wwPDB X-ray Structure Validation Summary Report (i)

Jul 19, 2022 – 01:16 pm BST

PDB ID	:	7NDT
Title	:	UL40:01 TCR in complex with HLA-E with a non-natural amino acid
Authors	:	Pengelly, R.J.; Robinson, R.A.
Deposited on	:	2021-02-02
Resolution	:	3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

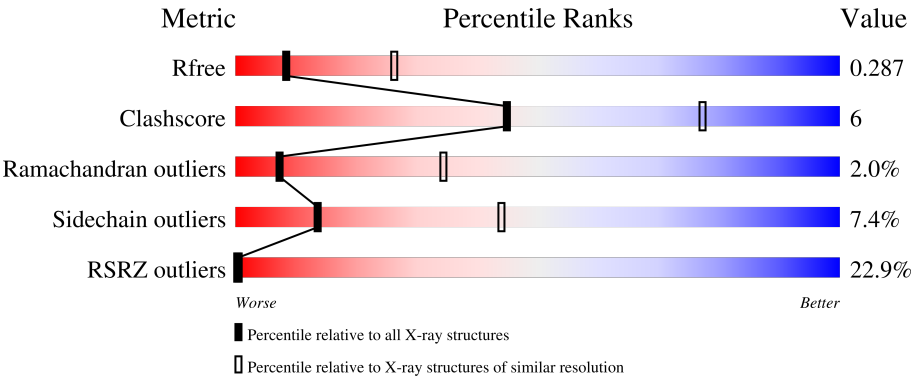
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.00 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.



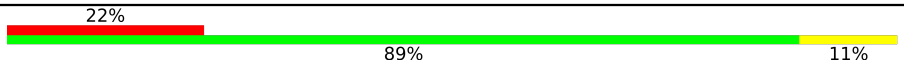
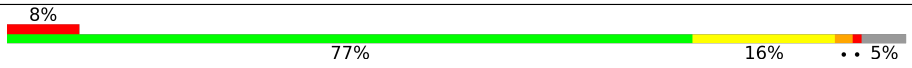
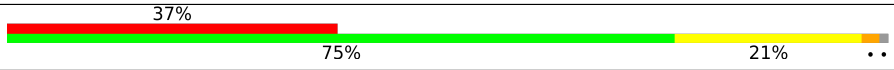
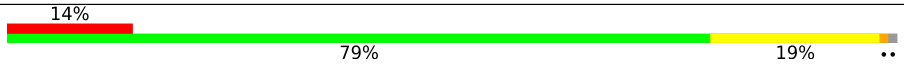
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	23% 81% 16%
1	FFF	277	30% 76% 18%
2	BBB	100	12% 77% 19%
2	GGG	100	13% 79% 17%
3	CCC	9	33% 67% 33%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	HHH	9	
4	DDD	198	
4	III	198	
5	EEE	243	
5	JJJ	243	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13024 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	271	Total	C	N	O	S	0	0	0
			2208	1380	395	425	8			
1	FFF	270	Total	C	N	O	S	0	0	0
			2203	1378	394	423	8			

There are 4 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
FFF	0	MET	-	initiating methionine	UNP P13747
FFF	116	CYS	PHE	conflict	UNP P13747

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	GGG	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a protein called UL40(15-23 H4C).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	CCC	9	Total	C	N	O	S	0	0	0
			71	46	12	11	2			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	HHH	9	Total	C	N	O	S	0	0	0
			71	46	12	11	2			

- Molecule 4 is a protein called T cell receptor alpha variable 26-1,T cell receptor alpha joining 37,T cell receptor alpha chain constant.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	DDD	190	Total	C	N	O	S	0	0	0
			1483	919	256	299	9			
4	III	189	Total	C	N	O	S	0	0	0
			1474	913	255	297	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DDD	0	MET	-	initiating methionine	UNP A0A087WT03
DDD	1	ALA	-	expression tag	UNP A0A087WT03
DDD	9	PRO	THR	engineered mutation	UNP A0A087WT03
DDD	13	VAL	CYS	engineered mutation	UNP A0A087WT03
DDD	107	VAL	-	linker	UNP A0A087WT03
DDD	108	ARG	-	linker	UNP A0A087WT03
DDD	129	ASP	-	linker	UNP A0A087X096
DDD	176	CYS	THR	engineered mutation	UNP P01848
III	0	MET	-	initiating methionine	UNP A0A087WT03
III	1	ALA	-	expression tag	UNP A0A087WT03
III	9	PRO	THR	engineered mutation	UNP A0A087WT03
III	13	VAL	CYS	engineered mutation	UNP A0A087WT03
III	107	VAL	-	linker	UNP A0A087WT03
III	108	ARG	-	linker	UNP A0A087WT03
III	129	ASP	-	linker	UNP A0A087X096
III	176	CYS	THR	engineered mutation	UNP P01848

- Molecule 5 is a protein called T cell receptor beta variable 14,T cell receptor beta joining 2-3,T cell receptor beta constant 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	EEE	240	Total	C	N	O	S	0	0	0
			1924	1212	336	369	7			
5	JJJ	241	Total	C	N	O	S	0	0	0
			1929	1215	337	370	7			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EEE	0	MET	-	initiating methionine	UNP A0A5B0
EEE	109	ASP	-	linker	UNP A0A5B0
EEE	113	ARG	-	linker	UNP A0A5B0
EEE	129	GLU	-	linker	UNP A0A0B4J200
EEE	138	GLU	LYS	engineered mutation	UNP A0A5B9
EEE	185	CYS	SER	engineered mutation	UNP A0A5B9
EEE	203	ALA	CYS	engineered mutation	UNP A0A5B9
JJJ	0	MET	-	initiating methionine	UNP A0A5B0
JJJ	109	ASP	-	linker	UNP A0A5B0
JJJ	113	ARG	-	linker	UNP A0A5B0
JJJ	129	GLU	-	linker	UNP A0A0B4J200
JJJ	138	GLU	LYS	engineered mutation	UNP A0A5B9
JJJ	185	CYS	SER	engineered mutation	UNP A0A5B9
JJJ	203	ALA	CYS	engineered mutation	UNP A0A5B9

- Molecule 6 is water.

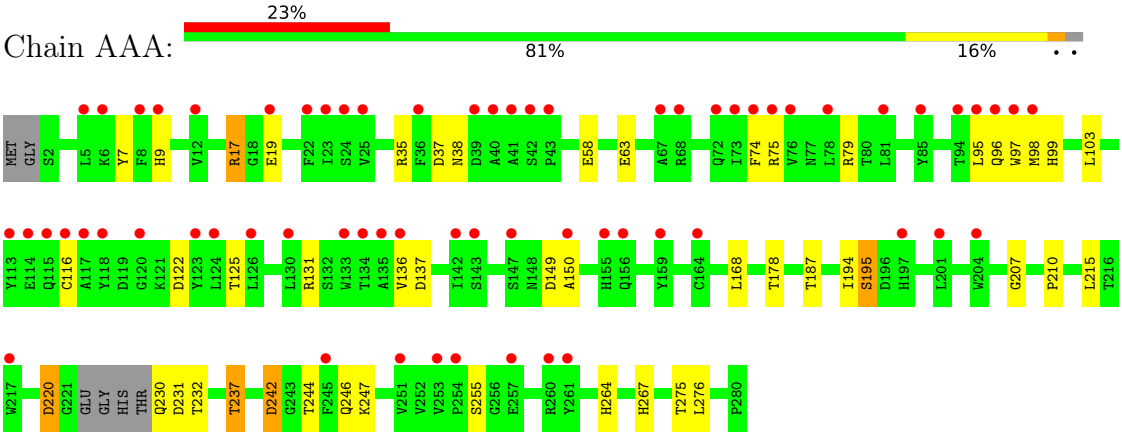
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	EEE	1	Total O 1 1	0	0
6	FFF	1	Total O 1 1	0	0
6	III	1	Total O 1 1	0	0

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.

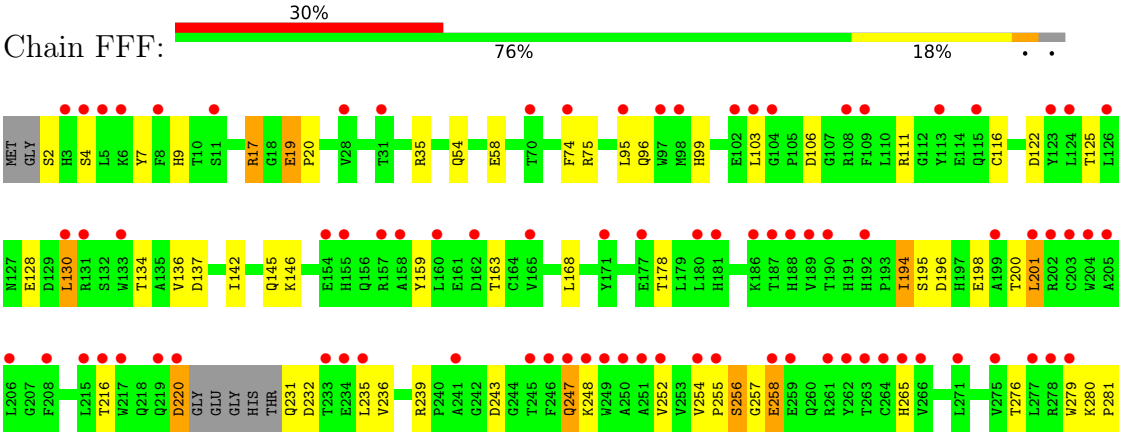
• Molecule 1: HLA class I histocompatibility antigen, alpha chain E

Chain AAA:



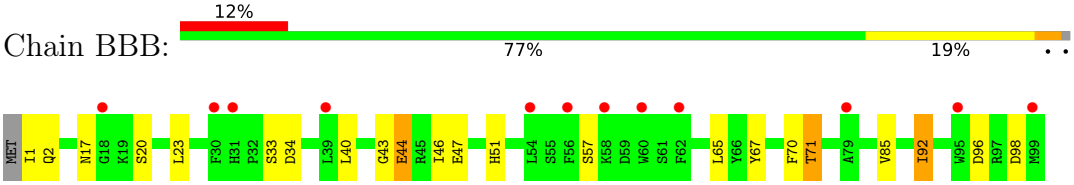
• Molecule 1: HLA class I histocompatibility antigen, alpha chain E

Chain FFF:



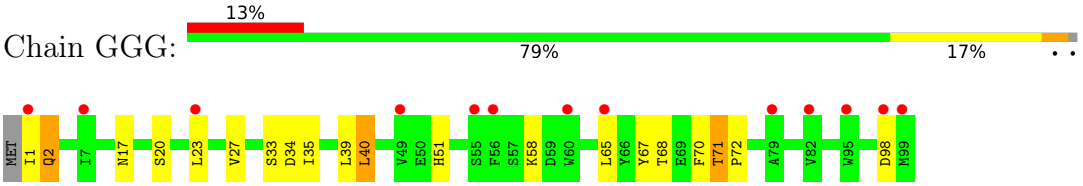
• Molecule 2: Beta-2-microglobulin

Chain BBB:



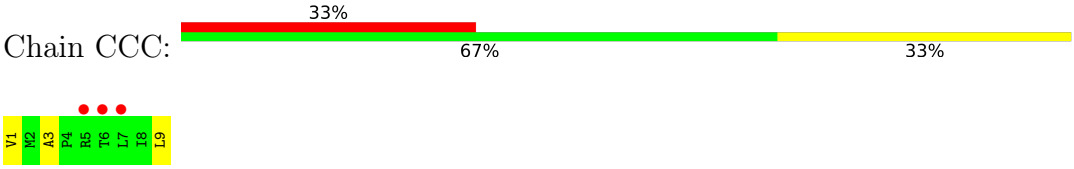
• Molecule 2: Beta-2-microglobulin

Chain GGG:



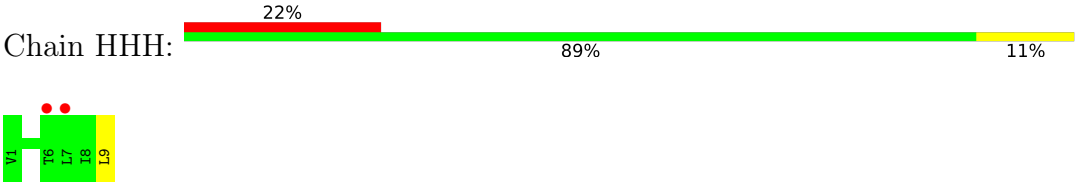
• Molecule 3: UL40(15-23 H4C)

Chain CCC:



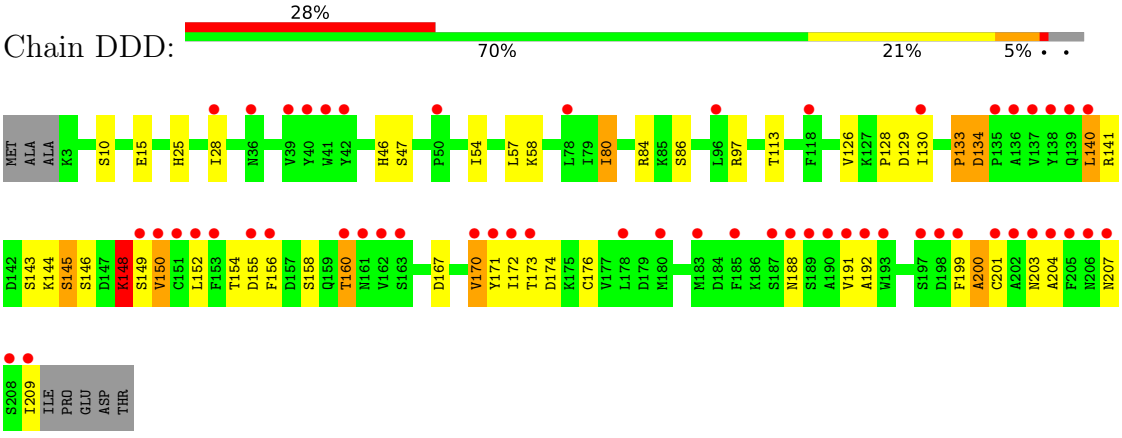
• Molecule 3: UL40(15-23 H4C)

Chain HHH:



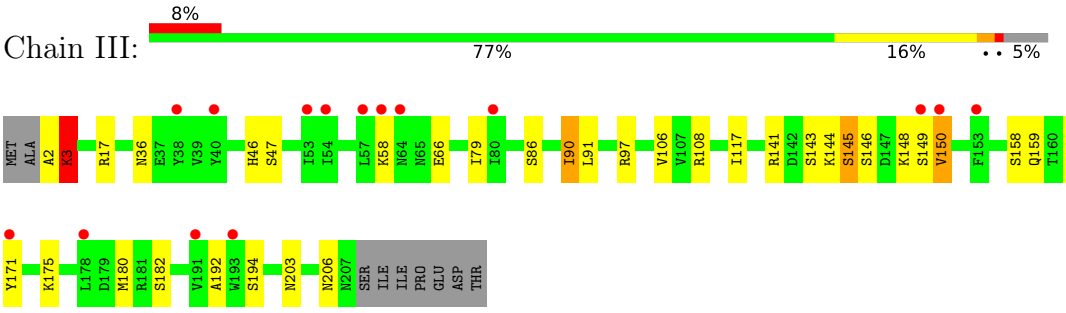
• Molecule 4: T cell receptor alpha variable 26-1,T cell receptor alpha joining 37,T cell receptor alpha chain constant

Chain DDD:



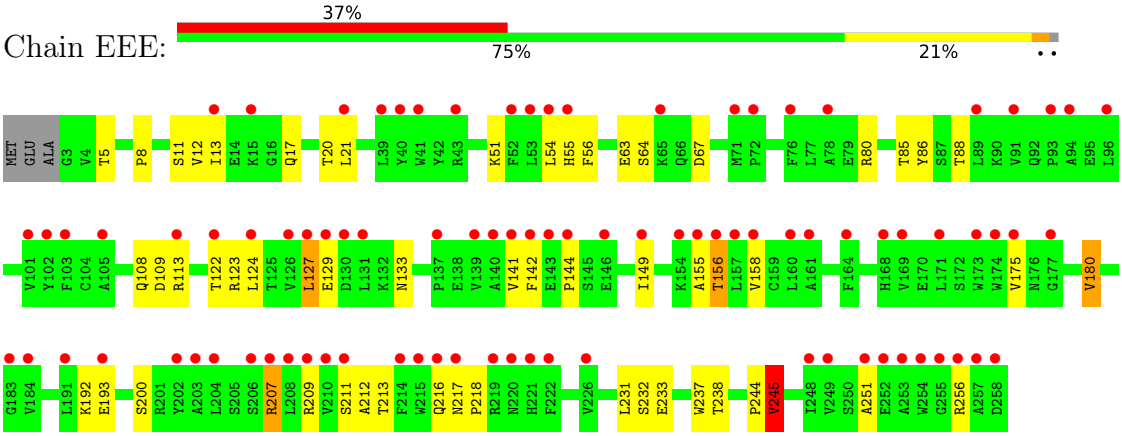
• Molecule 4: T cell receptor alpha variable 26-1,T cell receptor alpha joining 37,T cell receptor alpha chain constant

Chain III:



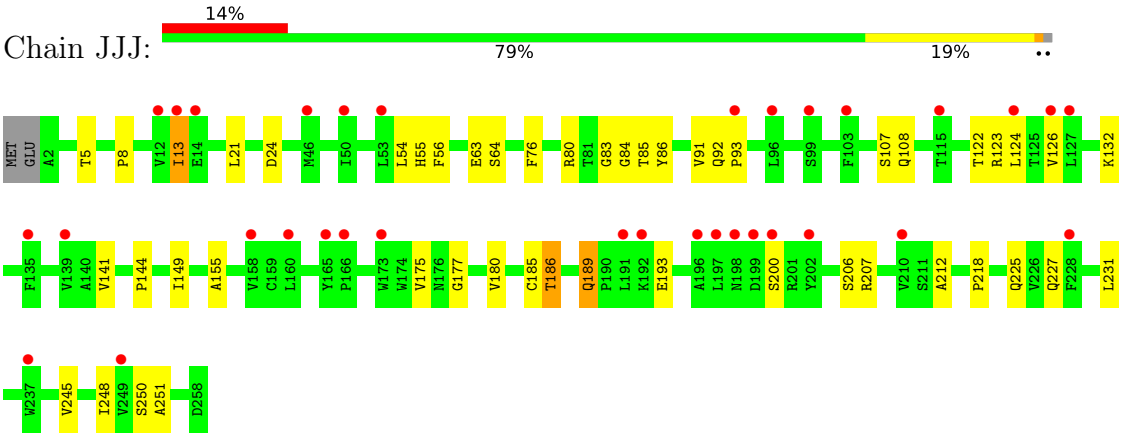
• Molecule 5: T cell receptor beta variable 14,T cell receptor beta joining 2-3,T cell receptor beta constant 2

Chain EEE:



• Molecule 5: T cell receptor beta variable 14,T cell receptor beta joining 2-3,T cell receptor beta constant 2

Chain JJJ:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	117.61Å 76.58Å 130.34Å 90.00° 107.64° 90.00°	Depositor
Resolution (Å)	65.27 – 3.00 65.19 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (65.27-3.00) 99.5 (65.19-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.03 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.221 , 0.269 0.235 , 0.287	Depositor DCC
R_{free} test set	2195 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	110.1	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	13024	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 3.94% 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	0.63	0/2272	0.76	0/3088
1	FFF	0.64	0/2267	0.75	0/3083
2	BBB	0.64	0/852	0.75	0/1152
2	GGG	0.65	0/852	0.73	0/1152
3	CCC	0.59	0/61	0.81	0/82
3	HHH	0.59	0/61	0.78	0/82
4	DDD	0.65	0/1512	0.78	0/2053
4	III	0.64	0/1503	0.79	0/2041
5	EEE	0.63	0/1976	0.76	0/2685
5	JJJ	0.63	0/1981	0.74	0/2692
All	All	0.63	0/13337	0.76	0/18110

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	AAA	2208	0	2053	29	0
1	FFF	2203	0	2050	25	0
2	BBB	829	0	794	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	GGG	829	0	794	9	0
3	CCC	71	0	74	2	0
3	HHH	71	0	74	0	0
4	DDD	1483	0	1428	33	0
4	III	1474	0	1417	13	0
5	EEE	1924	0	1830	35	0
5	JJJ	1929	0	1835	25	0
6	EEE	1	0	0	0	0
6	FFF	1	0	0	1	0
6	III	1	0	0	0	0
All	All	13024	0	12349	165	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.

The worst 5 of 165 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:AAA:242:ASP:OD1	1:AAA:244:THR:HG22	1.77	0.82
5:JJJ:83:GLY:O	5:JJJ:85:THR:N	2.17	0.78
1:AAA:187:THR:HB	1:AAA:276:LEU:HD11	1.65	0.76
4:III:3:LYS:HD2	4:III:106:VAL:HG21	1.69	0.74
1:AAA:79:ARG:NH1	5:EEE:63:GLU:OE2	2.23	0.70

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	267/277 (96%)	247 (92%)	16 (6%)	4 (2%)	10 42
1	FFF	266/277 (96%)	243 (91%)	14 (5%)	9 (3%)	3 20

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	BBB	97/100 (97%)	89 (92%)	4 (4%)	4 (4%)	3 16
2	GGG	97/100 (97%)	90 (93%)	5 (5%)	2 (2%)	7 33
3	CCC	7/9 (78%)	7 (100%)	0	0	100 100
3	HHH	7/9 (78%)	7 (100%)	0	0	100 100
4	DDD	188/198 (95%)	160 (85%)	20 (11%)	8 (4%)	2 15
4	III	187/198 (94%)	161 (86%)	23 (12%)	3 (2%)	9 40
5	EEE	238/243 (98%)	209 (88%)	28 (12%)	1 (0%)	34 72
5	JJJ	239/243 (98%)	215 (90%)	23 (10%)	1 (0%)	34 72
All	All	1593/1654 (96%)	1428 (90%)	133 (8%)	32 (2%)	7 34

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	195	SER
2	BBB	44	GLU
5	EEE	245	VAL
1	FFF	195	SER
1	FFF	256	SER

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	AAA	234/238 (98%)	221 (94%)	13 (6%)	21 56
1	FFF	234/238 (98%)	213 (91%)	21 (9%)	9 35
2	BBB	94/95 (99%)	85 (90%)	9 (10%)	8 32
2	GGG	94/95 (99%)	88 (94%)	6 (6%)	17 51
3	CCC	7/7 (100%)	7 (100%)	0	100 100
3	HHH	7/7 (100%)	7 (100%)	0	100 100
4	DDD	171/177 (97%)	155 (91%)	16 (9%)	8 32
4	III	169/177 (96%)	152 (90%)	17 (10%)	7 29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	EEE	211/213 (99%)	196 (93%)	15 (7%)	14 46
5	JJJ	211/213 (99%)	202 (96%)	9 (4%)	29 66
All	All	1432/1460 (98%)	1326 (93%)	106 (7%)	13 44

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	FFF	35	ARG
1	FFF	247	GLN
5	JJJ	123	ARG
1	FFF	58	GLU
1	FFF	200	THR

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)

2 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	QM8	CCC	9	3,1	8,9,9	0.87	1 (12%)	9,10,10	1.28	1 (11%)
3	QM8	HHH	9	3,1	8,9,9	0.87	1 (12%)	9,10,10	1.63	3 (33%)

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	3,1	-	2/9/9/9	-
3	QM8	HHH	9	3,1	-	2/9/9/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	CCC	9	QM8	OXT-C	-2.17	1.23	1.30
3	HHH	9	QM8	OXT-C	-2.11	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	HHH	9	QM8	OXT-C-O	-2.57	118.26	124.09
3	HHH	9	QM8	CB-CA-N	-2.37	103.95	110.17
3	HHH	9	QM8	OXT-C-CA	2.29	121.17	113.38
3	CCC	9	QM8	CD-CE-SZ	-2.24	105.76	112.96

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

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	271/277 (97%)	1.20	65 (23%)	0	0	40, 56, 88, 101	0
1	FFF	270/277 (97%)	1.53	83 (30%)	0	0	57, 81, 124, 140	0
2	BBB	99/100 (99%)	0.81	12 (12%)	4	1	45, 61, 83, 94	0
2	GGG	99/100 (99%)	0.92	13 (13%)	3	1	58, 73, 91, 96	0
3	CCC	8/9 (88%)	2.15	3 (37%)	0	0	51, 54, 61, 62	0
3	HHH	8/9 (88%)	1.38	2 (25%)	0	0	59, 61, 67, 67	0
4	DDD	190/198 (95%)	1.83	55 (28%)	0	0	53, 80, 123, 140	0
4	III	189/198 (95%)	0.79	15 (7%)	12	4	49, 60, 86, 93	0
5	EEE	240/243 (98%)	1.75	89 (37%)	0	0	51, 94, 129, 153	0
5	JJJ	241/243 (99%)	1.09	33 (13%)	3	1	51, 61, 88, 111	0
All	All	1615/1654 (97%)	1.31	370 (22%)	0	0	40, 69, 115, 153	0

The worst 5 of 370 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	DDD	209	ILE	14.1
4	DDD	205	PHE	10.0
1	FFF	201	LEU	8.5
1	FFF	215	LEU	8.5
4	DDD	140	LEU	8.4

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, 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	0.88	0.49	64,68,69,72	0
3	QM8	HHH	9	10/10	0.92	0.55	68,72,75,76	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.