



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 10:54 AM EDT

PDB ID : 2OWL / pdb_00002owl
Title : Crystal structure of E. coli RdgC
Authors : Briggs, G.S.; McEwan, P.A.; Yu, J.; Moore, T.; Emsley, J.; Lloyd, R.G.
Deposited on : 2007-02-16
Resolution : 2.40 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

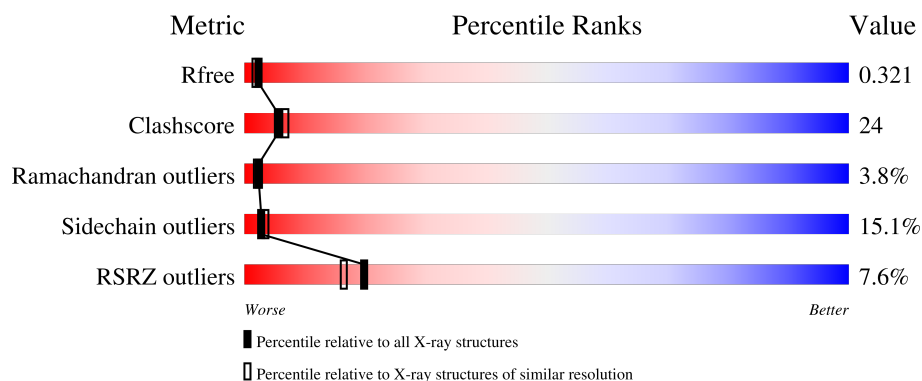
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	303	6% 44% 41% 13% .
1	B	303	8% 43% 37% 18% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4806 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 Recombination-associated protein rdgC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	Se	0	0	0
			2365	1489	406	452	5	13			
1	B	301	Total	C	N	O	S	Se	0	0	0
			2357	1484	405	451	5	12			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P36767
A	8	MSE	MET	modified residue	UNP P36767
A	23	MSE	MET	modified residue	UNP P36767
A	30	MSE	MET	modified residue	UNP P36767
A	40	MSE	MET	modified residue	UNP P36767
A	43	MSE	MET	modified residue	UNP P36767
A	49	MSE	MET	modified residue	UNP P36767
A	127	MSE	MET	modified residue	UNP P36767
A	128	MSE	MET	modified residue	UNP P36767
A	138	MSE	MET	modified residue	UNP P36767
A	168	MSE	MET	modified residue	UNP P36767
A	244	MSE	MET	modified residue	UNP P36767
A	282	MSE	MET	modified residue	UNP P36767
B	1	MSE	MET	modified residue	UNP P36767
B	8	MSE	MET	modified residue	UNP P36767
B	23	MSE	MET	modified residue	UNP P36767
B	30	MSE	MET	modified residue	UNP P36767
B	40	MSE	MET	modified residue	UNP P36767
B	43	MSE	MET	modified residue	UNP P36767
B	49	MSE	MET	modified residue	UNP P36767
B	127	MSE	MET	modified residue	UNP P36767
B	128	MSE	MET	modified residue	UNP P36767
B	138	MSE	MET	modified residue	UNP P36767
B	168	MSE	MET	modified residue	UNP P36767
B	244	MSE	MET	modified residue	UNP P36767

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Chain	Residue	Modelled	Actual	Comment	Reference
B	282	MSE	MET	modified residue	UNP P36767

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0

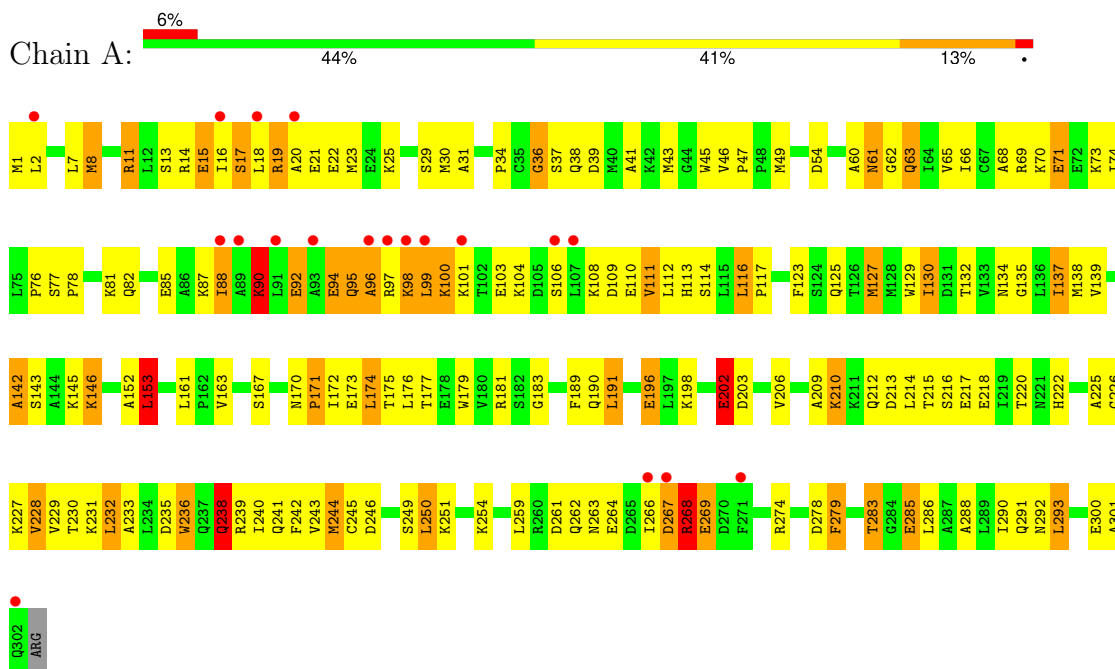
- Molecule 3 is water.

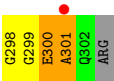
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	49	Total O 49 49	0	0
3	B	33	Total O 33 33	0	0

3 Residue-property plots

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: Recombination-associated protein rdgC





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.42Å 95.68Å 171.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.80 – 2.40 19.80 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (19.80-2.40) 98.0 (19.80-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.232 , 0.326 0.227 , 0.321	Depositor DCC
R_{free} test set	3355 reflections (9.89%)	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4806	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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: CA

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	1.99	66/2386 (2.8%)	1.70	36/3190 (1.1%)
1	B	1.78	41/2378 (1.7%)	1.61	26/3180 (0.8%)
All	All	1.89	107/4764 (2.2%)	1.66	62/6370 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	4

All (107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	229	VAL	CA-CB	15.23	1.71	1.53
1	A	226	GLY	N-CA	11.13	1.61	1.45
1	B	243	VAL	CA-CB	9.85	1.66	1.54
1	B	164	VAL	CA-CB	9.60	1.66	1.54
1	A	172	ILE	CA-CB	8.87	1.64	1.54
1	A	236	TRP	N-CA	-8.69	1.35	1.46
1	B	301	ALA	CA-CB	8.29	1.67	1.53
1	B	116	LEU	CA-C	8.24	1.61	1.52
1	A	233	ALA	CA-CB	-8.14	1.40	1.53
1	A	143	SER	N-CA	8.04	1.55	1.46
1	B	280	ILE	CA-CB	8.03	1.63	1.54
1	A	229	VAL	CA-C	-7.84	1.44	1.53
1	B	295	GLU	CA-C	7.82	1.63	1.52
1	A	293	LEU	CA-C	7.51	1.62	1.52
1	A	190	GLN	CA-C	7.46	1.61	1.52
1	A	236	TRP	CA-C	7.40	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	LYS	CE-NZ	7.36	1.71	1.49
1	B	300	GLU	N-CA	-7.19	1.37	1.45
1	A	190	GLN	N-CA	-7.03	1.37	1.46
1	A	179	TRP	C-O	-6.80	1.16	1.24
1	A	161	LEU	CA-C	-6.78	1.44	1.52
1	A	209	ALA	N-CA	6.71	1.54	1.46
1	A	65	VAL	N-CA	-6.68	1.38	1.46
1	B	126	THR	CA-CB	6.66	1.63	1.53
1	A	285	GLU	CA-C	6.66	1.61	1.52
1	B	290	ILE	CA-CB	6.65	1.62	1.54
1	A	142	ALA	CA-C	6.64	1.61	1.52
1	B	186	ALA	CA-CB	-6.60	1.42	1.53
1	A	243	VAL	N-CA	6.53	1.54	1.46
1	A	196	GLU	C-O	-6.50	1.16	1.24
1	B	290	ILE	C-O	6.49	1.31	1.24
1	A	291	GLN	N-CA	-6.46	1.38	1.46
1	A	241	GLN	CA-C	6.37	1.61	1.52
1	A	279	PHE	CA-C	-6.34	1.44	1.52
1	B	74	ILE	CA-CB	6.31	1.63	1.54
1	A	189	PHE	CA-C	-6.28	1.45	1.52
1	A	300	GLU	N-CA	-6.28	1.37	1.45
1	B	298	GLY	C-O	6.23	1.32	1.23
1	B	222	HIS	N-CA	6.22	1.53	1.46
1	A	240	ILE	N-CA	6.20	1.54	1.46
1	A	283	THR	C-O	6.19	1.31	1.24
1	A	167	SER	N-CA	-6.15	1.38	1.46
1	A	189	PHE	CA-CB	6.14	1.64	1.53
1	A	130	ILE	N-CA	-6.13	1.38	1.46
1	A	31	ALA	CA-CB	-6.07	1.43	1.53
1	A	176	LEU	CA-C	-6.05	1.44	1.52
1	A	177	THR	CA-CB	6.02	1.62	1.53
1	A	71	GLU	CA-C	-5.97	1.45	1.52
1	B	178	GLU	C-O	-5.96	1.17	1.24
1	B	189	PHE	CA-C	-5.93	1.45	1.52
1	A	227	LYS	N-CA	5.92	1.53	1.46
1	A	238	GLN	CB-CG	5.92	1.70	1.52
1	B	294	ILE	CA-CB	5.91	1.61	1.54
1	B	178	GLU	CA-C	-5.89	1.45	1.52
1	A	230	THR	CA-CB	5.79	1.62	1.54
1	B	228	VAL	CA-CB	5.78	1.61	1.54
1	A	153	LEU	CG-CD1	5.74	1.71	1.52
1	A	259	LEU	CA-C	-5.71	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	16	ILE	CA-CB	5.71	1.62	1.54
1	B	46	VAL	CA-CB	5.68	1.64	1.54
1	B	249	SER	C-O	-5.65	1.16	1.23
1	B	69	ARG	N-CA	-5.63	1.39	1.46
1	B	211	LYS	CA-C	-5.60	1.45	1.53
1	B	245	CYS	C-O	-5.58	1.16	1.23
1	A	214	LEU	C-O	5.57	1.30	1.24
1	A	123	PHE	N-CA	5.55	1.52	1.46
1	A	250	LEU	CA-C	-5.55	1.46	1.52
1	A	214	LEU	N-CA	5.49	1.53	1.46
1	A	34	PRO	C-O	-5.46	1.17	1.23
1	A	290	ILE	CA-CB	5.44	1.61	1.54
1	A	127	MSE	CA-CB	-5.43	1.45	1.53
1	B	283	THR	CA-CB	5.42	1.61	1.53
1	B	211	LYS	CD-CE	5.42	1.68	1.52
1	B	163	VAL	C-O	5.41	1.29	1.24
1	B	230	THR	CA-C	5.41	1.60	1.52
1	B	43	MSE	SE-CE	5.39	2.11	1.95
1	A	249	SER	CA-C	5.37	1.59	1.52
1	A	11	ARG	N-CA	-5.35	1.39	1.46
1	B	286	LEU	N-CA	5.35	1.53	1.46
1	A	210	LYS	N-CA	5.34	1.52	1.45
1	B	291	GLN	CG-CD	5.32	1.65	1.52
1	A	65	VAL	CA-C	5.31	1.58	1.52
1	B	287	ALA	C-O	-5.31	1.18	1.24
1	A	189	PHE	C-O	-5.30	1.17	1.23
1	A	202	GLU	C-O	5.30	1.30	1.23
1	A	209	ALA	C-O	-5.30	1.17	1.24
1	B	8	MSE	C-O	-5.29	1.17	1.24
1	B	194	GLU	CA-C	5.24	1.58	1.52
1	A	74	ILE	CA-CB	5.24	1.61	1.54
1	A	286	LEU	N-CA	5.23	1.52	1.46
1	A	235	ASP	C-O	-5.22	1.17	1.24
1	B	213	ASP	N-CA	-5.22	1.40	1.46
1	A	171	PRO	C-O	5.21	1.29	1.23
1	B	66	ILE	CA-CB	5.20	1.62	1.54
1	A	288	ALA	C-O	-5.19	1.17	1.24
1	A	135	GLY	N-CA	5.19	1.53	1.45
1	A	254	LYS	N-CA	5.18	1.52	1.46
1	A	63	GLN	C-O	-5.17	1.17	1.24
1	A	301	ALA	C-O	5.16	1.30	1.24
1	B	211	LYS	CE-NZ	5.14	1.64	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	228	VAL	CA-C	5.14	1.58	1.52
1	A	245	CYS	N-CA	5.13	1.52	1.46
1	A	206	VAL	CA-C	5.10	1.58	1.52
1	A	152	ALA	CA-CB	5.05	1.61	1.53
1	A	233	ALA	N-CA	5.04	1.52	1.46
1	B	233	ALA	N-CA	5.04	1.52	1.46
1	B	192	LEU	N-CA	5.04	1.52	1.46

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	LEU	N-CA-C	12.22	124.68	111.36
1	B	14	ARG	N-CA-C	8.80	122.52	109.24
1	A	259	LEU	N-CA-C	-8.29	102.76	113.12
1	A	191	LEU	N-CA-C	7.98	121.85	109.96
1	B	34	PRO	N-CA-C	7.94	123.65	111.34
1	B	134	ASN	N-CA-C	7.08	121.74	113.18
1	B	80	ILE	N-CA-C	-6.95	103.00	110.23
1	A	176	LEU	N-CA-C	6.88	119.62	111.71
1	B	36	GLY	N-CA-C	-6.84	103.39	112.82
1	A	170	ASN	CA-C-N	-6.79	112.77	119.76
1	A	170	ASN	C-N-CA	-6.79	112.77	119.76
1	A	8	MSE	CG-SE-CE	6.72	113.71	98.92
1	B	200	LEU	N-CA-C	6.68	118.64	111.36
1	B	144	ALA	N-CA-C	6.52	119.21	111.71
1	A	142	ALA	N-CA-C	6.42	119.26	111.82
1	A	123	PHE	N-CA-C	6.40	120.25	109.76
1	B	120	PHE	N-CA-C	-6.38	100.54	110.17
1	B	100	LYS	N-CA-C	-6.29	105.98	113.21
1	B	39	ASP	N-CA-C	6.27	117.91	111.14
1	B	21	GLU	N-CA-C	-6.01	97.99	110.80
1	A	36	GLY	N-CA-C	-6.01	103.17	112.85
1	A	246	ASP	N-CA-C	5.94	123.46	110.80
1	A	216	SER	N-CA-C	-5.86	99.83	108.79
1	A	225	ALA	O-C-N	-5.79	114.59	122.36
1	B	247	ASP	N-CA-C	-5.76	106.21	113.18
1	A	225	ALA	CA-C-N	-5.76	110.12	121.41
1	A	225	ALA	C-N-CA	-5.76	110.12	121.41
1	B	288	ALA	N-CA-C	5.68	117.95	111.02
1	B	173	GLU	CB-CA-C	-5.66	101.99	110.88
1	B	297	LEU	N-CA-C	5.65	119.80	113.02
1	A	29	SER	N-CA-C	5.62	119.75	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	13	SER	N-CA-C	5.61	117.39	111.28
1	A	175	THR	N-CA-C	-5.48	105.39	111.36
1	A	243	VAL	CB-CA-C	5.48	118.48	110.98
1	A	176	LEU	N-CA-CB	5.45	118.61	110.22
1	B	9	VAL	N-CA-C	5.44	116.42	108.53
1	A	134	ASN	N-CA-C	5.44	119.66	113.19
1	B	293	LEU	N-CA-C	5.43	120.02	112.90
1	A	70	LYS	CA-C-N	-5.38	115.40	122.99
1	A	70	LYS	C-N-CA	-5.38	115.40	122.99
1	A	14	ARG	N-CA-C	5.32	118.96	111.52
1	B	6	ASN	N-CA-C	-5.32	101.04	108.96
1	B	91	LEU	CB-CA-C	5.31	117.80	111.22
1	A	228	VAL	CA-C-N	5.25	129.46	122.01
1	A	228	VAL	C-N-CA	5.25	129.46	122.01
1	B	249	SER	N-CA-C	5.22	118.24	110.52
1	B	285	GLU	N-CA-CB	-5.21	102.51	110.07
1	A	268	ARG	N-CA-C	-5.20	105.76	113.40
1	B	11	ARG	CG-CD-NE	-5.19	100.58	112.00
1	A	244	MSE	CG-SE-CE	5.17	110.31	98.92
1	A	225	ALA	N-CA-C	-5.11	103.86	110.19
1	B	222	HIS	N-CA-C	5.09	117.48	111.33
1	A	210	LYS	CD-CE-NZ	5.07	128.13	111.90
1	A	238	GLN	CA-C-N	5.05	131.04	122.36
1	A	238	GLN	C-N-CA	5.05	131.04	122.36
1	A	210	LYS	CG-CD-CE	5.03	122.87	111.30
1	B	126	THR	CA-C-O	-5.03	113.91	120.25
1	A	8	MSE	N-CA-C	-5.03	100.70	108.90
1	B	15	GLU	N-CA-C	5.03	121.51	110.80
1	A	232	LEU	CB-CA-C	-5.01	102.12	110.14
1	A	13	SER	CA-C-N	5.00	129.30	122.34
1	A	13	SER	C-N-CA	5.00	129.30	122.34

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	17	SER	Peptide
1	B	264	GLU	Peptide
1	B	300	GLU	Peptide
1	B	95	GLN	Peptide

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	2365	0	2413	109	0
1	B	2357	0	2400	124	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	49	0	0	3	0
3	B	33	0	0	0	0
All	All	4806	0	4813	226	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 24.

All (226) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LYS:CE	1:A:90:LYS:NZ	1.71	1.53
1:A:244:MSE:CE	1:A:293:LEU:HD21	1.60	1.30
1:B:138:MSE:HE2	1:B:290:ILE:CD1	1.69	1.20
1:B:138:MSE:CE	1:B:290:ILE:HD13	1.81	1.09
1:A:244:MSE:HE3	1:A:293:LEU:HD11	1.29	1.07
1:B:268:ARG:HG3	1:B:268:ARG:HH11	1.14	1.04
1:A:244:MSE:HE3	1:A:293:LEU:CD1	1.87	1.03
1:B:138:MSE:HE2	1:B:290:ILE:HD13	1.36	1.00
1:A:244:MSE:HE1	1:A:293:LEU:HD21	1.01	0.99
1:B:138:MSE:HE2	1:B:290:ILE:HD11	1.41	0.99
1:A:244:MSE:CE	1:A:293:LEU:CD2	2.41	0.98
1:A:244:MSE:HE1	1:A:293:LEU:CD2	1.95	0.97
1:B:9:VAL:HG22	1:B:138:MSE:HE3	1.46	0.96
1:A:236:TRP:HE1	1:A:292:ASN:HD22	1.15	0.95
1:B:138:MSE:CE	1:B:290:ILE:CD1	2.43	0.94
1:A:7:LEU:HD11	1:A:138:MSE:HG3	1.50	0.93
1:B:102:THR:HA	1:B:105:ASP:HB3	1.50	0.91
1:A:263:ASN:HB3	1:A:266:ILE:HD13	1.52	0.90
1:A:222:HIS:HE1	1:B:222:HIS:HE1	1.18	0.89
1:A:244:MSE:HE3	1:A:293:LEU:HD21	1.61	0.82
1:B:236:TRP:HE1	1:B:292:ASN:HD22	1.26	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:TRP:CE3	1:B:138:MSE:HG3	2.15	0.81
1:B:242:PHE:HE2	1:B:244:MSE:CE	1.94	0.81
1:B:242:PHE:HE2	1:B:244:MSE:HE2	1.45	0.81
1:A:63:GLN:HE21	1:A:129:TRP:HE1	1.30	0.79
1:B:168:MSE:HE1	1:B:294:ILE:HA	1.66	0.78
1:B:268:ARG:HG3	1:B:268:ARG:NH1	1.93	0.78
1:A:99:LEU:HB3	1:A:100:LYS:HB2	1.64	0.78
1:B:138:MSE:HE1	1:B:290:ILE:HD13	1.66	0.78
1:B:236:TRP:HE1	1:B:292:ASN:ND2	1.82	0.77
1:B:39:ASP:O	1:B:40:MSE:HB3	1.85	0.77
1:B:261:ASP:O	1:B:264:GLU:HB2	1.84	0.77
1:A:69:ARG:HD2	1:A:125:GLN:HE21	1.51	0.76
1:B:8:MSE:HE3	1:B:249:SER:HB3	1.66	0.75
1:B:104:LYS:HE3	1:B:108:LYS:HE2	1.69	0.75
1:B:242:PHE:CE2	1:B:244:MSE:HE2	2.20	0.75
1:A:217:GLU:HA	1:A:220:THR:HB	1.69	0.75
1:B:129:TRP:CZ3	1:B:138:MSE:HG3	2.22	0.74
1:B:268:ARG:HH11	1:B:268:ARG:CG	1.98	0.74
1:A:244:MSE:HE3	1:A:293:LEU:CD2	2.14	0.74
1:B:39:ASP:O	1:B:40:MSE:CB	2.35	0.74
1:A:222:HIS:CE1	1:B:222:HIS:HE1	2.03	0.73
1:A:60:ALA:O	1:A:61:ASN:HB2	1.87	0.73
1:A:62:GLY:O	1:A:132:THR:OG1	2.05	0.72
1:B:242:PHE:CE2	1:B:244:MSE:CE	2.72	0.72
1:B:2:LEU:HD12	1:B:3:TRP:HD1	1.55	0.72
1:B:104:LYS:HD3	1:B:105:ASP:N	2.03	0.72
1:A:63:GLN:NE2	1:A:129:TRP:HE1	1.86	0.72
1:A:267:ASP:HB3	1:A:269:GLU:HG3	1.72	0.72
1:A:95:GLN:HE21	1:A:95:GLN:HA	1.53	0.72
1:A:222:HIS:HE1	1:B:222:HIS:CE1	2.07	0.71
1:B:85:GLU:HA	1:B:88:ILE:HG12	1.73	0.71
1:A:15:GLU:HG2	1:A:16:ILE:H	1.57	0.70
1:B:9:VAL:HG22	1:B:138:MSE:CE	2.22	0.69
1:A:7:LEU:HD11	1:A:138:MSE:CG	2.22	0.69
1:A:90:LYS:NZ	1:A:90:LYS:CD	2.56	0.69
1:A:15:GLU:HG2	1:A:16:ILE:N	2.08	0.68
1:A:110:GLU:O	1:A:114:SER:HB2	1.93	0.68
1:B:2:LEU:HD12	1:B:3:TRP:CD1	2.29	0.67
1:B:134:ASN:N	1:B:134:ASN:HD22	1.92	0.67
1:A:244:MSE:HE3	1:A:293:LEU:CG	2.25	0.67
1:A:183:GLY:HA2	1:A:215:THR:HG22	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:PHE:CE2	1:A:244:MSE:HE2	2.31	0.66
1:A:112:LEU:O	1:A:116:LEU:HB2	1.96	0.66
1:A:85:GLU:HA	1:A:88:ILE:HG22	1.78	0.65
1:A:94:GLU:HA	1:A:94:GLU:OE2	1.96	0.65
1:A:63:GLN:HE21	1:A:129:TRP:NE1	1.94	0.65
1:B:36:GLY:N	1:B:39:ASP:OD2	2.18	0.64
1:B:168:MSE:HE3	1:B:299:GLY:H	1.62	0.64
1:B:244:MSE:CE	1:B:293:LEU:HD21	2.28	0.64
1:B:295:GLU:O	1:B:296:GLY:C	2.39	0.64
1:A:41:ALA:HA	1:A:71:GLU:O	1.99	0.63
1:A:236:TRP:HE1	1:A:292:ASN:ND2	1.94	0.62
1:B:273:GLN:HA	1:B:276:ASP:OD2	1.98	0.62
1:B:214:LEU:HA	1:B:219:ILE:HG13	1.81	0.62
1:B:104:LYS:HE3	1:B:108:LYS:CE	2.29	0.62
1:B:88:ILE:HG13	1:B:89:ALA:N	2.13	0.62
1:A:1:MSE:HG2	1:A:2:LEU:N	2.15	0.62
1:A:130:ILE:HG12	1:A:137:ILE:HD13	1.80	0.62
1:A:238:GLN:OE1	1:A:238:GLN:HA	2.00	0.61
1:A:39:ASP:O	1:A:73:LYS:NZ	2.27	0.60
1:A:98:LYS:HZ2	1:A:99:LEU:H	1.49	0.59
1:B:40:MSE:HE3	1:B:73:LYS:HB2	1.84	0.59
1:A:16:ILE:CD1	1:A:18:LEU:HB3	2.33	0.59
1:A:100:LYS:H	1:A:103:GLU:HB2	1.68	0.58
1:B:99:LEU:C	1:B:101:LYS:H	2.10	0.58
1:A:212:GLN:HG3	1:A:213:ASP:N	2.18	0.58
1:A:239:ARG:NE	1:A:285:GLU:OE2	2.32	0.58
1:B:168:MSE:CE	1:B:294:ILE:HA	2.34	0.58
1:B:88:ILE:HG13	1:B:89:ALA:H	1.67	0.58
1:A:76:PRO:HG2	1:B:74:ILE:HD13	1.87	0.57
1:A:38:GLN:HE22	1:A:113:HIS:HA	1.69	0.57
1:A:218:GLU:OE1	1:B:227:LYS:NZ	2.38	0.56
1:B:220:THR:HA	1:B:223:ILE:HD12	1.87	0.56
1:A:100:LYS:N	1:A:103:GLU:HG3	2.20	0.56
1:B:43:MSE:HB2	1:B:70:LYS:HD3	1.86	0.56
1:A:196:GLU:HB3	1:A:231:LYS:HB2	1.88	0.56
1:A:92:GLU:HG2	1:A:96:ALA:HA	1.87	0.56
1:B:272:ALA:O	1:B:276:ASP:OD2	2.23	0.55
1:B:244:MSE:HE1	1:B:293:LEU:HD21	1.87	0.55
1:B:168:MSE:HE2	1:B:297:LEU:HB2	1.89	0.55
1:A:7:LEU:HD23	1:A:250:LEU:HD22	1.89	0.54
1:A:202:GLU:O	1:A:203:ASP:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:CYS:SG	1:B:147:ALA:HB2	2.48	0.54
1:A:88:ILE:HG13	1:A:104:LYS:HD3	1.88	0.54
1:A:266:ILE:O	1:A:268:ARG:N	2.40	0.54
1:A:98:LYS:HG2	1:A:99:LEU:H	1.72	0.54
1:B:102:THR:HA	1:B:105:ASP:CB	2.32	0.54
1:A:36:GLY:N	1:A:39:ASP:OD2	2.31	0.54
1:B:244:MSE:HE1	1:B:250:LEU:HG	1.91	0.53
1:B:295:GLU:O	1:B:297:LEU:N	2.42	0.53
1:B:59:VAL:HG22	1:B:64:ILE:HG12	1.91	0.53
1:B:90:LYS:C	1:B:92:GLU:H	2.15	0.53
1:B:99:LEU:O	1:B:103:GLU:HB2	2.09	0.52
1:A:210:LYS:O	1:B:205:GLY:HA2	2.10	0.52
1:B:14:ARG:CZ	1:B:14:ARG:HB2	2.38	0.52
1:B:100:LYS:O	1:B:104:LYS:HD2	2.10	0.52
1:A:261:ASP:O	1:A:262:GLN:C	2.53	0.52
1:A:99:LEU:CB	1:A:100:LYS:HB2	2.37	0.52
1:A:108:LYS:O	1:A:111:VAL:HG22	2.08	0.51
1:B:242:PHE:HB3	1:B:253:LEU:HD23	1.92	0.51
1:A:16:ILE:HG13	1:A:18:LEU:HD23	1.91	0.51
1:A:267:ASP:HB3	1:A:269:GLU:CG	2.39	0.51
1:B:191:LEU:CD2	1:B:232:LEU:HD21	2.41	0.51
1:B:18:LEU:HD22	1:B:158:LEU:HD22	1.93	0.50
1:B:212:GLN:HG2	1:B:219:ILE:HD11	1.93	0.50
1:A:98:LYS:NZ	1:A:99:LEU:H	2.08	0.50
1:B:20:ALA:O	1:B:21:GLU:HG3	2.10	0.50
1:B:236:TRP:CZ3	1:B:285:GLU:OE2	2.65	0.50
1:A:263:ASN:HB3	1:A:266:ILE:CD1	2.35	0.50
1:A:37:SER:HB2	1:A:117:PRO:HA	1.93	0.50
1:A:77:SER:N	1:A:78:PRO:CD	2.75	0.50
1:B:130:ILE:HG12	1:B:137:ILE:HG12	1.94	0.50
1:A:98:LYS:HG2	1:A:99:LEU:N	2.26	0.50
1:A:11:ARG:O	1:A:163:VAL:HA	2.12	0.49
1:A:1:MSE:HE2	1:A:278:ASP:HB3	1.94	0.49
1:B:41:ALA:HA	1:B:71:GLU:O	2.12	0.49
1:A:261:ASP:O	1:A:264:GLU:HB2	2.13	0.49
1:B:134:ASN:N	1:B:134:ASN:ND2	2.60	0.49
1:B:168:MSE:HE1	1:B:294:ILE:HG23	1.95	0.48
1:A:20:ALA:HA	1:A:23:MSE:HB3	1.95	0.48
1:B:265:ASP:HB2	1:B:266:ILE:HD12	1.94	0.48
1:A:279:PHE:CE1	1:A:283:THR:HG21	2.48	0.48
1:B:68:ALA:O	1:B:125:GLN:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:ASN:ND2	1:B:277:ALA:HB1	2.28	0.48
1:A:43:MSE:HE2	1:A:68:ALA:HB1	1.96	0.48
1:B:201:LEU:H	1:B:201:LEU:CD1	2.27	0.48
1:A:99:LEU:CA	1:A:100:LYS:HB2	2.44	0.48
1:A:242:PHE:HE2	1:A:244:MSE:HE2	1.75	0.48
1:B:239:ARG:NH1	1:B:285:GLU:OE2	2.46	0.47
1:B:262:GLN:O	1:B:262:GLN:HG2	2.14	0.47
1:B:168:MSE:HE1	1:B:294:ILE:CA	2.42	0.47
1:A:8:MSE:CE	1:A:142:ALA:O	2.63	0.47
1:A:69:ARG:HD2	1:A:125:GLN:NE2	2.25	0.47
1:A:104:LYS:O	1:A:108:LYS:HB2	2.15	0.47
1:A:181:ARG:O	1:A:181:ARG:HG2	2.14	0.47
1:B:268:ARG:HG2	1:B:269:GLU:N	2.30	0.47
1:A:268:ARG:HE	1:A:268:ARG:HB3	1.52	0.47
1:B:70:LYS:NZ	1:B:72:GLU:OE2	2.48	0.47
1:A:81:LYS:O	1:A:85:GLU:HG3	2.14	0.46
1:A:8:MSE:HE2	3:A:312:HOH:O	2.14	0.46
1:A:60:ALA:O	1:A:61:ASN:CB	2.58	0.46
1:B:76:PRO:CB	1:B:78:PRO:HD2	2.45	0.46
1:A:45:TRP:CZ2	1:A:153:LEU:HD13	2.51	0.46
1:A:238:GLN:OE1	1:A:238:GLN:CA	2.63	0.46
1:B:76:PRO:C	1:B:78:PRO:HD2	2.41	0.46
1:A:19:ARG:O	1:A:23:MSE:N	2.47	0.46
1:B:99:LEU:HD12	1:B:103:GLU:OE1	2.16	0.45
1:B:236:TRP:HZ3	1:B:285:GLU:OE2	1.98	0.45
1:B:129:TRP:CE3	1:B:138:MSE:CG	2.92	0.45
1:B:2:LEU:CD1	1:B:3:TRP:CD1	2.98	0.45
1:B:266:ILE:HG22	1:B:266:ILE:O	2.16	0.45
1:B:168:MSE:HE3	1:B:299:GLY:N	2.30	0.45
1:B:131:ASP:C	1:B:131:ASP:OD1	2.58	0.45
1:B:255:PHE:HB2	1:B:260:ARG:HD3	1.97	0.45
1:B:101:LYS:HG2	1:B:102:THR:H	1.82	0.45
1:B:9:VAL:CG2	1:B:138:MSE:CE	2.94	0.44
1:B:12:LEU:HD11	1:B:16:ILE:HD12	1.99	0.44
1:B:99:LEU:C	1:B:101:LYS:N	2.76	0.44
1:A:146:LYS:NZ	3:A:310:HOH:O	2.26	0.44
1:B:95:GLN:O	1:B:96:ALA:CB	2.66	0.44
1:B:219:ILE:O	1:B:222:HIS:HB2	2.18	0.44
1:B:217:GLU:O	1:B:221:ASN:HB2	2.18	0.44
1:A:99:LEU:HD22	1:A:100:LYS:HD2	2.00	0.43
1:B:66:ILE:HG21	1:B:66:ILE:HD13	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:PRO:HG2	1:A:174:LEU:HD22	1.99	0.43
1:B:265:ASP:OD1	1:B:266:ILE:N	2.39	0.43
1:A:8:MSE:HE3	1:A:142:ALA:C	2.42	0.43
1:A:25:LYS:O	3:A:328:HOH:O	2.21	0.43
1:B:281:LEU:O	1:B:285:GLU:HB2	2.18	0.43
1:A:106:SER:O	1:A:110:GLU:HG3	2.19	0.43
1:B:129:TRP:CE2	1:B:283:THR:HG22	2.54	0.43
1:A:274:ARG:HA	1:A:274:ARG:HD2	1.68	0.43
1:B:77:SER:HA	1:B:80:ILE:HD12	2.00	0.43
1:A:191:LEU:CD2	1:A:232:LEU:HD21	2.49	0.42
1:A:16:ILE:HD12	1:A:18:LEU:HB3	2.01	0.42
1:A:95:GLN:HE21	1:A:95:GLN:CA	2.27	0.42
1:B:87:LYS:NZ	1:B:110:GLU:OE2	2.48	0.42
1:B:224:GLU:C	1:B:226:GLY:H	2.26	0.42
1:B:200:LEU:HD23	1:B:200:LEU:HA	1.88	0.42
1:B:9:VAL:HG13	1:B:138:MSE:CE	2.49	0.42
1:B:19:ARG:O	1:B:22:GLU:N	2.51	0.42
1:B:77:SER:N	1:B:78:PRO:CD	2.83	0.42
1:B:176:LEU:HB3	1:B:229:VAL:HB	2.02	0.42
1:A:1:MSE:CE	1:A:278:ASP:HB3	2.50	0.41
1:A:49:MSE:HB3	1:A:49:MSE:HE2	1.67	0.41
1:B:268:ARG:HG2	1:B:269:GLU:H	1.84	0.41
1:A:202:GLU:O	1:A:203:ASP:CB	2.68	0.41
1:B:102:THR:CA	1:B:105:ASP:HB3	2.34	0.41
1:B:199:SER:OG	1:B:204:GLY:HA3	2.19	0.41
1:B:19:ARG:HG3	1:B:22:GLU:OE1	2.19	0.41
1:A:218:GLU:HG2	1:B:222:HIS:CD2	2.56	0.41
1:B:101:LYS:CG	1:B:102:THR:N	2.84	0.41
1:B:194:GLU:HB3	1:B:233:ALA:HB2	2.03	0.41
1:A:129:TRP:CZ2	1:A:283:THR:HB	2.55	0.41
1:B:173:GLU:CD	1:B:173:GLU:H	2.29	0.41
1:B:247:ASP:OD1	1:B:247:ASP:C	2.63	0.41
1:A:16:ILE:O	1:A:18:LEU:N	2.53	0.41
1:A:146:LYS:O	1:A:146:LYS:HG3	2.20	0.41
1:A:183:GLY:HA2	1:A:215:THR:CG2	2.48	0.41
1:B:28:ALA:HA	1:B:56:LEU:HD11	2.03	0.41
1:B:134:ASN:HD22	1:B:134:ASN:H	1.68	0.41
1:A:198:LYS:N	1:A:228:VAL:O	2.46	0.40
1:A:46:VAL:HB	1:A:47:PRO:HD2	2.03	0.40
1:B:269:GLU:O	1:B:269:GLU:HG2	2.13	0.40
1:B:103:GLU:O	1:B:107:LEU:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	300/303 (99%)	267 (89%)	25 (8%)	8 (3%)	4	4
1	B	299/303 (99%)	257 (86%)	27 (9%)	15 (5%)	1	1
All	All	599/606 (99%)	524 (88%)	52 (9%)	23 (4%)	2	2

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	ALA
1	A	100	LYS
1	B	37	SER
1	B	96	ALA
1	B	98	LYS
1	A	99	LEU
1	A	267	ASP
1	B	15	GLU
1	B	24	GLU
1	B	40	MSE
1	B	89	ALA
1	B	133	VAL
1	B	262	GLN
1	A	15	GLU
1	A	17	SER
1	B	21	GLU
1	B	301	ALA
1	A	101	LYS
1	B	17	SER
1	B	296	GLY
1	A	61	ASN
1	B	20	ALA

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Mol	Chain	Res	Type
1	B	95	GLN

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	258/246 (105%)	226 (88%)	32 (12%)	4	6
1	B	257/246 (104%)	211 (82%)	46 (18%)	2	2
All	All	515/492 (105%)	437 (85%)	78 (15%)	3	3

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	SER
1	A	19	ARG
1	A	21	GLU
1	A	22	GLU
1	A	30	MSE
1	A	54	ASP
1	A	66	ILE
1	A	82	GLN
1	A	87	LYS
1	A	88	ILE
1	A	90	LYS
1	A	92	GLU
1	A	94	GLU
1	A	95	GLN
1	A	97	ARG
1	A	98	LYS
1	A	109	ASP
1	A	111	VAL
1	A	116	LEU
1	A	127	MSE
1	A	137	ILE
1	A	139	VAL

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Mol	Chain	Res	Type
1	A	145	LYS
1	A	146	LYS
1	A	153	LEU
1	A	173	GLU
1	A	174	LEU
1	A	202	GLU
1	A	238	GLN
1	A	251	LYS
1	A	268	ARG
1	A	269	GLU
1	B	2	LEU
1	B	8	MSE
1	B	12	LEU
1	B	14	ARG
1	B	15	GLU
1	B	16	ILE
1	B	19	ARG
1	B	21	GLU
1	B	25	LYS
1	B	29	SER
1	B	42	LYS
1	B	49	MSE
1	B	54	ASP
1	B	81	LYS
1	B	84	LEU
1	B	90	LYS
1	B	94	GLU
1	B	98	LYS
1	B	99	LEU
1	B	102	THR
1	B	103	GLU
1	B	104	LYS
1	B	105	ASP
1	B	107	LEU
1	B	112	LEU
1	B	122	ARG
1	B	125	GLN
1	B	134	ASN
1	B	138	MSE
1	B	146	LYS
1	B	157	SER
1	B	160	SER

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Mol	Chain	Res	Type
1	B	164	VAL
1	B	168	MSE
1	B	176	LEU
1	B	184	SER
1	B	187	GLN
1	B	197	LEU
1	B	201	LEU
1	B	202	GLU
1	B	220	THR
1	B	221	ASN
1	B	268	ARG
1	B	269	GLU
1	B	274	ARG
1	B	276	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	63	GLN
1	A	95	GLN
1	A	125	GLN
1	A	222	HIS
1	A	237	GLN
1	A	291	GLN
1	A	292	ASN
1	B	26	GLN
1	B	82	GLN
1	B	95	GLN
1	B	113	HIS
1	B	134	ASN
1	B	221	ASN
1	B	222	HIS
1	B	263	ASN
1	B	291	GLN
1	B	292	ASN
1	B	302	GLN

5.3.3 RNA ⓘ

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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	289/303 (95%)	0.20	19 (6%)	24 20	16, 41, 107, 127	0
1	B	289/303 (95%)	0.30	25 (8%)	16 13	28, 47, 101, 118	0
All	All	578/606 (95%)	0.25	44 (7%)	20 16	16, 45, 106, 127	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	93	ALA	4.7
1	B	266	ILE	4.2
1	A	99	LEU	3.7
1	A	18	LEU	3.7
1	B	90	LYS	3.6
1	B	91	LEU	3.4
1	A	20	ALA	3.2
1	A	89	ALA	2.9
1	B	18	LEU	2.9
1	B	276	ASP	2.9
1	A	16	ILE	2.8
1	A	93	ALA	2.8
1	B	267	ASP	2.8
1	A	96	ALA	2.7
1	B	88	ILE	2.7
1	B	89	ALA	2.6
1	A	302	GLN	2.6
1	A	91	LEU	2.6
1	B	301	ALA	2.5
1	B	100	LYS	2.5
1	B	92	GLU	2.4
1	B	20	ALA	2.4
1	B	202	GLU	2.4
1	B	98	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	107	LEU	2.4
1	B	16	ILE	2.4
1	B	268	ARG	2.4
1	A	106	SER	2.3
1	B	106	SER	2.3
1	B	271	PHE	2.3
1	B	96	ALA	2.2
1	A	266	ILE	2.2
1	A	97	ARG	2.2
1	A	101	LYS	2.2
1	B	86	ALA	2.2
1	B	107	LEU	2.2
1	A	88	ILE	2.1
1	B	97	ARG	2.1
1	A	267	ASP	2.1
1	A	2	LEU	2.1
1	A	98	LYS	2.1
1	B	99	LEU	2.0
1	A	271	PHE	2.0
1	B	102	THR	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(Å ²)	Q<0.9
2	CA	A	304	1/1	0.89	0.15	59,59,59,59	0
2	CA	B	304	1/1	0.95	0.16	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.