WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2023 – 12:27 PM EST

|		
PDB ID	:	8FIF
Title	:	A2.3 Nanobody In Complex With Microcystin-LR
Authors	:	Arenas, R.; Tabares-da Rosa, S.; Gonzalez-Sapienza, G.; Wilson, D.K.
Deposited on	:	2022-12-16
Resolution	:	2.35 Å(reported)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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.
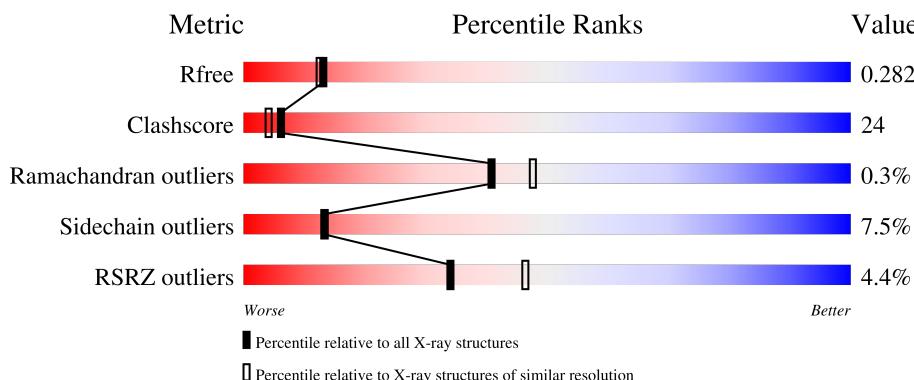
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 <=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	129	54% 37% · 7%
1	B	129	10% 50% 36% 5% 9%
1	C	129	% 67% 26% · 7%
2	D	7	14% 29% 43% 29%
2	F	7	14% 57% 29% 14%
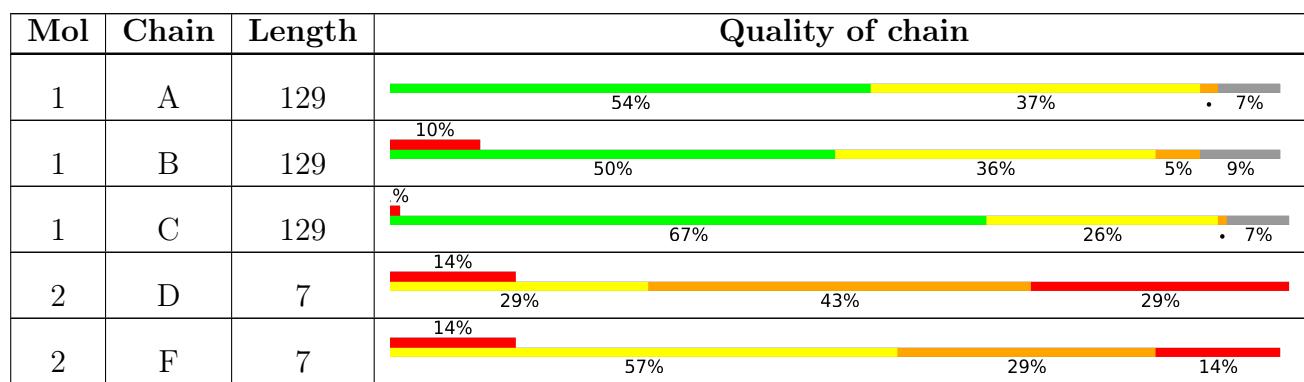
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Mol	Chain	Length	Quality of chain
2	G	7	43% 43% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MAA	D	7	X	-	-	-
2	MAA	F	7	X	-	-	-
2	ACB	G	3	X	-	-	-
2	MAA	G	7	X	-	-	-

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 3123 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 Single Domain Camelid Nanobody VHH A2.3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	120	Total	C	N	O	S	0	0	0
			927	579	165	179	4			
1	B	118	Total	C	N	O	S	0	0	0
			914	571	163	176	4			
1	C	120	Total	C	N	O	S	0	0	0
			927	579	165	179	4			

- Molecule 2 is a protein called Microcystin-LR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	7	Total	C	N	O	0	0	0
			71	49	10	12			
2	F	7	Total	C	N	O	0	0	0
			71	49	10	12			
2	G	7	Total	C	N	O	0	0	0
			71	49	10	12			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	40	Total	O	0	0
			40	40		
3	B	44	Total	O	0	0
			44	44		
3	C	47	Total	O	0	0
			47	47		
3	D	4	Total	O	0	0
			4	4		
3	F	1	Total	O	0	0
			1	1		
3	G	6	Total	O	0	0
			6	6		

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: Single Domain Camelid Nanobody VHH A2.3
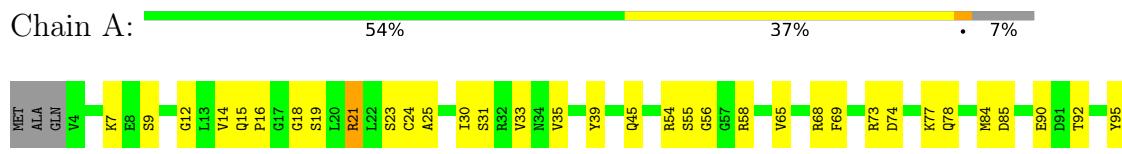
Chain A:

• Molecule 1: Single Domain Camelid Nanobody VHH A2.3

Chain B:

• Molecule 1: Single Domain Camelid Nanobody VHH A2.3

Chain C:

• Molecule 2: Microcystin-LR

Chain D:

• Molecule 2: Microcystin-LR

Chain F:

• Molecule 2: Microcystin-LR

Chain G:
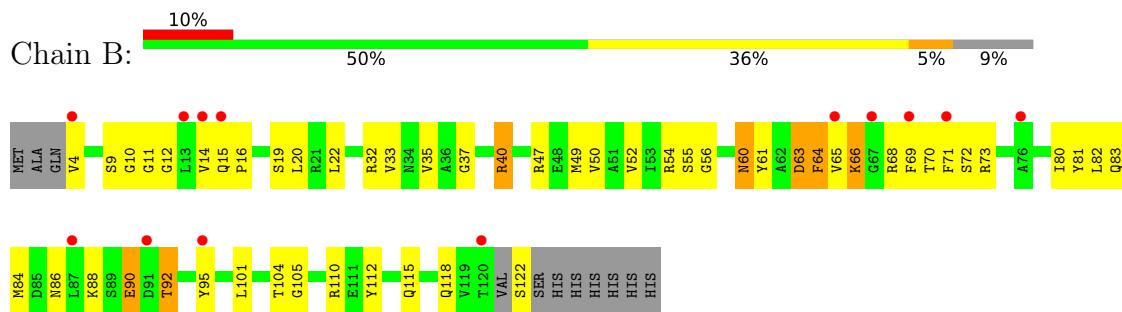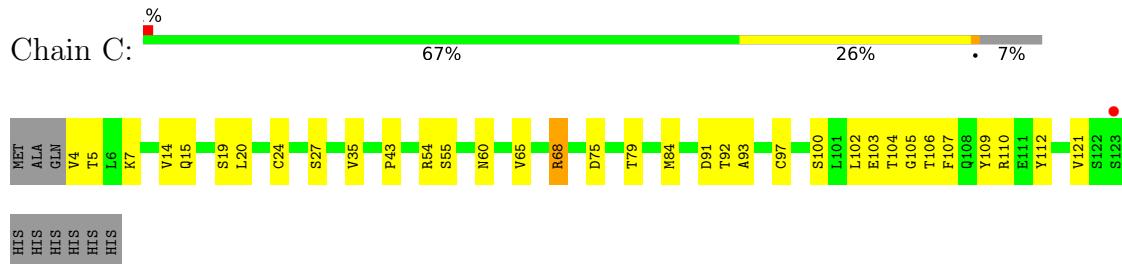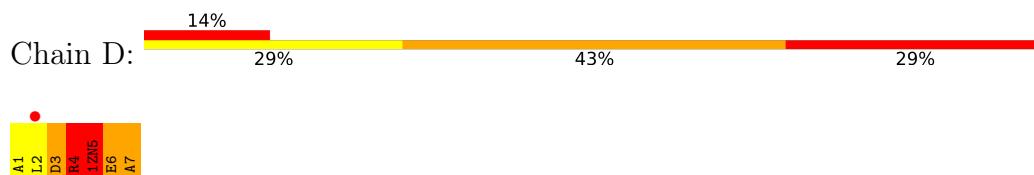
4 Data and refinement statistics (i)

| Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	38.10Å 101.32Å 102.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.69 – 2.35 35.66 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.7 (35.69-2.35) 98.7 (35.66-2.35)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.236 , 0.280 0.242 , 0.282	Depositor DCC
R_{free} test set	847 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	57.7	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 39.0	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3123	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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   ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 1ZN, FGA, MAA, DAL, ACB

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	0.52	0/944	0.95	0/1273
1	B	0.48	0/930	0.92	1/1252 (0.1%)
1	C	0.53	0/944	0.95	1/1273 (0.1%)
2	D	0.97	0/17	3.20	1/19 (5.3%)
2	F	1.46	1/17 (5.9%)	2.81	3/19 (15.8%)
2	G	1.34	0/17	2.55	1/19 (5.3%)
All	All	0.54	1/2869 (0.0%)	1.00	7/3855 (0.2%)

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	2
1	B	0	2
1	C	0	1
2	D	1	2
2	F	1	1
2	G	2	2
All	All	4	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	4	ARG	NE-CZ	-5.05	1.26	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	4	ARG	CD-NE-CZ	10.81	138.73	123.60
2	G	4	ARG	NE-CZ-NH1	8.54	124.57	120.30
2	F	4	ARG	CD-NE-CZ	6.53	132.75	123.60
1	B	60	ASN	CB-CA-C	6.29	122.97	110.40
1	C	68	ARG	NE-CZ-NH2	-5.78	117.41	120.30
2	F	4	ARG	CG-CD-NE	-5.22	100.83	111.80
2	F	4	ARG	NE-CZ-NH2	5.07	122.83	120.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	7	MAA	CA
2	F	7	MAA	CA
2	G	3	ACB	CB
2	G	7	MAA	CA

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	ARG	Sidechain
1	A	54	ARG	Sidechain
1	B	40	ARG	Sidechain
1	B	54	ARG	Sidechain
1	C	110	ARG	Sidechain
2	D	5	1ZN	Mainchain,Peptide
2	F	5	1ZN	Mainchain
2	G	5	1ZN	Mainchain,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	A	927	0	897	54	0
1	B	914	0	882	51	0
1	C	927	0	897	34	0
2	D	71	0	63	8	0
2	F	71	0	64	4	0
2	G	71	0	63	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	40	0	0	27	0
3	B	44	0	0	22	0
3	C	47	0	0	17	0
3	D	4	0	0	2	0
3	F	1	0	0	0	0
3	G	6	0	0	2	0
All	All	3123	0	2866	143	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 24.

All (143) 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:80:ILE:HA	3:B:203:HOH:O	1.31	1.23
1:B:73:ARG:HA	3:B:203:HOH:O	1.34	1.23
1:C:106:THR:HG22	3:C:234:HOH:O	1.57	1.04
1:A:33:VAL:HA	3:A:225:HOH:O	1.65	0.96
1:B:11:GLY:HA2	3:B:224:HOH:O	1.65	0.95
1:A:101:LEU:HD23	3:A:225:HOH:O	1.68	0.93
1:A:19:SER:N	3:A:203:HOH:O	2.01	0.92
1:C:14:VAL:O	3:C:201:HOH:O	1.89	0.90
1:C:14:VAL:C	3:C:201:HOH:O	2.10	0.90
1:A:23:SER:HB2	3:A:218:HOH:O	1.70	0.90
1:A:69:PHE:CE1	3:A:224:HOH:O	2.25	0.89
1:A:96:TYR:O	3:A:201:HOH:O	1.90	0.89
1:B:122:SER:HB2	3:B:214:HOH:O	1.70	0.89
1:C:43:PRO:O	3:C:202:HOH:O	1.93	0.86
1:B:16:PRO:HD3	3:B:214:HOH:O	1.76	0.85
1:A:100:SER:O	3:A:202:HOH:O	1.95	0.84
1:A:21:ARG:HH11	1:A:21:ARG:HG3	1.43	0.82
1:A:18:GLY:C	3:A:203:HOH:O	2.18	0.82
2:D:2:LEU:HD23	3:D:103:HOH:O	1.79	0.81
2:G:2:LEU:N	2:G:7:MAA:O	2.12	0.81
1:B:69:PHE:HB3	1:B:82:LEU:HD11	1.62	0.80
1:A:31:SER:HB2	3:A:206:HOH:O	1.80	0.80
1:A:69:PHE:HE1	3:A:224:HOH:O	1.64	0.80
2:D:6:FGA:O	3:D:101:HOH:O	1.99	0.79
1:B:22:LEU:HD11	1:B:84:MET:SD	2.24	0.78
1:B:82:LEU:HD13	3:B:228:HOH:O	1.83	0.78
1:B:66:LYS:HA	3:B:235:HOH:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:THR:HB	3:B:209:HOH:O	1.88	0.73
1:C:103:GLU:OE2	1:C:112:TYR:OH	2.07	0.71
1:A:78:GLN:OE1	2:D:4:ARG:NH2	2.23	0.71
2:F:2:LEU:HG	2:F:3:ACB:N	2.06	0.70
1:C:5:THR:HG22	3:C:205:HOH:O	1.94	0.68
1:A:18:GLY:HA3	3:A:203:HOH:O	1.93	0.68
1:A:7:LYS:HD2	1:A:25:ALA:O	1.93	0.68
1:A:31:SER:CB	3:A:206:HOH:O	2.41	0.68
2:G:7:MAA:HM2	3:G:101:HOH:O	1.94	0.67
1:A:108:GLN:NE2	1:B:10:GLY:O	2.28	0.66
1:A:18:GLY:CA	3:A:203:HOH:O	2.44	0.66
1:C:35:VAL:HG22	1:C:100:SER:HB3	1.77	0.65
1:C:15:GLN:C	3:C:201:HOH:O	2.33	0.65
1:B:92:THR:HG1	1:B:122:SER:N	1.95	0.65
1:C:14:VAL:HG13	1:C:20:LEU:HD21	1.78	0.64
1:C:60:ASN:HB3	3:C:242:HOH:O	1.98	0.64
1:A:101:LEU:CD2	3:A:225:HOH:O	2.38	0.64
1:B:82:LEU:HB2	3:B:228:HOH:O	1.98	0.64
1:C:5:THR:HA	3:C:205:HOH:O	1.97	0.63
1:B:22:LEU:O	1:B:81:TYR:HA	1.98	0.63
1:A:73:ARG:NH2	2:D:3:ACB:OXT	2.24	0.63
1:A:101:LEU:HA	3:A:202:HOH:O	1.99	0.62
1:C:103:GLU:HG2	3:C:243:HOH:O	1.98	0.61
1:B:37:GLY:HA3	1:B:52:VAL:HG12	1.82	0.61
1:B:82:LEU:CD1	3:B:228:HOH:O	2.43	0.61
1:C:4:VAL:HA	1:C:27:SER:O	2.00	0.60
1:A:15:GLN:HB2	3:A:226:HOH:O	2.00	0.60
1:C:75:ASP:CG	2:G:3:ACB:H42	2.22	0.59
1:A:101:LEU:HA	3:A:225:HOH:O	2.03	0.58
1:B:65:VAL:HG13	3:B:240:HOH:O	2.04	0.58
1:B:11:GLY:HA2	1:B:20:LEU:HD13	1.86	0.58
1:B:65:VAL:HA	3:B:240:HOH:O	2.04	0.58
1:A:30:ILE:O	2:D:4:ARG:NE	2.35	0.58
1:B:69:PHE:HA	1:B:83:GLN:O	2.05	0.57
1:B:63:ASP:HA	3:B:238:HOH:O	2.04	0.57
1:B:61:TYR:HD2	3:B:241:HOH:O	1.87	0.56
1:B:40:ARG:HG2	1:B:95:TYR:CZ	2.41	0.56
1:C:15:GLN:CA	3:C:201:HOH:O	2.52	0.56
1:A:117:THR:HB	3:A:205:HOH:O	2.05	0.56
1:C:65:VAL:O	1:C:68:ARG:HD3	2.05	0.56
1:A:58:ARG:HB2	3:A:220:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:DAL:C	2:D:7:MAA:O	2.54	0.56
1:B:66:LYS:HB2	1:B:68:ARG:HG3	1.87	0.55
1:A:96:TYR:C	3:A:201:HOH:O	2.40	0.55
2:F:5:1ZN:H16	2:F:5:1ZN:H2	1.89	0.55
1:C:14:VAL:HG23	3:C:201:HOH:O	2.07	0.55
2:D:5:1ZN:H2	2:D:5:1ZN:H16	1.88	0.55
1:C:15:GLN:N	3:C:201:HOH:O	2.37	0.54
1:B:32:ARG:HG3	1:B:33:VAL:N	2.22	0.54
1:A:16:PRO:HD3	1:A:122:SER:O	2.08	0.54
1:B:88:LYS:HB2	1:B:90:GLU:OE2	2.08	0.54
1:A:55:SER:O	1:A:56:GLY:C	2.46	0.53
1:B:40:ARG:CZ	3:B:212:HOH:O	2.56	0.53
1:A:73:ARG:HH21	2:D:3:ACB:C	2.21	0.53
1:C:24:CYS:O	1:C:79:THR:HA	2.10	0.52
2:G:1:DAL:N	3:G:101:HOH:O	2.34	0.52
1:B:110:ARG:NH2	3:B:204:HOH:O	2.43	0.52
1:B:69:PHE:CE2	1:B:84:MET:HE3	2.45	0.52
1:B:86:ASN:O	1:B:88:LYS:HE3	2.09	0.52
1:C:54:ARG:NH1	3:C:204:HOH:O	2.35	0.52
1:A:102:LEU:HG	1:A:109:TYR:CE1	2.45	0.51
1:A:95:TYR:O	1:A:116:GLY:HA2	2.11	0.50
1:B:69:PHE:CD1	1:B:84:MET:HA	2.48	0.49
1:A:39:TYR:O	3:A:201:HOH:O	2.19	0.49
1:C:97:CYS:HA	3:C:239:HOH:O	2.13	0.49
2:F:5:1ZN:H16	2:F:5:1ZN:C1	2.43	0.49
1:B:82:LEU:CB	3:B:228:HOH:O	2.57	0.49
1:C:106:THR:CG2	3:C:234:HOH:O	2.35	0.48
1:A:90:GLU:HB3	3:A:212:HOH:O	2.12	0.48
1:C:14:VAL:CG1	1:C:20:LEU:HD21	2.44	0.48
1:A:7:LYS:O	1:A:24:CYS:HA	2.12	0.47
1:C:102:LEU:HB2	1:C:109:TYR:CE1	2.48	0.47
1:A:12:GLY:HA2	1:C:107:PHE:CE1	2.50	0.47
1:B:66:LYS:C	1:B:68:ARG:H	2.16	0.47
1:A:21:ARG:HH11	1:A:21:ARG:CG	2.21	0.46
1:C:75:ASP:OD2	2:G:3:ACB:H42	2.15	0.46
1:C:103:GLU:CG	3:C:243:HOH:O	2.60	0.46
1:B:4:VAL:HA	3:B:231:HOH:O	2.14	0.46
1:A:16:PRO:CD	1:A:122:SER:O	2.64	0.46
1:A:84:MET:HB3	3:A:224:HOH:O	2.15	0.46
1:A:96:TYR:N	3:A:201:HOH:O	2.47	0.46
1:A:115:GLN:O	1:C:109:TYR:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ARG:HG3	1:B:33:VAL:H	1.80	0.46
1:B:64:PHE:N	3:B:206:HOH:O	2.49	0.46
1:B:101:LEU:HD12	1:B:112:TYR:CE1	2.50	0.46
1:C:55:SER:O	2:G:5:1ZN:O	2.33	0.46
1:A:12:GLY:HA2	1:C:107:PHE:CD1	2.51	0.45
1:A:19:SER:OG	1:A:85:ASP:OD1	2.29	0.45
1:A:102:LEU:HD11	1:B:118:GLN:HB2	1.99	0.45
1:B:49:MET:SD	1:B:50:VAL:N	2.90	0.44
1:B:65:VAL:HG12	1:B:66:LYS:O	2.17	0.44
1:C:68:ARG:NH2	1:C:91:ASP:OD2	2.49	0.44
1:B:20:LEU:HD13	3:B:224:HOH:O	2.17	0.44
1:A:117:THR:CB	3:A:205:HOH:O	2.62	0.44
1:A:74:ASP:OD2	1:A:77:LYS:HD3	2.17	0.44
1:B:55:SER:O	1:B:56:GLY:C	2.55	0.43
1:A:65:VAL:O	1:A:68:ARG:HD3	2.18	0.43
1:A:107:PHE:CG	1:B:12:GLY:HA2	2.53	0.43
1:B:40:ARG:HG3	1:B:50:VAL:HG21	2.01	0.42
1:B:104:THR:HG23	1:B:105:GLY:N	2.35	0.42
1:A:45:GLN:N	1:A:45:GLN:CD	2.73	0.41
1:B:22:LEU:HD12	1:B:82:LEU:HB3	2.02	0.41
1:B:71:PHE:HA	3:B:228:HOH:O	2.20	0.41
1:B:69:PHE:CE2	1:B:84:MET:CE	3.03	0.41
1:C:121:VAL:HG13	3:C:201:HOH:O	2.19	0.41
1:A:14:VAL:HB	3:A:203:HOH:O	2.20	0.41
1:B:73:ARG:HH21	2:F:3:ACB:C	2.33	0.41
1:A:92:THR:HA	1:A:119:VAL:O	2.20	0.41
1:B:40:ARG:O	1:B:47:ARG:HA	2.21	0.40
1:B:64:PHE:HD2	3:B:212:HOH:O	2.04	0.40
1:A:35:VAL:CG2	1:A:98:TYR:HE2	2.34	0.40
1:A:68:ARG:HB3	1:A:85:ASP:O	2.22	0.40
1:C:19:SER:HA	1:C:84:MET:O	2.21	0.40
1:A:74:ASP:HA	3:A:228:HOH:O	2.19	0.40
1:C:92:THR:O	1:C:93:ALA:HB2	2.22	0.40
1:A:14:VAL:O	1:A:121:VAL:HA	2.21	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	118/129 (92%)	110 (93%)	8 (7%)	0	100	100
1	B	115/129 (89%)	105 (91%)	10 (9%)	0	100	100
1	C	118/129 (92%)	111 (94%)	6 (5%)	1 (1%)	19	20
2	D	1/7 (14%)	0	1 (100%)	0	100	100
2	F	1/7 (14%)	0	1 (100%)	0	100	100
2	G	1/7 (14%)	0	1 (100%)	0	100	100
All	All	354/408 (87%)	326 (92%)	27 (8%)	1 (0%)	41	47

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	105	GLY

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	96/104 (92%)	92 (96%)	4 (4%)	30	36
1	B	94/104 (90%)	80 (85%)	14 (15%)	3	3
1	C	96/104 (92%)	94 (98%)	2 (2%)	53	65
2	D	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	F	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	G	2/2 (100%)	2 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	292/318 (92%)	270 (92%)	22 (8%)	13 13

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	21	ARG
1	A	100	SER
1	A	123	SER
1	B	9	SER
1	B	14	VAL
1	B	15	GLN
1	B	19	SER
1	B	35	VAL
1	B	60	ASN
1	B	63	ASP
1	B	64	PHE
1	B	66	LYS
1	B	70	THR
1	B	72	SER
1	B	90	GLU
1	B	92	THR
1	B	115	GLN
1	C	7	LYS
1	C	104	THR
2	D	4	ARG
2	F	4	ARG

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

Mol	Chain	Res	Type
1	B	78	GLN
1	B	115	GLN
1	B	118	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

15 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MAA	F	7	2	4,5,6	4.71	2 (50%)	1,5,7	3.91	1 (100%)
2	FGA	G	6	2	7,8,9	0.49	0	7,9,11	1.44	1 (14%)
2	DAL	F	1	2	3,4,5	0.35	0	2,4,6	2.16	1 (50%)
2	DAL	G	1	2	3,4,5	0.81	0	2,4,6	2.26	1 (50%)
2	MAA	D	7	2	4,5,6	4.66	2 (50%)	1,5,7	6.39	1 (100%)
2	FGA	F	6	2	7,8,9	1.69	2 (28%)	7,9,11	2.34	2 (28%)
2	DAL	D	1	2	3,4,5	1.14	0	2,4,6	0.32	0
2	1ZN	F	5	2	23,23,24	1.23	2 (8%)	24,29,31	1.87	8 (33%)
2	1ZN	D	5	2	23,23,24	1.28	3 (13%)	24,29,31	1.51	5 (20%)
2	FGA	D	6	2	7,8,9	0.78	0	7,9,11	1.67	3 (42%)
2	1ZN	G	5	2	23,23,24	1.09	2 (8%)	24,29,31	1.49	4 (16%)
2	MAA	G	7	2	4,5,6	5.13	2 (50%)	1,5,7	3.66	1 (100%)
2	ACB	F	3	2	7,8,9	0.66	0	8,10,12	3.26	3 (37%)
2	ACB	D	3	2	7,8,9	0.75	0	8,10,12	1.57	2 (25%)
2	ACB	G	3	2	7,8,9	1.76	2 (28%)	8,10,12	2.35	3 (37%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAA	F	7	2	1/1/1/3	0/1/4/6	-
2	FGA	G	6	2	-	5/7/8/9	-
2	DAL	F	1	2	-	0/0/2/4	-
2	DAL	G	1	2	-	0/0/2/4	-
2	MAA	D	7	2	1/1/1/3	0/1/4/6	-
2	FGA	F	6	2	-	1/7/8/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DAL	D	1	2	-	0/0/2/4	-
2	1ZN	F	5	2	-	3/22/25/27	0/1/1/1
2	1ZN	D	5	2	-	3/22/25/27	0/1/1/1
2	FGA	D	6	2	-	5/7/8/9	-
2	MAA	G	7	2	1/1/1/3	1/1/4/6	-
2	1ZN	G	5	2	-	4/22/25/27	0/1/1/1
2	ACB	F	3	2	-	3/9/10/12	-
2	ACB	D	3	2	-	0/9/10/12	-
2	ACB	G	3	2	1/1/3/4	4/9/10/12	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	7	MAA	CA-N	-7.90	1.33	1.47
2	D	7	MAA	CB-CA	-6.76	1.33	1.51
2	F	7	MAA	CB-CA	-6.73	1.33	1.51
2	F	7	MAA	CA-N	-6.58	1.35	1.47
2	G	7	MAA	CB-CA	-6.45	1.34	1.51
2	D	7	MAA	CA-N	-6.35	1.36	1.47
2	F	6	FGA	O-C	3.67	1.33	1.22
2	F	5	1ZN	C15-C13	3.47	1.53	1.45
2	F	5	1ZN	C18-CA	-3.43	1.51	1.55
2	G	3	ACB	O-C	3.06	1.31	1.22
2	G	5	1ZN	C18-CA	-2.76	1.52	1.55
2	D	5	1ZN	C18-CA	-2.75	1.52	1.55
2	D	5	1ZN	C3-C2	2.67	1.56	1.52
2	F	6	FGA	OXT-C	-2.39	1.22	1.30
2	G	5	1ZN	CA-C16	2.15	1.52	1.50
2	G	3	ACB	OXT-C	-2.15	1.23	1.30
2	D	5	1ZN	C15-C13	2.08	1.50	1.45

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	3	ACB	C4-CB-CA	7.47	118.88	110.94
2	D	7	MAA	CB-CA-N	6.39	125.23	110.18
2	F	5	1ZN	C2-C10-C12	-4.65	101.86	110.24
2	F	6	FGA	OXT-C-O	-4.57	113.72	124.09
2	G	3	ACB	CB-CA-C	4.52	117.48	110.59
2	F	3	ACB	OXT-C-O	-4.34	114.24	124.09
2	F	7	MAA	CB-CA-N	3.91	119.38	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	7	MAA	CB-CA-N	3.66	118.81	110.18
2	G	5	1ZN	C2-C10-C12	-3.48	103.97	110.24
2	F	5	1ZN	C14-C13-C15	3.43	123.48	118.08
2	G	5	1ZN	C11-C10-C12	3.42	115.73	110.05
2	F	5	1ZN	C11-C10-C2	-3.38	106.76	111.80
2	F	6	FGA	OXT-C-CA	3.37	124.86	113.38
2	F	5	1ZN	C11-C10-C12	3.19	115.35	110.05
2	G	1	DAL	O-C-CA	-3.09	114.50	124.28
2	D	5	1ZN	C3-C2-C10	3.08	122.64	115.45
2	D	5	1ZN	O-C-C18	-3.08	116.73	124.91
2	G	3	ACB	OD1-CG-CB	-3.07	116.75	124.91
2	F	5	1ZN	CA-C18-C	2.93	114.35	110.72
2	F	1	DAL	O-C-CA	-2.89	115.13	124.28
2	D	5	1ZN	C7-C6-C5	2.52	124.03	120.19
2	G	5	1ZN	CA-C18-C	-2.46	107.67	110.72
2	G	5	1ZN	C1-O1-C2	-2.44	107.45	114.03
2	G	6	FGA	OXT-C-O	-2.42	118.59	124.09
2	F	5	1ZN	O-C-C18	-2.42	118.49	124.91
2	D	3	ACB	OXT-C-O	-2.40	118.63	124.09
2	D	5	1ZN	CA-C18-C	-2.38	107.77	110.72
2	D	6	FGA	CB-CA-N	2.33	116.27	110.17
2	D	3	ACB	OXT-C-CA	2.32	122.33	114.22
2	D	6	FGA	OXT-C-CA	2.32	121.27	113.38
2	F	3	ACB	CB-CA-C	-2.27	107.13	110.59
2	D	6	FGA	OXT-C-O	-2.13	119.26	124.09
2	F	5	1ZN	C4-C3-C2	-2.12	110.32	113.42
2	D	5	1ZN	C11-C10-C2	2.11	114.94	111.80
2	F	5	1ZN	C1-O1-C2	2.09	119.65	114.03
2	G	3	ACB	OXT-C-CA	2.04	121.35	114.22

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	3	ACB	CB
2	D	7	MAA	CA
2	F	7	MAA	CA
2	G	7	MAA	CA

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	3	ACB	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
2	F	3	ACB	OXT-C-CA-N
2	F	3	ACB	OXT-C-CA-CB
2	G	3	ACB	C-CA-CB-CG
2	G	3	ACB	C-CA-CB-C4
2	G	3	ACB	N-CA-CB-CG
2	G	3	ACB	N-CA-CB-C4
2	G	5	1ZN	C19-C18-CA-C16
2	D	6	FGA	O-C-CA-N
2	D	6	FGA	N-CA-CB-CG
2	D	6	FGA	CA-CB-CG-CD
2	F	6	FGA	C-CA-CB-CG
2	G	6	FGA	N-CA-CB-CG
2	G	6	FGA	C-CA-CB-CG
2	G	6	FGA	CA-CB-CG-CD
2	G	7	MAA	CB-CA-N-CM
2	D	6	FGA	OXT-C-CA-N
2	G	6	FGA	O-C-CA-N
2	F	5	1ZN	C12-C13-C15-C16
2	D	6	FGA	C-CA-CB-CG
2	F	5	1ZN	C2-C3-C4-C5
2	F	5	1ZN	C2-C3-C4-C9
2	G	5	1ZN	C2-C3-C4-C9
2	D	5	1ZN	O-C-C18-CA
2	G	5	1ZN	O-C-C18-CA
2	G	5	1ZN	C2-C3-C4-C5
2	D	5	1ZN	C2-C3-C4-C5
2	D	5	1ZN	C2-C3-C4-C9
2	G	6	FGA	OXT-C-CA-N

There are no ring outliers.

11 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	DAL	1	0
2	D	7	MAA	1	0
2	D	1	DAL	1	0
2	F	5	1ZN	2	0
2	D	5	1ZN	1	0
2	D	6	FGA	1	0
2	G	5	1ZN	1	0
2	G	7	MAA	2	0
2	F	3	ACB	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	ACB	2	0
2	G	3	ACB	2	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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(Å²)	Q<0.9
1	A	120/129 (93%)	-0.11	0	100	100	39, 54, 85, 90	0
1	B	118/129 (91%)	0.52	13 (11%)	5	8	42, 72, 102, 124	0
1	C	120/129 (93%)	-0.17	1 (0%)	86	91	34, 51, 77, 96	0
2	D	2/7 (28%)	1.28	1 (50%)	0	0	67, 67, 67, 93	0
2	F	2/7 (28%)	2.50	1 (50%)	0	0	70, 70, 70, 122	0
2	G	2/7 (28%)	0.45	0	100	100	59, 59, 59, 106	0
All	All	364/408 (89%)	0.10	16 (4%)	34	46	34, 59, 94, 124	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	2	LEU	4.9
1	B	14	VAL	3.5
1	B	120	THR	3.1
1	B	13	LEU	3.0
1	B	76	ALA	2.9
1	B	87	LEU	2.8
1	B	67	GLY	2.7
1	B	65	VAL	2.6
1	B	91	ASP	2.6
2	D	2	LEU	2.5
1	B	4	VAL	2.2
1	B	69	PHE	2.2
1	B	95	TYR	2.2
1	B	15	GLN	2.0
1	C	123	SER	2.0
1	B	71	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	DAL	D	1	5/6	0.64	0.23	72,79,92,99	0
2	DAL	G	1	5/6	0.74	0.17	75,80,89,98	0
2	MAA	D	7	6/7	0.79	0.18	81,91,101,119	0
2	DAL	F	1	5/6	0.82	0.19	70,87,101,104	0
2	FGA	D	6	9/10	0.86	0.20	70,89,109,115	0
2	MAA	G	7	6/7	0.87	0.14	69,92,105,106	0
2	FGA	G	6	9/10	0.88	0.13	72,84,107,111	0
2	FGA	F	6	9/10	0.89	0.13	72,85,95,110	0
2	ACB	G	3	9/10	0.92	0.14	65,68,75,95	0
2	MAA	F	7	6/7	0.92	0.19	97,100,108,114	0
2	ACB	F	3	9/10	0.92	0.22	52,77,85,88	0
2	1ZN	D	5	23/24	0.94	0.15	45,60,69,82	0
2	1ZN	F	5	23/24	0.94	0.15	42,58,70,73	0
2	ACB	D	3	9/10	0.95	0.20	65,78,96,106	0
2	1ZN	G	5	23/24	0.96	0.15	43,57,68,75	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.