



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2023 – 02:54 am GMT

PDB ID : 1UMR  
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.; Michelan-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](mailto: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 : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

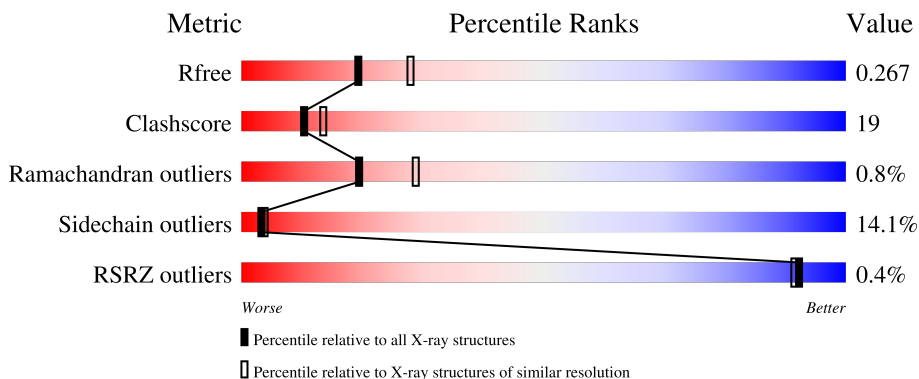
# 1 Overall quality at a glance

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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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  $\geq 3$ , 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	
1	B	135	
2	C	125	
2	D	125	

## 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
			Total	C	N	O	S			
1	A	135	1105	711	182	202	10	0	0	0
1	B	135	1105	711	182	202	10	0	0	0

- Molecule 2 is a protein called CONVULXIN BETA.

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

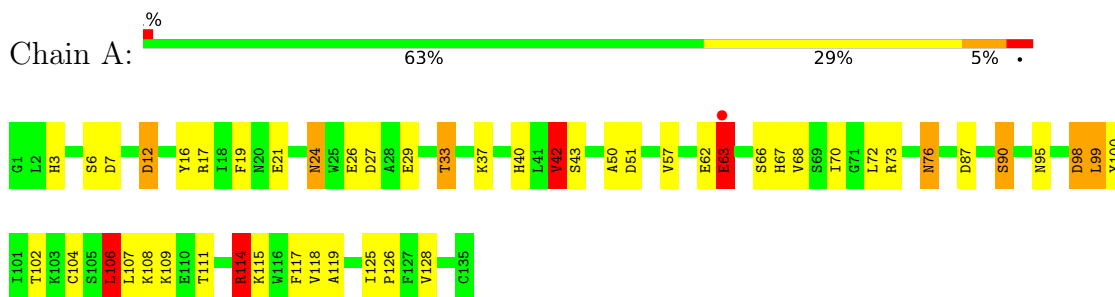
- Molecule 3 is water.

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		

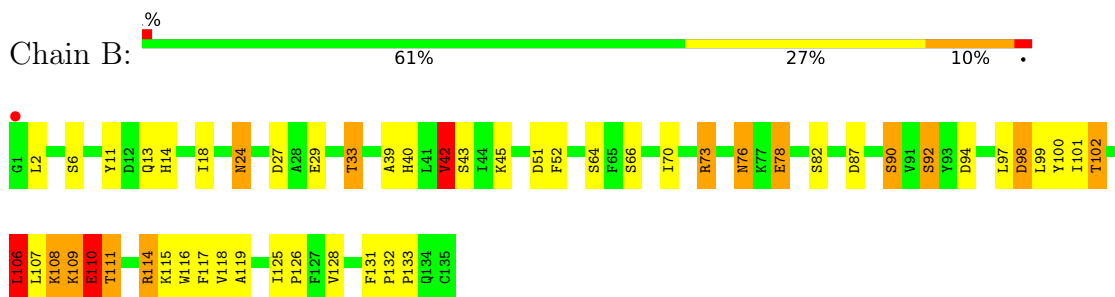
### 3 Residue-property plots

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.

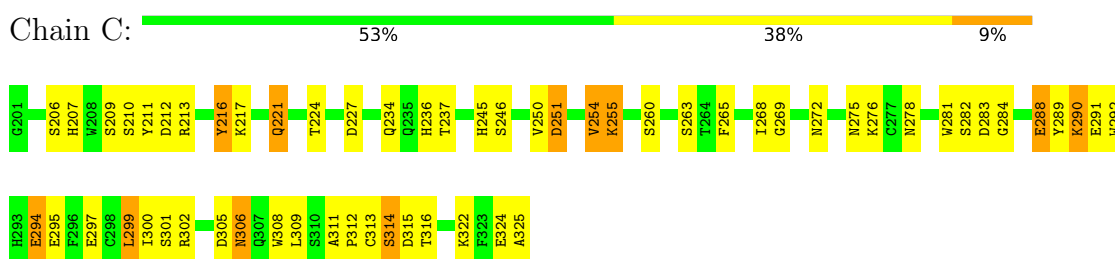
- Molecule 1: CONVULXIN ALPHA



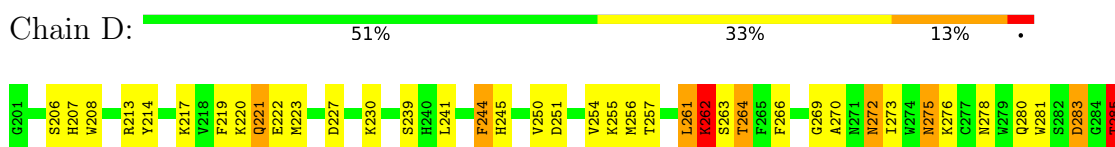
- Molecule 1: CONVULXIN ALPHA



- Molecule 2: CONVULXIN BETA



- Molecule 2: CONVULXIN BETA



K286	F287	E288	Y289	K290	E291	W292	H293	E294	F295	F296	E297	C298	L299	I300	S301	R302	S303	M306	Q307	W308	L309	S314	B315	T316	Y317	S318	F319	V320	C321	R322	F323	E324	A325
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.91Å 131.91Å 112.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 29.50 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.6 (30.00-2.40) 97.6 (29.50-2.40)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.187 , 0.264 0.196 , 0.267	Depositor DCC
$R_{free}$ test set	1845 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.4	Xtrriage
Anisotropy	0.061	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 51.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.027 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4515	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	1.66	10/1138 (0.9%)	1.64	18/1538 (1.2%)
1	B	1.55	8/1138 (0.7%)	1.39	11/1538 (0.7%)
2	C	1.62	12/1094 (1.1%)	1.42	15/1483 (1.0%)
2	D	1.92	17/1094 (1.6%)	1.38	14/1483 (0.9%)
All	All	1.69	47/4464 (1.1%)	1.46	58/6042 (1.0%)

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	0	1

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	GLU	CD-OE2	19.65	1.47	1.25
2	D	288	GLU	CD-OE2	17.13	1.44	1.25
2	D	295	GLU	CD-OE2	15.79	1.43	1.25
2	D	294	GLU	CD-OE2	14.16	1.41	1.25
2	D	295	GLU	CD-OE1	12.73	1.39	1.25
2	D	288	GLU	CD-OE1	12.10	1.39	1.25
2	D	295	GLU	CG-CD	11.36	1.69	1.51
1	B	108	LYS	CE-NZ	10.31	1.74	1.49
2	D	294	GLU	CD-OE1	9.99	1.36	1.25
1	B	92	SER	CB-OG	8.44	1.53	1.42
2	C	305	ASP	CB-CG	-7.42	1.36	1.51
1	B	11	TYR	CD1-CE1	7.31	1.50	1.39
1	A	16	TYR	CE2-CZ	7.17	1.47	1.38
1	A	73	ARG	NE-CZ	7.00	1.42	1.33
2	D	264	THR	CA-CB	6.93	1.71	1.53
1	B	78	GLU	CD-OE1	6.91	1.33	1.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	VAL	CB-CG1	6.83	1.67	1.52
2	D	305	ASP	CB-CG	-6.72	1.37	1.51
2	C	289	TYR	CD2-CE2	6.70	1.49	1.39
1	B	52	PHE	CE2-CZ	6.56	1.49	1.37
2	C	276	LYS	CE-NZ	6.35	1.65	1.49
2	D	262	LYS	CD-CE	6.14	1.66	1.51
2	D	320	VAL	CA-CB	-6.13	1.41	1.54
1	B	45	LYS	CB-CG	6.08	1.69	1.52
2	C	255	LYS	CD-CE	5.90	1.66	1.51
2	C	325	ALA	CA-CB	5.89	1.64	1.52
2	D	295	GLU	CB-CG	5.88	1.63	1.52
1	A	37	LYS	CE-NZ	5.85	1.63	1.49
2	C	265	PHE	CE2-CZ	5.82	1.48	1.37
2	C	313	CYS	CB-SG	5.67	1.91	1.82
2	D	244	PHE	CD2-CE2	5.55	1.50	1.39
1	A	50	ALA	CA-CB	5.47	1.64	1.52
2	D	288	GLU	CG-CD	5.45	1.60	1.51
2	C	216	TYR	CZ-OH	5.43	1.47	1.37
2	C	311	ALA	CA-CB	5.38	1.63	1.52
2	D	306	ASN	CB-CG	-5.37	1.38	1.51
1	A	100	TYR	CE2-CZ	5.36	1.45	1.38
2	C	324	GLU	CD-OE2	-5.27	1.19	1.25
2	D	297	GLU	CD-OE1	5.27	1.31	1.25
1	A	16	TYR	CG-CD2	5.26	1.46	1.39
1	A	42	VAL	CB-CG2	-5.26	1.41	1.52
1	B	73	ARG	NE-CZ	5.25	1.39	1.33
1	A	70	ILE	CA-CB	-5.22	1.42	1.54
2	C	265	PHE	CD1-CE1	5.15	1.49	1.39
1	B	110	GLU	CG-CD	5.13	1.59	1.51
2	C	297	GLU	CD-OE1	5.12	1.31	1.25
2	D	324	GLU	CD-OE1	-5.01	1.20	1.25

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	ARG	NE-CZ-NH2	-18.53	111.03	120.30
1	A	114	ARG	NE-CZ-NH1	15.04	127.82	120.30
1	A	63	GLU	OE1-CD-OE2	-14.59	105.79	123.30
1	A	12	ASP	CB-CG-OD2	14.05	130.94	118.30
1	A	73	ARG	NE-CZ-NH1	13.32	126.96	120.30
2	C	288	GLU	OE1-CD-OE2	-12.43	108.39	123.30
2	D	295	GLU	OE1-CD-OE2	12.33	138.10	123.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	305	ASP	CB-CG-OD1	-11.13	108.28	118.30
1	B	51	ASP	CB-CG-OD2	10.45	127.70	118.30
1	B	98	ASP	CB-CG-OD2	9.64	126.98	118.30
1	B	73	ARG	NE-CZ-NH1	9.19	124.90	120.30
2	C	305	ASP	CB-CG-OD2	8.79	126.22	118.30
1	A	87	ASP	CB-CG-OD2	8.40	125.86	118.30
2	D	213	ARG	NE-CZ-NH2	8.05	124.33	120.30
1	B	106	LEU	CA-CB-CG	8.04	133.79	115.30
1	B	42	VAL	CB-CA-C	-7.96	96.27	111.40
2	C	302	ARG	NE-CZ-NH2	7.70	124.15	120.30
2	C	302	ARG	NE-CZ-NH1	-7.69	116.46	120.30
1	A	12	ASP	CB-CG-OD1	-7.66	111.41	118.30
1	A	42	VAL	CB-CA-C	-7.46	97.22	111.40
2	C	305	ASP	CB-CA-C	-7.39	95.61	110.40
2	D	305	ASP	CB-CG-OD1	-7.34	111.69	118.30
1	B	102	THR	OG1-CB-CG2	-7.05	93.78	110.00
1	A	51	ASP	CB-CG-OD2	7.02	124.62	118.30
1	B	42	VAL	CG1-CB-CG2	6.90	121.93	110.90
1	A	114	ARG	C-N-CA	-6.83	104.63	121.70
1	A	106	LEU	CA-CB-CG	6.82	130.99	115.30
2	C	251	ASP	CB-CG-OD2	6.73	124.36	118.30
2	C	227	ASP	CB-CG-OD2	6.66	124.29	118.30
1	A	98	ASP	CB-CG-OD2	6.62	124.25	118.30
2	C	306	ASN	CB-CA-C	-6.60	97.20	110.40
1	A	73	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	B	87	ASP	CB-CG-OD2	6.50	124.15	118.30
1	B	94	ASP	CB-CG-OD2	6.49	124.14	118.30
2	D	283	ASP	CB-CG-OD2	6.49	124.14	118.30
1	A	104	CYS	CA-CB-SG	-6.38	102.51	114.00
1	B	114	ARG	C-N-CA	-6.34	105.84	121.70
2	C	213	ARG	NE-CZ-NH1	-6.29	117.15	120.30
1	A	73	ARG	CD-NE-CZ	6.25	132.35	123.60
2	D	305	ASP	CB-CG-OD2	6.12	123.81	118.30
2	D	285	THR	N-CA-CB	-6.09	98.72	110.30
2	D	305	ASP	CB-CA-C	-6.05	98.30	110.40
2	C	288	GLU	CG-CD-OE2	5.91	130.12	118.30
2	D	213	ARG	NE-CZ-NH1	-5.83	117.38	120.30
2	C	324	GLU	OE1-CD-OE2	-5.68	116.48	123.30
2	C	269	GLY	N-CA-C	5.66	127.25	113.10
2	D	251	ASP	CB-CG-OD2	5.56	123.30	118.30
1	B	33	THR	N-CA-CB	-5.55	99.75	110.30
2	D	262	LYS	CD-CE-NZ	5.54	124.44	111.70

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	302	ARG	CG-CD-NE	5.54	123.43	111.80
1	A	114	ARG	CG-CD-NE	-5.48	100.29	111.80
2	D	295	GLU	CG-CD-OE2	-5.47	107.35	118.30
2	D	302	ARG	NE-CZ-NH2	5.47	123.03	120.30
2	D	261	LEU	CA-CB-CG	5.41	127.73	115.30
1	A	33	THR	N-CA-CB	-5.37	100.09	110.30
1	A	114	ARG	CD-NE-CZ	5.19	130.87	123.60
2	C	217	LYS	CD-CE-NZ	-5.15	99.85	111.70
2	D	269	GLY	N-CA-C	5.04	125.70	113.10

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	44	0
2	C	1054	0	938	31	0
2	D	1054	0	938	60	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	3	0
All	All	4515	0	3982	155	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 (155) 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
2:D:223:MET:CE	2:D:227:ASP:HB3	2.10	0.82
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:B:24:ASN:C	1:B:24:ASN:HD22	1.83	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
1:A:24:ASN:HD22	1:A:24:ASN:C	1.87	0.77
1:B:110:GLU:HG2	3:B:2047:HOH:O	1.84	0.77
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
2:D:290:LYS:HD2	2:D:290:LYS:C	2.09	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
2:D:207:HIS:ND1	3:D:2005:HOH:O	2.26	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
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:290:LYS:HE2	2:C:290:LYS:C	2.23	0.59
1:A:17:ARG:HD3	1:A:19:PHE:CZ	2.38	0.59
1:A:72:LEU:HD13	2:C:292:TRP:CZ2	2.40	0.57
2:C:206:SER:O	2:C:207:HIS:HB2	2.04	0.57
2:D:223:MET:HE2	2:D:227:ASP:HB3	1.86	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:257:THR:HB	2:D:261:LEU:HD22	1.89	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
2:D:223:MET:HE2	2:D:227:ASP:CB	2.38	0.54
2:D:275:ASN:ND2	2:D:275:ASN:H	2.05	0.54
1:A:24:ASN:C	1:A:24:ASN:ND2	2.61	0.53
2:C:221:GLN:HE21	2:C:221:GLN:N	1.83	0.53
1:B:24:ASN:C	1:B:24:ASN:ND2	2.55	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
2:D:290:LYS:C	2:D:290:LYS:CD	2.77	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: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:THR:CB	1:A:118:VAL:HG12	2.36	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: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: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
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
1:A:98:ASP:O	1:A:99:LEU:C	2.54	0.46
2:D:272:ASN:N	2:D:272:ASN:ND2	2.63	0.46
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:223:MET:HE1	2:D:227:ASP:HB3	1.93	0.45
1:B:82:SER:HA	2:D:276:LYS:HD3	1.98	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

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:206:SER:O	2:C:207:HIS:CB	2.67	0.43
2:C:282:SER:C	2:C:284:GLY:H	2.21	0.43
2:D:239:SER:HA	2:D:323:PHE:HB3	1.99	0.43
1:A:63:GLU:CD	1:B:108:LYS:NZ	2.73	0.42
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
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:78:GLU:H	1:B:78:GLU:CD	2.22	0.41
2:C:312:PRO:C	2:C:314:SER:H	2.22	0.41
2:C:299:LEU:HD12	2:C:299:LEU:HA	1.73	0.41
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
1:B:13:GLN:O	1:B:133:PRO:HD2	2.21	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
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:211:TYR:O	2:C:212:ASP:C	2.60	0.40
2:D:283:ASP:OD2	2:D:283:ASP:C	2.59	0.40
2:D:320:VAL:CG1	2:D:321:CYS:N	2.84	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 [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	133/135 (98%)	123 (92%)	9 (7%)	1 (1%)	19	29
1	B	133/135 (98%)	123 (92%)	8 (6%)	2 (2%)	10	14
2	C	123/125 (98%)	113 (92%)	9 (7%)	1 (1%)	19	29
2	D	123/125 (98%)	114 (93%)	9 (7%)	0	100	100
All	All	512/520 (98%)	473 (92%)	35 (7%)	4 (1%)	19	29

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 [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	122/122 (100%)	109 (89%)	13 (11%)	6	9
1	B	122/122 (100%)	106 (87%)	16 (13%)	4	4
2	C	116/116 (100%)	98 (84%)	18 (16%)	2	3
2	D	116/116 (100%)	96 (83%)	20 (17%)	2	2
All	All	476/476 (100%)	409 (86%)	67 (14%)	3	4

All (67) 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

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	111	THR
1	A	114	ARG
1	A	115	LYS
1	B	2	LEU
1	B	6	SER
1	B	24	ASN
1	B	33	THR
1	B	42	VAL
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	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	309	LEU
2	C	314	SER

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	C	316	THR
2	D	220	LYS
2	D	221	GLN
2	D	230	LYS
2	D	255	LYS
2	D	256	MET
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	299	LEU
2	D	301	SER
2	D	305	ASP
2	D	309	LEU
2	D	314	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	24	ASN
1	A	40	HIS
1	A	60	ASN
1	A	67	HIS
1	A	76	ASN
1	B	3	HIS
1	B	24	ASN
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	D	221	GLN
2	D	234	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	236	HIS
2	D	245	HIS
2	D	272	ASN
2	D	275	ASN
2	D	306	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	135/135 (100%)	-0.66	1 (0%) 87 86	33, 44, 62, 82	0
1	B	135/135 (100%)	-0.65	1 (0%) 87 86	33, 44, 66, 81	0
2	C	125/125 (100%)	-0.70	0 100 100	33, 44, 65, 78	0
2	D	125/125 (100%)	-0.62	0 100 100	34, 47, 65, 84	0
All	All	520/520 (100%)	-0.66	2 (0%) 92 91	33, 45, 65, 84	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	63	GLU	2.2
1	B	1	GLY	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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.