



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Sep 7, 2017 – 03:14 AM EDT

PDB ID : 5WEL
EMDB ID: : EMD-8820
Title : GluA2 bound to antagonist ZK and GSG1L in digitonin, state 2
Authors : Twomey, E.C.; Yelshanskaya, M.V.; Grassucci, R.A.; Frank, J.; Sobolevsky, A.I.
Deposited on : unknown
Resolution : 4.40 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-20029824

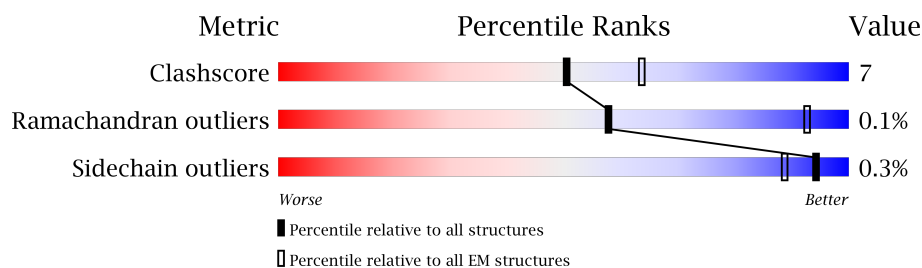
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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	
1	B	1057	
1	C	1057	
1	D	1057	

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
3	AJP	A	1302	-	-	X	-
3	AJP	C	1302	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27638 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 Chimera of Glutamate receptor 2, Germ cell-specific gene 1-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	962	Total	C	N	O	S	0	0
			7555	4864	1248	1401	42		
1	B	780	Total	C	N	O	S	0	0
			6125	3932	1011	1152	30		
1	C	962	Total	C	N	O	S	0	0
			7555	4864	1248	1401	42		
1	D	780	Total	C	N	O	S	0	0
			6125	3932	1011	1152	30		

There are 60 discrepancies between the modelled and reference sequences:

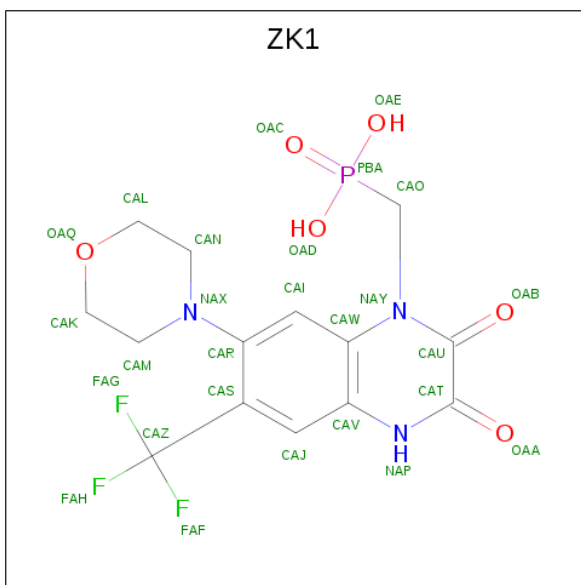
Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	engineered mutation	UNP P19491
A	382	LEU	VAL	engineered mutation	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	engineered mutation	UNP P19491
A	385	ASP	ASN	engineered mutation	UNP P19491
A	392	GLN	ASN	engineered mutation	UNP P19491
A	827	GLY	-	linker	UNP P19491
A	828	THR	-	linker	UNP P19491
A	829	GLY	-	linker	UNP P19491
A	1151	LEU	VAL	engineered mutation	UNP D3Z7H4
B	241	GLU	ASN	engineered mutation	UNP P19491
B	382	LEU	VAL	engineered mutation	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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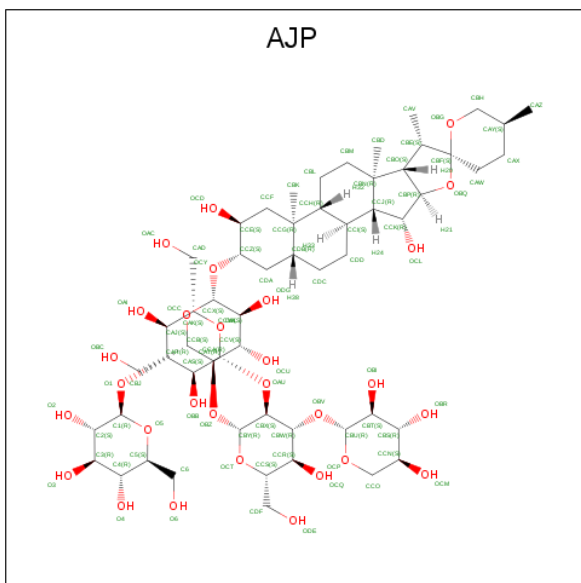
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	engineered mutation	UNP P19491
B	385	ASP	ASN	engineered mutation	UNP P19491
B	392	GLN	ASN	engineered mutation	UNP P19491
B	827	GLY	-	linker	UNP P19491
B	828	THR	-	linker	UNP P19491
B	829	GLY	-	linker	UNP P19491
B	1151	LEU	VAL	engineered mutation	UNP D3Z7H4
C	241	GLU	ASN	engineered mutation	UNP P19491
C	382	LEU	VAL	engineered mutation	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	engineered mutation	UNP P19491
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C	392	GLN	ASN	engineered mutation	UNP P19491
C	827	GLY	-	linker	UNP P19491
C	828	THR	-	linker	UNP P19491
C	829	GLY	-	linker	UNP P19491
C	1151	LEU	VAL	engineered mutation	UNP D3Z7H4
D	241	GLU	ASN	engineered mutation	UNP P19491
D	382	LEU	VAL	engineered mutation	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	engineered mutation	UNP P19491
D	385	ASP	ASN	engineered mutation	UNP P19491
D	392	GLN	ASN	engineered mutation	UNP P19491
D	827	GLY	-	linker	UNP P19491
D	828	THR	-	linker	UNP P19491
D	829	GLY	-	linker	UNP P19491
D	1151	LEU	VAL	engineered mutation	UNP D3Z7H4

- 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 27	C 14	F 3	N 3	O 6	P 1	0
2	B	1	Total 27	C 14	F 3	N 3	O 6	P 1	0
2	C	1	Total 27	C 14	F 3	N 3	O 6	P 1	0
2	D	1	Total 27	C 14	F 3	N 3	O 6	P 1	0

- Molecule 3 is Digitonin (three-letter code: AJP) (formula: $C_{56}H_{92}O_{29}$).

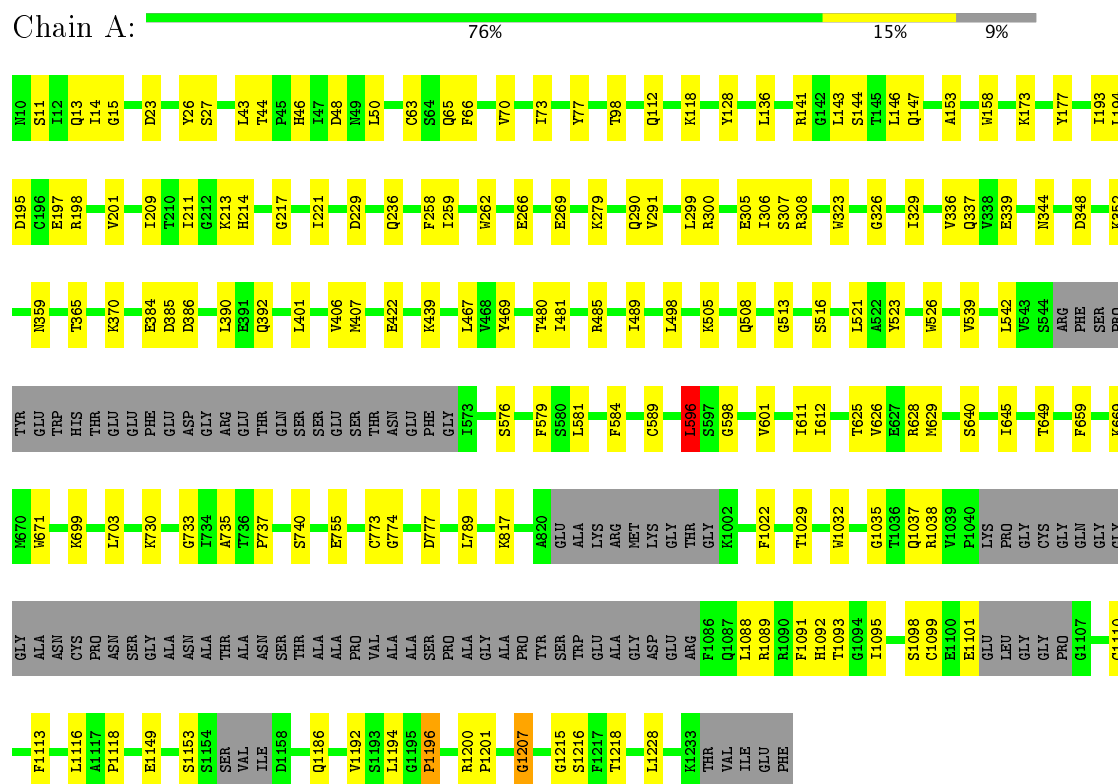


Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			85	56	29	
3	C	1	Total	C	O	0
			85	56	29	

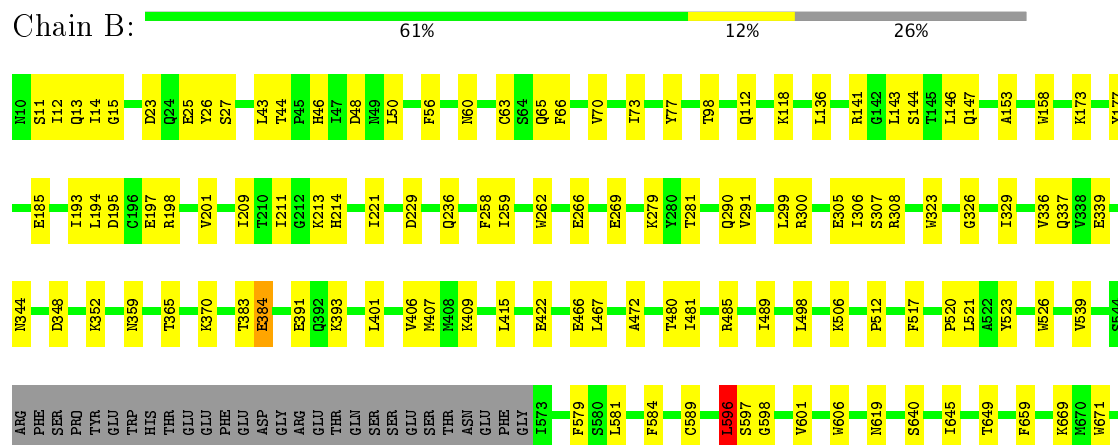
3 Residue-property plots

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.

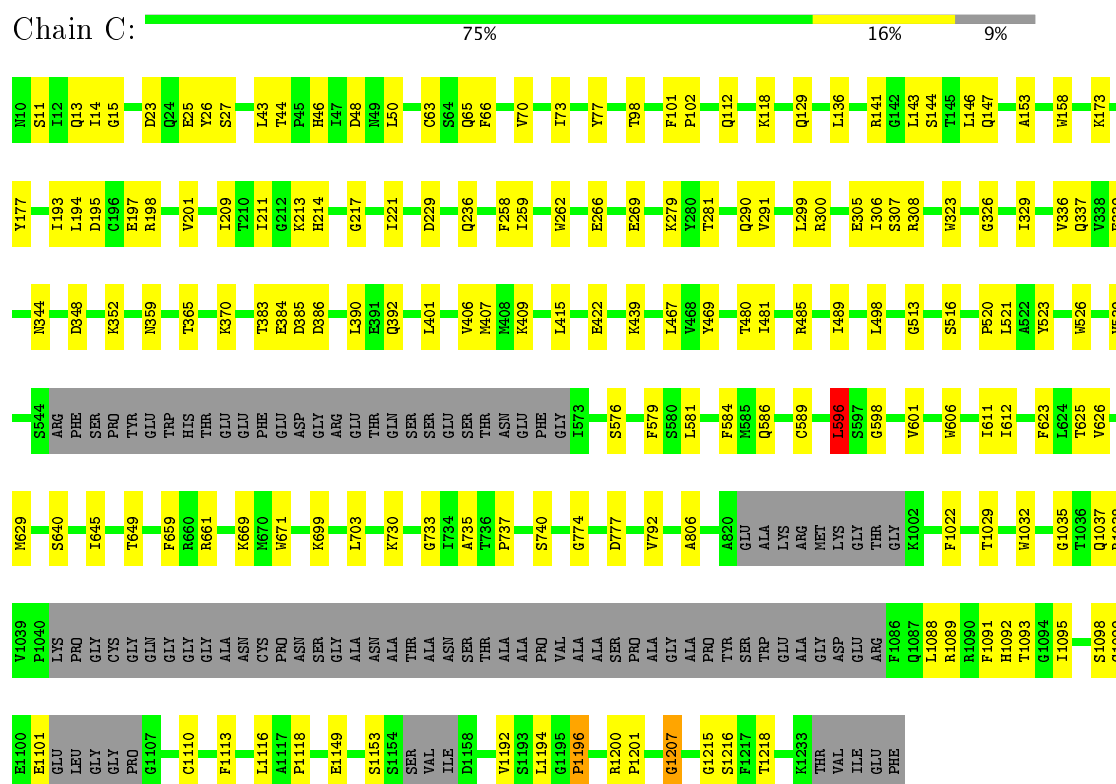
- Molecule 1: Chimera of Glutamate receptor 2, Germ cell-specific gene 1-like protein



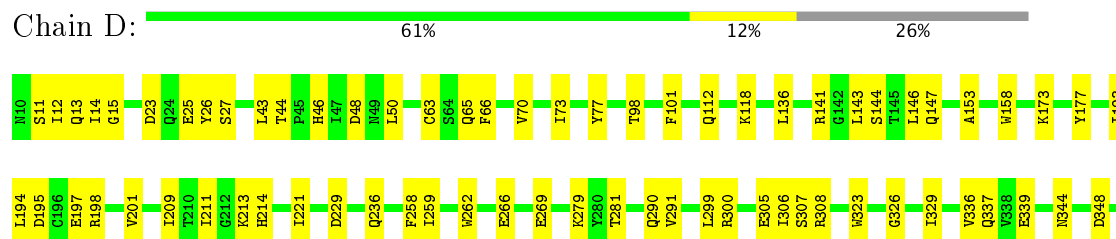
- Molecule 1: Chimera of Glutamate receptor 2, Germ cell-specific gene 1-like protein



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



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



K352	SER	K669	PHE	GLY	HIS
K359	PRO	K670	ALA	ASP	SER
T365	THR	K671	THR	GLU	TRP
K370	TRP	K699	ALA	ARG	LEU
K374	HIS	L703	PHE	GLN	MET
K380	THR	D719	LEU	LEU	CYS
K383	GLU	G733	ARG	ARG	GLU
K384	PHE	I734	THR	THR	LEU
E391	ASP	A735	THR	PHE	LEU
Q392	GLY	I736	HIS	GLY	LEU
K393	ARG	P737	GLN	ILE	CYS
L401	THR	K738	THR	THR	HIS
V406	GLN	A775	ARG	ASP	SER
N407	SER	G779	VAL	CYS	GLY
N408	SER	T784	PRO	LEU	LEU
K409	GLU	S788	LYS	GLU	LYS
L415	PHE	L789	PRO	GLU	ALA
E422	GLY	S790	GLY	GLY	ASN
E466	LEU	K817	GLY	LYS	THR
L467	LEU	SER	ALA	CYS	VAL
A472	LEU	F576	ASN	ASN	THR
T480	LEU	F579	CYS	CYS	LEU
I481	LEU	S580	PRO	PRO	SER
R485	LEU	L581	ILE	PHE	GLY
L489	LEU	F584	ASP	ILE	LEU
K506	LEU	N585	LEU	ASP	LEU
P512	LEU	Q586	ALA	ALA	GLY
F517	LEU	C589	ALA	PRO	MET
L521	LEU	L596	ALA	ALA	VAL
V523	LEU	S597	ASN	GLU	HIS
I525	LEU	G598	THR	LYS	MET
N526	LEU	V601	SER	GLY	MET
V539	LEU	A622	THR	VAL	TYR
S544	LEU	E634	ALA	LEU	THR
R661	LEU	S640	PRO	TRP	GLN
PHE	LEU	I645	ALA	VAL	VAL
	LEU	N646	SER	VAL	PHE
	LEU	T649	THR	VAL	GLN
	LEU	F659	TYR	THR	VAL
	LEU	R660	SER	GLU	SER
	LEU		TRP	LEU	ASP
	LEU		GLU	LEU	TRP
	LEU		VAL	VAL	ARG
	LEU		ALA	PRO	PRO

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	41926	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	67	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: AJP, 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	0.29	0/7718	0.51	5/10438 (0.0%)
1	B	0.29	0/6253	0.51	1/8450 (0.0%)
1	C	0.29	0/7718	0.51	4/10438 (0.0%)
1	D	0.29	0/6253	0.51	2/8450 (0.0%)
All	All	0.29	0/27942	0.51	12/37776 (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	A	0	5
1	B	0	1
1	C	0	5
1	D	0	2
All	All	0	13

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	596	LEU	CA-CB-CG	7.89	133.44	115.30
1	C	596	LEU	CA-CB-CG	7.88	133.43	115.30
1	D	596	LEU	CA-CB-CG	7.87	133.39	115.30
1	B	596	LEU	CA-CB-CG	7.86	133.38	115.30
1	C	612	ILE	O-C-N	-6.41	112.44	122.70

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1196	PRO	Peptide
1	A	1207	GLY	Peptide
1	A	384	GLU	Peptide
1	A	773	CYS	Mainchain
1	A	817	LYS	Peptide

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	7555	0	7536	105	0
1	B	6125	0	6110	77	0
1	C	7555	0	7536	109	0
1	D	6125	0	6110	76	0
2	A	27	0	13	1	0
2	B	27	0	13	2	0
2	C	27	0	13	1	0
2	D	27	0	13	1	0
3	A	85	0	0	23	0
3	C	85	0	0	24	0
All	All	27638	0	27344	373	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 7.

The worst 5 of 373 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:C:740:SER:HA	3:C:1302:AJP:ODE	1.26	1.29
1:C:469:TYR:HB3	3:C:1302:AJP:CBD	1.65	1.26
1:C:740:SER:CA	3:C:1302:AJP:ODE	1.94	1.15
1:A:740:SER:HA	3:A:1302:AJP:ODE	1.45	1.15
1:A:469:TYR:HB3	3:A:1302:AJP:CBD	1.81	1.11

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	950/1057 (90%)	893 (94%)	55 (6%)	2 (0%)	51	85
1	B	776/1057 (73%)	721 (93%)	54 (7%)	1 (0%)	55	89
1	C	950/1057 (90%)	889 (94%)	59 (6%)	2 (0%)	51	85
1	D	776/1057 (73%)	721 (93%)	55 (7%)	0	100	100
All	All	3452/4228 (82%)	3224 (93%)	223 (6%)	5 (0%)	58	89

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	384	GLU
1	A	385	ASP
1	A	386	ASP
1	C	385	ASP
1	C	386	ASP

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	816/888 (92%)	814 (100%)	2 (0%)	94	96
1	B	662/888 (74%)	660 (100%)	2 (0%)	94	96
1	C	816/888 (92%)	814 (100%)	2 (0%)	94	96
1	D	662/888 (74%)	660 (100%)	2 (0%)	94	96
All	All	2956/3552 (83%)	2948 (100%)	8 (0%)	94	96

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	596	LEU
1	D	596	LEU
1	C	596	LEU
1	B	300	ARG
1	C	300	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	392	GLN
1	C	65	GLN
1	D	392	GLN
1	B	642	GLN
1	C	147	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 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	1301	-	28,29,29	3.13	11 (39%)	36,45,45	1.53	5 (13%)
3	AJP	A	1302	-	95,95,95	0.79	4 (4%)	142,149,149	1.32	19 (13%)
2	ZK1	B	1301	-	28,29,29	3.15	11 (39%)	36,45,45	1.72	8 (22%)
2	ZK1	C	1301	-	28,29,29	3.12	10 (35%)	36,45,45	1.60	5 (13%)
3	AJP	C	1302	-	95,95,95	0.79	4 (4%)	142,149,149	1.32	19 (13%)
2	ZK1	D	1301	-	28,29,29	3.16	11 (39%)	36,45,45	1.78	7 (19%)

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	1301	-	-	0/13/23/23	0/3/3/3
3	AJP	A	1302	-	-	0/28/220/220	0/11/11/11
2	ZK1	B	1301	-	-	0/13/23/23	0/3/3/3
2	ZK1	C	1301	-	-	0/13/23/23	0/3/3/3
3	AJP	C	1302	-	-	0/28/220/220	0/11/11/11
2	ZK1	D	1301	-	-	0/13/23/23	0/3/3/3

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1301	ZK1	PBA-OAD	-3.63	1.46	1.54
2	B	1301	ZK1	PBA-OAD	-3.62	1.46	1.54
2	C	1301	ZK1	PBA-OAD	-3.61	1.46	1.54
2	A	1301	ZK1	PBA-OAD	-3.59	1.46	1.54
3	A	1302	AJP	CCI-CCJ	-2.70	1.50	1.54

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1301	ZK1	CAI-CAR-NAX	-4.15	117.02	122.69
2	B	1301	ZK1	CAI-CAR-NAX	-3.95	117.29	122.69
3	A	1302	AJP	CCX-OCY-CCZ	-3.89	109.32	115.32
3	C	1302	AJP	CCX-OCY-CCZ	-3.87	109.35	115.32
3	C	1302	AJP	C1-O1-CAR	-3.51	109.45	118.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301	ZK1	1	0
3	A	1302	AJP	23	0
2	B	1301	ZK1	2	0
2	C	1301	ZK1	1	0
3	C	1302	AJP	24	0
2	D	1301	ZK1	1	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.