



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:23 AM UTC

PDB ID : 1IKF / pdb_00001ikf
Title : A CONFORMATION OF CYCLOSPORIN A IN AQUEOUS ENVIRONMENT REVEALED BY THE X-RAY STRUCTURE OF A CYCLOSPORIN-FAB COMPLEX
Authors : Vix, O.; Altschuh, D.; Rees, B.; Thierry, J.-C.
Deposited on : 1993-12-09
Resolution : 2.50 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

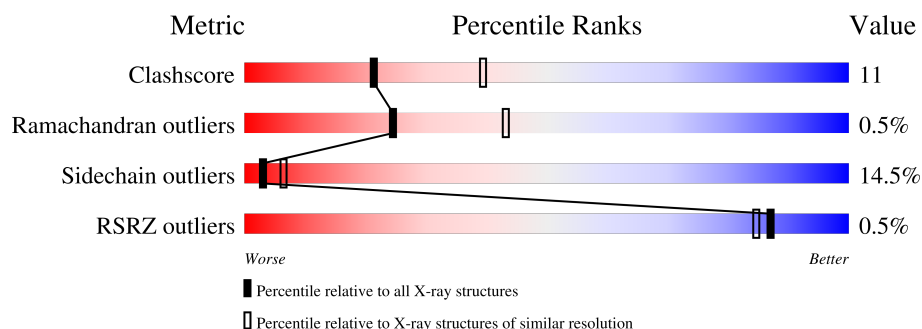
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	L	214	59% 34% 5%
2	H	228	57% 32% 11%
3	C	11	27% 9% 55% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3651 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 IGG1-KAPPA R45-45-11 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1652	1024	281	340	7			

- Molecule 2 is a protein called IGG1-KAPPA R45-45-11 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	228	Total	C	N	O	S	0	0	0
			1742	1107	288	338	9			

- Molecule 3 is a protein called CYCLOSPORIN A.

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

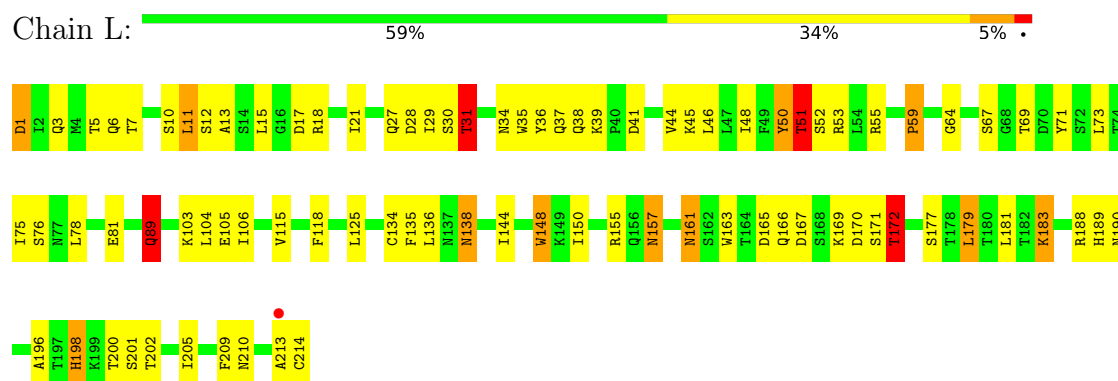
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	96	Total	O	0	0
			96	96		
4	H	69	Total	O	0	0
			69	69		
4	C	7	Total	O	0	0
			7	7		

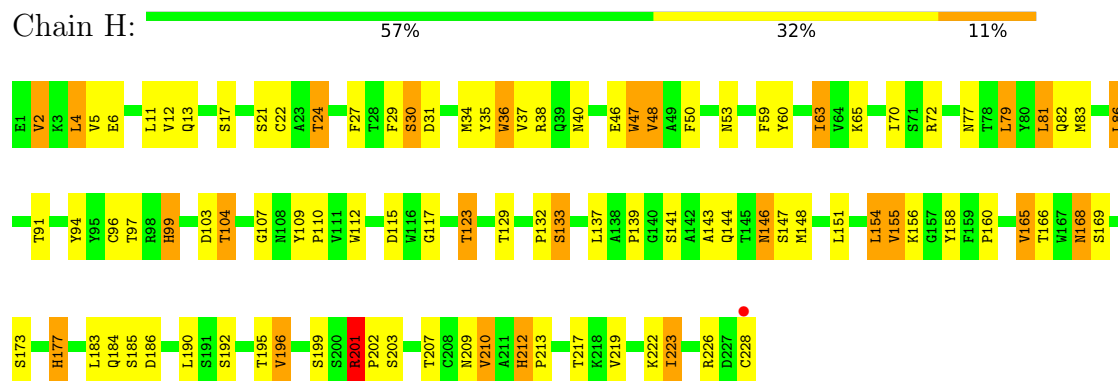
3 Residue-property plots

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.

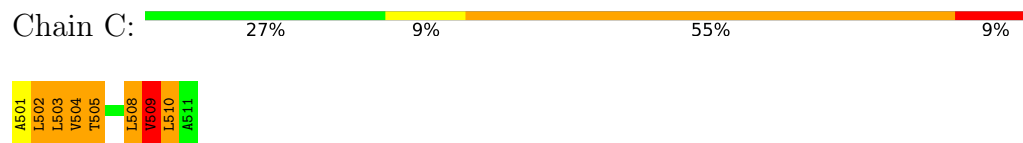
• Molecule 1: IGG1-KAPPA R45-45-11 FAB (LIGHT CHAIN)



• Molecule 2: IGG1-KAPPA R45-45-11 FAB (HEAVY CHAIN)



• Molecule 3: CYCLOSPORIN A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.60Å 70.20Å 118.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50 8.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.50) 81.7 (8.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.164 , (Not available) 0.170 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 53.6	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3651	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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: SAR, ABA, BMT, MVA, DAL, MLE

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	L	1.05	3/1685 (0.2%)	1.94	44/2286 (1.9%)
2	H	1.10	6/1788 (0.3%)	2.02	62/2439 (2.5%)
3	C	0.81	0/10	2.33	1/11 (9.1%)
All	All	1.08	9/3483 (0.3%)	1.98	107/4736 (2.3%)

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
2	H	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	223	ILE	CA-CB	9.13	1.64	1.54
1	L	198	HIS	CD2-NE2	-7.22	1.29	1.37
1	L	189	HIS	CD2-NE2	-6.88	1.30	1.37
1	L	31	THR	CA-CB	6.51	1.62	1.53
2	H	212	HIS	CD2-NE2	-6.49	1.30	1.37
2	H	210	VAL	CA-CB	6.44	1.64	1.54
2	H	177	HIS	CD2-NE2	-6.34	1.30	1.37
2	H	99	HIS	CD2-NE2	-6.34	1.30	1.37
2	H	155	VAL	CA-CB	5.32	1.60	1.53

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	1	ASP	CA-CB-CG	11.23	123.83	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	50	PHE	CA-CB-CG	11.15	124.95	113.80
2	H	209	ASN	OD1-CG-ND2	-10.28	112.32	122.60
2	H	168	ASN	OD1-CG-ND2	-10.18	112.42	122.60
2	H	31	ASP	CA-CB-CG	9.49	122.09	112.60
2	H	168	ASN	CB-CG-ND2	9.03	129.95	116.40
2	H	77	ASN	CA-CB-CG	8.38	120.98	112.60
2	H	77	ASN	OD1-CG-ND2	-8.33	114.27	122.60
1	L	209	PHE	CA-CB-CG	8.18	121.98	113.80
2	H	156	LYS	N-CA-C	8.05	122.55	109.59
1	L	31	THR	N-CA-CB	-7.62	102.45	113.65
2	H	168	ASN	CA-CB-CG	7.55	120.15	112.60
2	H	48	VAL	CG1-CB-CG2	-7.41	94.50	110.80
1	L	76	SER	N-CA-C	-7.32	98.06	109.25
2	H	82	GLN	OE1-CD-NE2	-7.31	115.29	122.60
1	L	172	THR	N-CA-CB	-7.07	99.50	110.46
1	L	41	ASP	CA-CB-CG	6.96	119.56	112.60
1	L	170	ASP	CA-CB-CG	6.88	119.48	112.60
2	H	196	VAL	N-CA-CB	-6.81	101.67	111.21
1	L	210	ASN	O-C-N	-6.57	115.54	123.29
2	H	112	TRP	CG-CD2-CE3	6.55	140.46	133.90
2	H	177	HIS	CB-CG-CD2	-6.54	122.70	131.20
1	L	210	ASN	OD1-CG-ND2	-6.53	116.07	122.60
2	H	223	ILE	CB-CA-C	6.48	118.81	110.96
1	L	6	GLN	OE1-CD-NE2	-6.47	116.13	122.60
1	L	31	THR	CA-CB-CG2	6.36	121.32	110.50
1	L	189	HIS	CB-CG-CD2	-6.36	122.94	131.20
1	L	167	ASP	CA-CB-CG	6.29	118.89	112.60
2	H	212	HIS	CB-CG-CD2	-6.25	123.07	131.20
2	H	201	ARG	N-CA-C	-6.23	99.92	109.64
1	L	59	PRO	N-CA-C	6.22	120.98	111.15
2	H	117	GLY	O-C-N	-6.19	116.84	122.96
2	H	40	ASN	CA-CB-CG	6.18	118.78	112.60
2	H	196	VAL	O-C-N	-6.08	114.17	121.10
2	H	217	THR	CA-CB-OG1	-6.07	100.50	109.60
1	L	161	ASN	OD1-CG-ND2	-6.05	116.55	122.60
2	H	184	GLN	CG-CD-NE2	5.98	125.37	116.40
2	H	104	THR	N-CA-C	-5.93	100.95	110.14
2	H	36	TRP	CG-CD2-CE3	5.81	139.71	133.90
1	L	51	THR	N-CA-C	5.80	123.16	110.80
2	H	222	LYS	CA-C-N	-5.76	115.17	122.37
2	H	222	LYS	C-N-CA	-5.76	115.17	122.37
2	H	24	THR	O-C-N	-5.75	116.45	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	44	VAL	O-C-N	-5.71	117.01	123.18
2	H	99	HIS	CB-CG-CD2	-5.71	123.77	131.20
3	C	509	VAL	N-CA-CB	-5.70	101.81	111.50
2	H	48	VAL	CA-CB-CG2	5.69	120.07	110.40
1	L	213	ALA	N-CA-C	-5.66	101.79	109.54
1	L	35	TRP	CG-CD2-CE3	5.64	139.54	133.90
2	H	154	LEU	CA-C-N	-5.64	115.58	123.13
2	H	154	LEU	C-N-CA	-5.64	115.58	123.13
1	L	148	TRP	CE2-CD2-CG	-5.63	100.44	107.20
2	H	165	VAL	O-C-N	-5.62	115.51	122.88
1	L	89	GLN	OE1-CD-NE2	-5.61	117.00	122.60
2	H	223	ILE	CA-C-O	5.58	127.17	120.65
2	H	63	ILE	N-CA-C	5.57	120.92	109.34
2	H	201	ARG	NE-CZ-NH1	5.57	127.06	121.50
1	L	31	THR	CA-CB-OG1	-5.56	101.26	109.60
1	L	17	ASP	CA-CB-CG	5.52	118.12	112.60
1	L	75	ILE	N-CA-C	-5.52	99.01	106.85
1	L	190	ASN	CA-CB-CG	5.51	118.11	112.60
1	L	18	ARG	N-CA-C	-5.50	100.22	109.07
2	H	82	GLN	N-CA-C	-5.48	100.37	109.46
1	L	171	SER	N-CA-C	5.47	119.54	112.86
2	H	36	TRP	CB-CG-CD1	-5.47	118.69	126.90
2	H	213	PRO	O-C-N	-5.47	115.94	122.24
2	H	82	GLN	CG-CD-NE2	5.47	124.61	116.40
1	L	28	ASP	CA-CB-CG	5.46	118.06	112.60
2	H	212	HIS	CB-CG-ND1	5.46	130.88	122.70
1	L	118	PHE	CA-C-N	5.45	126.00	120.38
1	L	118	PHE	C-N-CA	5.45	126.00	120.38
1	L	37	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	L	163	TRP	CB-CG-CD1	-5.42	118.76	126.90
2	H	99	HIS	CB-CG-ND1	5.42	130.83	122.70
2	H	186	ASP	CA-CB-CG	5.42	118.02	112.60
1	L	210	ASN	N-CA-C	-5.40	100.37	109.07
1	L	148	TRP	CD1-CG-CD2	5.36	114.88	106.30
1	L	5	THR	O-C-N	-5.36	117.00	123.27
2	H	155	VAL	CB-CA-C	5.35	117.95	110.99
1	L	157	ASN	CA-CB-CG	5.33	117.93	112.60
1	L	188	ARG	CA-CB-CG	5.33	124.76	114.10
2	H	37	VAL	O-C-N	-5.31	117.32	123.00
2	H	47	TRP	CA-C-N	-5.31	117.51	122.66
2	H	47	TRP	C-N-CA	-5.31	117.51	122.66
2	H	133	SER	N-CA-C	-5.28	100.64	109.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	207	THR	CA-C-N	-5.26	115.46	122.72
2	H	207	THR	C-N-CA	-5.26	115.46	122.72
1	L	138	ASN	OD1-CG-ND2	-5.25	117.36	122.60
2	H	4	LEU	N-CA-C	-5.24	99.86	108.41
1	L	38	GLN	N-CA-C	-5.24	99.99	108.52
2	H	36	TRP	CE2-CD2-CG	-5.24	100.92	107.20
1	L	73	LEU	N-CA-C	-5.23	99.88	108.41
2	H	2	VAL	N-CA-C	-5.23	100.95	108.53
1	L	148	TRP	CG-CD1-NE1	-5.22	103.42	110.20
2	H	223	ILE	N-CA-C	-5.20	100.27	108.23
2	H	29	PHE	CA-CB-CG	5.14	118.94	113.80
2	H	141	SER	N-CA-C	5.13	119.01	112.34
2	H	184	GLN	OE1-CD-NE2	-5.12	117.48	122.60
1	L	5	THR	N-CA-CB	-5.10	102.77	110.77
2	H	47	TRP	CE2-CD2-CG	-5.10	101.08	107.20
1	L	163	TRP	CG-CD2-CE3	5.09	138.99	133.90
1	L	11	LEU	O-C-N	-5.08	117.38	123.27
2	H	209	ASN	N-CA-C	-5.07	100.26	108.52
2	H	169	SER	N-CA-C	5.04	119.28	113.38
2	H	112	TRP	CE2-CD2-CG	-5.04	101.16	107.20
2	H	123	THR	N-CA-C	-5.03	100.97	109.07
2	H	146	ASN	CA-CB-CG	5.02	117.62	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	35	TYR	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1652	0	1594	33	0
2	H	1742	0	1699	37	0
3	C	85	0	109	8	0
4	C	7	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	69	0	0	0	0
4	L	96	0	0	4	0
All	All	3651	0	3402	75	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 11.

All (75) 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:H:201:ARG:HG2	2:H:202:PRO:HA	1.66	0.77
1:L:106:ILE:H	1:L:166:GLN:HE22	1.36	0.73
2:H:53:ASN:HA	2:H:72:ARG:NH1	2.03	0.73
2:H:201:ARG:HH11	2:H:201:ARG:HB3	1.55	0.70
1:L:138:ASN:HD22	1:L:172:THR:HG21	1.61	0.66
1:L:34:ASN:HD22	1:L:89:GLN:HE22	1.45	0.64
1:L:31:THR:HG23	1:L:51:THR:CG2	2.31	0.61
2:H:91:THR:HG23	2:H:123:THR:HA	1.83	0.60
3:C:501:DAL:C	3:C:503:MLE:HN1	2.33	0.59
2:H:160:PRO:O	2:H:212:HIS:HE1	1.86	0.59
1:L:125:LEU:HD22	1:L:183:LYS:HG3	1.83	0.58
1:L:138:ASN:HA	1:L:172:THR:HG23	1.86	0.58
2:H:165:VAL:HG21	2:H:190:LEU:HD11	1.85	0.58
1:L:48:ILE:HG22	4:L:2031:HOH:O	2.01	0.58
2:H:24:THR:HB	2:H:27:PHE:CZ	2.39	0.58
3:C:504:MVA:HN3	3:C:505:BMT:HG2	1.87	0.57
1:L:12:SER:HA	1:L:105:GLU:O	2.06	0.56
2:H:12:VAL:HG21	2:H:86:LEU:HD23	1.89	0.55
2:H:38:ARG:HD3	2:H:48:VAL:HG11	1.90	0.54
2:H:47:TRP:HH2	2:H:59:PHE:HD1	1.56	0.53
2:H:104:THR:HB	2:H:107:GLY:O	2.07	0.53
1:L:30:SER:O	1:L:31:THR:HB	2.09	0.53
2:H:6:GLU:HG3	2:H:96:CYS:SG	2.50	0.52
2:H:60:TYR:OH	2:H:70:ILE:HG22	2.10	0.52
1:L:31:THR:HG22	1:L:50:TYR:CE1	2.46	0.50
1:L:34:ASN:HD22	1:L:89:GLN:NE2	2.10	0.50
1:L:165:ASP:HB3	4:L:2088:HOH:O	2.10	0.50
1:L:52:SER:HA	1:L:64:GLY:O	2.12	0.50
2:H:38:ARG:NH2	2:H:63:ILE:HD12	2.27	0.50
1:L:78:LEU:HD21	1:L:104:LEU:HD21	1.94	0.50
1:L:115:VAL:HA	1:L:135:PHE:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:4:LEU:HD13	2:H:24:THR:HG22	1.94	0.49
1:L:134:CYS:HB2	1:L:148:TRP:CH2	2.47	0.49
2:H:38:ARG:HG2	2:H:46:GLU:HB3	1.96	0.47
1:L:198:HIS:HD2	1:L:200:THR:OG1	1.96	0.47
1:L:31:THR:HG23	1:L:51:THR:HG22	1.96	0.47
1:L:196:ALA:HB3	1:L:205:ILE:HB	1.95	0.47
1:L:15:LEU:HD22	1:L:15:LEU:H	1.80	0.46
1:L:27:GLN:O	1:L:69:THR:HG22	2.16	0.46
2:H:148:MET:HE3	2:H:195:THR:HG22	1.97	0.46
3:C:501:DAL:HA	3:C:502:MLE:HN1	1.70	0.46
2:H:30:SER:O	2:H:53:ASN:HB2	2.15	0.45
2:H:47:TRP:HH2	2:H:59:PHE:CD1	2.35	0.45
1:L:161:ASN:ND2	1:L:177:SER:OG	2.50	0.45
3:C:502:MLE:N	3:C:503:MLE:HN1	2.32	0.45
2:H:2:VAL:HG13	2:H:27:PHE:CD1	2.51	0.45
2:H:107:GLY:HA2	3:C:510:MLE:HD22	1.99	0.45
2:H:83:MET:HE1	2:H:94:TYR:CZ	2.52	0.45
3:C:509:VAL:HA	3:C:510:MLE:HN1	1.80	0.45
2:H:36:TRP:CD1	2:H:81:LEU:HG	2.53	0.44
1:L:29:ILE:HD11	1:L:71:TYR:CE2	2.53	0.44
1:L:13:ALA:HB3	1:L:78:LEU:HD11	1.98	0.44
1:L:36:TYR:HE2	1:L:89:GLN:HE21	1.64	0.44
2:H:104:THR:HG21	3:C:508:MLE:HD21	2.00	0.43
2:H:5:VAL:O	2:H:22:CYS:HA	2.17	0.43
1:L:138:ASN:HA	1:L:172:THR:CG2	2.47	0.43
1:L:27:GLN:C	1:L:69:THR:HG22	2.44	0.43
4:L:2067:HOH:O	2:H:139:PRO:HA	2.19	0.43
1:L:53:ARG:HH12	2:H:104:THR:HA	1.84	0.43
2:H:109:TYR:HA	2:H:110:PRO:HD3	1.85	0.43
2:H:34:MET:HB3	2:H:79:LEU:HG	2.00	0.43
1:L:144:ILE:HG13	1:L:198:HIS:HB2	2.01	0.43
1:L:150:ILE:HD11	1:L:179:LEU:HD11	2.01	0.43
2:H:2:VAL:HG13	2:H:27:PHE:CE1	2.54	0.42
1:L:10:SER:HA	1:L:103:LYS:O	2.19	0.42
2:H:17:SER:HA	2:H:83:MET:O	2.19	0.42
2:H:132:PRO:HB3	2:H:158:TYR:HB3	2.02	0.42
2:H:144:GLN:HB3	2:H:146:ASN:OD1	2.19	0.41
2:H:144:GLN:HE21	2:H:226:ARG:NH2	2.18	0.41
2:H:177:HIS:O	2:H:192:SER:HA	2.20	0.41
1:L:31:THR:O	1:L:51:THR:HG22	2.20	0.41
2:H:97:THR:HA	2:H:115:ASP:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:155:ARG:HA	4:L:2081:HOH:O	2.19	0.41
3:C:503:MLE:HA	3:C:504:MVA:HN1	1.76	0.40
2:H:60:TYR:HB2	2:H:65:LYS:HG3	2.04	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	L	212/214 (99%)	199 (94%)	12 (6%)	1 (0%)	24	43
2	H	226/228 (99%)	217 (96%)	8 (4%)	1 (0%)	30	49
3	C	1/11 (9%)	1 (100%)	0	0	100	100
All	All	439/453 (97%)	417 (95%)	20 (5%)	2 (0%)	24	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	51	THR
2	H	143	ALA

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	L	190/190 (100%)	164 (86%)	26 (14%)	3	7
2	H	195/195 (100%)	166 (85%)	29 (15%)	3	6
3	C	1/1 (100%)	0	1 (100%)	0	0
All	All	386/386 (100%)	330 (86%)	56 (14%)	3	6

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASP
1	L	3	GLN
1	L	7	THR
1	L	11	LEU
1	L	21	ILE
1	L	31	THR
1	L	39	LYS
1	L	45	LYS
1	L	46	LEU
1	L	50	TYR
1	L	51	THR
1	L	55	ARG
1	L	59	PRO
1	L	67	SER
1	L	81	GLU
1	L	89	GLN
1	L	136	LEU
1	L	157	ASN
1	L	169	LYS
1	L	172	THR
1	L	179	LEU
1	L	181	LEU
1	L	183	LYS
1	L	201	SER
1	L	202	THR
1	L	214	CYS
2	H	11	LEU
2	H	13	GLN
2	H	21	SER
2	H	30	SER
2	H	79	LEU
2	H	81	LEU
2	H	86	LEU
2	H	99	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	103	ASP
2	H	129	THR
2	H	133	SER
2	H	137	LEU
2	H	147	SER
2	H	151	LEU
2	H	154	LEU
2	H	155	VAL
2	H	166	THR
2	H	168	ASN
2	H	173	SER
2	H	183	LEU
2	H	185	SER
2	H	196	VAL
2	H	199	SER
2	H	201	ARG
2	H	203	SER
2	H	210	VAL
2	H	219	VAL
2	H	223	ILE
2	H	228	CYS
3	C	509	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	27	GLN
1	L	38	GLN
1	L	89	GLN
1	L	138	ASN
1	L	145	ASN
1	L	157	ASN
1	L	161	ASN
1	L	166	GLN
1	L	190	ASN
1	L	198	HIS
2	H	39	GLN
2	H	82	GLN
2	H	108	ASN
2	H	212	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

9 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$
3	MLE	C	510	3	7,8,9	0.89	0	7,9,11	1.21	2 (28%)
3	MLE	C	508	3	7,8,9	0.82	0	7,9,11	1.21	1 (14%)
3	MLE	C	503	3	7,8,9	0.86	0	7,9,11	1.70	2 (28%)
3	MLE	C	502	3	7,8,9	0.93	0	7,9,11	1.23	1 (14%)
3	SAR	C	507	3	3,4,5	0.76	0	1,3,5	0.67	0
3	ABA	C	506	3	4,5,6	0.64	0	1,5,7	0.29	0
3	BMT	C	505	3	11,12,13	1.95	3 (27%)	11,14,16	2.10	3 (27%)
3	MVA	C	504	3	6,7,8	0.86	0	6,8,10	2.01	1 (16%)

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
3	MLE	C	510	3	-	0/5/8/10	-
3	MLE	C	508	3	-	2/5/8/10	-
3	MLE	C	503	3	-	2/5/8/10	-
3	MLE	C	502	3	-	2/5/8/10	-
3	SAR	C	507	3	-	1/1/2/3	-
3	ABA	C	506	3	-	0/3/4/6	-
3	BMT	C	505	3	-	5/14/16/18	-
3	MVA	C	504	3	-	4/6/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	505	BMT	CE-CZ	3.67	1.56	1.29
3	C	505	BMT	CG2-CB	3.55	1.59	1.53
3	C	505	BMT	CA-N	-2.42	1.43	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	505	BMT	O-C-CA	-3.94	114.44	124.86
3	C	504	MVA	CB-CA-C	-3.71	108.17	112.96
3	C	505	BMT	CD1-CG2-CD2	-3.14	105.49	110.48
3	C	505	BMT	CG2-CD2-CE	3.04	118.86	114.11
3	C	503	MLE	CB-CA-C	-2.95	106.45	110.99
3	C	502	MLE	O-C-CA	-2.73	117.74	124.77
3	C	508	MLE	CN-N-CA	2.61	121.51	113.70
3	C	510	MLE	O-C-CA	-2.32	118.80	124.77
3	C	503	MLE	CB-CA-N	2.31	114.11	110.59
3	C	510	MLE	CN-N-CA	2.02	119.73	113.70

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	504	MVA	CB-CA-N-CN
3	C	504	MVA	N-CA-CB-CG1
3	C	504	MVA	N-CA-CB-CG2
3	C	504	MVA	C-CA-CB-CG1
3	C	505	BMT	O-C-CA-CB
3	C	505	BMT	CE-CD2-CG2-CB
3	C	505	BMT	CE-CD2-CG2-CD1
3	C	505	BMT	CD2-CE-CZ-CH
3	C	507	SAR	C-CA-N-CN
3	C	508	MLE	C-CA-CB-CG
3	C	508	MLE	N-CA-CB-CG
3	C	503	MLE	CA-CB-CG-CD1
3	C	503	MLE	CA-CB-CG-CD2
3	C	502	MLE	N-CA-CB-CG
3	C	505	BMT	CB-CA-N-CN
3	C	502	MLE	C-CA-CB-CG

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	510	MLE	2	0
3	C	508	MLE	1	0
3	C	503	MLE	3	0
3	C	502	MLE	2	0
3	C	505	BMT	1	0
3	C	504	MVA	2	0

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

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	L	214/214 (100%)	-0.78	1 (0%) 87 85	2, 7, 26, 59	0
2	H	228/228 (100%)	-0.67	1 (0%) 88 86	2, 8, 32, 58	0
3	C	2/11 (18%)	-0.13	0 100 100	18, 18, 18, 30	0
All	All	444/453 (98%)	-0.72	2 (0%) 87 85	2, 8, 30, 59	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	228	CYS	2.9
1	L	213	ALA	2.3

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
3	DAL	C	501	5/6	0.75	0.08	25,25,28,28	0
3	MLE	C	503	9/10	0.80	0.10	13,16,19,20	0
3	MLE	C	502	9/10	0.82	0.10	18,19,22,23	0
3	SAR	C	507	5/6	0.91	0.08	10,14,15,17	0
3	BMT	C	505	13/14	0.92	0.07	5,13,19,19	0
3	MLE	C	510	9/10	0.92	0.06	16,21,25,25	0
3	MVA	C	504	8/9	0.93	0.07	2,9,12,14	0
3	MLE	C	508	9/10	0.95	0.05	7,15,19,21	0
3	ABA	C	506	6/7	0.97	0.05	5,7,8,10	0

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.