Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:28 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)

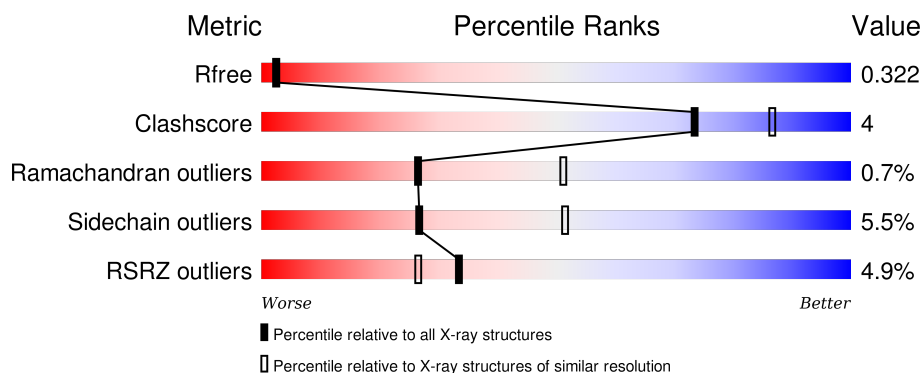
1 Overall quality at a glance ⓘ

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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 <=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	7% / 83% / 15% / •
1	C	267	5% / 87% / 12% / •
1	E	267	7% / 82% / 15% / ••
1	G	267	7% / 84% / 13% / ••
2	B	99	2% / 89% / 9% / •

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Mol	Chain	Length	Quality of chain
2	D	99	89% ⟨green⟩ 11% ⟨yellow⟩
2	F	99	2% 84% ⟨green⟩ 16% ⟨yellow⟩
2	H	99	% 93% ⟨green⟩ 7% ⟨yellow⟩
3	I	15	60% ⟨green⟩ 40% ⟨yellow⟩
3	J	15	80% ⟨green⟩ 20% ⟨yellow⟩
3	K	15	73% ⟨green⟩ 27% ⟨yellow⟩
3	L	15	80% ⟨green⟩ 20% ⟨yellow⟩

2 Entry composition (i)

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 1958	C 1253	N 329	O 368	S 8	0	0	0
1	C	263	Total 1935	C 1240	N 325	O 362	S 8	0	0	0
1	E	263	Total 1931	C 1239	N 322	O 362	S 8	0	0	0
1	G	263	Total 1933	C 1239	N 323	O 363	S 8	0	0	0

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

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

- Molecule 3 is a protein called monomeric peptide inhibitor.

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

- 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 errors 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
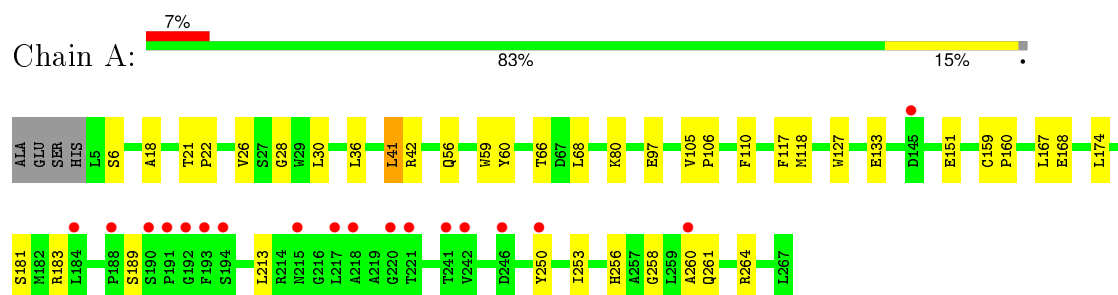
- Molecule 1: IgG receptor FcRn large subunit p51

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M182 R183 P188 S189 S190 P191 G192 F193 S194 V195 I196 F203 Y204 P205 P206 R211 A218 A219 G220 T221 V242 K243 S244 G245 D246 C252 I253 H256 A257 G258 V265 E266 L267

● Molecule 2: Beta-2-microglobulin

Chain B:

2%
89%	9%	•

I1 N24 C25 E36 L39 E50 L54 S57 L64 L65 T73 E74 R97 D98 M99

● Molecule 2: Beta-2-microglobulin

Chain D:

89%	11%

I1 R12 S20 E36 E44 L54 L64 F70 N83 D96 R97 D98 M99

● Molecule 2: Beta-2-microglobulin

Chain F:

2%
84%	16%

I1 R12 N24 C25 Y26 V27 V37 D38 L39 L64 L65 E69 F70 R81 V82 V85 R97 D98 M99

● Molecule 2: Beta-2-microglobulin

Chain H:

%
93%	7%

I1 N17 E36 L54 S57 L64 F70 T71 P72 D98 M99

● Molecule 3: monomeric peptide inhibitor

Chain I:

60%	40%

?0 R1 F2 G9 L10 C13 ?14

● Molecule 3: monomeric peptide inhibitor

Chain J:

80%	20%

?0 R1 F2 ?3 ?14

● Molecule 3: monomeric peptide inhibitor

Chain K:

73%	27%

• Molecule 3: monomeric peptide inhibitor

Chain L:

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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
Estimated twinning fraction	0.043 for -k,-h,-l	Xtriage
L-test for twinning [2]	$< |L| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 51331 reflections	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.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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 (i)

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:C:141:TRP:O	1:C:144:GLN:HB2	2.12	0.50
1:A:42:ARG:HD2	4:A:274:HOH:O	2.11	0.50
2:F:25:CYS:HB2	2:F:39:LEU:HD21	1.93	0.50
1:A:56:GLN:HG3	1:A:60:TYR:CB	2.42	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
1:G:211:ARG:HG3	1:G:253:ILE:HB	2.00	0.43
2:F:37:VAL:HG22	2:F:82:VAL:HG22	2.01	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
2:D:36:GLU:HB2	2:D:83:ASN:HB2	2.02	0.42
1:A:105:VAL:HA	1:A:106:PRO:HD3	1.78	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)
2:F:97:ARG:C	2:F:99:MET:H	2.24	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: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%)	39	65
1	C	261/267 (98%)	248 (95%)	12 (5%)	1 (0%)	39	65
1	E	261/267 (98%)	247 (95%)	10 (4%)	4 (2%)	13	26
1	G	261/267 (98%)	247 (95%)	13 (5%)	1 (0%)	39	65
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%)	19	39
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%)	26	51

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 (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	186/220 (84%)	176 (95%)	10 (5%)	27	52
1	C	181/220 (82%)	176 (97%)	5 (3%)	51	78
1	E	179/220 (81%)	167 (93%)	12 (7%)	20	40
1	G	179/220 (81%)	168 (94%)	11 (6%)	23	46
2	B	88/94 (94%)	82 (93%)	6 (7%)	20	39
2	D	87/94 (93%)	80 (92%)	7 (8%)	15	29
2	F	88/94 (94%)	84 (96%)	4 (4%)	34	62
2	H	82/94 (87%)	77 (94%)	5 (6%)	23	46
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%)	6	10
3	L	8/8 (100%)	8 (100%)	0	100	100
All	All	1102/1288 (86%)	1041 (94%)	61 (6%)	27	51

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 (i)

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	7,8,9	0.40	0	4,9,11	0.95	0
3	LE1	I	3	3	3,7,8	0.62	0	3,10,12	0.78	0
3	SAR	I	9	3	4,4,5	0.65	0	2,3,5	1.11	0
3	MLE	J	10	3	7,8,9	0.41	0	4,9,11	0.93	0
3	LE1	J	3	3	3,7,8	0.61	0	3,10,12	0.80	0
3	SAR	J	9	3	4,4,5	0.59	0	2,3,5	1.15	0
3	MLE	K	10	3	7,8,9	0.43	0	4,9,11	1.00	0
3	LE1	K	3	3	3,7,8	0.59	0	3,10,12	1.01	0
3	SAR	K	9	3	4,4,5	0.66	0	2,3,5	1.12	0
3	MLE	L	10	3	7,8,9	0.44	0	4,9,11	1.00	0
3	LE1	L	3	3	3,7,8	0.63	0	3,10,12	1.02	0
3	SAR	L	9	3	4,4,5	0.71	0	2,3,5	1.06	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.

There are no bond angle outliers.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	263/267 (98%)	0.52	18 (6%)	20	15	20, 34, 51, 54	0
1	C	263/267 (98%)	0.34	13 (4%)	33	26	18, 31, 48, 50	0
1	E	263/267 (98%)	0.48	19 (7%)	18	13	19, 37, 53, 57	0
1	G	263/267 (98%)	0.46	18 (6%)	20	15	18, 33, 55, 60	0
2	B	99/99 (100%)	0.19	2 (2%)	68	63	20, 30, 40, 48	0
2	D	99/99 (100%)	-0.05	0	100	100	19, 25, 33, 40	0
2	F	99/99 (100%)	0.04	2 (2%)	68	63	21, 27, 35, 42	0
2	H	99/99 (100%)	0.28	1 (1%)	84	81	24, 34, 40, 49	0
3	I	10/15 (66%)	0.24	0	100	100	29, 33, 40, 41	0
3	J	10/15 (66%)	0.11	0	100	100	26, 29, 33, 37	0
3	K	10/15 (66%)	0.49	0	100	100	32, 32, 36, 37	0
3	L	10/15 (66%)	0.35	0	100	100	25, 29, 36, 38	0
All	All	1488/1524 (97%)	0.36	73 (4%)	33	26	18, 32, 50, 60	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	191	PRO	6.7
1	A	218	ALA	5.9
1	A	192	GLY	5.6
1	E	100	PRO	5.3
1	A	220	GLY	5.2
1	E	191	PRO	5.0
1	E	186	ALA	4.7
1	C	145	ASP	4.2
1	G	193	PHE	4.1
1	G	220	GLY	3.9
1	E	192	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	244	SER	3.8
1	G	245	GLY	3.6
1	E	241	THR	3.5
2	B	74	GLU	3.5
1	C	191	PRO	3.4
1	A	221	THR	3.4
1	E	101	ASP	3.4
1	A	191	PRO	3.3
1	A	242	VAL	3.3
1	C	100	PRO	3.3
1	E	188	PRO	3.2
1	G	221	THR	3.2
1	E	248	HIS	3.2
1	G	195	VAL	3.2
1	G	102	ASN	3.1
1	E	250	TYR	3.1
1	A	194	SER	3.1
1	G	189	SER	3.1
1	A	241	THR	3.1
1	G	242	VAL	3.0
1	A	193	PHE	2.9
1	E	145	ASP	2.9
1	C	188	PRO	2.9
1	A	217	LEU	2.8
1	C	192	GLY	2.8
1	C	222	GLY	2.8
1	A	188	PRO	2.8
1	C	193	PHE	2.7
1	G	196	LEU	2.7
2	B	73	THR	2.7
1	A	145	ASP	2.7
1	E	195	VAL	2.6
1	E	190	SER	2.6
1	G	246	ASP	2.6
1	G	243	LYS	2.6
1	E	126	THR	2.6
1	G	145	ASP	2.6
1	C	99	GLY	2.5
1	C	190	SER	2.5
1	A	184	LEU	2.4
1	E	99	GLY	2.4
1	C	104	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	100	PRO	2.4
1	A	250	TYR	2.3
1	C	250	TYR	2.3
1	C	196	LEU	2.3
2	F	98	ASP	2.3
1	G	192	GLY	2.3
1	A	215	ASN	2.2
1	E	247	GLU	2.2
2	H	98	ASP	2.2
1	G	244	SER	2.2
1	A	246	ASP	2.2
1	E	215	ASN	2.2
1	G	218	ALA	2.2
1	G	188	PRO	2.1
1	E	246	ASP	2.1
1	A	260	ALA	2.1
2	F	69	GLU	2.1
1	E	240	LEU	2.0
1	A	190	SER	2.0
1	C	247	GLU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($\mathring{A}^2$)	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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.