wwPDB X-ray Structure Validation Summary Report (i)

Dec 15, 2022 – 03:28 pm GMT

PDB ID	:	6YMQ
Title	:	TREM2 extracellular domain (19-131) in complex with single-chain variable 4 (scFv-4)
Authors	:	Szykowska, A.; Preger, C.; Scacioc, A.; Mukhopadhyay, S.M.M.; McKinley, G.; Graslund, S.; Wigren, E.; Persson, H.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.; Bountra, C.; Di Daniel, E.; Davis, J.B.; Burgess-Brown, N.; Bullock, A.
Deposited on	:	2020-04-09
Resolution	:	3.07 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 (i)) were used in the production of this report:

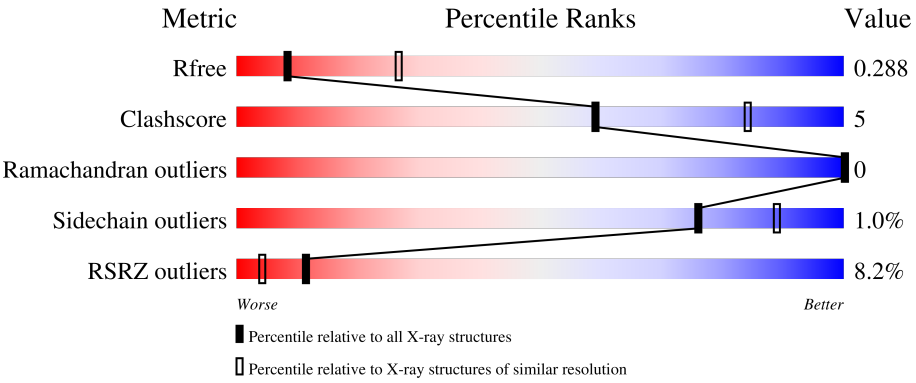
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

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 3.07 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	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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	A	245	3% 79% 14% 7%
1	B	245	3% 81% 12% 7%
1	C	245	3% 82% 11% 7%
1	D	245	5% 78% 16% 7%

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Mol	Chain	Length	Quality of chain
1	E	245	16% 84% 10% 6%
1	F	245	13% 80% 13% 7%
2	D000	125	21% 90% 10%
2	G	125	4% 79% 12% 9%
2	H	125	2% 80% 10% 10%
2	I	125	% 78% 12% 10%
2	J	125	2% 86% 10%
2	K	125	18% 69% 19% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MPD	J	202	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15730 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 Single-chain variable 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1745	1103	288	346	8			
1	B	228	Total	C	N	O	S	0	0	0
			1746	1106	288	344	8			
1	C	228	Total	C	N	O	S	0	0	0
			1744	1100	289	347	8			
1	D	229	Total	C	N	O	S	0	0	0
			1742	1102	289	343	8			
1	E	230	Total	C	N	O	S	0	0	0
			1709	1082	284	336	7			
1	F	229	Total	C	N	O	S	0	0	0
			1727	1086	286	347	8			

- Molecule 2 is a protein called Triggering receptor expressed on myeloid cells 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	114	Total	C	N	O	S	0	0	0
			887	552	166	164	5			
2	H	112	Total	C	N	O	S	0	0	0
			878	547	164	162	5			
2	I	113	Total	C	N	O	S	0	0	0
			883	550	165	163	5			
2	J	112	Total	C	N	O	S	0	0	0
			863	539	159	160	5			
2	K	112	Total	C	N	O	S	0	0	0
			841	525	157	154	5			
2	D000	112	Total	C	N	O	S	0	0	0
			860	537	157	161	5			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	16	GLU	-	expression tag	UNP Q9NZC2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	17	THR	-	expression tag	UNP Q9NZC2
G	18	GLY	-	expression tag	UNP Q9NZC2
G	132	GLY	-	expression tag	UNP Q9NZC2
G	133	THR	-	expression tag	UNP Q9NZC2
G	134	LYS	-	expression tag	UNP Q9NZC2
G	135	HIS	-	expression tag	UNP Q9NZC2
G	136	HIS	-	expression tag	UNP Q9NZC2
G	137	HIS	-	expression tag	UNP Q9NZC2
G	138	HIS	-	expression tag	UNP Q9NZC2
G	139	HIS	-	expression tag	UNP Q9NZC2
G	140	HIS	-	expression tag	UNP Q9NZC2
H	16	GLU	-	expression tag	UNP Q9NZC2
H	17	THR	-	expression tag	UNP Q9NZC2
H	18	GLY	-	expression tag	UNP Q9NZC2
H	132	GLY	-	expression tag	UNP Q9NZC2
H	133	THR	-	expression tag	UNP Q9NZC2
H	134	LYS	-	expression tag	UNP Q9NZC2
H	135	HIS	-	expression tag	UNP Q9NZC2
H	136	HIS	-	expression tag	UNP Q9NZC2
H	137	HIS	-	expression tag	UNP Q9NZC2
H	138	HIS	-	expression tag	UNP Q9NZC2
H	139	HIS	-	expression tag	UNP Q9NZC2
H	140	HIS	-	expression tag	UNP Q9NZC2
I	16	GLU	-	expression tag	UNP Q9NZC2
I	17	THR	-	expression tag	UNP Q9NZC2
I	18	GLY	-	expression tag	UNP Q9NZC2
I	132	GLY	-	expression tag	UNP Q9NZC2
I	133	THR	-	expression tag	UNP Q9NZC2
I	134	LYS	-	expression tag	UNP Q9NZC2
I	135	HIS	-	expression tag	UNP Q9NZC2
I	136	HIS	-	expression tag	UNP Q9NZC2
I	137	HIS	-	expression tag	UNP Q9NZC2
I	138	HIS	-	expression tag	UNP Q9NZC2
I	139	HIS	-	expression tag	UNP Q9NZC2
I	140	HIS	-	expression tag	UNP Q9NZC2
J	16	GLU	-	expression tag	UNP Q9NZC2
J	17	THR	-	expression tag	UNP Q9NZC2
J	18	GLY	-	expression tag	UNP Q9NZC2
J	132	GLY	-	expression tag	UNP Q9NZC2
J	133	THR	-	expression tag	UNP Q9NZC2
J	134	LYS	-	expression tag	UNP Q9NZC2
J	135	HIS	-	expression tag	UNP Q9NZC2

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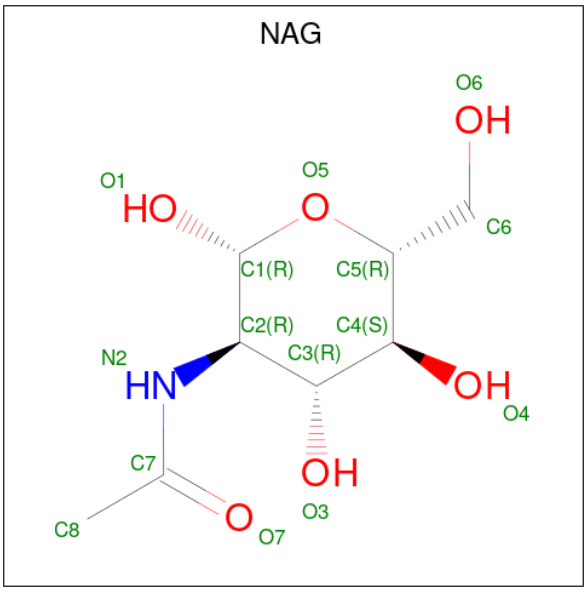
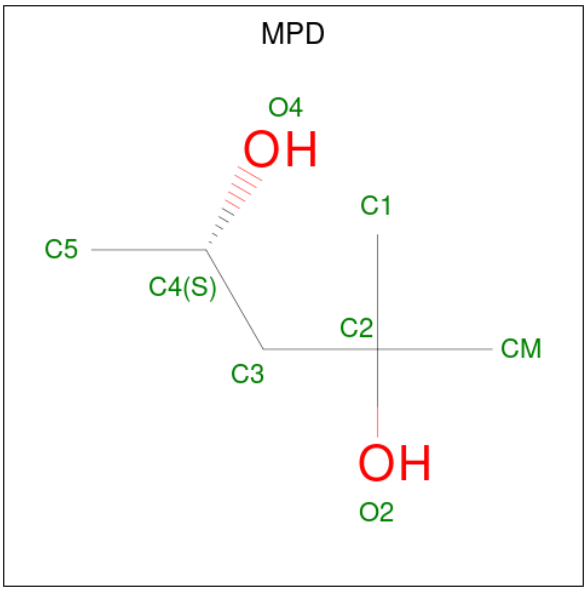
Chain	Residue	Modelled	Actual	Comment	Reference
J	136	HIS	-	expression tag	UNP Q9NZC2
J	137	HIS	-	expression tag	UNP Q9NZC2
J	138	HIS	-	expression tag	UNP Q9NZC2
J	139	HIS	-	expression tag	UNP Q9NZC2
J	140	HIS	-	expression tag	UNP Q9NZC2
K	16	GLU	-	expression tag	UNP Q9NZC2
K	17	THR	-	expression tag	UNP Q9NZC2
K	18	GLY	-	expression tag	UNP Q9NZC2
K	132	GLY	-	expression tag	UNP Q9NZC2
K	133	THR	-	expression tag	UNP Q9NZC2
K	134	LYS	-	expression tag	UNP Q9NZC2
K	135	HIS	-	expression tag	UNP Q9NZC2
K	136	HIS	-	expression tag	UNP Q9NZC2
K	137	HIS	-	expression tag	UNP Q9NZC2
K	138	HIS	-	expression tag	UNP Q9NZC2
K	139	HIS	-	expression tag	UNP Q9NZC2
K	140	HIS	-	expression tag	UNP Q9NZC2
D000	16	GLU	-	expression tag	UNP Q9NZC2
D000	17	THR	-	expression tag	UNP Q9NZC2
D000	18	GLY	-	expression tag	UNP Q9NZC2
D000	132	GLY	-	expression tag	UNP Q9NZC2
D000	133	THR	-	expression tag	UNP Q9NZC2
D000	134	LYS	-	expression tag	UNP Q9NZC2
D000	135	HIS	-	expression tag	UNP Q9NZC2
D000	136	HIS	-	expression tag	UNP Q9NZC2
D000	137	HIS	-	expression tag	UNP Q9NZC2
D000	138	HIS	-	expression tag	UNP Q9NZC2
D000	139	HIS	-	expression tag	UNP Q9NZC2
D000	140	HIS	-	expression tag	UNP Q9NZC2

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total C N O 14 8 1 5	0	0
3	H	1	Total C N O 14 8 1 5	0	0
3	I	1	Total C N O 14 8 1 5	0	0
3	J	1	Total C N O 14 8 1 5	0	0
3	K	1	Total C N O 14 8 1 5	0	0
3	D000	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	J	1	Total C O 8 6 2	0	0

- Molecule 5 is water.

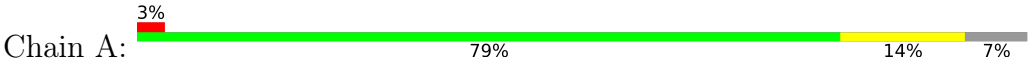
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total O 4 4	0	0
5	D	4	Total O 4 4	0	0
5	G	1	Total O 1 1	0	0
5	H	1	Total O 1 1	0	0
5	I	1	Total O 1 1	0	0
5	J	2	Total O 2 2	0	0

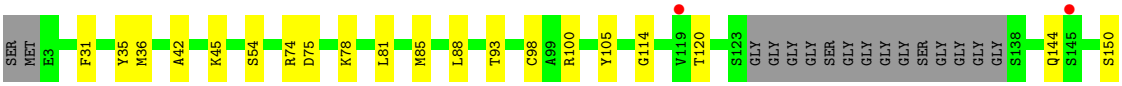
3 Residue-property plots

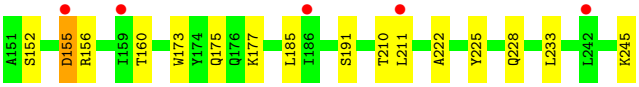
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Single-chain variable 4

Chain A:

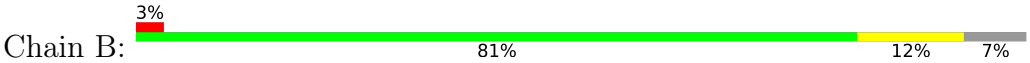


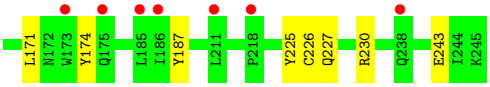




• Molecule 1: Single-chain variable 4

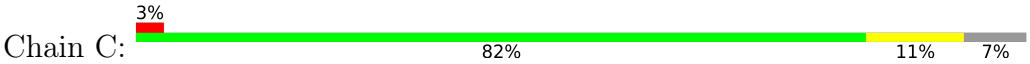
Chain B:

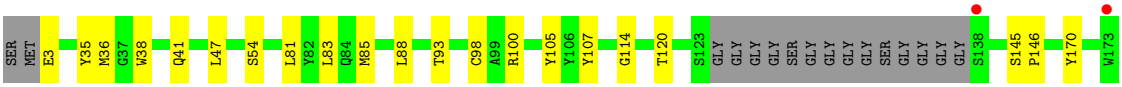


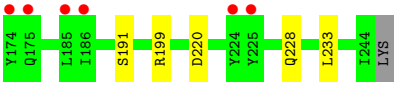


• Molecule 1: Single-chain variable 4

Chain C:

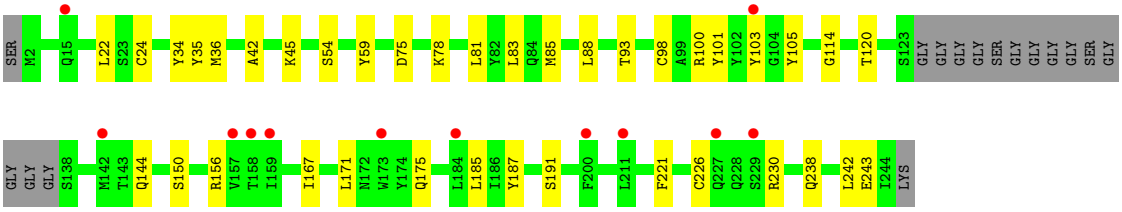






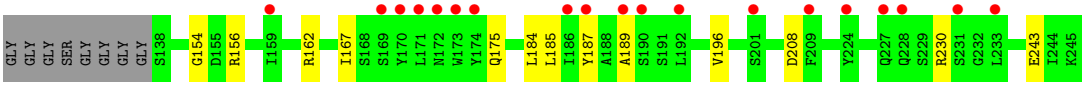
• Molecule 1: Single-chain variable 4

Chain D:



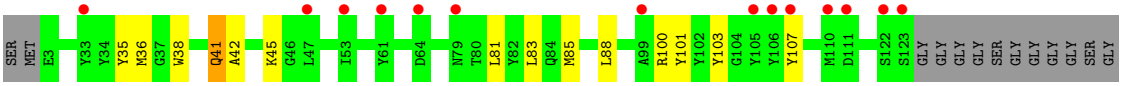
• Molecule 1: Single-chain variable 4

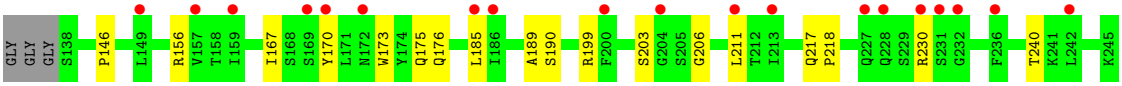
Chain E:



• Molecule 1: Single-chain variable 4

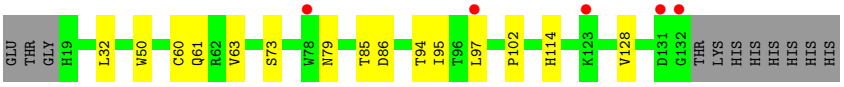
Chain F:





• Molecule 2: Triggering receptor expressed on myeloid cells 2

Chain G:

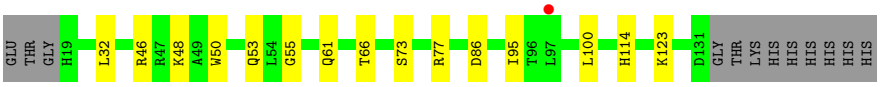


• Molecule 2: Triggering receptor expressed on myeloid cells 2

Chain H:

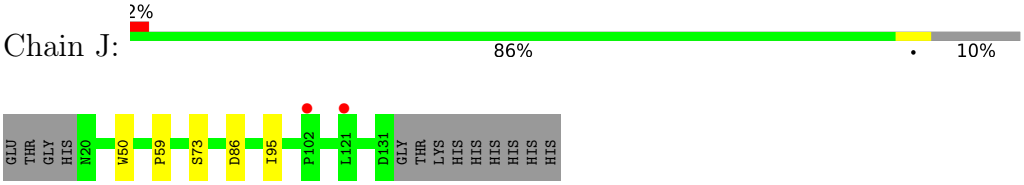
• Molecule 2: Triggering receptor expressed on myeloid cells 2

Chain I:



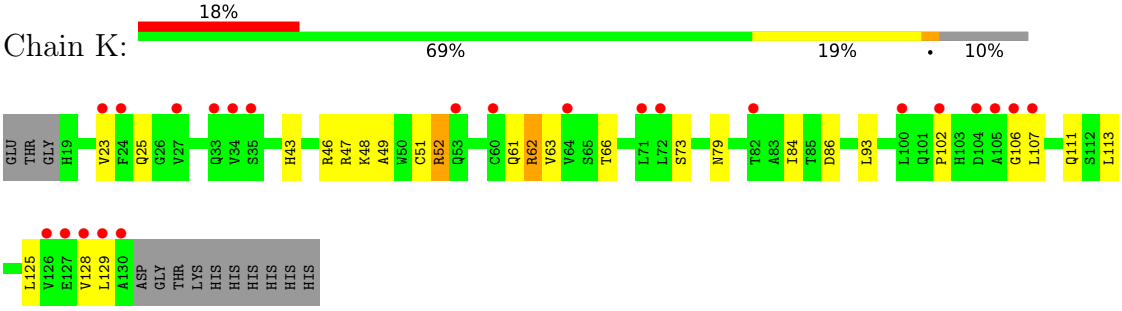
• Molecule 2: Triggering receptor expressed on myeloid cells 2

Chain J:



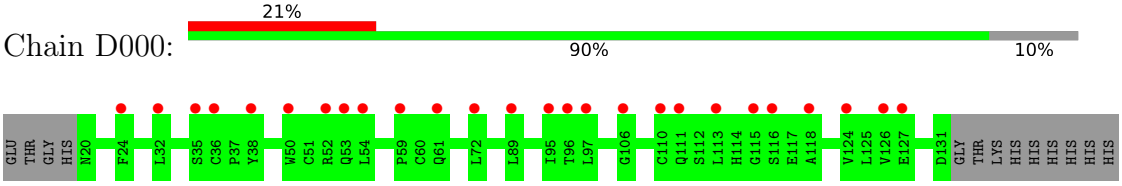
• Molecule 2: Triggering receptor expressed on myeloid cells 2

Chain K:



• Molecule 2: Triggering receptor expressed on myeloid cells 2

Chain D000:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	167.51Å 180.77Å 125.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.99 – 3.07 125.51 – 3.07	Depositor EDS
% Data completeness (in resolution range)	99.8 (75.99-3.07) 89.3 (125.51-3.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.274 , 0.288 0.274 , 0.288	Depositor DCC
R_{free} test set	3515 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	59.2	Xtriage
Anisotropy	0.641	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 26.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	15730	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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: MPD, NAG

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	0.25	0/1789	0.44	0/2428
1	B	0.25	0/1789	0.44	0/2427
1	C	0.25	0/1788	0.45	0/2427
1	D	0.25	0/1786	0.44	0/2424
1	E	0.25	0/1753	0.44	0/2384
1	F	0.25	0/1770	0.45	0/2404
2	D000	0.23	0/878	0.43	0/1195
2	G	0.22	0/904	0.42	0/1225
2	H	0.23	0/896	0.42	0/1216
2	I	0.23	0/901	0.41	0/1223
2	J	0.23	0/881	0.42	0/1199
2	K	0.23	0/859	0.43	0/1170
All	All	0.24	0/15994	0.43	0/21722

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	A	1745	0	1618	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1746	0	1635	16	0
1	C	1744	0	1617	13	0
1	D	1742	0	1624	24	0
1	E	1709	0	1552	16	0
1	F	1727	0	1589	18	0
2	D000	860	0	0	0	0
2	G	887	0	868	9	0
2	H	878	0	863	7	0
2	I	883	0	866	9	0
2	J	863	0	832	3	0
2	K	841	0	782	15	0
3	D000	14	0	0	0	0
3	G	14	0	13	0	0
3	H	14	0	13	0	0
3	I	14	0	13	1	0
3	J	14	0	13	0	0
3	K	14	0	13	0	0
4	J	8	0	14	0	0
5	A	4	0	0	0	0
5	D	4	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	2	0	0	0	0
All	All	15730	0	13925	137	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 5.

The worst 5 of 137 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:D:156:ARG:HH22	1:F:189:ALA:HB3	1.54	0.71
1:E:184:LEU:HD21	1:E:187:TYR:HB3	1.77	0.66
2:I:73:SER:HB3	2:I:86:ASP:HB3	1.80	0.64
1:E:109:HIS:CG	1:E:187:TYR:HB2	2.33	0.64
1:D:144:GLN:O	1:D:238:GLN:NE2	2.32	0.63

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	225/245 (92%)	208 (92%)	17 (8%)	0	100	100
1	B	224/245 (91%)	206 (92%)	18 (8%)	0	100	100
1	C	224/245 (91%)	201 (90%)	23 (10%)	0	100	100
1	D	225/245 (92%)	206 (92%)	19 (8%)	0	100	100
1	E	226/245 (92%)	210 (93%)	16 (7%)	0	100	100
1	F	225/245 (92%)	205 (91%)	20 (9%)	0	100	100
2	D000	110/125 (88%)	102 (93%)	8 (7%)	0	100	100
2	G	111/125 (89%)	107 (96%)	4 (4%)	0	100	100
2	H	110/125 (88%)	105 (96%)	5 (4%)	0	100	100
2	I	111/125 (89%)	105 (95%)	6 (5%)	0	100	100
2	J	110/125 (88%)	104 (94%)	6 (6%)	0	100	100
2	K	110/125 (88%)	103 (94%)	7 (6%)	0	100	100
All	All	2011/2220 (91%)	1862 (93%)	149 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	183/196 (93%)	181 (99%)	2 (1%)	73	88
1	B	182/196 (93%)	180 (99%)	2 (1%)	73	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	183/196 (93%)	181 (99%)	2 (1%)	73 88
1	D	182/196 (93%)	181 (100%)	1 (0%)	88 94
1	E	171/196 (87%)	168 (98%)	3 (2%)	59 80
1	F	181/196 (92%)	179 (99%)	2 (1%)	73 88
2	D000	92/107 (86%)	92 (100%)	0	100 100
2	G	96/107 (90%)	96 (100%)	0	100 100
2	H	96/107 (90%)	95 (99%)	1 (1%)	76 89
2	I	96/107 (90%)	96 (100%)	0	100 100
2	J	92/107 (86%)	92 (100%)	0	100 100
2	K	84/107 (78%)	81 (96%)	3 (4%)	35 66
All	All	1638/1818 (90%)	1622 (99%)	16 (1%)	76 89

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	41	GLN
1	E	100	ARG
2	K	52	ARG
1	E	93	THR
2	H	20	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	238	GLN
1	E	238	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

7 ligands 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	NAG	H	201	2	14,14,15	0.27	0	17,19,21	0.44	0
4	MPD	J	202	-	7,7,7	0.26	0	9,10,10	0.22	0
3	NAG	I	201	-	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	J	201	2	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	D000	201	2	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	G	201	-	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	K	201	2	14,14,15	0.29	0	17,19,21	0.46	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	NAG	H	201	2	-	2/6/23/26	0/1/1/1
4	MPD	J	202	-	-	1/5/5/5	-
3	NAG	I	201	-	-	2/6/23/26	0/1/1/1
3	NAG	J	201	2	-	2/6/23/26	0/1/1/1
3	NAG	D000	201	2	-	2/6/23/26	0/1/1/1
3	NAG	G	201	-	-	2/6/23/26	0/1/1/1
3	NAG	K	201	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	201	NAG	C4-C5-C6-O6
3	K	201	NAG	O5-C5-C6-O6
3	J	201	NAG	O5-C5-C6-O6
3	K	201	NAG	C4-C5-C6-O6
3	I	201	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	201	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	131:ASP	C	132:GLY	N	3.13

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	A	229/245 (93%)	0.46	7 (3%) 49 25	55, 75, 104, 116	0
1	B	228/245 (93%)	0.53	8 (3%) 44 22	54, 79, 121, 133	0
1	C	228/245 (93%)	0.47	8 (3%) 44 22	55, 85, 135, 145	0
1	D	229/245 (93%)	0.59	12 (5%) 27 12	58, 80, 110, 122	0
1	E	230/245 (93%)	0.89	40 (17%) 1 0	68, 113, 138, 145	0
1	F	229/245 (93%)	0.88	33 (14%) 2 1	72, 113, 132, 139	0
2	D000	112/125 (89%)	1.31	26 (23%) 0 0	103, 116, 124, 132	0
2	G	114/125 (91%)	0.45	5 (4%) 34 17	53, 61, 73, 85	0
2	H	112/125 (89%)	0.53	3 (2%) 54 29	55, 65, 80, 89	0
2	I	113/125 (90%)	0.41	1 (0%) 84 68	53, 64, 81, 97	0
2	J	112/125 (89%)	0.35	2 (1%) 68 46	52, 61, 79, 92	0
2	K	112/125 (89%)	1.04	23 (20%) 1 0	107, 122, 131, 142	0
All	All	2048/2220 (92%)	0.65	168 (8%) 11 4	52, 84, 130, 145	0

The worst 5 of 168 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D000	52	ARG	5.8
2	D000	54	LEU	5.6
2	K	107	LEU	5.5
2	D000	24	PHE	5.4
1	F	170	TYR	5.1

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (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	NAG	K	201	14/15	0.67	0.32	116,122,128,129	0
3	NAG	D000	201	14/15	0.71	0.35	117,120,122,123	0
4	MPD	J	202	8/8	0.71	0.49	69,69,69,69	0
3	NAG	I	201	14/15	0.75	0.25	71,74,78,78	0
3	NAG	J	201	14/15	0.81	0.23	71,74,76,77	0
3	NAG	G	201	14/15	0.81	0.20	78,81,82,83	0
3	NAG	H	201	14/15	0.86	0.19	78,79,83,84	0

6.5 Other polymers (i)

There are no such residues in this entry.