



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:54 PM UTC

PDB ID : 4RXN / pdb_00004rxn
Title : CRYSTALLOGRAPHIC REFINEMENT OF RUBREDOXIN AT 1.2
ANGSTROMS RESOLUTION
Authors : Watenpaugh, K.D.; Sieker, L.C.; Jensen, L.H.
Deposited on : 1984-10-15
Resolution : 1.20 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

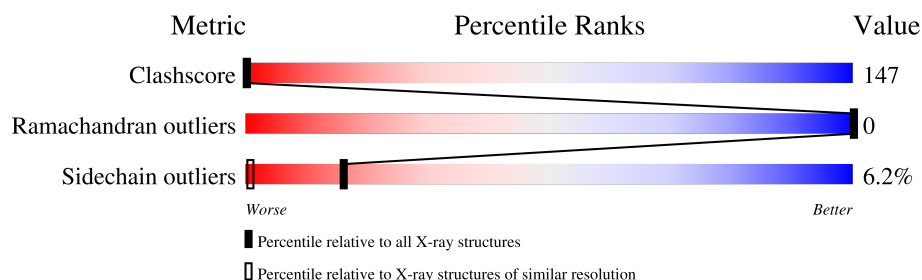
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.20 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))
Clashscore	190562	1265 (1.20-1.20)
Ramachandran outliers	187476	1226 (1.20-1.20)
Sidechain outliers	187428	1226 (1.20-1.20)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	54	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 884 atoms, of which 334 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 RUBREDOXIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	54	Total	C	H	N	O	S	0	0	0
			756	263	334	60	94	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	ASP	ASN	conflict	UNP P00268
A	22	ASP	ASN	conflict	UNP P00268
A	48	GLU	GLN	conflict	UNP P00268

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		

- Molecule 3 is water.

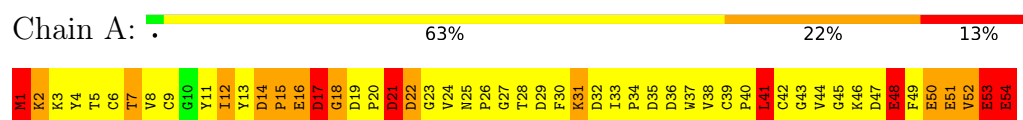
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	127	Total	O	0	0
			127	127		

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. 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. 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.

Note EDS was not executed.

- Molecule 1: RUBREDOXIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	64.29Å 64.29Å 32.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 1.20	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	0.128 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	884	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

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: FE

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	8.18	137/433 (31.6%)	6.03	163/588 (27.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	9

All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	GLU	N-CA	92.54	2.60	1.46
1	A	51	GLU	CG-CD	35.53	2.40	1.52
1	A	52	VAL	CA-C	33.93	1.87	1.53
1	A	50	GLU	CG-CD	26.73	2.18	1.52
1	A	53	GLU	CA-C	23.96	1.82	1.52
1	A	17	ASP	CB-CG	23.55	2.10	1.52
1	A	48	GLU	CD-OE1	22.92	1.68	1.25
1	A	16	GLU	CA-CB	22.32	1.92	1.53
1	A	1	MET	SD-CE	21.86	2.34	1.79
1	A	53	GLU	CD-OE2	21.46	1.66	1.25
1	A	21	ASP	CG-OD2	20.69	1.64	1.25
1	A	32	ASP	CG-OD2	-20.39	0.86	1.25
1	A	1	MET	N-CA	19.44	1.83	1.46
1	A	1	MET	CB-CG	19.04	2.09	1.52
1	A	12	ILE	CG1-CD1	-18.82	0.78	1.51
1	A	1	MET	C-N	18.61	1.58	1.33
1	A	1	MET	CA-C	18.02	1.90	1.52
1	A	2	LYS	CB-CG	-17.95	0.98	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	GLU	C-O	17.08	1.44	1.24
1	A	50	GLU	CD-OE1	16.94	1.57	1.25
1	A	17	ASP	N-CA	-15.98	1.25	1.46
1	A	51	GLU	CB-CG	-15.81	1.05	1.52
1	A	7	THR	C-O	14.29	1.42	1.24
1	A	7	THR	CA-CB	14.26	1.78	1.53
1	A	12	ILE	N-CA	-14.22	1.28	1.46
1	A	26	PRO	CA-C	-13.72	1.36	1.52
1	A	2	LYS	CA-CB	13.67	1.75	1.53
1	A	41	LEU	CG-CD1	13.54	1.97	1.52
1	A	49	PHE	C-O	12.93	1.39	1.23
1	A	44	VAL	N-CA	-12.91	1.31	1.46
1	A	16	GLU	CA-C	-12.54	1.35	1.52
1	A	41	LEU	C-O	12.37	1.38	1.24
1	A	17	ASP	CG-OD1	11.66	1.47	1.25
1	A	44	VAL	CA-CB	11.56	1.69	1.54
1	A	42	CYS	N-CA	-11.53	1.31	1.45
1	A	17	ASP	CG-OD2	-11.18	1.04	1.25
1	A	1	MET	C-O	-11.03	1.01	1.23
1	A	5	THR	CB-CG2	-10.82	1.16	1.52
1	A	1	MET	CG-SD	10.78	2.07	1.80
1	A	45	GLY	C-N	10.74	1.48	1.33
1	A	44	VAL	CA-C	10.69	1.65	1.52
1	A	27	GLY	C-N	10.37	1.48	1.33
1	A	42	CYS	CA-C	-10.19	1.39	1.52
1	A	16	GLU	C-N	-10.04	1.18	1.33
1	A	54	GLU	N-CA	10.02	1.65	1.46
1	A	29	ASP	CA-CB	9.89	1.69	1.53
1	A	21	ASP	C-N	9.87	1.46	1.33
1	A	12	ILE	CA-CB	9.83	1.66	1.54
1	A	51	GLU	CD-OE1	9.83	1.44	1.25
1	A	17	ASP	CA-C	9.74	1.66	1.52
1	A	52	VAL	CA-CB	-9.68	1.42	1.53
1	A	36	ASP	CG-OD1	9.63	1.43	1.25
1	A	16	GLU	CB-CG	-9.61	1.23	1.52
1	A	45	GLY	N-CA	9.59	1.58	1.45
1	A	20	PRO	C-N	9.47	1.46	1.33
1	A	31	LYS	CA-CB	-9.34	1.36	1.53
1	A	42	CYS	C-O	9.29	1.35	1.23
1	A	46	LYS	C-N	9.27	1.46	1.33
1	A	47	ASP	C-N	9.20	1.46	1.33
1	A	22	ASP	CA-C	-8.88	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	GLU	CA-CB	-8.88	1.40	1.53
1	A	9	CYS	C-O	8.62	1.34	1.24
1	A	14	ASP	C-O	8.57	1.34	1.24
1	A	37	TRP	CA-C	8.57	1.64	1.52
1	A	11	TYR	CA-C	8.51	1.63	1.52
1	A	32	ASP	CB-CG	8.35	1.73	1.52
1	A	47	ASP	CG-OD2	8.27	1.41	1.25
1	A	22	ASP	CB-CG	8.25	1.72	1.52
1	A	21	ASP	CB-CG	8.18	1.72	1.52
1	A	33	ILE	N-CA	-8.15	1.37	1.47
1	A	54	GLU	CA-CB	8.12	1.69	1.53
1	A	27	GLY	C-O	-8.03	1.13	1.24
1	A	38	VAL	C-N	8.01	1.46	1.33
1	A	15	PRO	C-N	8.00	1.45	1.33
1	A	22	ASP	CG-OD1	7.93	1.40	1.25
1	A	26	PRO	CA-CB	7.92	1.64	1.53
1	A	6	CYS	CA-C	7.84	1.63	1.52
1	A	30	PHE	N-CA	7.66	1.55	1.46
1	A	35	ASP	CG-OD1	7.65	1.39	1.25
1	A	21	ASP	CA-C	-7.63	1.41	1.52
1	A	22	ASP	C-N	-7.51	1.23	1.33
1	A	42	CYS	C-N	7.49	1.45	1.33
1	A	31	LYS	CB-CG	-7.49	1.29	1.52
1	A	26	PRO	N-CA	7.44	1.56	1.47
1	A	49	PHE	CA-CB	-7.28	1.42	1.53
1	A	34	PRO	N-CD	7.27	1.57	1.47
1	A	14	ASP	CG-OD2	7.27	1.39	1.25
1	A	32	ASP	CA-C	-7.26	1.42	1.52
1	A	48	GLU	CA-C	-7.07	1.42	1.52
1	A	18	GLY	C-O	7.05	1.32	1.24
1	A	31	LYS	CG-CD	6.97	1.73	1.52
1	A	37	TRP	CD2-CE2	6.96	1.53	1.41
1	A	21	ASP	C-O	-6.93	1.15	1.24
1	A	5	THR	C-O	6.86	1.32	1.24
1	A	52	VAL	CB-CG1	-6.82	1.30	1.52
1	A	54	GLU	CA-C	6.82	1.67	1.52
1	A	29	ASP	CG-OD1	-6.80	1.12	1.25
1	A	49	PHE	CA-C	-6.74	1.43	1.52
1	A	34	PRO	CA-C	6.57	1.60	1.52
1	A	19	ASP	C-N	6.50	1.42	1.34
1	A	14	ASP	C-N	-6.34	1.24	1.33
1	A	51	GLU	CD-OE2	-6.22	1.13	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	50	GLU	N-CA	6.18	1.53	1.45
1	A	24	VAL	C-O	6.04	1.31	1.24
1	A	51	GLU	CA-C	-5.97	1.45	1.52
1	A	28	THR	C-O	5.95	1.31	1.24
1	A	8	VAL	N-CA	-5.84	1.38	1.46
1	A	2	LYS	C-O	5.84	1.31	1.23
1	A	20	PRO	CA-CB	5.84	1.62	1.53
1	A	13	TYR	C-O	-5.80	1.17	1.24
1	A	13	TYR	C-N	5.79	1.42	1.33
1	A	36	ASP	CB-CG	-5.79	1.37	1.52
1	A	11	TYR	CB-CG	5.72	1.64	1.51
1	A	7	THR	N-CA	5.68	1.53	1.46
1	A	15	PRO	N-CA	5.68	1.55	1.47
1	A	2	LYS	CG-CD	5.66	1.69	1.52
1	A	43	GLY	CA-C	-5.66	1.43	1.51
1	A	40	PRO	N-CA	5.59	1.54	1.47
1	A	25	ASN	CA-C	5.49	1.60	1.53
1	A	16	GLU	CD-OE2	5.42	1.35	1.25
1	A	12	ILE	CA-C	5.41	1.59	1.52
1	A	41	LEU	CA-C	-5.38	1.46	1.52
1	A	46	LYS	CA-CB	5.36	1.62	1.53
1	A	28	THR	CA-CB	5.34	1.60	1.53
1	A	47	ASP	CG-OD1	5.32	1.35	1.25
1	A	20	PRO	C-O	-5.30	1.17	1.24
1	A	11	TYR	CE1-CZ	5.26	1.50	1.38
1	A	15	PRO	CA-CB	5.24	1.61	1.53
1	A	37	TRP	NE1-CE2	-5.19	1.31	1.37
1	A	2	LYS	CA-C	-5.16	1.46	1.52
1	A	37	TRP	CD2-CE3	-5.16	1.32	1.40
1	A	11	TYR	CA-CB	-5.11	1.45	1.53
1	A	7	THR	CB-OG1	5.09	1.51	1.43
1	A	52	VAL	C-O	5.08	1.31	1.23
1	A	22	ASP	CA-CB	5.03	1.60	1.53
1	A	47	ASP	CA-C	-5.01	1.45	1.52
1	A	40	PRO	CA-C	5.01	1.59	1.52

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	GLU	N-CA-C	-38.71	46.14	109.24
1	A	53	GLU	CG-CD-OE2	-30.23	48.88	118.40
1	A	53	GLU	O-C-N	-27.85	91.80	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	MET	N-CA-CB	24.85	152.74	110.50
1	A	51	GLU	CG-CD-OE1	-24.79	61.38	118.40
1	A	2	LYS	CA-CB-CG	24.36	162.82	114.10
1	A	50	GLU	OE1-CD-OE2	20.84	172.91	122.90
1	A	53	GLU	CA-C-O	19.02	141.16	120.43
1	A	17	ASP	CB-CG-OD1	-18.73	75.32	118.40
1	A	14	ASP	CA-CB-CG	-17.51	95.09	112.60
1	A	54	GLU	CB-CA-C	-17.47	76.91	110.10
1	A	51	GLU	CG-CD-OE2	-16.92	79.48	118.40
1	A	32	ASP	OD1-CG-OD2	16.56	162.65	122.90
1	A	50	GLU	CG-CD-OE1	-16.23	81.08	118.40
1	A	21	ASP	N-CA-C	15.36	132.30	112.34
1	A	53	GLU	CB-CA-C	15.34	135.06	109.75
1	A	1	MET	CA-CB-CG	-14.72	84.66	114.10
1	A	18	GLY	CA-C-N	14.69	136.03	122.37
1	A	18	GLY	C-N-CA	14.69	136.03	122.37
1	A	27	GLY	CA-C-O	14.53	136.85	119.13
1	A	1	MET	CA-C-N	-14.52	97.36	122.92
1	A	1	MET	C-N-CA	-14.52	97.36	122.92
1	A	53	GLU	CB-CG-CD	-14.41	88.10	112.60
1	A	48	GLU	CG-CD-OE2	14.40	151.52	118.40
1	A	22	ASP	CA-CB-CG	13.20	125.80	112.60
1	A	21	ASP	CA-C-O	13.11	135.08	119.61
1	A	18	GLY	O-C-N	-13.02	108.17	122.62
1	A	49	PHE	O-C-N	-12.85	108.67	123.06
1	A	31	LYS	CD-CE-NZ	-12.67	71.36	111.90
1	A	5	THR	CA-CB-CG2	12.63	131.97	110.50
1	A	41	LEU	O-C-N	-12.33	107.81	122.11
1	A	48	GLU	OE1-CD-OE2	-12.17	93.69	122.90
1	A	14	ASP	CB-CG-OD2	-12.04	90.71	118.40
1	A	16	GLU	N-CA-C	11.48	126.55	112.54
1	A	53	GLU	N-CA-CB	-11.42	91.82	110.43
1	A	2	LYS	N-CA-CB	-11.40	93.30	110.85
1	A	21	ASP	OD1-CG-OD2	-11.40	95.55	122.90
1	A	53	GLU	CA-C-N	-11.39	101.20	121.70
1	A	53	GLU	C-N-CA	-11.39	101.20	121.70
1	A	16	GLU	CA-CB-CG	-10.97	92.15	114.10
1	A	50	GLU	CG-CD-OE2	-10.95	93.21	118.40
1	A	16	GLU	O-C-N	10.94	137.08	122.43
1	A	45	GLY	CA-C-O	10.78	138.36	122.62
1	A	47	ASP	OD1-CG-OD2	-10.64	97.37	122.90
1	A	47	ASP	CB-CG-OD2	10.43	142.38	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	ASP	CB-CG-OD1	-10.21	94.91	118.40
1	A	32	ASP	CB-CG-OD1	-10.15	95.05	118.40
1	A	41	LEU	CD1-CG-CD2	10.13	133.09	110.80
1	A	36	ASP	CB-CG-OD2	10.11	141.64	118.40
1	A	7	THR	OG1-CB-CG2	10.04	129.39	109.30
1	A	32	ASP	CA-CB-CG	10.00	122.60	112.60
1	A	42	CYS	O-C-N	-9.94	110.45	122.48
1	A	17	ASP	N-CA-CB	9.69	124.86	110.33
1	A	5	THR	OG1-CB-CG2	9.53	128.36	109.30
1	A	1	MET	CB-CA-C	-9.51	92.04	110.10
1	A	41	LEU	CA-C-O	-9.49	110.83	120.80
1	A	40	PRO	CA-N-CD	-9.48	98.73	112.00
1	A	12	ILE	N-CA-C	9.17	121.10	107.80
1	A	1	MET	N-CA-C	-9.09	85.56	111.00
1	A	52	VAL	CA-C-N	9.04	135.19	122.72
1	A	52	VAL	C-N-CA	9.04	135.19	122.72
1	A	22	ASP	N-CA-C	9.02	123.00	112.72
1	A	17	ASP	CA-C-O	9.01	130.14	119.60
1	A	51	GLU	CB-CA-C	-9.00	94.27	109.65
1	A	29	ASP	OD1-CG-OD2	-8.99	101.33	122.90
1	A	17	ASP	N-CA-C	8.98	124.67	112.90
1	A	46	LYS	N-CA-C	8.61	122.88	112.38
1	A	14	ASP	CA-C-O	-8.44	112.65	119.99
1	A	27	GLY	N-CA-C	8.34	126.89	115.30
1	A	20	PRO	CA-C-O	8.32	132.85	119.86
1	A	14	ASP	O-C-N	8.31	129.64	120.83
1	A	19	ASP	O-C-N	-8.25	115.17	121.19
1	A	16	GLU	N-CA-CB	-8.17	96.82	110.39
1	A	52	VAL	N-CA-C	-8.16	94.67	107.15
1	A	15	PRO	N-CD-CG	-8.13	91.00	103.20
1	A	3	LYS	CG-CD-CE	8.05	129.82	111.30
1	A	36	ASP	OD1-CG-OD2	-8.00	103.70	122.90
1	A	29	ASP	CB-CG-OD1	7.91	136.58	118.40
1	A	38	VAL	CA-C-O	7.77	129.83	121.67
1	A	53	GLU	OE1-CD-OE2	7.75	141.51	122.90
1	A	33	ILE	CB-CA-C	-7.75	102.52	110.89
1	A	1	MET	CA-C-O	7.68	133.85	120.80
1	A	51	GLU	CA-C-O	7.64	129.71	121.16
1	A	14	ASP	CB-CG-OD1	7.62	135.93	118.40
1	A	36	ASP	CA-CB-CG	-7.61	104.99	112.60
1	A	12	ILE	CA-CB-CG2	7.48	123.21	110.50
1	A	15	PRO	CB-CG-CD	7.48	130.03	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	PRO	N-CD-CG	7.21	114.01	103.20
1	A	7	THR	O-C-N	7.18	132.92	122.43
1	A	5	THR	CA-CB-OG1	-7.18	98.83	109.60
1	A	12	ILE	CB-CA-C	-7.18	100.48	110.96
1	A	9	CYS	O-C-N	-7.17	114.81	122.19
1	A	27	GLY	O-C-N	-7.17	113.45	122.41
1	A	11	TYR	CA-C-N	-7.08	113.91	123.12
1	A	11	TYR	C-N-CA	-7.08	113.91	123.12
1	A	32	ASP	CB-CG-OD2	-7.06	102.15	118.40
1	A	17	ASP	CB-CG-OD2	-7.06	102.16	118.40
1	A	51	GLU	OE1-CD-OE2	6.90	139.46	122.90
1	A	11	TYR	CG-CD1-CE1	-6.88	110.89	121.20
1	A	33	ILE	CA-C-N	6.83	126.87	119.90
1	A	33	ILE	C-N-CA	6.83	126.87	119.90
1	A	39	CYS	CA-C-N	6.71	126.50	119.05
1	A	39	CYS	C-N-CA	6.71	126.50	119.05
1	A	7	THR	CA-CB-OG1	-6.69	99.56	109.60
1	A	49	PHE	CA-C-N	6.68	133.05	122.62
1	A	49	PHE	C-N-CA	6.68	133.05	122.62
1	A	1	MET	CB-CG-SD	-6.67	92.69	112.70
1	A	26	PRO	N-CD-CG	-6.66	93.21	103.20
1	A	37	TRP	CE2-CD2-CG	-6.66	99.21	107.20
1	A	17	ASP	OD1-CG-OD2	6.65	138.86	122.90
1	A	22	ASP	N-CA-CB	-6.63	100.82	110.70
1	A	7	THR	CA-C-O	-6.60	110.66	119.11
1	A	17	ASP	CB-CA-C	-6.59	96.43	109.67
1	A	16	GLU	CB-CG-CD	-6.51	101.53	112.60
1	A	46	LYS	CA-C-O	6.50	127.36	119.49
1	A	32	ASP	O-C-N	-6.46	113.46	122.37
1	A	31	LYS	CA-C-O	-6.32	111.84	119.49
1	A	40	PRO	N-CA-C	-6.27	104.81	113.53
1	A	41	LEU	CA-C-N	6.26	132.37	122.11
1	A	41	LEU	C-N-CA	6.26	132.37	122.11
1	A	47	ASP	CA-CB-CG	-6.26	106.34	112.60
1	A	19	ASP	CA-C-O	6.24	127.21	121.34
1	A	41	LEU	CB-CG-CD1	-6.20	92.09	110.70
1	A	22	ASP	O-C-N	6.15	129.92	122.35
1	A	43	GLY	N-CA-C	6.09	123.72	115.32
1	A	47	ASP	CA-C-O	6.06	126.92	119.05
1	A	1	MET	CG-SD-CE	6.04	114.20	100.90
1	A	30	PHE	CE1-CZ-CE2	6.04	130.87	120.00
1	A	42	CYS	CA-C-O	5.98	125.37	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	ASP	O-C-N	-5.97	114.22	122.46
1	A	15	PRO	O-C-N	-5.97	114.95	122.17
1	A	5	THR	N-CA-CB	-5.95	100.48	110.83
1	A	54	GLU	CA-CB-CG	5.95	125.99	114.10
1	A	41	LEU	CB-CA-C	5.94	120.66	110.86
1	A	20	PRO	O-C-N	-5.91	115.13	122.23
1	A	37	TRP	O-C-N	5.89	129.82	122.86
1	A	26	PRO	N-CA-CB	-5.89	98.38	103.32
1	A	20	PRO	N-CA-C	5.87	121.69	113.53
1	A	31	LYS	CA-CB-CG	5.82	125.75	114.10
1	A	39	CYS	O-C-N	5.79	126.46	121.30
1	A	34	PRO	N-CA-CB	5.79	108.34	103.25
1	A	11	TYR	CD1-CG-CD2	5.76	126.74	118.10
1	A	30	PHE	N-CA-C	5.69	117.93	111.11
1	A	23	GLY	O-C-N	-5.65	115.35	122.41
1	A	44	VAL	N-CA-CB	5.56	120.22	110.49
1	A	4	TYR	CB-CG-CD2	5.50	129.06	120.80
1	A	44	VAL	CA-C-O	-5.49	114.84	121.54
1	A	49	PHE	CD1-CE1-CZ	-5.49	110.12	120.00
1	A	32	ASP	N-CA-CB	-5.44	102.11	110.44
1	A	33	ILE	O-C-N	-5.40	115.13	121.07
1	A	52	VAL	CG1-CB-CG2	5.32	122.49	110.80
1	A	12	ILE	CA-C-O	-5.31	114.85	120.53
1	A	7	THR	CB-CA-C	5.26	120.41	109.95
1	A	54	GLU	N-CA-C	-5.25	96.30	111.00
1	A	31	LYS	CB-CG-CD	5.20	123.25	111.30
1	A	43	GLY	CA-C-O	5.17	124.85	119.06
1	A	37	TRP	CB-CG-CD2	-5.17	119.57	126.80
1	A	33	ILE	N-CA-CB	5.15	114.87	110.08
1	A	41	LEU	N-CA-C	-5.15	104.60	111.24
1	A	4	TYR	OH-CZ-CE2	-5.10	104.61	119.90
1	A	49	PHE	CG-CD1-CE1	5.09	129.35	120.70
1	A	37	TRP	CG-CD2-CE3	5.05	138.95	133.90
1	A	31	LYS	CG-CD-CE	5.02	122.85	111.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	5	THR	CB

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	MET	Mainchain
1	A	14	ASP	Sidechain
1	A	17	ASP	Sidechain
1	A	18	GLY	Mainchain
1	A	21	ASP	Sidechain
1	A	41	LEU	Mainchain
1	A	48	GLU	Sidechain
1	A	53	GLU	Sidechain,Mainchain

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	422	334	0	62	1
2	A	1	0	0	0	0
3	A	127	0	0	12	1
All	All	550	334	0	62	1

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 147.

All (62) 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:2:LYS:CA	1:A:2:LYS:CB	1.75	1.64
1:A:7:THR:CA	1:A:7:THR:CB	1.78	1.60
1:A:53:GLU:CA	1:A:53:GLU:C	1.82	1.51
1:A:52:VAL:CA	1:A:52:VAL:C	1.87	1.46
1:A:16:GLU:CA	1:A:16:GLU:CB	1.92	1.45
1:A:1:MET:CA	1:A:1:MET:C	1.90	1.44
1:A:41:LEU:CG	1:A:41:LEU:CD1	1.97	1.42
1:A:1:MET:SD	1:A:1:MET:CG	2.07	1.41
1:A:1:MET:CA	1:A:1:MET:N	1.83	1.40
1:A:21:ASP:OD2	1:A:21:ASP:CG	1.64	1.38
1:A:48:GLU:OE1	1:A:48:GLU:CD	1.68	1.36
1:A:41:LEU:CD1	3:A:128:HOH:O	1.71	1.32
1:A:53:GLU:C	1:A:53:GLU:N	1.87	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ILE:CD1	1:A:12:ILE:CB	2.10	1.30
1:A:1:MET:CG	1:A:1:MET:CB	2.09	1.30
1:A:17:ASP:CB	1:A:17:ASP:CG	2.10	1.24
1:A:1:MET:SD	1:A:1:MET:CE	2.34	1.16
1:A:50:GLU:CD	1:A:50:GLU:CG	2.18	1.16
1:A:16:GLU:CA	1:A:16:GLU:CG	2.32	1.06
1:A:41:LEU:CG	3:A:128:HOH:O	2.08	1.00
1:A:1:MET:CA	1:A:1:MET:CG	2.43	0.96
1:A:51:GLU:OE1	1:A:51:GLU:CG	2.13	0.96
1:A:51:GLU:CG	1:A:51:GLU:CD	2.40	0.94
1:A:1:MET:C	1:A:1:MET:CB	2.43	0.92
1:A:54:GLU:CG	3:A:160:HOH:O	2.18	0.90
1:A:2:LYS:CB	1:A:2:LYS:N	2.37	0.87
1:A:17:ASP:CB	1:A:17:ASP:OD1	2.24	0.85
1:A:41:LEU:CD1	1:A:41:LEU:CB	2.54	0.85
1:A:12:ILE:CD1	1:A:12:ILE:CG1	0.78	0.78
1:A:15:PRO:O	3:A:150:HOH:O	2.07	0.73
1:A:52:VAL:C	1:A:52:VAL:N	2.47	0.72
1:A:54:GLU:OE2	3:A:111:HOH:O	2.06	0.72
1:A:51:GLU:O	3:A:157:HOH:O	2.09	0.71
1:A:2:LYS:CD	3:A:163:HOH:O	2.40	0.70
1:A:1:MET:CA	1:A:2:LYS:N	2.55	0.70
1:A:16:GLU:CB	1:A:16:GLU:N	2.56	0.69
1:A:7:THR:CA	1:A:7:THR:CG2	2.69	0.68
1:A:15:PRO:CA	3:A:150:HOH:O	2.42	0.68
1:A:2:LYS:CB	1:A:2:LYS:C	2.66	0.67
1:A:1:MET:C	1:A:1:MET:N	2.53	0.65
1:A:53:GLU:CA	1:A:53:GLU:N	2.59	0.65
1:A:21:ASP:OD2	1:A:21:ASP:OD1	2.12	0.64
1:A:51:GLU:CG	1:A:51:GLU:OE2	2.46	0.64
1:A:12:ILE:CD1	1:A:12:ILE:CG2	2.78	0.61
1:A:50:GLU:CG	1:A:50:GLU:OE1	2.48	0.61
1:A:7:THR:CB	1:A:7:THR:N	2.63	0.61
1:A:52:VAL:C	1:A:52:VAL:CG1	2.73	0.60
1:A:52:VAL:C	1:A:52:VAL:CB	2.70	0.60
1:A:22:ASP:OD2	3:A:110:HOH:O	2.16	0.59
1:A:48:GLU:OE1	1:A:48:GLU:OE2	2.17	0.59
1:A:7:THR:CA	1:A:7:THR:OG1	2.52	0.56
1:A:41:LEU:CD2	3:A:124:HOH:O	2.53	0.56
1:A:16:GLU:CB	1:A:16:GLU:C	2.74	0.54
1:A:50:GLU:CG	1:A:50:GLU:OE2	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:SD	1:A:1:MET:CB	3.01	0.49
1:A:53:GLU:N	1:A:53:GLU:O	2.47	0.46
1:A:51:GLU:CB	3:A:141:HOH:O	2.64	0.45
1:A:17:ASP:CB	1:A:17:ASP:OD2	2.53	0.45
1:A:51:GLU:OE2	1:A:51:GLU:CB	2.66	0.43
1:A:1:MET:N	3:A:120:HOH:O	2.53	0.42
1:A:16:GLU:CG	1:A:16:GLU:N	2.78	0.41
1:A:51:GLU:CD	1:A:53:GLU:CD	2.89	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:GLU:OE1	3:A:93:HOH:O[5_554]	1.85	0.35

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	52/54 (96%)	51 (98%)	1 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	48/48 (100%)	45 (94%)	3 (6%)	16 1

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	31	LYS
1	A	54	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

Of 1 ligands modelled in this entry, 1 is 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	16:GLU	C	17:ASP	N	1.18

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.