



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:12 PM GMT

PDB ID : 1SK6  
Title : Crystal structure of the adenylyl cyclase domain of anthrax edema factor (EF) in complex with calmodulin, 3',5' cyclic AMP (cAMP), and pyrophosphate  
Authors : Guo, Q.; Shen, Y.; Zhukovskaya, N.L.; Tang, W.J.  
Deposited on : 2004-03-04  
Resolution : 3.20 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

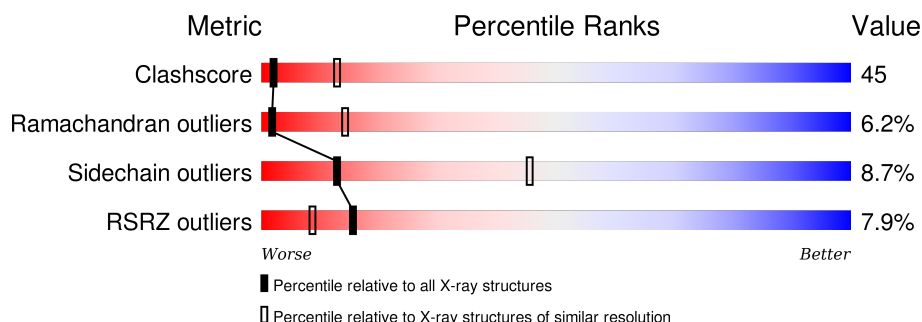
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	A	510	<div> <div>2%</div> <div>36% 50% 8% 6%</div> </div>
1	B	510	<div> <div>5%</div> <div>23% 52% 12% 11%</div> </div>
1	C	510	<div> <div>4%</div> <div>38% 47% 8% 5%</div> </div>
2	D	148	<div> <div>17%</div> <div>41% 48% 7%</div> </div>
2	E	148	<div> <div>28%</div> <div>45% 41% 11%</div> </div>
2	F	148	<div> <div>17%</div> <div>39% 49% 9%</div> </div>

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	CA	D	801	-	-	-	X
3	CA	F	805	-	-	-	X
4	YB	A	907	-	-	-	X
4	YB	B	905	-	-	-	X
4	YB	B	908	-	-	-	X
5	CMP	A	289	X	-	-	-
5	CMP	B	290	X	-	-	-
5	CMP	C	910	X	-	-	-
6	POP	A	893	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15050 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 protein called Calmodulin-sensitive adenylyate cyclase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3924	2511	668	742	3			
1	B	454	Total	C	N	O	S	0	0	0
			3706	2370	628	705	3			
1	C	483	Total	C	N	O	S	0	0	0
			3937	2519	670	745	3			

- Molecule 2 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	143	Total	C	N	O	S	0	0	0
			1125	690	181	245	9			
2	E	143	Total	C	N	O	S	0	0	0
			1125	690	181	245	9			
2	F	143	Total	C	N	O	S	0	0	0
			1125	690	181	245	9			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total	Ca	0	0
			2	2		
3	F	2	Total	Ca	0	0
			2	2		
3	E	2	Total	Ca	0	0
			2	2		

- Molecule 4 is YTTERBIUM (III) ION (three-letter code: YB) (formula: Yb).

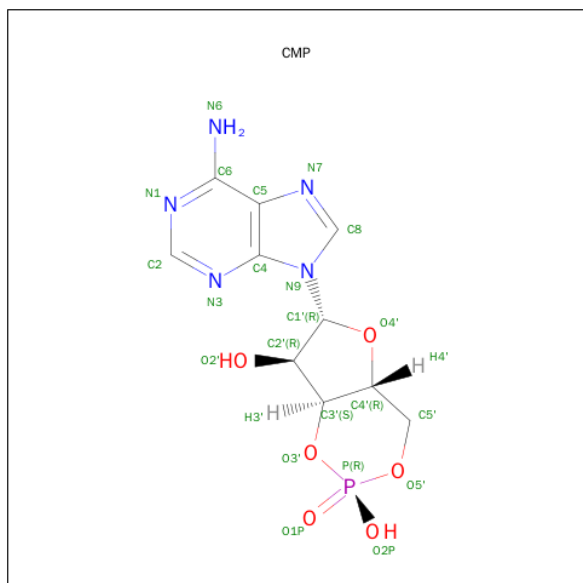
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Yb	0	0
			3	3		

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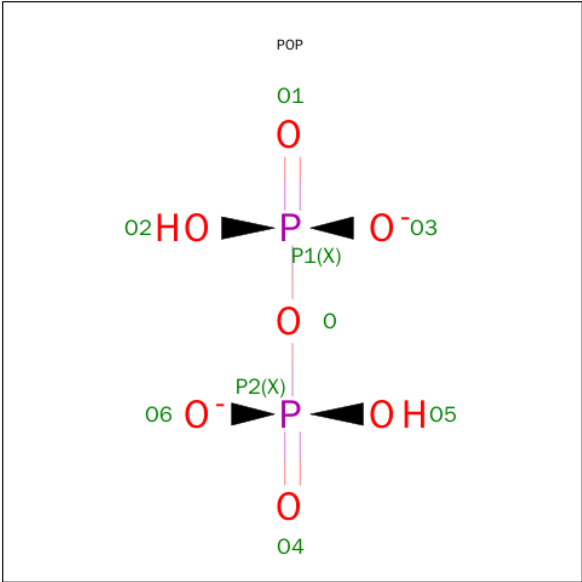
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Yb	0	0
			3	3		
4	C	3	Total	Yb	0	0
			3	3		

- Molecule 5 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (three-letter code: CMP) (formula:  $C_{10}H_{12}N_5O_6P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
5	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
5	C	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

- Molecule 6 is PYROPHOSPHATE 2- (three-letter code: POP) (formula:  $H_2O_7P_2$ ).

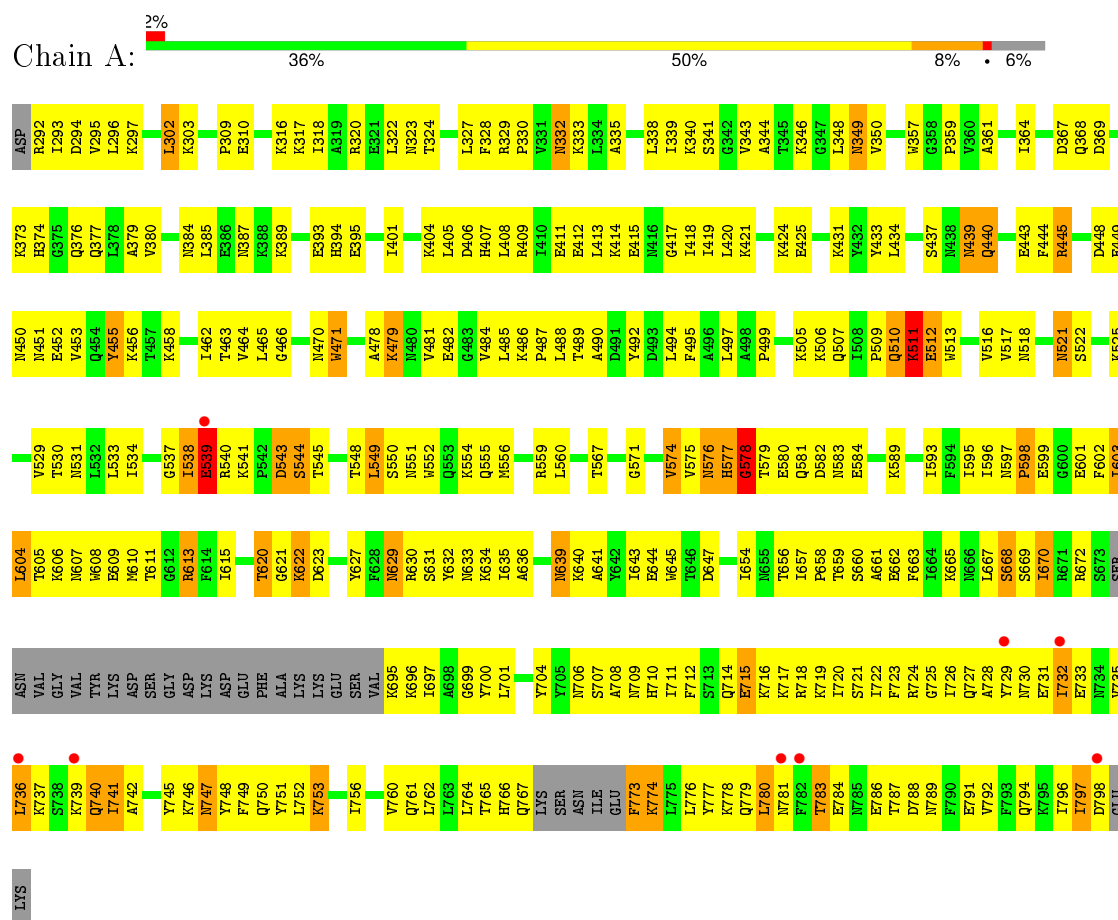


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			9	7	2		
6	B	1	Total	O	P	0	0
			9	7	2		
6	C	1	Total	O	P	0	0
			9	7	2		

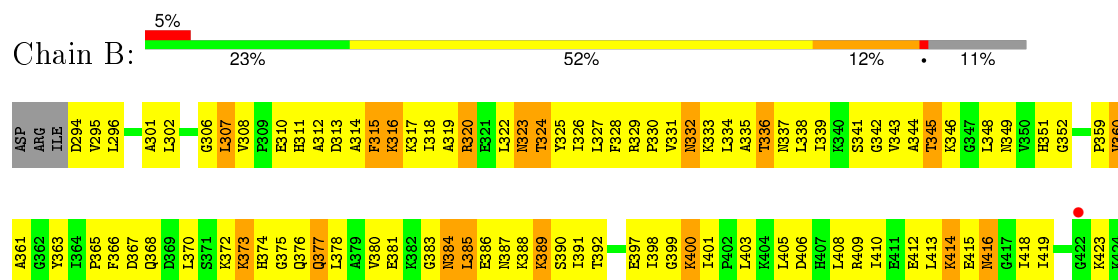
### 3 Residue-property plots

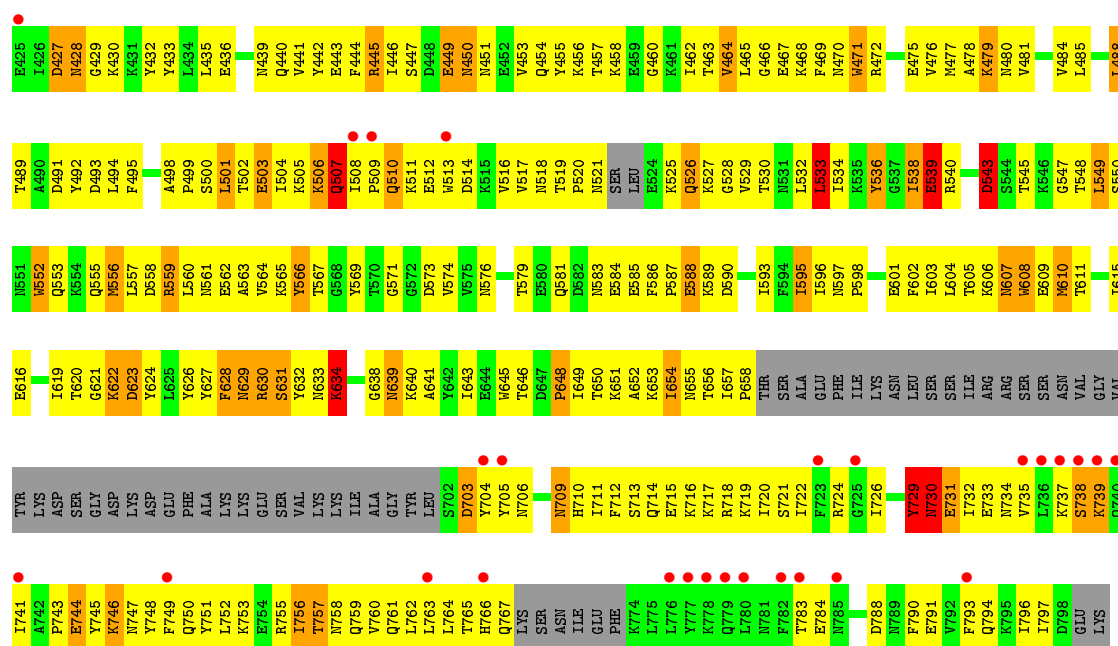
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Calmodulin-sensitive adenylate cyclase

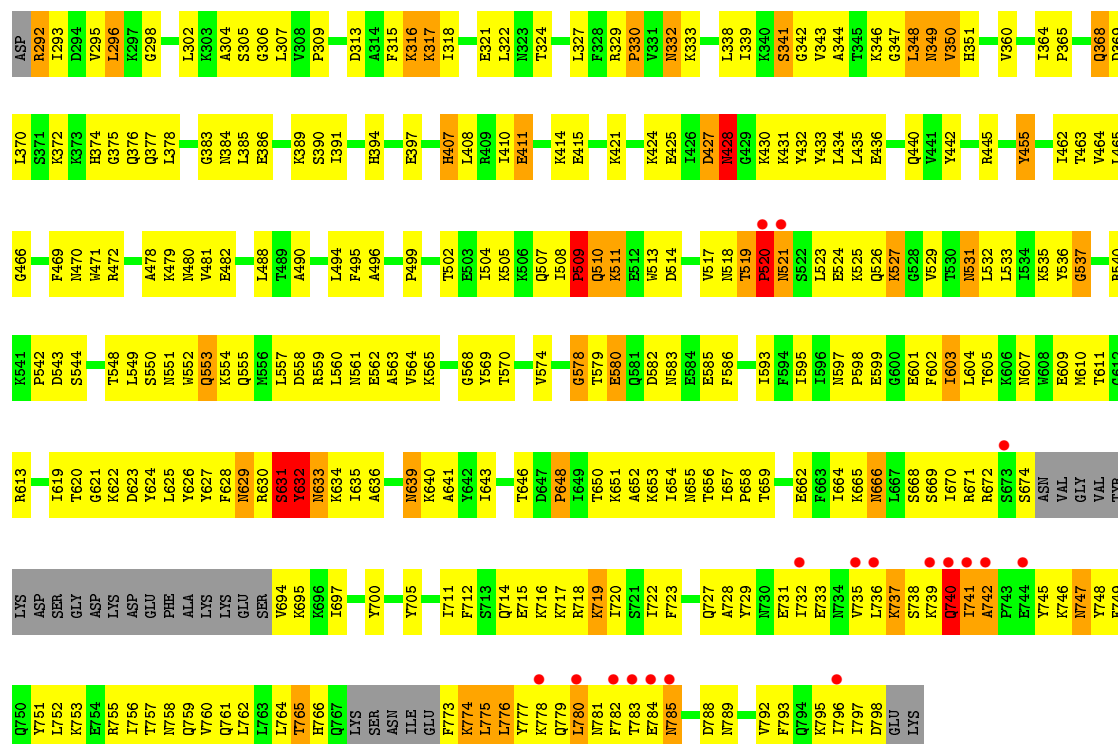


- Molecule 1: Calmodulin-sensitive adenylate cyclase





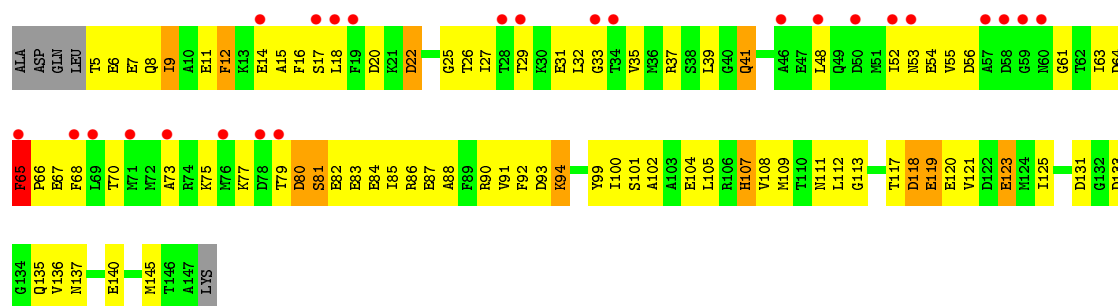
• Molecule 1: Calmodulin-sensitive adenylylate cyclase



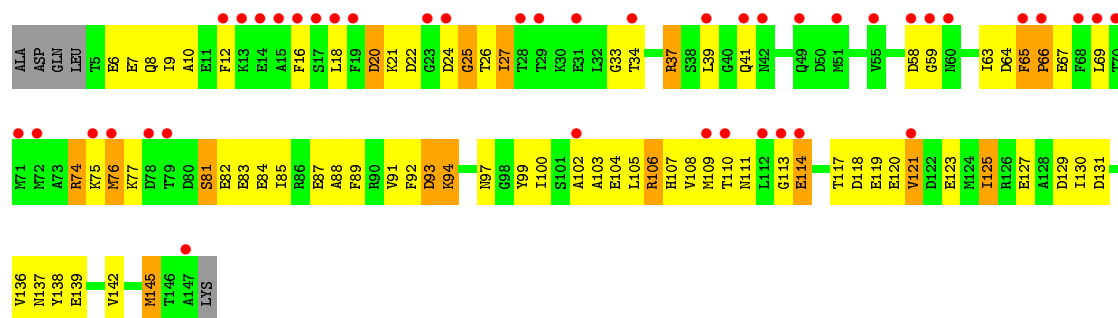
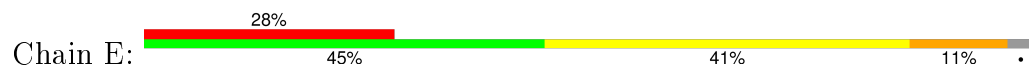
• Molecule 2: Calmodulin



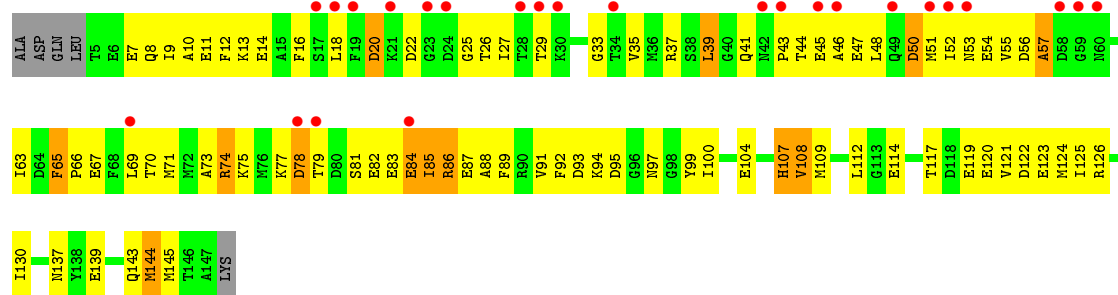




• Molecule 2: Calmodulin



• Molecule 2: Calmodulin



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.87Å 166.45Å 342.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 43.11 – 3.29	Depositor EDS
% Data completeness (in resolution range)	96.2 (50.00-3.20) 95.7 (43.11-3.29)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.75 (at 3.32Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.250 , 0.307 0.268 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	71.0	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 54.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 50500 reflections	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	15050	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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: CA, YB, POP, CMP

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	A	0.57	5/3999 (0.1%)	0.91	25/5382 (0.5%)
1	B	0.64	5/3778 (0.1%)	0.97	22/5088 (0.4%)
1	C	0.84	8/4012 (0.2%)	1.30	36/5400 (0.7%)
2	D	0.39	0/1137	0.56	0/1527
2	E	0.36	0/1137	0.54	0/1527
2	F	0.45	1/1137 (0.1%)	0.62	0/1527
All	All	0.64	19/15200 (0.1%)	0.99	83/20451 (0.4%)

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	1
1	C	1	5
All	All	1	8

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	520	PRO	N-CD	20.86	1.77	1.47
1	C	773	PHE	C-N	20.19	1.80	1.34
1	C	632	TYR	N-CA	19.71	1.85	1.46
1	C	741	ILE	N-CA	15.98	1.78	1.46
1	C	521	ASN	N-CA	14.19	1.74	1.46

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	773	PHE	O-C-N	-46.13	48.88	122.70
1	C	773	PHE	CB-CA-C	22.71	155.82	110.40
1	C	773	PHE	N-CA-C	-22.63	49.90	111.00
1	C	520	PRO	CA-N-CD	-18.66	85.37	111.50
1	B	730	ASN	N-CA-CB	-17.00	80.00	110.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	773	PHE	CA

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	511	LYS	Peptide
1	A	773	PHE	Peptide
1	B	729	TYR	Peptide
1	C	427	ASP	Peptide
1	C	510	GLN	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	3924	0	3967	345	0
1	B	3706	0	3728	472	0
1	C	3937	0	3980	329	0
2	D	1125	0	1049	82	0
2	E	1125	0	1049	92	0
2	F	1125	0	1048	102	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
5	A	22	0	10	6	0
5	B	22	0	10	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	22	0	10	3	0
6	A	9	0	0	3	0
6	B	9	0	0	1	0
6	C	9	0	0	1	0
All	All	15050	0	14851	1356	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 45.

The worst 5 of 1356 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)
5:B:290:CMP:C2	5:B:290:CMP:H2	0.97	1.49
5:A:289:CMP:H2	5:A:289:CMP:C2	0.97	1.48
5:C:910:CMP:C2	5:C:910:CMP:H2	0.97	1.47
1:B:730:ASN:CA	1:B:730:ASN:N	1.73	1.46
1:C:741:ILE:CA	1:C:741:ILE:N	1.78	1.46

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	
1	A	475/510 (93%)	371 (78%)	83 (18%)	21 (4%)	3	24
1	B	448/510 (88%)	308 (69%)	116 (26%)	24 (5%)	2	19
1	C	477/510 (94%)	358 (75%)	98 (20%)	21 (4%)	3	24
2	D	141/148 (95%)	85 (60%)	43 (30%)	13 (9%)	1	5
2	E	141/148 (95%)	87 (62%)	37 (26%)	17 (12%)	0	2
2	F	141/148 (95%)	88 (62%)	36 (26%)	17 (12%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1823/1974 (92%)	1297 (71%)	413 (23%)	113 (6%)	2 14

5 of 113 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	GLN
1	A	521	ASN
1	A	539	GLU
1	A	669	SER
2	D	81	SER

### 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
1	A	429/455 (94%)	395 (92%)	34 (8%)	15 53
1	B	405/455 (89%)	350 (86%)	55 (14%)	5 22
1	C	431/455 (95%)	397 (92%)	34 (8%)	15 53
2	D	121/126 (96%)	112 (93%)	9 (7%)	17 56
2	E	121/126 (96%)	114 (94%)	7 (6%)	25 66
2	F	121/126 (96%)	119 (98%)	2 (2%)	68 90
All	All	1628/1743 (93%)	1487 (91%)	141 (9%)	13 45

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	440	GLN
1	B	552	TRP
1	C	632	TYR
1	B	450	ASN
1	B	533	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	470	ASN
1	B	709	ASN
1	C	759	GLN
1	B	518	ASN
1	B	555	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 21 ligands modelled in this entry, 15 are monoatomic - leaving 6 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$
5	CMP	A	289	4	19,25,25	1.70	5 (26%)	18,39,39	5.83	9 (50%)
6	POP	A	893	4	8,8,8	1.99	2 (25%)	13,13,13	1.03	1 (7%)
5	CMP	B	290	4	19,25,25	1.38	4 (21%)	18,39,39	5.29	10 (55%)
6	POP	B	894	4	8,8,8	2.17	3 (37%)	13,13,13	1.07	1 (7%)
6	POP	C	895	4	8,8,8	1.77	3 (37%)	13,13,13	1.07	1 (7%)
5	CMP	C	910	4	19,25,25	1.26	1 (5%)	18,39,39	5.01	10 (55%)

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
5	CMP	A	289	4	1/1/5/5	0/0/31/31	0/4/4/4
6	POP	A	893	4	-	0/6/6/6	0/0/0/0
5	CMP	B	290	4	1/1/5/5	0/0/31/31	0/4/4/4
6	POP	B	894	4	-	0/6/6/6	0/0/0/0
6	POP	C	895	4	-	0/6/6/6	0/0/0/0
5	CMP	C	910	4	1/1/5/5	0/0/31/31	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	289	CMP	P-O3'	-4.46	1.50	1.58
6	B	894	POP	P2-O	-4.11	1.51	1.61
6	A	893	POP	P2-O	-3.53	1.53	1.61
6	B	894	POP	P1-O	-3.15	1.53	1.61
6	C	895	POP	P1-O	-3.07	1.54	1.61

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	290	CMP	N3-C2-N1	-11.84	119.83	128.89
5	A	289	CMP	N3-C2-N1	-11.24	120.28	128.89
5	C	910	CMP	N3-C2-N1	-10.73	120.67	128.89
5	A	289	CMP	C4'-O4'-C1'	-5.54	103.64	109.72
5	A	289	CMP	C3'-C2'-C1'	-3.75	90.97	99.98

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	910	CMP	C1'
5	A	289	CMP	C1'
5	B	290	CMP	C1'

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	289	CMP	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	893	POP	3	0
5	B	290	CMP	5	0
6	B	894	POP	1	0
6	C	895	POP	1	0
5	C	910	CMP	3	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.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	481/510 (94%)	-0.07	8 (1%) 73 60	10, 43, 95, 99	0
1	B	454/510 (89%)	0.17	28 (6%) 24 13	10, 51, 95, 98	0
1	C	483/510 (94%)	-0.04	18 (3%) 45 30	10, 43, 95, 97	0
2	D	143/148 (96%)	0.84	25 (17%) 2 1	18, 95, 95, 98	0
2	E	143/148 (96%)	1.35	42 (29%) 1 0	39, 95, 96, 98	0
2	F	143/148 (96%)	0.82	25 (17%) 2 1	17, 95, 95, 97	0
All	All	1847/1974 (93%)	0.24	146 (7%) 15 9	10, 55, 95, 99	0

The worst 5 of 146 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	79	THR	9.3
2	E	59	GLY	7.9
2	E	79	THR	7.3
2	E	71	MET	7.2
1	B	740	GLN	7.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	YB	B	908	1/1	0.95	0.36	4.15	49,49,49,49	1
4	YB	B	905	1/1	0.98	0.35	3.86	31,31,31,31	1
4	YB	A	907	1/1	0.95	0.35	3.67	49,49,49,49	1
3	CA	F	805	1/1	0.96	0.33	3.19	21,21,21,21	0
6	POP	A	893	9/9	0.94	0.29	2.89	96,101,104,105	0
3	CA	D	801	1/1	0.98	0.35	2.20	13,13,13,13	0
6	POP	C	895	9/9	0.88	0.30	1.65	50,52,61,62	0
6	POP	B	894	9/9	0.93	0.26	1.41	51,52,54,55	0
5	CMP	C	910	22/22	0.87	0.28	1.23	15,22,44,45	0
3	CA	E	803	1/1	0.99	0.32	1.17	23,23,23,23	0
5	CMP	A	289	22/22	0.91	0.25	1.13	11,18,39,43	0
5	CMP	B	290	22/22	0.92	0.24	0.56	16,25,44,46	0
3	CA	F	804	1/1	0.99	0.11	-1.95	26,26,26,26	0
3	CA	D	800	1/1	0.97	0.15	-2.90	11,11,11,11	0
3	CA	E	802	1/1	0.96	0.04	-3.16	43,43,43,43	0
4	YB	C	909	1/1	0.93	0.42	-	72,72,72,72	1
4	YB	C	906	1/1	0.97	0.40	-	31,31,31,31	1
4	YB	A	901	1/1	0.97	0.27	-	50,50,50,50	1
4	YB	B	902	1/1	0.98	0.34	-	107,107,107,107	1
4	YB	A	904	1/1	0.95	0.37	-	42,42,42,42	1
4	YB	C	903	1/1	0.97	0.45	-	72,72,72,72	1

## 6.5 Other polymers

There are no such residues in this entry.