



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:25 PM GMT

PDB ID : 4RXN
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

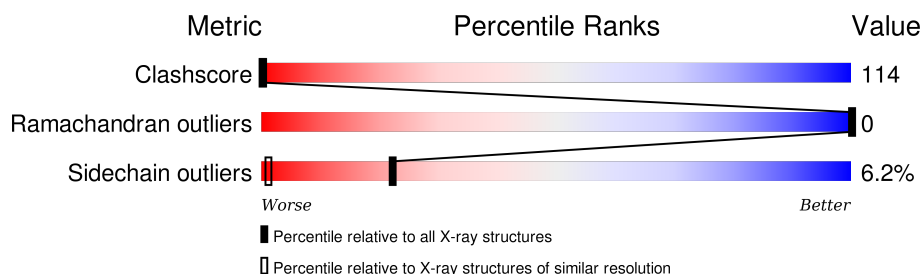
1 Overall quality at a glance

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	102246	1607 (1.26-1.14)
Ramachandran outliers	100387	1540 (1.26-1.14)
Sidechain outliers	100360	1538 (1.26-1.14)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	54	

2 Entry composition

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 (three-letter code: FE) (formula: Fe).

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

- Molecule 3 is water.

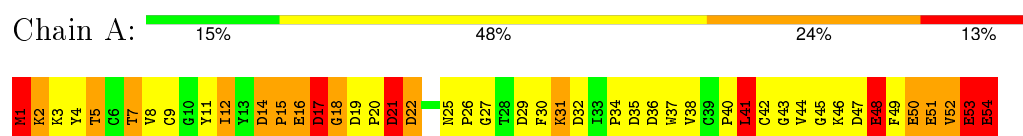
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	127	Total	O	0	0
			127	127		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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.

Note EDS was not executed.

- Molecule 1: RUBREDOXIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	64.29 Å 64.29 Å 32.49 Å 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 ⓘ

5.1 Standard geometry ⓘ

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	7.44	104/433 (24.0%)	6.61	135/588 (23.0%)

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	A	1	9

All (104) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	GLU	CG-CD	59.28	2.40	1.51
1	A	53	GLU	N-CA	56.79	2.60	1.46
1	A	50	GLU	CG-CD	44.61	2.18	1.51
1	A	48	GLU	CD-OE1	39.31	1.68	1.25
1	A	53	GLU	CD-OE2	36.79	1.66	1.25
1	A	50	GLU	CD-OE1	28.98	1.57	1.25
1	A	17	ASP	CB-CG	28.18	2.10	1.51
1	A	51	GLU	CB-CG	-24.81	1.05	1.52
1	A	2	LYS	CB-CG	-19.98	0.98	1.52
1	A	1	MET	N-CA	18.41	1.83	1.46
1	A	1	MET	CB-CG	18.20	2.09	1.51
1	A	16	GLU	CA-CB	17.39	1.92	1.53
1	A	21	ASP	CG-OD2	17.09	1.64	1.25
1	A	32	ASP	CG-OD2	-16.84	0.86	1.25
1	A	51	GLU	CD-OE1	16.70	1.44	1.25
1	A	16	GLU	CB-CG	-15.02	1.23	1.52
1	A	1	MET	CA-C	14.56	1.90	1.52
1	A	52	VAL	CA-C	13.21	1.87	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	41	LEU	CG-CD1	12.26	1.97	1.51
1	A	1	MET	C-O	-11.50	1.01	1.23
1	A	53	GLU	CA-C	11.25	1.82	1.52
1	A	53	GLU	C-O	11.22	1.44	1.23
1	A	51	GLU	CD-OE2	-11.01	1.13	1.25
1	A	52	VAL	CB-CG1	-10.86	1.30	1.52
1	A	5	THR	CB-CG2	-10.76	1.16	1.52
1	A	1	MET	C-N	10.69	1.58	1.34
1	A	12	ILE	CG1-CD1	-10.45	0.78	1.50
1	A	17	ASP	N-CA	-10.41	1.25	1.46
1	A	7	THR	C-O	10.21	1.42	1.23
1	A	1	MET	CG-SD	10.21	2.07	1.81
1	A	32	ASP	CB-CG	10.09	1.73	1.51
1	A	1	MET	SD-CE	10.06	2.34	1.77
1	A	22	ASP	CB-CG	9.97	1.72	1.51
1	A	21	ASP	CB-CG	9.88	1.72	1.51
1	A	37	TRP	CD2-CE2	9.85	1.53	1.41
1	A	2	LYS	CA-CB	9.85	1.75	1.53
1	A	7	THR	CA-CB	9.66	1.78	1.53
1	A	17	ASP	CG-OD1	9.63	1.47	1.25
1	A	11	TYR	CE1-CZ	9.48	1.50	1.38
1	A	54	GLU	N-CA	9.47	1.65	1.46
1	A	17	ASP	CG-OD2	-9.23	1.04	1.25
1	A	16	GLU	CD-OE2	9.09	1.35	1.25
1	A	12	ILE	N-CA	-8.81	1.28	1.46
1	A	4	TYR	CE1-CZ	-8.79	1.27	1.38
1	A	49	PHE	C-O	8.63	1.39	1.23
1	A	11	TYR	CB-CG	8.40	1.64	1.51
1	A	11	TYR	CE2-CZ	-8.38	1.27	1.38
1	A	31	LYS	CB-CG	-8.36	1.29	1.52
1	A	45	GLY	N-CA	8.07	1.58	1.46
1	A	4	TYR	CD2-CE2	8.01	1.51	1.39
1	A	26	PRO	CA-C	-7.98	1.36	1.52
1	A	41	LEU	C-O	7.97	1.38	1.23
1	A	36	ASP	CG-OD1	7.96	1.43	1.25
1	A	31	LYS	CA-CB	-7.82	1.36	1.53
1	A	42	CYS	N-CA	-7.64	1.31	1.46
1	A	44	VAL	N-CA	-7.59	1.31	1.46
1	A	4	TYR	CG-CD1	7.59	1.49	1.39
1	A	34	PRO	N-CD	7.20	1.57	1.47
1	A	29	ASP	CA-CB	7.18	1.69	1.53
1	A	54	GLU	CA-CB	7.16	1.69	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	VAL	CA-CB	6.89	1.69	1.54
1	A	16	GLU	CA-C	-6.85	1.35	1.52
1	A	47	ASP	CG-OD2	6.83	1.41	1.25
1	A	36	ASP	CB-CG	-6.75	1.37	1.51
1	A	16	GLU	C-N	-6.69	1.18	1.34
1	A	42	CYS	C-N	6.66	1.45	1.33
1	A	22	ASP	CG-OD1	6.55	1.40	1.25
1	A	42	CYS	C-O	6.42	1.35	1.23
1	A	35	ASP	CG-OD1	6.32	1.39	1.25
1	A	37	TRP	CE3-CZ3	6.28	1.49	1.38
1	A	27	GLY	C-O	-6.26	1.13	1.23
1	A	45	GLY	C-N	6.26	1.48	1.34
1	A	31	LYS	CG-CD	6.15	1.73	1.52
1	A	27	GLY	C-N	6.10	1.48	1.34
1	A	53	GLU	CA-CB	-6.01	1.40	1.53
1	A	14	ASP	CG-OD2	6.01	1.39	1.25
1	A	31	LYS	CE-NZ	5.98	1.64	1.49
1	A	9	CYS	C-O	5.95	1.34	1.23
1	A	4	TYR	CZ-OH	5.92	1.48	1.37
1	A	30	PHE	CG-CD1	5.90	1.47	1.38
1	A	14	ASP	C-O	5.78	1.34	1.23
1	A	52	VAL	CA-CB	-5.75	1.42	1.54
1	A	16	GLU	CD-OE1	5.75	1.31	1.25
1	A	8	VAL	CB-CG2	5.74	1.65	1.52
1	A	18	GLY	C-O	5.67	1.32	1.23
1	A	29	ASP	CG-OD1	-5.62	1.12	1.25
1	A	49	PHE	CG-CD2	-5.60	1.30	1.38
1	A	22	ASP	C-N	-5.57	1.23	1.33
1	A	37	TRP	CD2-CE3	-5.57	1.32	1.40
1	A	20	PRO	C-N	5.52	1.46	1.34
1	A	54	GLU	CA-C	5.51	1.67	1.52
1	A	46	LYS	C-N	5.49	1.46	1.34
1	A	49	PHE	CA-CB	-5.37	1.42	1.53
1	A	21	ASP	C-N	5.33	1.46	1.34
1	A	26	PRO	N-CA	5.27	1.56	1.47
1	A	11	TYR	CZ-OH	5.27	1.46	1.37
1	A	38	VAL	C-N	5.22	1.46	1.34
1	A	26	PRO	CA-CB	5.22	1.64	1.53
1	A	43	GLY	CA-C	-5.19	1.43	1.51
1	A	47	ASP	C-N	5.17	1.46	1.34
1	A	42	CYS	CA-C	-5.14	1.39	1.52
1	A	17	ASP	CA-C	5.11	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	ASP	CA-C	-5.08	1.39	1.52
1	A	14	ASP	C-N	-5.06	1.24	1.34

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	ASP	CB-CG-OD1	-47.76	75.32	118.30
1	A	50	GLU	OE1-CD-OE2	41.34	172.91	123.30
1	A	53	GLU	CG-CD-OE2	-34.71	48.88	118.30
1	A	14	ASP	CB-CG-OD2	-30.66	90.71	118.30
1	A	51	GLU	CG-CD-OE1	-28.46	61.38	118.30
1	A	47	ASP	CB-CG-OD2	26.76	142.38	118.30
1	A	22	ASP	CB-CG-OD1	-25.99	94.91	118.30
1	A	36	ASP	CB-CG-OD2	25.94	141.64	118.30
1	A	32	ASP	CB-CG-OD1	-25.83	95.05	118.30
1	A	48	GLU	OE1-CD-OE2	-24.67	93.69	123.30
1	A	53	GLU	N-CA-C	-24.02	46.14	111.00
1	A	1	MET	N-CA-CB	23.41	152.74	110.60
1	A	2	LYS	CA-CB-CG	22.46	162.82	113.40
1	A	32	ASP	OD1-CG-OD2	20.71	162.65	123.30
1	A	29	ASP	CB-CG-OD1	20.31	136.58	118.30
1	A	14	ASP	CB-CG-OD1	19.59	135.93	118.30
1	A	51	GLU	CG-CD-OE2	-19.41	79.48	118.30
1	A	53	GLU	O-C-N	-19.31	91.80	122.70
1	A	50	GLU	CG-CD-OE1	-18.61	81.08	118.30
1	A	32	ASP	CB-CG-OD2	-17.94	102.15	118.30
1	A	17	ASP	CB-CG-OD2	-17.93	102.16	118.30
1	A	31	LYS	CD-CE-NZ	-17.54	71.36	111.70
1	A	1	MET	CA-CB-CG	-16.85	84.66	113.30
1	A	54	GLU	CB-CA-C	-16.75	76.91	110.40
1	A	48	GLU	CG-CD-OE2	16.61	151.52	118.30
1	A	53	GLU	OE1-CD-OE2	15.17	141.51	123.30
1	A	21	ASP	OD1-CG-OD2	-14.61	95.55	123.30
1	A	5	THR	CA-CB-CG2	13.98	131.97	112.40
1	A	47	ASP	OD1-CG-OD2	-13.65	97.37	123.30
1	A	51	GLU	OE1-CD-OE2	13.46	139.46	123.30
1	A	4	TYR	CB-CG-CD2	13.43	129.06	121.00
1	A	11	TYR	CG-CD1-CE1	-13.02	110.89	121.30
1	A	50	GLU	CG-CD-OE2	-12.54	93.21	118.30
1	A	53	GLU	CB-CA-C	12.33	135.06	110.40
1	A	29	ASP	OD1-CG-OD2	-11.56	101.33	123.30
1	A	41	LEU	CB-CG-CD1	-11.12	92.09	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	MET	CA-C-N	-10.74	93.56	117.20
1	A	19	ASP	CB-CG-OD2	10.73	127.96	118.30
1	A	11	TYR	CB-CG-CD2	-10.58	114.65	121.00
1	A	53	GLU	N-CA-CB	-10.43	91.82	110.60
1	A	36	ASP	OD1-CG-OD2	-10.32	103.70	123.30
1	A	37	TRP	CE2-CD2-CG	-10.12	99.21	107.30
1	A	53	GLU	CA-C-O	10.03	141.16	120.10
1	A	45	GLY	CA-C-O	9.87	138.36	120.60
1	A	16	GLU	OE1-CD-OE2	-9.78	111.56	123.30
1	A	1	MET	C-N-CA	-9.73	97.36	121.70
1	A	53	GLU	CB-CG-CD	-9.66	88.10	114.20
1	A	16	GLU	CA-CB-CG	-9.66	92.15	113.40
1	A	22	ASP	CB-CG-OD2	9.65	126.98	118.30
1	A	2	LYS	N-CA-CB	-9.61	93.30	110.60
1	A	1	MET	N-CA-C	-9.42	85.56	111.00
1	A	41	LEU	O-C-N	-9.31	107.81	122.70
1	A	1	MET	CB-CA-C	-9.18	92.04	110.40
1	A	40	PRO	CA-N-CD	-9.12	98.73	111.50
1	A	18	GLY	O-C-N	-9.08	108.17	122.70
1	A	4	TYR	CZ-CE2-CD2	-9.04	111.66	119.80
1	A	27	GLY	CA-C-O	9.03	136.85	120.60
1	A	16	GLU	O-C-N	8.99	137.08	122.70
1	A	49	PHE	O-C-N	-8.77	108.67	122.70
1	A	1	MET	CG-SD-CE	8.75	114.20	100.20
1	A	7	THR	OG1-CB-CG2	8.43	129.39	110.00
1	A	14	ASP	CA-CB-CG	-8.32	95.09	113.40
1	A	49	PHE	CD1-CE1-CZ	-8.31	110.12	120.10
1	A	53	GLU	C-N-CA	-8.20	101.20	121.70
1	A	17	ASP	OD1-CG-OD2	8.19	138.86	123.30
1	A	15	PRO	N-CD-CG	-8.13	91.00	103.20
1	A	51	GLU	CB-CA-C	-8.07	94.27	110.40
1	A	11	TYR	CD1-CG-CD2	8.04	126.74	117.90
1	A	5	THR	OG1-CB-CG2	7.98	128.36	110.00
1	A	17	ASP	N-CA-CB	7.92	124.86	110.60
1	A	21	ASP	N-CA-C	7.89	132.30	111.00
1	A	49	PHE	CG-CD1-CE1	7.78	129.35	120.80
1	A	16	GLU	N-CA-CB	-7.65	96.82	110.60
1	A	35	ASP	CB-CG-OD2	7.57	125.11	118.30
1	A	41	LEU	CD1-CG-CD2	7.53	133.09	110.50
1	A	42	CYS	O-C-N	-7.50	110.45	123.20
1	A	52	VAL	CG1-CB-CG2	7.25	122.49	110.90
1	A	40	PRO	N-CD-CG	7.21	114.01	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	PHE	CD1-CE1-CZ	-7.14	111.53	120.10
1	A	21	ASP	CB-CG-OD1	7.14	124.72	118.30
1	A	21	ASP	CA-C-O	7.13	135.08	120.10
1	A	4	TYR	CB-CG-CD1	-7.07	116.76	121.00
1	A	17	ASP	CB-CA-C	-6.99	96.43	110.40
1	A	11	TYR	CG-CD2-CE2	-6.98	115.71	121.30
1	A	17	ASP	CA-C-N	-6.75	102.70	116.20
1	A	26	PRO	N-CD-CG	-6.66	93.21	103.20
1	A	1	MET	CB-CG-SD	-6.57	92.69	112.40
1	A	4	TYR	CG-CD2-CE2	6.56	126.55	121.30
1	A	1	MET	CA-C-O	6.55	133.85	120.10
1	A	37	TRP	CD1-CG-CD2	6.40	111.42	106.30
1	A	7	THR	O-C-N	6.39	132.92	122.70
1	A	12	ILE	CA-CB-CG2	6.16	123.21	110.90
1	A	52	VAL	N-CA-C	-6.05	94.67	111.00
1	A	30	PHE	CE1-CZ-CE2	6.04	130.87	120.00
1	A	15	PRO	CB-CG-CD	6.03	130.03	106.50
1	A	3	LYS	CG-CD-CE	5.97	129.82	111.90
1	A	9	CYS	CA-C-N	5.95	128.10	116.20
1	A	11	TYR	CB-CG-CD1	-5.95	117.43	121.00
1	A	22	ASP	OD1-CG-OD2	5.78	134.29	123.30
1	A	27	GLY	O-C-N	-5.78	113.45	122.70
1	A	32	ASP	O-C-N	-5.78	113.46	122.70
1	A	16	GLU	N-CA-C	5.76	126.55	111.00
1	A	4	TYR	OH-CZ-CE2	-5.74	104.61	120.10
1	A	18	GLY	C-N-CA	5.73	136.03	121.70
1	A	54	GLU	CA-CB-CG	5.72	125.99	113.40
1	A	41	LEU	CB-CG-CD2	5.71	120.72	111.00
1	A	53	GLU	CG-CD-OE1	5.68	129.67	118.30
1	A	22	ASP	CA-CB-CG	5.64	125.80	113.40
1	A	21	ASP	CA-C-N	-5.63	104.82	117.20
1	A	16	GLU	CA-C-N	-5.62	104.83	117.20
1	A	37	TRP	CG-CD2-CE3	5.61	138.95	133.90
1	A	31	LYS	CA-CB-CG	5.61	125.75	113.40
1	A	11	TYR	CZ-CE2-CD2	5.56	124.81	119.80
1	A	21	ASP	CB-CG-OD2	-5.56	113.29	118.30
1	A	12	ILE	CB-CA-C	-5.56	100.48	111.60
1	A	44	VAL	CG1-CB-CG2	5.54	119.76	110.90
1	A	27	GLY	N-CA-C	5.52	126.89	113.10
1	A	41	LEU	CB-CA-C	5.51	120.66	110.20
1	A	12	ILE	CG1-CB-CG2	-5.45	99.41	111.40
1	A	54	GLU	N-CA-C	-5.44	96.30	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	ASP	N-CA-CB	-5.43	100.82	110.60
1	A	45	GLY	CA-C-N	-5.42	105.28	117.20
1	A	37	TRP	CB-CG-CD2	-5.41	119.57	126.60
1	A	54	GLU	CA-C-O	5.41	131.46	120.10
1	A	52	VAL	C-N-CA	5.40	135.19	121.70
1	A	16	GLU	CG-CD-OE2	5.38	129.05	118.30
1	A	19	ASP	CB-CG-OD1	-5.35	113.48	118.30
1	A	47	ASP	O-C-N	-5.30	114.22	122.70
1	A	20	PRO	CA-C-O	5.27	132.85	120.20
1	A	41	LEU	CA-C-N	5.20	128.64	117.20
1	A	8	VAL	CA-CB-CG2	-5.20	103.10	110.90
1	A	5	THR	N-CA-CB	-5.17	100.48	110.30
1	A	25	ASN	CB-CG-OD1	-5.16	111.27	121.60
1	A	18	GLY	CA-C-N	5.11	128.45	117.20
1	A	17	ASP	N-CA-C	5.06	124.67	111.00

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 ⓘ

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	368	90	1
2	A	1	0	0	0	0
3	A	127	0	0	23	1
All	All	550	334	368	90	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 114.

All (90) 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	1.46
1:A:16:GLU:CB	1:A:16:GLU:CA	1.92	1.45
1:A:41:LEU:CG	1:A:41:LEU:CD1	1.97	1.42
1:A:52:VAL:CA	1:A:52:VAL:C	1.87	1.42
1:A:1:MET:SD	1:A:1:MET:CG	2.07	1.41
1:A:1:MET:C	1:A:1:MET:CA	1.90	1.40
1:A:1:MET:N	1:A:1:MET:CA	1.83	1.40
1:A:21:ASP:OD2	1:A:21:ASP:CG	1.64	1.34
1:A:48:GLU:CD	1:A:48:GLU:OE1	1.68	1.32
1:A:41:LEU:CD1	3:A:128:HOH:O	1.71	1.32
1:A:12:ILE:CD1	1:A:12:ILE:CB	2.10	1.30
1:A:1:MET:CB	1:A:1:MET:CG	2.09	1.30
1:A:53:GLU:N	1:A:53:GLU:C	1.87	1.27
1:A:17:ASP:CB	1:A:17:ASP:CG	2.10	1.19
1:A:1:MET:SD	1:A:1:MET:CE	2.34	1.16
1:A:1:MET:HA	1:A:1:MET:CG	1.74	1.15
1:A:50:GLU:CG	1:A:50:GLU:CD	2.18	1.11
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:41:LEU:HD11	3:A:128:HOH:O	1.40	1.00
1:A:2:LYS:HD3	3:A:163:HOH:O	1.63	0.96
1:A:1:MET:CG	1:A:1:MET:CA	2.43	0.96
1:A:51:GLU:OE1	1:A:51:GLU:CG	2.13	0.96
1:A:12:ILE:HD11	1:A:12:ILE:CG1	1.43	0.95
1:A:12:ILE:CG1	1:A:12:ILE:HD12	1.43	0.95
1:A:12:ILE:HD13	1:A:12:ILE:CG1	1.43	0.93
1:A:12:ILE:CD1	1:A:12:ILE:HG12	1.42	0.93
1:A:12:ILE:CD1	1:A:12:ILE:HG13	1.42	0.92
1:A:54:GLU:CG	3:A:160:HOH:O	2.18	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:GLU:CG	1:A:51:GLU:CD	2.40	0.89
1:A:15:PRO:HA	3:A:150:HOH:O	1.73	0.87
1:A:54:GLU:HG3	3:A:160:HOH:O	1.75	0.87
1:A:1:MET:C	1:A:1:MET:CB	2.43	0.87
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:CB	1:A:41:LEU:CD1	2.54	0.85
1:A:51:GLU:HB3	3:A:141:HOH:O	1.83	0.79
1:A:12:ILE:CD1	1:A:12:ILE:CG1	0.78	0.78
1:A:2:LYS:HB2	1:A:2:LYS:CA	2.08	0.77
1:A:16:GLU:HG2	1:A:16:GLU:CA	2.13	0.75
1:A:2:LYS:CA	1:A:2:LYS:HB3	2.08	0.75
1:A:54:GLU:HG2	3:A:160:HOH:O	1.82	0.75
1:A:15:PRO:O	3:A:150:HOH:O	2.07	0.73
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: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:1:MET:HG3	1:A:1:MET:HA	1.73	0.69
1:A:7:THR:CA	1:A:7:THR:CG2	2.69	0.68
1:A:52:VAL:N	1:A:52:VAL:C	2.47	0.68
1:A:52:VAL:C	1:A:52:VAL:HG12	2.15	0.67
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:41:LEU:HB3	1:A:41:LEU:CD1	2.26	0.64
1:A:41:LEU:HG	3:A:128:HOH:O	1.86	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:1:MET:C	1:A:1:MET:N	2.53	0.60
1:A:22:ASP:OD2	3:A:110:HOH:O	2.16	0.59
1:A:48:GLU:OE2	1:A:48:GLU:OE1	2.17	0.59
1:A:52:VAL:CG1	1:A:52:VAL:C	2.73	0.57
1:A:52:VAL:CB	1:A:52:VAL:C	2.70	0.56
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:15:PRO:CA	3:A:150:HOH:O	2.42	0.55
1:A:1:MET:HE3	3:A:147:HOH:O	2.09	0.52
1:A:2:LYS:C	1:A:2:LYS:CB	2.66	0.52
1:A:2:LYS:CD	3:A:163:HOH:O	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:GLU:CG	1:A:48:GLU:OE1	2.56	0.50
1:A:50:GLU:CG	1:A:50:GLU:OE2	2.60	0.49
1:A:1:MET:SD	1:A:1:MET:CB	3.01	0.49
1:A:2:LYS:HE2	3:A:166:HOH:O	2.13	0.48
1:A:12:ILE:HD13	1:A:12:ILE:CG2	2.42	0.48
1:A:41:LEU:HD23	3:A:124:HOH:O	2.13	0.48
1:A:2:LYS:HG3	3:A:141:HOH:O	2.14	0.48
1:A:12:ILE:HD13	1:A:12:ILE:HG21	1.96	0.48
1:A:53:GLU:HG3	3:A:121:HOH:O	2.13	0.47
1:A:17:ASP:CB	1:A:17:ASP:OD2	2.53	0.47
1:A:5:THR:HG22	1:A:52:VAL:CG2	2.45	0.46
1:A:51:GLU:HB3	1:A:51:GLU:OE2	2.15	0.46
1:A:53:GLU:O	1:A:53:GLU:N	2.47	0.46
1:A:53:GLU:CA	1:A:54:GLU:N	2.70	0.45
1:A:17:ASP:HB2	1:A:17:ASP:OD1	2.12	0.43
1:A:51:GLU:CB	1:A:51:GLU:OE2	2.66	0.43
1:A:41:LEU:HB3	3:A:156:HOH:O	2.20	0.42
1:A:16:GLU:N	1:A:16:GLU:CG	2.78	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 [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	52/54 (96%)	51 (98%)	1 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	48/48 (100%)	45 (94%)	3 (6%)	22 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

Some 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 carbohydrates 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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.