



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:18 PM BST

PDB ID : 5FTM
EMDB ID: : EMD-3298
Title : Cryo-EM structure of human p97 bound to ATPgS (Conformation II)
Authors : Banerjee, S.; Bartesaghi, A.; Merk, A.; Rao, P.; Bulfer, S.L.; Yan, Y.; Green, N.; Mroczkowski, B.; Neitz, R.J.; Wipf, P.; Falconieri, V.; Deshaies, R.J.; Milne, J.L.S.; Hury, D.; Arkin, M.; Subramaniam, S.
Deposited on : 2016-01-14
Resolution : 3.20 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

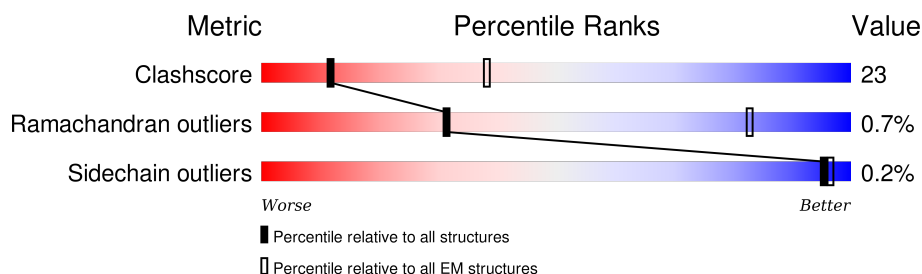
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	806	52% 37% • 10%
1	B	806	53% 37% • 10%
1	C	806	52% 37% • 10%
1	D	806	53% 37% • 10%
1	E	806	53% 36% • 10%
1	F	806	53% 36% • 10%

2 Entry composition [i](#)

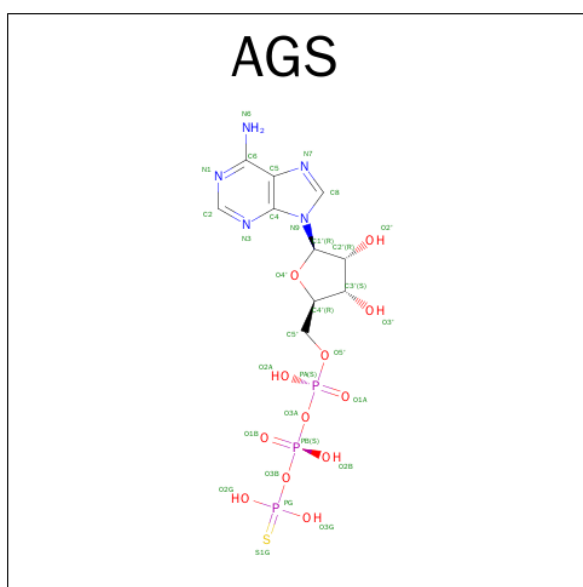
There are 4 unique types of molecules in this entry. The entry contains 34554 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE.

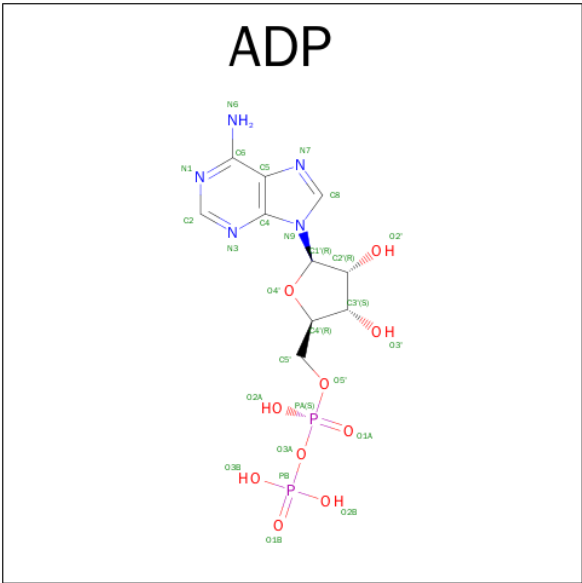
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	728	Total	C	N	O	S	0	0
			5700	3586	1005	1079	30		
1	B	728	Total	C	N	O	S	0	0
			5700	3586	1005	1079	30		
1	C	728	Total	C	N	O	S	0	0
			5700	3586	1005	1079	30		
1	D	728	Total	C	N	O	S	0	0
			5700	3586	1005	1079	30		
1	E	728	Total	C	N	O	S	0	0
			5700	3586	1005	1079	30		
1	F	728	Total	C	N	O	S	0	0
			5700	3586	1005	1079	30		

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	F	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

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Mol	Chain	Residues	Atoms					AltConf
3	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

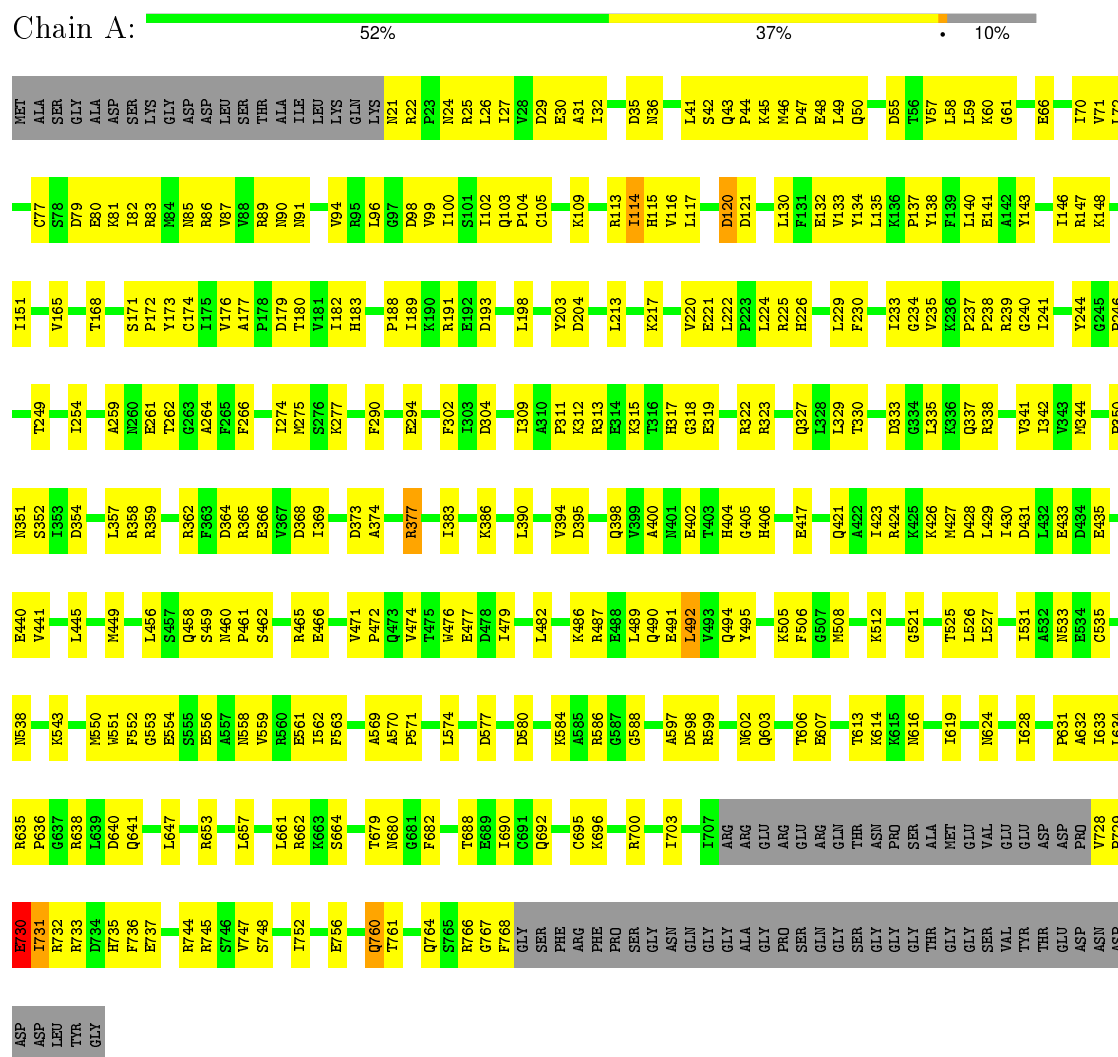
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	D	1	Total	Mg	0
			1	1	
4	E	1	Total	Mg	0
			1	1	
4	B	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	
4	A	1	Total	Mg	0
			1	1	
4	F	1	Total	Mg	0
			1	1	

3 Residue-property plots

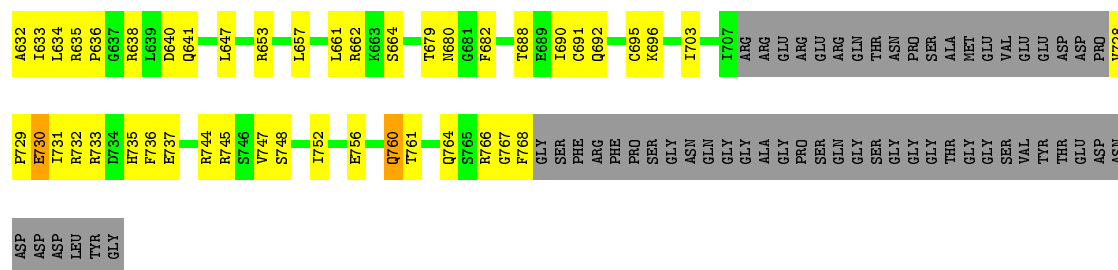
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE



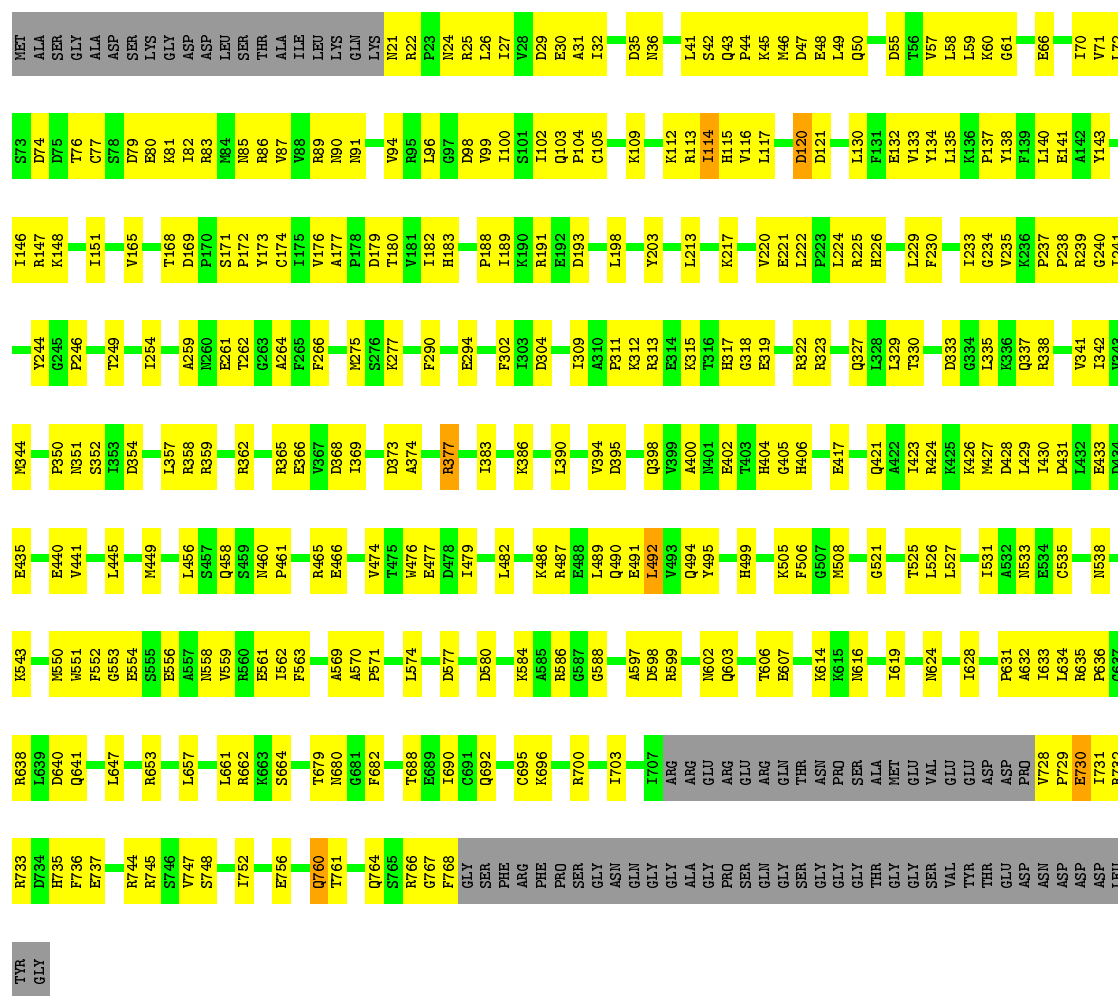
- Molecule 1: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE





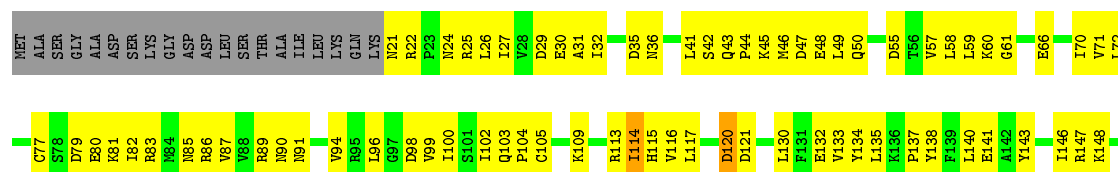
• Molecule 1: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE

Chain D: 53% 37% 10%



• Molecule 1: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE

Chain E: 53% 36% 10%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE, Not provided	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	950	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4K X 4K)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AGS, ADP

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	0.59	0/5793	0.69	3/7822 (0.0%)
1	B	0.59	0/5793	0.68	1/7822 (0.0%)
1	C	0.59	0/5793	0.68	1/7822 (0.0%)
1	D	0.59	0/5793	0.68	1/7822 (0.0%)
1	E	0.59	0/5793	0.68	1/7822 (0.0%)
1	F	0.59	0/5793	0.68	1/7822 (0.0%)
All	All	0.59	0/34758	0.68	8/46932 (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	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
All	All	0	12

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	730	GLU	CB-CA-C	7.15	124.70	110.40
1	A	731	ILE	N-CA-C	-6.49	93.49	111.00
1	C	104	PRO	C-N-CA	-5.82	107.14	121.70
1	B	104	PRO	C-N-CA	-5.82	107.15	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	104	PRO	C-N-CA	-5.82	107.16	121.70

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	359	ARG	Sidechain
1	A	377	ARG	Sidechain
1	B	359	ARG	Sidechain
1	B	377	ARG	Sidechain
1	C	359	ARG	Sidechain

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	5700	0	5769	285	0
1	B	5700	0	5769	285	0
1	C	5700	0	5769	287	0
1	D	5700	0	5769	285	0
1	E	5700	0	5769	288	0
1	F	5700	0	5769	288	0
2	A	31	0	12	6	0
2	B	31	0	12	6	0
2	C	31	0	12	6	0
2	D	31	0	12	6	0
2	E	31	0	12	6	0
2	F	31	0	12	6	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	0	0
3	E	27	0	12	0	0
3	F	27	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
All	All	34554	0	34758	1584	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 23.

The worst 5 of 1584 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:F:312:LYS:HD3	1:F:315:LYS:HD3	1.29	1.15
1:E:312:LYS:HD3	1:E:315:LYS:HD3	1.29	1.15
1:D:312:LYS:HD3	1:D:315:LYS:HD3	1.29	1.12
1:A:312:LYS:HD3	1:A:315:LYS:HD3	1.29	1.12
1:C:312:LYS:HD2	1:C:315:LYS:HB2	1.32	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	724/806 (90%)	664 (92%)	55 (8%)	5 (1%)	26	72
1	B	724/806 (90%)	664 (92%)	55 (8%)	5 (1%)	26	72
1	C	724/806 (90%)	664 (92%)	55 (8%)	5 (1%)	26	72
1	D	724/806 (90%)	664 (92%)	55 (8%)	5 (1%)	26	72
1	E	724/806 (90%)	664 (92%)	54 (8%)	6 (1%)	24	69
1	F	724/806 (90%)	664 (92%)	55 (8%)	5 (1%)	26	72
All	All	4344/4836 (90%)	3984 (92%)	329 (8%)	31 (1%)	31	72

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	730	GLU
1	C	730	GLU
1	D	730	GLU
1	E	730	GLU
1	F	730	GLU

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	619/678 (91%)	618 (100%)	1 (0%)	95	99
1	B	619/678 (91%)	618 (100%)	1 (0%)	95	99
1	C	619/678 (91%)	618 (100%)	1 (0%)	95	99
1	D	619/678 (91%)	618 (100%)	1 (0%)	95	99
1	E	619/678 (91%)	618 (100%)	1 (0%)	95	99
1	F	619/678 (91%)	618 (100%)	1 (0%)	95	99
All	All	3714/4068 (91%)	3708 (100%)	6 (0%)	95	99

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	492	LEU
1	F	492	LEU
1	D	492	LEU
1	B	492	LEU
1	E	492	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	692	GLN
1	D	499	HIS

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Mol	Chain	Res	Type
1	F	533	ASN
1	D	36	ASN
1	D	533	ASN

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](#)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

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	AGS	A	901	4	26,33,33	2.22	4 (15%)	24,52,52	1.80	2 (8%)
3	ADP	A	902	-	24,29,29	1.11	2 (8%)	23,45,45	1.79	2 (8%)
2	AGS	B	901	4	26,33,33	2.21	4 (15%)	24,52,52	1.79	2 (8%)
3	ADP	B	902	-	24,29,29	1.11	2 (8%)	23,45,45	1.79	2 (8%)
2	AGS	C	901	4	26,33,33	2.21	4 (15%)	24,52,52	1.79	2 (8%)
3	ADP	C	902	-	24,29,29	1.11	2 (8%)	23,45,45	1.80	2 (8%)
2	AGS	D	901	4	26,33,33	2.22	4 (15%)	24,52,52	1.81	2 (8%)
3	ADP	D	902	-	24,29,29	1.11	2 (8%)	23,45,45	1.79	2 (8%)
2	AGS	E	901	4	26,33,33	2.21	4 (15%)	24,52,52	1.81	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	E	902	-	24,29,29	1.11	2 (8%)	23,45,45	1.79	2 (8%)
2	AGS	F	901	4	26,33,33	2.21	4 (15%)	24,52,52	1.80	2 (8%)
3	ADP	F	902	-	24,29,29	1.10	2 (8%)	23,45,45	1.79	2 (8%)

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	AGS	A	901	4	-	0/17/38/38	0/3/3/3
3	ADP	A	902	-	-	0/12/32/32	0/3/3/3
2	AGS	B	901	4	-	0/17/38/38	0/3/3/3
3	ADP	B	902	-	-	0/12/32/32	0/3/3/3
2	AGS	C	901	4	-	0/17/38/38	0/3/3/3
3	ADP	C	902	-	-	0/12/32/32	0/3/3/3
2	AGS	D	901	4	-	0/17/38/38	0/3/3/3
3	ADP	D	902	-	-	0/12/32/32	0/3/3/3
2	AGS	E	901	4	-	0/17/38/38	0/3/3/3
3	ADP	E	902	-	-	0/12/32/32	0/3/3/3
2	AGS	F	901	4	-	0/17/38/38	0/3/3/3
3	ADP	F	902	-	-	0/12/32/32	0/3/3/3

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	901	AGS	PG-O3G	-2.60	1.48	1.55
2	F	901	AGS	PG-O3G	-2.60	1.48	1.55
2	A	901	AGS	PG-O3G	-2.59	1.48	1.55
2	D	901	AGS	PG-O3G	-2.59	1.48	1.55
2	C	901	AGS	PG-O3G	-2.58	1.48	1.55

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	901	AGS	N3-C2-N1	-6.61	123.68	128.87
2	E	901	AGS	N3-C2-N1	-6.59	123.70	128.87
2	F	901	AGS	N3-C2-N1	-6.58	123.71	128.87
2	A	901	AGS	N3-C2-N1	-6.57	123.71	128.87
2	B	901	AGS	N3-C2-N1	-6.53	123.75	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	AGS	6	0
2	B	901	AGS	6	0
2	C	901	AGS	6	0
2	D	901	AGS	6	0
2	E	901	AGS	6	0
2	F	901	AGS	6	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.