



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 07:18 PM UTC

PDB ID : 3M17 / pdb_00003m17
Title : Crystal structure of human FcRn with a monomeric peptide inhibitor
Authors : Mezo, A.R.; Sridhar, V.; Badger, J.; Sakorafas, P.; Nienaber, V.
Deposited on : 2010-03-04
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
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

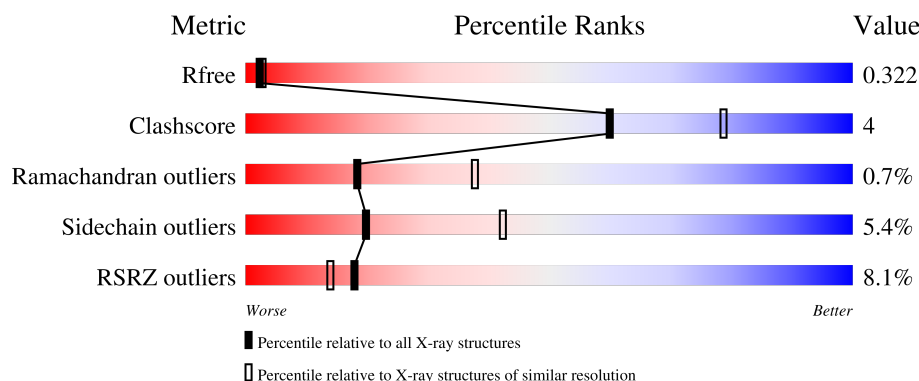
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	267	15% 83% 15% .
1	C	267	6% 86% 12% .
1	E	267	10% 81% 16% ..
1	G	267	12% 84% 14% ..
2	B	99	2% 89% 10% .

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Mol	Chain	Length	Quality of chain
2	D	99	91% 9%
2	F	99	3% 86% 13%
2	H	99	2% 94% 6%
3	I	15	53% 47%
3	J	15	80% 13% 7%
3	K	15	73% 20% 7%
3	L	15	67% 33%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11581 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 IgG receptor FcRn large subunit p51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			1958	1253	329	368	8			
1	C	263	Total	C	N	O	S	0	0	0
			1935	1240	325	362	8			
1	E	263	Total	C	N	O	S	0	0	0
			1931	1239	322	362	8			
1	G	263	Total	C	N	O	S	0	0	0
			1933	1239	323	363	8			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			808	514	135	156	3			
2	D	99	Total	C	N	O	S	0	0	0
			804	512	135	154	3			
2	F	99	Total	C	N	O	S	0	0	0
			807	513	135	156	3			
2	H	99	Total	C	N	O	S	0	0	0
			786	503	135	145	3			

- Molecule 3 is a protein called monomeric peptide inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	15	Total	C	N	O	S	0	0	1
			109	72	19	16	2			
3	J	15	Total	C	N	O	S	0	0	1
			109	72	19	16	2			
3	K	15	Total	C	N	O	S	0	0	1
			109	72	19	16	2			
3	L	15	Total	C	N	O	S	0	0	1
			109	72	19	16	2			

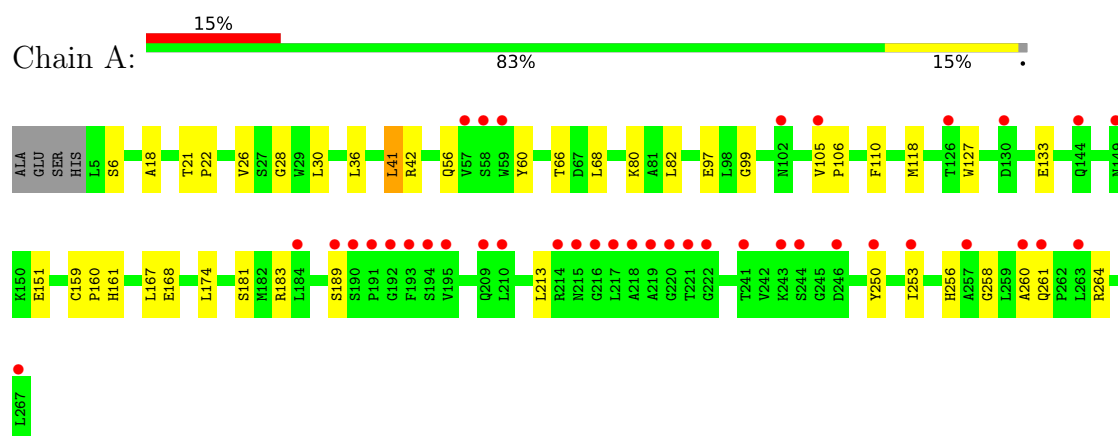
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total 13	O 13	0	0
4	B	15	Total 15	O 15	0	0
4	C	40	Total 40	O 40	0	0
4	D	28	Total 28	O 28	0	0
4	E	21	Total 21	O 21	0	0
4	F	21	Total 21	O 21	0	0
4	G	24	Total 24	O 24	0	0
4	H	18	Total 18	O 18	0	0
4	I	1	Total 1	O 1	0	0
4	J	2	Total 2	O 2	0	0

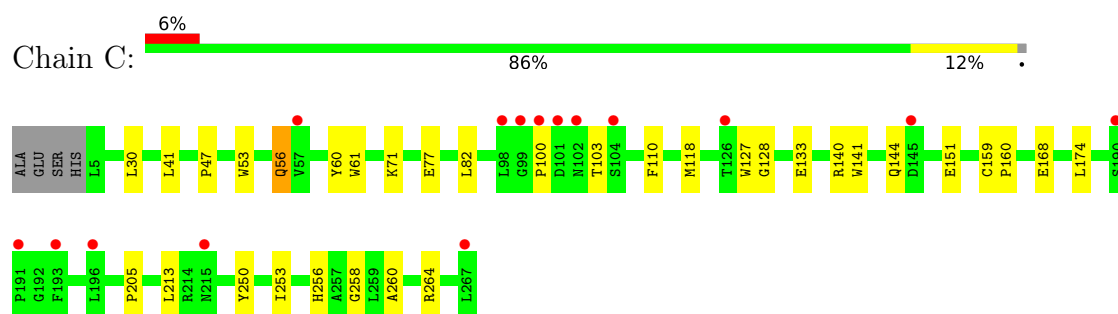
3 Residue-property plots [i](#)

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

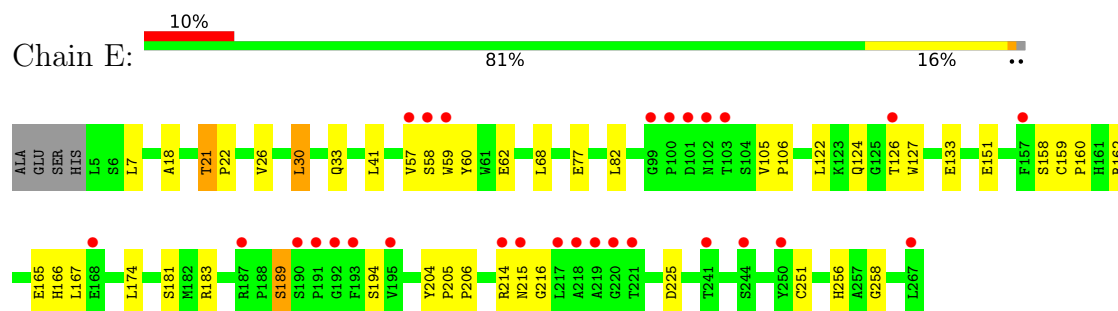
- Molecule 1: IgG receptor FcRn large subunit p51



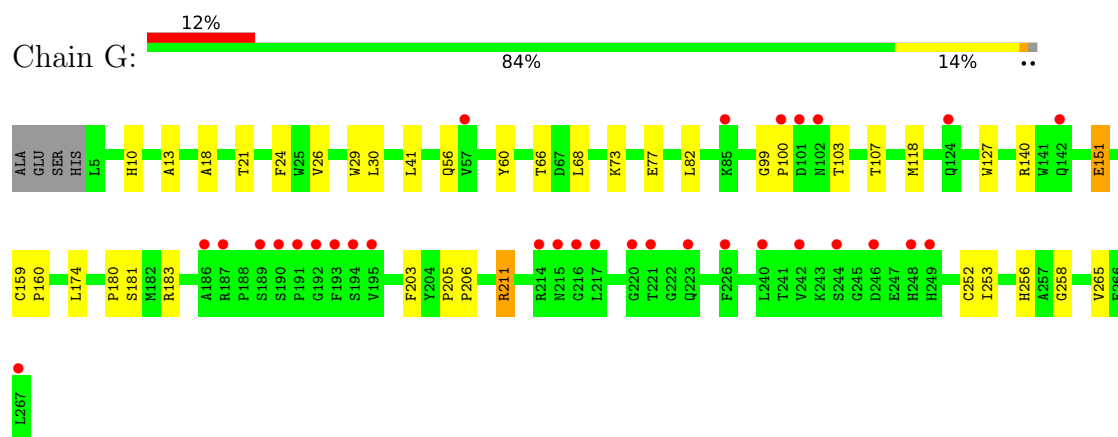
- Molecule 1: IgG receptor FcRn large subunit p51



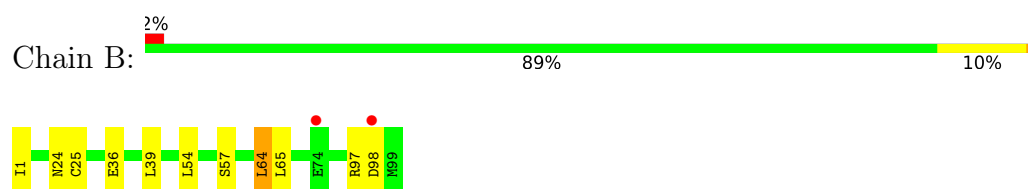
- Molecule 1: IgG receptor FcRn large subunit p51



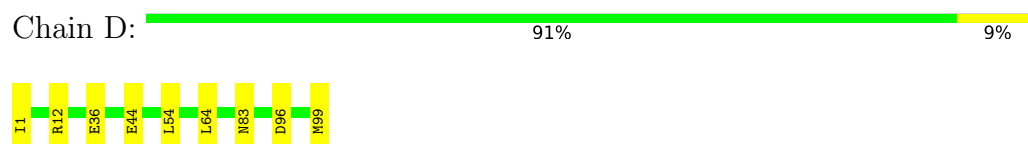
- Molecule 1: IgG receptor FcRn large subunit p51



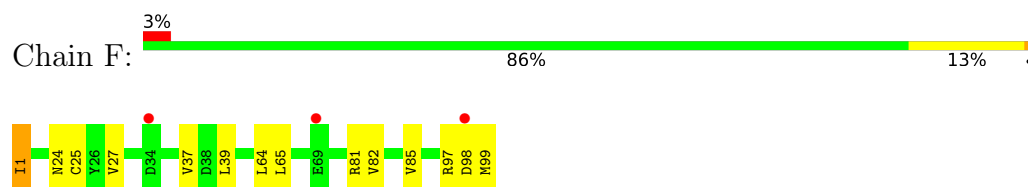
- Molecule 2: Beta-2-microglobulin



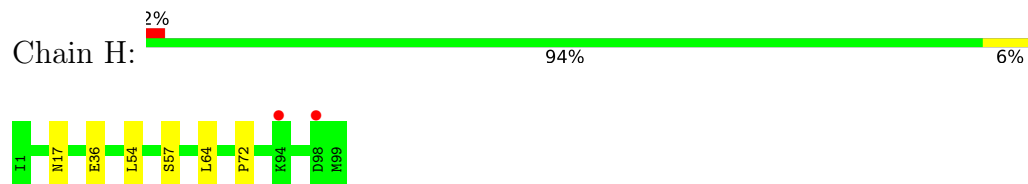
- Molecule 2: Beta-2-microglobulin



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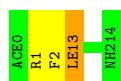


- Molecule 3: monomeric peptide inhibitor



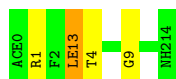
- Molecule 3: monomeric peptide inhibitor

Chain J:  80% 13% 7%



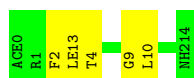
- Molecule 3: monomeric peptide inhibitor

Chain K:  73% 20% 7%



- Molecule 3: monomeric peptide inhibitor

Chain L:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	114.32Å 118.30Å 248.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.10 – 2.60 41.10 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (41.10-2.60) 98.5 (41.10-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.261 , 0.325 0.259 , 0.322	Depositor DCC
R_{free} test set	2606 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.043 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11581	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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: SAR, MLE, LE1, ACE, NH2

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	0.41	0/2020	0.76	2/2764 (0.1%)
1	C	0.43	0/1995	0.76	0/2731
1	E	0.41	0/1991	0.75	0/2726
1	G	0.41	0/1995	0.75	2/2732 (0.1%)
2	B	0.41	0/831	0.71	0/1130
2	D	0.40	0/827	0.68	0/1125
2	F	0.41	0/830	0.68	0/1129
2	H	0.41	0/809	0.66	0/1102
3	I	0.30	0/86	0.40	0/112
3	J	0.37	0/86	0.60	0/112
3	K	0.37	0/86	0.60	0/112
3	L	0.36	0/86	0.57	0/112
All	All	0.41	0/11642	0.73	4/15887 (0.0%)

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
3	I	0	1
3	J	0	2
3	K	0	1
3	L	0	1
All	All	0	5

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	99	GLY	CA-C-N	6.45	127.90	119.84
1	G	99	GLY	C-N-CA	6.45	127.90	119.84
1	A	99	GLY	CA-C-N	5.77	127.06	119.84
1	A	99	GLY	C-N-CA	5.77	127.06	119.84

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	I	2	PHE	Mainchain
3	J	2	PHE	Mainchain
3	J	3	LE1	Mainchain
3	K	3	LE1	Mainchain
3	L	2	PHE	Mainchain

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	1958	0	1753	22	0
1	C	1935	0	1729	16	0
1	E	1931	0	1716	24	0
1	G	1933	0	1708	16	0
2	B	808	0	741	4	0
2	D	804	0	737	2	0
2	F	807	0	739	7	0
2	H	786	0	716	1	0
3	I	109	0	99	2	0
3	J	109	0	99	0	0
3	K	109	0	99	1	0
3	L	109	0	99	1	0
4	A	13	0	0	1	0
4	B	15	0	0	1	0
4	C	40	0	0	0	0
4	D	28	0	0	0	0
4	E	21	0	0	3	0
4	F	21	0	0	3	0
4	G	24	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	18	0	0	0	0
4	I	1	0	0	0	0
4	J	2	0	0	0	0
All	All	11581	0	10235	92	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 4.

All (92) 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:A:6:SER:HB3	1:A:97:GLU:HB3	1.65	0.77
1:G:18:ALA:O	1:G:21:THR:HB	1.88	0.73
1:A:168:GLU:HA	1:C:260:ALA:HB3	1.73	0.71
1:A:256:HIS:CD2	1:A:258:GLY:H	2.10	0.70
1:A:159:CYS:HB3	1:A:160:PRO:HD3	1.77	0.67
3:I:1:ARG:HG2	3:I:14:NH2:N	2.11	0.66
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.76	0.65
1:C:56:GLN:HG3	1:C:60:TYR:HB3	1.77	0.65
1:C:205:PRO:O	1:C:256:HIS:HE1	1.78	0.65
1:C:110:PHE:HB2	1:C:118:MET:HB2	1.78	0.64
2:B:64:LEU:HA	4:B:173:HOH:O	1.98	0.63
1:C:256:HIS:CD2	1:C:258:GLY:H	2.19	0.61
1:E:256:HIS:CD2	1:E:258:GLY:H	2.20	0.60
1:G:256:HIS:CD2	1:G:258:GLY:H	2.19	0.60
2:B:97:ARG:O	2:B:98:ASP:HB2	2.02	0.58
1:E:106:PRO:HG2	1:E:122:LEU:HD22	1.85	0.58
1:E:159:CYS:HB3	1:E:160:PRO:HD3	1.87	0.57
1:G:159:CYS:HB3	1:G:160:PRO:HD3	1.86	0.57
1:E:205:PRO:O	1:E:256:HIS:HE1	1.86	0.57
1:G:77:GLU:HG3	1:G:140:ARG:HE	1.69	0.57
1:E:214:ARG:C	1:E:216:GLY:H	2.12	0.57
1:A:18:ALA:O	1:A:21:THR:HB	2.05	0.56
2:H:17:ASN:HA	2:H:72:PRO:O	2.07	0.55
1:A:41:LEU:HG	2:F:85:VAL:HA	1.88	0.55
2:F:1:ILE:HB	4:F:163:HOH:O	2.06	0.55
1:G:205:PRO:O	1:G:256:HIS:HE1	1.90	0.54
1:A:213:LEU:O	1:A:250:TYR:HA	2.06	0.54
1:C:56:GLN:HG3	1:C:60:TYR:CB	2.39	0.53
1:E:127:TRP:HZ2	1:E:151:GLU:HG3	1.74	0.52
1:G:127:TRP:HZ2	1:G:151:GLU:HG3	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:PHE:HB2	1:A:118:MET:HB2	1.92	0.52
1:A:42:ARG:HD2	4:A:274:HOH:O	2.11	0.50
1:C:141:TRP:O	1:C:144:GLN:HB2	2.12	0.50
1:A:56:GLN:HG3	1:A:60:TYR:CB	2.42	0.50
2:F:25:CYS:HB2	2:F:39:LEU:HD21	1.93	0.50
1:A:22:PRO:HA	1:A:41:LEU:HD13	1.93	0.49
2:D:96:ASP:HB3	2:D:99:MET:HB2	1.93	0.49
1:A:56:GLN:HG3	1:A:60:TYR:HB3	1.95	0.49
1:E:205:PRO:HB2	1:E:206:PRO:HD2	1.95	0.49
1:C:77:GLU:HG3	1:C:140:ARG:HE	1.77	0.48
1:E:189:SER:H	1:E:194:SER:HA	1.79	0.48
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.94	0.48
2:F:24:ASN:HB3	2:F:65:LEU:HD11	1.96	0.47
1:A:253:ILE:HD12	1:A:264:ARG:HG2	1.96	0.47
2:F:81:ARG:HD3	4:F:103:HOH:O	2.13	0.47
1:G:252:CYS:HB3	1:G:265:VAL:HB	1.96	0.47
1:C:159:CYS:HB3	1:C:160:PRO:HD3	1.97	0.47
1:E:60:TYR:OH	1:E:166:HIS:NE2	2.45	0.47
3:L:4:THR:HA	3:L:9:SAR:O	2.15	0.47
1:E:59:TRP:HA	4:E:288:HOH:O	2.15	0.47
1:E:165:GLU:HG3	4:E:269:HOH:O	2.14	0.46
1:C:47:PRO:HB3	1:C:61:TRP:CZ2	2.50	0.46
1:C:127:TRP:HZ2	1:C:151:GLU:HG3	1.80	0.46
1:E:158:SER:O	1:E:162:ARG:HG3	2.16	0.46
2:F:97:ARG:C	2:F:99:MET:H	2.24	0.45
1:G:73:LYS:O	1:G:77:GLU:HB2	2.15	0.45
1:C:213:LEU:O	1:C:250:TYR:HA	2.17	0.45
1:G:205:PRO:HB2	1:G:206:PRO:HD2	1.98	0.45
1:G:10:HIS:CD2	1:G:29:TRP:CD1	3.05	0.44
1:E:127:TRP:CZ2	1:E:151:GLU:HG3	2.52	0.44
1:G:26:VAL:HG21	1:G:68:LEU:HD22	2.00	0.44
1:E:105:VAL:HA	1:E:106:PRO:HD3	1.83	0.44
1:E:33:GLN:HB2	1:E:204:TYR:OH	2.17	0.44
1:E:22:PRO:HA	1:E:41:LEU:HD13	1.99	0.43
1:E:18:ALA:O	1:E:21:THR:HB	2.18	0.43
1:G:56:GLN:HG3	1:G:60:TYR:CB	2.49	0.43
1:E:124:GLN:HB3	4:E:268:HOH:O	2.19	0.43
1:G:13:ALA:HB2	1:G:24:PHE:HD1	1.83	0.43
2:F:37:VAL:HG22	2:F:82:VAL:HG22	2.01	0.43
1:G:211:ARG:HG3	1:G:253:ILE:HB	2.00	0.43
1:C:118:MET:HA	1:C:128:GLY:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:TRP:HZ2	1:A:151:GLU:HG3	1.84	0.42
1:E:26:VAL:HG21	1:E:68:LEU:HD22	2.01	0.42
3:K:4:THR:HA	3:K:9:SAR:O	2.20	0.42
1:A:105:VAL:HA	1:A:106:PRO:HD3	1.78	0.42
2:D:36:GLU:HB2	2:D:83:ASN:HB2	2.02	0.42
3:I:9:SAR:HA3	3:I:10:MLE:HN1	1.76	0.42
1:G:180:PRO:HB3	1:G:203:PHE:HB3	2.02	0.42
1:A:181:SER:OG	1:C:53:TRP:HB3	2.19	0.41
1:E:214:ARG:O	1:E:216:GLY:N	2.42	0.41
1:E:30:LEU:HD21	1:E:166:HIS:CG	2.56	0.41
1:A:6:SER:CB	1:A:97:GLU:HB3	2.45	0.41
1:E:214:ARG:C	1:E:216:GLY:N	2.76	0.41
1:G:66:THR:HG22	4:G:268:HOH:O	2.20	0.41
1:A:26:VAL:HG21	1:A:68:LEU:HD22	2.02	0.41
1:A:22:PRO:HD3	1:A:41:LEU:HD22	2.03	0.41
1:A:28:GLY:HA3	1:A:36:LEU:HB3	2.01	0.41
1:A:66:THR:HG22	4:F:126:HOH:O	2.21	0.41
1:A:260:ALA:HB3	1:C:168:GLU:HA	2.01	0.40
1:C:253:ILE:CD1	1:C:264:ARG:HG2	2.52	0.40
1:E:62:GLU:H	1:E:62:GLU:CD	2.28	0.40
1:E:256:HIS:HD2	1:E:258:GLY:H	1.67	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	261/267 (98%)	244 (94%)	16 (6%)	1 (0%)	30	51
1	C	261/267 (98%)	248 (95%)	12 (5%)	1 (0%)	30	51
1	E	261/267 (98%)	247 (95%)	10 (4%)	4 (2%)	8	18
1	G	261/267 (98%)	247 (95%)	13 (5%)	1 (0%)	30	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
2	D	97/99 (98%)	97 (100%)	0	0	100	100
2	F	97/99 (98%)	92 (95%)	4 (4%)	1 (1%)	12	28
2	H	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
3	I	10/15 (67%)	9 (90%)	0	1 (10%)	0	0
3	J	10/15 (67%)	8 (80%)	1 (10%)	1 (10%)	0	0
3	K	10/15 (67%)	9 (90%)	1 (10%)	0	100	100
3	L	10/15 (67%)	9 (90%)	1 (10%)	0	100	100
All	All	1472/1524 (97%)	1398 (95%)	64 (4%)	10 (1%)	18	38

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	98	ASP
1	A	189	SER
1	E	58	SER
1	E	189	SER
1	E	215	ASN
3	J	1	ARG
1	C	100	PRO
3	I	13	CYS
1	G	100	PRO
1	E	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	186/220 (84%)	176 (95%)	10 (5%)	20	42
1	C	181/220 (82%)	173 (96%)	8 (4%)	25	50
1	E	179/220 (81%)	166 (93%)	13 (7%)	13	29
1	G	179/220 (81%)	168 (94%)	11 (6%)	17	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	88/94 (94%)	83 (94%)	5 (6%)	18	40
2	D	87/94 (93%)	82 (94%)	5 (6%)	18	40
2	F	88/94 (94%)	85 (97%)	3 (3%)	32	60
2	H	82/94 (87%)	78 (95%)	4 (5%)	22	47
3	I	8/8 (100%)	8 (100%)	0	100	100
3	J	8/8 (100%)	8 (100%)	0	100	100
3	K	8/8 (100%)	7 (88%)	1 (12%)	4	9
3	L	8/8 (100%)	8 (100%)	0	100	100
All	All	1102/1288 (86%)	1042 (95%)	60 (5%)	20	42

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	41	LEU
1	A	80	LYS
1	A	82	LEU
1	A	133	GLU
1	A	161	HIS
1	A	167	LEU
1	A	174	LEU
1	A	183	ARG
1	A	261	GLN
2	B	1	ILE
2	B	36	GLU
2	B	54	LEU
2	B	57	SER
2	B	64	LEU
1	C	30	LEU
1	C	41	LEU
1	C	56	GLN
1	C	71	LYS
1	C	82	LEU
1	C	103	THR
1	C	133	GLU
1	C	174	LEU
2	D	1	ILE
2	D	12	ARG
2	D	44	GLU

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Mol	Chain	Res	Type
2	D	54	LEU
2	D	64	LEU
1	E	7	LEU
1	E	21	THR
1	E	30	LEU
1	E	77	GLU
1	E	82	LEU
1	E	126	THR
1	E	133	GLU
1	E	167	LEU
1	E	174	LEU
1	E	181	SER
1	E	183	ARG
1	E	225	ASP
1	E	251	CYS
2	F	1	ILE
2	F	27	VAL
2	F	64	LEU
1	G	30	LEU
1	G	41	LEU
1	G	82	LEU
1	G	103	THR
1	G	107	THR
1	G	118	MET
1	G	151	GLU
1	G	174	LEU
1	G	181	SER
1	G	183	ARG
1	G	211	ARG
2	H	36	GLU
2	H	54	LEU
2	H	57	SER
2	H	64	LEU
3	K	1	ARG

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

Mol	Chain	Res	Type
1	A	10	HIS
1	A	173	ASN
1	A	256	HIS
2	B	8	GLN

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Mol	Chain	Res	Type
1	C	10	HIS
1	C	256	HIS
1	E	56	GLN
1	E	173	ASN
1	E	256	HIS
1	G	56	GLN
1	G	173	ASN
1	G	256	HIS
2	H	13	HIS
3	K	6	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	LE1	K	3	3	3,7,8	0.63	0	3,10,12	1.89	1 (33%)
3	LE1	I	3	3	3,7,8	0.65	0	3,10,12	2.25	1 (33%)
3	SAR	K	9	3	3,4,5	0.64	0	1,3,5	1.63	0
3	MLE	J	10	3	7,8,9	0.43	0	7,9,11	1.09	0
3	SAR	J	9	3	3,4,5	0.59	0	1,3,5	1.60	0
3	MLE	I	10	3	7,8,9	0.42	0	7,9,11	1.17	0
3	SAR	L	9	3	3,4,5	0.69	0	1,3,5	1.56	0
3	MLE	K	10	3	7,8,9	0.47	0	7,9,11	1.15	0
3	LE1	L	3	3	3,7,8	0.67	0	3,10,12	1.93	1 (33%)
3	LE1	J	3	3	3,7,8	0.66	0	3,10,12	1.66	1 (33%)
3	MLE	L	10	3	7,8,9	0.49	0	7,9,11	1.63	1 (14%)
3	SAR	I	9	3	3,4,5	0.66	0	1,3,5	1.61	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
3	LE1	K	3	3	-	0/4/8/10	-
3	LE1	I	3	3	-	0/4/8/10	-
3	SAR	K	9	3	-	1/1/2/3	-
3	MLE	J	10	3	-	0/5/8/10	-
3	SAR	J	9	3	-	1/1/2/3	-
3	MLE	I	10	3	-	0/5/8/10	-
3	SAR	L	9	3	-	1/1/2/3	-
3	MLE	K	10	3	-	0/5/8/10	-
3	LE1	L	3	3	-	0/4/8/10	-
3	LE1	J	3	3	-	0/4/8/10	-
3	MLE	L	10	3	-	1/5/8/10	-
3	SAR	I	9	3	-	1/1/2/3	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	L	10	MLE	CB-CA-N	3.44	115.82	110.59
3	I	3	LE1	C-CA-N	-3.21	105.47	110.34
3	L	3	LE1	C-CA-N	-2.53	106.50	110.34
3	K	3	LE1	C-CA-N	-2.46	106.61	110.34
3	J	3	LE1	C-CA-N	-2.24	106.94	110.34

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	9	SAR	C-CA-N-CN
3	J	9	SAR	C-CA-N-CN
3	K	9	SAR	C-CA-N-CN
3	L	9	SAR	C-CA-N-CN
3	L	10	MLE	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	9	SAR	1	0
3	I	10	MLE	1	0
3	L	9	SAR	1	0
3	I	9	SAR	1	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	A	263/267 (98%)	0.92	39 (14%) 5 4	20, 34, 51, 54	0
1	C	263/267 (98%)	0.64	15 (5%) 29 24	18, 31, 48, 50	0
1	E	263/267 (98%)	0.91	28 (10%) 11 9	19, 37, 53, 57	0
1	G	263/267 (98%)	0.80	31 (11%) 9 7	18, 33, 55, 60	0
2	B	99/99 (100%)	0.39	2 (2%) 65 60	20, 30, 40, 48	0
2	D	99/99 (100%)	0.15	0 100 100	19, 25, 33, 40	0
2	F	99/99 (100%)	0.32	3 (3%) 52 47	21, 27, 35, 42	0
2	H	99/99 (100%)	0.50	2 (2%) 65 60	24, 34, 40, 49	0
3	I	10/15 (66%)	0.50	0 100 100	29, 33, 40, 41	0
3	J	10/15 (66%)	0.19	0 100 100	26, 29, 33, 37	0
3	K	10/15 (66%)	0.68	0 100 100	32, 32, 36, 37	0
3	L	10/15 (66%)	0.46	0 100 100	25, 29, 36, 38	0
All	All	1488/1524 (97%)	0.68	120 (8%) 18 14	18, 32, 50, 60	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	218	ALA	5.3
1	G	102	ASN	4.5
1	E	191	PRO	4.4
1	E	102	ASN	4.4
1	G	195	VAL	4.3
1	G	191	PRO	4.2
1	A	267	LEU	4.2
1	C	215	ASN	4.2
1	A	217	LEU	4.2
1	C	193	PHE	4.1
1	E	101	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
2	F	98	ASP	3.7
1	G	221	THR	3.7
1	A	194	SER	3.7
1	A	191	PRO	3.7
1	A	215	ASN	3.7
1	E	193	PHE	3.6
1	G	193	PHE	3.6
1	E	217	LEU	3.6
1	C	145	ASP	3.6
1	C	267	LEU	3.6
1	E	215	ASN	3.5
1	C	104	SER	3.5
1	E	187	ARG	3.5
1	G	215	ASN	3.4
1	E	100	PRO	3.4
1	A	209	GLN	3.3
1	A	193	PHE	3.3
2	H	98	ASP	3.3
1	E	57	VAL	3.3
1	E	244	SER	3.2
1	G	190	SER	3.2
1	A	244	SER	3.2
1	G	214	ARG	3.1
1	C	190	SER	3.1
1	A	260	ALA	3.0
1	A	220	GLY	3.0
1	E	192	GLY	3.0
1	C	101	ASP	2.9
1	A	58	SER	2.9
1	G	194	SER	2.9
1	C	99	GLY	2.9
1	A	210	LEU	2.9
1	G	248	HIS	2.9
1	E	221	THR	2.8
1	A	130	ASP	2.8
1	E	103	THR	2.8
2	F	69	GLU	2.8
1	A	189	SER	2.7
1	A	243	LYS	2.7
1	A	219	ALA	2.7
1	E	241	THR	2.7
1	E	190	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	216	GLY	2.7
1	G	100	PRO	2.7
1	G	57	VAL	2.7
1	G	226	PHE	2.7
1	E	59	TRP	2.6
1	E	267	LEU	2.6
1	A	190	SER	2.6
1	A	195	VAL	2.6
1	A	184	LEU	2.6
1	A	102	ASN	2.6
1	A	105	VAL	2.6
1	A	241	THR	2.6
1	E	99	GLY	2.6
1	E	214	ARG	2.5
1	A	246	ASP	2.5
1	G	85	LYS	2.5
1	C	196	LEU	2.5
1	G	249	HIS	2.5
1	E	219	ALA	2.5
1	G	220	GLY	2.5
2	H	94	LYS	2.4
1	A	192	GLY	2.4
1	E	168	GLU	2.4
1	G	142	GLN	2.4
1	A	257	ALA	2.4
1	E	58	SER	2.4
1	G	101	ASP	2.4
1	E	157	PHE	2.4
1	E	126	THR	2.3
1	G	246	ASP	2.3
2	F	34	ASP	2.3
1	E	195	VAL	2.3
1	C	126	THR	2.3
1	A	216	GLY	2.3
1	A	57	VAL	2.3
1	G	124	GLN	2.3
1	G	223	GLN	2.3
1	A	222	GLY	2.3
1	A	263	LEU	2.3
1	G	242	VAL	2.3
1	E	218	ALA	2.2
1	A	221	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	74	GLU	2.2
1	A	149	ASN	2.2
1	C	98	LEU	2.2
1	C	57	VAL	2.2
1	A	126	THR	2.2
1	A	250	TYR	2.2
1	E	250	TYR	2.2
1	G	217	LEU	2.2
1	A	214	ARG	2.2
1	C	100	PRO	2.2
1	G	189	SER	2.2
1	C	191	PRO	2.1
1	A	253	ILE	2.1
1	A	59	TRP	2.1
1	G	240	LEU	2.1
1	A	144	GLN	2.1
1	C	102	ASN	2.1
1	G	187	ARG	2.0
2	B	98	ASP	2.0
1	G	186	ALA	2.0
1	G	244	SER	2.0
1	A	261	GLN	2.0
1	G	267	LEU	2.0
1	E	220	GLY	2.0
1	G	192	GLY	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
3	LE1	I	3	8/9	0.63	0.20	38,39,39,40	0
3	SAR	I	9	5/6	0.86	0.13	29,30,30,31	0
3	MLE	L	10	9/10	0.87	0.12	28,29,29,30	0
3	SAR	K	9	5/6	0.88	0.11	32,32,32,32	0
3	SAR	L	9	5/6	0.90	0.10	27,27,28,28	0
3	MLE	K	10	9/10	0.90	0.12	32,33,33,33	0
3	MLE	I	10	9/10	0.91	0.10	31,32,32,32	0
3	SAR	J	9	5/6	0.92	0.14	27,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	LE1	K	3	8/9	0.92	0.10	31,31,31,32	0
3	MLE	J	10	9/10	0.93	0.09	29,29,30,30	0
3	LE1	J	3	8/9	0.94	0.09	29,29,30,30	0
3	LE1	L	3	8/9	0.94	0.09	31,31,32,32	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.