



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:13 PM UTC

PDB ID : 7QFC / pdb_00007qfc
Title : Crystal structure of cytotoxin 13 from Naja naja, orthorhombic form
Authors : Samygina, V.R.; Dubova, K.M.; Bourenkov, G.; Utkin, Y.N.; Dubovskii, P.V.
Deposited on : 2021-12-05
Resolution : 2.60 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

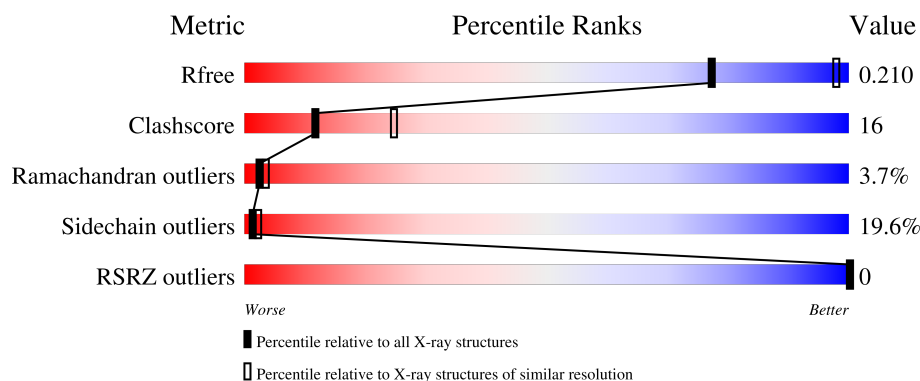
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	AAA	60	52% 38% 8% .
1	BBB	60	58% 28% 12% .
1	CCC	60	53% 32% 12% .
1	DDD	60	63% 25% 10% .
1	EEE	60	63% 20% 15% .

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Mol	Chain	Length	Quality of chain
1	FFF	60	 A horizontal bar chart showing the quality of chain 1 (FFF, length 60). The bar is divided into three segments: green (37%), yellow (48%), and orange (15%).

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2801 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 Cytotoxin 13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	60	Total	C	N	O	S	0	0	0
			464	294	81	79	10			
1	BBB	60	Total	C	N	O	S	0	0	0
			464	294	81	79	10			
1	CCC	60	Total	C	N	O	S	0	0	0
			464	294	81	79	10			
1	DDD	60	Total	C	N	O	S	0	0	0
			464	294	81	79	10			
1	EEE	60	Total	C	N	O	S	0	0	0
			464	294	81	79	10			
1	FFF	60	Total	C	N	O	S	0	0	0
			464	294	81	79	10			

- Molecule 2 is water.

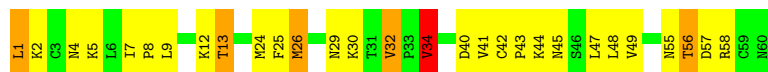
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	7	Total	O	0	0
			7	7		
2	BBB	3	Total	O	0	0
			3	3		
2	CCC	4	Total	O	0	0
			4	4		
2	DDD	1	Total	O	0	0
			1	1		
2	EEE	1	Total	O	0	0
			1	1		
2	FFF	1	Total	O	0	0
			1	1		

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: Cytotoxin 13

Chain AAA: 



• Molecule 1: Cytotoxin 13

Chain BBB: 



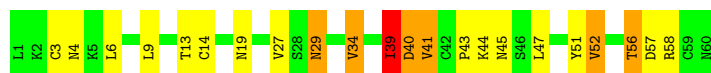
• Molecule 1: Cytotoxin 13

Chain CCC: 



• Molecule 1: Cytotoxin 13

Chain DDD: 

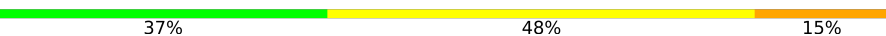


• Molecule 1: Cytotoxin 13

Chain EEE: 



• Molecule 1: Cytotoxin 13

Chain FFF: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	88.76Å 97.17Å 131.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.89 – 2.60 14.89 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (14.89-2.60) 99.2 (14.89-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.205 , 0.255 0.210 , 0.210	Depositor DCC
R_{free} test set	913 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	79.7	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 59.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2801	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% 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	AAA	1.35	3/471 (0.6%)	1.76	13/632 (2.1%)
1	BBB	1.14	1/471 (0.2%)	1.65	4/632 (0.6%)
1	CCC	1.22	2/471 (0.4%)	1.67	8/632 (1.3%)
1	DDD	1.17	0/471	1.67	5/632 (0.8%)
1	EEE	1.10	0/471	1.55	3/632 (0.5%)
1	FFF	1.22	1/471 (0.2%)	1.59	3/632 (0.5%)
All	All	1.20	7/2826 (0.2%)	1.65	36/3792 (0.9%)

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	CCC	0	1
1	DDD	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	55	ASN	C-O	-7.09	1.13	1.23
1	AAA	43	PRO	C-O	-6.90	1.16	1.23
1	AAA	45	ASN	C-O	-6.34	1.16	1.24
1	BBB	55	ASN	C-O	-6.01	1.17	1.24
1	CCC	1	LEU	N-CA	5.36	1.56	1.46
1	CCC	55	ASN	C-O	-5.20	1.16	1.23
1	FFF	50	LYS	C-O	5.01	1.30	1.23

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	34	VAL	N-CA-CB	-10.08	100.33	112.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DDD	34	VAL	N-CA-CB	-9.80	101.43	112.21
1	BBB	34	VAL	N-CA-CB	-8.09	101.19	112.35
1	AAA	13	THR	CB-CA-C	7.34	122.48	110.22
1	DDD	6	LEU	CA-C-N	-7.22	117.69	122.60
1	DDD	6	LEU	C-N-CA	-7.22	117.69	122.60
1	CCC	56	THR	CA-CB-OG1	-6.99	99.11	109.60
1	CCC	34	VAL	N-CA-CB	-6.68	103.64	112.26
1	BBB	25	PHE	CA-CB-CG	6.37	120.17	113.80
1	AAA	25	PHE	CA-CB-CG	6.23	120.03	113.80
1	AAA	30	LYS	N-CA-C	-6.15	105.73	113.18
1	CCC	19	ASN	CA-CB-CG	-5.96	106.64	112.60
1	DDD	52	VAL	CB-CA-C	5.96	119.23	110.77
1	FFF	47	LEU	CA-C-O	-5.86	114.35	120.92
1	CCC	45	ASN	CA-CB-CG	5.83	118.43	112.60
1	CCC	13	THR	CA-CB-OG1	-5.72	101.02	109.60
1	FFF	5	LYS	CA-C-N	5.47	128.39	120.79
1	FFF	5	LYS	C-N-CA	5.47	128.39	120.79
1	BBB	34	VAL	CB-CA-C	5.45	116.82	110.88
1	DDD	19	ASN	CB-CA-C	5.41	119.78	111.02
1	EEE	47	LEU	CA-C-O	-5.41	115.32	121.00
1	AAA	34	VAL	N-CA-C	-5.33	108.09	113.47
1	AAA	2	LYS	CB-CA-C	5.27	118.43	109.84
1	EEE	39	ILE	CA-C-N	5.26	127.78	120.63
1	EEE	39	ILE	C-N-CA	5.26	127.78	120.63
1	BBB	13	THR	CA-CB-OG1	-5.26	101.71	109.60
1	AAA	34	VAL	CB-CA-C	5.24	116.27	110.62
1	AAA	30	LYS	CB-CA-C	5.21	120.32	109.95
1	AAA	8	PRO	CA-C-N	5.20	127.50	120.38
1	AAA	8	PRO	C-N-CA	5.20	127.50	120.38
1	AAA	56	THR	CA-CB-OG1	-5.17	101.84	109.60
1	CCC	6	LEU	CA-C-O	-5.16	114.98	121.02
1	CCC	7	ILE	N-CA-CB	5.15	118.42	111.21
1	AAA	25	PHE	CA-C-N	5.14	128.15	120.95
1	AAA	25	PHE	C-N-CA	5.14	128.15	120.95
1	CCC	30	LYS	N-CA-C	-5.02	107.13	113.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	CCC	20	LEU	Peptide
1	DDD	39	ILE	Peptide

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	AAA	464	0	492	10	0
1	BBB	464	0	492	24	0
1	CCC	464	0	492	18	0
1	DDD	464	0	492	11	0
1	EEE	464	0	492	13	0
1	FFF	464	0	492	23	0
2	AAA	7	0	0	0	0
2	BBB	3	0	0	0	0
2	CCC	4	0	0	0	0
2	DDD	1	0	0	0	0
2	EEE	1	0	0	0	0
2	FFF	1	0	0	0	0
All	All	2801	0	2952	91	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 16.

All (91) 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:CCC:26:MET:HE3	1:EEE:26:MET:HE2	1.34	1.04
1:CCC:45:ASN:ND2	1:CCC:51:TYR:H	1.81	0.79
1:FFF:5:LYS:HG2	1:FFF:11:TYR:HA	1.65	0.76
1:BBB:4:ASN:ND2	1:BBB:58:ARG:HE	1.86	0.73
1:CCC:26:MET:CE	1:EEE:26:MET:HE2	2.17	0.73
1:CCC:31:THR:HG21	1:DDD:9:LEU:HD11	1.73	0.71
1:BBB:4:ASN:HD21	1:BBB:58:ARG:HE	1.38	0.70
1:CCC:45:ASN:HD21	1:CCC:51:TYR:H	1.41	0.69
1:CCC:29:ASN:HD22	1:CCC:30:LYS:N	1.91	0.68
1:FFF:25:PHE:CD1	1:FFF:29:ASN:HA	2.30	0.67
1:AAA:26:MET:HE1	1:AAA:49:VAL:HG22	1.76	0.67
1:DDD:29:ASN:C	1:DDD:29:ASN:HD22	2.04	0.66
1:FFF:21:CYS:HB2	1:FFF:54:CYS:SG	2.36	0.66
1:AAA:4:ASN:HD21	1:AAA:58:ARG:HE	1.42	0.65
1:BBB:26:MET:CA	1:BBB:26:MET:HE2	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FFF:23:LYS:HB2	1:FFF:25:PHE:CE2	2.32	0.65
1:CCC:45:ASN:HD22	1:CCC:50:LYS:HA	1.59	0.65
1:CCC:29:ASN:HD22	1:CCC:29:ASN:C	2.06	0.63
1:DDD:43:PRO:HB2	1:DDD:51:TYR:CE2	2.36	0.61
1:AAA:40:ASP:OD2	1:AAA:41:VAL:N	2.34	0.60
1:DDD:43:PRO:HB2	1:DDD:51:TYR:CD2	2.37	0.60
1:CCC:24:MET:HE1	1:EEE:24:MET:HE2	1.84	0.59
1:CCC:45:ASN:ND2	1:CCC:50:LYS:HA	2.18	0.59
1:EEE:29:ASN:ND2	1:EEE:32:VAL:O	2.35	0.59
1:FFF:26:MET:HA	1:FFF:26:MET:HE2	1.86	0.57
1:FFF:25:PHE:CG	1:FFF:29:ASN:HA	2.40	0.57
1:DDD:45:ASN:ND2	1:DDD:51:TYR:H	2.03	0.56
1:BBB:26:MET:HE2	1:BBB:26:MET:N	2.21	0.56
1:AAA:26:MET:HE3	1:AAA:48:LEU:O	2.04	0.56
1:EEE:29:ASN:C	1:EEE:31:THR:H	2.16	0.54
1:BBB:26:MET:HE2	1:BBB:26:MET:HA	1.88	0.53
1:EEE:40:ASP:OD2	1:EEE:40:ASP:N	2.23	0.53
1:FFF:57:ASP:OD1	1:FFF:57:ASP:N	2.41	0.53
1:FFF:32:VAL:HG23	1:FFF:33:PRO:HD2	1.90	0.53
1:EEE:2:LYS:HG3	1:EEE:13:THR:HG22	1.91	0.53
1:BBB:29:ASN:HD21	1:BBB:30:LYS:HE2	1.74	0.52
1:FFF:1:LEU:HD21	1:FFF:56:THR:O	2.10	0.52
1:FFF:1:LEU:HD23	1:FFF:2:LYS:N	2.26	0.50
1:EEE:1:LEU:HD11	1:EEE:55:ASN:HA	1.93	0.50
1:FFF:2:LYS:HA	1:FFF:13:THR:HG22	1.92	0.50
1:BBB:46:SER:HB2	1:FFF:35:LYS:HE3	1.93	0.50
1:BBB:26:MET:HE3	1:BBB:34:VAL:HG11	1.94	0.49
1:FFF:26:MET:O	1:FFF:27:VAL:HB	2.11	0.49
1:DDD:3:CYS:SG	1:DDD:14:CYS:SG	3.10	0.49
1:BBB:29:ASN:C	1:BBB:29:ASN:HD22	2.21	0.49
1:BBB:46:SER:OG	1:BBB:47:LEU:N	2.47	0.48
1:CCC:7:ILE:O	1:CCC:9:LEU:N	2.46	0.48
1:FFF:23:LYS:HB2	1:FFF:25:PHE:HE2	1.78	0.47
1:AAA:1:LEU:HD23	1:AAA:1:LEU:HA	1.82	0.47
1:CCC:29:ASN:C	1:CCC:29:ASN:ND2	2.70	0.47
1:DDD:4:ASN:HD21	1:DDD:58:ARG:NE	2.12	0.47
1:CCC:23:LYS:O	1:CCC:51:TYR:HA	2.15	0.46
1:EEE:2:LYS:CG	1:EEE:13:THR:HG22	2.45	0.46
1:FFF:1:LEU:HD12	1:FFF:19:ASN:HA	1.98	0.46
1:BBB:25:PHE:CE1	1:BBB:33:PRO:HG3	2.51	0.46
1:FFF:2:LYS:HG2	1:FFF:13:THR:CG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:24:MET:HE2	1:AAA:34:VAL:HG12	1.98	0.45
1:FFF:9:LEU:HD23	1:FFF:9:LEU:HA	1.90	0.44
1:FFF:20:LEU:HD12	1:FFF:41:VAL:HA	1.99	0.44
1:BBB:26:MET:CA	1:BBB:26:MET:CE	2.95	0.44
1:BBB:4:ASN:HD21	1:BBB:58:ARG:NE	2.10	0.43
1:BBB:55:ASN:OD1	1:BBB:55:ASN:C	2.61	0.43
1:BBB:26:MET:HA	1:BBB:26:MET:CE	2.46	0.43
1:EEE:24:MET:HE3	1:EEE:51:TYR:OH	2.18	0.43
1:AAA:24:MET:HE2	1:AAA:34:VAL:CG1	2.49	0.43
1:AAA:56:THR:O	1:AAA:57:ASP:C	2.62	0.43
1:BBB:25:PHE:C	1:BBB:26:MET:HE2	2.44	0.42
1:BBB:56:THR:HG22	1:BBB:59:CYS:HB3	2.01	0.42
1:CCC:32:VAL:HA	1:CCC:33:PRO:HD3	1.75	0.42
1:CCC:27:VAL:HG12	1:CCC:28:SER:N	2.33	0.42
1:BBB:19:ASN:O	1:BBB:20:LEU:HD23	2.20	0.42
1:DDD:29:ASN:C	1:DDD:29:ASN:ND2	2.76	0.42
1:DDD:43:PRO:HG2	1:DDD:51:TYR:CE1	2.55	0.42
1:AAA:32:VAL:HG21	1:BBB:32:VAL:HG13	2.01	0.41
1:FFF:4:ASN:OD1	1:FFF:60:ASN:ND2	2.52	0.41
1:FFF:2:LYS:HG2	1:FFF:13:THR:HG22	2.03	0.41
1:FFF:5:LYS:HA	1:FFF:36:ARG:HB2	2.01	0.41
1:AAA:32:VAL:CG2	1:BBB:32:VAL:HG13	2.50	0.41
1:CCC:56:THR:O	1:CCC:57:ASP:C	2.63	0.41
1:BBB:30:LYS:HB3	1:CCC:27:VAL:HG21	2.03	0.41
1:BBB:21:CYS:HB3	1:BBB:60:ASN:CG	2.46	0.41
1:FFF:11:TYR:O	1:FFF:12:LYS:HB3	2.20	0.41
1:EEE:26:MET:N	1:EEE:26:MET:SD	2.93	0.41
1:BBB:29:ASN:C	1:BBB:29:ASN:ND2	2.79	0.40
1:BBB:45:ASN:ND2	1:BBB:51:TYR:H	2.19	0.40
1:EEE:11:TYR:CG	1:EEE:58:ARG:NH1	2.89	0.40
1:FFF:30:LYS:O	1:FFF:31:THR:O	2.39	0.40
1:CCC:21:CYS:HA	1:CCC:37:GLY:O	2.21	0.40
1:DDD:4:ASN:ND2	1:DDD:58:ARG:HG2	2.37	0.40
1:DDD:39:ILE:HG12	1:DDD:41:VAL:O	2.21	0.40
1:EEE:46:SER:OG	1:EEE:47:LEU:N	2.55	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	AAA	58/60 (97%)	55 (95%)	3 (5%)	0	100	100
1	BBB	58/60 (97%)	50 (86%)	6 (10%)	2 (3%)	3	4
1	CCC	58/60 (97%)	54 (93%)	4 (7%)	0	100	100
1	DDD	58/60 (97%)	52 (90%)	3 (5%)	3 (5%)	1	2
1	EEE	58/60 (97%)	48 (83%)	7 (12%)	3 (5%)	1	2
1	FFF	58/60 (97%)	47 (81%)	6 (10%)	5 (9%)	0	0
All	All	348/360 (97%)	306 (88%)	29 (8%)	13 (4%)	2	3

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	DDD	40	ASP
1	BBB	46	SER
1	DDD	56	THR
1	FFF	9	LEU
1	FFF	40	ASP
1	BBB	40	ASP
1	FFF	15	PRO
1	FFF	31	THR
1	DDD	27	VAL
1	EEE	9	LEU
1	EEE	28	SER
1	EEE	29	ASN
1	FFF	58	ARG

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	AAA	56/56 (100%)	43 (77%)	13 (23%)	1	1
1	BBB	56/56 (100%)	48 (86%)	8 (14%)	3	6
1	CCC	56/56 (100%)	47 (84%)	9 (16%)	2	4
1	DDD	56/56 (100%)	45 (80%)	11 (20%)	1	2
1	EEE	56/56 (100%)	43 (77%)	13 (23%)	1	1
1	FFF	56/56 (100%)	44 (79%)	12 (21%)	1	2
All	All	336/336 (100%)	270 (80%)	66 (20%)	1	2

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	1	LEU
1	AAA	5	LYS
1	AAA	7	ILE
1	AAA	9	LEU
1	AAA	12	LYS
1	AAA	13	THR
1	AAA	26	MET
1	AAA	29	ASN
1	AAA	32	VAL
1	AAA	34	VAL
1	AAA	42	CYS
1	AAA	44	LYS
1	AAA	47	LEU
1	BBB	1	LEU
1	BBB	26	MET
1	BBB	28	SER
1	BBB	29	ASN
1	BBB	34	VAL
1	BBB	40	ASP
1	BBB	41	VAL
1	BBB	56	THR
1	CCC	1	LEU
1	CCC	26	MET
1	CCC	29	ASN
1	CCC	30	LYS
1	CCC	32	VAL
1	CCC	34	VAL

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Mol	Chain	Res	Type
1	CCC	36	ARG
1	CCC	44	LYS
1	CCC	56	THR
1	DDD	13	THR
1	DDD	29	ASN
1	DDD	34	VAL
1	DDD	39	ILE
1	DDD	40	ASP
1	DDD	41	VAL
1	DDD	44	LYS
1	DDD	47	LEU
1	DDD	52	VAL
1	DDD	56	THR
1	DDD	57	ASP
1	EEE	24	MET
1	EEE	26	MET
1	EEE	28	SER
1	EEE	30	LYS
1	EEE	31	THR
1	EEE	32	VAL
1	EEE	34	VAL
1	EEE	40	ASP
1	EEE	42	CYS
1	EEE	45	ASN
1	EEE	46	SER
1	EEE	47	LEU
1	EEE	55	ASN
1	FFF	4	ASN
1	FFF	12	LYS
1	FFF	24	MET
1	FFF	30	LYS
1	FFF	32	VAL
1	FFF	34	VAL
1	FFF	42	CYS
1	FFF	44	LYS
1	FFF	47	LEU
1	FFF	52	VAL
1	FFF	57	ASP
1	FFF	59	CYS

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	AAA	60/60 (100%)	-0.69	0 100 100	58, 72, 93, 100	0
1	BBB	60/60 (100%)	-0.66	0 100 100	59, 78, 109, 119	0
1	CCC	60/60 (100%)	-0.51	0 100 100	68, 77, 108, 127	0
1	DDD	60/60 (100%)	-0.36	0 100 100	72, 95, 132, 141	0
1	EEE	60/60 (100%)	-0.29	0 100 100	77, 123, 158, 171	0
1	FFF	60/60 (100%)	-0.00	0 100 100	72, 149, 178, 194	0
All	All	360/360 (100%)	-0.42	0 100 100	58, 90, 164, 194	0

There are no RSRZ outliers to report.

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.