



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:22 PM BST

PDB ID : 5FTN
EMDB ID: : EMD-3299
Title : Cryo-EM structure of human p97 bound to ATPgS (Conformation III)
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 : 3.30 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

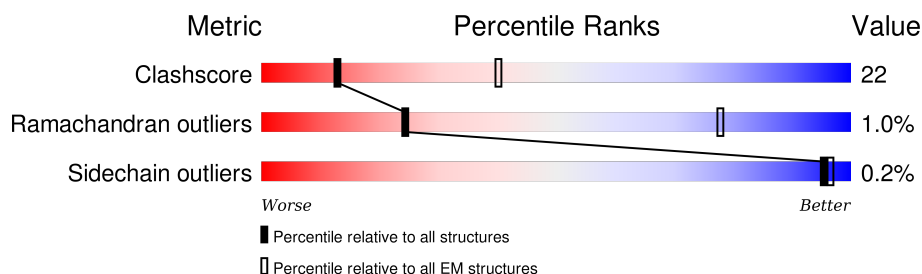
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	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	59% 31% • 9%
1	B	806	59% 31% • 9%
1	C	806	59% 31% • 9%
1	D	806	59% 31% • 9%
1	E	806	59% 31% • 9%
1	F	806	59% 31% • 9%

2 Entry composition [i](#)

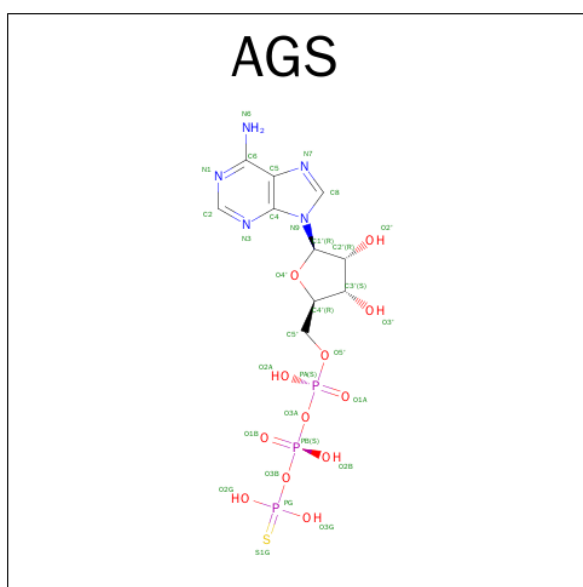
There are 3 unique types of molecules in this entry. The entry contains 34956 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	737	Total	C	N	O	S	0	0
			5762	3627	1014	1091	30		
1	B	737	Total	C	N	O	S	0	0
			5762	3627	1014	1091	30		
1	C	737	Total	C	N	O	S	0	0
			5762	3627	1014	1091	30		
1	D	737	Total	C	N	O	S	0	0
			5762	3627	1014	1091	30		
1	E	737	Total	C	N	O	S	0	0
			5762	3627	1014	1091	30		
1	F	737	Total	C	N	O	S	0	0
			5762	3627	1014	1091	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
			62	20	10	24	6	2	
2	A	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	B	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	B	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	C	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	C	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	D	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	D	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	E	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	E	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	F	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	F	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	

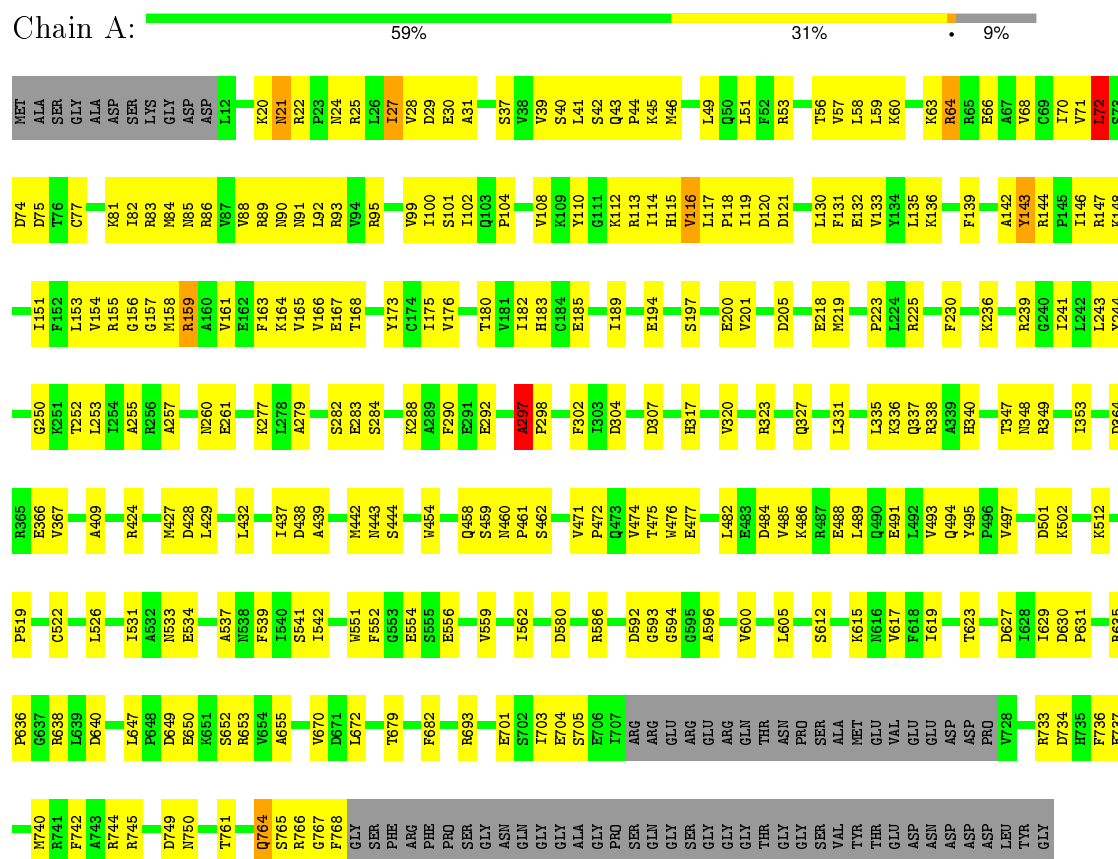
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
3	D	2	Total	Mg	0
			2	2	
3	E	2	Total	Mg	0
			2	2	
3	B	2	Total	Mg	0
			2	2	
3	C	2	Total	Mg	0
			2	2	
3	A	2	Total	Mg	0
			2	2	
3	F	2	Total	Mg	0
			2	2	

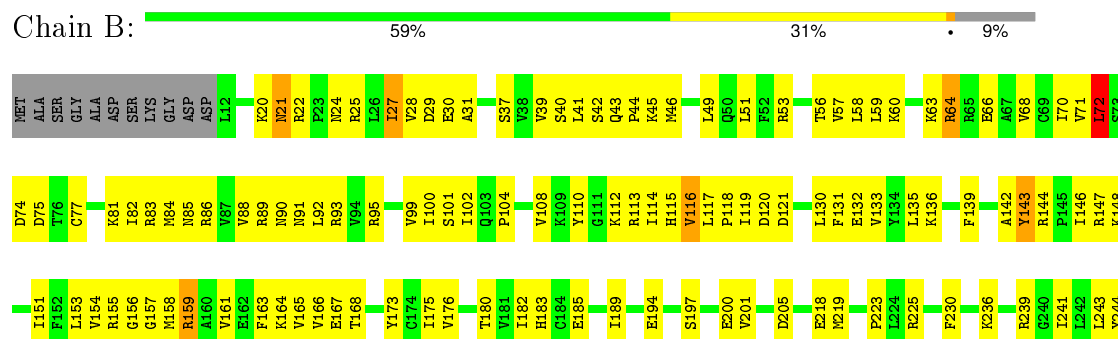
3 Residue-property plots

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



M740	R741	F742	A743	R744	R745	D749	N750	T761	O764	S765	R766	F767	F768	GLY	SER	PHE	ARG	PHE	PRO	SER	GLY	ASN	GLN	GLY	GLY	ALA	GLY	PRO	SER	GLN	GLY	SER	ARG	ARG	GLU	GLU	GLY	SER	ARG	GLY	GLY	GLN	THR	GLY	ASN	PRO	SER	VAL	THR	THR	GLU	ASP	ASP	ASP	ASP	LEU	TYR	GLY
P636	G637	R638	L639	D640	L647	F648	D649	S652	R653	V654	A655	V670	D671	L672	T679	F682	R693	E701	S702	I703	E704	S705	F706	I707	ARG	ARG	ARG	ARG	ARG	GLN	THR	ASN	PRO	SER	ALA	ALA	MET	GLU	VAL	GLU	ASP	GLU	ASP	ASP	ASP	ASP	PRO	V728	R733	D734	F736	E737						
P519	C522	L526	L531	A532	E533	E534	A537	N538	F539	S541	I542	V551	F552	G553	E554	S555	E556	V559	I562	D580	R586	D592	G593	G594	G595	A596	V600	L605	S612	R615	N616	V617	F618	I619	T623	D627	I628	I629	D630	P631	R635																	
R366	E366	V367	A409	R424	M427	D428	L429	L432	I437	D438	A439	M442	N443	S444	W454	Q458	S459	M460	P461	S462	V471	P472	Q473	V474	T475	W476	E477	L482	E483	D484	V485	K486	R487	E488	L489	Q490	E491	I492	V493	Q494	Y495	P496	V497	D501	K502	K512												
D74	D75	C77	K81	I82	R83	R84	N85	R86	V87	V88	R89	I90	N91	L92	R93	V94	A95	V99	I100	S101	I102	Q103	P104	V108	K109	I110	E111	K112	R113	I114	H115	V116	L117	P118	I119	D120	D121	L130	F131	E132	V133	V134	L135	K136	F139	A142	Y143	R144	F145	I146	R147	K148						
I151	F152	L153	V154	R155	G156	G157	M158	R159	A160	V161	F162	F163	K164	V165	V166	E167	T168	Y173	C174	I175	V176	T180	V181	I182	H183	G184	E185	I189	E194	S197	E200	V201	D205	E218	M219	P223	L224	R225	F230	K236	R239	G240	I241	L242	I243	Y244												
G250	K251	T252	L253	L254	A255	K256	A257	N260	E261	K277	L278	A279	S282	E283	S284	K288	A289	F290	E291	E292	K297	P298	F302	I303	D304	D307	E317	V320	R323	Q327	L331	L335	K336	Q337	R338	A339	R340	T347	N348	R349	T353	D364																

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	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

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	0.50	0/5855	0.65	3/7905 (0.0%)
1	B	0.50	0/5855	0.65	3/7905 (0.0%)
1	C	0.50	0/5855	0.65	3/7905 (0.0%)
1	D	0.50	0/5855	0.65	3/7905 (0.0%)
1	E	0.50	0/5855	0.65	3/7905 (0.0%)
1	F	0.50	0/5855	0.65	3/7905 (0.0%)
All	All	0.50	0/35130	0.65	18/47430 (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	6
1	B	0	6
1	C	0	6
1	D	0	6
1	E	0	6
1	F	0	6
All	All	0	36

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	143	TYR	C-N-CA	5.73	136.03	121.70
1	C	143	TYR	C-N-CA	5.73	136.02	121.70
1	A	143	TYR	C-N-CA	5.71	135.98	121.70
1	D	143	TYR	C-N-CA	5.71	135.98	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	143	TYR	C-N-CA	5.71	135.98	121.70

There are no chirality outliers.

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	ALA	Peptide
1	A	144	ARG	Peptide
1	A	156	GLY	Peptide
1	A	64	ARG	Peptide
1	A	72	LEU	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	5762	0	5841	259	0
1	B	5762	0	5841	258	0
1	C	5762	0	5841	261	0
1	D	5762	0	5841	261	0
1	E	5762	0	5841	258	0
1	F	5762	0	5841	261	0
2	A	62	0	24	10	0
2	B	62	0	24	10	0
2	C	62	0	24	10	0
2	D	62	0	24	9	0
2	E	62	0	24	10	0
2	F	62	0	24	10	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
All	All	34956	0	35190	1518	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 22.

The worst 5 of 1518 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:B:113:ARG:NH2	1:B:131:PHE:CE2	2.26	1.03
1:C:113:ARG:NH2	1:C:131:PHE:CE2	2.26	1.03
1:D:113:ARG:NH2	1:D:131:PHE:CE2	2.26	1.03
1:A:113:ARG:NH2	1:A:131:PHE:CE2	2.26	1.03
1:F:113:ARG:NH2	1:F:131:PHE:CE2	2.26	1.02

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	733/806 (91%)	672 (92%)	54 (7%)	7 (1%)	19	58
1	B	733/806 (91%)	671 (92%)	55 (8%)	7 (1%)	19	58
1	C	733/806 (91%)	672 (92%)	54 (7%)	7 (1%)	19	58
1	D	733/806 (91%)	672 (92%)	54 (7%)	7 (1%)	19	58
1	E	733/806 (91%)	672 (92%)	54 (7%)	7 (1%)	19	58
1	F	733/806 (91%)	672 (92%)	54 (7%)	7 (1%)	19	58
All	All	4398/4836 (91%)	4031 (92%)	325 (7%)	42 (1%)	24	58

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	297	ALA
1	B	297	ALA
1	C	297	ALA
1	D	297	ALA
1	E	297	ALA

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	626/678 (92%)	625 (100%)	1 (0%)	95	98
1	B	626/678 (92%)	625 (100%)	1 (0%)	95	98
1	C	626/678 (92%)	625 (100%)	1 (0%)	95	98
1	D	626/678 (92%)	625 (100%)	1 (0%)	95	98
1	E	626/678 (92%)	625 (100%)	1 (0%)	95	98
1	F	626/678 (92%)	625 (100%)	1 (0%)	95	98
All	All	3756/4068 (92%)	3750 (100%)	6 (0%)	95	98

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

Mol	Chain	Res	Type
1	C	474	VAL
1	F	474	VAL
1	D	474	VAL
1	B	474	VAL
1	E	474	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	337	GLN
1	D	317	HIS
1	F	327	GLN
1	D	91	ASN
1	D	327	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 ⓘ

Of 24 ligands modelled in this entry, 12 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	-	26,33,33	2.19	4 (15%)	24,52,52	1.76	2 (8%)
2	AGS	A	902	-	26,33,33	2.19	4 (15%)	24,52,52	1.80	2 (8%)
2	AGS	B	901	-	26,33,33	2.19	4 (15%)	24,52,52	1.75	2 (8%)
2	AGS	B	902	-	26,33,33	2.19	4 (15%)	24,52,52	1.81	2 (8%)
2	AGS	C	901	-	26,33,33	2.20	4 (15%)	24,52,52	1.76	2 (8%)
2	AGS	C	902	-	26,33,33	2.20	4 (15%)	24,52,52	1.80	2 (8%)
2	AGS	D	901	-	26,33,33	2.19	4 (15%)	24,52,52	1.76	2 (8%)
2	AGS	D	902	-	26,33,33	2.20	4 (15%)	24,52,52	1.80	2 (8%)
2	AGS	E	901	-	26,33,33	2.20	4 (15%)	24,52,52	1.76	2 (8%)
2	AGS	E	902	-	26,33,33	2.20	4 (15%)	24,52,52	1.79	2 (8%)
2	AGS	F	901	-	26,33,33	2.19	4 (15%)	24,52,52	1.75	2 (8%)
2	AGS	F	902	-	26,33,33	2.19	4 (15%)	24,52,52	1.80	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	-	-	0/17/38/38	0/3/3/3
2	AGS	A	902	-	-	0/17/38/38	0/3/3/3
2	AGS	B	901	-	-	0/17/38/38	0/3/3/3
2	AGS	B	902	-	-	0/17/38/38	0/3/3/3
2	AGS	C	901	-	-	0/17/38/38	0/3/3/3
2	AGS	C	902	-	-	0/17/38/38	0/3/3/3
2	AGS	D	901	-	-	0/17/38/38	0/3/3/3
2	AGS	D	902	-	-	0/17/38/38	0/3/3/3
2	AGS	E	901	-	-	0/17/38/38	0/3/3/3
2	AGS	E	902	-	-	0/17/38/38	0/3/3/3
2	AGS	F	901	-	-	0/17/38/38	0/3/3/3
2	AGS	F	902	-	-	0/17/38/38	0/3/3/3

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	901	AGS	PG-O3G	-2.62	1.48	1.55
2	E	901	AGS	PG-O3G	-2.62	1.48	1.55
2	A	901	AGS	PG-O3G	-2.62	1.48	1.55
2	D	901	AGS	PG-O3G	-2.62	1.48	1.55
2	F	901	AGS	PG-O3G	-2.62	1.48	1.55

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	902	AGS	N3-C2-N1	-6.60	123.68	128.87
2	C	902	AGS	N3-C2-N1	-6.54	123.73	128.87
2	F	902	AGS	N3-C2-N1	-6.54	123.73	128.87
2	A	902	AGS	N3-C2-N1	-6.54	123.74	128.87
2	D	902	AGS	N3-C2-N1	-6.54	123.74	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 59 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	AGS	8	0
2	A	902	AGS	2	0
2	B	901	AGS	8	0
2	B	902	AGS	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	901	AGS	7	0
2	C	902	AGS	3	0
2	D	901	AGS	7	0
2	D	902	AGS	2	0
2	E	901	AGS	7	0
2	E	902	AGS	3	0
2	F	901	AGS	8	0
2	F	902	AGS	2	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.