



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:00 PM UTC

PDB ID : 1UMR / pdb_00001umr
Title : Crystal structure of the platelet activator convulxin, a disulfide linked a4b4 cyclic tetramer from the venom of Crotalus durissus terrificus
Authors : Murakami, M.T.; Zela, S.P.; Gava, L.M.; Michelin-Duarte, S.; Cintra, A.C.O.; Arni, R.K.
Deposited on : 2003-08-28
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

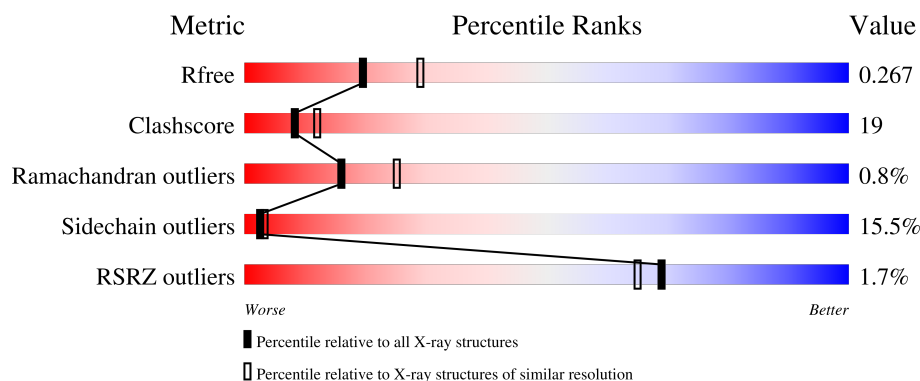
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	135	62% 30% 5% •
1	B	135	54% 31% 13% •
2	C	125	2% 53% 36% 10% •
2	D	125	3% 44% 39% 12% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4515 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 CONVULXIN ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	135	Total	C	N	O	S	0	0	0
			1105	711	182	202	10			
1	B	135	Total	C	N	O	S	0	0	0
			1105	711	182	202	10			

- Molecule 2 is a protein called CONVULXIN BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	125	Total	C	N	O	S	0	0	0
			1054	677	171	196	10			
2	D	125	Total	C	N	O	S	0	0	0
			1054	677	171	196	10			

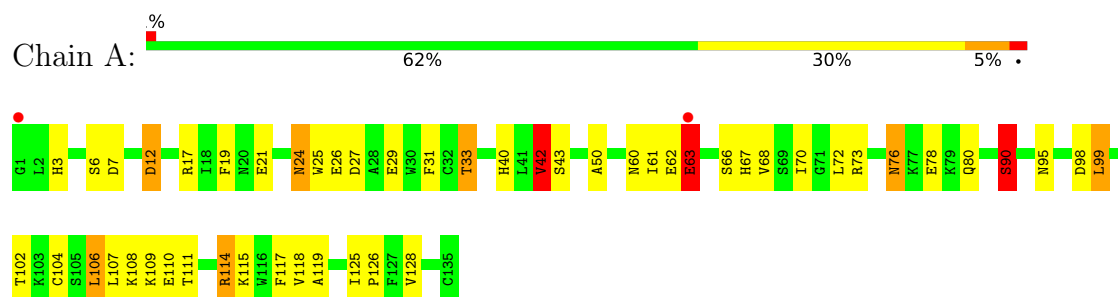
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	49	Total	O	0	0
			49	49		
3	B	57	Total	O	0	0
			57	57		
3	C	43	Total	O	0	0
			43	43		
3	D	48	Total	O	0	0
			48	48		

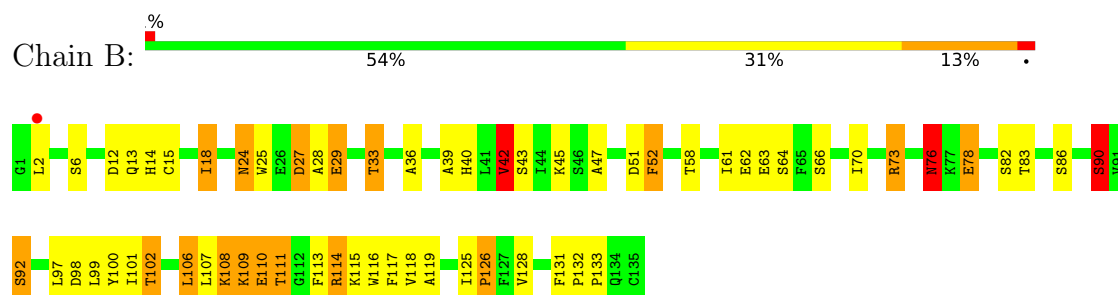
3 Residue-property plots [i](#)

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 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.

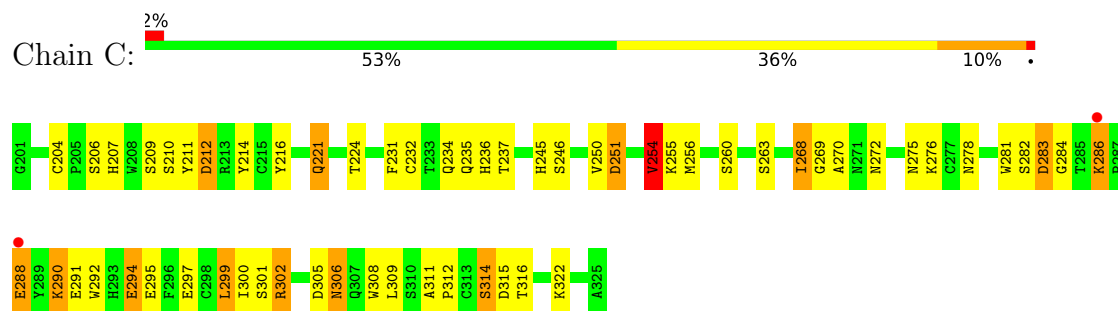
• Molecule 1: CONVULXIN ALPHA



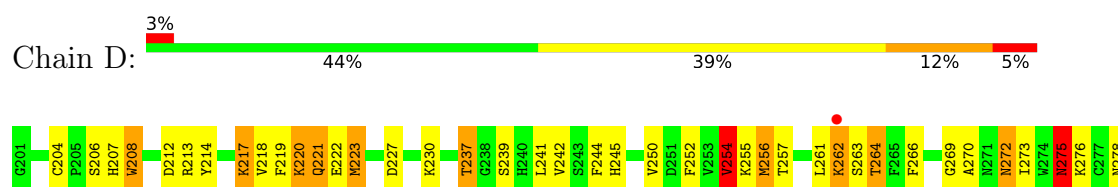
• Molecule 1: CONVULXIN ALPHA



• Molecule 2: CONVULXIN BETA



• Molecule 2: CONVULXIN BETA





4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	131.91Å 131.91Å 112.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 30.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.6 (30.00-2.40) 97.5 (30.00-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.187 , 0.264 0.197 , 0.267	Depositor DCC
R_{free} test set	1845 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4515	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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

5.1 Standard geometry

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	1.76	8/1138 (0.7%)	1.75	23/1538 (1.5%)
1	B	1.73	17/1138 (1.5%)	1.68	15/1538 (1.0%)
2	C	1.75	11/1094 (1.0%)	1.68	17/1483 (1.1%)
2	D	1.86	21/1094 (1.9%)	1.64	21/1483 (1.4%)
All	All	1.78	57/4464 (1.3%)	1.69	76/6042 (1.3%)

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	A	0	1

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	GLU	CD-OE2	11.53	1.47	1.25
2	D	264	THR	CA-CB	10.26	1.71	1.53
2	D	288	GLU	CD-OE2	10.08	1.44	1.25
2	D	242	VAL	CA-CB	9.35	1.64	1.54
2	D	295	GLU	CD-OE2	9.30	1.43	1.25
2	D	311	ALA	C-O	-8.84	1.15	1.24
2	C	256	MET	SD-CE	-8.62	1.57	1.79
1	A	70	ILE	CA-CB	-8.54	1.42	1.54
1	B	108	LYS	CE-NZ	8.49	1.74	1.49
2	D	294	GLU	CD-OE2	8.36	1.41	1.25
1	A	73	ARG	NE-CZ	8.28	1.42	1.33
2	D	309	LEU	C-O	-8.19	1.16	1.24
2	D	320	VAL	CA-CB	-7.74	1.41	1.55
2	D	295	GLU	CD-OE1	7.53	1.39	1.25
2	C	311	ALA	CA-CB	7.22	1.63	1.53
2	D	288	GLU	CD-OE1	7.16	1.39	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	268	ILE	CA-CB	-7.01	1.45	1.54
1	A	50	ALA	CA-CB	6.84	1.64	1.53
2	D	295	GLU	CG-CD	6.78	1.69	1.52
1	B	47	ALA	C-O	-6.52	1.16	1.24
2	C	305	ASP	CB-CG	-6.35	1.36	1.52
1	A	61	ILE	CA-C	6.35	1.59	1.52
1	B	73	ARG	NE-CZ	6.20	1.39	1.33
1	B	27	ASP	C-O	-6.13	1.16	1.24
2	D	242	VAL	N-CA	-6.06	1.38	1.46
1	B	90	SER	CA-C	6.03	1.60	1.52
1	B	83	THR	CA-C	-6.00	1.44	1.52
2	D	294	GLU	CD-OE1	5.94	1.36	1.25
2	C	305	ASP	C-O	5.93	1.31	1.23
1	B	28	ALA	C-O	5.92	1.31	1.24
2	C	288	GLU	CA-C	5.90	1.60	1.52
1	B	113	PHE	C-O	-5.90	1.16	1.23
1	A	90	SER	CA-C	5.79	1.60	1.52
2	D	305	ASP	CB-CG	-5.77	1.37	1.52
1	B	29	GLU	C-O	5.76	1.30	1.24
2	D	242	VAL	CA-C	5.64	1.59	1.52
1	B	18	ILE	CA-CB	-5.59	1.47	1.54
1	B	126	PRO	CA-C	5.57	1.59	1.52
1	B	15	CYS	CA-C	5.57	1.59	1.52
2	C	268	ILE	C-O	-5.54	1.17	1.24
1	B	92	SER	CB-OG	5.54	1.53	1.42
1	B	45	LYS	CB-CG	5.51	1.69	1.52
2	D	256	MET	SD-CE	-5.50	1.65	1.79
1	A	31	PHE	CA-C	5.47	1.60	1.52
2	D	254	VAL	CA-C	5.46	1.59	1.52
1	B	58	THR	CA-C	5.37	1.59	1.52
2	D	285	THR	CA-CB	-5.36	1.45	1.53
2	D	306	ASN	CB-CG	-5.34	1.38	1.52
1	A	70	ILE	CA-C	5.21	1.59	1.52
1	B	52	PHE	CA-C	5.21	1.59	1.52
2	C	276	LYS	CE-NZ	5.19	1.65	1.49
2	D	237	THR	CA-CB	5.12	1.61	1.53
2	C	214	TYR	C-O	5.12	1.30	1.23
1	B	76	ASN	C-O	-5.08	1.17	1.23
2	C	235	GLN	C-O	-5.08	1.18	1.24
2	D	275	ASN	C-O	-5.05	1.17	1.24
2	C	270	ALA	CA-CB	-5.02	1.44	1.53

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	ARG	CA-C-N	-10.07	104.63	123.27
1	A	114	ARG	C-N-CA	-10.07	104.63	123.27
1	B	114	ARG	CA-C-N	-9.64	105.84	123.01
1	B	114	ARG	C-N-CA	-9.64	105.84	123.01
1	B	42	VAL	CB-CA-C	-9.23	96.27	111.51
1	A	114	ARG	NE-CZ-NH2	-9.07	111.03	119.20
1	A	42	VAL	CB-CA-C	-8.58	97.22	111.29
1	B	92	SER	N-CA-C	-8.21	103.71	114.31
1	B	102	THR	OG1-CB-CG2	-7.76	93.78	109.30
2	D	319	PHE	N-CA-C	7.69	118.77	108.38
2	D	285	THR	N-CA-CB	-7.59	98.72	110.56
1	B	86	SER	N-CA-C	-7.58	103.49	112.89
1	A	60	ASN	CA-C-N	-7.54	110.42	120.91
1	A	60	ASN	C-N-CA	-7.54	110.42	120.91
2	D	275	ASN	N-CA-C	-7.34	102.98	112.23
1	A	63	GLU	OE1-CD-OE2	-7.13	105.79	122.90
2	D	305	ASP	CB-CA-C	-6.62	98.30	110.62
1	A	33	THR	N-CA-CB	-6.58	100.09	110.28
2	C	306	ASN	N-CA-C	6.42	120.58	112.87
2	C	212	ASP	CA-C-N	-6.42	113.04	122.86
2	C	212	ASP	C-N-CA	-6.42	113.04	122.86
1	B	33	THR	N-CA-CB	-6.41	99.75	110.39
2	D	295	GLU	OE1-CD-OE2	6.33	138.10	122.90
1	A	114	ARG	NE-CZ-NH1	6.32	127.82	121.50
2	D	306	ASN	N-CA-C	6.31	120.24	112.54
2	C	305	ASP	CB-CA-C	-6.28	95.61	109.56
1	A	80	GLN	N-CA-C	-6.09	100.33	108.74
1	A	114	ARG	O-C-N	-6.06	115.67	122.34
2	D	302	ARG	N-CA-C	6.06	118.16	109.14
2	C	288	GLU	OE1-CD-OE2	-6.05	108.39	122.90
2	C	254	VAL	N-CA-CB	6.02	118.73	110.54
2	D	264	THR	CB-CA-C	6.00	120.08	109.65
2	C	254	VAL	N-CA-C	5.95	116.69	110.62
2	C	306	ASN	CB-CA-C	-5.94	97.20	110.21
2	D	293	HIS	N-CA-C	-5.94	101.05	109.96
1	B	12	ASP	CA-C-N	-5.94	113.11	122.79
1	B	12	ASP	C-N-CA	-5.94	113.11	122.79
2	C	269	GLY	N-CA-C	5.94	127.25	113.18
2	D	305	ASP	CA-C-N	5.92	130.60	120.72
2	D	305	ASP	C-N-CA	5.92	130.60	120.72
2	D	212	ASP	CA-C-N	-5.89	113.85	122.86
2	D	212	ASP	C-N-CA	-5.89	113.85	122.86
2	D	294	GLU	N-CA-CB	-5.85	101.75	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	315	ASP	N-CA-C	-5.74	102.27	110.59
2	C	204	CYS	N-CA-C	-5.71	102.41	110.29
2	C	286	LYS	CB-CA-C	5.71	116.33	109.31
2	D	213	ARG	NE-CZ-NH2	5.69	124.33	119.20
1	A	73	ARG	CD-NE-CZ	5.68	132.35	124.40
2	D	204	CYS	N-CA-C	-5.67	103.02	110.39
2	D	208	TRP	N-CA-C	-5.65	100.93	109.85
1	A	25	TRP	CA-C-N	-5.63	111.30	121.14
1	A	25	TRP	C-N-CA	-5.63	111.30	121.14
1	B	63	GLU	N-CA-C	5.61	117.39	111.28
2	C	251	ASP	N-CA-C	-5.59	105.27	111.36
1	B	42	VAL	N-CA-CB	5.57	119.11	110.14
2	C	302	ARG	NE-CZ-NH2	5.50	124.15	119.20
1	B	78	GLU	N-CA-C	5.48	117.40	110.33
1	A	73	ARG	NE-CZ-NH1	5.46	126.96	121.50
1	A	12	ASP	CB-CG-OD2	5.45	130.94	118.40
2	D	218	VAL	N-CA-C	5.44	116.07	108.89
1	B	36	ALA	N-CA-C	5.41	116.75	108.42
1	A	78	GLU	CA-C-N	5.34	127.43	120.28
1	A	78	GLU	C-N-CA	5.34	127.43	120.28
2	C	297	GLU	N-CA-C	5.33	118.50	109.76
1	A	114	ARG	CG-CD-NE	-5.32	100.29	112.00
2	D	269	GLY	N-CA-C	5.28	125.70	113.18
1	A	12	ASP	CA-C-N	-5.22	114.28	122.79
1	A	12	ASP	C-N-CA	-5.22	114.28	122.79
2	C	302	ARG	CG-CD-NE	5.19	123.43	112.00
1	B	25	TRP	N-CA-C	-5.18	105.32	111.69
1	A	104	CYS	CA-CB-SG	-5.17	102.51	114.40
2	C	288	GLU	CG-CD-OE2	5.10	130.12	118.40
1	B	42	VAL	CG1-CB-CG2	5.06	121.93	110.80
1	A	114	ARG	N-CA-C	5.05	120.83	114.31
2	C	302	ARG	NE-CZ-NH1	-5.04	116.46	121.50
2	D	252	PHE	CB-CA-C	-5.02	102.45	110.79

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	63	GLU	Sidechain

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	1105	0	1053	39	0
1	B	1105	0	1053	47	0
2	C	1054	0	938	33	0
2	D	1054	0	938	59	0
3	A	49	0	0	3	0
3	B	57	0	0	5	0
3	C	43	0	0	1	0
3	D	48	0	0	2	0
All	All	4515	0	3982	159	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 19.

All (159) 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:108:LYS:CE	1:B:108:LYS:NZ	1.74	1.46
2:C:221:GLN:HE21	2:C:221:GLN:H	0.97	0.90
2:C:251:ASP:OD1	2:C:306:ASN:ND2	2.04	0.89
2:D:283:ASP:OD2	2:D:285:THR:HB	1.72	0.89
2:D:280:GLN:OE1	2:D:286:LYS:HE3	1.74	0.87
1:A:102:THR:HB	1:A:118:VAL:HG12	1.56	0.85
2:D:217:LYS:HD3	2:D:219:PHE:CZ	2.12	0.85
1:B:76:ASN:HD22	1:B:76:ASN:H	1.22	0.84
1:B:29:GLU:OE2	1:B:40:HIS:HD2	1.60	0.84
1:B:24:ASN:C	1:B:24:ASN:HD22	1.83	0.84
2:D:223:MET:CE	2:D:227:ASP:HB3	2.10	0.82
1:A:24:ASN:HD22	1:A:24:ASN:C	1.87	0.81
1:A:76:ASN:H	1:A:76:ASN:HD22	1.29	0.80
1:A:106:LEU:HD13	1:A:119:ALA:HB2	1.63	0.80
2:C:236:HIS:HD2	2:C:237:THR:O	1.65	0.80
1:A:29:GLU:OE1	1:A:40:HIS:HD2	1.65	0.80
2:C:221:GLN:H	2:C:221:GLN:NE2	1.77	0.79
1:A:108:LYS:NZ	2:D:222:GLU:OE1	2.15	0.78
2:D:221:GLN:HE21	2:D:221:GLN:H	1.28	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:GLU:HG2	3:B:2047:HOH:O	1.84	0.77
2:D:290:LYS:HD2	2:D:290:LYS:C	2.09	0.76
1:B:76:ASN:HD21	2:D:278:ASN:H	1.32	0.75
1:B:110:GLU:CG	3:B:2047:HOH:O	2.37	0.73
2:D:270:ALA:HB3	2:D:299:LEU:HD22	1.70	0.72
1:B:76:ASN:H	1:B:76:ASN:ND2	1.88	0.72
1:B:106:LEU:HD13	1:B:119:ALA:HB2	1.71	0.72
1:A:76:ASN:HD21	2:C:278:ASN:H	1.41	0.69
1:A:106:LEU:CD2	1:A:117:PHE:HB2	2.23	0.68
1:A:63:GLU:OE2	1:B:108:LYS:NZ	2.26	0.67
2:D:275:ASN:ND2	3:D:2030:HOH:O	2.28	0.66
1:A:24:ASN:ND2	1:A:27:ASP:H	1.94	0.66
2:D:206:SER:O	2:D:207:HIS:HB2	1.96	0.66
1:B:110:GLU:CB	3:B:2047:HOH:O	2.43	0.65
1:B:106:LEU:HD13	1:B:119:ALA:CB	2.27	0.65
2:C:290:LYS:HE2	2:C:290:LYS:C	2.23	0.64
1:A:68:VAL:HG11	1:A:128:VAL:HG23	1.79	0.63
1:B:73:ARG:HD3	3:B:2034:HOH:O	1.98	0.63
1:A:125:ILE:HB	1:A:126:PRO:HD2	1.80	0.63
1:A:109:LYS:HD3	3:A:2025:HOH:O	1.98	0.63
2:D:275:ASN:H	2:D:275:ASN:HD22	1.48	0.62
1:B:114:ARG:O	2:D:291:GLU:OE1	2.18	0.62
1:B:24:ASN:ND2	1:B:27:ASP:H	1.97	0.62
2:C:290:LYS:CE	2:C:292:TRP:H	2.14	0.61
2:D:272:ASN:HD22	2:D:272:ASN:N	1.97	0.61
2:D:294:GLU:O	2:D:294:GLU:HG3	1.99	0.60
1:A:17:ARG:HD3	1:A:19:PHE:CZ	2.38	0.59
2:D:290:LYS:C	2:D:290:LYS:CD	2.77	0.57
1:A:72:LEU:HD13	2:C:292:TRP:CZ2	2.40	0.57
1:B:24:ASN:C	1:B:24:ASN:ND2	2.55	0.56
2:D:266:PHE:CZ	2:D:301:SER:HB3	2.40	0.56
1:B:125:ILE:HB	1:B:126:PRO:HD2	1.87	0.56
2:D:272:ASN:HD22	2:D:272:ASN:H	1.54	0.56
1:A:106:LEU:HD13	1:A:119:ALA:CB	2.32	0.56
1:A:43:SER:HA	2:C:281:TRP:CZ3	2.41	0.56
1:A:76:ASN:H	1:A:76:ASN:ND2	1.99	0.56
2:D:223:MET:HE2	2:D:227:ASP:HB3	1.87	0.56
2:D:257:THR:HB	2:D:261:LEU:HD22	1.89	0.55
2:C:206:SER:O	2:C:207:HIS:HB2	2.04	0.55
2:D:223:MET:O	2:D:316:THR:HA	2.07	0.54
1:B:43:SER:HA	2:D:281:TRP:CE3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:275:ASN:ND2	2:D:275:ASN:H	2.05	0.54
2:D:223:MET:HE2	2:D:227:ASP:CB	2.38	0.53
2:C:221:GLN:HE21	2:C:221:GLN:N	1.83	0.53
1:B:24:ASN:HD21	1:B:27:ASP:H	1.57	0.53
1:B:42:VAL:HG22	1:B:128:VAL:HB	1.91	0.52
2:D:250:VAL:O	2:D:254:VAL:HG13	2.10	0.52
1:A:42:VAL:HG22	1:A:128:VAL:HB	1.90	0.52
1:B:102:THR:HB	1:B:118:VAL:HG12	1.91	0.52
1:A:43:SER:HA	2:C:281:TRP:CE3	2.46	0.51
2:D:320:VAL:HG12	2:D:321:CYS:N	2.27	0.50
1:B:18:ILE:HB	1:B:128:VAL:HG22	1.94	0.50
1:A:98:ASP:O	1:A:99:LEU:C	2.54	0.50
1:A:114:ARG:O	2:C:291:GLU:OE1	2.30	0.50
2:C:250:VAL:O	2:C:254:VAL:HG13	2.12	0.50
1:A:106:LEU:HD23	1:A:117:PHE:HB2	1.94	0.49
1:B:116:TRP:CZ3	2:D:290:LYS:HA	2.47	0.49
2:D:294:GLU:O	2:D:294:GLU:CG	2.58	0.49
1:B:14:HIS:HE1	3:B:2004:HOH:O	1.93	0.49
1:A:90:SER:O	2:C:245:HIS:HE1	1.96	0.49
2:C:245:HIS:HD2	3:C:2025:HOH:O	1.96	0.49
1:B:90:SER:O	2:D:245:HIS:HE1	1.96	0.49
2:D:291:GLU:O	2:D:291:GLU:HG3	2.13	0.49
1:A:102:THR:CB	1:A:118:VAL:HG12	2.36	0.48
2:C:282:SER:C	2:C:284:GLY:H	2.21	0.48
2:C:272:ASN:N	2:C:272:ASN:HD22	2.11	0.48
1:A:106:LEU:HD22	1:A:117:PHE:HB2	1.96	0.47
1:A:3:HIS:HD2	3:A:2049:HOH:O	1.96	0.47
1:A:62:GLU:HB3	3:A:2024:HOH:O	2.13	0.47
1:A:63:GLU:CD	1:B:108:LYS:NZ	2.73	0.47
1:B:108:LYS:HD2	1:B:117:PHE:CD2	2.49	0.47
1:A:24:ASN:HD22	1:A:27:ASP:H	1.62	0.47
2:D:221:GLN:H	2:D:221:GLN:NE2	2.04	0.47
2:D:281:TRP:HD1	2:D:285:THR:HG22	1.80	0.47
2:D:295:GLU:OE2	2:D:297:GLU:OE2	2.33	0.47
2:D:217:LYS:HD3	2:D:219:PHE:CE2	2.49	0.47
2:D:261:LEU:HD11	2:D:318:SER:HB3	1.97	0.47
1:B:78:GLU:H	1:B:78:GLU:CD	2.22	0.46
2:C:312:PRO:C	2:C:314:SER:H	2.22	0.46
1:A:24:ASN:C	1:A:24:ASN:ND2	2.61	0.46
1:A:66:SER:O	1:A:67:HIS:HD2	1.99	0.46
2:D:223:MET:CE	2:D:227:ASP:CB	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:VAL:HG23	1:B:70:ILE:HG22	1.98	0.46
1:A:76:ASN:ND2	1:A:76:ASN:N	2.63	0.46
2:C:294:GLU:H	2:D:262:LYS:NZ	2.14	0.46
2:D:223:MET:HE1	2:D:227:ASP:HB3	1.93	0.45
2:D:286:LYS:HD2	2:D:286:LYS:HA	1.79	0.45
1:A:6:SER:O	1:A:7:ASP:HB2	2.16	0.45
2:D:283:ASP:OD2	2:D:283:ASP:C	2.59	0.45
1:B:82:SER:HA	2:D:276:LYS:HD3	1.98	0.45
2:C:211:TYR:O	2:C:212:ASP:C	2.60	0.45
2:C:268:ILE:HG21	2:C:268:ILE:HD13	1.70	0.45
2:D:206:SER:O	2:D:207:HIS:CB	2.61	0.45
1:A:108:LYS:HD2	1:A:117:PHE:CE2	2.52	0.45
1:B:109:LYS:O	1:B:111:THR:N	2.49	0.45
2:D:261:LEU:HD11	2:D:318:SER:CB	2.46	0.45
1:A:68:VAL:CG1	1:A:128:VAL:HG23	2.45	0.44
1:A:95:ASN:HB2	2:C:308:TRP:CE2	2.52	0.44
1:B:118:VAL:HG12	1:B:119:ALA:N	2.31	0.44
2:D:244:PHE:CG	2:D:250:VAL:HG22	2.53	0.44
1:B:108:LYS:HD2	1:B:117:PHE:CE2	2.52	0.44
1:B:76:ASN:HD21	2:D:278:ASN:N	2.09	0.43
1:B:114:ARG:HD2	1:B:114:ARG:HA	1.50	0.43
2:C:216:TYR:CE2	2:C:322:LYS:HD2	2.53	0.43
2:D:278:ASN:OD1	2:D:286:LYS:HE2	2.18	0.43
2:D:208:TRP:CE3	2:D:217:LYS:HB2	2.53	0.43
2:D:214:TYR:CD2	2:D:324:GLU:HA	2.53	0.43
2:D:275:ASN:ND2	2:D:275:ASN:N	2.66	0.43
1:B:98:ASP:HA	1:B:101:ILE:HD12	2.01	0.43
2:C:206:SER:O	2:C:207:HIS:CB	2.67	0.43
2:D:239:SER:HA	2:D:323:PHE:HB3	1.99	0.43
2:D:272:ASN:N	2:D:272:ASN:ND2	2.63	0.43
1:B:76:ASN:ND2	1:B:76:ASN:N	2.59	0.42
2:C:236:HIS:CD2	2:C:237:THR:O	2.57	0.42
2:D:261:LEU:O	3:D:2025:HOH:O	2.22	0.42
2:C:290:LYS:NZ	2:C:292:TRP:H	2.16	0.42
1:A:102:THR:O	1:A:118:VAL:CG1	2.67	0.42
1:B:109:LYS:C	1:B:111:THR:N	2.76	0.42
2:D:273:ILE:HG21	2:D:299:LEU:HD13	2.02	0.42
2:D:305:ASP:HB3	2:D:307:GLN:H	1.85	0.42
1:B:109:LYS:C	1:B:111:THR:H	2.28	0.42
2:C:299:LEU:HD12	2:C:299:LEU:HA	1.73	0.41
1:B:51:ASP:O	1:B:52:PHE:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:290:LYS:HD3	2:D:292:TRP:H	1.86	0.41
1:B:39:ALA:HB2	1:B:131:PHE:HB3	2.02	0.41
1:B:102:THR:CB	1:B:118:VAL:HG12	2.50	0.41
2:C:246:SER:O	2:C:250:VAL:HG23	2.21	0.41
2:C:283:ASP:OD2	2:C:283:ASP:C	2.64	0.41
1:B:13:GLN:O	1:B:133:PRO:HD2	2.21	0.41
2:C:231:PHE:O	2:C:232:CYS:C	2.64	0.41
2:D:241:LEU:HD23	2:D:241:LEU:HA	1.90	0.41
1:B:106:LEU:HD22	1:B:117:PHE:HB2	2.02	0.41
1:B:125:ILE:CB	1:B:126:PRO:HD2	2.48	0.41
2:C:234:GLN:HE21	2:C:234:GLN:HB2	1.71	0.41
2:D:220:LYS:O	2:D:221:GLN:C	2.64	0.41
1:B:43:SER:HA	2:D:281:TRP:CZ3	2.55	0.40
1:A:102:THR:HB	1:A:118:VAL:CG1	2.39	0.40
2:C:224:THR:HA	2:C:315:ASP:O	2.22	0.40
2:D:281:TRP:CD1	2:D:285:THR:HG22	2.56	0.40
1:B:97:LEU:O	1:B:100:TYR:N	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	133/135 (98%)	123 (92%)	9 (7%)	1 (1%)	16	25
1	B	133/135 (98%)	123 (92%)	8 (6%)	2 (2%)	8	12
2	C	123/125 (98%)	113 (92%)	9 (7%)	1 (1%)	16	25
2	D	123/125 (98%)	114 (93%)	9 (7%)	0	100	100
All	All	512/520 (98%)	473 (92%)	35 (7%)	4 (1%)	16	25

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	B	110	GLU
2	C	283	ASP
1	B	132	PRO

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	122/122 (100%)	109 (89%)	13 (11%)	6	10
1	B	122/122 (100%)	104 (85%)	18 (15%)	3	4
2	C	116/116 (100%)	96 (83%)	20 (17%)	2	2
2	D	116/116 (100%)	93 (80%)	23 (20%)	1	2
All	All	476/476 (100%)	402 (84%)	74 (16%)	2	3

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLU
1	A	24	ASN
1	A	26	GLU
1	A	33	THR
1	A	42	VAL
1	A	76	ASN
1	A	90	SER
1	A	99	LEU
1	A	106	LEU
1	A	107	LEU
1	A	110	GLU
1	A	111	THR
1	A	115	LYS
1	B	2	LEU
1	B	6	SER
1	B	24	ASN
1	B	33	THR
1	B	42	VAL

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Mol	Chain	Res	Type
1	B	61	ILE
1	B	62	GLU
1	B	64	SER
1	B	66	SER
1	B	76	ASN
1	B	90	SER
1	B	92	SER
1	B	99	LEU
1	B	106	LEU
1	B	107	LEU
1	B	109	LYS
1	B	111	THR
1	B	115	LYS
2	C	209	SER
2	C	210	SER
2	C	221	GLN
2	C	254	VAL
2	C	255	LYS
2	C	260	SER
2	C	263	SER
2	C	275	ASN
2	C	286	LYS
2	C	288	GLU
2	C	290	LYS
2	C	294	GLU
2	C	295	GLU
2	C	299	LEU
2	C	300	ILE
2	C	301	SER
2	C	302	ARG
2	C	309	LEU
2	C	314	SER
2	C	316	THR
2	D	217	LYS
2	D	220	LYS
2	D	221	GLN
2	D	223	MET
2	D	230	LYS
2	D	237	THR
2	D	254	VAL
2	D	255	LYS
2	D	256	MET

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Mol	Chain	Res	Type
2	D	262	LYS
2	D	263	SER
2	D	264	THR
2	D	272	ASN
2	D	275	ASN
2	D	285	THR
2	D	286	LYS
2	D	288	GLU
2	D	290	LYS
2	D	294	GLU
2	D	295	GLU
2	D	299	LEU
2	D	305	ASP
2	D	314	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	35	GLN
1	A	40	HIS
1	A	67	HIS
1	A	76	ASN
1	B	3	HIS
1	B	24	ASN
1	B	35	GLN
1	B	40	HIS
1	B	76	ASN
2	C	221	GLN
2	C	234	GLN
2	C	236	HIS
2	C	245	HIS
2	C	272	ASN
2	C	278	ASN
2	C	293	HIS
2	C	307	GLN
2	D	221	GLN
2	D	234	GLN
2	D	236	HIS
2	D	245	HIS
2	D	272	ASN
2	D	275	ASN

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Mol	Chain	Res	Type
2	D	306	ASN
2	D	307	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 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	135/135 (100%)	-0.34	2 (1%) 72 68	33, 44, 62, 82	0
1	B	135/135 (100%)	-0.41	1 (0%) 84 81	33, 44, 66, 81	0
2	C	125/125 (100%)	-0.29	2 (1%) 70 66	33, 44, 65, 78	0
2	D	125/125 (100%)	-0.09	4 (3%) 50 46	34, 47, 65, 84	0
All	All	520/520 (100%)	-0.28	9 (1%) 69 65	33, 45, 65, 84	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	262	LYS	5.0
1	A	1	GLY	4.7
1	A	63	GLU	4.4
1	B	2	LEU	4.1
2	D	294	GLU	3.8
2	D	295	GLU	3.8
2	D	288	GLU	3.4
2	C	288	GLU	3.1
2	C	286	LYS	2.9

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.