



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2017 – 01:46 AM EDT

PDB ID : 1M63
Title : Crystal structure of calcineurin-cyclophilin-cyclosporin shows common but distinct recognition of immunophilin-drug complexes
Authors : Huai, Q.; Kim, H.-Y.; Liu, Y.; Zhao, Y.; Mondragon, A.; Liu, J.O.; Ke, H.
Deposited on : unknown
Resolution : 2.80 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

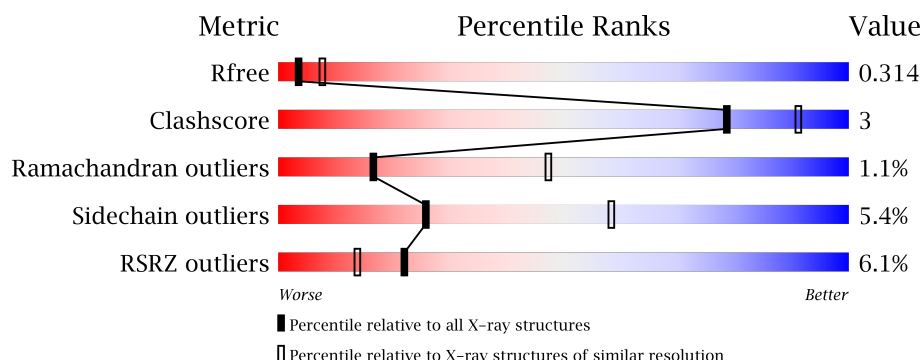
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



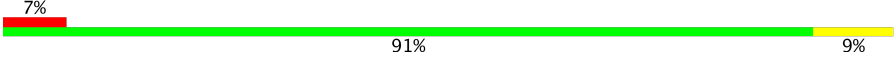
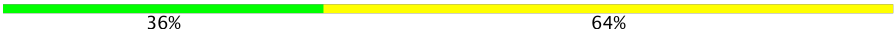

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	372	<div> <div>5%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>..</div> </div> </div>
1	E	372	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>..</div> </div> </div>
2	B	169	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>7%</div> </div> </div>
2	F	169	<div> <div>20%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>5%</div> </div> </div>
3	C	165	<div> <div></div> <div> <div></div> <div>88%</div> <div>12%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	G	165	
4	D	11	
4	H	11	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11185 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 SERINE/THREONINE PROTEIN PHOSPHATASE 2B CATALYTIC SUBUNIT, ALPHA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	0	0
			3014	1940	503	549	22			
1	E	359	Total	C	N	O	S	0	0	0
			2917	1879	488	529	21			

- Molecule 2 is a protein called CALCINEURIN B SUBUNIT ISOFORM 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	158	Total	C	N	O	S	0	0	0
			1263	797	211	249	6			
2	F	160	Total	C	N	O	S	0	0	0
			1277	805	213	251	8			

- Molecule 3 is a protein called PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	165	Total	C	N	O	S	0	0	0
			1266	802	218	237	9			
3	G	165	Total	C	N	O	S	0	0	0
			1266	802	218	237	9			

- Molecule 4 is a protein called CYCLOSPORIN A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	11	Total	C	N	O	0	0	0
			85	62	11	12			
4	H	11	Total	C	N	O	0	0	0
			85	62	11	12			

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Zn 1	0	0
5	E	1	Total 1	Zn 1	0	0

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	Fe 1	0	0
6	E	1	Total 1	Fe 1	0	0

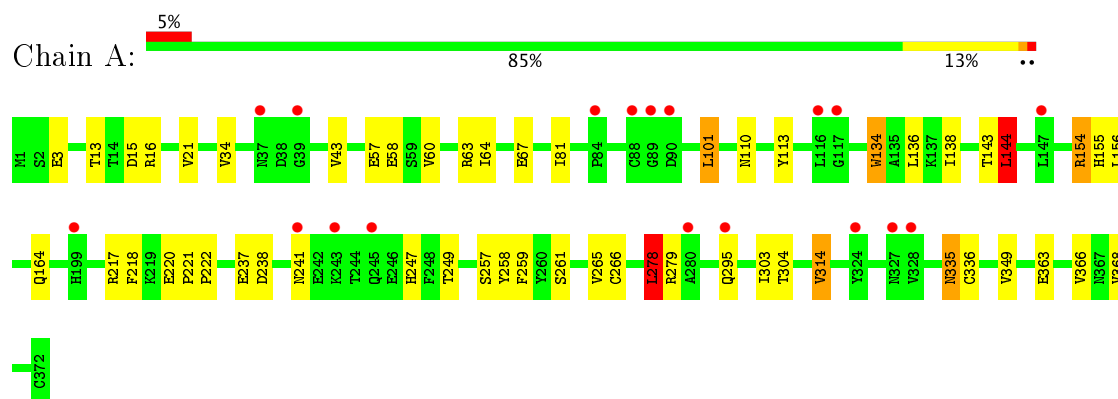
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	4	Total 4	Ca 4	0	0
7	F	4	Total 4	Ca 4	0	0

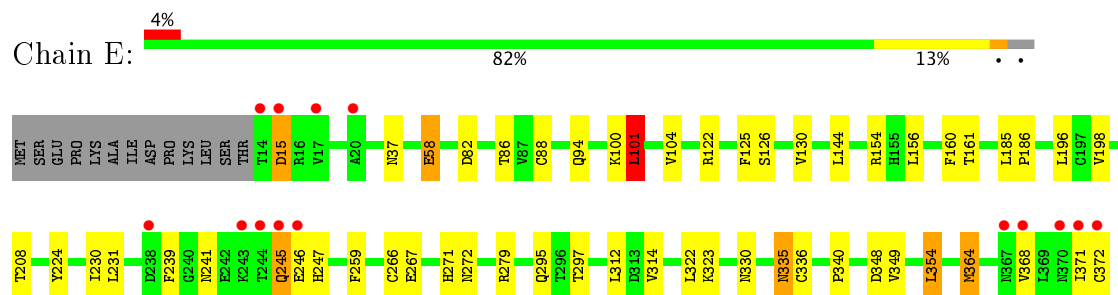
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

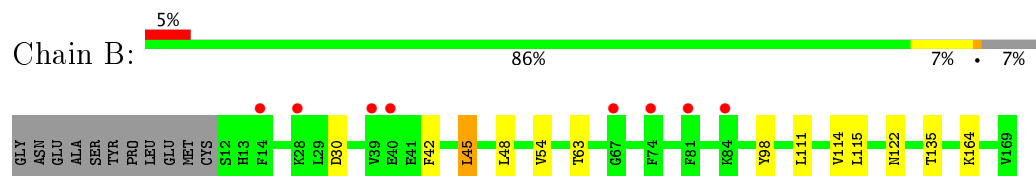
- Molecule 1: SERINE/THREONINE PROTEIN PHOSPHATASE 2B CATALYTIC SUBUNIT, ALPHA ISOFORM



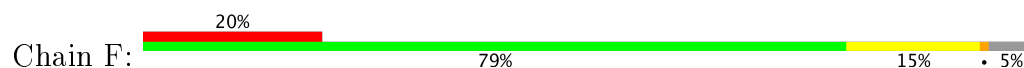
- Molecule 1: SERINE/THREONINE PROTEIN PHOSPHATASE 2B CATALYTIC SUBUNIT, ALPHA ISOFORM

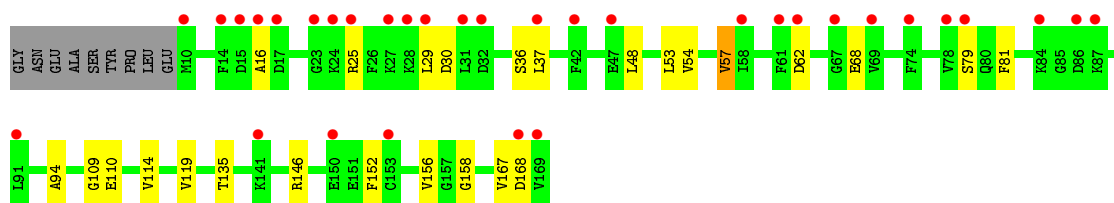


- Molecule 2: CALCINEURIN B SUBUNIT ISOFORM 1



- Molecule 2: CALCINEURIN B SUBUNIT ISOFORM 1





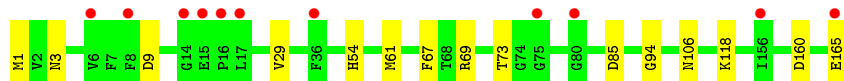
● Molecule 3: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A

Chain C: 88% 12%



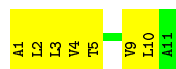
● Molecule 3: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A

Chain G: 7% 91% 9%



● Molecule 4: CYCLOSPORIN A

Chain D: 36% 64%



● Molecule 4: CYCLOSPORIN A

Chain H: 64% 36%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	108.66Å 108.66Å 316.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.80 34.76 – 2.80	Depositor EDS
% Data completeness (in resolution range)	0.9 (40.00-2.80) 91.0 (34.76-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.260 , 0.322 0.262 , 0.314	Depositor DCC
R_{free} test set	4379 reflections (10.07%)	DCC
Wilson B-factor (Å ²)	55.2	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 22.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11185	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 2.00% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ABA, ZN, MLE, DAL, CA, MVA, FE, BMT, SAR

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	0.72	0/3095	0.80	4/4198 (0.1%)
1	E	0.71	0/2996	0.80	2/4064 (0.0%)
2	B	0.72	0/1280	0.73	0/1711
2	F	0.72	0/1294	0.74	0/1729
3	C	0.69	0/1294	0.78	0/1733
3	G	0.69	0/1294	0.76	0/1733
4	D	0.67	0/10	0.88	0/11
4	H	0.49	0/10	0.75	0/11
All	All	0.71	0/11273	0.78	6/15190 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	LEU	CA-CB-CG	6.97	131.33	115.30
1	E	144	LEU	CA-CB-CG	6.69	130.68	115.30
1	E	101	LEU	CA-CB-CG	6.50	130.25	115.30
1	A	144	LEU	CA-CB-CG	5.62	128.23	115.30
1	A	278	LEU	CA-CB-CG	5.51	127.97	115.30
1	A	314	VAL	CG1-CB-CG2	5.36	119.48	110.90

There are no chirality outliers.

There are no planarity outliers.

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	3014	0	2960	16	0
1	E	2917	0	2854	21	0
2	B	1263	0	1246	8	0
2	F	1277	0	1260	12	0
3	C	1266	0	1237	11	0
3	G	1266	0	1237	7	0
4	D	85	0	110	9	0
4	H	85	0	109	3	0
5	A	1	0	0	0	0
5	E	1	0	0	0	0
6	A	1	0	0	0	0
6	E	1	0	0	0	0
7	B	4	0	0	0	0
7	F	4	0	0	0	0
All	All	11185	0	11013	73	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 3.

All (73) 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)
3:C:63:GLN:HE21	4:D:4:MVA:HG12	1.38	0.87
2:B:45:LEU:H	2:B:45:LEU:HD12	1.47	0.79
3:C:85:ASP:H	3:C:106:ASN:HD22	1.33	0.77
2:B:122:ASN:HD22	4:D:5:BMT:HH2	1.53	0.74
1:E:349:VAL:HG22	2:F:135:THR:HG21	1.80	0.64
3:G:1:MET:H2	3:G:3:ASN:HD22	1.44	0.63
1:E:335:ASN:HD22	1:E:336:CYS:H	1.47	0.62
1:E:348:ASP:HB2	2:F:135:THR:HG23	1.83	0.60
3:G:1:MET:N	3:G:3:ASN:HD22	2.02	0.58
1:E:208:THR:HA	1:E:272:ASN:HD21	1.69	0.58
1:E:230:ILE:HG22	1:E:231:LEU:HD12	1.87	0.57
3:G:94:GLY:HA2	3:G:118:LYS:HA	1.90	0.54
3:G:9:ASP:HB2	3:G:160:ASP:HB3	1.89	0.54
3:C:85:ASP:H	3:C:106:ASN:ND2	2.04	0.52
1:E:323:LYS:HG3	1:E:330:ASN:HB2	1.91	0.51
2:B:45:LEU:HD13	2:B:48:LEU:HD22	1.93	0.51
3:C:145:PHE:HB2	3:C:156:ILE:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:141:ALA:O	3:C:144:ARG:HG2	2.12	0.50
2:B:111:LEU:O	2:B:115:LEU:HG	2.12	0.49
3:C:63:GLN:NE2	4:D:4:MVA:HG12	2.17	0.49
1:E:88:CYS:SG	1:E:101:LEU:HD11	2.53	0.48
2:F:110:GLU:O	2:F:114:VAL:HG23	2.12	0.48
1:A:349:VAL:HG22	2:B:135:THR:HG21	1.95	0.48
2:F:48:LEU:O	2:F:54:VAL:HG21	2.13	0.48
1:A:154:ARG:HG2	1:A:220:GLU:OE1	2.13	0.48
4:D:9:VAL:HA	4:D:10:MLE:HN1	1.65	0.47
2:B:98:TYR:HA	2:B:114:VAL:HG21	1.96	0.47
1:A:238:ASP:HB3	1:A:241:ASN:HB2	1.95	0.47
3:C:113:PHE:CD1	4:D:4:MVA:HG11	2.50	0.47
4:D:1:DAL:HA	4:D:2:MLE:HN1	1.57	0.47
2:F:81:PHE:HB3	2:F:167:VAL:HG22	1.96	0.47
1:A:257:SER:OG	1:A:258:TYR:N	2.46	0.47
1:A:34:VAL:HG11	1:A:64:ILE:HD11	1.97	0.46
3:C:87:ASN:O	3:C:127:VAL:HG13	2.16	0.46
1:A:113:TYR:HB2	1:A:144:LEU:HD22	1.98	0.46
3:C:18:GLY:HA3	3:C:138:ILE:HD12	1.98	0.46
1:A:217:ARG:HG2	1:A:218:PHE:H	1.80	0.45
2:B:164:LYS:NZ	3:C:71:ASN:HD22	2.15	0.45
1:E:100:LYS:O	1:E:104:VAL:HG23	2.16	0.45
2:F:36:SER:HB2	2:F:68:GLU:HB3	1.98	0.45
1:E:185:LEU:HA	1:E:186:PRO:HD3	1.85	0.45
1:E:267:GLU:O	1:E:271:HIS:HB2	2.16	0.45
3:G:54:HIS:H	3:G:54:HIS:CD2	2.35	0.45
1:E:371:ILE:HG13	1:E:371:ILE:H	1.60	0.45
1:E:372:CYS:HB3	2:F:25:ARG:HG2	1.99	0.45
1:A:221:PRO:HA	1:A:222:PRO:HD3	1.76	0.44
1:A:57:GLU:HB2	1:A:60:VAL:HG12	1.98	0.44
2:F:29:LEU:HD13	2:F:37:LEU:HD21	1.99	0.44
2:F:152:PHE:O	2:F:156:VAL:HG22	2.18	0.43
1:A:16:ARG:NH2	1:A:21:VAL:HG23	2.34	0.43
1:A:335:ASN:HD22	1:A:336:CYS:H	1.66	0.43
1:A:278:LEU:HD12	1:A:303:ILE:HB	1.99	0.43
1:A:63:ARG:O	1:A:67:GLU:HB2	2.19	0.43
1:E:364:MET:O	1:E:368:VAL:HG23	2.19	0.42
1:A:134:TRP:O	1:A:138:ILE:HG13	2.19	0.42
4:H:9:VAL:HA	4:H:10:MLE:HN1	1.64	0.42
1:A:43:VAL:HG11	1:A:136:LEU:HD23	2.01	0.42
4:D:2:MLE:HA	4:D:3:MLE:HN1	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:241:ASN:HD22	1:E:241:ASN:N	2.18	0.42
1:E:354:LEU:HD21	2:F:94:ALA:HB1	2.01	0.42
3:G:73:THR:HG22	4:H:7:SAR:HA3	2.02	0.42
1:E:312:LEU:HD13	4:H:2:MLE:HD21	2.02	0.42
3:C:55:ARG:HB3	3:C:63:GLN:HB3	2.01	0.41
1:E:126:SER:O	1:E:130:VAL:HG23	2.20	0.41
4:D:4:MVA:HA	4:D:5:BMT:HN1	1.77	0.41
1:E:86:THR:HG23	1:E:323:LYS:HB3	2.02	0.41
2:F:53:LEU:O	2:F:57:VAL:HG23	2.21	0.40
1:E:125:PHE:HZ	1:E:340:PRO:HB2	1.86	0.40
1:E:15:ASP:HB3	2:F:109:GLY:H	1.85	0.40
2:B:122:ASN:ND2	4:D:5:BMT:HH2	2.29	0.40
3:G:85:ASP:H	3:G:106:ASN:HD22	1.69	0.40
1:A:261:SER:O	1:A:265:VAL:HG23	2.21	0.40
1:E:160:PHE:HB3	1:E:161:THR:H	1.77	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	370/372 (100%)	337 (91%)	30 (8%)	3 (1%)	22	55
1	E	357/372 (96%)	318 (89%)	32 (9%)	7 (2%)	9	28
2	B	156/169 (92%)	145 (93%)	11 (7%)	0	100	100
2	F	158/169 (94%)	141 (89%)	14 (9%)	3 (2%)	9	30
3	C	163/165 (99%)	155 (95%)	6 (4%)	2 (1%)	15	44
3	G	163/165 (99%)	147 (90%)	16 (10%)	0	100	100
4	D	1/11 (9%)	1 (100%)	0	0	100	100
4	H	1/11 (9%)	1 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1369/1434 (96%)	1245 (91%)	109 (8%)	15 (1%)	17	47

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	81	GLU
1	E	245	GLN
1	E	239	PHE
1	E	246	GLU
1	E	295	GLN
1	A	304	THR
1	E	58	GLU
1	E	94	GLN
2	F	158	GLY
1	A	237	GLU
2	F	16	ALA
1	A	3	GLU
3	C	25	PHE
1	E	122	ARG
2	F	57	VAL

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	333/333 (100%)	308 (92%)	25 (8%)	16	41
1	E	321/333 (96%)	300 (94%)	21 (6%)	20	49
2	B	141/150 (94%)	136 (96%)	5 (4%)	41	75
2	F	143/150 (95%)	137 (96%)	6 (4%)	34	68
3	C	133/133 (100%)	130 (98%)	3 (2%)	56	86
3	G	133/133 (100%)	128 (96%)	5 (4%)	38	72
4	D	1/1 (100%)	1 (100%)	0	100	100
4	H	1/1 (100%)	1 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1206/1234 (98%)	1141 (95%)	65 (5%)	26 58

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	15	ASP
1	A	58	GLU
1	A	81	ILE
1	A	101	LEU
1	A	110	ASN
1	A	134	TRP
1	A	143	THR
1	A	144	LEU
1	A	154	ARG
1	A	155	HIS
1	A	156	LEU
1	A	164	GLN
1	A	247	HIS
1	A	249	THR
1	A	259	PHE
1	A	266	CYS
1	A	278	LEU
1	A	279	ARG
1	A	295	GLN
1	A	314	VAL
1	A	335	ASN
1	A	363	GLU
1	A	366	VAL
1	A	368	VAL
2	B	30	ASP
2	B	42	PHE
2	B	45	LEU
2	B	54	VAL
2	B	63	THR
3	C	29	VAL
3	C	61	MET
3	C	120	GLU
1	E	15	ASP
1	E	37	ASN
1	E	58	GLU
1	E	82	ASP

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Mol	Chain	Res	Type
1	E	101	LEU
1	E	154	ARG
1	E	156	LEU
1	E	196	LEU
1	E	198	VAL
1	E	224	TYR
1	E	245	GLN
1	E	247	HIS
1	E	259	PHE
1	E	266	CYS
1	E	279	ARG
1	E	297	THR
1	E	314	VAL
1	E	322	LEU
1	E	335	ASN
1	E	354	LEU
1	E	364	MET
2	F	30	ASP
2	F	62	ASP
2	F	79	SER
2	F	119	VAL
2	F	146	ARG
2	F	168	ASP
3	G	29	VAL
3	G	61	MET
3	G	67	PHE
3	G	69	ARG
3	G	165	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	GLN
1	A	295	GLN
1	A	316	ASN
1	A	335	ASN
2	B	122	ASN
3	C	63	GLN
3	C	71	ASN
3	C	106	ASN
1	E	37	ASN
1	E	241	ASN

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Mol	Chain	Res	Type
1	E	335	ASN
2	F	51	ASN
2	F	55	GLN
3	G	3	ASN
3	G	54	HIS
3	G	106	ASN
3	G	111	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

18 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
4	DAL	D	1	4	4,4,5	1.39	1 (25%)	1,4,6	0.03	0
4	MLE	D	10	4	8,8,9	1.18	1 (12%)	7,9,11	1.19	1 (14%)
4	MLE	D	2	4	8,8,9	1.76	1 (12%)	7,9,11	1.58	1 (14%)
4	MLE	D	3	4	8,8,9	1.37	1 (12%)	7,9,11	1.65	1 (14%)
4	MVA	D	4	4	7,7,8	1.73	2 (28%)	7,8,10	1.44	2 (28%)
4	BMT	D	5	4	12,12,13	1.15	1 (8%)	11,14,16	1.16	1 (9%)
4	ABA	D	6	4	5,5,6	1.31	1 (20%)	3,5,7	1.40	0
4	SAR	D	7	4	4,4,5	0.96	0	1,3,5	1.97	0
4	MLE	D	8	4	8,8,9	0.81	0	7,9,11	1.21	0
4	DAL	H	1	4	4,4,5	1.56	1 (25%)	1,4,6	0.15	0
4	MLE	H	10	4	8,8,9	1.55	1 (12%)	7,9,11	1.22	0
4	MLE	H	2	4	8,8,9	1.35	1 (12%)	7,9,11	2.31	2 (28%)
4	MLE	H	3	4	8,8,9	1.61	1 (12%)	7,9,11	1.47	3 (42%)
4	MVA	H	4	4	7,7,8	1.62	2 (28%)	7,8,10	1.57	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BMT	H	5	4	12,12,13	1.22	1 (8%)	11,14,16	1.22	1 (9%)
4	ABA	H	6	4	5,5,6	1.23	1 (20%)	3,5,7	1.38	0
4	SAR	H	7	4	4,4,5	0.89	0	1,3,5	1.95	0
4	MLE	H	8	4	8,8,9	1.31	1 (12%)	7,9,11	1.11	0

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
4	DAL	D	1	4	-	0/0/2/4	0/0/0/0
4	MLE	D	10	4	-	0/4/8/10	0/0/0/0
4	MLE	D	2	4	-	0/4/8/10	0/0/0/0
4	MLE	D	3	4	-	0/4/8/10	0/0/0/0
4	MVA	D	4	4	-	0/5/8/10	0/0/0/0
4	BMT	D	5	4	-	0/13/16/18	0/0/0/0
4	ABA	D	6	4	-	0/2/4/6	0/0/0/0
4	SAR	D	7	4	-	0/1/2/3	0/0/0/0
4	MLE	D	8	4	-	0/4/8/10	0/0/0/0
4	DAL	H	1	4	-	0/0/2/4	0/0/0/0
4	MLE	H	10	4	-	0/4/8/10	0/0/0/0
4	MLE	H	2	4	-	0/4/8/10	0/0/0/0
4	MLE	H	3	4	-	0/4/8/10	0/0/0/0
4	MVA	H	4	4	-	0/5/8/10	0/0/0/0
4	BMT	H	5	4	-	0/13/16/18	0/0/0/0
4	ABA	H	6	4	-	0/2/4/6	0/0/0/0
4	SAR	H	7	4	-	0/1/2/3	0/0/0/0
4	MLE	H	8	4	-	0/4/8/10	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	5	BMT	CG2-CB	2.04	1.57	1.53
4	H	4	MVA	CB-CA	2.17	1.58	1.54
4	D	10	MLE	CA-C	2.44	1.53	1.50
4	H	6	ABA	CA-C	2.49	1.53	1.50
4	D	1	DAL	CA-C	2.49	1.53	1.50
4	D	6	ABA	CA-C	2.52	1.53	1.50
4	D	4	MVA	CA-C	2.53	1.53	1.50
4	D	4	MVA	CB-CA	2.68	1.58	1.54
4	D	5	BMT	CG2-CB	2.71	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	DAL	CA-C	2.91	1.54	1.50
4	H	8	MLE	CA-C	2.95	1.54	1.50
4	D	3	MLE	CA-C	3.04	1.54	1.50
4	H	4	MVA	CA-C	3.16	1.54	1.50
4	H	2	MLE	CA-C	3.24	1.54	1.50
4	H	10	MLE	CA-C	3.70	1.55	1.50
4	D	2	MLE	CA-C	4.03	1.55	1.50
4	H	3	MLE	CA-C	4.04	1.55	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	4	MVA	CB-CA-C	-2.81	109.49	113.07
4	D	10	MLE	O-C-CA	-2.34	119.69	125.15
4	H	3	MLE	O-C-CA	-2.28	119.84	125.15
4	D	4	MVA	CB-CA-C	-2.13	110.36	113.07
4	D	4	MVA	O-C-CA	-2.10	119.61	125.22
4	H	2	MLE	O-C-CA	-2.09	120.28	125.15
4	H	3	MLE	CN-N-CA	2.03	120.21	113.60
4	H	3	MLE	CG-CB-CA	2.10	120.80	115.27
4	H	5	BMT	CN-N-CA	2.22	120.32	113.58
4	D	5	BMT	CN-N-CA	2.28	120.48	113.58
4	D	3	MLE	CG-CB-CA	2.84	122.76	115.27
4	D	2	MLE	CG-CB-CA	3.10	123.45	115.27
4	H	2	MLE	CG-CB-CA	5.43	129.61	115.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	DAL	1	0
4	D	10	MLE	1	0
4	D	2	MLE	2	0
4	D	3	MLE	1	0
4	D	4	MVA	4	0
4	D	5	BMT	3	0
4	H	10	MLE	1	0
4	H	2	MLE	1	0
4	H	7	SAR	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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(Å ²)	Q<0.9
1	A	372/372 (100%)	0.16	18 (4%) 31 21	18, 52, 97, 100	0
1	E	359/372 (96%)	0.12	14 (3%) 40 29	24, 65, 99, 100	0
2	B	158/169 (93%)	0.22	8 (5%) 29 19	23, 92, 100, 100	0
2	F	160/169 (94%)	0.88	33 (20%) 1 1	58, 98, 100, 100	0
3	C	165/165 (100%)	-0.43	0 100 100	15, 33, 51, 76	0
3	G	165/165 (100%)	0.22	11 (6%) 19 11	28, 76, 99, 100	0
4	D	2/11 (18%)	-0.78	0 100 100	17, 17, 17, 30	0
4	H	2/11 (18%)	-0.59	0 100 100	49, 49, 49, 53	0
All	All	1383/1434 (96%)	0.17	84 (6%) 22 14	15, 63, 100, 100	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	370	ASN	6.3
1	A	327	ASN	6.1
1	E	244	THR	5.8
2	F	69	VAL	5.8
2	B	14	PHE	4.9
3	G	16	PRO	4.7
2	F	61	PHE	4.7
2	F	37	LEU	4.6
1	A	295	GLN	4.3
2	F	28	LYS	4.2
2	F	58	ILE	4.1
2	B	84	LYS	4.1
2	F	16	ALA	4.1
2	F	29	LEU	4.0
2	F	74	PHE	3.9
2	F	31	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	243	LYS	3.8
2	F	169	VAL	3.8
2	F	27	LYS	3.7
3	G	17	LEU	3.7
2	F	14	PHE	3.7
1	E	371	ILE	3.6
1	A	328	VAL	3.6
1	A	89	GLY	3.5
3	G	156	ILE	3.5
2	B	39	VAL	3.5
1	E	17	VAL	3.5
2	F	32	ASP	3.4
1	E	367	ASN	3.4
2	F	10	MET	3.4
2	F	78	VAL	3.3
3	G	36	PHE	3.3
1	E	372	CYS	3.3
2	B	74	PHE	3.3
1	E	14	THR	3.3
3	G	15	GLU	3.2
1	E	20	ALA	3.2
2	B	67	GLY	3.2
3	G	80	GLY	3.0
1	A	117	GLY	2.9
1	A	245	GLN	2.9
2	F	24	LYS	2.8
2	F	23	GLY	2.8
2	F	42	PHE	2.7
2	F	168	ASP	2.6
1	A	199	HIS	2.6
2	F	17	ASP	2.6
1	A	84	PRO	2.6
2	F	62	ASP	2.6
3	G	8	PHE	2.5
2	F	86	ASP	2.5
1	E	15	ASP	2.5
1	A	280	ALA	2.5
1	E	246	GLU	2.5
3	G	14	GLY	2.5
1	A	147	LEU	2.4
2	F	25	ARG	2.4
1	E	238	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	243	LYS	2.3
3	G	6	VAL	2.3
1	E	368	VAL	2.3
1	A	88	CYS	2.3
2	F	153	CYS	2.3
2	F	67	GLY	2.2
1	A	90	ASP	2.2
2	F	84	LYS	2.2
2	F	87	LYS	2.2
2	B	81	PHE	2.2
1	A	324	TYR	2.2
2	F	150	GLU	2.2
1	A	241	ASN	2.2
1	A	39	GLY	2.1
2	F	91	LEU	2.1
2	B	28	LYS	2.1
3	G	75	GLY	2.1
2	F	47	GLU	2.1
1	E	245	GLN	2.1
2	B	40	GLU	2.1
2	F	141	LYS	2.1
3	G	165	GLU	2.1
1	A	37	ASN	2.1
2	F	79	SER	2.0
2	F	15	ASP	2.0
1	A	116	LEU	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	MLE	H	3	9/10	0.97	0.18	-	25,37,46,48	0
4	ABA	D	6	6/7	0.99	0.15	-	16,21,24,26	0
4	MVA	D	4	8/9	0.98	0.14	-	6,12,19,20	0
4	ABA	H	6	6/7	0.97	0.15	-	48,53,56,57	0
4	DAL	H	1	5/6	0.97	0.15	-	51,51,51,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	MVA	H	4	8/9	0.98	0.17	-	39,40,42,43	0
4	MLE	D	8	9/10	0.97	0.18	-	10,16,23,24	0
4	MLE	H	2	9/10	0.97	0.21	-	43,48,50,51	0
4	MLE	D	10	9/10	0.97	0.15	-	13,16,21,25	0
4	MLE	D	2	9/10	0.95	0.22	-	17,24,33,35	0
4	MLE	H	10	9/10	0.95	0.21	-	46,49,55,56	0
4	BMT	H	5	13/14	0.96	0.18	-	24,28,43,44	0
4	SAR	H	7	5/6	0.95	0.21	-	52,54,58,59	0
4	DAL	D	1	5/6	0.96	0.13	-	29,30,34,37	0
4	MLE	D	3	9/10	0.97	0.14	-	17,19,24,28	0
4	BMT	D	5	13/14	0.96	0.20	-	8,13,25,26	0
4	MLE	H	8	9/10	0.94	0.21	-	53,57,58,59	0
4	SAR	D	7	5/6	0.99	0.19	-	23,25,26,30	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
6	FE	E	505	1/1	0.96	0.20	0.27	55,55,55,55	0
6	FE	A	505	1/1	0.93	0.24	-0.30	42,42,42,42	0
7	CA	F	501	1/1	0.92	0.11	-0.77	93,93,93,93	0
7	CA	B	503	1/1	0.98	0.12	-0.82	46,46,46,46	0
5	ZN	A	504	1/1	0.94	0.23	-0.85	52,52,52,52	0
5	ZN	E	504	1/1	0.99	0.17	-1.02	46,46,46,46	0
7	CA	F	500	1/1	0.93	0.07	-1.20	95,95,95,95	0
7	CA	F	502	1/1	0.86	0.10	-1.40	97,97,97,97	0
7	CA	B	502	1/1	0.95	0.09	-1.52	58,58,58,58	0
7	CA	F	503	1/1	0.72	0.07	-1.84	99,99,99,99	0
7	CA	B	500	1/1	0.41	0.09	-2.22	100,100,100,100	0
7	CA	B	501	1/1	0.94	0.04	-2.23	94,94,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.