



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 03:05 PM GMT

PDB ID : 3GCM  
Title : Crystal Structure of E. coli polynucleotide phosphorylase bound to RNA and RNase E  
Authors : Nurmohamed, S.; Luisi, B.L.  
Deposited on : 2009-02-22  
Resolution : 2.50 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

---

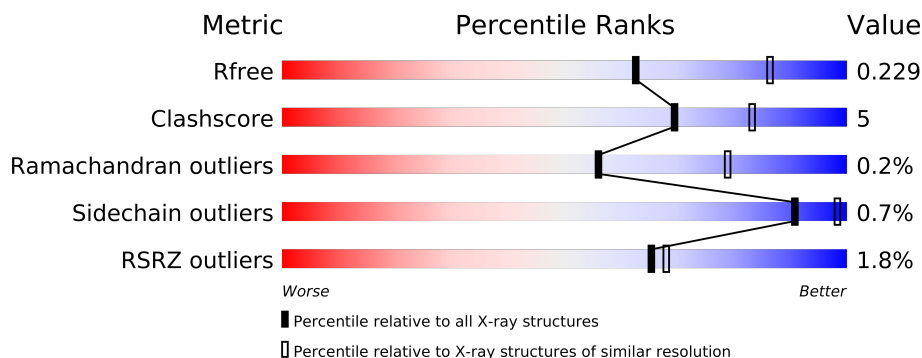
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
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 2.50 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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	549	
1	B	549	
1	C	549	
2	D	41	
2	E	41	
2	F	41	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	FLC	A	550	-	X
3	FLC	B	552	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
3	FLC	B	554	-	X
5	5GP	B	550	-	X
5	5GP	B	551	-	X
5	5GP	C	550	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13916 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.

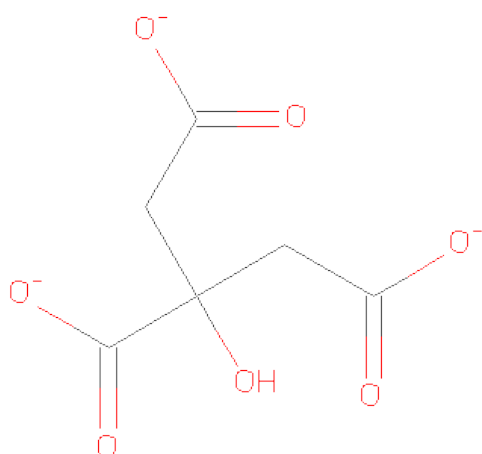
- Molecule 1 is a protein called Polyribonucleotide nucleotidyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	544	Total	C	N	O	S	8	4	0
			4151	2604	724	802	21			
1	B	544	Total	C	N	O	S	0	5	0
			4170	2614	732	803	21			
1	C	544	Total	C	N	O	S	0	2	0
			4142	2598	721	802	21			

- Molecule 2 is a protein called Ribonuclease E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	21	Total	C	N	O	0	0	0
			134	80	30	24			
2	E	20	Total	C	N	O	0	0	0
			130	78	29	23			
2	F	21	Total	C	N	O	0	0	0
			138	82	31	25			

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: C<sub>6</sub>H<sub>5</sub>O<sub>7</sub>).



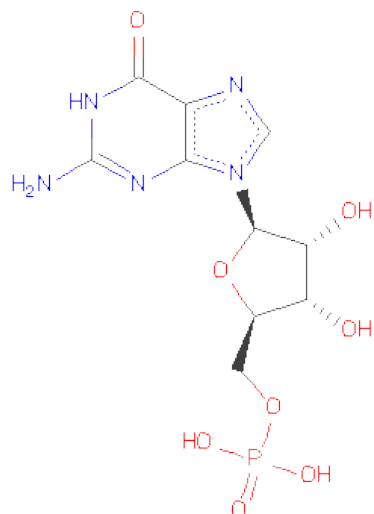
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula:

C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			20	10	5	5		
5	B	1	Total	C	N	O	0	0
			20	10	5	5		
5	C	1	Total	C	N	O	0	0
			20	10	5	5		

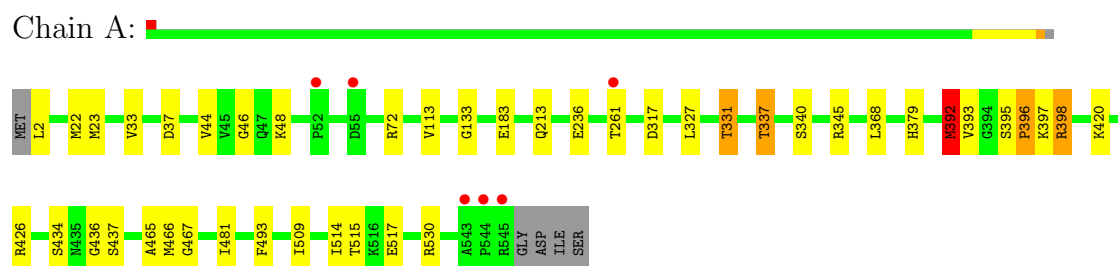
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	334	Total	O	0	0
			334	334		
6	D	8	Total	O	0	0
			8	8		
6	B	280	Total	O	0	0
			280	280		
6	E	9	Total	O	0	0
			9	9		
6	C	247	Total	O	0	0
			247	247		
6	F	6	Total	O	0	0
			6	6		

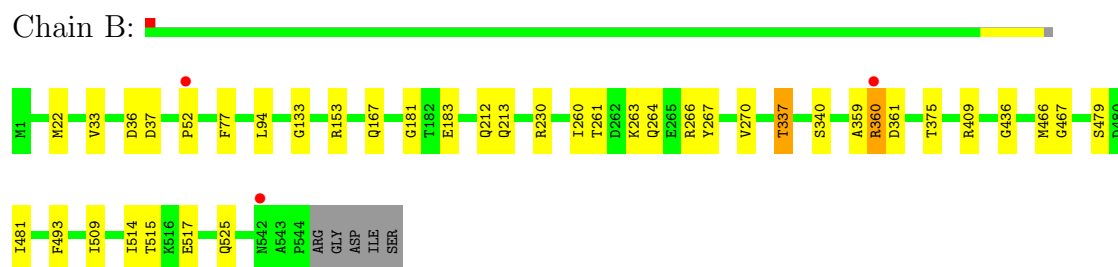
### 3 Residue-property plots

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.

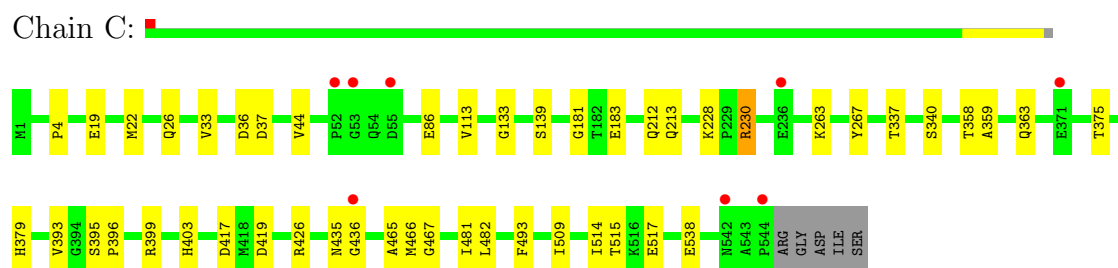
- Molecule 1: Polyribonucleotide nucleotidyltransferase



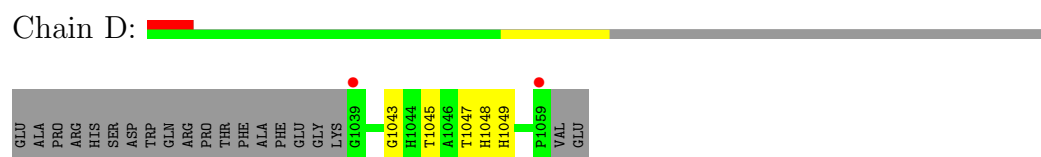
- Molecule 1: Polyribonucleotide nucleotidyltransferase



- Molecule 1: Polyribonucleotide nucleotidyltransferase

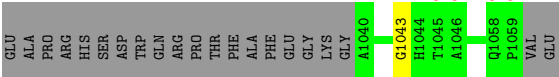


- Molecule 2: Ribonuclease E



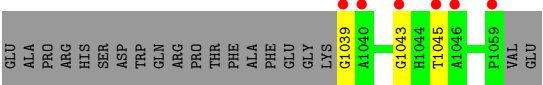
- Molecule 2: Ribonuclease E





● Molecule 2: Ribonuclease E

Chain F:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	176.34Å 176.34Å 189.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 43.46 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-2.50) 99.4 (43.46-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.166 , 0.221 0.201 , 0.229	Depositor DCC
$R_{free}$ test set	5134 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.9	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 13.4	EDS
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	0 of 102779 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13916	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: FLC, 5GP, 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	A	0.51	4/4226 (0.1%)	0.52	2/5728 (0.0%)
1	B	0.35	0/4245	0.47	0/5751
1	C	0.36	0/4211	0.47	0/5708
2	D	0.34	0/139	0.49	0/191
2	E	0.29	0/135	0.46	0/186
2	F	0.33	0/143	0.43	0/196
All	All	0.41	4/13099 (0.0%)	0.49	2/17760 (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	3
1	B	0	1
1	C	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	392[A]	MET	CA-C	-10.84	1.24	1.52
1	A	392[B]	MET	CA-C	-10.84	1.24	1.52
1	A	398[A]	ARG	N-CA	-9.54	1.27	1.46
1	A	398[B]	ARG	N-CA	-9.54	1.27	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398[A]	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	A	398[B]	ARG	NE-CZ-NH1	5.97	123.28	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	392[A]	MET	Mainchain
1	A	392[B]	MET	Mainchain
1	A	436	GLY	Peptide
1	B	436	GLY	Peptide
1	C	436	GLY	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	A	4151	0	4170	35	0
1	B	4170	0	4203	33	0
1	C	4142	0	4160	47	0
2	D	134	0	119	4	0
2	E	130	0	116	3	0
2	F	138	0	125	6	0
3	A	26	0	10	0	0
3	B	52	0	20	6	0
3	C	26	0	10	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	B	40	0	24	4	0
5	C	20	0	12	0	0
6	A	334	0	0	12	0
6	B	280	0	0	10	0
6	C	247	0	0	11	0
6	D	8	0	0	1	0
6	E	9	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	6	0	0	0	0
All	All	13916	0	12969	123	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 5.

All (123) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:550:5GP:C5'	5:B:551:5GP:H8	1.75	1.18
5:B:550:5GP:H5'1	5:B:551:5GP:C8	1.78	1.10
1:B:264:GLN:NE2	1:C:26:GLN:HA	1.74	1.02
5:B:550:5GP:H5'1	5:B:551:5GP:H8	0.94	0.93
1:B:77:PHE:HB2	5:B:550:5GP:H2'	1.50	0.92
1:B:264:GLN:HE21	1:C:26:GLN:HA	1.37	0.85
1:B:515:THR:CG2	6:B:608:HOH:O	2.30	0.80
1:C:337:THR:HG21	1:C:340:SER:HB3	1.64	0.79
1:A:236:GLU:HG3	6:A:646:HOH:O	1.84	0.78
3:B:552:FLC:HG1	6:B:1067:HOH:O	1.82	0.78
1:A:337:THR:HG21	1:A:340:SER:HB3	1.68	0.76
1:A:72[A]:ARG:HD3	6:A:689:HOH:O	1.87	0.74
1:B:337:THR:HG21	1:B:340:SER:HB3	1.71	0.73
3:B:552:FLC:CG	6:B:1067:HOH:O	2.37	0.70
2:E:1043:GLY:HA3	1:C:22:MET:HE3	1.73	0.70
6:C:1044:HOH:O	2:F:1045:THR:HG21	1.91	0.70
1:C:393:VAL:HG12	1:C:393:VAL:O	1.91	0.69
2:E:1043:GLY:HA3	1:C:22:MET:CE	2.22	0.68
6:C:1044:HOH:O	2:F:1045:THR:CG2	2.41	0.67
1:A:2:LEU:HG	1:A:22:MET:HG3	1.75	0.67
1:C:358:THR:HG22	1:C:359:ALA:H	1.60	0.66
1:B:515:THR:HG23	6:B:608:HOH:O	1.92	0.66
1:C:538:GLU:HG3	6:C:627:HOH:O	1.95	0.65
1:B:263:LYS:O	1:B:267:TYR:HD2	1.79	0.65
1:B:479:SER:OG	1:B:525:GLN:NE2	2.29	0.65
1:B:36:ASP:O	1:B:37:ASP:HB2	1.97	0.63
1:C:263:LYS:O	1:C:267:TYR:HD2	1.80	0.63
1:B:261:THR:HG21	6:B:702:HOH:O	1.99	0.62
1:B:466:MET:HB2	1:B:493:PHE:HB3	1.82	0.61
1:A:515:THR:HG22	1:A:517:GLU:H	1.66	0.60
1:A:331:THR:HG22	2:D:1048:HIS:HB2	1.84	0.60
1:B:153:ARG:HH21	3:B:552:FLC:CBC	2.14	0.59
1:C:435:ASN:HD21	1:C:482:LEU:HG	1.67	0.59
1:B:515:THR:HG22	1:B:517:GLU:H	1.67	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:466:MET:HB2	1:A:493:PHE:HB3	1.84	0.59
1:A:395:SER:O	1:A:396:PRO:C	2.36	0.59
1:C:358:THR:HG22	1:C:359:ALA:N	2.17	0.58
1:A:379:HIS:HE1	6:A:602:HOH:O	1.87	0.57
1:B:33:VAL:HG21	1:B:133:GLY:HA2	1.85	0.57
1:B:375:THR:HG22	6:B:697:HOH:O	2.04	0.57
1:C:139:SER:O	1:C:230:ARG:NH2	2.36	0.55
1:A:397:LYS:HE3	6:A:694:HOH:O	2.07	0.55
1:C:4:PRO:HB2	1:C:19:GLU:HG3	1.86	0.55
1:A:33:VAL:HG21	1:A:133:GLY:HA2	1.89	0.55
1:A:72[A]:ARG:HH22	1:A:368:LEU:HA	1.72	0.54
1:C:228:LYS:O	1:C:230:ARG:NH1	2.41	0.54
1:C:395:SER:HB2	1:C:396:PRO:HD2	1.88	0.54
1:B:94:LEU:HD11	3:B:552:FLC:HG2	1.90	0.53
1:A:327:LEU:CD2	1:A:345:ARG:HG3	2.38	0.53
1:A:420:LYS:O	1:A:420:LYS:HG3	2.08	0.53
1:C:515:THR:HG22	1:C:517:GLU:H	1.74	0.53
1:C:426:ARG:HD3	6:C:612:HOH:O	2.09	0.53
1:C:33:VAL:HG21	1:C:133:GLY:HA2	1.90	0.53
1:B:263:LYS:O	1:B:267:TYR:CD2	2.63	0.52
1:A:426:ARG:HD3	6:A:565:HOH:O	2.09	0.52
1:B:266:ARG:O	1:B:270:VAL:HG23	2.09	0.52
1:A:261:THR:HG22	1:A:317:ASP:HA	1.91	0.52
1:B:264:GLN:HE22	1:C:26:GLN:HA	1.66	0.51
1:C:466:MET:HB2	1:C:493:PHE:HB3	1.93	0.51
1:C:379:HIS:CD2	1:C:426:ARG:HE	2.30	0.50
1:A:22:MET:HE3	1:A:23:MET:HG3	1.94	0.49
1:B:181:GLY:H	1:B:212:GLN:HE22	1.60	0.49
1:B:183:GLU:HA	1:B:213:GLN:HE22	1.78	0.49
1:A:327:LEU:HD23	1:A:345:ARG:HG3	1.93	0.49
2:D:1049:HIS:CE1	6:D:1112:HOH:O	2.64	0.49
1:C:375:THR:HG23	6:C:614:HOH:O	2.11	0.49
1:A:22:MET:CE	2:F:1043:GLY:HA3	2.43	0.48
1:B:359:ALA:O	1:B:360:ARG:C	2.51	0.48
1:A:46:GLY:O	6:A:561:HOH:O	2.20	0.48
1:A:183:GLU:HA	1:A:213:GLN:HE22	1.79	0.48
1:B:509:ILE:HD13	1:B:514:ILE:HG21	1.94	0.48
1:A:437:SER:HB2	1:A:465:ALA:HB2	1.95	0.48
1:B:359:ALA:O	1:B:361:ASP:N	2.46	0.48
1:A:379:HIS:CD2	1:A:426:ARG:HE	2.32	0.47
1:A:48:LYS:CD	6:A:653:HOH:O	2.62	0.47
1:A:37:ASP:OD1	2:F:1039:GLY:HA3	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:48:LYS:HD2	6:A:653:HOH:O	2.14	0.47
1:A:509:ILE:HD13	1:A:514:ILE:HG21	1.96	0.47
1:A:72[A]:ARG:HD2	6:A:775:HOH:O	2.13	0.47
1:B:267:TYR:O	1:B:270:VAL:N	2.48	0.47
1:C:465:ALA:HB3	6:C:573:HOH:O	2.15	0.47
1:C:379:HIS:HD2	1:C:426:ARG:HE	1.63	0.47
1:C:263:LYS:HG2	1:C:267:TYR:CE2	2.50	0.47
1:C:509:ILE:HD13	1:C:514:ILE:HG21	1.97	0.46
1:C:393:VAL:CG1	1:C:393:VAL:O	2.61	0.46
1:B:167:GLN:NE2	6:B:657:HOH:O	2.48	0.46
1:C:515:THR:HG22	6:C:1025:HOH:O	2.15	0.46
1:C:183:GLU:HA	1:C:213:GLN:HE22	1.80	0.46
1:A:530:ARG:HD3	6:A:607:HOH:O	2.16	0.46
1:A:379:HIS:HD2	1:A:426:ARG:HE	1.64	0.45
1:C:22:MET:HE2	1:C:22:MET:HB3	1.70	0.45
1:C:33:VAL:HG21	1:C:133:GLY:CA	2.46	0.45
1:C:435:ASN:ND2	1:C:482:LEU:HG	2.31	0.45
1:C:181:GLY:H	1:C:212:GLN:HE22	1.64	0.45
1:C:395:SER:HB2	1:C:396:PRO:CD	2.47	0.45
1:C:467:GLY:HA3	1:C:481:ILE:HG21	1.98	0.45
6:A:685:HOH:O	2:D:1047:THR:HG21	2.17	0.45
1:B:261:THR:CG2	6:B:702:HOH:O	2.61	0.44
1:C:44:VAL:HG22	1:C:113:VAL:HG22	1.98	0.44
1:B:337:THR:HG22	6:B:596:HOH:O	2.16	0.44
2:E:1043:GLY:HA3	1:C:22:MET:HE1	1.98	0.44
6:C:1044:HOH:O	2:F:1045:THR:HG22	2.13	0.44
1:A:467:GLY:HA3	1:A:481:ILE:HG21	1.99	0.44
1:C:515:THR:CG2	6:C:1025:HOH:O	2.66	0.44
1:C:263:LYS:CG	1:C:267:TYR:CE2	3.01	0.44
1:C:363:GLN:NE2	6:C:703:HOH:O	2.51	0.43
1:B:409:ARG:NH1	3:B:552:FLC:HA2	2.33	0.43
1:C:263:LYS:HG3	1:C:267:TYR:HE2	1.83	0.42
1:A:379:HIS:HD2	1:A:426:ARG:HH21	1.67	0.42
1:C:399[A]:ARG:HG2	1:C:403:HIS:CE1	2.54	0.42
1:A:22:MET:HE1	2:F:1043:GLY:HA3	2.00	0.42
1:C:417:ASP:OD2	1:C:419:ASP:HB2	2.20	0.42
1:C:36:ASP:O	1:C:37:ASP:HB2	2.20	0.42
1:A:44:VAL:HG22	1:A:113:VAL:HG22	2.01	0.42
1:C:515:THR:HG21	6:C:700:HOH:O	2.20	0.41
1:B:467:GLY:HA3	1:B:481:ILE:HG21	2.02	0.41
1:B:515:THR:HG22	1:B:517:GLU:N	2.34	0.41
1:C:358:THR:CG2	1:C:359:ALA:H	2.31	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:260:ILE:O	1:B:266:ARG:HD3	2.20	0.41
1:C:399[A]:ARG:HD3	1:C:403:HIS:CE1	2.55	0.41
3:B:552:FLC:HG2	6:B:1067:HOH:O	2.12	0.41
1:A:72[B]:ARG:CD	6:A:689:HOH:O	2.69	0.40
2:D:1043:GLY:HA3	1:B:22:MET:SD	2.61	0.40

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	
1	A	546/549 (100%)	532 (97%)	11 (2%)	3 (0%)	38	60
1	B	547/549 (100%)	530 (97%)	15 (3%)	2 (0%)	43	66
1	C	544/549 (99%)	532 (98%)	12 (2%)	0	100	100
2	D	19/41 (46%)	18 (95%)	1 (5%)	0	100	100
2	E	18/41 (44%)	18 (100%)	0	0	100	100
2	F	19/41 (46%)	19 (100%)	0	0	100	100
All	All	1693/1770 (96%)	1649 (97%)	39 (2%)	5 (0%)	56	73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	360	ARG
1	A	392[A]	MET
1	A	392[B]	MET
1	A	396	PRO
1	B	52	PRO

### 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	441/446 (99%)	435 (99%)	6 (1%)	78	94
1	B	444/446 (100%)	442 (100%)	2 (0%)	94	99
1	C	440/446 (99%)	438 (100%)	2 (0%)	94	99
2	D	10/28 (36%)	9 (90%)	1 (10%)	11	20
2	E	10/28 (36%)	10 (100%)	0	100	100
2	F	11/28 (39%)	11 (100%)	0	100	100
All	All	1356/1422 (95%)	1345 (99%)	11 (1%)	91	98

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	331	THR
1	A	337	THR
1	A	393	VAL
1	A	398[A]	ARG
1	A	398[B]	ARG
1	A	434	SER
2	D	1045	THR
1	B	230	ARG
1	B	337	THR
1	C	86	GLU
1	C	230	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	GLN
1	A	213	GLN
1	A	269	GLN
1	A	303	ASN
1	A	363	GLN
1	A	379	HIS
1	B	47	GLN
1	B	62	ASN
1	B	167	GLN
1	B	212	GLN
1	B	213	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	264	GLN
1	B	363	GLN
1	B	525	GLN
1	C	3	ASN
1	C	47	GLN
1	C	62	ASN
1	C	167	GLN
1	C	212	GLN
1	C	213	GLN
1	C	363	GLN
1	C	379	HIS
2	F	1049	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 14 ligands modelled in this entry, 3 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
3	FLC	A	550	-	5,12,12	2.11	2 (40%)	7,17,17	1.27	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FLC	A	551	-	5,12,12	2.20	2 (40%)	7,17,17	0.92	0
5	5GP	B	550	-	22,22,26	0.76	0	30,33,40	5.13	4 (13%)
5	5GP	B	551	-	22,22,26	0.79	0	30,33,40	6.11	4 (13%)
3	FLC	B	552	-	5,12,12	2.26	2 (40%)	7,17,17	1.22	0
3	FLC	B	553	-	5,12,12	2.12	2 (40%)	7,17,17	0.81	0
3	FLC	B	554	-	5,12,12	2.07	2 (40%)	7,17,17	1.15	1 (14%)
3	FLC	B	555	-	5,12,12	2.28	2 (40%)	7,17,17	0.69	0
5	5GP	C	550	-	22,22,26	0.77	0	30,33,40	6.12	2 (6%)
3	FLC	C	551	-	5,12,12	2.03	2 (40%)	7,17,17	1.25	2 (28%)
3	FLC	C	552	-	5,12,12	2.14	2 (40%)	7,17,17	0.94	0

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
3	FLC	A	550	-	-	0/6/16/16	0/0/0/0
3	FLC	A	551	-	-	0/6/16/16	0/0/0/0
5	5GP	B	550	-	-	0/6/22/26	0/1/3/3
5	5GP	B	551	-	-	0/6/22/26	0/1/3/3
3	FLC	B	552	-	-	0/6/16/16	0/0/0/0
3	FLC	B	553	-	-	0/6/16/16	0/0/0/0
3	FLC	B	554	-	-	0/6/16/16	0/0/0/0
3	FLC	B	555	-	-	0/6/16/16	0/0/0/0
5	5GP	C	550	-	-	0/6/22/26	0/1/3/3
3	FLC	C	551	-	-	0/6/16/16	0/0/0/0
3	FLC	C	552	-	-	0/6/16/16	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	552	FLC	CG-CGC	3.79	1.52	1.49
3	B	555	FLC	CA-CAC	3.51	1.51	1.49
3	A	551	FLC	CA-CAC	3.51	1.51	1.49
3	B	555	FLC	CG-CGC	3.47	1.51	1.49
3	B	553	FLC	CA-CAC	3.33	1.51	1.49
3	C	552	FLC	CA-CAC	3.31	1.51	1.49
3	B	554	FLC	CG-CGC	3.27	1.51	1.49
3	A	550	FLC	CA-CAC	3.22	1.51	1.49

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	552	FLC	CG-CGC	3.20	1.51	1.49
3	A	551	FLC	CG-CGC	3.17	1.51	1.49
3	A	550	FLC	CG-CGC	3.16	1.51	1.49
3	B	553	FLC	CG-CGC	3.11	1.51	1.49
3	B	552	FLC	CA-CAC	3.07	1.51	1.49
3	C	551	FLC	CA-CAC	3.04	1.51	1.49
3	C	551	FLC	CG-CGC	3.03	1.51	1.49
3	B	554	FLC	CA-CAC	2.90	1.51	1.49

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	550	5GP	C6-C5-N7	-33.02	129.69	134.14
5	B	551	5GP	C6-C5-N7	-32.89	129.71	134.14
5	B	550	5GP	C6-C5-N7	-27.25	130.47	134.14
5	B	550	5GP	C6-N1-C2	2.93	124.63	119.51
5	C	550	5GP	C6-N1-C2	2.84	124.48	119.51
5	B	551	5GP	C6-N1-C2	2.82	124.44	119.51
5	B	550	5GP	C4'-O4'-C1'	-2.55	106.98	109.75
5	B	550	5GP	O4'-C1'-N9	2.41	110.68	108.44
3	A	550	FLC	CB-CG-CGC	-2.38	111.46	115.01
3	C	551	FLC	CB-CG-CGC	-2.32	111.54	115.01
3	C	551	FLC	CB-CA-CAC	-2.21	111.71	115.01
5	B	551	5GP	C8-N9-C4	-2.18	105.23	106.90
3	A	550	FLC	CB-CA-CAC	-2.17	111.77	115.01
5	B	551	5GP	C3'-C2'-C1'	2.12	104.23	100.91
3	B	554	FLC	CB-CA-CAC	-2.00	112.02	115.01

There are no chirality outliers.

There are no torsion outliers.

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 ⓘ

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(Å²)	Q<0.9	
1	A	544/549 (99%)	-0.27	6 (1%)	77	79	10, 21, 44, 62	1 (0%)
1	B	544/549 (99%)	-0.24	3 (0%)	86	88	11, 23, 46, 68	1 (0%)
1	C	544/549 (99%)	-0.19	8 (1%)	70	72	12, 25, 47, 64	1 (0%)
2	D	21/41 (51%)	0.39	2 (9%)	8	8	17, 37, 47, 52	0
2	E	20/41 (48%)	0.92	4 (20%)	2	1	33, 50, 62, 65	0
2	F	21/41 (51%)	1.34	6 (28%)	1	1	24, 48, 61, 61	0
All	All	1694/1770 (95%)	-0.19	29 (1%)	65	69	10, 24, 49, 68	3 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	1045	THR	4.5
2	F	1059	PRO	4.4
2	E	1045	THR	4.3
2	E	1059	PRO	4.0
2	F	1046	ALA	3.9
2	F	1039	GLY	3.8
1	B	52	PRO	3.4
2	D	1059	PRO	3.2
1	B	542	ASN	3.2
1	A	545	ARG	3.0
1	C	52	PRO	2.9
1	C	542	ASN	2.8
1	B	360	ARG	2.6
1	A	52	PRO	2.6
1	A	544	PRO	2.5
2	F	1040	ALA	2.5
1	A	55	ASP	2.5
2	F	1043	GLY	2.4
2	E	1046	ALA	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	436	GLY	2.3
1	C	55	ASP	2.2
1	C	544	PRO	2.2
2	D	1039	GLY	2.2
2	E	1058	GLN	2.2
1	C	236	GLU	2.1
1	C	53	GLY	2.1
1	A	543	ALA	2.1
1	A	261	THR	2.0
1	C	371	GLU	2.0

## 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 ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	FLC	B	552	13/13	0.33	6.46	60,62,64,64	0
5	5GP	B	550	20/24	0.47	6.15	18,20,23,25	20
5	5GP	B	551	20/24	0.36	5.11	15,16,18,21	20
3	FLC	B	554	13/13	0.26	4.55	77,80,81,81	0
5	5GP	C	550	20/24	0.47	4.44	23,24,29,31	20
3	FLC	A	550	13/13	0.16	2.64	46,49,50,50	0
3	FLC	B	555	13/13	0.20	1.66	40,47,54,57	0
3	FLC	B	553	13/13	0.18	1.34	41,48,52,54	0
3	FLC	A	551	13/13	0.19	1.30	30,42,51,54	0
3	FLC	C	551	13/13	0.17	0.52	45,48,51,53	0
4	MG	A	552	1/1	0.17	0.41	33,33,33,33	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	C	553	1/1	0.18	0.15	40,40,40,40	0
4	MG	B	556	1/1	0.15	-0.18	36,36,36,36	0
3	FLC	C	552	13/13	0.15	-0.26	30,43,51,55	0

## 6.5 Other polymers

There are no such residues in this entry.