



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 06:53 AM GMT

PDB ID : 1XPU
Title : Structural mechanism of inhibition of the Rho transcription termination factor by the antibiotic 5a-(3-formylphenylsulfanyl)-dihydrobicyclomycin(FPDB)
Authors : Skordalakes, E.; Brogan, A.P.; Park, B.S.; Kohn, H.; Berger, J.M.
Deposited on : 2004-10-09
Resolution : 3.05 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

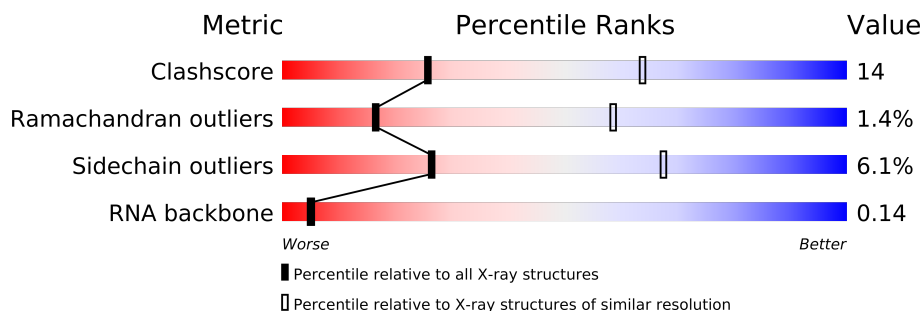
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	FAILED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.05 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	2629 (3.12-3.00)
Ramachandran outliers	78287	2536 (3.12-3.00)
Sidechain outliers	78261	2539 (3.12-3.00)
RNA backbone	1838	1006 (3.52-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	G	8	
1	H	8	
1	J	8	
1	K	8	
1	L	8	
1	M	8	
2	A	419	
2	B	419	
2	C	419	
2	D	419	
2	E	419	
2	F	419	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19873 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 RNA chain called 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			
1	M	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			
1	H	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			
1	J	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			
1	K	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			
1	L	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			

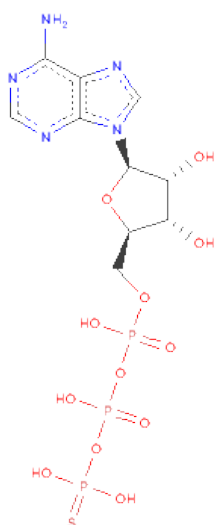
- Molecule 2 is a protein called Rho transcription termination factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	408	Total	C	N	O	S	0	0	0
			3213	2028	564	604	17			
2	B	408	Total	C	N	O	S	0	0	0
			3213	2028	564	604	17			
2	C	408	Total	C	N	O	S	0	0	0
			3213	2028	564	604	17			
2	D	408	Total	C	N	O	S	0	0	0
			3213	2028	564	604	17			
2	E	407	Total	C	N	O	S	0	0	0
			3206	2023	563	603	17			
2	F	408	Total	C	N	O	S	0	0	0
			3213	2028	564	604	17			

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

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

- Molecule 4 is PHOSPHOTHIOPHOSPHORICACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



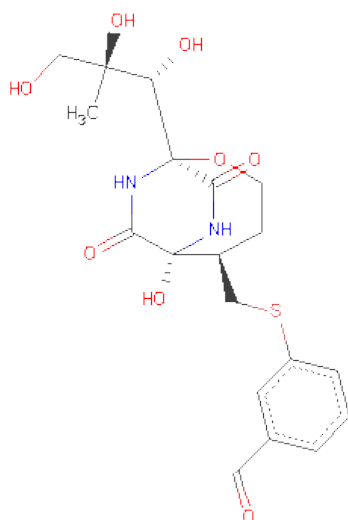
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	C	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	E	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	E	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 5 is 5A-(3-FORMYLPHENYLSULFANYL)-DIHYDROBICYCLOMYCIN (three-letter code: FPD) (formula: C₁₉H₂₄N₂O₈S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			30	19	2	8	1		
5	C	1	Total	C	N	O	S	0	0
			30	19	2	8	1		
5	D	1	Total	C	N	O	S	0	0
			30	19	2	8	1		
5	E	1	Total	C	N	O	S	0	0
			30	19	2	8	1		
5	F	1	Total	C	N	O	S	0	0
			30	19	2	8	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total O 2 2	0	0
6	B	5	Total O 5 5	0	0
6	C	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	4	Total 4	O 4	0	0
6	E	3	Total 3	O 3	0	0
6	F	1	Total 1	O 1	0	0
6	G	1	Total 1	O 1	0	0
6	H	1	Total 1	O 1	0	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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

Note EDS failed to run properly.

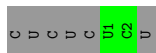
- Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'

Chain G: 



- Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'

Chain M: 



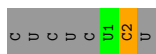
- Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'

Chain H: 



- Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'

Chain J: 



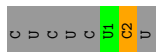
- Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'

Chain K: 



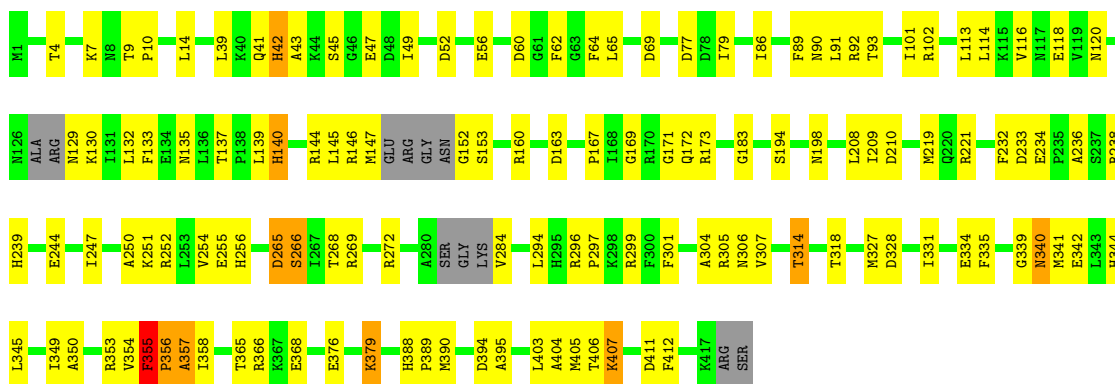
- Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'

Chain L: 



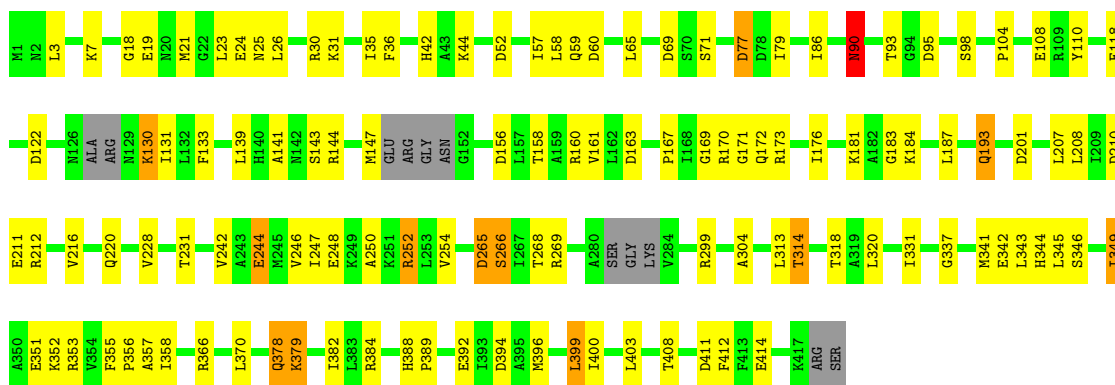
- Molecule 2: Rho transcription termination factor

Chain A: 



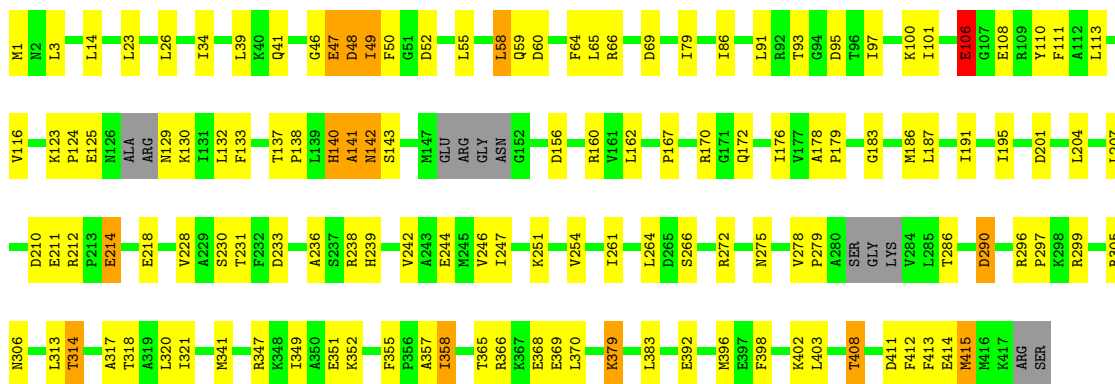
• Molecule 2: Rho transcription termination factor

Chain B:



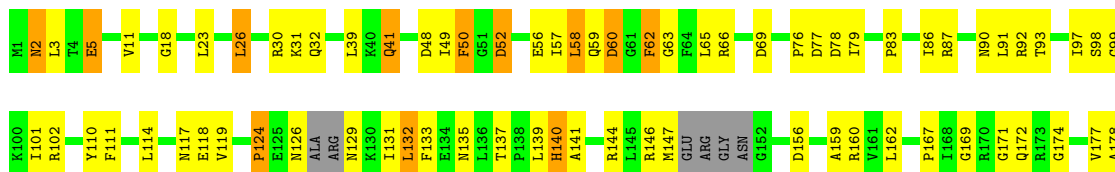
• Molecule 2: Rho transcription termination factor

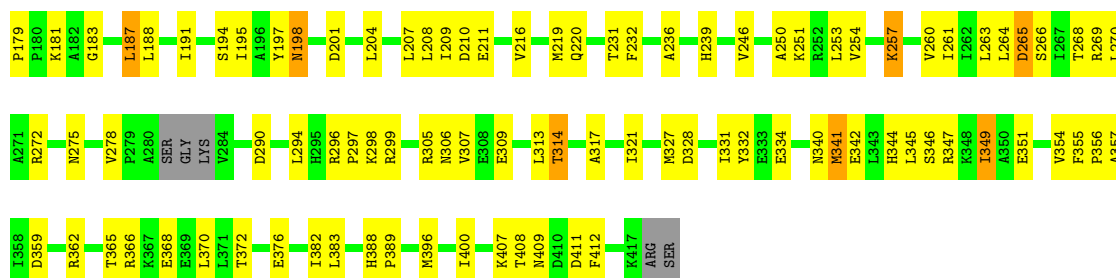
Chain C:



• Molecule 2: Rho transcription termination factor

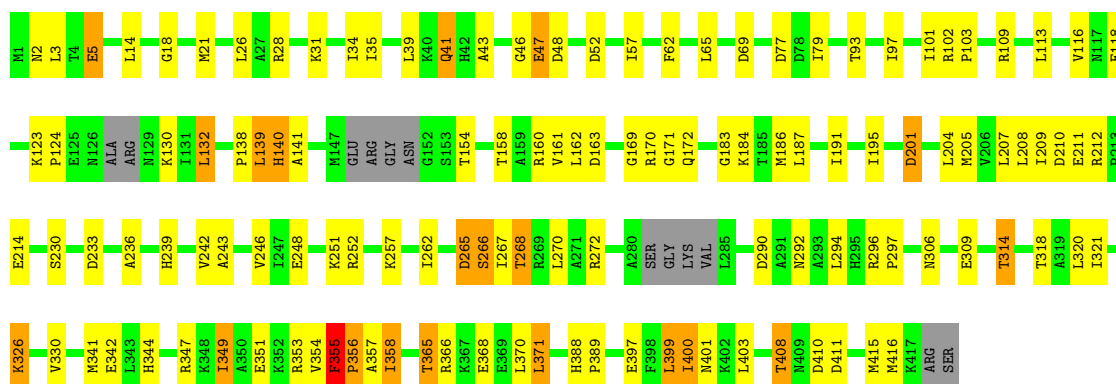
Chain D:





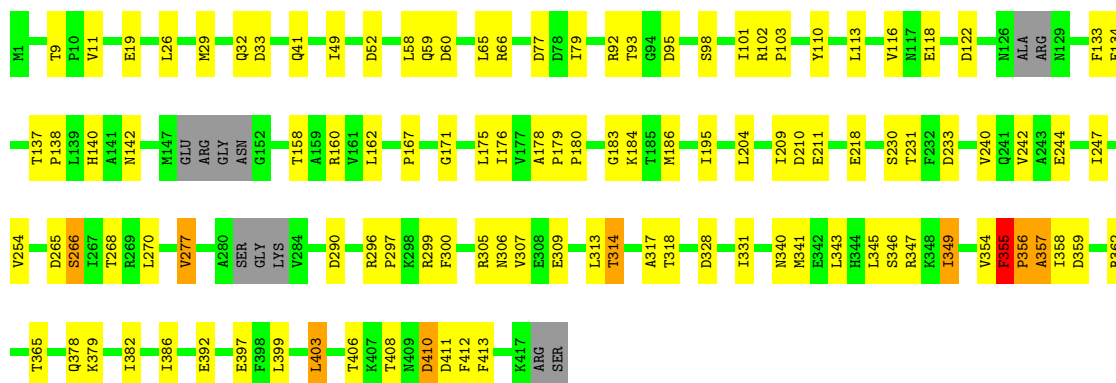
• Molecule 2: Rho transcription termination factor

Chain E:



• Molecule 2: Rho transcription termination factor

Chain F:



4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	119.48Å 206.94Å 148.61Å 90.00° 96.95° 90.00°	Depositor
Resolution (Å)	20.00 – 3.05	Depositor
% Data completeness (in resolution range)	86.5 (20.00-3.05)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.92 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.276 , 0.295	Depositor
Wilson B-factor (Å ²)	92.4	Xtriage
Anisotropy	0.209	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 60868 reflections (0.003%)	Xtriage
Total number of atoms	19873	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FPD, 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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	G	0.72	0/43	1.27	1/64 (1.6%)
1	H	0.88	0/43	1.42	1/64 (1.6%)
1	J	0.70	0/43	1.22	0/64
1	K	0.90	0/43	1.60	2/64 (3.1%)
1	L	0.67	0/43	1.08	0/64
1	M	0.81	0/43	1.21	0/64
2	A	0.30	0/3259	0.65	7/4387 (0.2%)
2	B	0.30	0/3259	0.67	12/4387 (0.3%)
2	C	0.30	0/3259	0.65	9/4387 (0.2%)
2	D	0.30	0/3259	0.65	9/4387 (0.2%)
2	E	0.30	0/3252	0.67	11/4377 (0.3%)
2	F	0.30	0/3259	0.64	11/4387 (0.3%)
All	All	0.31	0/19805	0.67	63/26696 (0.2%)

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
2	A	0	1
2	E	0	1
2	F	0	1
All	All	0	3

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	1	U	P-O3'-C3'	6.60	127.61	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	77	ASP	CB-CG-OD2	6.21	123.89	118.30
2	D	77	ASP	CB-CG-OD2	6.21	123.89	118.30
2	F	233	ASP	CB-CG-OD2	6.08	123.77	118.30
2	F	290	ASP	CB-CG-OD2	6.04	123.73	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	355	PHE	Peptide
2	E	355	PHE	Peptide
2	F	355	PHE	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	40	0	22	0	0
1	H	40	0	22	2	0
1	J	40	0	22	3	0
1	K	40	0	22	2	0
1	L	40	0	22	2	0
1	M	40	0	22	0	0
2	A	3213	0	3289	106	0
2	B	3213	0	3288	76	0
2	C	3213	0	3289	81	0
2	D	3213	0	3289	118	0
2	E	3206	0	3279	87	0
2	F	3213	0	3288	62	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	31	0	12	4	0
4	B	31	0	12	6	0
4	C	31	0	12	7	0
4	D	31	0	12	5	0
4	E	62	0	24	16	0
5	B	30	0	24	6	0
5	C	30	0	24	9	0
5	D	30	0	24	8	0
5	E	30	0	24	11	0
5	F	30	0	24	3	0
6	A	2	0	0	0	0
6	B	5	0	0	1	0
6	C	3	0	0	0	0
6	D	4	0	0	1	0
6	E	3	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
All	All	19873	0	20046	539	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

The worst 5 of 539 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:366:ARG:NE	4:D:4600:AGS:S1G	2.12	1.22
2:A:366:ARG:NE	4:B:2600:AGS:S1G	2.13	1.20
2:D:356:PRO:HG3	2:D:400:ILE:HD11	1.26	1.15
2:B:366:ARG:NE	4:C:3600:AGS:S1G	2.23	1.11
2:D:366:ARG:NE	4:E:5600:AGS:S1G	2.24	1.11

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. 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	
2	A	400/419 (96%)	368 (92%)	25 (6%)	7 (2%)	13	52
2	B	400/419 (96%)	366 (92%)	32 (8%)	2 (0%)	38	82
2	C	400/419 (96%)	364 (91%)	29 (7%)	7 (2%)	13	52
2	D	400/419 (96%)	358 (90%)	37 (9%)	5 (1%)	18	60
2	E	399/419 (95%)	368 (92%)	25 (6%)	6 (2%)	15	57
2	F	400/419 (96%)	366 (92%)	28 (7%)	6 (2%)	15	57
All	All	2399/2514 (95%)	2190 (91%)	176 (7%)	33 (1%)	16	58

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	47	GLU
2	C	140	HIS
2	E	356	PRO
2	E	358	ILE
2	F	355	PHE

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 X-ray entries followed by that with respect to entries of similar resolution. 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	
2	A	351/359 (98%)	331 (94%)	20 (6%)	29	70
2	B	351/359 (98%)	331 (94%)	20 (6%)	29	70
2	C	351/359 (98%)	327 (93%)	24 (7%)	22	62
2	D	351/359 (98%)	329 (94%)	22 (6%)	25	66
2	E	350/359 (98%)	325 (93%)	25 (7%)	21	60
2	F	351/359 (98%)	333 (95%)	18 (5%)	33	75
All	All	2105/2154 (98%)	1976 (94%)	129 (6%)	26	67

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	352	LYS
2	D	140	HIS

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Mol	Chain	Res	Type
2	F	210	ASP
2	C	383	LEU
2	D	5	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	142	ASN
2	C	275	ASN
2	E	374	GLN
2	C	172	GLN
2	C	193	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	G	2/8 (25%)	1 (50%)	1 (50%)
1	H	2/8 (25%)	1 (50%)	1 (50%)
1	J	1/8 (12%)	1 (100%)	0
1	K	2/8 (25%)	1 (50%)	1 (50%)
1	L	1/8 (12%)	1 (100%)	0
1	M	1/8 (12%)	0	0
All	All	9/48 (18%)	5 (55%)	3 (33%)

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	G	2	C
1	H	2	C
1	J	2	C
1	K	2	C
1	L	2	C

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	G	1	U
1	H	1	U
1	K	1	U

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 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 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$
4	AGS	A	1600	3	33,33,33	1.97	5 (15%)	52,52,52	2.82	10 (19%)
4	AGS	B	2600	3	33,33,33	1.87	4 (12%)	52,52,52	4.31	9 (17%)
5	FPD	B	2701	3	32,32,32	1.22	4 (12%)	49,49,49	3.67	12 (24%)
4	AGS	C	3600	-	33,33,33	1.92	4 (12%)	52,52,52	3.60	9 (17%)
5	FPD	C	3701	-	32,32,32	1.16	2 (6%)	49,49,49	3.58	12 (24%)
4	AGS	D	4600	3	33,33,33	1.86	4 (12%)	52,52,52	4.27	9 (17%)
5	FPD	D	4701	-	32,32,32	1.11	3 (9%)	49,49,49	3.38	11 (22%)
4	AGS	E	5600	-	33,33,33	1.84	4 (12%)	52,52,52	4.31	10 (19%)
5	FPD	E	5701	-	32,32,32	1.12	3 (9%)	49,49,49	3.63	12 (24%)
4	AGS	E	6600	3,2	33,33,33	2.00	4 (12%)	52,52,52	2.04	11 (21%)
5	FPD	F	6701	3	32,32,32	1.16	4 (12%)	49,49,49	3.41	10 (20%)

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
4	AGS	A	1600	3	-	0/21/38/38	0/1/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AGS	B	2600	3	-	0/21/38/38	0/1/3/3
5	FPD	B	2701	3	-	1/20/57/57	0/1/3/3
4	AGS	C	3600	-	-	0/21/38/38	0/1/3/3
5	FPD	C	3701	-	-	1/20/57/57	0/1/3/3
4	AGS	D	4600	3	-	0/21/38/38	0/1/3/3
5	FPD	D	4701	-	-	1/20/57/57	0/1/3/3
4	AGS	E	5600	-	-	0/21/38/38	0/1/3/3
5	FPD	E	5701	-	-	1/20/57/57	0/1/3/3
4	AGS	E	6600	3,2	-	0/21/38/38	0/1/3/3
5	FPD	F	6701	3	-	1/20/57/57	0/1/3/3

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1600	AGS	PG-S1G	7.62	2.04	1.90
4	E	6600	AGS	PG-S1G	7.57	2.04	1.90
4	C	3600	AGS	PG-S1G	7.01	2.03	1.90
4	B	2600	AGS	PG-S1G	6.61	2.02	1.90
4	D	4600	AGS	PG-S1G	6.56	2.02	1.90

The worst 5 of 115 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	5600	AGS	O3B-PG-S1G	-28.75	101.78	114.53
4	B	2600	AGS	O3B-PG-S1G	-28.61	101.84	114.53
4	D	4600	AGS	O3B-PG-S1G	-28.37	101.94	114.53
4	C	3600	AGS	O3B-PG-S1G	-22.91	104.36	114.53
5	E	5701	FPD	C9-C10-C11	-18.33	103.28	108.88

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	4701	FPD	C1-C4-C5-N2
5	B	2701	FPD	C1-C4-C5-N2
5	E	5701	FPD	C1-C4-C5-N2
5	C	3701	FPD	C1-C4-C5-N2
5	F	6701	FPD	C1-C4-C5-N2

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.