



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2020 – 07:50 pm BST

PDB ID : 1XQ7
Title : Cyclophilin from Trypanosoma cruzi bound to cyclosporin A
Authors : Caruthers, J.M.; Hol, W.G.J.; Structural Genomics of Pathogenic Protozoa Consortium (SGPP)
Deposited on : 2004-10-11
Resolution : 2.07 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

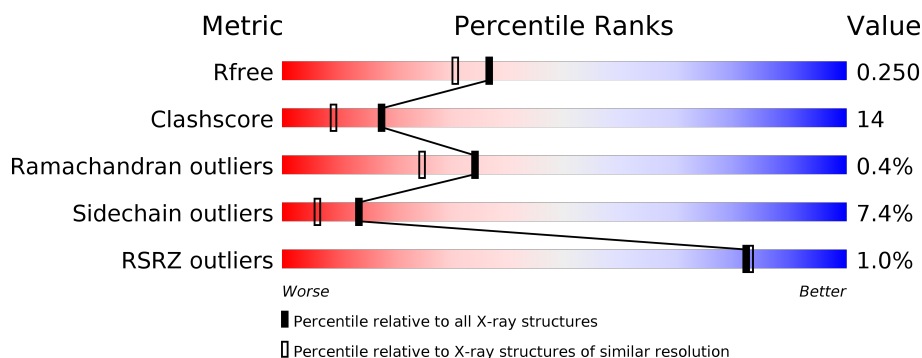
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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 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	166	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>5%</div> </div> </div>
1	B	166	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>20%</div> <div>.</div> </div> </div>
1	C	166	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div>..</div> </div> </div>
2	D	11	<div> <div>9%</div> <div>82%</div> <div>9%</div> </div>
2	E	11	<div> <div>9%</div> <div>73%</div> <div>18%</div> </div>
2	F	11	<div> <div>45%</div> <div>55%</div> </div>

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	MVA	D	4	-	-	X	-
2	BMT	D	5	-	-	X	-
2	MVA	E	4	-	-	X	-
2	BMT	E	5	-	-	X	-
2	MLE	F	10	-	-	X	-
2	MVA	F	4	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4356 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 PEPTIDYL-PROLYL CIS-TRANS ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	0	0
			1271	811	218	237	5			
1	B	166	Total	C	N	O	S	0	0	0
			1271	811	218	237	5			
1	C	166	Total	C	N	O	S	0	0	0
			1271	811	218	237	5			

- Molecule 2 is a protein called CYCLOSPORIN A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	11	Total	C	N	O	0	0	0
			85	62	11	12			
2	E	11	Total	C	N	O	0	0	0
			85	62	11	12			
2	F	11	Total	C	N	O	0	0	0
			85	62	11	12			

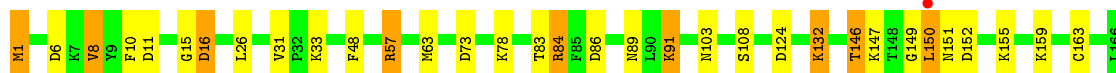
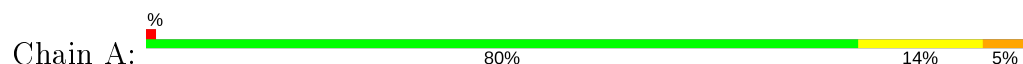
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	96	Total	O	0	0
			96	96		
3	B	87	Total	O	0	0
			87	87		
3	C	97	Total	O	0	0
			97	97		
3	E	2	Total	O	0	0
			2	2		
3	F	6	Total	O	0	0
			6	6		

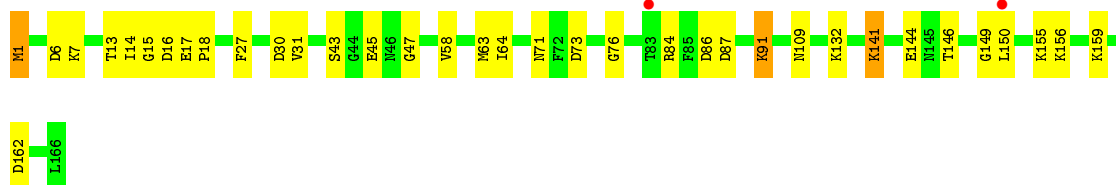
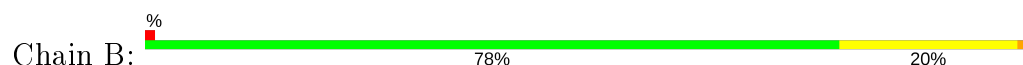
3 Residue-property plots [i](#)

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.

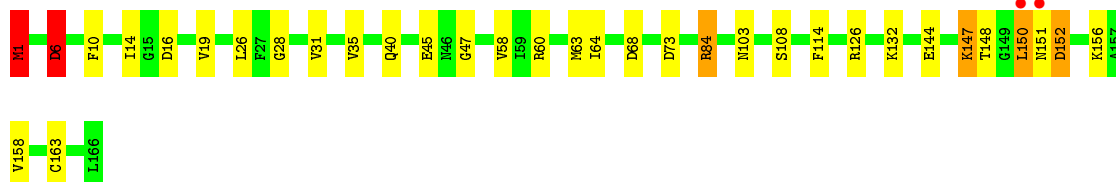
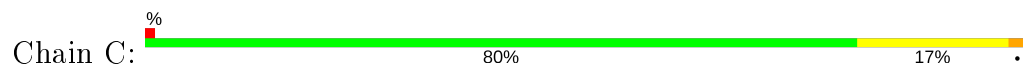
• Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE



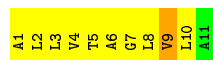
• Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE



• Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE

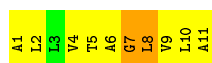


• Molecule 2: CYCLOSPORIN A

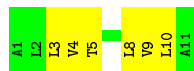


• Molecule 2: CYCLOSPORIN A





● Molecule 2: CYCLOSPORIN A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	52.27Å 57.06Å 58.81Å 110.49° 108.21° 105.40°	Depositor
Resolution (Å)	49.39 – 2.07 15.75 – 2.07	Depositor EDS
% Data completeness (in resolution range)	94.4 (49.39-2.07) 94.6 (15.75-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.169 , 0.235 0.186 , 0.250	Depositor DCC
R_{free} test set	1590 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,h+k+l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4356	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.46% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ABA, MLE, DAL, MVA, 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	1.09	1/1298 (0.1%)	1.09	10/1751 (0.6%)
1	B	1.06	1/1298 (0.1%)	1.06	7/1751 (0.4%)
1	C	1.04	1/1298 (0.1%)	1.06	5/1751 (0.3%)
2	D	0.97	0/10	1.16	0/11
2	E	0.82	0/10	1.68	0/11
2	F	1.15	0/10	1.03	0/11
All	All	1.06	3/3924 (0.1%)	1.07	22/5286 (0.4%)

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	C	0	1
2	E	0	2
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1	MET	CG-SD	5.86	1.96	1.81
1	B	27	PHE	CE2-CZ	5.40	1.47	1.37
1	A	132	LYS	CE-NZ	5.33	1.62	1.49

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	6	ASP	CB-CG-OD2	10.20	127.48	118.30
1	A	150	LEU	CA-CB-CG	8.75	135.43	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	ASP	CB-CG-OD2	8.25	125.73	118.30
1	C	152	ASP	CB-CG-OD2	8.20	125.68	118.30
1	B	162	ASP	CB-CG-OD2	7.82	125.33	118.30
1	B	87	ASP	CB-CG-OD2	7.58	125.12	118.30
1	A	57	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	C	16	ASP	CB-CG-OD2	6.90	124.51	118.30
1	A	57	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	B	30	ASP	CB-CG-OD2	6.78	124.40	118.30
1	A	124	ASP	CB-CG-OD2	6.32	123.99	118.30
1	B	73	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	132	LYS	CD-CE-NZ	5.77	124.97	111.70
1	A	152	ASP	CB-CG-OD2	5.76	123.48	118.30
1	A	86	ASP	CB-CG-OD2	5.63	123.37	118.30
1	B	6	ASP	CB-CG-OD2	5.51	123.26	118.30
1	C	73	ASP	CB-CG-OD1	5.44	123.20	118.30
1	A	16	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	16	ASP	CB-CG-OD2	5.33	123.10	118.30
1	B	86	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	73	ASP	CB-CG-OD2	5.16	122.94	118.30
1	C	68	ASP	CB-CG-OD2	5.12	122.91	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	151	ASN	Peptide
2	E	7	SAR	Peptide
2	E	8	MLE	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	1271	0	1264	26	0
1	B	1271	0	1264	19	0
1	C	1271	0	1264	20	0
2	D	85	0	110	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	85	0	110	24	0
2	F	85	0	109	15	0
3	A	96	0	0	8	0
3	B	87	0	0	7	0
3	C	97	0	0	3	0
3	E	2	0	0	2	0
3	F	6	0	0	3	0
All	All	4356	0	4121	112	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 14.

All (112) 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)
2:D:4:MVA:C	2:D:5:BMT:H	1.22	1.49
2:E:4:MVA:C	2:E:5:BMT:H	1.27	1.47
2:D:4:MVA:C	2:D:5:BMT:N	1.82	1.39
1:A:132:LYS:HD2	3:B:2027:HOH:O	1.29	1.25
2:E:4:MVA:C	2:E:5:BMT:N	2.10	1.15
1:B:43:SER:OG	1:B:45:GLU:HG3	1.57	1.04
1:A:149:GLY:CA	1:A:155:LYS:HE2	1.88	1.03
2:E:9:VAL:N	2:E:10:MLE:HN1	1.82	0.93
2:E:4:MVA:CA	2:E:5:BMT:H	1.80	0.92
1:A:33:LYS:HD2	3:A:2053:HOH:O	1.74	0.88
1:A:33:LYS:HB2	3:A:2053:HOH:O	1.73	0.87
1:A:33:LYS:CB	3:A:2053:HOH:O	2.23	0.87
1:A:84:ARG:CZ	3:A:2048:HOH:O	2.25	0.84
1:B:149:GLY:HA3	1:B:155:LYS:HE2	1.61	0.83
2:D:5:BMT:O	2:D:5:BMT:HN3	1.79	0.82
2:F:3:MLE:HB2	2:F:4:MVA:HN1	1.62	0.81
2:E:9:VAL:H	2:E:10:MLE:HN1	1.43	0.81
1:C:147:LYS:HE2	1:C:148:THR:H	1.44	0.81
1:A:149:GLY:N	1:A:155:LYS:HE2	1.96	0.80
2:D:4:MVA:C	2:D:5:BMT:CN	2.59	0.80
2:F:3:MLE:HN3	3:F:2001:HOH:O	1.81	0.80
1:A:149:GLY:HA3	1:A:155:LYS:HE2	1.63	0.78
1:C:150:LEU:H	1:C:150:LEU:HD13	1.48	0.78
2:E:4:MVA:HA	2:E:5:BMT:HN1	1.66	0.76
1:B:43:SER:HG	1:B:45:GLU:HG3	1.47	0.76
1:B:141:LYS:HE2	1:B:144:GLU:OE2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:GLY:CA	1:B:155:LYS:HE2	2.20	0.71
1:A:84:ARG:NH1	3:A:2048:HOH:O	2.24	0.71
2:F:9:VAL:HB	2:F:10:MLE:HN1	1.74	0.69
2:D:6:ABA:N	2:D:7:SAR:HN1	2.08	0.69
2:E:11:ALA:HB1	3:E:2001:HOH:O	1.93	0.67
2:F:3:MLE:HB2	2:F:4:MVA:CN	2.24	0.67
1:B:58:VAL:HG13	1:B:64:ILE:HG22	1.76	0.66
2:E:4:MVA:O	2:E:5:BMT:N	2.29	0.66
2:E:4:MVA:HA	2:E:5:BMT:CN	2.27	0.64
2:E:4:MVA:CA	2:E:5:BMT:N	2.54	0.64
2:D:5:BMT:O	2:D:5:BMT:CN	2.39	0.64
1:C:6:ASP:HB3	3:C:2008:HOH:O	1.98	0.63
2:F:9:VAL:N	2:F:10:MLE:HN1	2.15	0.62
2:F:10:MLE:HN3	3:F:2005:HOH:O	2.00	0.61
1:C:6:ASP:OD1	1:C:26:LEU:HB2	2.01	0.61
1:A:15:GLY:O	1:A:16:ASP:HB2	1.99	0.61
1:A:132:LYS:CD	3:B:2027:HOH:O	2.08	0.59
2:E:9:VAL:N	2:E:10:MLE:CN	2.62	0.58
2:E:7:SAR:O	2:E:8:MLE:HD22	2.03	0.58
1:A:89:ASN:ND2	1:A:91:LYS:H	2.02	0.57
1:A:1:MET:HE1	3:B:2033:HOH:O	2.05	0.57
2:D:4:MVA:HA	2:D:5:BMT:HN1	1.87	0.57
1:A:1:MET:HB3	1:B:47:GLY:C	2.26	0.56
1:C:150:LEU:HD13	1:C:150:LEU:N	2.17	0.56
1:A:103:ASN:O	2:D:5:BMT:HA	2.06	0.56
2:D:4:MVA:CA	2:D:5:BMT:HN1	2.37	0.55
1:A:1:MET:HB3	1:B:47:GLY:O	2.06	0.55
1:A:33:LYS:CD	3:A:2053:HOH:O	2.42	0.55
1:B:58:VAL:CG1	1:B:144:GLU:HA	2.38	0.54
1:A:8:VAL:HG13	1:A:26:LEU:HD11	1.88	0.54
1:C:14:ILE:HD12	1:C:19:VAL:HG11	1.88	0.54
1:B:13:THR:HG22	1:B:18:PRO:HA	1.89	0.54
2:F:5:BMT:HZ	2:F:8:MLE:O	2.07	0.53
1:C:14:ILE:HG12	1:C:158:VAL:HG22	1.90	0.53
2:E:4:MVA:HA	2:E:5:BMT:N	2.24	0.53
1:A:10:PHE:HD1	1:A:163:CYS:HB3	1.74	0.53
1:A:146:THR:HG22	3:A:2034:HOH:O	2.08	0.52
2:F:9:VAL:CB	2:F:10:MLE:HN1	2.31	0.52
2:D:8:MLE:O	2:D:9:VAL:HB	2.09	0.51
2:E:4:MVA:O	2:E:5:BMT:CA	2.59	0.50
1:B:150:LEU:HB2	3:B:2082:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:3:MLE:CB	2:F:4:MVA:HN1	2.28	0.50
1:C:84:ARG:HG2	1:C:108:SER:HA	1.94	0.50
2:E:4:MVA:O	2:E:5:BMT:HA	2.11	0.50
1:C:58:VAL:HG13	1:C:64:ILE:HG22	1.93	0.49
1:B:71:ASN:HD22	1:B:76:GLY:HA3	1.77	0.49
2:E:10:MLE:HD22	2:E:10:MLE:HN3	1.95	0.48
1:C:60:ARG:HH11	1:C:60:ARG:HG2	1.77	0.48
1:B:91:LYS:HE3	3:B:2021:HOH:O	2.12	0.48
1:C:156:LYS:HG2	3:C:2045:HOH:O	2.14	0.48
1:B:15:GLY:HA3	1:B:156:LYS:HD2	1.96	0.46
2:E:4:MVA:C	2:E:5:BMT:CA	2.92	0.46
1:B:7:LYS:HE3	3:B:2008:HOH:O	2.15	0.46
2:E:8:MLE:HD12	2:E:9:VAL:H	1.80	0.46
1:B:43:SER:OG	1:B:45:GLU:CG	2.47	0.46
1:C:1:MET:N	3:C:2002:HOH:O	2.38	0.45
2:F:3:MLE:CB	2:F:4:MVA:CN	2.92	0.45
2:D:4:MVA:C	2:D:5:BMT:CA	2.87	0.45
1:B:1:MET:HB3	1:C:47:GLY:HA2	2.00	0.44
1:A:57:ARG:NH2	2:D:4:MVA:HA	2.32	0.44
1:C:28:GLY:HA2	1:C:35:VAL:HG21	1.99	0.44
1:A:146:THR:CG2	3:A:2034:HOH:O	2.66	0.44
2:F:9:VAL:O	2:F:10:MLE:HB3	2.18	0.44
2:E:4:MVA:C	2:E:5:BMT:HD12	2.48	0.43
2:D:9:VAL:HA	2:D:10:MLE:HN1	1.39	0.43
2:F:10:MLE:HN2	3:F:2002:HOH:O	2.19	0.43
1:A:84:ARG:HG2	1:A:108:SER:HA	2.00	0.43
1:A:1:MET:CE	3:B:2033:HOH:O	2.63	0.42
1:B:84:ARG:HA	1:B:109:ASN:O	2.19	0.42
1:C:60:ARG:NH1	1:C:60:ARG:HG2	2.34	0.42
1:C:103:ASN:O	2:F:5:BMT:HA	2.19	0.42
1:C:40:GLN:HG2	1:C:45:GLU:CD	2.39	0.42
2:E:8:MLE:CB	3:E:2002:HOH:O	2.68	0.42
1:B:14:ILE:O	1:B:17:GLU:HB3	2.19	0.42
2:E:7:SAR:HA2	2:E:8:MLE:HN1	1.61	0.42
1:C:10:PHE:HD1	1:C:163:CYS:HB3	1.84	0.42
2:D:1:DAL:HA	2:D:2:MLE:HN1	1.81	0.42
1:A:48:PHE:CZ	1:A:78:LYS:HE3	2.55	0.41
2:E:1:DAL:HA	2:E:2:MLE:HN1	1.37	0.41
2:F:4:MVA:HA	2:F:5:BMT:HN1	1.65	0.41
2:D:2:MLE:HA	2:D:3:MLE:HN1	1.76	0.41
1:C:150:LEU:H	1:C:150:LEU:CD1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:PHE:CD1	2:F:4:MVA:HG11	2.55	0.41
2:E:4:MVA:CA	2:E:5:BMT:CN	2.97	0.40
1:A:15:GLY:O	1:A:16:ASP:CB	2.69	0.40
2:E:6:ABA:HA	2:E:7:SAR:HN1	1.82	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	164/166 (99%)	158 (96%)	6 (4%)	0	100	100
1	B	164/166 (99%)	157 (96%)	7 (4%)	0	100	100
1	C	164/166 (99%)	157 (96%)	6 (4%)	1 (1%)	25	15
2	D	1/11 (9%)	0	0	1 (100%)	0	0
2	E	1/11 (9%)	1 (100%)	0	0	100	100
2	F	1/11 (9%)	1 (100%)	0	0	100	100
All	All	495/531 (93%)	474 (96%)	19 (4%)	2 (0%)	34	25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	152	ASP
2	D	9	VAL

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	138/138 (100%)	125 (91%)	13 (9%)	8	3
1	B	138/138 (100%)	130 (94%)	8 (6%)	20	11
1	C	138/138 (100%)	128 (93%)	10 (7%)	14	7
2	D	1/1 (100%)	1 (100%)	0	100	100
2	E	1/1 (100%)	1 (100%)	0	100	100
2	F	1/1 (100%)	1 (100%)	0	100	100
All	All	417/417 (100%)	386 (93%)	31 (7%)	13	6

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	6	ASP
1	A	8	VAL
1	A	31	VAL
1	A	63	MET
1	A	83	THR
1	A	84	ARG
1	A	91	LYS
1	A	146	THR
1	A	147	LYS
1	A	150	LEU
1	A	151	ASN
1	A	159	LYS
1	B	1	MET
1	B	31	VAL
1	B	63	MET
1	B	91	LYS
1	B	132	LYS
1	B	141	LYS
1	B	146	THR
1	B	159	LYS
1	C	1	MET
1	C	6	ASP
1	C	31	VAL
1	C	63	MET
1	C	84	ARG
1	C	126	ARG

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Mol	Chain	Res	Type
1	C	132	LYS
1	C	144	GLU
1	C	147	LYS
1	C	150	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	145	ASN
1	B	46	ASN
1	B	71	ASN
1	B	145	ASN
1	C	46	ASN
1	C	145	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

27 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	MLE	F	2	2	7,8,9	2.03	2 (28%)	6,9,11	1.18	1 (16%)
2	MLE	D	2	2	7,8,9	2.29	2 (28%)	6,9,11	1.66	2 (33%)
2	SAR	F	7	2	4,4,5	2.06	1 (25%)	1,3,5	2.99	1 (100%)
2	MLE	F	3	2	7,8,9	1.84	1 (14%)	6,9,11	1.41	2 (33%)
2	MLE	E	10	2	7,8,9	2.04	1 (14%)	6,9,11	1.30	0
2	MVA	F	4	2	6,7,8	2.41	1 (16%)	7,8,10	1.31	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MLE	E	8	2	7,8,9	2.30	1 (14%)	6,9,11	1.94	1 (16%)
2	MLE	D	8	2	7,8,9	2.30	1 (14%)	6,9,11	1.42	1 (16%)
2	SAR	E	7	2	4,4,5	1.79	1 (25%)	1,3,5	2.61	1 (100%)
2	MLE	D	3	2	7,8,9	1.90	1 (14%)	6,9,11	1.77	1 (16%)
2	MLE	E	3	2	7,8,9	1.78	1 (14%)	6,9,11	1.51	1 (16%)
2	ABA	F	6	2	4,5,6	0.59	0	1,5,7	0.30	0
2	MVA	D	4	2	6,7,8	2.08	1 (16%)	7,8,10	2.38	2 (28%)
2	MLE	D	10	2	7,8,9	2.08	1 (14%)	6,9,11	1.73	3 (50%)
2	MLE	F	10	2	7,8,9	2.04	1 (14%)	6,9,11	1.23	1 (16%)
2	ABA	E	6	2	4,5,6	0.68	0	1,5,7	0.18	0
2	BMT	D	5	2	11,12,13	1.40	3 (27%)	12,14,16	3.04	8 (66%)
2	BMT	E	5	2	11,12,13	1.14	1 (9%)	12,14,16	1.56	2 (16%)
2	MLE	F	8	2	7,8,9	1.91	1 (14%)	6,9,11	1.29	1 (16%)
2	BMT	F	5	2	11,12,13	1.09	1 (9%)	12,14,16	1.39	1 (8%)
2	MVA	E	4	2	6,7,8	2.25	1 (16%)	7,8,10	2.65	3 (42%)
2	ABA	D	6	2	4,5,6	0.60	0	1,5,7	0.64	0
2	MLE	E	2	2	7,8,9	2.17	2 (28%)	6,9,11	0.88	0
2	SAR	D	7	2	4,4,5	1.87	1 (25%)	1,3,5	2.34	1 (100%)

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	MLE	F	2	2	-	0/5/8/10	-
2	MLE	D	2	2	-	3/5/8/10	-
2	SAR	F	7	2	-	1/1/2/3	-
2	MLE	F	3	2	-	0/5/8/10	-
2	MLE	E	10	2	-	1/5/8/10	-
2	MVA	F	4	2	-	2/6/8/10	-
2	MLE	E	8	2	-	4/5/8/10	-
2	MLE	D	8	2	-	2/5/8/10	-
2	SAR	E	7	2	-	1/1/2/3	-
2	MLE	D	3	2	-	0/5/8/10	-
2	MLE	E	3	2	-	0/5/8/10	-
2	ABA	F	6	2	-	0/3/4/6	-
2	MVA	D	4	2	-	3/6/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLE	D	10	2	-	0/5/8/10	-
2	MLE	F	10	2	-	0/5/8/10	-
2	ABA	E	6	2	-	0/3/4/6	-
2	BMT	D	5	2	-	4/13/16/18	-
2	BMT	E	5	2	-	2/13/16/18	-
2	MLE	F	8	2	-	1/5/8/10	-
2	BMT	F	5	2	-	1/13/16/18	-
2	MVA	E	4	2	-	5/6/8/10	-
2	ABA	D	6	2	-	1/3/4/6	-
2	MLE	E	2	2	-	4/5/8/10	-
2	SAR	D	7	2	-	1/1/2/3	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	8	MLE	O-C	5.98	1.43	1.19
2	F	4	MVA	O-C	5.74	1.42	1.19
2	E	8	MLE	O-C	5.61	1.42	1.19
2	E	4	MVA	O-C	5.47	1.41	1.19
2	E	2	MLE	O-C	5.32	1.41	1.19
2	E	10	MLE	O-C	5.31	1.41	1.19
2	D	2	MLE	O-C	5.22	1.40	1.19
2	F	10	MLE	O-C	5.19	1.40	1.19
2	D	10	MLE	O-C	5.15	1.40	1.19
2	F	8	MLE	O-C	5.03	1.40	1.19
2	D	4	MVA	O-C	4.90	1.39	1.19
2	F	2	MLE	O-C	4.87	1.39	1.19
2	D	3	MLE	O-C	4.86	1.39	1.19
2	F	3	MLE	O-C	4.81	1.39	1.19
2	E	3	MLE	O-C	4.52	1.38	1.19
2	F	7	SAR	O-C	4.05	1.42	1.19
2	D	7	SAR	O-C	3.62	1.40	1.19
2	E	7	SAR	O-C	3.52	1.39	1.19
2	D	2	MLE	CA-N	2.87	1.52	1.47
2	D	5	BMT	CG2-CB	2.72	1.58	1.53
2	E	5	BMT	CE-CZ	2.67	1.49	1.29
2	D	5	BMT	CE-CZ	2.52	1.48	1.29
2	D	5	BMT	CA-N	2.49	1.51	1.47
2	F	5	BMT	CE-CZ	2.35	1.47	1.29
2	E	2	MLE	CA-N	2.09	1.51	1.47
2	F	2	MLE	CA-N	2.03	1.51	1.47

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	5	BMT	CB-CA-N	-5.96	99.56	111.41
2	E	4	MVA	CB-CA-C	-5.53	106.10	113.04
2	D	4	MVA	CB-CA-C	-4.94	106.84	113.04
2	E	8	MLE	CN-N-CA	4.48	127.58	113.64
2	D	5	BMT	O-C-CA	-3.78	114.30	124.83
2	D	5	BMT	CD2-CG2-CB	3.72	117.63	110.39
2	D	5	BMT	OG1-CB-CA	-3.54	101.80	109.32
2	E	5	BMT	CG2-CD2-CE	-3.54	108.55	113.98
2	D	4	MVA	CB-CA-N	3.52	115.76	111.17
2	D	5	BMT	C-CA-N	-3.33	99.73	110.88
2	F	5	BMT	CG2-CD2-CE	-3.27	108.96	113.98
2	E	3	MLE	O-C-CA	-3.27	116.21	124.78
2	D	5	BMT	CD1-CG2-CB	3.16	117.39	111.54
2	F	7	SAR	O-C-CA	-2.99	116.77	125.42
2	E	4	MVA	CB-CA-N	2.88	114.93	111.17
2	E	5	BMT	OG1-CB-CA	-2.88	103.21	109.32
2	D	3	MLE	O-C-CA	-2.75	117.57	124.78
2	D	10	MLE	CN-N-CA	2.64	121.86	113.64
2	E	7	SAR	O-C-CA	-2.61	117.86	125.42
2	D	5	BMT	CD1-CG2-CD2	-2.60	106.17	110.54
2	F	10	MLE	CN-N-CA	2.41	121.14	113.64
2	D	2	MLE	O-C-CA	-2.38	118.54	124.78
2	D	7	SAR	O-C-CA	-2.34	118.64	125.42
2	D	10	MLE	CG-CB-CA	-2.31	109.57	115.34
2	F	3	MLE	O-C-CA	-2.28	118.79	124.78
2	F	2	MLE	O-C-CA	-2.21	118.98	124.78
2	F	8	MLE	O-C-CA	-2.20	119.01	124.78
2	F	3	MLE	CN-N-CA	2.17	120.40	113.64
2	D	2	MLE	CN-N-CA	2.09	120.14	113.64
2	D	8	MLE	CG-CB-CA	-2.09	110.13	115.34
2	D	10	MLE	O-C-CA	-2.08	119.32	124.78
2	F	4	MVA	CB-CA-N	2.07	113.87	111.17
2	E	4	MVA	CG1-CB-CA	-2.05	108.08	111.21
2	D	5	BMT	CD2-CE-CZ	-2.01	117.95	127.25

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	MLE	O-C-CA-CB
2	D	6	ABA	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	E	8	MLE	C-CA-CB-CG
2	E	7	SAR	C-CA-N-CN
2	D	5	BMT	CB-CA-N-CN
2	D	5	BMT	CD2-CE-CZ-CH
2	F	8	MLE	O-C-CA-CB
2	E	4	MVA	CB-CA-N-CN
2	E	4	MVA	N-CA-CB-CG1
2	E	4	MVA	N-CA-CB-CG2
2	E	4	MVA	C-CA-CB-CG1
2	E	4	MVA	C-CA-CB-CG2
2	F	4	MVA	CB-CA-N-CN
2	F	4	MVA	N-CA-CB-CG2
2	E	2	MLE	C-CA-CB-CG
2	D	8	MLE	N-CA-CB-CG
2	E	8	MLE	N-CA-CB-CG
2	E	8	MLE	CA-CB-CG-CD1
2	E	2	MLE	CA-CB-CG-CD1
2	E	8	MLE	CA-CB-CG-CD2
2	E	5	BMT	CD2-CE-CZ-CH
2	E	2	MLE	N-CA-CB-CG
2	E	2	MLE	CA-CB-CG-CD2
2	D	2	MLE	CA-CB-CG-CD2
2	D	5	BMT	C-CA-CB-CG2
2	D	4	MVA	N-CA-CB-CG2
2	D	5	BMT	C-CA-CB-OG1
2	E	5	BMT	CB-CA-N-CN
2	F	5	BMT	CB-CA-N-CN
2	D	4	MVA	CB-CA-N-CN
2	E	10	MLE	CA-CB-CG-CD2
2	D	8	MLE	C-CA-CB-CG
2	D	2	MLE	CA-CB-CG-CD1
2	D	4	MVA	O-C-CA-CB
2	F	7	SAR	C-CA-N-CN
2	D	7	SAR	C-CA-N-CN

There are no ring outliers.

20 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	MLE	2	0
2	F	3	MLE	5	0
2	E	10	MLE	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	4	MVA	6	0
2	E	8	MLE	4	0
2	D	8	MLE	1	0
2	E	7	SAR	3	0
2	D	3	MLE	1	0
2	D	4	MVA	7	0
2	D	10	MLE	1	0
2	F	10	MLE	6	0
2	E	6	ABA	1	0
2	D	5	BMT	9	0
2	E	5	BMT	13	0
2	F	8	MLE	1	0
2	F	5	BMT	3	0
2	E	4	MVA	13	0
2	D	6	ABA	1	0
2	E	2	MLE	1	0
2	D	7	SAR	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	1
2	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	4:MVA	C	5:BMT	N	2.10
1	D	4:MVA	C	5:BMT	N	1.82

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	166/166 (100%)	-0.23	1 (0%) 89 90	14, 22, 31, 36	0
1	B	166/166 (100%)	-0.25	2 (1%) 79 80	13, 21, 31, 39	0
1	C	166/166 (100%)	-0.23	2 (1%) 79 80	13, 22, 31, 38	0
2	D	2/11 (18%)	0.60	0 100 100	45, 45, 45, 50	0
2	E	2/11 (18%)	0.40	0 100 100	52, 52, 52, 57	0
2	F	2/11 (18%)	0.66	0 100 100	47, 47, 47, 50	0
All	All	504/531 (94%)	-0.23	5 (0%) 82 83	13, 22, 32, 57	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	150	LEU	5.0
1	A	150	LEU	4.4
1	C	151	ASN	2.6
1	B	83	THR	2.5
1	B	150	LEU	2.4

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	MLE	D	2	9/10	0.78	0.20	40,44,48,51	0
2	MLE	D	10	9/10	0.84	0.13	45,46,48,49	0
2	MLE	D	8	9/10	0.86	0.18	46,47,50,50	0
2	MLE	E	10	9/10	0.86	0.12	54,55,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MLE	E	8	9/10	0.87	0.18	45,47,54,55	0
2	DAL	E	1	5/6	0.87	0.17	51,51,53,55	0
2	DAL	D	1	5/6	0.88	0.23	49,49,50,50	0
2	MLE	F	2	9/10	0.89	0.13	39,44,46,48	0
2	MLE	F	10	9/10	0.90	0.13	47,49,55,57	0
2	DAL	F	1	5/6	0.91	0.10	47,48,49,49	0
2	BMT	D	5	13/14	0.93	0.14	31,33,39,41	0
2	ABA	F	6	6/7	0.93	0.14	35,35,36,36	0
2	MLE	E	2	9/10	0.93	0.13	40,44,47,48	0
2	SAR	D	7	5/6	0.93	0.10	41,42,45,45	0
2	SAR	F	7	5/6	0.94	0.12	35,36,40,41	0
2	ABA	D	6	6/7	0.94	0.17	37,39,40,41	0
2	SAR	E	7	5/6	0.94	0.11	36,37,43,45	0
2	MLE	F	8	9/10	0.95	0.10	36,41,42,42	0
2	MLE	E	3	9/10	0.95	0.14	36,39,41,42	0
2	MLE	D	3	9/10	0.96	0.12	32,36,38,39	0
2	BMT	F	5	13/14	0.96	0.13	32,35,45,48	0
2	MVA	E	4	8/9	0.96	0.14	31,35,36,36	0
2	MVA	D	4	8/9	0.96	0.21	29,30,31,32	0
2	MLE	F	3	9/10	0.96	0.15	36,38,41,43	0
2	BMT	E	5	13/14	0.96	0.12	26,30,42,44	0
2	ABA	E	6	6/7	0.97	0.10	32,35,36,36	0
2	MVA	F	4	8/9	0.97	0.13	31,34,35,36	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.