



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 04:36 pm BST

PDB ID : 1FG4
Title : STRUCTURE OF TRYPAREDOXIN II
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Deposited on : 2000-07-28
Resolution : 1.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

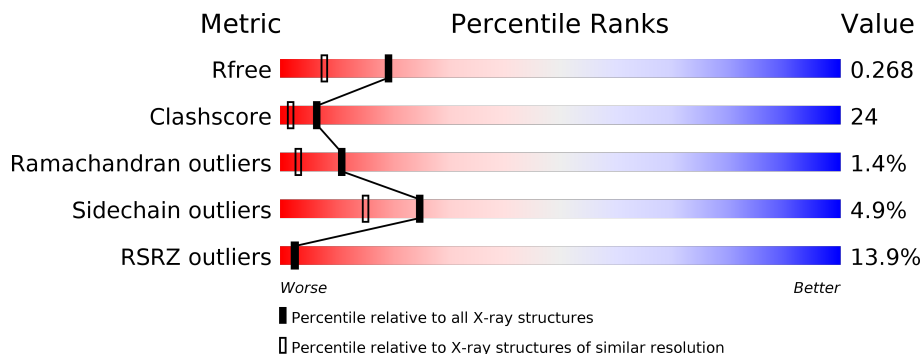
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 1.90 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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	149	
1	B	149	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2471 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 TRYPAREDOXIN II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	145	1153	758	179	210	6	0	0	0
1	B	143	1140	750	177	207	6	0	0	0

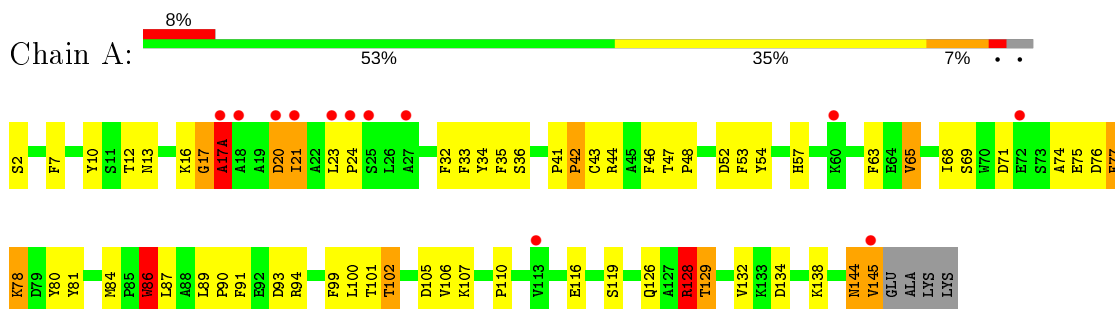
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	105	105	105	0	0
2	B	73	73	73	0	0

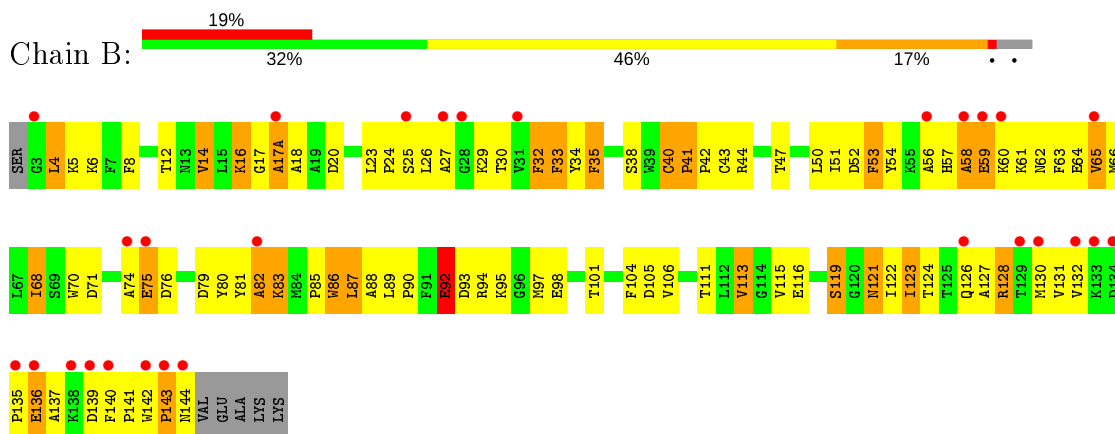
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: TRYPAREDOXIN II



- Molecule 1: TRYPAREDOXIN II



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	109.28Å 109.28Å 55.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.00 – 1.90 27.75 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.0 (77.00-1.90) 93.0 (27.75-1.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.69 (at 1.91Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.204 , 0.263 0.209 , 0.268	Depositor DCC
R_{free} test set	1253 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	21.0	Xtrriage
Anisotropy	0.409	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2471	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage'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

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	1.69	14/1190 (1.2%)	2.53	71/1617 (4.4%)
1	B	1.43	5/1177 (0.4%)	2.46	66/1599 (4.1%)
All	All	1.56	19/2367 (0.8%)	2.49	137/3216 (4.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	TYR	CG-CD2	7.74	1.49	1.39
1	B	40	CYS	CB-SG	-7.46	1.69	1.82
1	A	34	TYR	CE1-CZ	7.06	1.47	1.38
1	A	69	SER	CA-CB	6.24	1.62	1.52
1	B	41	PRO	CA-CB	6.21	1.66	1.53
1	A	35	PHE	CG-CD1	-5.95	1.29	1.38
1	A	128	ARG	CZ-NH1	5.87	1.40	1.33
1	A	86	TRP	CD2-CE2	-5.69	1.34	1.41
1	A	110	PRO	CA-C	5.68	1.64	1.52
1	A	128	ARG	CG-CD	-5.60	1.38	1.51
1	A	53	PHE	CD2-CE2	5.18	1.49	1.39
1	A	10	TYR	CG-CD2	-5.15	1.32	1.39
1	A	32	PHE	C-O	5.11	1.33	1.23
1	A	36	SER	CA-CB	5.09	1.60	1.52
1	B	41	PRO	N-CD	5.07	1.54	1.47
1	A	43	CYS	CB-SG	5.06	1.90	1.82
1	B	5	LYS	N-CA	-5.04	1.36	1.46
1	A	99	PHE	CG-CD1	5.04	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	14	VAL	CB-CG1	5.03	1.63	1.52

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	ARG	NE-CZ-NH1	14.88	127.74	120.30
1	A	44	ARG	NE-CZ-NH2	-13.43	113.58	120.30
1	A	134	ASP	CB-CG-OD2	13.35	130.31	118.30
1	B	92	GLU	OE1-CD-OE2	-13.21	107.44	123.30
1	A	71	ASP	CB-CG-OD1	13.02	130.02	118.30
1	B	71	ASP	CB-CG-OD2	12.34	129.40	118.30
1	B	44	ARG	NE-CZ-NH1	12.09	126.34	120.30
1	A	76	ASP	CB-CG-OD2	11.89	129.00	118.30
1	B	33	PHE	CB-CG-CD1	-11.87	112.49	120.80
1	B	79	ASP	CB-CG-OD1	-11.53	107.92	118.30
1	B	88	ALA	CB-CA-C	-11.34	93.09	110.10
1	A	20	ASP	CB-CG-OD2	-11.14	108.27	118.30
1	A	128	ARG	NE-CZ-NH2	-10.79	114.91	120.30
1	B	92	GLU	CG-CD-OE1	10.77	139.84	118.30
1	A	144	ASN	OD1-CG-ND2	-10.54	97.66	121.90
1	B	12	THR	CA-CB-CG2	-10.27	98.03	112.40
1	A	116	GLU	OE1-CD-OE2	10.16	135.49	123.30
1	B	33	PHE	CZ-CE2-CD2	-10.15	107.92	120.10
1	A	138	LYS	CA-CB-CG	10.08	135.57	113.40
1	A	63	PHE	CB-CG-CD1	10.02	127.81	120.80
1	A	94	ARG	NE-CZ-NH2	-9.73	115.44	120.30
1	B	35	PHE	CB-CG-CD2	-9.66	114.04	120.80
1	A	144	ASN	CB-CG-ND2	9.59	139.72	116.70
1	B	33	PHE	CG-CD1-CE1	-9.56	110.28	120.80
1	A	145	VAL	CA-CB-CG1	-9.53	96.61	110.90
1	B	80	TYR	N-CA-CB	-8.96	94.47	110.60
1	B	14	VAL	CA-CB-CG2	8.93	124.30	110.90
1	B	94	ARG	NE-CZ-NH1	-8.79	115.90	120.30
1	B	52	ASP	CB-CG-OD2	-8.78	110.40	118.30
1	A	34	TYR	CB-CG-CD1	8.55	126.13	121.00
1	A	44	ARG	CD-NE-CZ	8.49	135.48	123.60
1	B	93	ASP	CB-CG-OD2	8.48	125.94	118.30
1	A	34	TYR	CZ-CE2-CD2	8.43	127.38	119.80
1	A	144	ASN	CA-C-O	8.26	137.45	120.10
1	B	34	TYR	CB-CG-CD1	-8.15	116.11	121.00
1	A	65	VAL	CG1-CB-CG2	8.10	123.86	110.90
1	B	83	LYS	N-CA-CB	-8.10	96.02	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	VAL	CA-C-O	7.87	136.63	120.10
1	B	101	THR	CA-CB-CG2	-7.86	101.39	112.40
1	B	139	ASP	CB-CG-OD1	-7.72	111.35	118.30
1	B	8	PHE	CB-CG-CD1	7.68	126.18	120.80
1	B	105	ASP	CB-CG-OD1	7.67	125.20	118.30
1	A	35	PHE	CB-CG-CD2	-7.56	115.51	120.80
1	A	34	TYR	CG-CD1-CE1	7.45	127.26	121.30
1	A	46	PHE	CB-CG-CD2	-7.35	115.66	120.80
1	B	94	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	A	101	THR	O-C-N	7.30	134.38	122.70
1	B	32	PHE	CB-CG-CD2	-7.23	115.74	120.80
1	A	12	THR	CA-CB-CG2	-7.08	102.48	112.40
1	A	102	THR	OG1-CB-CG2	-7.02	93.86	110.00
1	A	7	PHE	CB-CG-CD2	-6.97	115.92	120.80
1	A	52	ASP	CB-CG-OD2	-6.95	112.05	118.30
1	A	128	ARG	CB-CG-CD	6.88	129.49	111.60
1	B	92	GLU	CB-CG-CD	6.79	132.53	114.20
1	A	63	PHE	CB-CG-CD2	-6.76	116.07	120.80
1	B	113	VAL	CA-CB-CG2	-6.73	100.81	110.90
1	A	35	PHE	CB-CG-CD1	6.72	125.51	120.80
1	B	79	ASP	CA-C-O	-6.70	106.03	120.10
1	A	20	ASP	CA-C-O	6.63	134.02	120.10
1	A	144	ASN	O-C-N	-6.57	112.19	122.70
1	B	139	ASP	CB-CG-OD2	6.52	124.17	118.30
1	B	71	ASP	CB-CG-OD1	-6.52	112.43	118.30
1	B	111	THR	O-C-N	6.52	133.14	122.70
1	A	34	TYR	CG-CD2-CE2	-6.51	116.09	121.30
1	A	53	PHE	CB-CG-CD2	-6.47	116.27	120.80
1	B	33	PHE	CA-C-O	-6.38	106.69	120.10
1	B	66	MET	N-CA-CB	-6.38	99.11	110.60
1	B	76	ASP	CB-CG-OD1	-6.38	112.56	118.30
1	B	98	GLU	CG-CD-OE1	6.36	131.02	118.30
1	A	99	PHE	CG-CD1-CE1	-6.31	113.86	120.80
1	B	35	PHE	O-C-N	6.17	132.57	122.70
1	A	107	LYS	CB-CG-CD	6.16	127.62	111.60
1	A	20	ASP	OD1-CG-OD2	6.07	134.84	123.30
1	A	102	THR	CA-CB-OG1	6.05	121.70	109.00
1	B	66	MET	CA-CB-CG	6.01	123.52	113.30
1	B	87	LEU	O-C-N	6.01	132.32	122.70
1	B	68	ILE	O-C-N	5.99	132.29	122.70
1	A	33	PHE	CB-CG-CD2	5.98	124.99	120.80
1	A	128	ARG	NH1-CZ-NH2	5.97	125.97	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	33	PHE	O-C-N	5.96	132.24	122.70
1	A	134	ASP	OD1-CG-OD2	-5.95	111.99	123.30
1	A	80	TYR	CB-CG-CD2	-5.93	117.44	121.00
1	B	122	ILE	CA-CB-CG1	-5.92	99.75	111.00
1	B	18	ALA	CB-CA-C	-5.92	101.23	110.10
1	A	77	PHE	CB-CG-CD2	5.90	124.93	120.80
1	A	99	PHE	CD1-CE1-CZ	5.90	127.18	120.10
1	B	32	PHE	C-N-CA	-5.89	106.98	121.70
1	A	17	GLY	CA-C-N	-5.88	104.26	117.20
1	B	33	PHE	CD1-CG-CD2	5.88	125.95	118.30
1	B	79	ASP	OD1-CG-OD2	5.88	134.47	123.30
1	A	65	VAL	N-CA-CB	5.87	124.42	111.50
1	B	116	GLU	CG-CD-OE2	-5.86	106.58	118.30
1	A	86	TRP	CD2-CE2-CZ2	5.85	129.32	122.30
1	B	122	ILE	O-C-N	5.83	132.03	122.70
1	A	21	ILE	CB-CG1-CD1	-5.83	97.58	113.90
1	B	115	VAL	O-C-N	5.83	132.03	122.70
1	A	126	GLN	CA-CB-CG	-5.82	100.61	113.40
1	A	91	PHE	CB-CG-CD1	-5.81	116.73	120.80
1	B	50	LEU	CB-CG-CD2	-5.75	101.23	111.00
1	B	86	TRP	CA-C-O	5.74	132.15	120.10
1	A	54	TYR	C-N-CA	-5.65	107.57	121.70
1	B	87	LEU	CA-C-O	-5.59	108.37	120.10
1	A	129	THR	CA-CB-OG1	-5.58	97.27	109.00
1	A	78	LYS	CA-C-O	-5.57	108.40	120.10
1	A	84	MET	CA-CB-CG	-5.56	103.85	113.30
1	B	34	TYR	CZ-CE2-CD2	-5.51	114.84	119.80
1	B	106	VAL	O-C-N	5.47	131.46	122.70
1	B	136	GLU	CA-C-N	5.47	129.24	117.20
1	A	57	HIS	CB-CA-C	-5.45	99.50	110.40
1	B	56	ALA	CB-CA-C	-5.44	101.94	110.10
1	A	77	PHE	CB-CG-CD1	-5.39	117.03	120.80
1	A	21	ILE	N-CA-CB	-5.39	98.40	110.80
1	B	136	GLU	CA-C-O	-5.37	108.83	120.10
1	A	110	PRO	O-C-N	5.32	131.22	122.70
1	A	126	GLN	CG-CD-NE2	-5.30	103.99	116.70
1	A	71	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	A	17(A)	ALA	C-N-CA	-5.26	108.55	121.70
1	B	115	VAL	CB-CA-C	-5.26	101.41	111.40
1	A	81	TYR	CZ-CE2-CD2	5.25	124.52	119.80
1	B	38	SER	CA-CB-OG	5.25	125.36	111.20
1	B	33	PHE	CG-CD2-CE2	5.23	126.55	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	TRP	CB-CG-CD2	5.21	133.37	126.60
1	A	35	PHE	CD1-CE1-CZ	-5.20	113.86	120.10
1	B	95	LYS	CA-C-O	5.17	130.96	120.10
1	B	123	ILE	CB-CA-C	-5.16	101.29	111.60
1	A	42	PRO	N-CD-CG	-5.16	95.47	103.20
1	A	100	LEU	CA-C-O	-5.12	109.36	120.10
1	B	14	VAL	CA-CB-CG1	-5.11	103.23	110.90
1	B	98	GLU	CG-CD-OE2	-5.10	108.09	118.30
1	B	53	PHE	CB-CA-C	-5.10	100.20	110.40
1	A	68	ILE	CA-C-O	5.09	130.78	120.10
1	A	93	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	126	GLN	CA-C-O	5.08	130.77	120.10
1	B	106	VAL	CG1-CB-CG2	-5.08	102.77	110.90
1	B	116	GLU	OE1-CD-OE2	5.04	129.34	123.30
1	B	35	PHE	CD1-CG-CD2	5.02	124.82	118.30
1	A	126	GLN	CB-CG-CD	5.00	124.61	111.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	4	LEU	Mainchain
1	B	6	LYS	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	1153	0	1128	44	0
1	B	1140	0	1114	70	0
2	A	105	0	0	10	2
2	B	73	0	0	6	2
All	All	2471	0	2242	107	2

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 (107) 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:16:LYS:HB2	1:A:21:ILE:HD11	1.39	1.04
1:A:77:PHE:HD2	1:A:78:LYS:HE2	1.31	0.94
1:A:128:ARG:HD2	2:A:245:HOH:O	1.66	0.94
1:B:82:ALA:HA	2:B:168:HOH:O	1.69	0.92
1:A:16:LYS:HB2	1:A:21:ILE:CD1	2.04	0.87
1:A:129:THR:HG23	2:A:236:HOH:O	1.76	0.84
1:A:144:ASN:HB3	1:A:145:VAL:HG23	1.57	0.84
1:B:119:SER:OG	1:B:121:ASN:ND2	2.12	0.82
1:B:14:VAL:O	1:B:20:ASP:HB2	1.84	0.78
1:B:126:GLN:HE21	1:B:130:MET:HG3	1.48	0.77
1:A:77:PHE:CD2	1:A:78:LYS:HE2	2.17	0.76
1:A:16:LYS:HD2	1:A:21:ILE:HD11	1.71	0.72
1:A:16:LYS:CB	1:A:21:ILE:HD11	2.21	0.69
1:B:121:ASN:HD22	1:B:121:ASN:N	1.89	0.69
1:A:105:ASP:OD1	2:A:247:HOH:O	2.12	0.68
1:B:65:VAL:HG13	1:B:86:TRP:CB	2.24	0.67
1:B:23:LEU:HD12	1:B:24:PRO:HD2	1.75	0.67
1:B:57:HIS:HB3	1:B:61:LYS:HG2	1.77	0.66
1:A:145:VAL:HG11	1:B:97:MET:CE	2.28	0.64
1:B:136:GLU:O	1:B:137:ALA:HB3	1.95	0.64
1:B:121:ASN:HD22	1:B:121:ASN:H	1.44	0.63
1:A:128:ARG:NE	2:A:165:HOH:O	2.31	0.63
1:B:40:CYS:CB	1:B:43:CYS:HG	2.12	0.62
1:B:92:GLU:H	1:B:92:GLU:CD	2.03	0.62
1:A:106:VAL:HA	2:A:185:HOH:O	2.00	0.62
1:B:127:ALA:O	1:B:131:VAL:HG23	2.01	0.61
1:A:145:VAL:CG1	1:B:97:MET:SD	2.89	0.60
1:B:126:GLN:NE2	1:B:130:MET:HG3	2.18	0.59
1:B:124:THR:HA	1:B:144:ASN:OD1	2.03	0.58
1:A:23:LEU:N	1:A:24:PRO:CD	2.67	0.58
1:B:126:GLN:NE2	1:B:142:TRP:HB3	2.19	0.58
1:A:145:VAL:HG13	2:A:254:HOH:O	2.03	0.58
1:B:126:GLN:HE21	1:B:142:TRP:HB3	1.69	0.57
1:B:54:TYR:CE1	1:B:65:VAL:HG12	2.39	0.57
1:A:145:VAL:HG11	1:B:97:MET:SD	2.45	0.56
1:B:17:GLY:O	1:B:17(A):ALA:C	2.44	0.56
1:B:75:GLU:H	1:B:75:GLU:CD	2.09	0.56
1:A:145:VAL:CG1	1:B:97:MET:CE	2.83	0.56
1:B:113:VAL:HG23	1:B:113:VAL:O	2.06	0.55
1:A:74:ALA:O	1:A:78:LYS:HG2	2.07	0.55
1:A:78:LYS:HD3	2:A:206:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:VAL:HG11	1:B:97:MET:HE2	1.87	0.54
1:B:141:PRO:HD2	1:B:143:PRO:HD3	1.88	0.54
1:A:145:VAL:HG12	1:B:97:MET:SD	2.48	0.54
1:B:127:ALA:O	1:B:128:ARG:C	2.44	0.53
1:B:16:LYS:HD2	1:B:87:LEU:CD2	2.38	0.53
1:A:102:THR:HG22	2:A:229:HOH:O	2.08	0.53
1:B:89:LEU:HD12	1:B:90:PRO:HD2	1.89	0.53
1:A:2:SER:HB2	1:A:119:SER:O	2.09	0.53
1:B:140:PHE:CE1	1:B:141:PRO:HB3	2.44	0.52
1:A:89:LEU:HD12	1:A:90:PRO:HD2	1.92	0.51
1:B:30:THR:HG23	1:B:123:ILE:HD12	1.91	0.51
1:B:75:GLU:CD	1:B:75:GLU:N	2.65	0.50
1:B:58:ALA:O	1:B:62:ASN:N	2.45	0.50
1:A:145:VAL:HB	1:B:70:TRP:CD1	2.47	0.50
1:B:135:PRO:HB2	2:B:218:HOH:O	2.13	0.49
1:A:17:GLY:O	1:A:17(A):ALA:C	2.50	0.49
1:A:65:VAL:O	1:A:86:TRP:HB2	2.11	0.49
1:B:16:LYS:HD2	1:B:87:LEU:HD21	1.95	0.49
1:B:81:TYR:OH	1:B:86:TRP:O	2.15	0.49
1:A:128:ARG:HD2	2:A:175:HOH:O	2.12	0.48
1:A:47:THR:N	1:A:48:PRO:HD2	2.27	0.48
1:B:41:PRO:N	1:B:42:PRO:HD2	2.29	0.47
1:B:65:VAL:O	1:B:86:TRP:HB2	2.14	0.47
1:B:54:TYR:CD2	1:B:85:PRO:HG2	2.50	0.47
1:B:121:ASN:ND2	1:B:121:ASN:N	2.60	0.47
1:B:104:PHE:CD1	1:B:113:VAL:HG21	2.50	0.46
1:B:32:PHE:HA	1:B:113:VAL:O	2.15	0.46
1:B:59:GLU:HG2	1:B:60:LYS:N	2.30	0.46
1:A:75:GLU:H	1:A:75:GLU:CD	2.19	0.46
1:A:47:THR:N	1:A:48:PRO:CD	2.79	0.45
1:B:65:VAL:HG13	1:B:86:TRP:CG	2.51	0.45
1:A:41:PRO:HB2	1:A:42:PRO:CD	2.46	0.45
1:B:35:PHE:HA	1:B:68:ILE:O	2.16	0.45
1:B:97:MET:HB3	1:B:97:MET:HE3	1.71	0.45
1:A:21:ILE:HD13	1:A:21:ILE:HG21	1.70	0.45
1:B:68:ILE:HG22	1:B:97:MET:HG2	1.99	0.44
1:A:128:ARG:HH12	1:A:132:VAL:HG21	1.83	0.44
1:A:47:THR:HB	1:A:48:PRO:HD3	2.00	0.44
1:B:130:MET:HB3	1:B:130:MET:HE2	1.79	0.44
1:B:33:PHE:N	1:B:113:VAL:O	2.41	0.43
1:B:54:TYR:HE2	1:B:85:PRO:HB2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:GLU:CG	1:B:60:LYS:N	2.82	0.43
1:A:13:ASN:HA	1:A:21:ILE:O	2.19	0.42
1:B:54:TYR:CE2	1:B:85:PRO:HB2	2.55	0.42
1:B:92:GLU:N	1:B:92:GLU:CD	2.71	0.42
1:A:102:THR:HG23	2:A:194:HOH:O	2.19	0.42
1:A:41:PRO:HB2	1:A:42:PRO:HD3	2.02	0.42
1:B:65:VAL:HG13	1:B:86:TRP:HB3	1.97	0.42
1:B:64:GLU:HA	2:B:219:HOH:O	2.19	0.42
1:B:74:ALA:O	1:B:75:GLU:C	2.57	0.42
1:A:21:ILE:CD1	1:A:87:LEU:HD22	2.49	0.42
1:B:61:LYS:HE3	1:B:137:ALA:HB1	2.02	0.42
1:B:29:LYS:HG2	1:B:62:ASN:CG	2.40	0.42
1:B:4:LEU:O	1:B:4:LEU:HG	2.20	0.42
1:B:53:PHE:HB2	2:B:220:HOH:O	2.19	0.42
1:B:25:SER:HA	2:B:208:HOH:O	2.20	0.41
1:B:26:LEU:O	1:B:27:ALA:C	2.57	0.41
1:B:81:TYR:O	1:B:83:LYS:N	2.52	0.41
1:A:128:ARG:HD3	1:A:128:ARG:HH11	1.68	0.41
1:B:14:VAL:O	1:B:20:ASP:CB	2.62	0.41
1:B:57:HIS:O	1:B:58:ALA:C	2.58	0.41
1:B:30:THR:O	1:B:63:PHE:HA	2.21	0.41
1:A:145:VAL:CG2	2:B:166:HOH:O	2.69	0.41
1:B:47:THR:O	1:B:51:ILE:HG13	2.21	0.41
1:A:16:LYS:CD	1:A:21:ILE:HD11	2.46	0.41
1:A:13:ASN:HB3	1:A:20:ASP:HB2	2.01	0.40

All (2) 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)
2:A:245:HOH:O	2:B:215:HOH:O[3_555]	2.13	0.07
2:A:175:HOH:O	2:B:215:HOH:O[3_555]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	143/149 (96%)	137 (96%)	5 (4%)	1 (1%)	22	12
1	B	141/149 (95%)	130 (92%)	8 (6%)	3 (2%)	7	1
All	All	284/298 (95%)	267 (94%)	13 (5%)	4 (1%)	11	3

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17(A)	ALA
1	B	17(A)	ALA
1	B	82	ALA
1	B	58	ALA

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	123/126 (98%)	121 (98%)	2 (2%)	62	60
1	B	121/126 (96%)	111 (92%)	10 (8%)	11	4
All	All	244/252 (97%)	232 (95%)	12 (5%)	25	15

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	TRP
1	A	128	ARG
1	B	16	LYS
1	B	59	GLU
1	B	65	VAL
1	B	75	GLU
1	B	92	GLU
1	B	119	SER
1	B	121	ASN

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Mol	Chain	Res	Type
1	B	128	ARG
1	B	132	VAL
1	B	143	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	13	ASN
1	B	121	ASN
1	B	126	GLN

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](#)

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	145/149 (97%)	0.45	12 (8%) 11 13	10, 20, 40, 62	0
1	B	143/149 (95%)	1.02	28 (19%) 1 1	13, 33, 56, 63	0
All	All	288/298 (96%)	0.73	40 (13%) 2 3	10, 25, 53, 63	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	17(A)	ALA	5.9
1	B	134	ASP	5.3
1	B	139	ASP	5.2
1	B	142	TRP	4.6
1	B	17(A)	ALA	4.5
1	B	28	GLY	4.0
1	B	27	ALA	3.8
1	A	24	PRO	3.4
1	B	136	GLU	3.4
1	B	130	MET	3.3
1	A	18	ALA	3.2
1	B	3	GLY	3.1
1	B	60	LYS	3.0
1	B	135	PRO	3.0
1	A	20	ASP	3.0
1	A	145	VAL	3.0
1	B	144	ASN	3.0
1	B	59	GLU	2.9
1	A	72	GLU	2.9
1	B	143	PRO	2.8
1	B	133	LYS	2.8
1	A	113	VAL	2.7
1	B	58	ALA	2.7
1	B	132	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	25	SER	2.6
1	B	138	LYS	2.6
1	B	126	GLN	2.6
1	A	25	SER	2.6
1	B	74	ALA	2.5
1	B	56	ALA	2.3
1	B	31	VAL	2.3
1	B	140	PHE	2.3
1	B	82	ALA	2.3
1	B	129	THR	2.3
1	A	21	ILE	2.2
1	B	65	VAL	2.1
1	B	75	GLU	2.1
1	A	23	LEU	2.1
1	A	27	ALA	2.1
1	A	60	LYS	2.1

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 carbohydrates 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.