



wwPDB/EMDatabank EM Map/Model Validation Summary Report

Feb 20, 2018 – 04:30 am GMT


PDB ID : 5UP2
EMDB ID: : EMD-8581
Title : Triheteromeric NMDA receptor GluN1/GluN2A/GluN2B in complex with glycine, glutamate, Ro 25-6981, MK-801 and a GluN2B-specific Fab, at pH 6.5
Authors : Lu, W.; Du, J.; Goehring, A.; Gouaux, E.
Deposited on : 2017-02-01
Resolution : 6.00 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the  symbol.

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

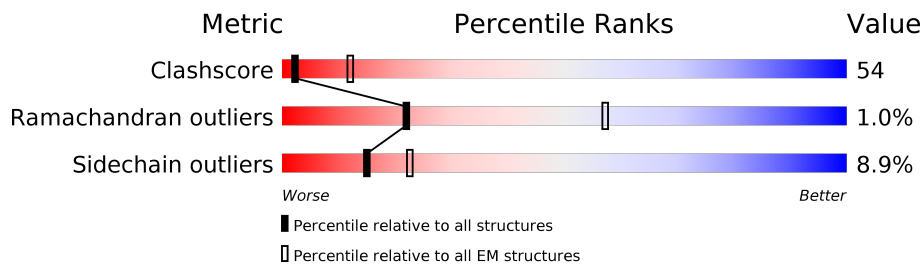
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.00 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)	EM structures (#Entries)
Clashscore	136279	1886
Ramachandran outliers	132675	1663
Sidechain outliers	132484	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	836	50% 41% 5%
1	C	836	58% 33% 5%
2	B	831	45% 45% 6%
3	D	837	61% 30% 5%
4	F	216	90% 9%
4	G	216	91% 8%

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 24161 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 N-methyl-D-aspartate receptor subunit NR1-8a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	796	Total	C	N	O	S	0	0
			5745	3691	978	1047	29		
1	C	798	Total	C	N	O	S	0	0
			5442	3460	938	1018	26		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ALA	CYS	conflict	UNP C0KD18
A	300	GLN	ASN	conflict	UNP C0KD18
A	350	GLN	ASN	conflict	UNP C0KD18
A	368	ASP	ASN	conflict	UNP C0KD18
A	440	ASP	ASN	conflict	UNP C0KD18
A	469	ASP	ASN	conflict	UNP C0KD18
A	493	ALA	LYS	conflict	UNP C0KD18
A	494	ALA	LYS	conflict	UNP C0KD18
A	495	ALA	GLU	conflict	UNP C0KD18
A	592	ALA	GLU	conflict	UNP C0KD18
A	593	ALA	GLU	conflict	UNP C0KD18
A	594	ALA	GLU	conflict	UNP C0KD18
A	610	ARG	GLY	conflict	UNP C0KD18
A	617	LEU	ILE	conflict	UNP C0KD18
A	636	LEU	GLY	conflict	UNP C0KD18
A	656	ARG	ASP	conflict	UNP C0KD18
A	741	ASP	LYS	conflict	UNP C0KD18
A	769	GLU	ASN	conflict	UNP C0KD18
A	816	TYR	MET	conflict	UNP C0KD18
C	22	ALA	CYS	conflict	UNP C0KD18
C	300	GLN	ASN	conflict	UNP C0KD18
C	350	GLN	ASN	conflict	UNP C0KD18
C	368	ASP	ASN	conflict	UNP C0KD18
C	440	ASP	ASN	conflict	UNP C0KD18
C	469	ASP	ASN	conflict	UNP C0KD18
C	493	ALA	LYS	conflict	UNP C0KD18

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Chain	Residue	Modelled	Actual	Comment	Reference
C	494	ALA	LYS	conflict	UNP C0KD18
C	495	ALA	GLU	conflict	UNP C0KD18
C	592	ALA	GLU	conflict	UNP C0KD18
C	593	ALA	GLU	conflict	UNP C0KD18
C	594	ALA	GLU	conflict	UNP C0KD18
C	610	ARG	GLY	conflict	UNP C0KD18
C	617	LEU	ILE	conflict	UNP C0KD18
C	636	LEU	GLY	conflict	UNP C0KD18
C	656	ARG	ASP	conflict	UNP C0KD18
C	741	ASP	LYS	conflict	UNP C0KD18
C	769	GLU	ASN	conflict	UNP C0KD18
C	816	TYR	MET	conflict	UNP C0KD18

- Molecule 2 is a protein called N-methyl-D-aspartate receptor subunit NR2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	795	5573	3592	931	1019	31	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	67	GLN	ASN	conflict	UNP B7ZSK1
B	372	ALA	ASN	conflict	UNP B7ZSK1
B	?	-	THR	deletion	UNP B7ZSK1
B	?	-	ALA	deletion	UNP B7ZSK1
B	?	-	SER	deletion	UNP B7ZSK1
B	?	-	LEU	deletion	UNP B7ZSK1
B	431	ALA	ASN	conflict	UNP B7ZSK1
B	529	ALA	ASN	conflict	UNP B7ZSK1
B	605	LEU	VAL	conflict	UNP B7ZSK1
B	644	ARG	GLU	conflict	UNP B7ZSK1
B	645	ARG	GLU	conflict	UNP B7ZSK1
B	675	GLN	ASN	conflict	UNP B7ZSK1
B	831	LYS	-	expression tag	UNP B7ZSK1

- Molecule 3 is a protein called Ionotropic glutamate receptor subunit NR2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	794	5130	3283	865	957	25	0	0

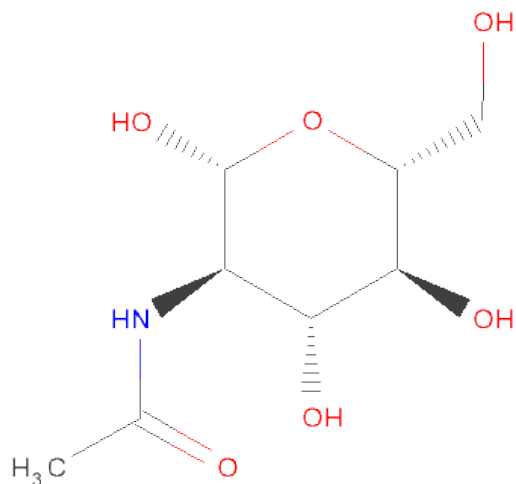
There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	20	SER	MET	conflict	UNP A7XY94
D	21	ARG	GLY	conflict	UNP A7XY94
D	22	ALA	CYS	conflict	UNP A7XY94
D	64	GLU	ALA	conflict	UNP A7XY94
D	69	GLN	ASN	conflict	UNP A7XY94
D	343	ASP	ASN	conflict	UNP A7XY94
D	?	-	LYS	deletion	UNP A7XY94
D	?	-	TYR	deletion	UNP A7XY94
D	?	-	TYR	deletion	UNP A7XY94
D	?	-	VAL	deletion	UNP A7XY94
D	486	VAL	THR	conflict	UNP A7XY94
D	581	ALA	CYS	conflict	UNP A7XY94
D	611	LEU	VAL	conflict	UNP A7XY94
D	650	ARG	GLU	conflict	UNP A7XY94
D	651	ARG	GLU	conflict	UNP A7XY94
D	836	TYR	PHE	conflict	UNP A7XY94
D	837	LYS	-	expression tag	UNP A7XY94

- Molecule 4 is a protein called GluN2B-specific Fab, termed 11D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	214	Total	C	N	O	0	0
			1070	642	214	214		
4	G	215	Total	C	N	O	0	0
			1075	645	215	215		

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).

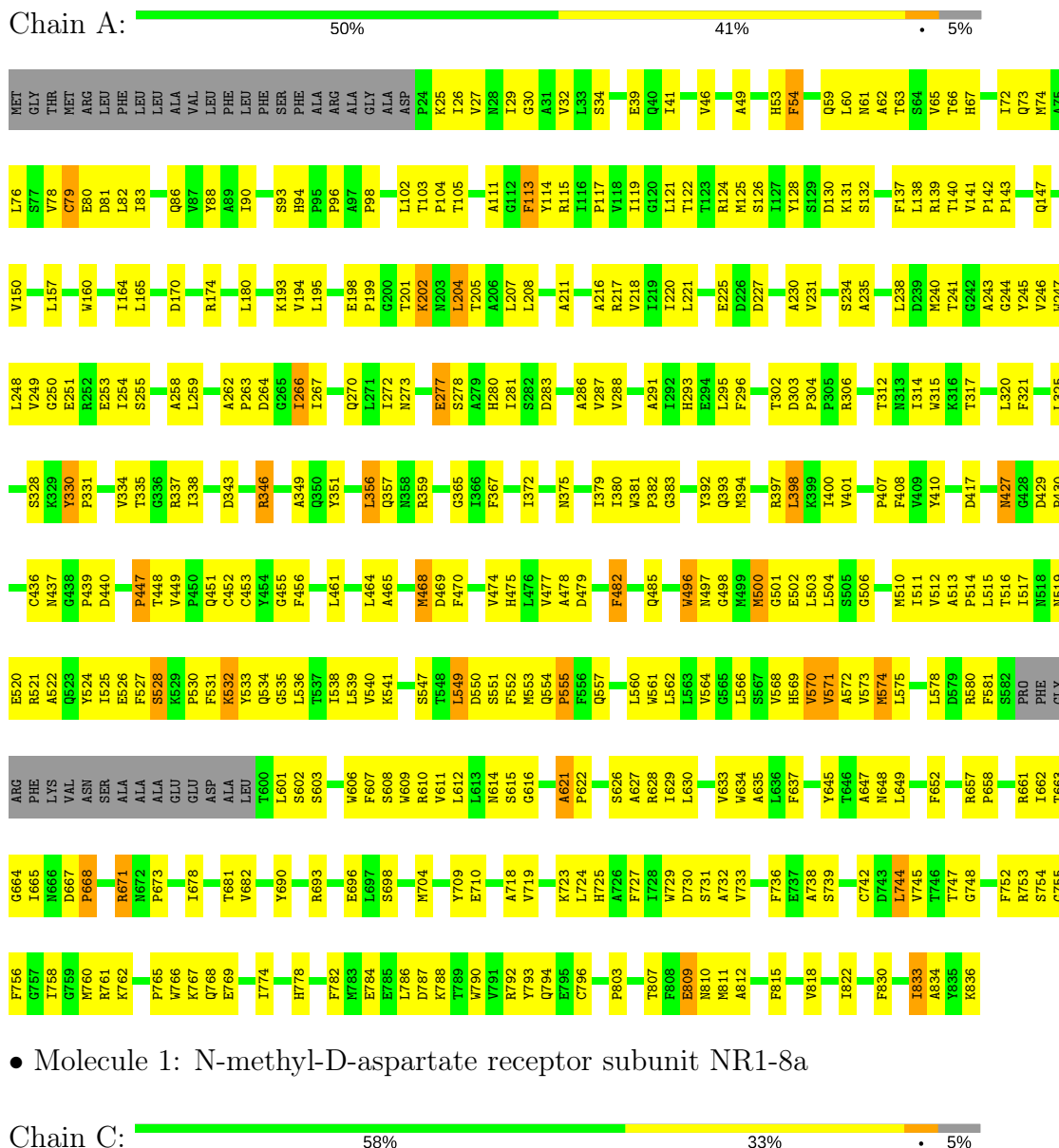


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	A	1	28	16	2	10	0
5	A	1	28	16	2	10	0
5	C	1	56	32	4	20	0
5	C	1	56	32	4	20	0
5	C	1	56	32	4	20	0
5	C	1	56	32	4	20	0
5	D	1	42	24	3	15	0
5	D	1	42	24	3	15	0
5	D	1	42	24	3	15	0

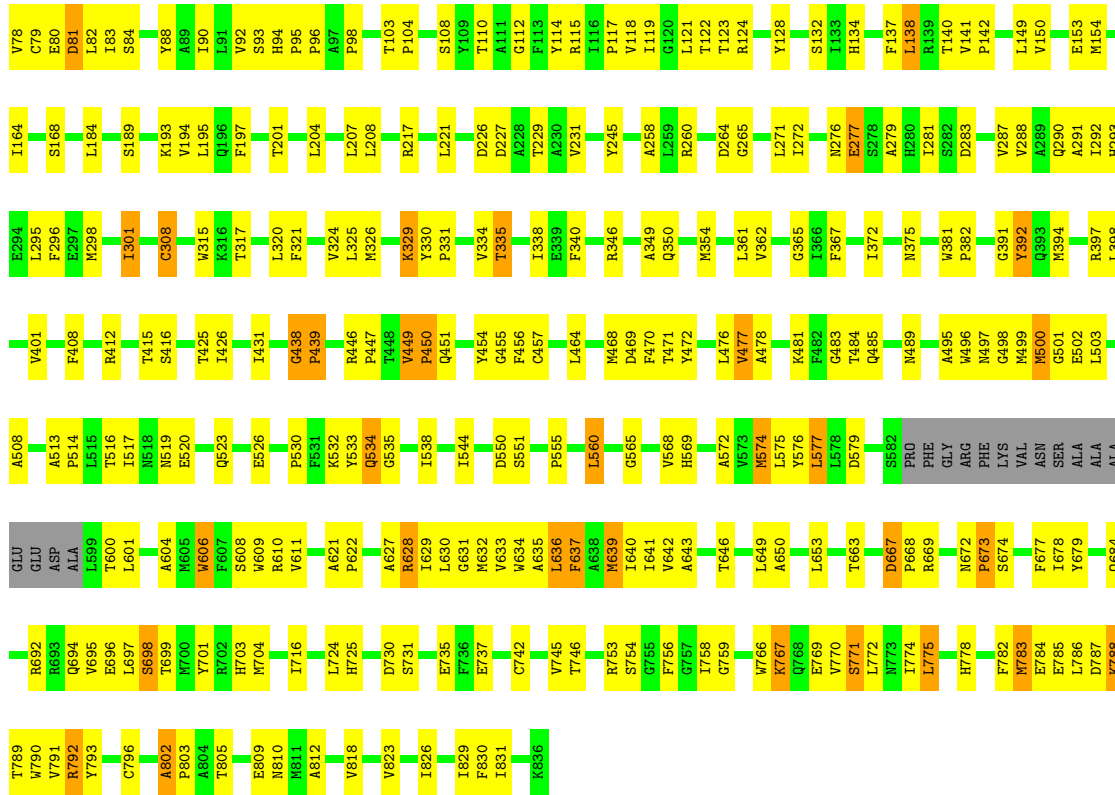
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated with issues in geometry. 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. 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.

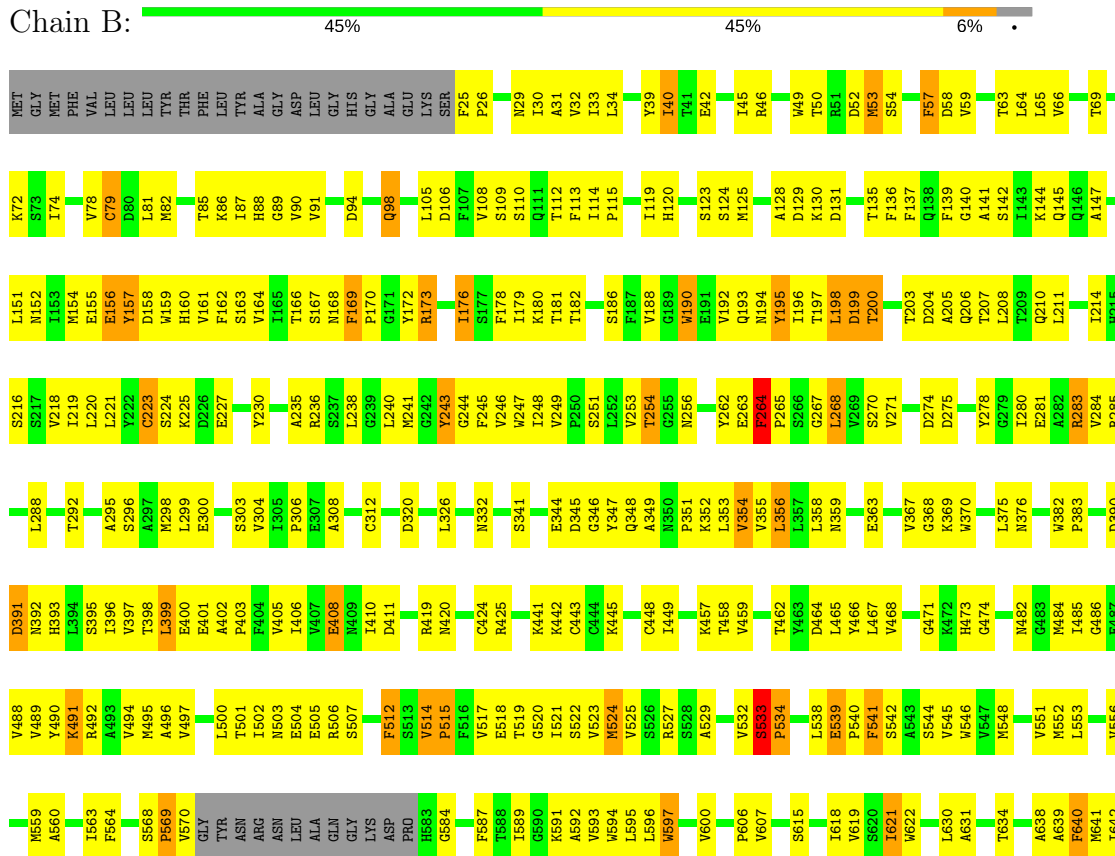
- Molecule 1: N-methyl-D-aspartate receptor subunit NR1-8a



- Molecule 1: N-methyl-D-aspartate receptor subunit NR1-8a



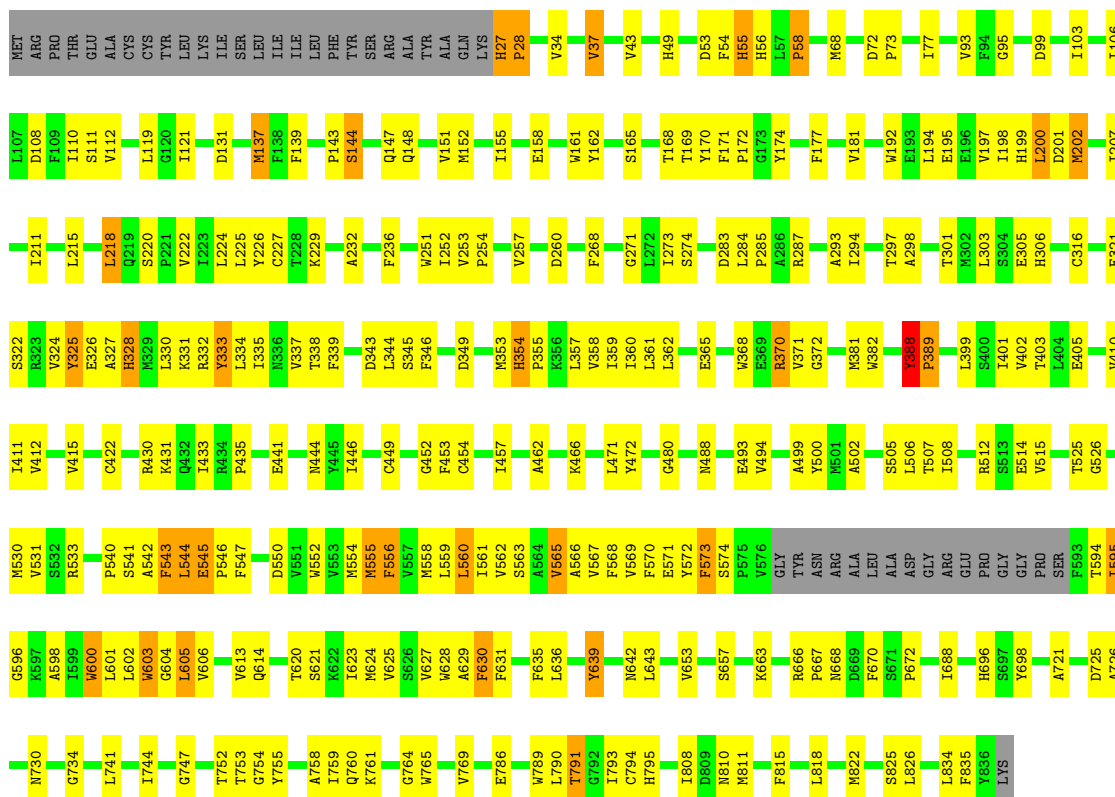
• Molecule 2: N-methyl-D-aspartate receptor subunit NR2A





- Molecule 3: Iontropic glutamate receptor subunit NR2B

Chain D: 61% 30% 5%



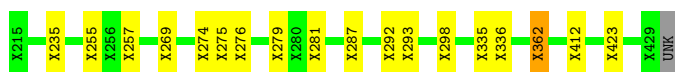
- Molecule 4: GluN2B-specific Fab, termed 11D1

Chain F: 90% 9%



- Molecule 4: GluN2B-specific Fab, termed 11D1

Chain G: 91% 8%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	302052	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	0.84	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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:
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 >2	RMSZ	# Z >2
1	A	0.49	0/5877	0.72	2/8041 (0.0%)
1	C	0.33	0/5549	0.67	6/7614 (0.1%)
2	B	0.54	0/5697	0.78	10/7814 (0.1%)
3	D	0.38	0/5233	0.68	3/7227 (0.0%)
All	All	0.45	0/22356	0.72	21/30696 (0.1%)

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	A	0	1
1	C	0	1
4	F	0	1
4	G	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	533	SER	C-N-CD	-14.68	88.31	120.60
2	B	514	VAL	C-N-CD	-11.49	95.31	120.60
1	C	438	GLY	C-N-CD	-10.63	97.22	120.60
1	A	621	ALA	C-N-CD	-9.79	99.07	120.60
3	D	27	HIS	C-N-CD	-8.33	102.28	120.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	570	VAL	Mainchain
1	C	792	ARG	Mainchain
4	F	67	UNK	Mainchain
4	G	362	UNK	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	A	5745	0	5276	784	0
1	C	5442	0	4757	512	0
2	B	5573	0	4942	878	0
3	D	5130	0	4104	438	0
4	F	1070	0	235	10	0
4	G	1075	0	235	11	0
5	A	28	0	25	4	0
5	C	56	0	50	5	0
5	D	42	0	38	2	0
All	All	24161	0	19662	2358	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 54.

The worst 5 of 2358 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:630:LEU:HD22	2:B:816:MET:SD	1.39	1.62
1:A:682:VAL:HG21	1:A:729:TRP:CH2	1.17	1.60
2:B:403:PRO:CG	2:B:722:VAL:HG22	1.11	1.57
1:A:506:GLY:CA	1:A:761:ARG:NH2	1.68	1.57
1:A:121:LEU:HD13	1:A:281:ILE:CG1	1.34	1.55

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 PDB entries followed by that with respect to all EM entries.

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	792/836 (95%)	756 (96%)	31 (4%)	5 (1%)	27	70
1	C	794/836 (95%)	758 (96%)	30 (4%)	6 (1%)	21	65
2	B	791/831 (95%)	733 (93%)	44 (6%)	14 (2%)	9	47
3	D	790/837 (94%)	752 (95%)	31 (4%)	7 (1%)	19	61
All	All	3167/3340 (95%)	2999 (95%)	136 (4%)	32 (1%)	22	59

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	447	PRO
2	B	169	PHE
2	B	515	PRO
2	B	534	PRO
1	C	392	TYR

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 PDB entries followed by that with respect to all EM entries.

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	534/714 (75%)	499 (93%)	35 (7%)	18	49
1	C	461/714 (65%)	421 (91%)	40 (9%)	11	38
2	B	490/724 (68%)	437 (89%)	53 (11%)	7	28
3	D	375/735 (51%)	338 (90%)	37 (10%)	8	32
All	All	1860/2887 (64%)	1695 (91%)	165 (9%)	15	37

5 of 165 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	662	HIS
1	C	79	CYS
3	D	568	PHE
2	B	692	TYR
2	B	788	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	503	ASN
1	C	53	HIS
3	D	306	HIS
2	B	659	GLN
1	A	293	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

9 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
5	NAG	A	901	1,5	14,14,15	0.29	0	17,19,21	0.65	0
5	NAG	A	902	5	14,14,15	0.29	0	17,19,21	0.66	0
5	NAG	C	901	1,5	14,14,15	0.29	0	17,19,21	0.65	0
5	NAG	C	902	5	14,14,15	0.28	0	17,19,21	0.65	0
5	NAG	C	903	1,5	14,14,15	0.28	0	17,19,21	0.66	0
5	NAG	C	904	5	14,14,15	0.28	0	17,19,21	0.65	0
5	NAG	D	1001	3,5	14,14,15	0.29	0	17,19,21	0.66	0
5	NAG	D	1002	5	14,14,15	0.29	0	17,19,21	0.65	0
5	NAG	D	1003	3	14,14,15	0.28	0	17,19,21	0.66	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
5	NAG	A	901	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	902	5	-	0/6/23/26	0/1/1/1
5	NAG	C	901	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	902	5	-	0/6/23/26	0/1/1/1
5	NAG	C	903	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	904	5	-	0/6/23/26	0/1/1/1
5	NAG	D	1001	3,5	-	0/6/23/26	0/1/1/1
5	NAG	D	1002	5	-	0/6/23/26	0/1/1/1
5	NAG	D	1003	3	-	0/6/23/26	0/1/1/1

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 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	902	NAG	4	0
5	C	902	NAG	2	0
5	C	904	NAG	3	0
5	D	1002	NAG	2	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
4	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	348:UNK	C	349:UNK	N	14.40