



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:39 PM UTC

PDB ID : 2DB0 / pdb_00002db0
Title : Crystal structure of PH0542
Authors : Nishino, A.; Handa, N.; Kishishita, S.; Murayama, K.; Shirouzu, M.; RIKEN
Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-12-14
Resolution : 2.20 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
Xtrriage (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

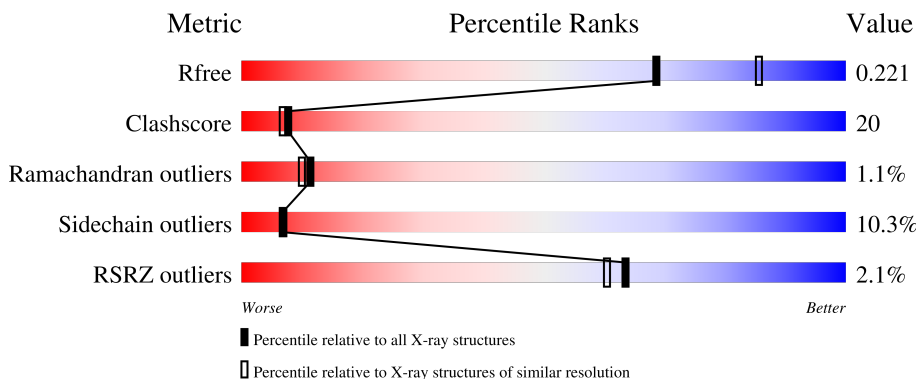
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	253	 2% 36% 44% 14% • 6%
1	B	253	 2% 31% 45% 16% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3908 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 253aa long hypothetical protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	239	1899	1221	316	352	10	0	0	0
1	B	240	1908	1226	317	355	10	0	0	0

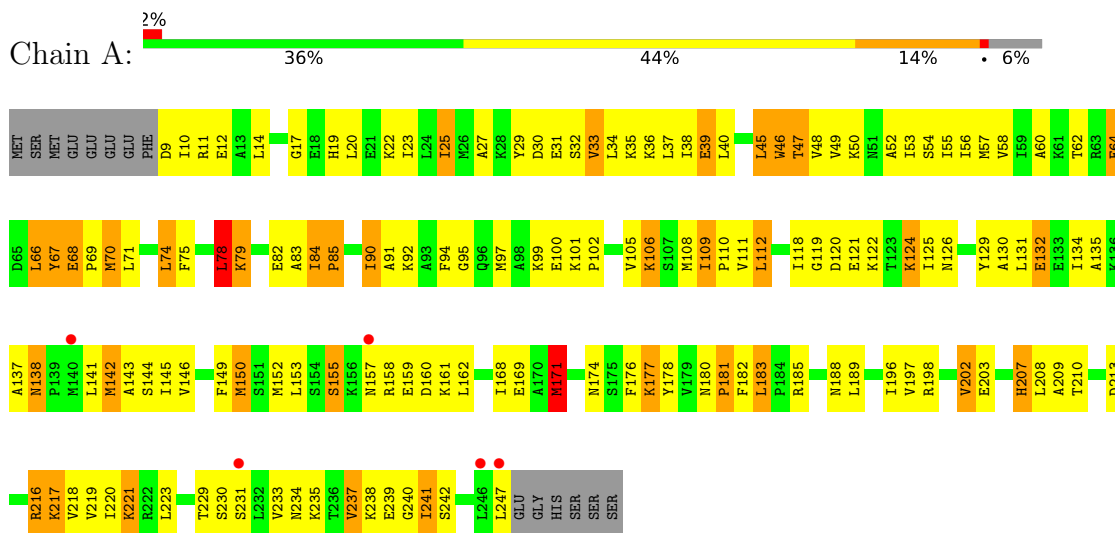
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	58	Total	O	0	0
			58	58		
2	B	43	Total	O	0	0
			43	43		

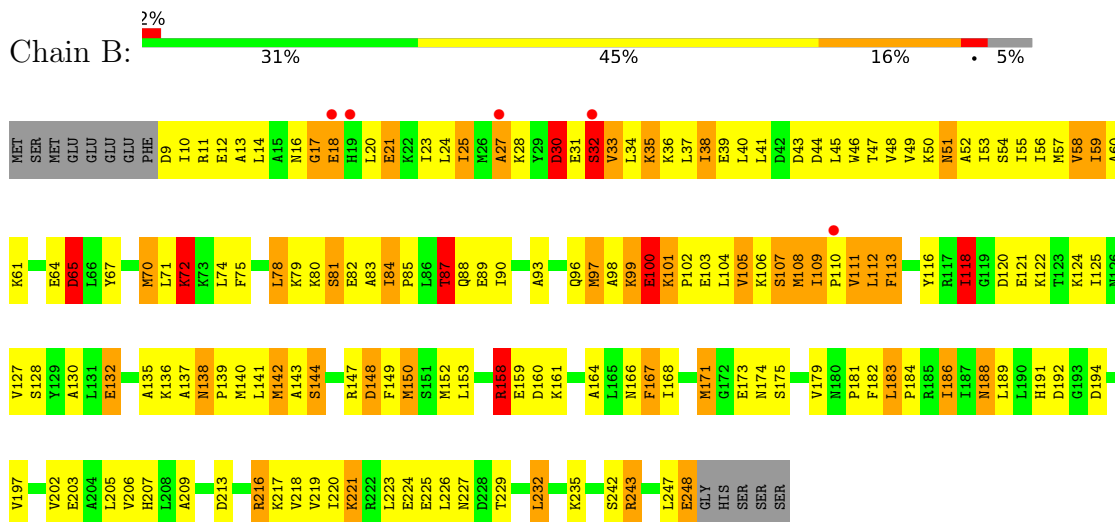
3 Residue-property plots

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: 253aa long hypothetical protein



- Molecule 1: 253aa long hypothetical protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	78.80Å 90.78Å 66.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.20) 99.2 (50.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.73 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.205 , 0.268 (Not available) , 0.221	Depositor DCC
R_{free} test set	1246 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtrriage
Anisotropy	0.252	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3908	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.50% 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

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	2.64	109/1922 (5.7%)	1.78	29/2586 (1.1%)
1	B	2.60	107/1931 (5.5%)	1.89	42/2598 (1.6%)
All	All	2.62	216/3853 (5.6%)	1.84	71/5184 (1.4%)

All (216) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	142	MET	SD-CE	-23.28	1.21	1.79
1	A	97	MET	SD-CE	-15.78	1.40	1.79
1	A	142	MET	SD-CE	-14.41	1.43	1.79
1	B	152	MET	SD-CE	-13.14	1.46	1.79
1	A	130	ALA	C-O	-12.59	1.09	1.24
1	A	53	ILE	CA-CB	12.10	1.67	1.54
1	A	90	ILE	CA-CB	-11.58	1.41	1.54
1	B	97	MET	SD-CE	-11.48	1.50	1.79
1	B	140	MET	SD-CE	-10.81	1.52	1.79
1	A	169	GLU	C-O	-10.64	1.10	1.24
1	A	134	ILE	CA-CB	-10.61	1.41	1.54
1	A	49	VAL	CA-CB	-10.42	1.42	1.54
1	B	186	ILE	CA-CB	-10.15	1.42	1.54
1	A	198	ARG	C-O	-9.84	1.12	1.24
1	B	96	GLN	C-O	9.81	1.35	1.24
1	A	23	ILE	CA-CB	-9.63	1.41	1.54
1	A	38	ILE	CA-CB	-9.62	1.42	1.54
1	B	53	ILE	CA-C	-9.44	1.41	1.52
1	A	196	ILE	CA-CB	9.37	1.67	1.54
1	B	188	ASN	CG-ND2	9.26	1.52	1.33
1	A	82	GLU	CA-CB	9.21	1.66	1.54
1	B	150	MET	SD-CE	-9.19	1.56	1.79
1	A	120	ASP	C-O	9.15	1.34	1.23
1	A	52	ALA	CA-CB	9.03	1.67	1.53
1	B	18	GLU	CA-C	8.99	1.63	1.53
1	B	203	GLU	C-O	-8.95	1.13	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	88	GLN	C-O	-8.87	1.13	1.24
1	A	196	ILE	C-O	-8.83	1.12	1.24
1	B	197	VAL	C-O	-8.80	1.14	1.24
1	B	183	LEU	N-CA	-8.58	1.38	1.46
1	A	135	ALA	C-O	-8.41	1.14	1.24
1	B	78	LEU	C-O	8.36	1.34	1.24
1	B	209	ALA	CA-CB	-8.30	1.39	1.53
1	A	150	MET	SD-CE	8.20	2.00	1.79
1	A	60	ALA	CA-CB	8.19	1.66	1.53
1	A	122	LYS	CA-C	8.13	1.63	1.52
1	A	216	ARG	C-O	-8.12	1.14	1.24
1	B	27	ALA	CA-CB	8.11	1.66	1.53
1	A	56	ILE	CA-C	-8.05	1.42	1.52
1	A	208	LEU	CA-C	7.97	1.63	1.52
1	A	207	HIS	N-CA	-7.87	1.36	1.46
1	B	57	MET	SD-CE	-7.82	1.59	1.79
1	A	109	ILE	CA-C	7.71	1.59	1.52
1	B	50	LYS	CA-C	-7.64	1.43	1.52
1	B	18	GLU	CA-CB	7.61	1.61	1.52
1	B	99	LYS	C-O	-7.60	1.15	1.24
1	B	219	VAL	CA-C	-7.59	1.43	1.52
1	A	149	PHE	C-O	-7.56	1.15	1.24
1	B	191	HIS	CA-CB	7.56	1.65	1.53
1	A	124	LYS	CE-NZ	7.53	1.72	1.49
1	B	58	VAL	C-O	-7.49	1.15	1.24
1	B	30	ASP	CA-C	7.44	1.61	1.52
1	B	109	ILE	C-O	-7.41	1.18	1.24
1	B	65	ASP	CA-C	7.40	1.62	1.52
1	B	109	ILE	CA-CB	-7.34	1.50	1.54
1	B	127	VAL	CA-C	-7.34	1.43	1.52
1	B	113	PHE	CA-C	7.30	1.64	1.52
1	A	33	VAL	C-O	-7.28	1.16	1.24
1	A	145	ILE	CA-CB	7.28	1.63	1.54
1	A	97	MET	CA-C	-7.27	1.42	1.52
1	A	70	MET	C-O	-7.25	1.15	1.24
1	A	17	GLY	C-O	-7.14	1.16	1.24
1	A	83	ALA	CA-C	-7.10	1.44	1.52
1	B	52	ALA	N-CA	7.08	1.55	1.46
1	B	93	ALA	CA-CB	-7.06	1.42	1.53
1	B	218	VAL	C-O	7.01	1.32	1.24
1	A	108	MET	SD-CE	-6.97	1.62	1.79
1	A	78	LEU	CG-CD2	-6.95	1.29	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	LEU	CA-C	6.95	1.62	1.52
1	B	135	ALA	CA-CB	6.88	1.64	1.53
1	B	28	LYS	CA-C	6.85	1.62	1.52
1	A	48	VAL	CA-CB	6.83	1.62	1.54
1	B	38	ILE	CB-CG2	6.80	1.75	1.52
1	A	35	LYS	CA-C	-6.79	1.43	1.52
1	B	118	ILE	C-O	6.78	1.33	1.24
1	B	45	LEU	CA-C	-6.78	1.44	1.52
1	A	94	PHE	CA-C	6.76	1.61	1.52
1	A	105	VAL	CA-CB	-6.75	1.46	1.54
1	B	167	PHE	C-O	-6.72	1.16	1.24
1	B	36	LYS	CA-C	6.72	1.61	1.52
1	A	189	LEU	CA-C	-6.71	1.43	1.52
1	B	217	LYS	C-O	-6.63	1.16	1.24
1	B	219	VAL	C-O	-6.61	1.16	1.24
1	A	131	LEU	C-O	-6.59	1.15	1.24
1	A	218	VAL	C-O	6.59	1.31	1.24
1	B	183	LEU	CA-CB	-6.53	1.46	1.53
1	B	171	MET	N-CA	-6.52	1.37	1.45
1	B	84	ILE	CA-C	6.50	1.59	1.52
1	A	40	LEU	CA-C	6.49	1.61	1.52
1	B	49	VAL	C-O	-6.48	1.16	1.24
1	A	57	MET	C-O	6.48	1.32	1.24
1	A	161	LYS	C-O	-6.48	1.16	1.24
1	A	39	GLU	CA-C	-6.47	1.44	1.52
1	B	164	ALA	N-CA	6.45	1.54	1.46
1	A	197	VAL	CA-CB	-6.40	1.45	1.54
1	B	173	GLU	C-O	-6.39	1.16	1.24
1	B	111	VAL	CA-C	6.39	1.60	1.52
1	B	229	THR	CA-CB	-6.39	1.42	1.53
1	B	105	VAL	CA-CB	-6.38	1.47	1.54
1	B	46	TRP	CA-C	-6.38	1.44	1.52
1	A	10	ILE	C-O	-6.37	1.16	1.24
1	A	142	MET	CB-CG	6.33	1.71	1.52
1	B	137	ALA	C-O	-6.32	1.16	1.24
1	B	49	VAL	CA-CB	-6.31	1.47	1.54
1	A	121	GLU	CA-C	-6.26	1.44	1.52
1	A	171	MET	SD-CE	-6.25	1.64	1.79
1	B	235	LYS	N-CA	6.22	1.54	1.46
1	A	158	ARG	CA-C	6.19	1.61	1.52
1	B	14	LEU	CA-C	-6.10	1.45	1.52
1	A	176	PHE	C-O	6.05	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	ILE	CA-C	6.04	1.59	1.52
1	A	105	VAL	C-O	6.00	1.30	1.24
1	A	84	ILE	CB-CG2	5.96	1.72	1.52
1	B	148	ASP	C-O	-5.96	1.17	1.24
1	B	122	LYS	CD-CE	5.95	1.70	1.52
1	B	48	VAL	CA-CB	5.93	1.61	1.54
1	A	210	THR	CA-CB	5.91	1.63	1.53
1	B	140	MET	CG-SD	5.87	1.95	1.80
1	A	10	ILE	CA-CB	-5.85	1.48	1.54
1	B	38	ILE	C-O	5.85	1.30	1.24
1	A	238	LYS	C-O	-5.84	1.17	1.24
1	A	50	LYS	CB-CG	5.83	1.70	1.52
1	B	181	PRO	CG-CD	5.83	1.70	1.50
1	B	132	GLU	C-O	-5.82	1.17	1.24
1	A	171	MET	CG-SD	-5.81	1.66	1.80
1	A	54	SER	CA-CB	5.81	1.62	1.53
1	B	60	ALA	CA-CB	5.77	1.64	1.53
1	A	112	LEU	CB-CG	5.76	1.65	1.53
1	A	99	LYS	C-O	5.75	1.31	1.24
1	A	55	ILE	CA-CB	-5.74	1.47	1.54
1	B	160	ASP	N-CA	-5.73	1.39	1.46
1	B	171	MET	SD-CE	-5.72	1.65	1.79
1	A	92	LYS	CE-NZ	5.69	1.66	1.49
1	B	81	SER	CA-C	5.69	1.60	1.52
1	A	240	GLY	CA-C	-5.69	1.43	1.51
1	A	74	LEU	C-O	-5.68	1.17	1.24
1	A	57	MET	CB-CG	5.68	1.69	1.52
1	A	111	VAL	CA-C	-5.67	1.46	1.52
1	B	225	GLU	C-O	5.67	1.31	1.24
1	B	173	GLU	CA-C	-5.66	1.45	1.52
1	B	72	LYS	C-O	5.64	1.30	1.24
1	A	124	LYS	C-O	5.63	1.30	1.24
1	B	50	LYS	C-O	-5.63	1.17	1.24
1	B	111	VAL	CA-CB	5.63	1.62	1.54
1	A	35	LYS	CB-CG	5.60	1.69	1.52
1	B	87	THR	C-O	-5.58	1.17	1.24
1	A	14	LEU	N-CA	5.57	1.53	1.46
1	A	149	PHE	CA-C	5.57	1.59	1.52
1	A	37	LEU	C-O	-5.57	1.17	1.24
1	A	153	LEU	C-O	5.57	1.31	1.24
1	A	112	LEU	N-CA	-5.55	1.39	1.46
1	B	232	LEU	C-O	-5.54	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	ASN	CA-CB	-5.53	1.46	1.53
1	B	21	GLU	CA-C	5.53	1.60	1.52
1	B	48	VAL	CB-CG1	5.51	1.70	1.52
1	A	106	LYS	CE-NZ	-5.50	1.32	1.49
1	A	129	TYR	C-O	-5.49	1.17	1.24
1	A	68	GLU	N-CA	-5.49	1.41	1.46
1	B	136	LYS	C-O	-5.48	1.17	1.24
1	B	121	GLU	CD-OE1	5.48	1.35	1.25
1	A	162	LEU	C-O	-5.47	1.17	1.24
1	A	111	VAL	C-O	-5.47	1.18	1.24
1	A	152	MET	SD-CE	-5.47	1.65	1.79
1	B	161	LYS	CD-CE	-5.46	1.36	1.52
1	A	45	LEU	C-O	-5.44	1.17	1.24
1	A	46	TRP	CB-CG	-5.42	1.33	1.50
1	B	125	ILE	C-O	-5.39	1.17	1.24
1	A	134	ILE	N-CA	5.38	1.52	1.46
1	B	158	ARG	N-CA	-5.37	1.39	1.46
1	A	137	ALA	C-O	-5.37	1.17	1.24
1	A	35	LYS	CG-CD	5.36	1.68	1.52
1	B	205	LEU	C-O	-5.33	1.18	1.24
1	B	232	LEU	CG-CD2	-5.31	1.35	1.52
1	A	152	MET	CB-CG	5.29	1.68	1.52
1	B	44	ASP	CA-C	5.28	1.59	1.52
1	B	149	PHE	CA-C	5.27	1.59	1.52
1	A	109	ILE	N-CA	-5.24	1.40	1.46
1	A	155	SER	N-CA	5.23	1.52	1.46
1	B	100	GLU	C-O	-5.22	1.17	1.24
1	B	219	VAL	C-N	-5.20	1.27	1.33
1	B	112	LEU	C-O	-5.17	1.18	1.24
1	B	89	GLU	N-CA	-5.17	1.40	1.46
1	B	38	ILE	N-CA	-5.16	1.40	1.46
1	B	135	ALA	C-O	-5.16	1.18	1.24
1	B	74	LEU	C-O	5.15	1.30	1.24
1	B	130	ALA	CA-C	-5.15	1.46	1.52
1	A	47	THR	CA-C	-5.14	1.45	1.52
1	A	137	ALA	CA-CB	5.13	1.61	1.53
1	A	85	PRO	C-O	-5.13	1.18	1.24
1	B	72	LYS	N-CA	-5.13	1.40	1.46
1	A	122	LYS	CG-CD	5.12	1.67	1.52
1	B	166	ASN	CA-CB	5.12	1.61	1.53
1	A	33	VAL	N-CA	5.12	1.52	1.46
1	A	70	MET	C-N	-5.12	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	120	ASP	CA-CB	5.11	1.60	1.53
1	A	161	LYS	CA-C	-5.09	1.46	1.52
1	B	51	ASN	N-CA	5.08	1.52	1.46
1	A	36	LYS	C-O	-5.07	1.18	1.24
1	B	70	MET	C-O	-5.07	1.18	1.24
1	B	223	LEU	CA-C	-5.07	1.45	1.52
1	A	142	MET	N-CA	-5.07	1.40	1.46
1	A	197	VAL	N-CA	-5.06	1.39	1.46
1	A	36	LYS	C-N	-5.06	1.27	1.33
1	B	141	LEU	CA-C	5.04	1.59	1.52
1	B	229	THR	CB-CG2	5.04	1.69	1.52
1	A	39	GLU	CD-OE1	5.04	1.34	1.25
1	B	109	ILE	CA-C	5.04	1.57	1.52
1	B	103	GLU	C-O	-5.04	1.18	1.24
1	A	67	TYR	N-CA	-5.03	1.40	1.46
1	B	207	HIS	CA-CB	-5.03	1.45	1.53
1	B	70	MET	CA-C	-5.02	1.46	1.52
1	B	186	ILE	CA-C	-5.01	1.46	1.52
1	A	54	SER	C-O	-5.01	1.18	1.24
1	A	118	ILE	CA-CB	-5.01	1.47	1.54
1	A	125	ILE	CA-CB	-5.01	1.48	1.54
1	B	149	PHE	N-CA	5.00	1.52	1.46

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	143	ALA	N-CA-C	-10.37	99.16	112.23
1	B	216	ARG	NE-CZ-NH2	-8.54	111.51	119.20
1	A	58	VAL	N-CA-C	-8.50	102.14	110.72
1	B	159	GLU	N-CA-C	8.13	121.06	111.71
1	B	103	GLU	N-CA-C	-7.35	102.66	111.69
1	B	229	THR	OG1-CB-CG2	-7.27	94.77	109.30
1	A	71	LEU	N-CA-C	-7.25	103.31	111.14
1	B	83	ALA	N-CA-C	7.01	119.54	108.67
1	B	80	LYS	N-CA-C	6.66	121.14	112.89
1	B	138	ASN	O-C-N	6.44	126.14	121.12
1	A	33	VAL	N-CA-C	6.41	116.56	110.53
1	B	38	ILE	N-CA-C	-6.31	104.36	110.42
1	B	192	ASP	CA-C-N	6.28	127.07	120.03
1	B	192	ASP	C-N-CA	6.28	127.07	120.03
1	A	9	ASP	CA-C-N	6.27	128.69	120.60
1	A	9	ASP	C-N-CA	6.27	128.69	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	ILE	N-CA-C	-6.21	104.28	110.62
1	B	217	LYS	N-CA-C	6.21	117.71	111.07
1	B	138	ASN	CA-C-N	6.21	125.69	119.24
1	B	138	ASN	C-N-CA	6.21	125.69	119.24
1	B	105	VAL	CB-CA-C	-6.20	104.06	111.81
1	B	235	LYS	N-CA-C	-6.15	104.66	111.36
1	B	46	TRP	N-CA-C	6.07	118.69	111.71
1	B	25	ILE	CA-C-N	6.00	128.91	120.28
1	B	25	ILE	C-N-CA	6.00	128.91	120.28
1	B	25	ILE	N-CA-CB	-5.94	104.14	110.62
1	B	107	SER	CA-CB-OG	5.91	122.93	111.10
1	A	229	THR	N-CA-C	5.91	118.95	111.69
1	B	174	ASN	N-CA-C	5.90	120.21	112.89
1	A	174	ASN	N-CA-C	5.88	120.18	112.89
1	B	98	ALA	CA-C-N	5.77	127.94	120.44
1	B	98	ALA	C-N-CA	5.77	127.94	120.44
1	B	173	GLU	CA-C-O	-5.76	114.44	120.55
1	B	153	LEU	N-CA-C	5.74	118.28	111.33
1	A	150	MET	N-CA-C	-5.73	105.12	111.71
1	A	95	GLY	CA-C-O	-5.68	115.20	121.05
1	B	50	LYS	CB-CA-C	-5.62	102.06	110.88
1	A	185	ARG	CB-CG-CD	5.61	124.20	111.30
1	B	221	LYS	N-CA-C	-5.56	105.23	112.23
1	A	202	VAL	N-CA-C	5.52	115.66	110.30
1	A	237	VAL	N-CA-C	-5.52	105.14	110.72
1	A	112	LEU	N-CA-C	5.48	117.69	111.11
1	B	36	LYS	N-CA-C	-5.45	105.42	111.36
1	A	120	ASP	N-CA-C	-5.39	100.87	109.23
1	B	32	SER	CB-CA-C	-5.39	101.52	110.68
1	A	55	ILE	N-CA-C	5.37	115.58	110.42
1	B	142	MET	N-CA-CB	5.37	118.02	110.12
1	B	111	VAL	CA-C-N	5.37	127.79	120.54
1	B	111	VAL	C-N-CA	5.37	127.79	120.54
1	B	33	VAL	N-CA-C	-5.28	105.24	111.00
1	A	91	ALA	N-CA-C	-5.27	105.62	111.36
1	A	71	LEU	CD1-CG-CD2	-5.27	99.21	110.80
1	A	78	LEU	CA-C-O	5.22	125.80	119.38
1	B	213	ASP	N-CA-C	5.20	117.03	111.36
1	A	79	LYS	CB-CG-CD	5.20	123.25	111.30
1	A	25	ILE	N-CA-C	-5.17	105.50	110.72
1	B	107	SER	N-CA-C	-5.17	105.73	111.36
1	B	161	LYS	CB-CG-CD	5.16	123.17	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	PRO	N-CA-C	5.15	120.62	113.98
1	B	218	VAL	CA-CB-CG1	5.15	119.15	110.40
1	A	10	ILE	CB-CA-C	-5.13	105.31	111.88
1	A	82	GLU	CA-CB-CG	-5.13	103.84	114.10
1	B	58	VAL	CA-C-N	5.12	127.48	120.46
1	B	58	VAL	C-N-CA	5.12	127.48	120.46
1	A	47	THR	CA-C-O	5.12	125.83	119.79
1	A	52	ALA	CA-C-O	5.11	126.18	120.82
1	A	132	GLU	N-CA-C	-5.08	105.92	111.82
1	B	25	ILE	N-CA-C	5.06	115.21	110.30
1	B	108	MET	N-CA-C	-5.05	107.12	113.28
1	A	109	ILE	CB-CG1-CD1	5.04	124.38	113.80
1	A	213	ASP	N-CA-C	-5.01	105.53	111.69

There are no chirality outliers.

There are no planarity outliers.

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	1899	0	2019	65	0
1	B	1908	0	2025	93	0
2	A	58	0	0	1	0
2	B	43	0	0	1	0
All	All	3908	0	4044	157	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 20.

All (157) 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:38:ILE:CG2	1:B:38:ILE:CB	1.75	1.63
1:A:124:LYS:CE	1:A:124:LYS:NZ	1.71	1.50
1:B:142:MET:CE	1:B:142:MET:SD	1.21	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLU:HG3	1:A:101:LYS:NZ	1.53	1.23
1:B:142:MET:SD	1:B:142:MET:HE2	1.78	1.13
1:B:142:MET:SD	1:B:142:MET:HE1	1.79	1.11
1:B:142:MET:SD	1:B:142:MET:HE3	1.79	1.10
1:B:216:ARG:HD2	1:B:248:GLU:OE2	1.59	1.01
1:B:142:MET:CE	1:B:142:MET:CG	2.38	1.00
1:A:217:LYS:O	1:A:221:LYS:HE2	1.64	0.96
1:B:56:ILE:HG21	1:B:70:MET:HE3	1.49	0.95
1:B:10:ILE:HG23	1:B:23:ILE:HD12	1.46	0.93
1:A:64:GLU:CG	1:A:101:LYS:NZ	2.34	0.90
1:B:30:ASP:OD2	1:B:32:SER:HB2	1.75	0.86
1:A:171:MET:HA	1:A:171:MET:HE2	1.59	0.84
1:B:9:ASP:OD2	1:B:12:GLU:HG3	1.78	0.84
1:A:64:GLU:HG3	1:A:101:LYS:HZ3	1.43	0.83
1:A:64:GLU:HG3	1:A:101:LYS:HZ2	1.40	0.83
1:A:216:ARG:HD3	2:A:302:HOH:O	1.83	0.77
1:B:106:LYS:HE2	1:B:148:ASP:OD2	1.84	0.76
1:B:10:ILE:HG23	1:B:23:ILE:CD1	2.17	0.74
1:B:81:SER:OG	1:B:87:THR:HG22	1.89	0.72
1:B:21:GLU:O	1:B:25:ILE:HG12	1.90	0.72
1:A:177:LYS:H	1:A:177:LYS:NZ	1.90	0.69
1:B:13:ALA:HB1	2:B:282:HOH:O	1.94	0.67
1:B:18:GLU:HA	1:B:20:LEU:CD1	2.24	0.67
1:B:158:ARG:HD2	1:B:194:ASP:OD1	1.94	0.67
1:B:38:ILE:CG2	1:B:38:ILE:CG1	2.71	0.66
1:B:38:ILE:O	1:B:41:LEU:HD13	1.96	0.66
1:A:157:ASN:HD22	1:A:160:ASP:CG	2.02	0.66
1:B:38:ILE:CG2	1:B:38:ILE:CA	2.71	0.65
1:B:41:LEU:HD12	1:B:41:LEU:N	2.11	0.65
1:A:19:HIS:O	1:A:22:LYS:HB3	1.95	0.65
1:B:118:ILE:HD11	1:B:124:LYS:HG3	1.80	0.63
1:B:150:MET:HG3	1:B:182:PHE:CD2	2.34	0.63
1:A:101:LYS:N	1:A:102:PRO:HD3	2.16	0.61
1:B:37:LEU:O	1:B:41:LEU:CD1	2.48	0.61
1:B:138:ASN:C	1:B:138:ASN:HD22	2.08	0.60
1:B:9:ASP:OD2	1:B:12:GLU:CG	2.50	0.59
1:B:41:LEU:CD1	1:B:41:LEU:H	2.15	0.59
1:A:78:LEU:HD13	1:A:90:ILE:HG21	1.83	0.59
1:A:188:ASN:HD21	1:B:102:PRO:HD2	1.66	0.58
1:A:138:ASN:C	1:A:138:ASN:HD22	2.11	0.58
1:A:64:GLU:CG	1:A:101:LYS:HZ1	2.14	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ALA:HA	1:B:33:VAL:HG23	1.84	0.58
1:B:78:LEU:HB2	1:B:90:ILE:HG21	1.85	0.57
1:B:64:GLU:OE1	1:B:101:LYS:NZ	2.34	0.57
1:B:183:LEU:HB3	1:B:184:PRO:HD3	1.87	0.57
1:B:109:ILE:HB	1:B:110:PRO:HD3	1.87	0.57
1:B:16:ASN:O	1:B:17:GLY:C	2.48	0.57
1:B:150:MET:HE1	1:B:168:ILE:HD11	1.88	0.56
1:B:27:ALA:HA	1:B:33:VAL:CG2	2.35	0.56
1:A:138:ASN:ND2	1:A:141:LEU:H	2.04	0.56
1:B:105:VAL:O	1:B:109:ILE:HG12	2.05	0.56
1:A:27:ALA:HA	1:A:33:VAL:HB	1.88	0.56
1:B:41:LEU:N	1:B:41:LEU:CD1	2.69	0.56
1:A:171:MET:HA	1:A:171:MET:CE	2.32	0.55
1:B:18:GLU:HA	1:B:20:LEU:HD12	1.89	0.55
1:B:16:ASN:O	1:B:17:GLY:O	2.24	0.55
1:A:142:MET:O	1:A:146:VAL:HG23	2.07	0.54
1:B:100:GLU:C	1:B:101:LYS:HD3	2.33	0.54
1:A:30:ASP:OD2	1:A:32:SER:OG	2.25	0.54
1:B:144:SER:O	1:B:148:ASP:OD2	2.26	0.53
1:A:177:LYS:H	1:A:177:LYS:HZ3	1.57	0.53
1:B:23:ILE:CG2	1:B:55:ILE:HD13	2.40	0.52
1:A:34:LEU:C	1:A:34:LEU:HD23	2.34	0.52
1:A:64:GLU:CA	1:A:64:GLU:OE2	2.58	0.51
1:B:20:LEU:HD23	1:B:55:ILE:HG13	1.93	0.51
1:B:40:LEU:O	1:B:43:ASP:HB2	2.10	0.51
1:B:18:GLU:CG	1:B:20:LEU:HD13	2.41	0.51
1:A:239:GLU:O	1:A:242:SER:OG	2.26	0.51
1:B:75:PHE:CE2	1:B:79:LYS:HE3	2.46	0.51
1:B:100:GLU:HB3	1:B:101:LYS:HD3	1.92	0.51
1:B:71:LEU:HD23	1:B:108:MET:HG3	1.93	0.50
1:A:235:LYS:O	1:A:239:GLU:HG3	2.12	0.50
1:B:10:ILE:CG2	1:B:23:ILE:HD12	2.31	0.49
1:A:157:ASN:HD21	1:A:159:GLU:HB2	1.77	0.49
1:B:150:MET:HA	1:B:150:MET:HE2	1.93	0.49
1:B:84:ILE:HB	1:B:85:PRO:HD3	1.95	0.49
1:A:67:TYR:OH	1:A:100:GLU:OE1	2.26	0.49
1:B:109:ILE:CB	1:B:110:PRO:HD3	2.42	0.49
1:B:220:ILE:O	1:B:224:GLU:HG3	2.13	0.49
1:B:72:LYS:C	1:B:72:LYS:HD3	2.38	0.49
1:A:34:LEU:HD21	1:A:66:LEU:HD21	1.95	0.49
1:B:41:LEU:HD12	1:B:41:LEU:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLY:HA2	1:A:124:LYS:HE2	1.95	0.48
1:B:64:GLU:O	1:B:65:ASP:C	2.57	0.48
1:B:116:TYR:OH	1:B:118:ILE:HD12	2.13	0.48
1:A:64:GLU:OE2	1:A:64:GLU:HA	2.12	0.48
1:A:209:ALA:HB1	1:A:216:ARG:HA	1.95	0.48
1:A:171:MET:O	1:A:207:HIS:HE1	1.97	0.48
1:A:180:ASN:HB3	1:A:181:PRO:HD3	1.96	0.47
1:B:20:LEU:HD21	1:B:51:ASN:HB3	1.96	0.47
1:B:24:LEU:CD1	1:B:59:ILE:HD11	2.45	0.47
1:B:183:LEU:HA	1:B:186:ILE:HD12	1.95	0.47
1:B:64:GLU:CD	1:B:101:LYS:HE3	2.39	0.47
1:A:101:LYS:N	1:A:102:PRO:CD	2.77	0.47
1:A:34:LEU:HD11	1:A:66:LEU:HD11	1.97	0.47
1:B:31:GLU:OE1	1:B:35:LYS:NZ	2.47	0.47
1:A:150:MET:HG3	1:A:182:PHE:CG	2.50	0.46
1:A:30:ASP:OD2	1:A:33:VAL:HG23	2.15	0.46
1:B:71:LEU:HD13	1:B:97:MET:SD	2.56	0.46
1:A:182:PHE:O	1:A:183:LEU:C	2.57	0.46
1:B:47:THR:HG22	1:B:51:ASN:ND2	2.31	0.46
1:B:128:SER:O	1:B:132:GLU:HG2	2.15	0.45
1:A:68:GLU:HB3	1:A:69:PRO:HD3	1.98	0.45
1:A:230:SER:HB3	1:A:233:VAL:HB	1.99	0.45
1:A:143:ALA:HB2	1:A:178:TYR:CE1	2.51	0.45
1:B:171:MET:HG3	1:B:179:VAL:HG21	1.98	0.45
1:B:71:LEU:HD12	1:B:71:LEU:HA	1.80	0.44
1:B:202:VAL:O	1:B:206:VAL:HG23	2.17	0.44
1:A:109:ILE:HB	1:A:110:PRO:HD3	2.00	0.44
1:A:64:GLU:CD	1:A:101:LYS:HZ1	2.25	0.44
1:B:142:MET:CE	1:B:142:MET:HG3	2.44	0.44
1:B:167:PHE:CE2	1:B:171:MET:HE3	2.53	0.44
1:A:33:VAL:O	1:A:34:LEU:C	2.61	0.43
1:B:11:ARG:C	1:B:11:ARG:HD3	2.43	0.43
1:B:100:GLU:C	1:B:101:LYS:CD	2.91	0.43
1:B:23:ILE:HG22	1:B:55:ILE:HD13	2.01	0.43
1:A:46:TRP:CZ3	1:A:47:THR:HG22	2.53	0.43
1:B:38:ILE:O	1:B:39:GLU:C	2.60	0.43
1:A:219:VAL:O	1:A:223:LEU:HG	2.19	0.43
1:B:101:LYS:HB3	1:B:104:LEU:HB3	1.99	0.43
1:A:75:PHE:CE1	1:A:112:LEU:HB2	2.53	0.42
1:A:106:LYS:HE2	1:A:144:SER:OG	2.19	0.42
1:A:11:ARG:C	1:A:11:ARG:HD3	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ILE:C	1:B:41:LEU:HD13	2.44	0.42
1:B:242:SER:O	1:B:243:ARG:C	2.62	0.42
1:B:247:LEU:HA	1:B:247:LEU:HD23	1.64	0.42
1:A:25:ILE:O	1:A:29:TYR:HD1	2.03	0.42
1:B:31:GLU:O	1:B:34:LEU:HB3	2.20	0.42
1:B:101:LYS:CD	1:B:101:LYS:N	2.82	0.42
1:A:106:LYS:CE	1:A:144:SER:OG	2.68	0.42
1:A:64:GLU:CD	1:A:101:LYS:NZ	2.78	0.41
1:B:118:ILE:HD12	1:B:118:ILE:HA	1.68	0.41
1:A:223:LEU:HB3	1:A:237:VAL:HG13	2.01	0.41
1:B:33:VAL:O	1:B:34:LEU:C	2.64	0.41
1:A:138:ASN:C	1:A:138:ASN:ND2	2.78	0.41
1:B:54:SER:O	1:B:58:VAL:HG23	2.19	0.41
1:B:70:MET:O	1:B:71:LEU:C	2.62	0.41
1:A:202:VAL:O	1:A:203:GLU:C	2.61	0.41
1:A:230:SER:O	1:A:234:ASN:OD1	2.38	0.41
1:A:237:VAL:HG12	1:A:241:ILE:HD12	2.03	0.41
1:B:56:ILE:HD13	1:B:70:MET:CE	2.51	0.41
1:B:182:PHE:O	1:B:183:LEU:C	2.58	0.41
1:A:78:LEU:HD12	1:A:126:ASN:HB3	2.02	0.41
1:A:70:MET:HE2	1:A:70:MET:HA	2.03	0.41
1:B:18:GLU:HG3	1:B:20:LEU:HD13	2.02	0.41
1:B:64:GLU:HG2	1:B:67:TYR:CE1	2.56	0.41
1:B:138:ASN:C	1:B:138:ASN:ND2	2.76	0.41
1:A:84:ILE:CG2	1:A:85:PRO:HD3	2.51	0.40
1:A:183:LEU:HD22	1:A:183:LEU:HA	1.61	0.40
1:A:168:ILE:HA	1:A:171:MET:HG2	2.02	0.40
1:B:109:ILE:O	1:B:113:PHE:HB2	2.21	0.40
1:B:10:ILE:H	1:B:10:ILE:HD12	1.86	0.40
1:A:70:MET:O	1:A:74:LEU:HG	2.21	0.40
1:A:216:ARG:O	1:A:220:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	237/253 (94%)	226 (95%)	9 (4%)	2 (1%)	16	16
1	B	238/253 (94%)	227 (95%)	8 (3%)	3 (1%)	9	8
All	All	475/506 (94%)	453 (95%)	17 (4%)	5 (1%)	11	10

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
1	B	17	GLY
1	B	65	ASP
1	B	111	VAL
1	A	155	SER

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	213/226 (94%)	196 (92%)	17 (8%)	11	13
1	B	214/226 (95%)	187 (87%)	27 (13%)	4	4
All	All	427/452 (94%)	383 (90%)	44 (10%)	7	7

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLU
1	A	20	LEU
1	A	39	GLU
1	A	45	LEU
1	A	62	THR
1	A	64	GLU
1	A	78	LEU
1	A	79	LYS

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Mol	Chain	Res	Type
1	A	132	GLU
1	A	171	MET
1	A	177	LYS
1	A	183	LEU
1	A	217	LYS
1	A	221	LYS
1	A	231	SER
1	A	241	ILE
1	A	247	LEU
1	B	30	ASP
1	B	32	SER
1	B	35	LYS
1	B	59	ILE
1	B	61	LYS
1	B	72	LYS
1	B	82	GLU
1	B	87	THR
1	B	99	LYS
1	B	100	GLU
1	B	101	LYS
1	B	107	SER
1	B	112	LEU
1	B	118	ILE
1	B	139	PRO
1	B	144	SER
1	B	147	ARG
1	B	158	ARG
1	B	175	SER
1	B	188	ASN
1	B	189	LEU
1	B	221	LYS
1	B	226	LEU
1	B	227	ASN
1	B	232	LEU
1	B	243	ARG
1	B	248	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
1	A	157	ASN

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Mol	Chain	Res	Type
1	A	174	ASN
1	A	180	ASN
1	A	188	ASN
1	A	207	HIS
1	A	234	ASN
1	B	51	ASN
1	B	88	GLN
1	B	126	ASN
1	B	138	ASN
1	B	174	ASN
1	B	227	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](#)

There are no chain breaks in this entry.

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	239/253 (94%)	-0.05	5 (2%) 63 60	16, 34, 62, 70	0
1	B	240/253 (94%)	0.15	5 (2%) 63 60	21, 39, 61, 74	0
All	All	479/506 (94%)	0.05	10 (2%) 63 60	16, 37, 61, 74	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	18	GLU	3.1
1	B	27	ALA	3.1
1	A	246	LEU	3.1
1	A	140	MET	2.7
1	A	247	LEU	2.5
1	B	32	SER	2.3
1	B	19	HIS	2.2
1	A	231	SER	2.1
1	B	110	PRO	2.0
1	A	157	ASN	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.