



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Nov 1, 2017 – 11:35 PM EDT

PDB ID : 5VHX
EMDB ID: : EMD-8686
Title : GluA2-1xGSG1L bound to ZK
Authors : Twomey, E.C.; Yelshanskaya, M.V.; Grassucci, R.A.; Frank, J.; Sobolevsky, A.I.
Deposited on : unknown
Resolution : 8.30 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

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

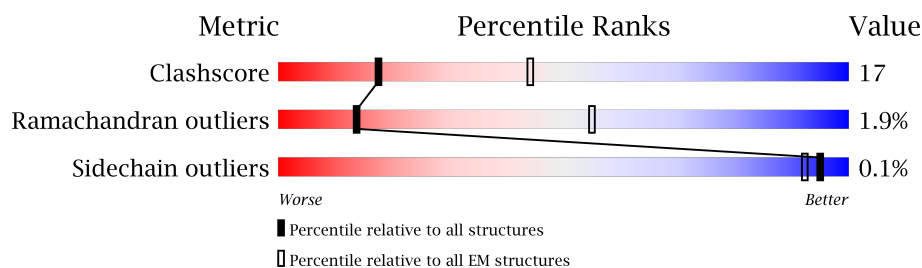
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.30 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	1057	46% 27% . 26%
1	B	1057	46% 27% . 26%
1	C	1057	47% 26% . 26%
1	D	1057	46% 28% . 26%
1	E	1057	8% 9% 83%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26164 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 Glutamate receptor 2,Germ cell-specific gene 1-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	783	Total	C	N	O	S	0	0
			6159	3950	1023	1156	30		
1	B	780	Total	C	N	O	S	0	0
			6137	3938	1017	1152	30		
1	C	783	Total	C	N	O	S	0	0
			6159	3950	1023	1156	30		
1	D	780	Total	C	N	O	S	0	0
			6137	3938	1017	1152	30		
1	E	179	Total	C	N	O	S	0	0
			1408	920	231	245	12		

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	conflict	UNP P19491
A	382	LEU	VAL	conflict	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	conflict	UNP P19491
A	385	ASP	ASN	conflict	UNP P19491
A	392	GLN	ASN	conflict	UNP P19491
A	827	GLY	-	linker	UNP P19491
A	828	THR	-	linker	UNP P19491
A	829	GLY	-	linker	UNP P19491
B	241	GLU	ASN	conflict	UNP P19491
B	382	LEU	VAL	conflict	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491
B	?	-	LEU	deletion	UNP P19491

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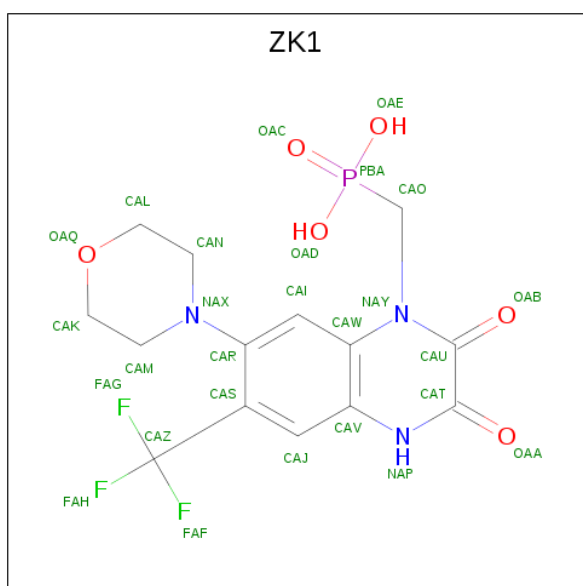
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	conflict	UNP P19491
B	385	ASP	ASN	conflict	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	827	GLY	-	linker	UNP P19491
B	828	THR	-	linker	UNP P19491
B	829	GLY	-	linker	UNP P19491
C	241	GLU	ASN	conflict	UNP P19491
C	382	LEU	VAL	conflict	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	384	GLU	GLY	conflict	UNP P19491
C	385	ASP	ASN	conflict	UNP P19491
C	392	GLN	ASN	conflict	UNP P19491
C	827	GLY	-	linker	UNP P19491
C	828	THR	-	linker	UNP P19491
C	829	GLY	-	linker	UNP P19491
D	241	GLU	ASN	conflict	UNP P19491
D	382	LEU	VAL	conflict	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	conflict	UNP P19491
D	385	ASP	ASN	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	827	GLY	-	linker	UNP P19491
D	828	THR	-	linker	UNP P19491
D	829	GLY	-	linker	UNP P19491
E	-588	GLU	ASN	conflict	UNP P19491
E	-447	LEU	VAL	conflict	UNP P19491
E	?	-	LEU	deletion	UNP P19491
E	?	-	THR	deletion	UNP P19491
E	?	-	GLU	deletion	UNP P19491
E	?	-	LEU	deletion	UNP P19491

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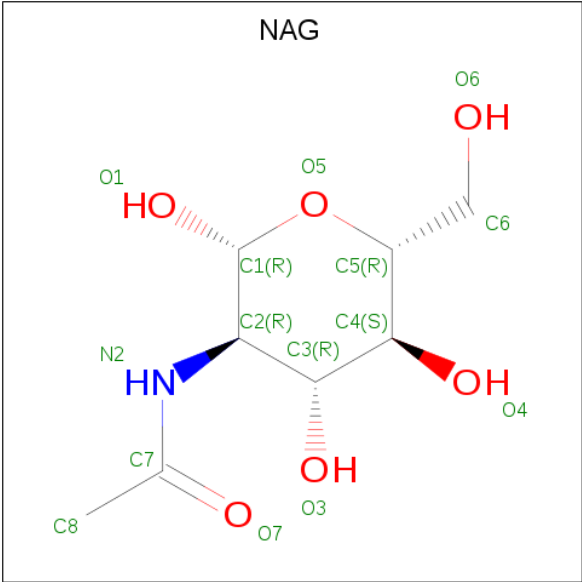
Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	PRO	deletion	UNP P19491
E	?	-	SER	deletion	UNP P19491
E	-445	GLU	GLY	conflict	UNP P19491
E	-444	ASP	ASN	conflict	UNP P19491
E	-437	GLN	ASN	conflict	UNP P19491
E	-2	GLY	-	linker	UNP P19491
E	-1	THR	-	linker	UNP P19491
E	0	GLY	-	linker	UNP P19491

- Molecule 2 is {[7-morpholin-4-yl-2,3-dioxo-6-(trifluoromethyl)-3,4-dihydroquinoxalin-1(2H)-yl]methyl}phosphonic acid (three-letter code: ZK1) (formula: C₁₄H₁₅F₃N₃O₆P).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
2	B	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
2	C	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
2	D	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).

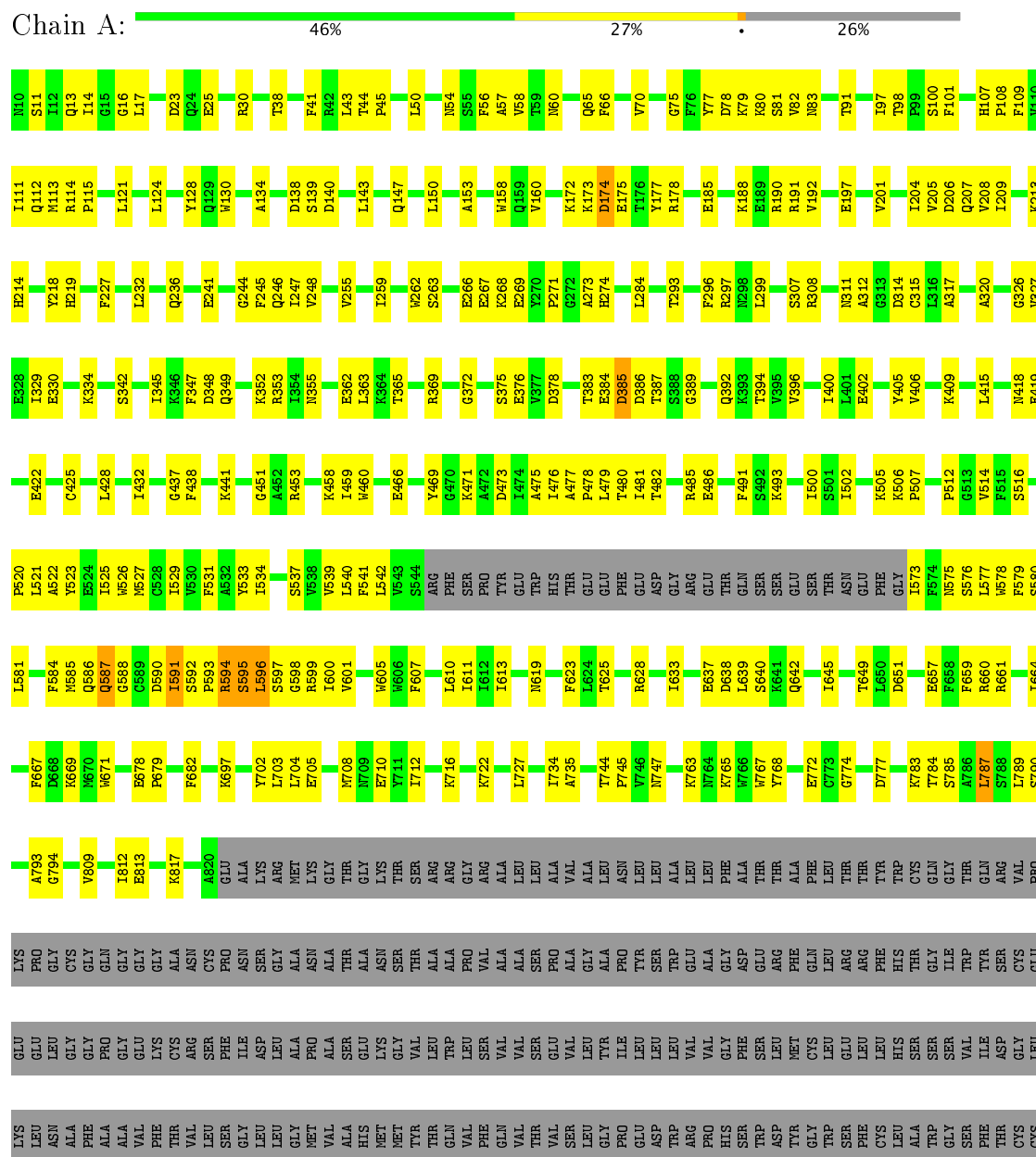


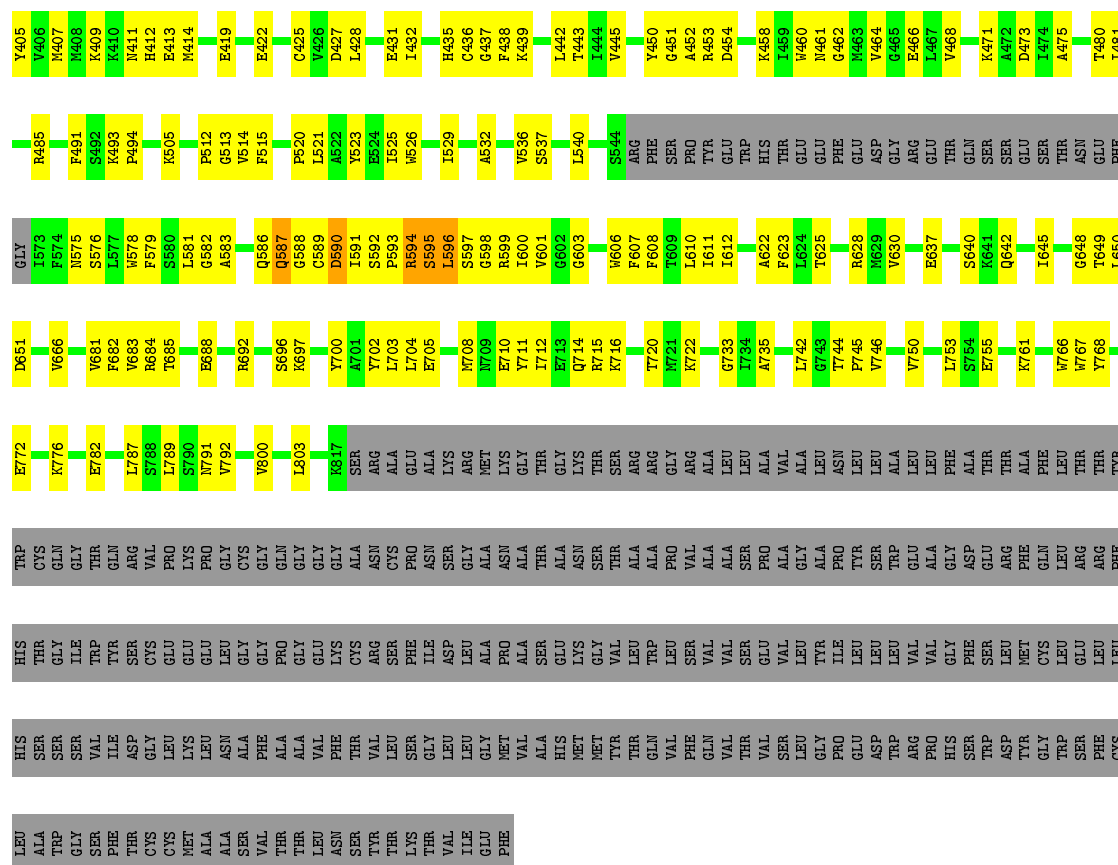
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	

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 by 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.

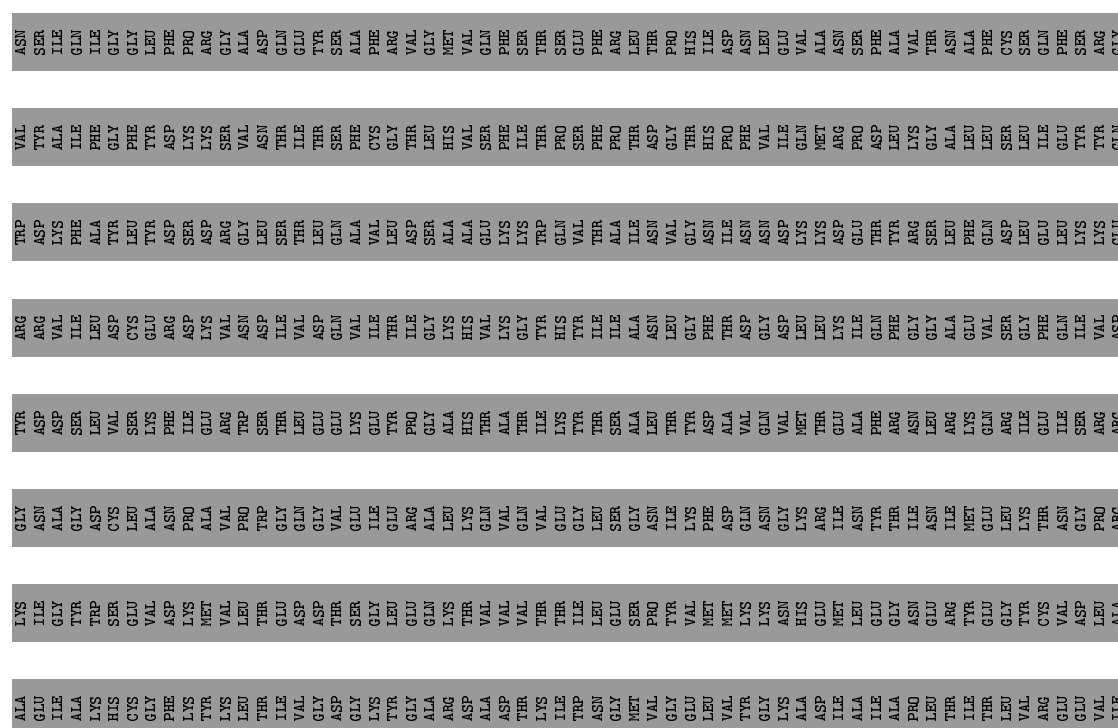
- Molecule 1: Glutamate receptor 2, Germ cell-specific gene 1-like protein





- Molecule 1: Glutamate receptor 2, Germ cell-specific gene 1-like protein

Chain E:  8% 9% 83%



K232	D157	F90	T29	SER	LYS	MET	LEU	GLU	ASP
THR	G188	H91	T30	ASN	GLY	TRP	ILE	TRP	PHE
VAL	L159	T92	K31	VAL	TYR	THR	ILE	HIS	SER
ILE	K160	G93	C32	ALA	ILE	THR	ILE	THR	LYS
GLU	L161	I94	G33	GLY	ILE	MET	SER	GLU	PRO
PHE	N162	W95	I34	VAL	ALA	ARG	TYR	PHE	PHE
	A163	Y96	T35	PHE	THR	SER	THR	THR	MET
	F164	S97	Q36	TYR	PRO	ALA	ALA	GLU	SER
	A165	C98	R37	ILE	LYS	GLU	ALA	ASP	LEU
	A166	E99	V38	LEU	GLY	PRO	ASN	GLY	GLY
	V167	E100	P39	VAL	SER	SER	LEU	ARG	ILE
	F168	GLU	LYS	GLY	SER	VAL	ALA	GLU	SER
	T169	LEU	PRO	GLY	LEU	PHE	ALA	THR	ILE
	V170	GLY	GLY	LEU	THR	VAL	PHE	GLN	MET
	L174	PRO	CYS	GLY	THR	ARG	THR	SER	ILE
	M177	GLN	GLN	ALA	VAL	THR	VAL	GLU	LYS
	V178	G106	GLY	MET	ASN	ALA	GLU	SER	PRO
	A179	E107	GLY	LEU	LEU	GLY	ARG	THR	GLN
	H180	K108	GLY	VAL	LEU	GLY	MET	ASN	LYS
	M181	C109	ALA	ALA	VAL	VAL	ALA	GLU	LYS
	M182	R110	ASN	LEU	VAL	ALA	VAL	ASN	SER
		S111	CYS	LEU	LYS	ARG	PRO	PHE	LYS
		F112	ILE	ILE	LYS	ARG	PRO	GLY	PRO
		I113	GLU	GLU	VAL	VAL	ILE	ILE	GLY
		D114	PRO	PHE	SER	ARG	GLU	PHE	VAL
	Q185	ASN	ASN	CYS	GLY	LYS	SER	ASN	PHE
	V186	SER	SER	TYR	GLN	LYS	ALA	SER	SER
		A116	GLY	TYR	GLY	LYS	ALA	LEU	PHE
	V189	P117	ALA	ASN	VAL	GLY	GLU	TRP	LEU
	T190	A118	ASN	SER	VAL	LYS	ASP	PHE	ASP
		S119	ALA	ARG	LEU	LYS	LEU	SER	PRO
	L193	E120	ALA	ALA	LYS	TYR	SER	SER	LEU
	G194	K121	ALA	GLU	LYS	ALA	LYS	LEU	ALA
	P195	G122	ASN	ALA	LYS	TYR	GLN	GLY	ALA
	E196	V123	SER	LYS	LYS	LEU	THR	ALA	TYR
	D197	L124	THR	ARG	ASN	LEU	GLU	PHE	GLU
	H198	W125	ALA	MET	LYS	ILE	ILE	ILE	ILE
	R199	I126	ALA	LYS	TRP	SER	ALA	GLN	TRP
		S127	PRO	GLY	TRP	THR	TYR	GLN	MET
	S202		VAL	THR	THR	MET	GLY	GLY	CYS
	W203	S130	ALA	ASP	ASN	GLY	THR	CYS	ILE
	D204	ALA	ALA	LYS	GLY	LEU	ASP	ILE	PHE
	Y205	L133	SER	GLY	TYR	ASP	ASP	ILE	ALA
		Y134	PRO	GLU	ILE	SER	SER	PRO	TYR
	F209	I135	ALA	CYS	GLY	GLY	GLY	ARG	ILE
		L136	GLY	R4	ALA	THR	SER	ARG	GLY
	W213	L137	ALA	G6	LYS	LYS	LYS	LEU	VAL
	G214	L138	PRO	R7	PRO	PRO	THR	SER	VAL
	S215		TYR	A8	ASP	CYS	GLU	SER	SER
	F216	L144	SER	L9	SER	PRO	PHE	VAL	VAL
	T217	W145	TRP		GLY	ASP	PHE	VAL	VAL
		C146	GLU	V12	SER	THR	ARG	ILE	LEU
	W220	L147	ALA	A18	LYS	MET	ARG	VAL	PHE
		E148	GLY		GLY	LYS	GLY	GLY	LEU
	S223	L149	ASP	F21	LYS	VAL	LYS	VAL	VAL
	V224		GLU	A22	THR	GLY	ILE	VAL	SER
		S152	ARG	F85	SER	GLY	ALA	TRP	ARG
	L227	S153	F86	T23	ALA	ASN	VAL	TRP	PHE
		SER	Q86	L27	LEU	LEU	PHE	TRP	SER
	Y230	VAL	L87		ASP	PHE	ASP	PHE	PRO
	T231	ILE		T28	LEU	THR	LYS	THR	TYR

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	16454	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 ($e^-/\text{\AA}^2$)	80	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, ZK1

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	0.32	0/6287	0.46	0/8493
1	B	0.32	0/6265	0.45	0/8464
1	C	0.32	0/6287	0.45	0/8493
1	D	0.32	0/6265	0.45	0/8464
1	E	0.29	0/1443	0.46	0/1959
All	All	0.32	0/26547	0.45	0/35873

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 [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	6159	0	6155	221	0
1	B	6137	0	6132	224	0
1	C	6159	0	6155	215	0
1	D	6137	0	6132	231	0
1	E	1408	0	1406	78	0
2	A	27	0	13	3	0
2	B	27	0	13	2	0
2	C	27	0	13	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	27	0	13	1	0
3	A	14	0	13	2	0
3	B	14	0	13	0	0
3	C	14	0	13	2	0
3	D	14	0	13	3	0
All	All	26164	0	26084	890	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 17.

The worst 5 of 890 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:E:205:TYR:OH	1:E:209:PHE:CE2	2.14	1.00
1:A:531:PHE:HE2	1:E:213:TRP:CD2	1.84	0.94
1:E:205:TYR:HH	1:E:209:PHE:HE2	1.15	0.88
1:E:98:CYS:HA	1:E:109:CYS:HA	1.55	0.88
1:C:337:GLN:HG3	1:C:346:LYS:HG2	1.58	0.85

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	779/1057 (74%)	729 (94%)	35 (4%)	15 (2%)	9	47
1	B	776/1057 (73%)	728 (94%)	37 (5%)	11 (1%)	13	54
1	C	779/1057 (74%)	726 (93%)	38 (5%)	15 (2%)	9	47
1	D	776/1057 (73%)	728 (94%)	35 (4%)	13 (2%)	11	50
1	E	171/1057 (16%)	150 (88%)	13 (8%)	8 (5%)	3	28
All	All	3281/5285 (62%)	3061 (93%)	158 (5%)	62 (2%)	14	47

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	385	ASP
1	A	591	ILE
1	B	395	VAL
1	B	512	PRO
1	C	591	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 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	666/888 (75%)	666 (100%)	0	100	100
1	B	664/888 (75%)	664 (100%)	0	100	100
1	C	666/888 (75%)	666 (100%)	0	100	100
1	D	664/888 (75%)	664 (100%)	0	100	100
1	E	152/888 (17%)	150 (99%)	2 (1%)	73	87
All	All	2812/4440 (63%)	2810 (100%)	2 (0%)	95	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	87	LEU
1	E	205	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	619	ASN
1	C	147	GLN
1	D	714	GLN
1	B	642	GLN
1	C	65	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 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
2	ZK1	A	1101	-	28,29,29	3.10	10 (35%)	36,45,45	1.66	7 (19%)
3	NAG	A	1102	-	14,14,15	0.26	0	15,19,21	0.39	0
2	ZK1	B	1101	-	28,29,29	3.14	11 (39%)	36,45,45	1.60	6 (16%)
3	NAG	B	1102	-	14,14,15	0.20	0	15,19,21	0.48	0
2	ZK1	C	1101	-	28,29,29	3.11	11 (39%)	36,45,45	1.65	7 (19%)
3	NAG	C	1102	-	14,14,15	0.19	0	15,19,21	0.49	0
2	ZK1	D	1101	-	28,29,29	3.15	11 (39%)	36,45,45	1.62	7 (19%)
3	NAG	D	1102	-	14,14,15	0.18	0	15,19,21	0.50	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
2	ZK1	A	1101	-	-	0/13/23/23	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1102	-	-	0/6/23/26	0/1/1/1
2	ZK1	B	1101	-	-	0/13/23/23	0/3/3/3
3	NAG	B	1102	-	-	0/6/23/26	0/1/1/1
2	ZK1	C	1101	-	-	0/13/23/23	0/3/3/3
3	NAG	C	1102	-	-	0/6/23/26	0/1/1/1
2	ZK1	D	1101	-	-	0/13/23/23	0/3/3/3
3	NAG	D	1102	-	-	0/6/23/26	0/1/1/1

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1101	ZK1	PBA-OAD	-3.68	1.46	1.54
2	A	1101	ZK1	PBA-OAD	-3.68	1.46	1.54
2	B	1101	ZK1	PBA-OAD	-3.66	1.46	1.54
2	D	1101	ZK1	PBA-OAD	-3.63	1.46	1.54
2	C	1101	ZK1	CAU-NAY	-2.09	1.35	1.38

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1101	ZK1	CAI-CAR-NAX	-3.32	118.15	122.69
2	B	1101	ZK1	CAI-CAR-NAX	-3.14	118.40	122.69
2	A	1101	ZK1	CAI-CAR-NAX	-3.00	118.58	122.69
2	C	1101	ZK1	CAI-CAR-NAX	-2.93	118.69	122.69
2	C	1101	ZK1	FAG-CAZ-CAS	-2.42	108.33	112.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	ZK1	3	0
3	A	1102	NAG	2	0
2	B	1101	ZK1	2	0
2	C	1101	ZK1	3	0
3	C	1102	NAG	2	0
2	D	1101	ZK1	1	0
3	D	1102	NAG	3	0

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.