



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:56 am GMT

PDB ID : 3M17
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

<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 : trunk28620
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) : recalc28949

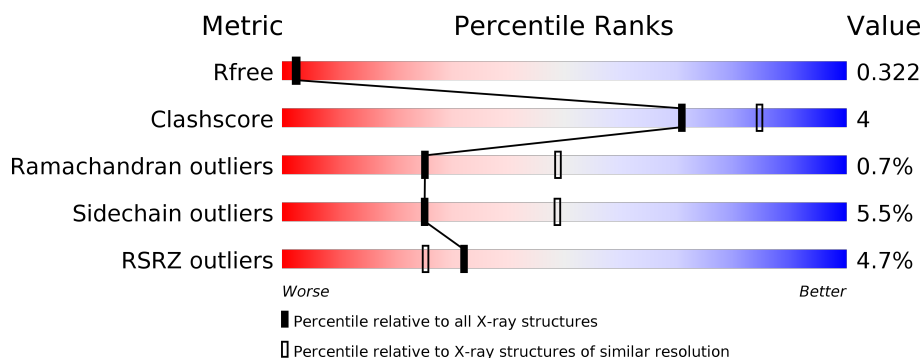
1 Overall quality at a glance

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}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (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 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	267	<div> <div>6%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
1	C	267	<div> <div>4%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
1	E	267	<div> <div>7%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>
1	G	267	<div> <div>7%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>
2	B	99	<div> <div>2%</div> <div>89%</div> <div>9%</div> <div>.</div> </div>
2	D	99	<div> <div>89%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	99	<div><div>%</div><div><div></div><div>84%</div><div>16%</div></div></div>
2	H	99	<div><div>%</div><div><div></div><div>93%</div><div>7%</div></div></div>
3	I	15	<div><div></div><div><div>60%</div><div>40%</div></div></div>
3	J	15	<div><div></div><div><div>80%</div><div>20%</div></div></div>
3	K	15	<div><div></div><div><div>73%</div><div>27%</div></div></div>
3	L	15	<div><div></div><div><div>80%</div><div>20%</div></div></div>

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			

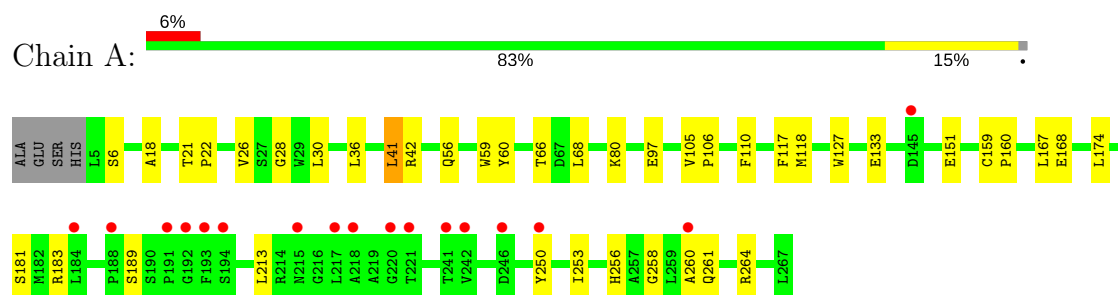
- Molecule 4 is water.

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

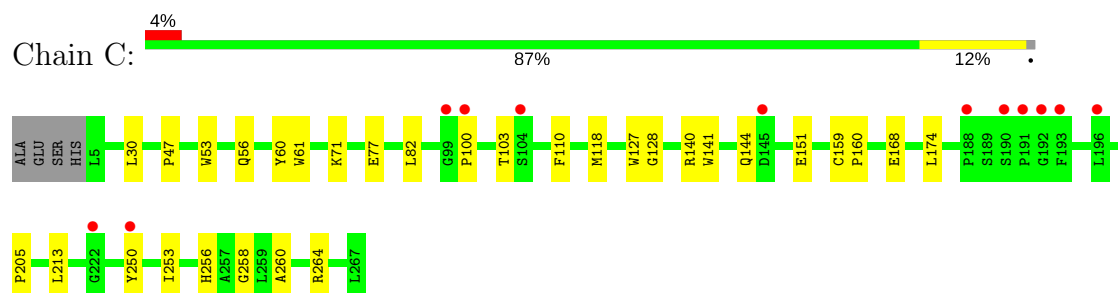
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA 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.

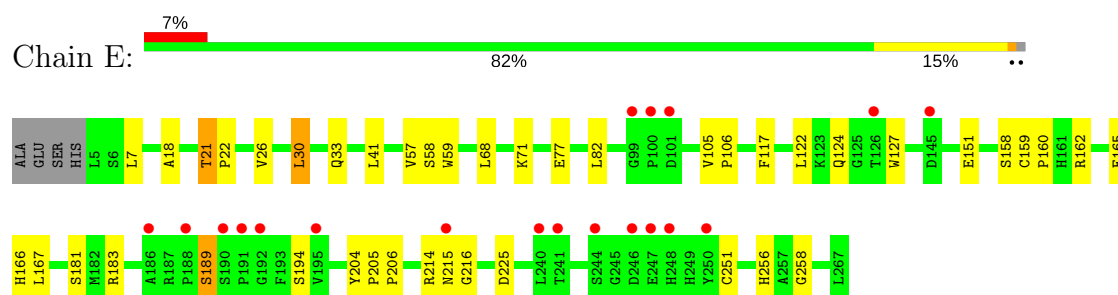
- Molecule 1: IgG receptor FcRn large subunit p51



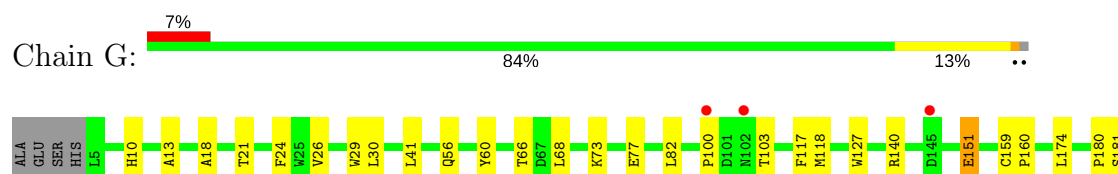
- Molecule 1: IgG receptor FcRn large subunit p51

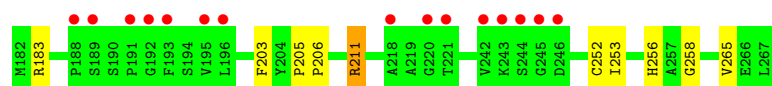


- Molecule 1: IgG receptor FcRn large subunit p51

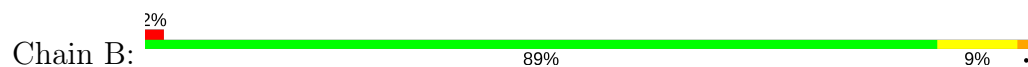


- Molecule 1: IgG receptor FcRn large subunit p51

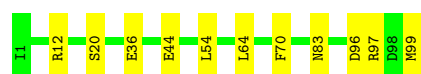




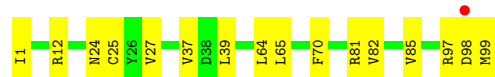
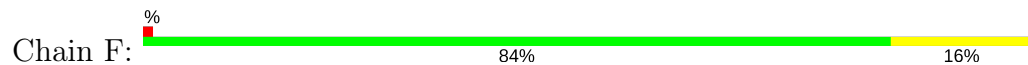
- Molecule 2: Beta-2-microglobulin



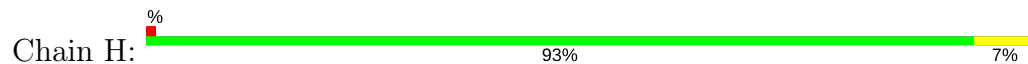
- Molecule 2: Beta-2-microglobulin



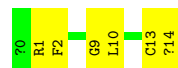
- Molecule 2: Beta-2-microglobulin



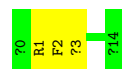
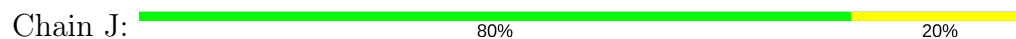
- Molecule 2: Beta-2-microglobulin



- Molecule 3: monomeric peptide inhibitor

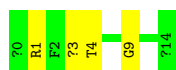


- Molecule 3: monomeric peptide inhibitor



- Molecule 3: monomeric peptide inhibitor





- Molecule 3: monomeric peptide inhibitor

Chain L:
80% 20%



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 40.55 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (41.10-2.60) 98.6 (40.55-2.60)	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 (5.35%)	DCC
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.4	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: LE1, NH2, SAR, ACE, 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	A	0.33	0/2020	0.48	0/2764
1	C	0.34	0/1995	0.49	0/2731
1	E	0.33	0/1991	0.49	0/2726
1	G	0.34	0/1995	0.49	0/2732
2	B	0.34	0/831	0.49	0/1130
2	D	0.34	0/827	0.51	0/1125
2	F	0.34	0/830	0.49	0/1129
2	H	0.34	0/809	0.47	0/1102
3	I	0.40	0/86	0.39	0/112
3	J	0.40	0/86	0.46	0/112
3	K	0.40	0/86	0.44	0/112
3	L	0.40	0/86	0.42	0/112
All	All	0.34	0/11642	0.49	0/15887

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.

There are no bond angle outliers.

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	21	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
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	89	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 (89) 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: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
1:A:110:PHE:HB2	1:A:118:MET:HB2	1.92	0.52
1:E:214:ARG:C	1:E:216:GLY:H	2.12	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:127:TRP:HZ2	1:C:151:GLU:HG3	1.80	0.46
1:C:47:PRO:HB3	1:C:61:TRP:CZ2	2.50	0.46
1:E:158:SER:O	1:E:162:ARG:HG3	2.16	0.46
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:GLY:HA3	1:A:36:LEU:HB3	2.01	0.41
2:F:97:ARG:C	2:F:99:MET:H	2.24	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:256:HIS:HD2	1:E:258:GLY:H	1.67	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	261/267 (98%)	244 (94%)	16 (6%)	1 (0%)	38	63
1	C	261/267 (98%)	248 (95%)	12 (5%)	1 (0%)	38	63
1	E	261/267 (98%)	247 (95%)	10 (4%)	4 (2%)	12	24
1	G	261/267 (98%)	247 (95%)	13 (5%)	1 (0%)	38	63
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%)	18	37
2	H	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
3	I	10/15 (67%)	9 (90%)	0	1 (10%)	1	0
3	J	10/15 (67%)	8 (80%)	1 (10%)	1 (10%)	1	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%)	25	49

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%)	26	49
1	C	181/220 (82%)	176 (97%)	5 (3%)	49	76
1	E	179/220 (81%)	167 (93%)	12 (7%)	19	38
1	G	179/220 (81%)	168 (94%)	11 (6%)	22	43
2	B	88/94 (94%)	82 (93%)	6 (7%)	18	37
2	D	87/94 (93%)	80 (92%)	7 (8%)	14	27
2	F	88/94 (94%)	84 (96%)	4 (4%)	32	59
2	H	82/94 (87%)	77 (94%)	5 (6%)	22	43
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%)	5	10
3	L	8/8 (100%)	8 (100%)	0	100	100
All	All	1102/1288 (86%)	1041 (94%)	61 (6%)	25	49

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU

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Mol	Chain	Res	Type
1	A	41	LEU
1	A	59	TRP
1	A	80	LYS
1	A	117	PHE
1	A	133	GLU
1	A	167	LEU
1	A	174	LEU
1	A	183	ARG
1	A	261	GLN
2	B	36	GLU
2	B	50	GLU
2	B	54	LEU
2	B	57	SER
2	B	64	LEU
2	B	98	ASP
1	C	30	LEU
1	C	71	LYS
1	C	82	LEU
1	C	103	THR
1	C	174	LEU
2	D	12	ARG
2	D	20	SER
2	D	44	GLU
2	D	54	LEU
2	D	64	LEU
2	D	70	PHE
2	D	97	ARG
1	E	7	LEU
1	E	21	THR
1	E	30	LEU
1	E	71	LYS
1	E	77	GLU
1	E	82	LEU
1	E	117	PHE
1	E	167	LEU
1	E	181	SER
1	E	183	ARG
1	E	225	ASP
1	E	251	CYS
2	F	12	ARG
2	F	27	VAL
2	F	64	LEU

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Mol	Chain	Res	Type
2	F	70	PHE
1	G	30	LEU
1	G	41	LEU
1	G	82	LEU
1	G	103	THR
1	G	117	PHE
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
2	H	70	PHE
3	K	1	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	173	ASN
1	A	256	HIS
1	C	256	HIS
2	D	2	GLN
1	E	56	GLN
1	E	173	ASN
1	E	256	HIS
1	G	173	ASN
1	G	256	HIS
2	H	8	GLN

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	MLE	I	10	3	8,8,9	0.45	0	7,9,11	1.08	0
3	LE1	I	3	3	4,7,8	0.73	0	4,10,12	1.82	1 (25%)
3	SAR	I	9	3	4,4,5	0.60	0	1,3,5	1.82	0
3	MLE	J	10	3	8,8,9	0.42	0	7,9,11	1.15	0
3	LE1	J	3	3	4,7,8	0.99	0	4,10,12	1.33	0
3	SAR	J	9	3	4,4,5	0.52	0	1,3,5	1.81	0
3	MLE	K	10	3	8,8,9	0.44	0	7,9,11	1.05	1 (14%)
3	LE1	K	3	3	4,7,8	0.92	0	4,10,12	1.58	1 (25%)
3	SAR	K	9	3	4,4,5	0.66	0	1,3,5	1.84	0
3	MLE	L	10	3	8,8,9	0.46	0	7,9,11	1.07	0
3	LE1	L	3	3	4,7,8	0.85	0	4,10,12	1.55	1 (25%)
3	SAR	L	9	3	4,4,5	0.69	0	1,3,5	1.76	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	MLE	I	10	3	-	0/4/8/10	0/0/0/0
3	LE1	I	3	3	-	0/4/8/10	0/0/0/0
3	SAR	I	9	3	-	0/1/2/3	0/0/0/0
3	MLE	J	10	3	-	0/4/8/10	0/0/0/0
3	LE1	J	3	3	-	0/4/8/10	0/0/0/0
3	SAR	J	9	3	-	0/1/2/3	0/0/0/0
3	MLE	K	10	3	-	0/4/8/10	0/0/0/0
3	LE1	K	3	3	-	0/4/8/10	0/0/0/0
3	SAR	K	9	3	-	0/1/2/3	0/0/0/0
3	MLE	L	10	3	-	0/4/8/10	0/0/0/0
3	LE1	L	3	3	-	0/4/8/10	0/0/0/0
3	SAR	L	9	3	-	0/1/2/3	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	I	3	LE1	O-C-CA	-2.92	118.89	125.01
3	K	3	LE1	O-C-CA	-2.50	119.77	125.01
3	L	3	LE1	O-C-CA	-2.26	120.28	125.01
3	K	10	MLE	O-C-CA	-2.02	120.43	125.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	10	MLE	1	0
3	I	9	SAR	1	0
3	K	9	SAR	1	0
3	L	9	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](#)

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%)	0.49	17 (6%) 20 14	20, 34, 51, 54	0
1	C	263/267 (98%)	0.30	12 (4%) 33 26	18, 31, 48, 50	0
1	E	263/267 (98%)	0.44	19 (7%) 16 12	19, 37, 53, 57	0
1	G	263/267 (98%)	0.42	18 (6%) 18 13	18, 33, 55, 60	0
2	B	99/99 (100%)	0.15	2 (2%) 65 59	20, 30, 40, 48	0
2	D	99/99 (100%)	-0.09	0 100 100	19, 25, 33, 40	0
2	F	99/99 (100%)	0.00	1 (1%) 82 79	21, 27, 35, 42	0
2	H	99/99 (100%)	0.24	1 (1%) 82 79	24, 34, 40, 49	0
3	I	10/15 (66%)	0.20	0 100 100	29, 33, 40, 41	0
3	J	10/15 (66%)	0.07	0 100 100	26, 29, 33, 37	0
3	K	10/15 (66%)	0.45	0 100 100	32, 32, 36, 37	0
3	L	10/15 (66%)	0.31	0 100 100	25, 29, 36, 38	0
All	All	1488/1524 (97%)	0.32	70 (4%) 32 25	18, 32, 50, 60	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	191	PRO	6.7
1	A	218	ALA	5.8
1	A	192	GLY	5.5
1	E	100	PRO	5.3
1	A	220	GLY	5.1
1	E	191	PRO	4.9
1	E	186	ALA	4.6
1	C	145	ASP	4.0
1	G	193	PHE	4.0
1	G	220	GLY	3.8
1	E	192	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	244	SER	3.7
1	G	245	GLY	3.6
1	E	241	THR	3.4
1	C	191	PRO	3.4
2	B	74	GLU	3.4
1	A	221	THR	3.3
1	A	191	PRO	3.3
1	A	242	VAL	3.2
1	C	100	PRO	3.2
1	E	101	ASP	3.2
1	E	188	PRO	3.2
1	G	221	THR	3.1
1	E	248	HIS	3.1
1	G	195	VAL	3.1
1	G	102	ASN	3.1
1	A	194	SER	3.1
1	E	250	TYR	3.0
1	G	189	SER	3.0
1	A	241	THR	3.0
1	G	242	VAL	2.9
1	A	193	PHE	2.9
1	C	188	PRO	2.9
1	A	217	LEU	2.8
1	E	145	ASP	2.8
1	C	192	GLY	2.8
1	C	222	GLY	2.7
1	A	188	PRO	2.7
1	C	193	PHE	2.7
1	G	196	LEU	2.7
2	B	73	THR	2.7
1	E	195	VAL	2.6
1	A	145	ASP	2.6
1	E	190	SER	2.6
1	G	243	LYS	2.5
1	E	126	THR	2.5
1	G	246	ASP	2.5
1	C	99	GLY	2.5
1	G	145	ASP	2.5
1	C	190	SER	2.4
1	A	184	LEU	2.4
1	E	99	GLY	2.3
1	C	104	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	100	PRO	2.3
1	C	196	LEU	2.3
1	A	250	TYR	2.3
1	C	250	TYR	2.3
2	F	98	ASP	2.2
1	G	192	GLY	2.2
1	A	215	ASN	2.2
1	G	244	SER	2.2
1	E	247	GLU	2.1
2	H	98	ASP	2.1
1	G	188	PRO	2.1
1	G	218	ALA	2.1
1	E	215	ASN	2.1
1	A	246	ASP	2.1
1	E	240	LEU	2.0
1	A	260	ALA	2.0
1	E	246	ASP	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. 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
3	MLE	I	10	9/10	0.95	0.20	-	31,32,32,32	0
3	LE1	L	3	8/9	0.94	0.10	-	31,31,32,32	0
3	MLE	J	10	9/10	0.94	0.17	-	29,29,30,30	0
3	LE1	J	3	8/9	0.95	0.12	-	29,29,30,30	0
3	LE1	K	3	8/9	0.94	0.15	-	31,31,31,32	0
3	SAR	K	9	5/6	0.94	0.12	-	32,32,32,32	0
3	MLE	L	10	9/10	0.89	0.24	-	28,29,29,30	0
3	SAR	L	9	5/6	0.96	0.13	-	27,27,28,28	0
3	LE1	I	3	8/9	0.77	0.24	-	38,39,39,40	0
3	SAR	J	9	5/6	0.96	0.17	-	27,28,28,28	0
3	SAR	I	9	5/6	0.93	0.14	-	29,30,30,31	0
3	MLE	K	10	9/10	0.90	0.21	-	32,33,33,33	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.