5.10	117.50	111.33
1	D	64	GLN	CG-CD-NE2	-5.07	108.80	116.40
1	J	88	ARG	NE-CZ-NH2	5.06	123.76	119.20
1	A	127	CYS	CA-CB-SG	5.05	126.02	114.40
1	E	40	ALA	O-C-N	5.03	127.89	122.15
1	L	31	ASN	N-CA-C	5.02	116.76	111.28
1	L	85	VAL	CB-CA-C	5.02	120.40	112.26
1	F	84	SER	N-CA-C	5.02	117.09	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	ILE	CA-CB-CG1	5.01	118.92	110.40
1	G	20	GLU	CG-CD-OE1	5.00	129.91	118.40

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	105	ASN	Mainchain
1	B	18	LYS	Peptide
1	D	61	ARG	Sidechain
1	D	69	GLY	Peptide
1	E	19	ARG	Peptide
1	G	3	SER	Peptide
1	G	47	LEU	Mainchain
1	H	19	ARG	Peptide
1	H	2	SER	Peptide
1	H	22	GLU	Peptide
1	J	22	GLU	Peptide
1	K	23	VAL	Peptide
1	L	15	LEU	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	1120	0	1131	15	0
1	B	1120	0	1131	18	0
1	C	1120	0	1131	7	0
1	D	1120	0	1131	9	0
1	E	1120	0	1131	10	0
1	F	1120	0	1131	6	0
1	G	1120	0	1131	7	0
1	H	1120	0	1131	11	0
1	I	1120	0	1131	11	0
1	J	1120	0	1131	11	0
1	K	1120	0	1131	11	0
1	L	1120	0	1131	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	4	0	6	0	0
3	A	34	0	0	0	0
3	B	23	0	0	0	0
3	C	27	0	0	1	0
3	D	17	0	0	1	0
3	E	16	0	0	0	0
3	F	19	0	0	0	0
3	G	11	0	0	0	0
3	H	9	0	0	0	0
3	I	6	0	0	1	0
3	J	17	0	0	0	0
3	K	14	0	0	0	0
3	L	8	0	0	0	0
All	All	13645	0	13578	112	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 4.

All (112) 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:I:79:ALA:HB1	1:J:85:VAL:HG13	1.50	0.90
1:L:16:LEU:HG	1:L:28:THR:HB	1.61	0.82
1:L:16:LEU:HD12	1:L:29:LEU:HB2	1.61	0.82
1:F:62:ILE:C	1:F:62:ILE:HD13	2.12	0.74
1:L:14:ASN:O	1:L:16:LEU:HD13	1.89	0.72
1:B:3:SER:HB2	1:B:48:ASP:HB2	1.72	0.71
1:F:79:ALA:HB1	1:G:85:VAL:HG22	1.78	0.66
1:D:79:ALA:HB1	1:H:85:VAL:HG22	1.76	0.66
1:I:85:VAL:HG22	1:K:79:ALA:HB1	1.77	0.65
1:I:77:PRO:HG2	1:I:81:THR:HB	1.78	0.65
1:A:20:GLU:HB2	1:A:21:PRO:HD2	1.77	0.64
1:C:77:PRO:HG2	1:C:81:THR:HB	1.79	0.64
1:K:145:ILE:O	1:K:145:ILE:HG22	1.98	0.64
1:H:5:ILE:HD13	1:H:45:ILE:HG21	1.80	0.64
1:A:85:VAL:HG22	1:C:79:ALA:HB1	1.80	0.63
1:D:20:GLU:HB2	1:D:21:PRO:CD	2.30	0.62
1:E:77:PRO:HG2	1:E:81:THR:HB	1.82	0.62
1:J:79:ALA:HB1	1:K:85:VAL:HG22	1.82	0.62
1:A:29:LEU:HD21	1:A:51:GLN:HG3	1.81	0.62
1:A:20:GLU:CB	1:A:21:PRO:HD2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:77:PRO:HG2	1:J:81:THR:HB	1.82	0.61
1:J:33:ASN:O	1:J:37:ILE:HG13	1.99	0.61
1:I:45:ILE:HD11	1:I:145:ILE:HD11	1.82	0.61
1:B:19:ARG:HB3	1:B:22:GLU:CG	2.33	0.59
1:A:79:ALA:HB1	1:B:85:VAL:HG22	1.85	0.59
1:B:77:PRO:HG2	1:B:81:THR:HB	1.84	0.58
1:G:77:PRO:HG2	1:G:81:THR:HB	1.86	0.58
1:H:77:PRO:HG2	1:H:81:THR:HB	1.85	0.58
1:B:79:ALA:HB1	1:C:85:VAL:HG22	1.86	0.57
1:D:20:GLU:HB2	1:D:21:PRO:HD2	1.86	0.57
1:A:77:PRO:HG2	1:A:81:THR:HB	1.86	0.57
1:B:4:THR:HB	1:B:46:THR:OG1	2.05	0.57
1:E:37:ILE:O	1:E:41:GLU:HG2	2.05	0.57
1:E:85:VAL:HG22	1:G:79:ALA:HB1	1.87	0.56
1:I:61:ARG:HG2	1:I:61:ARG:HH11	1.71	0.55
1:B:20:GLU:HB3	1:B:21:PRO:CD	2.37	0.55
1:G:132:LYS:HZ2	1:J:143:GLU:HG3	1.72	0.55
1:L:18:LYS:HE2	1:L:18:LYS:HA	1.90	0.54
1:D:8:ILE:HD11	1:D:62:ILE:HG22	1.88	0.54
1:G:11:PRO:HA	1:G:53:ASN:HD22	1.71	0.54
1:I:27:LEU:HD12	1:I:27:LEU:O	2.08	0.53
1:L:45:ILE:HD12	1:L:142:ILE:HD12	1.90	0.53
1:H:79:ALA:HB1	1:L:85:VAL:HG22	1.91	0.53
1:L:132:LYS:HG2	1:L:136:PHE:CZ	2.44	0.52
1:J:76:ASN:HD22	1:J:76:ASN:C	2.17	0.52
1:B:3:SER:CB	1:B:48:ASP:HB2	2.38	0.52
1:F:62:ILE:HD12	1:F:90:ALA:HB1	1.92	0.51
1:J:106:VAL:HG13	1:J:107:HIS:HD2	1.76	0.50
1:H:50:PHE:CE2	1:H:61:ARG:HG3	2.46	0.50
1:B:4:THR:HB	1:B:46:THR:O	2.11	0.50
1:H:18:LYS:CE	1:H:18:LYS:HA	2.42	0.50
1:E:79:ALA:HB1	1:F:85:VAL:HG22	1.93	0.50
1:K:77:PRO:HG3	1:K:118:LEU:HD12	1.93	0.49
1:I:35:GLN:HG2	3:I:203:HOH:O	2.13	0.49
1:L:16:LEU:HD12	1:L:29:LEU:CB	2.39	0.49
1:A:20:GLU:HB2	1:A:21:PRO:CD	2.40	0.49
1:B:29:LEU:CD2	1:B:51:GLN:HG3	2.43	0.49
1:B:18:LYS:C	1:B:19:ARG:HG2	2.37	0.49
1:B:18:LYS:HD2	1:C:66:GLN:OE1	2.13	0.49
1:L:4:THR:HG23	1:L:70:VAL:HA	1.96	0.48
1:E:115:HIS:HE1	1:E:117:TYR:CE2	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:45:ILE:HD11	1:I:145:ILE:CD1	2.42	0.48
1:D:8:ILE:CD1	1:D:62:ILE:CG2	2.93	0.47
1:G:132:LYS:NZ	1:J:143:GLU:HG3	2.29	0.47
1:K:4:THR:O	1:K:5:ILE:HG23	2.15	0.47
1:B:145:ILE:O	1:B:146:GLN:HG3	2.15	0.47
1:A:145:ILE:O	1:A:146:GLN:C	2.57	0.47
1:L:110:GLU:HG3	1:L:112:PHE:CE2	2.50	0.47
1:L:76:ASN:C	1:L:76:ASN:HD22	2.23	0.47
1:E:76:ASN:C	1:E:76:ASN:HD22	2.22	0.46
1:H:76:ASN:C	1:H:76:ASN:HD22	2.23	0.46
1:K:5:ILE:HG13	1:K:47:LEU:HD12	1.97	0.46
1:D:115:HIS:HB2	3:D:214:HOH:O	2.16	0.46
1:F:17:GLY:C	1:F:18:LYS:HD2	2.40	0.46
1:B:4:THR:HG22	1:B:5:ILE:N	2.30	0.46
1:A:29:LEU:CD2	1:A:51:GLN:HG3	2.46	0.45
1:A:106:VAL:HG23	1:A:107:HIS:HD2	1.81	0.45
1:K:16:LEU:HD23	1:K:24:TYR:CE1	2.51	0.45
1:E:27:LEU:HD12	1:E:31:ASN:HD22	1.82	0.45
1:B:142:ILE:O	1:B:146:GLN:N	2.48	0.45
1:A:20:GLU:CB	1:A:21:PRO:CD	2.94	0.45
1:A:146:GLN:HE21	1:A:146:GLN:HA	1.82	0.44
1:K:76:ASN:C	1:K:76:ASN:HD22	2.24	0.44
1:H:18:LYS:HA	1:H:18:LYS:HE3	1.99	0.44
1:C:145:ILE:CG2	1:C:146:GLN:N	2.81	0.43
1:B:21:PRO:HA	1:B:24:TYR:O	2.18	0.43
1:F:76:ASN:HD22	1:F:76:ASN:C	2.25	0.43
1:E:139:ASP:OD1	1:H:132:LYS:HE3	2.19	0.43
1:K:4:THR:O	1:K:5:ILE:CG2	2.67	0.43
1:A:34:ARG:O	1:A:34:ARG:HD2	2.19	0.43
1:K:2:SER:O	1:K:3:SER:CB	2.67	0.42
1:D:27:LEU:HD11	1:D:32:ILE:HG13	2.01	0.42
1:A:146:GLN:NE2	1:A:146:GLN:CA	2.82	0.42
1:D:20:GLU:CB	1:D:21:PRO:CD	2.98	0.42
1:G:111:ALA:HA	1:G:114:HIS:CE1	2.55	0.42
1:E:145:ILE:O	1:E:146:GLN:HB3	2.20	0.42
1:J:19:ARG:CG	1:J:23:VAL:HG22	2.50	0.42
1:A:13:LEU:C	1:A:29:LEU:HD22	2.45	0.42
1:D:2:SER:HB3	1:D:71:LYS:HG2	2.01	0.41
1:B:4:THR:CB	1:B:46:THR:OG1	2.66	0.41
1:H:50:PHE:CD2	1:H:61:ARG:HG3	2.55	0.41
1:J:145:ILE:O	1:J:146:GLN:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:4:THR:HA	1:I:46:THR:HG23	2.02	0.41
1:J:106:VAL:HG22	1:J:113:ARG:HB3	2.03	0.41
1:B:143:GLU:CD	1:K:132:LYS:HE2	2.46	0.41
1:C:20:GLU:O	1:C:22:GLU:N	2.54	0.41
1:C:118:LEU:HD13	3:C:202:HOH:O	2.19	0.41
1:I:45:ILE:HD12	1:I:142:ILE:HG12	2.02	0.41
1:H:106:VAL:HG12	1:H:113:ARG:HB3	2.02	0.41
1:I:38:ALA:HA	1:I:41:GLU:HG2	2.04	0.41
1:E:32:ILE:O	1:E:35:GLN:HG3	2.20	0.40
1:L:80:LEU:HD12	1:L:80:LEU:HA	1.85	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	143/145 (99%)	136 (95%)	5 (4%)	2 (1%)	9	17
1	B	143/145 (99%)	133 (93%)	8 (6%)	2 (1%)	9	17
1	C	143/145 (99%)	138 (96%)	5 (4%)	0	100	100
1	D	143/145 (99%)	134 (94%)	6 (4%)	3 (2%)	5	9
1	E	143/145 (99%)	134 (94%)	7 (5%)	2 (1%)	9	17
1	F	143/145 (99%)	134 (94%)	7 (5%)	2 (1%)	9	17
1	G	143/145 (99%)	131 (92%)	9 (6%)	3 (2%)	5	9
1	H	143/145 (99%)	133 (93%)	10 (7%)	0	100	100
1	I	143/145 (99%)	133 (93%)	9 (6%)	1 (1%)	18	34
1	J	143/145 (99%)	132 (92%)	8 (6%)	3 (2%)	5	9
1	K	143/145 (99%)	134 (94%)	7 (5%)	2 (1%)	9	17
1	L	143/145 (99%)	135 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1716/1740 (99%)	1607 (94%)	89 (5%)	20 (1%)	10	20

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	20	GLU
1	D	20	GLU
1	D	26	HIS
1	F	4	THR
1	K	21	PRO
1	A	24	TYR
1	D	21	PRO
1	F	22	GLU
1	G	24	TYR
1	J	19	ARG
1	E	22	GLU
1	K	3	SER
1	A	19	ARG
1	G	19	ARG
1	G	21	PRO
1	J	26	HIS
1	B	21	PRO
1	E	21	PRO
1	I	145	ILE
1	J	21	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	119/119 (100%)	111 (93%)	8 (7%)	15	31
1	B	119/119 (100%)	109 (92%)	10 (8%)	10	22
1	C	119/119 (100%)	109 (92%)	10 (8%)	10	22
1	D	119/119 (100%)	107 (90%)	12 (10%)	7	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	119/119 (100%)	111 (93%)	8 (7%)	15	31
1	F	119/119 (100%)	112 (94%)	7 (6%)	18	37
1	G	119/119 (100%)	107 (90%)	12 (10%)	7	15
1	H	119/119 (100%)	105 (88%)	14 (12%)	5	11
1	I	119/119 (100%)	106 (89%)	13 (11%)	6	13
1	J	119/119 (100%)	111 (93%)	8 (7%)	15	31
1	K	119/119 (100%)	110 (92%)	9 (8%)	12	26
1	L	119/119 (100%)	105 (88%)	14 (12%)	5	11
All	All	1428/1428 (100%)	1303 (91%)	125 (9%)	9	20

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLU
1	A	22	GLU
1	A	24	TYR
1	A	29	LEU
1	A	85	VAL
1	A	127	CYS
1	A	145	ILE
1	A	146	GLN
1	B	2	SER
1	B	4	THR
1	B	5	ILE
1	B	18	LYS
1	B	19	ARG
1	B	36	LEU
1	B	42	GLN
1	B	85	VAL
1	B	132	LYS
1	B	146	GLN
1	C	2	SER
1	C	13	LEU
1	C	24	TYR
1	C	29	LEU
1	C	34	ARG
1	C	36	LEU
1	C	61	ARG
1	C	67	THR

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Mol	Chain	Res	Type
1	C	85	VAL
1	C	145	ILE
1	D	13	LEU
1	D	18	LYS
1	D	19	ARG
1	D	27	LEU
1	D	29	LEU
1	D	36	LEU
1	D	61	ARG
1	D	71	LYS
1	D	85	VAL
1	D	106	VAL
1	D	109	ARG
1	D	132	LYS
1	E	13	LEU
1	E	18	LYS
1	E	29	LEU
1	E	35	GLN
1	E	36	LEU
1	E	85	VAL
1	E	106	VAL
1	E	109	ARG
1	F	13	LEU
1	F	29	LEU
1	F	34	ARG
1	F	36	LEU
1	F	62	ILE
1	F	85	VAL
1	F	132	LYS
1	G	2	SER
1	G	4	THR
1	G	13	LEU
1	G	20	GLU
1	G	27	LEU
1	G	29	LEU
1	G	36	LEU
1	G	44	SER
1	G	46	THR
1	G	85	VAL
1	G	106	VAL
1	G	146	GLN
1	H	5	ILE

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Mol	Chain	Res	Type
1	H	13	LEU
1	H	14	ASN
1	H	18	LYS
1	H	29	LEU
1	H	36	LEU
1	H	37	ILE
1	H	42	GLN
1	H	46	THR
1	H	61	ARG
1	H	71	LYS
1	H	85	VAL
1	H	144	LYS
1	H	146	GLN
1	I	13	LEU
1	I	18	LYS
1	I	20	GLU
1	I	24	TYR
1	I	27	LEU
1	I	29	LEU
1	I	36	LEU
1	I	45	ILE
1	I	61	ARG
1	I	85	VAL
1	I	127	CYS
1	I	145	ILE
1	I	146	GLN
1	J	4	THR
1	J	13	LEU
1	J	20	GLU
1	J	29	LEU
1	J	35	GLN
1	J	36	LEU
1	J	37	ILE
1	J	76	ASN
1	K	4	THR
1	K	13	LEU
1	K	26	HIS
1	K	29	LEU
1	K	36	LEU
1	K	61	ARG
1	K	85	VAL
1	K	106	VAL

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Mol	Chain	Res	Type
1	K	144	LYS
1	L	2	SER
1	L	13	LEU
1	L	14	ASN
1	L	27	LEU
1	L	29	LEU
1	L	30	ASP
1	L	35	GLN
1	L	36	LEU
1	L	45	ILE
1	L	61	ARG
1	L	80	LEU
1	L	85	VAL
1	L	110	GLU
1	L	132	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	HIS
1	A	114	HIS
1	A	146	GLN
1	B	35	GLN
1	B	64	GLN
1	B	146	GLN
1	C	14	ASN
1	C	114	HIS
1	C	146	GLN
1	D	12	ASN
1	D	35	GLN
1	D	114	HIS
1	E	31	ASN
1	E	35	GLN
1	E	39	GLN
1	E	76	ASN
1	E	115	HIS
1	E	146	GLN
1	F	35	GLN
1	F	76	ASN
1	G	26	HIS
1	G	35	GLN
1	G	53	ASN

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Mol	Chain	Res	Type
1	G	64	GLN
1	G	114	HIS
1	G	146	GLN
1	H	14	ASN
1	H	76	ASN
1	H	114	HIS
1	H	146	GLN
1	I	76	ASN
1	I	114	HIS
1	J	31	ASN
1	J	76	ASN
1	J	107	HIS
1	K	76	ASN
1	L	14	ASN
1	L	35	GLN
1	L	64	GLN
1	L	76	ASN
1	L	114	HIS

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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	EDO	A	201	-	3,3,3	0.48	0	2,2,2	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	201	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	145/145 (100%)	-0.02	8 (5%)	30	27	23, 34, 82, 108	0
1	B	145/145 (100%)	0.11	9 (6%)	26	23	24, 38, 82, 132	0
1	C	145/145 (100%)	-0.06	6 (4%)	41	37	24, 36, 73, 139	0
1	D	145/145 (100%)	0.53	13 (8%)	15	13	35, 50, 111, 139	0
1	E	145/145 (100%)	0.19	7 (4%)	35	31	32, 43, 96, 149	0
1	F	145/145 (100%)	-0.06	4 (2%)	55	50	28, 37, 83, 134	0
1	G	145/145 (100%)	0.24	8 (5%)	30	27	32, 47, 96, 130	0
1	H	145/145 (100%)	0.29	7 (4%)	35	31	35, 50, 110, 157	0
1	I	145/145 (100%)	0.80	12 (8%)	17	15	44, 62, 124, 142	0
1	J	145/145 (100%)	0.59	6 (4%)	41	37	39, 56, 114, 154	0
1	K	145/145 (100%)	0.47	9 (6%)	26	23	37, 52, 110, 156	0
1	L	145/145 (100%)	0.75	8 (5%)	30	27	40, 62, 112, 151	0
All	All	1740/1740 (100%)	0.32	97 (5%)	30	26	23, 49, 104, 157	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	23	VAL	7.3
1	C	24	TYR	5.6
1	F	24	TYR	5.1
1	B	4	THR	5.0
1	A	24	TYR	4.8
1	D	24	TYR	4.6
1	C	23	VAL	4.5
1	B	3	SER	4.5
1	G	24	TYR	4.5
1	A	23	VAL	4.4
1	B	24	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
1	K	21	PRO	4.2
1	G	23	VAL	4.2
1	K	23	VAL	4.2
1	E	23	VAL	4.1
1	J	21	PRO	4.1
1	D	3	SER	4.0
1	L	16	LEU	3.9
1	J	2	SER	3.9
1	L	23	VAL	3.8
1	K	24	TYR	3.8
1	B	19	ARG	3.8
1	A	2	SER	3.8
1	E	21	PRO	3.7
1	I	23	VAL	3.6
1	D	23	VAL	3.5
1	F	23	VAL	3.5
1	D	21	PRO	3.5
1	E	2	SER	3.4
1	F	21	PRO	3.3
1	J	3	SER	3.2
1	B	21	PRO	3.2
1	H	23	VAL	3.2
1	C	21	PRO	3.2
1	H	24	TYR	3.2
1	J	23	VAL	3.1
1	J	24	TYR	3.1
1	I	127	CYS	3.1
1	K	27	LEU	3.1
1	G	27	LEU	3.0
1	G	21	PRO	3.0
1	E	24	TYR	2.9
1	I	25	GLY	2.9
1	I	24	TYR	2.9
1	B	22	GLU	2.9
1	L	27	LEU	2.8
1	L	21	PRO	2.8
1	H	21	PRO	2.7
1	H	2	SER	2.7
1	L	131	ALA	2.7
1	D	34	ARG	2.6
1	A	21	PRO	2.6
1	G	2	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	26	HIS	2.6
1	L	24	TYR	2.5
1	I	4	THR	2.5
1	A	146	GLN	2.5
1	L	37	ILE	2.5
1	H	146	GLN	2.5
1	C	25	GLY	2.4
1	I	145	ILE	2.4
1	G	146	GLN	2.4
1	D	71	LYS	2.4
1	I	3	SER	2.3
1	B	25	GLY	2.3
1	A	19	ARG	2.3
1	D	145	ILE	2.3
1	I	19	ARG	2.3
1	I	27	LEU	2.3
1	E	3	SER	2.3
1	C	20	GLU	2.3
1	G	46	THR	2.3
1	D	19	ARG	2.3
1	I	136	PHE	2.3
1	B	2	SER	2.2
1	F	3	SER	2.2
1	I	45	ILE	2.2
1	H	18	LYS	2.2
1	G	3	SER	2.2
1	K	25	GLY	2.2
1	A	145	ILE	2.2
1	K	26	HIS	2.1
1	D	4	THR	2.1
1	K	5	ILE	2.1
1	I	47	LEU	2.1
1	A	22	GLU	2.1
1	K	145	ILE	2.1
1	D	2	SER	2.1
1	E	27	LEU	2.1
1	H	17	GLY	2.1
1	K	2	SER	2.1
1	C	34	ARG	2.0
1	J	18	LYS	2.0
1	L	45	ILE	2.0
1	D	146	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	45	ILE	2.0
1	E	44	SER	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	A	201	4/4	0.89	0.11	38,45,46,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.