wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 11:34 PM GMT

PDB ID	:	1XPR
Title	:	Structural mechanism of inhibition of the Rho transcription termination factor by the antibiotic 5a-formylbicyclomycin (FB)
Authors	:	Skordalakes, E.; Brogan, A.P.; Park, B.S.; Kohn, H.; Berger, J.M.
Deposited on	:	2004-10-09
Resolution	:	3.15 Å(reported)

This is a wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

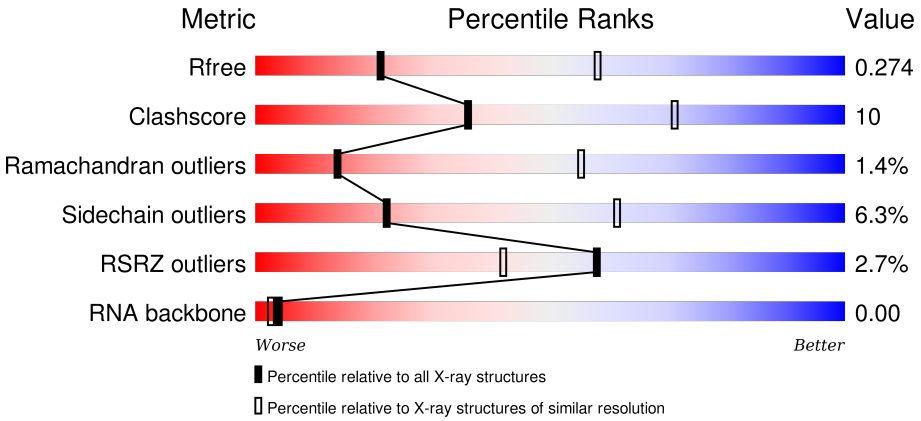
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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.



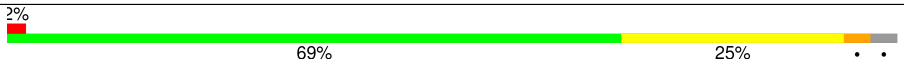
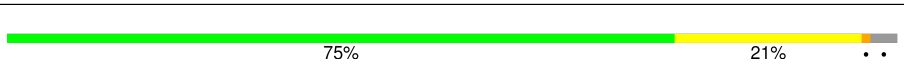
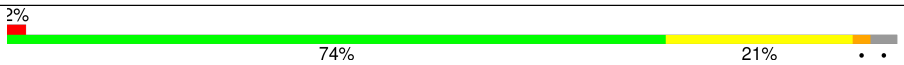
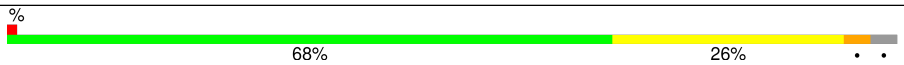
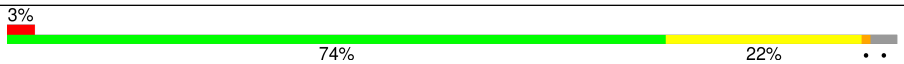
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)
RNA backbone	2183	1046 (3.62-2.70)

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. 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	G	8	25% 13% 13% 75%
1	H	8	25% 13% 13% 75%
1	J	8	13% 25% 75%
1	K	8	25% 13% 13% 75%

Continued on next page...

Continued from previous page...

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

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
4	AGS	B	2600	-	-	X	-
4	AGS	C	3600	-	-	-	X
4	AGS	D	4600	-	-	X	X
4	AGS	E	5600	-	-	-	X
4	AGS	F	6600	-	-	-	X
5	FB	B	2701	-	-	-	X
5	FB	C	3701	-	-	-	X
5	FB	D	4701	-	-	-	X
5	FB	E	5701	-	-	-	X
5	FB	F	6701	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19814 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			39	17	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			

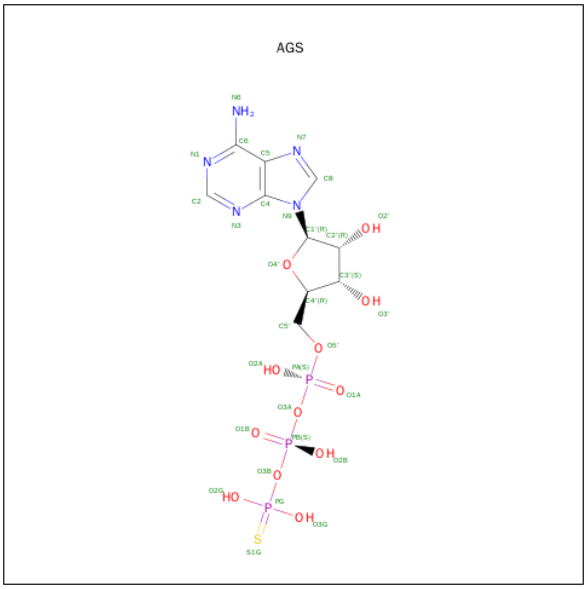
- Molecule 2 is a protein called Rho transcription termination factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	408	Total	C	N	O	S	0	0	0
			3210	2027	564	602	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 PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



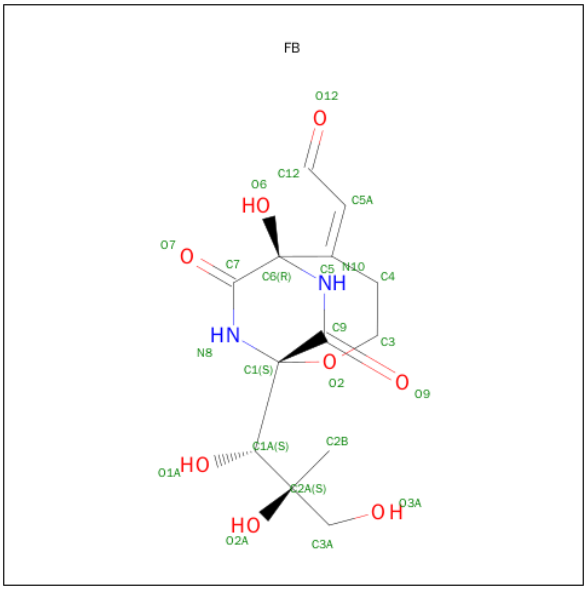
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P S 31 10 5 12 3 1	0	0
4	B	1	Total C N O P S 31 10 5 12 3 1	0	0
4	C	1	Total C N O P S 31 10 5 12 3 1	0	0
4	D	1	Total C N O P S 31 10 5 12 3 1	0	0
4	E	1	Total C N O P S 31 10 5 12 3 1	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 5 is 5A-FORMYLBICYCLOMYCIN (three-letter code: FB) (formula: $C_{13}H_{18}N_2O_8$).



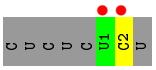
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			23	13	2	8		
5	C	1	Total	C	N	O	0	0
			23	13	2	8		
5	D	1	Total	C	N	O	0	0
			23	13	2	8		
5	E	1	Total	C	N	O	0	0
			23	13	2	8		
5	F	1	Total	C	N	O	0	0
			23	13	2	8		

3 Residue-property plots (i)

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.

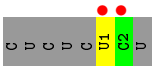
- Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'

Chain G:



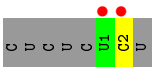
- Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'

Chain M:



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

Chain H:

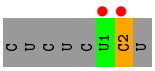


- Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'

Chain J:

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

Chain K:

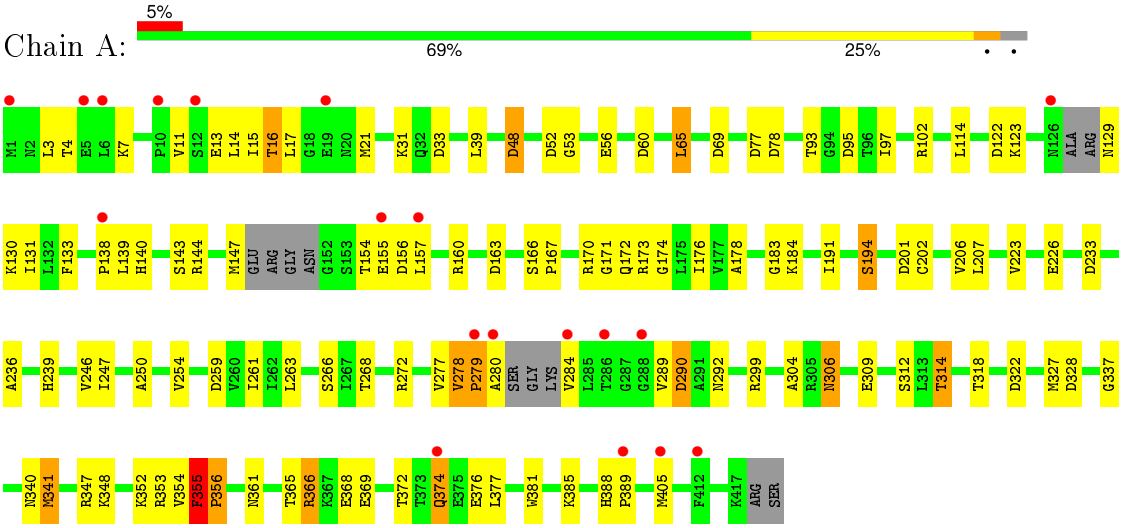


- Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'

Chain L:

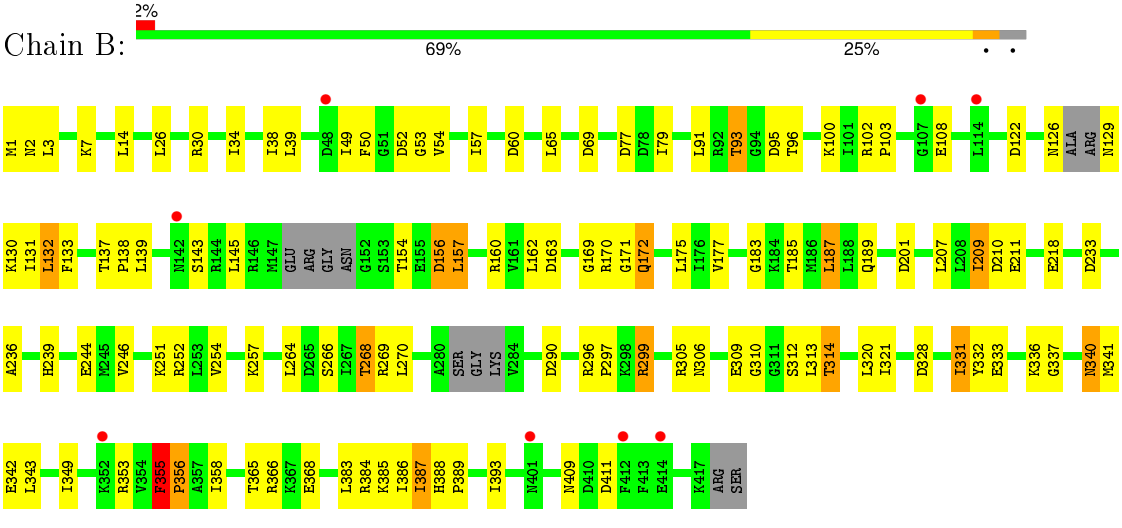
• Molecule 2: Rho transcription termination factor

Chain A:



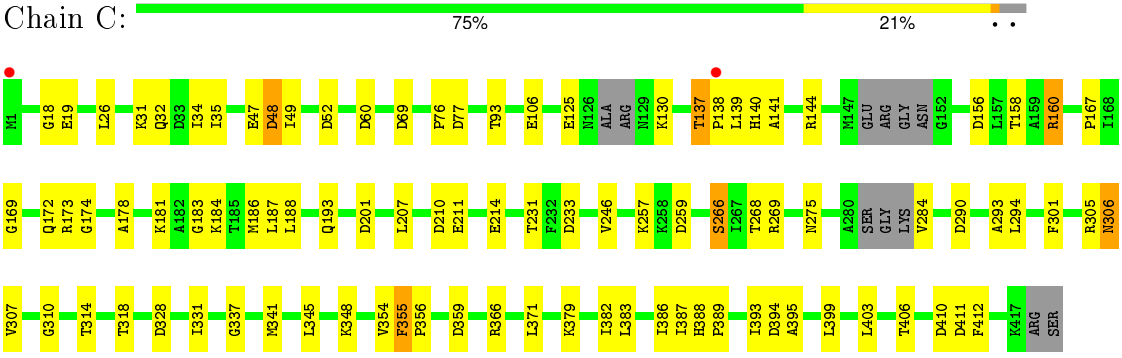
• Molecule 2: Rho transcription termination factor

Chain B:



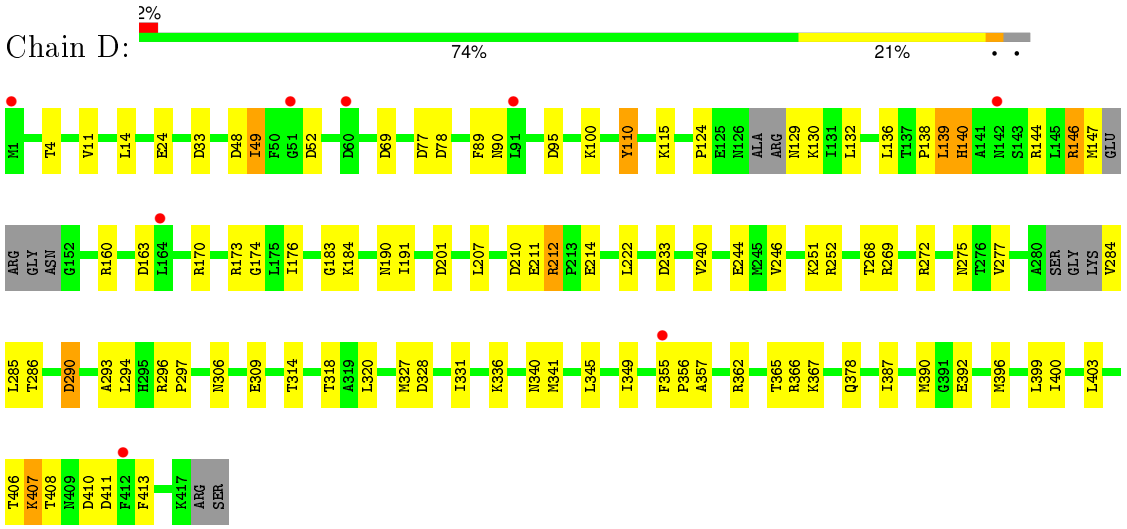
• Molecule 2: Rho transcription termination factor

Chain C:



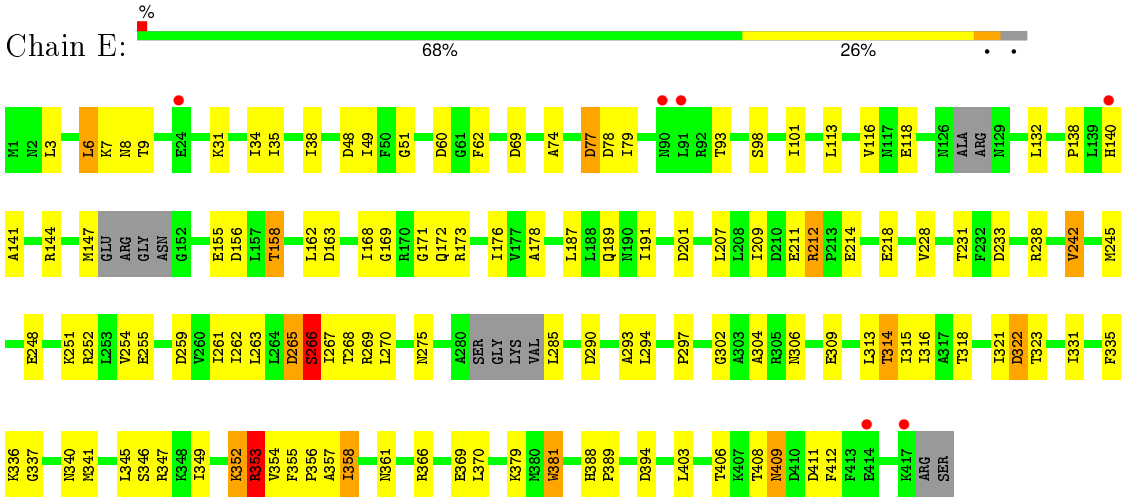
• Molecule 2: Rho transcription termination factor

Chain D:



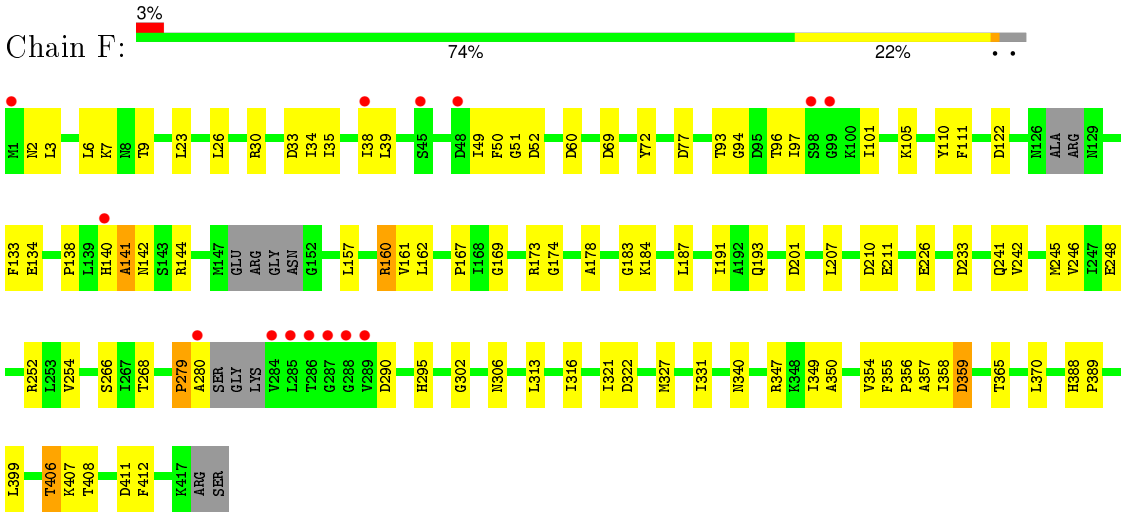
- Molecule 2: Rho transcription termination factor

Chain E:



- Molecule 2: Rho transcription termination factor

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	210.53Å 109.68Å 160.05Å 90.00° 108.16° 90.00°	Depositor
Resolution (Å)	20.00 – 3.15 39.26 – 3.10	Depositor EDS
% Data completeness (in resolution range)	86.5 (20.00-3.15) 85.8 (39.26-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.274 , 0.296 0.268 , 0.274	Depositor DCC
R_{free} test set	2614 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	100.9	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 66.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 54063 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	19814	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.73	0/43	1.04	0/64
1	H	0.79	0/43	1.15	0/64
1	J	0.70	0/43	1.02	0/64
1	K	0.72	0/43	0.94	0/64
1	L	0.79	0/43	1.52	0/64
1	M	0.75	0/41	1.12	0/60
2	A	0.31	0/3256	0.65	14/4383 (0.3%)
2	B	0.31	0/3259	0.65	10/4387 (0.2%)
2	C	0.30	0/3259	0.63	12/4387 (0.3%)
2	D	0.30	0/3259	0.64	14/4387 (0.3%)
2	E	0.30	0/3252	0.63	11/4377 (0.3%)
2	F	0.30	0/3259	0.64	10/4387 (0.2%)
All	All	0.31	0/19800	0.65	71/26688 (0.3%)

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	B	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	60	ASP	CB-CG-OD2	6.32	123.98	118.30
2	D	77	ASP	CB-CG-OD2	6.20	123.88	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	77	ASP	CB-CG-OD2	5.99	123.69	118.30
2	B	77	ASP	CB-CG-OD2	5.97	123.67	118.30
2	E	163	ASP	CB-CG-OD2	5.91	123.62	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	355	PHE	Peptide
2	B	355	PHE	Peptide

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	G	40	0	22	0	0
1	H	40	0	22	0	0
1	J	40	0	22	1	0
1	K	40	0	22	1	0
1	L	40	0	22	2	0
1	M	39	0	19	0	0
2	A	3210	0	3287	77	0
2	B	3213	0	3288	75	0
2	C	3213	0	3289	56	0
2	D	3213	0	3288	44	0
2	E	3206	0	3280	76	0
2	F	3213	0	3289	51	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
4	A	31	0	12	6	0
4	B	31	0	12	9	0
4	C	31	0	12	6	0
4	D	31	0	12	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	31	0	12	4	0
4	F	31	0	12	7	0
5	B	23	0	16	4	0
5	C	23	0	16	8	0
5	D	23	0	16	5	0
5	E	23	0	16	8	0
5	F	23	0	16	6	0
All	All	19814	0	20002	383	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 10.

The worst 5 of 383 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)
2:B:366:ARG:NE	4:C:3600:AGS:S1G	2.12	1.21
2:A:355:PHE:CE1	4:A:1600:AGS:H1'	1.82	1.12
2:C:366:ARG:HD2	4:D:4600:AGS:S1G	1.95	1.04
2:B:355:PHE:CZ	4:B:2600:AGS:H1'	1.94	1.03
2:C:140:HIS:HB3	2:C:306:ASN:HB3	1.38	1.03

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 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%)	356 (89%)	35 (9%)	9 (2%)	8 42
2	B	400/419 (96%)	362 (90%)	35 (9%)	3 (1%)	24 67
2	C	400/419 (96%)	372 (93%)	23 (6%)	5 (1%)	15 57
2	D	400/419 (96%)	374 (94%)	20 (5%)	6 (2%)	13 53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	399/419 (95%)	367 (92%)	28 (7%)	4 (1%)	19	63
2	F	400/419 (96%)	368 (92%)	26 (6%)	6 (2%)	13	53
All	All	2399/2514 (95%)	2199 (92%)	167 (7%)	33 (1%)	14	55

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	353	ARG
2	A	355	PHE
2	A	356	PRO
2	A	366	ARG
2	B	355	PHE

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 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	350/359 (98%)	329 (94%)	21 (6%)	24	63
2	B	351/359 (98%)	324 (92%)	27 (8%)	16	52
2	C	351/359 (98%)	334 (95%)	17 (5%)	31	71
2	D	351/359 (98%)	323 (92%)	28 (8%)	15	50
2	E	350/359 (98%)	327 (93%)	23 (7%)	21	59
2	F	351/359 (98%)	334 (95%)	17 (5%)	31	71
All	All	2104/2154 (98%)	1971 (94%)	133 (6%)	22	61

5 of 133 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	306	ASN
2	D	130	LYS
2	F	133	PHE
2	C	314	THR
2	D	49	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	20	ASN
2	C	120	ASN
2	F	241	GLN
2	C	41	GLN
2	C	90	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	G	1/8 (12%)	1 (100%)	0
1	H	1/8 (12%)	1 (100%)	0
1	J	1/8 (12%)	1 (100%)	0
1	K	1/8 (12%)	1 (100%)	0
1	L	1/8 (12%)	1 (100%)	0
1	M	1/8 (12%)	0	1 (100%)
All	All	6/48 (12%)	5 (83%)	1 (16%)

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 (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	M	1	U

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 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	24,33,33	2.48	5 (20%)	28,52,52	2.08	6 (21%)
4	AGS	B	2600	3	24,33,33	2.45	5 (20%)	28,52,52	2.10	6 (21%)
5	FB	B	2701	-	16,24,24	3.13	3 (18%)	10,38,38	9.58	2 (20%)
4	AGS	C	3600	3	24,33,33	2.33	6 (25%)	28,52,52	2.09	7 (25%)
5	FB	C	3701	-	16,24,24	2.91	3 (18%)	10,38,38	10.55	3 (30%)
4	AGS	D	4600	3	24,33,33	2.37	5 (20%)	28,52,52	2.11	5 (17%)
5	FB	D	4701	-	16,24,24	3.02	3 (18%)	10,38,38	11.79	2 (20%)
4	AGS	E	5600	3	24,33,33	2.39	5 (20%)	28,52,52	2.09	5 (17%)
5	FB	E	5701	-	16,24,24	2.72	3 (18%)	10,38,38	8.23	3 (30%)
4	AGS	F	6600	3	24,33,33	2.37	6 (25%)	28,52,52	2.12	5 (17%)
5	FB	F	6701	-	16,24,24	2.79	3 (18%)	10,38,38	8.49	3 (30%)

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	-	0/15/38/38	0/3/3/3
4	AGS	B	2600	3	-	0/15/38/38	0/3/3/3
5	FB	B	2701	-	-	0/9/53/53	0/0/2/2
4	AGS	C	3600	3	-	0/15/38/38	0/3/3/3
5	FB	C	3701	-	-	0/9/53/53	0/0/2/2
4	AGS	D	4600	3	-	0/15/38/38	0/3/3/3
5	FB	D	4701	-	-	0/9/53/53	0/0/2/2
4	AGS	E	5600	3	-	0/15/38/38	0/3/3/3
5	FB	E	5701	-	-	0/9/53/53	0/0/2/2
4	AGS	F	6600	3	-	0/15/38/38	0/3/3/3
5	FB	F	6701	-	-	0/9/53/53	0/0/2/2

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2701	FB	C5A-C12	-10.44	1.24	1.44
5	D	4701	FB	C5A-C12	-10.26	1.25	1.44
5	C	3701	FB	C5A-C12	-9.71	1.26	1.44
5	F	6701	FB	C5A-C12	-9.14	1.27	1.44
5	E	5701	FB	C5A-C12	-8.63	1.28	1.44

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	6600	AGS	N3-C2-N1	-8.11	122.68	128.89
4	D	4600	AGS	N3-C2-N1	-8.09	122.70	128.89
4	A	1600	AGS	N3-C2-N1	-8.07	122.72	128.89
4	E	5600	AGS	N3-C2-N1	-8.03	122.75	128.89
4	B	2600	AGS	N3-C2-N1	-8.03	122.75	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 72 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1600	AGS	6	0
4	B	2600	AGS	9	0
5	B	2701	FB	4	0
4	C	3600	AGS	6	0
5	C	3701	FB	8	0
4	D	4600	AGS	9	0
5	D	4701	FB	5	0
4	E	5600	AGS	4	0
5	E	5701	FB	8	0
4	F	6600	AGS	7	0
5	F	6701	FB	6	0

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	G	2/8 (25%)	7.18	2 (100%) 0 0	123, 123, 123, 123	0
1	H	2/8 (25%)	7.58	2 (100%) 0 0	123, 123, 123, 123	0
1	J	2/8 (25%)	3.48	1 (50%) 0 0	123, 123, 123, 123	0
1	K	2/8 (25%)	3.55	2 (100%) 0 0	123, 123, 123, 123	0
1	L	2/8 (25%)	1.70	0 100 100	122, 122, 122, 122	0
1	M	2/8 (25%)	6.91	2 (100%) 0 0	123, 123, 123, 123	0
2	A	408/419 (97%)	0.18	19 (4%) 35 20	40, 64, 112, 112	0
2	B	408/419 (97%)	0.02	8 (1%) 68 52	28, 52, 86, 112	0
2	C	408/419 (97%)	-0.14	2 (0%) 91 87	18, 37, 80, 94	0
2	D	408/419 (97%)	0.02	8 (1%) 68 52	29, 50, 82, 111	0
2	E	407/419 (97%)	0.04	6 (1%) 76 62	28, 50, 90, 112	0
2	F	408/419 (97%)	0.04	14 (3%) 49 32	33, 61, 97, 110	0
All	All	2459/2562 (95%)	0.05	66 (2%) 58 42	18, 54, 105, 123	0

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	2	C	8.7
1	M	2	C	8.6
1	G	2	C	8.6
1	H	1	U	6.4
1	G	1	U	5.8

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	FB	B	2701	23/23	0.66	0.59	5.92	43,53,53,53	0
4	AGS	C	3600	31/31	0.77	0.43	4.52	77,79,88,88	0
5	FB	D	4701	23/23	0.75	0.45	3.74	11,43,43,53	0
5	FB	E	5701	23/23	0.74	0.49	3.22	11,43,53,53	0
5	FB	F	6701	23/23	0.72	0.45	3.07	43,53,53,53	0
4	AGS	E	5600	31/31	0.79	0.41	2.91	77,79,87,87	0
5	FB	C	3701	23/23	0.80	0.39	2.69	11,43,43,53	0
4	AGS	F	6600	31/31	0.76	0.44	2.38	76,79,88,88	0
4	AGS	D	4600	31/31	0.74	0.45	2.23	77,79,87,87	0
4	AGS	B	2600	31/31	0.89	0.35	1.78	77,79,88,88	0
4	AGS	A	1600	31/31	0.66	0.34	1.74	77,80,89,89	0
3	MG	E	5601	1/1	0.95	0.63	-	60,60,60,60	0
3	MG	A	1601	1/1	0.90	0.23	-	62,62,62,62	0
3	MG	B	2601	1/1	0.95	0.47	-	59,59,59,59	0
3	MG	F	6601	1/1	0.90	0.58	-	62,62,62,62	0
3	MG	C	3601	1/1	0.86	0.76	-	77,77,77,77	0
3	MG	D	4601	1/1	0.86	0.46	-	36,36,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.