Full wwPDB X-ray Structure Validation Report (i)

Jul 19, 2022 – 01:09 pm BST

PDB ID	:	7NDU
Title	:	Gag:02 TCR in complex with HLA-E featuring a non-natural amino acid
Authors	:	Pengelly, R.J.; Robinson, R.A.
Deposited on	:	2021-02-02
Resolution	:	2.90 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 (i) 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 (1)) were used in the production of this report:

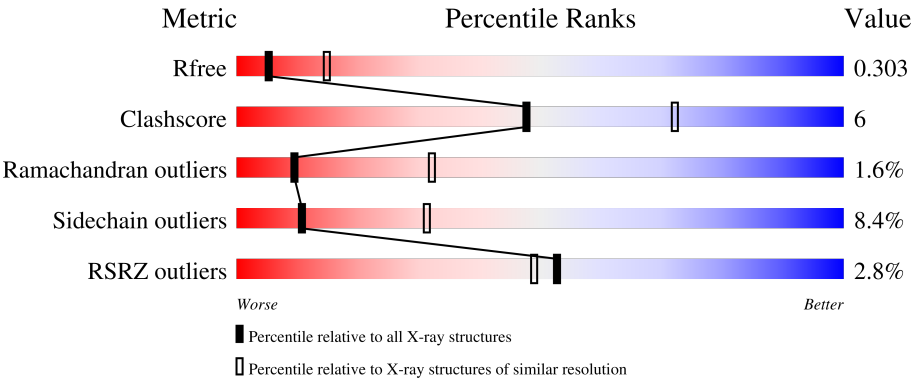
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	AAA	277	79% 18% .
2	BBB	100	76% 24%
3	CCC	9	89% 11%
4	DDD	199	6% 69% 20% . 8%
5	EEE	244	4% 84% 12% ..

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6545 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 HLA class I histocompatibility antigen, alpha chain E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	276	Total	C	N	O	S	0	1	0
			2248	1402	403	435	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	0	MET	-	initiating methionine	UNP P13747
AAA	116	CYS	PHE	conflict	UNP P13747

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Gag6V(276-284 H4C).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	CCC	9	Total	C	N	O	S	0	0	0
			75	48	12	13	2			

- Molecule 4 is a protein called T cell receptor alpha variable 4,T cell receptor alpha joining 23,M1-specific T cell receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	DDD	184	Total	C	N	O	S	0	2	0
			1441	899	239	295	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DDD	0	MET	-	initiating methionine	UNP A0A0B4J268
DDD	108	SER	-	linker	UNP A0A0B4J268
DDD	109	SER	-	linker	UNP A0A0B4J268
DDD	110	PHE	-	linker	UNP A0A0B4J268
DDD	129	ASN	-	linker	UNP A0A075B6U7
DDD	176	CYS	THR	engineered mutation	UNP P0DSE1

- Molecule 5 is a protein called T cell receptor beta variable 7-9,T cell receptor beta joining 1-2,Human nkt tcr beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	EEE	241	Total	C	N	O	S	0	0	0
			1944	1219	347	372	6			

There are 7 discrepancies between the modelled and reference sequences:

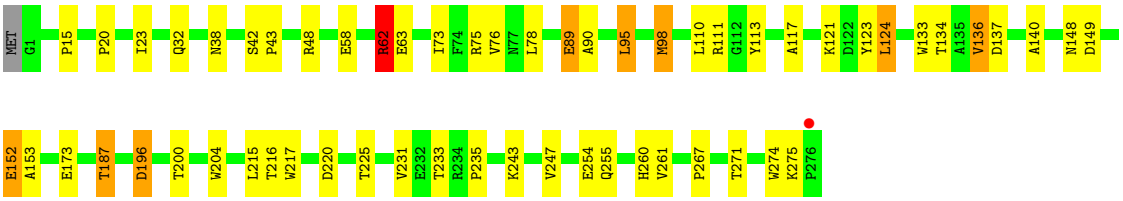
Chain	Residue	Modelled	Actual	Comment	Reference
EEE	0	MET	-	initiating methionine	UNP P04435
EEE	109	GLY	-	linker	UNP P04435
EEE	110	ARG	-	linker	UNP P04435
EEE	113	GLU	-	linker	UNP P04435
EEE	132	ASN	LYS	engineered mutation	UNP K7N5M4
EEE	133	LYS	ASN	engineered mutation	UNP K7N5M4
EEE	217	ASP	ASN	engineered mutation	UNP K7N5M4

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: HLA class I histocompatibility antigen, alpha chain E

Chain AAA:



• Molecule 2: Beta-2-microglobulin

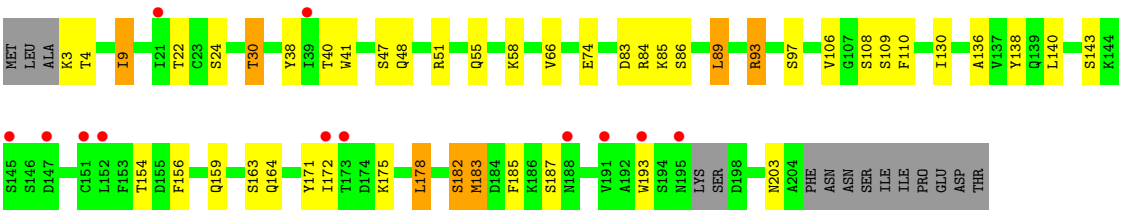
Chain BBB:

• Molecule 3: Gag6V(276-284 H4C)

Chain CCC:

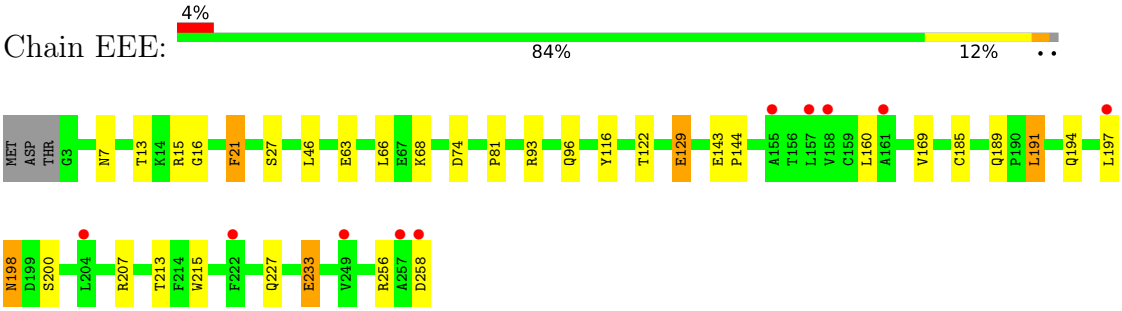
• Molecule 4: T cell receptor alpha variable 4,T cell receptor alpha joining 23,M1-specific T cell receptor alpha chain

Chain DDD:



• Molecule 5: T cell receptor beta variable 7-9,T cell receptor beta joining 1-2,Human nkt tcr beta chain

Chain EEE:


4%
84%
12%
MET
ASP
THR
G3
N7
T13
K14
R15
G16
F21
S27
L46
E63
L66
E67
K68
D74
P81
R93
Q96
Y116
T122
E129
E143
P144
A155
T156
L157
V158
C159
L160
A161
V169
C185
Q189
P190
L191
Q194
L197
N198
D199
S200
L204
R207
T213
F214
W215
F222
Q227
E233
V249
R256
A257
D258

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	88.98Å 88.98Å 293.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.60 – 2.90 61.52 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (61.60-2.90) 99.8 (61.52-2.90)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.242 , 0.301 0.245 , 0.303	Depositor DCC
R_{free} test set	1337 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	69.5	Xtriage
Anisotropy	0.554	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6545	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: QM8

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	AAA	0.71	0/2314	0.90	1/3146 (0.0%)
2	BBB	0.70	0/860	0.88	0/1162
3	CCC	0.62	0/66	1.03	0/88
4	DDD	0.71	0/1475	0.85	0/2001
5	EEE	0.70	0/1995	0.89	1/2708 (0.0%)
All	All	0.71	0/6710	0.88	2/9105 (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
1	AAA	0	1
4	DDD	0	2
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	EEE	81	PRO	C-N-CA	7.03	139.28	121.70
1	AAA	62	ARG	CG-CD-NE	5.62	123.61	111.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	136	VAL	Peptide

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Mol	Chain	Res	Type	Group
4	DDD	156	PHE	Peptide
4	DDD	3	LYS	Peptide

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	AAA	2248	0	2087	32	0
2	BBB	837	0	803	19	0
3	CCC	75	0	70	2	0
4	DDD	1441	0	1378	18	0
5	EEE	1944	0	1846	16	0
All	All	6545	0	6184	77	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 6.

All (77) 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:BBB:4:THR:HA	2:BBB:86:THR:HG21	1.52	0.92
1:AAA:187:THR:HG21	1:AAA:261:VAL:HG21	1.73	0.70
1:AAA:63:GLU:OE1	3:CCC:1:ARG:NH1	2.27	0.66
1:AAA:117:ALA:HB2	2:BBB:60:TRP:CE2	2.37	0.60
1:AAA:15:PRO:HG2	1:AAA:90:ALA:O	2.03	0.59
1:AAA:217:TRP:CD1	1:AAA:247:VAL:CG2	2.85	0.59
5:EEE:96:GLN:NE2	5:EEE:129:GLU:OE1	2.28	0.59
5:EEE:256:ARG:HD3	5:EEE:258:ASP:OD2	2.06	0.56
1:AAA:136:VAL:HG23	1:AAA:137:ASP:HB2	1.87	0.55
2:BBB:4:THR:HA	2:BBB:86:THR:CG2	2.32	0.55
5:EEE:233:GLU:HA	5:EEE:233:GLU:OE1	2.06	0.55
1:AAA:255:GLN:NE2	1:AAA:274:TRP:O	2.38	0.55
1:AAA:124:LEU:HD12	1:AAA:133:TRP:CE3	2.42	0.55
5:EEE:16:GLY:O	5:EEE:93:ARG:HA	2.08	0.54
4:DDD:4:THR:HG23	4:DDD:4:THR:O	2.07	0.53
4:DDD:58:LYS:HE3	4:DDD:84:ARG:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:EEE:143:GLU:OE1	5:EEE:256:ARG:NH2	2.41	0.53
2:BBB:4:THR:HG23	2:BBB:86:THR:HG23	1.90	0.53
1:AAA:32:GLN:NE2	2:BBB:53:ASP:OD2	2.42	0.52
5:EEE:207:ARG:N	5:EEE:207:ARG:HD3	2.25	0.52
1:AAA:48:ARG:NH1	2:BBB:53:ASP:OD2	2.43	0.51
1:AAA:98:MET:C	1:AAA:98:MET:SD	2.89	0.51
2:BBB:25:CYS:HB2	2:BBB:39:LEU:HD21	1.93	0.51
1:AAA:62:ARG:CZ	3:CCC:1:ARG:NE	2.74	0.51
4:DDD:9:ILE:N	4:DDD:9:ILE:HD13	2.25	0.50
1:AAA:78:LEU:HG	1:AAA:95:LEU:HD23	1.96	0.47
1:AAA:153:ALA:O	4:DDD:38:TYR:HE2	1.98	0.47
1:AAA:148:ASN:O	1:AAA:152:GLU:HG2	2.15	0.47
1:AAA:38:ASN:HA	1:AAA:43:PRO:HB3	1.97	0.47
4:DDD:182:SER:O	4:DDD:183:MET:HB2	2.15	0.46
1:AAA:233:THR:OG1	1:AAA:243:LYS:HE2	2.15	0.46
4:DDD:55:GLN:O	4:DDD:66:VAL:HG11	2.15	0.46
5:EEE:63:GLU:OE1	5:EEE:63:GLU:N	2.41	0.46
4:DDD:182:SER:O	4:DDD:183:MET:CB	2.64	0.46
1:AAA:73:ILE:O	1:AAA:76:VAL:HB	2.16	0.45
1:AAA:196:ASP:N	1:AAA:196:ASP:OD1	2.47	0.45
2:BBB:73:THR:OG1	2:BBB:76:ASP:HB2	2.16	0.45
2:BBB:84:HIS:C	2:BBB:86:THR:H	2.20	0.44
5:EEE:207:ARG:N	5:EEE:207:ARG:CD	2.80	0.44
4:DDD:83[B]:ASP:HB3	4:DDD:85:LYS:HG2	2.00	0.44
4:DDD:106:VAL:HG23	4:DDD:106:VAL:O	2.18	0.44
2:BBB:84:HIS:ND1	2:BBB:86:THR:HG22	2.32	0.44
1:AAA:15:PRO:HB3	1:AAA:89:GLU:O	2.18	0.44
1:AAA:187:THR:HA	1:AAA:204:TRP:O	2.18	0.44
1:AAA:215:LEU:HD22	1:AAA:261:VAL:HG22	2.00	0.43
4:DDD:136:ALA:HB3	4:DDD:138:TYR:CE2	2.53	0.43
5:EEE:144:PRO:HD2	5:EEE:215:TRP:CZ2	2.53	0.43
5:EEE:191:LEU:HD12	5:EEE:191:LEU:O	2.19	0.43
1:AAA:235:PRO:HG2	2:BBB:65:LEU:HD13	2.00	0.43
1:AAA:260:HIS:CD2	1:AAA:271:THR:HG22	2.54	0.42
4:DDD:171:TYR:HD2	4:DDD:193:TRP:NE1	2.18	0.42
1:AAA:121:LYS:HG3	2:BBB:1:ILE:HD13	2.02	0.42
1:AAA:123:TYR:CZ	1:AAA:140:ALA:HA	2.54	0.42
2:BBB:48:LYS:N	2:BBB:48:LYS:HD2	2.35	0.42
4:DDD:108:SER:C	4:DDD:110:PHE:H	2.23	0.42
1:AAA:95:LEU:HD13	1:AAA:95:LEU:HA	1.88	0.42
4:DDD:159:GLN:OE1	4:DDD:159:GLN:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:DDD:163:SER:O	4:DDD:172:ILE:HG21	2.20	0.41
1:AAA:152:GLU:HA	1:AAA:152:GLU:OE1	2.21	0.41
2:BBB:84:HIS:C	2:BBB:86:THR:N	2.74	0.41
4:DDD:4:THR:O	4:DDD:4:THR:CG2	2.68	0.41
1:AAA:217:TRP:CD1	1:AAA:247:VAL:HG23	2.56	0.41
1:AAA:217:TRP:CG	1:AAA:247:VAL:CG2	3.04	0.41
1:AAA:20:PRO:HD2	1:AAA:75:ARG:HD2	2.03	0.41
2:BBB:12:ARG:HG2	2:BBB:13:HIS:CE1	2.56	0.41
2:BBB:79:ALA:HB2	2:BBB:94:LYS:HA	2.02	0.41
5:EEE:194:GLN:O	5:EEE:200:SER:HB2	2.21	0.41
5:EEE:197:LEU:O	5:EEE:198:ASN:C	2.60	0.41
1:AAA:23:ILE:HD12	2:BBB:54:LEU:HD23	2.03	0.41
5:EEE:256:ARG:CD	5:EEE:258:ASP:OD2	2.68	0.41
2:BBB:29:GLY:HA2	2:BBB:61:SER:HB3	2.02	0.40
5:EEE:21:PHE:CD1	5:EEE:122:THR:HG21	2.56	0.40
5:EEE:169:VAL:HA	5:EEE:227:GLN:O	2.21	0.40
4:DDD:41:TRP:CG	4:DDD:89:LEU:HD23	2.57	0.40
4:DDD:178:LEU:HB3	5:EEE:185:CYS:HB2	2.03	0.40
2:BBB:5:PRO:HD3	2:BBB:86:THR:HG21	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	AAA	275/277 (99%)	253 (92%)	21 (8%)	1 (0%)	34 66
2	BBB	98/100 (98%)	89 (91%)	9 (9%)	0	100 100
3	CCC	7/9 (78%)	7 (100%)	0	0	100 100
4	DDD	182/199 (92%)	141 (78%)	33 (18%)	8 (4%)	2 10
5	EEE	239/244 (98%)	201 (84%)	34 (14%)	4 (2%)	9 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	801/829 (97%)	691 (86%)	97 (12%)	13 (2%)	9 32

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	DDD	47	SER
4	DDD	93	ARG
4	DDD	183	MET
5	EEE	66	LEU
4	DDD	30	THR
4	DDD	97	SER
4	DDD	164	GLN
4	DDD	185	PHE
5	EEE	116	TYR
5	EEE	198	ASN
1	AAA	267	PRO
5	EEE	68	LYS
4	DDD	130	ILE

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	AAA	238/238 (100%)	215 (90%)	23 (10%)	8 25
2	BBB	95/95 (100%)	91 (96%)	4 (4%)	30 63
3	CCC	8/8 (100%)	8 (100%)	0	100 100
4	DDD	168/180 (93%)	148 (88%)	20 (12%)	5 15
5	EEE	211/214 (99%)	198 (94%)	13 (6%)	18 47
All	All	720/735 (98%)	660 (92%)	60 (8%)	11 32

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

Mol	Chain	Res	Type
1	AAA	42	SER

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Mol	Chain	Res	Type
1	AAA	58	GLU
1	AAA	62	ARG
1	AAA	89	GLU
1	AAA	95	LEU
1	AAA	98	MET
1	AAA	110	LEU
1	AAA	111	ARG
1	AAA	113	TYR
1	AAA	124	LEU
1	AAA	134	THR
1	AAA	149	ASP
1	AAA	152	GLU
1	AAA	173	GLU
1	AAA	187	THR
1	AAA	196	ASP
1	AAA	200	THR
1	AAA	216	THR
1	AAA	220	ASP
1	AAA	225	THR
1	AAA	231	VAL
1	AAA	254	GLU
1	AAA	275	LYS
2	BBB	34	ASP
2	BBB	70	PHE
2	BBB	77	GLU
2	BBB	91	LYS
4	DDD	9	ILE
4	DDD	22	THR
4	DDD	24	SER
4	DDD	30	THR
4	DDD	40	THR
4	DDD	48	GLN
4	DDD	51	ARG
4	DDD	74	GLU
4	DDD	86	SER
4	DDD	89	LEU
4	DDD	93	ARG
4	DDD	109	SER
4	DDD	140	LEU
4	DDD	143	SER
4	DDD	154	THR
4	DDD	175	LYS

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Mol	Chain	Res	Type
4	DDD	178	LEU
4	DDD	182	SER
4	DDD	187	SER
4	DDD	203	ASN
5	EEE	7	ASN
5	EEE	13	THR
5	EEE	15	ARG
5	EEE	21	PHE
5	EEE	27	SER
5	EEE	46	LEU
5	EEE	74	ASP
5	EEE	129	GLU
5	EEE	160	LEU
5	EEE	189	GLN
5	EEE	191	LEU
5	EEE	213	THR
5	EEE	233	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	QM8	CCC	9	3	8,9,9	0.89	0	9,10,10	0.80	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	QM8	CCC	9	3	-	3/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	CCC	9	QM8	CG-CD-CE-SZ
3	CCC	9	QM8	CE-CD-CG-CB
3	CCC	9	QM8	CA-CB-CG-CD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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	AAA	276/277 (99%)	0.11	1 (0%) 92 93	52, 65, 78, 83	0
2	BBB	100/100 (100%)	0.16	0 100 100	52, 62, 77, 80	0
3	CCC	8/9 (88%)	0.72	0 100 100	69, 72, 74, 77	0
4	DDD	184/199 (92%)	0.46	12 (6%) 18 14	74, 93, 114, 123	0
5	EEE	241/244 (98%)	0.36	10 (4%) 37 32	59, 73, 102, 118	0
All	All	809/829 (97%)	0.28	23 (2%) 53 49	52, 70, 107, 123	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	EEE	257	ALA	5.7
4	DDD	195	ASN	4.1
5	EEE	222	PHE	3.8
4	DDD	152	LEU	3.5
5	EEE	258	ASP	3.5
4	DDD	172	ILE	3.3
4	DDD	21	ILE	3.0
5	EEE	157	LEU	3.0
4	DDD	145	SER	3.0
4	DDD	191	VAL	3.0
5	EEE	155	ALA	2.9
4	DDD	173	THR	2.7
5	EEE	158	VAL	2.6
5	EEE	161	ALA	2.5
4	DDD	193	TRP	2.5
4	DDD	39	ILE	2.4
5	EEE	249	VAL	2.4
5	EEE	197	LEU	2.3
5	EEE	204	LEU	2.2
1	AAA	276	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
4	DDD	188	ASN	2.1
4	DDD	147	ASP	2.1
4	DDD	151	CYS	2.1

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. The B-factors column lists the minimum, median, 95^{th} 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	QM8	CCC	9	10/10	0.84	0.42	77,79,81,84	0

6.3 Carbohydrates (i)

There are no monosaccharides 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.