



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:15 PM GMT

PDB ID : 1JGT  
Title : CRYSTAL STRUCTURE OF BETA-LACTAM SYNTHETASE  
Authors : Miller, M.T.; Bachmann, B.O.; Townsend, C.A.; Rosenzweig, A.C.  
Deposited on : 2001-06-26  
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure 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/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

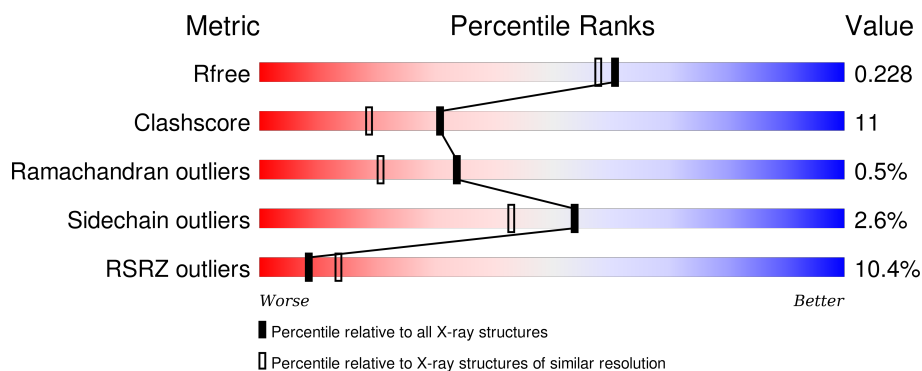
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	513	<div> <div>12%</div> <div>76%</div> <div>18%</div> <div>• •</div> </div>
1	B	513	<div> <div>8%</div> <div>80%</div> <div>17%</div> <div>• •</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
4	CMA	A	803	-	-	X	-
4	CMA	B	804	-	-	-	X
5	GOL	B	712	-	-	-	X
5	GOL	B	713	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8189 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.

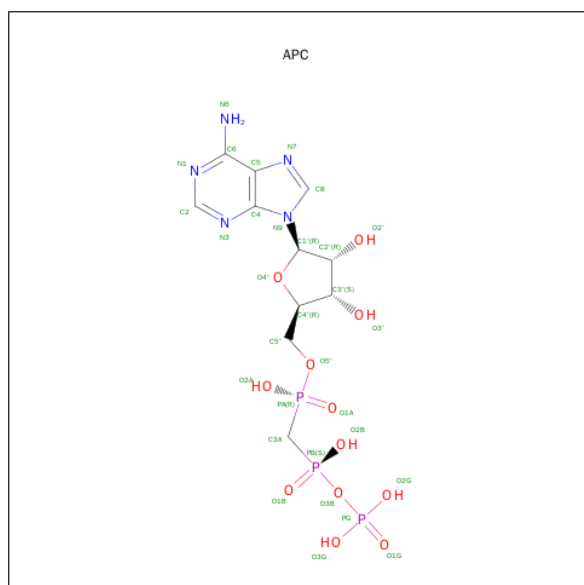
- Molecule 1 is a protein called BETA-LACTAM SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	0	0
			3690	2306	678	698	8			
1	B	500	Total	C	N	O	S	0	0	0
			3749	2337	691	713	8			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

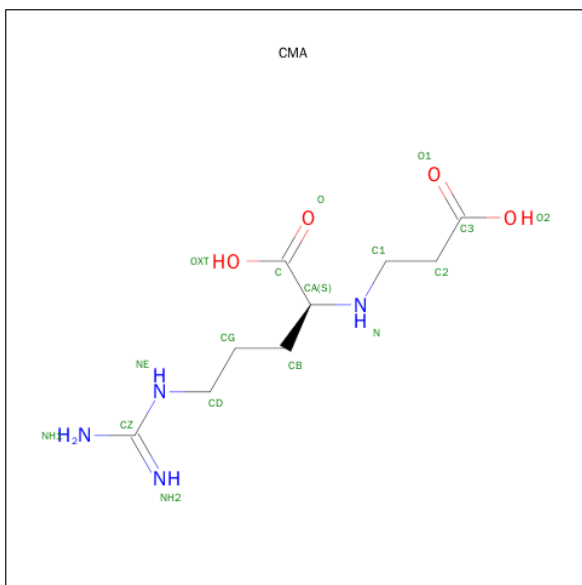
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (three-letter code: APC) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 4 is N2-(CARBOXYETHYL)-L-ARGININE (three-letter code: CMA) (formula:  $C_9H_{18}N_4O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	9	4	4		
4	B	1	Total	C	N	O	0	0
			17	9	4	4		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

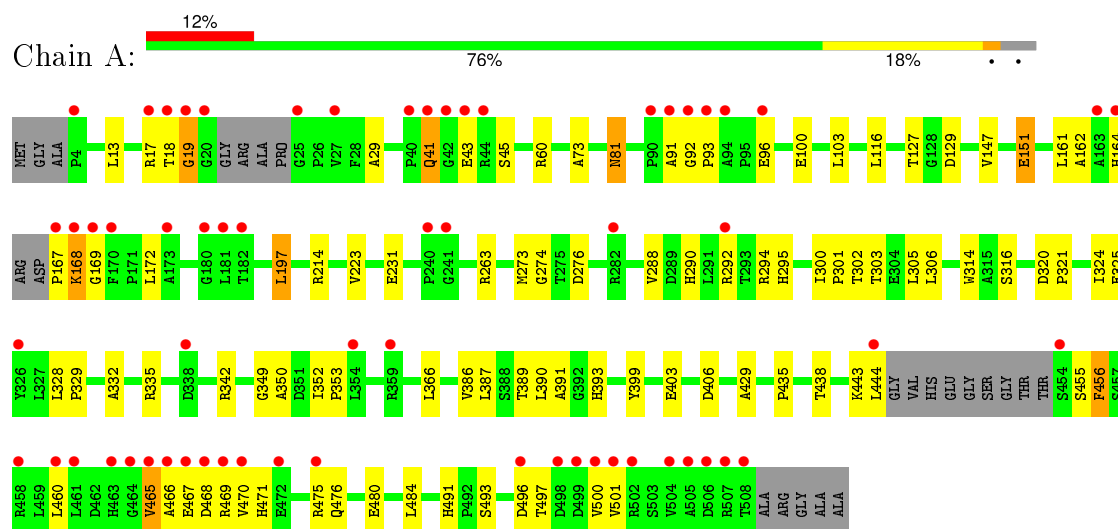
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	289	Total	O	0	0
			289	289		
6	B	333	Total	O	0	0
			333	333		

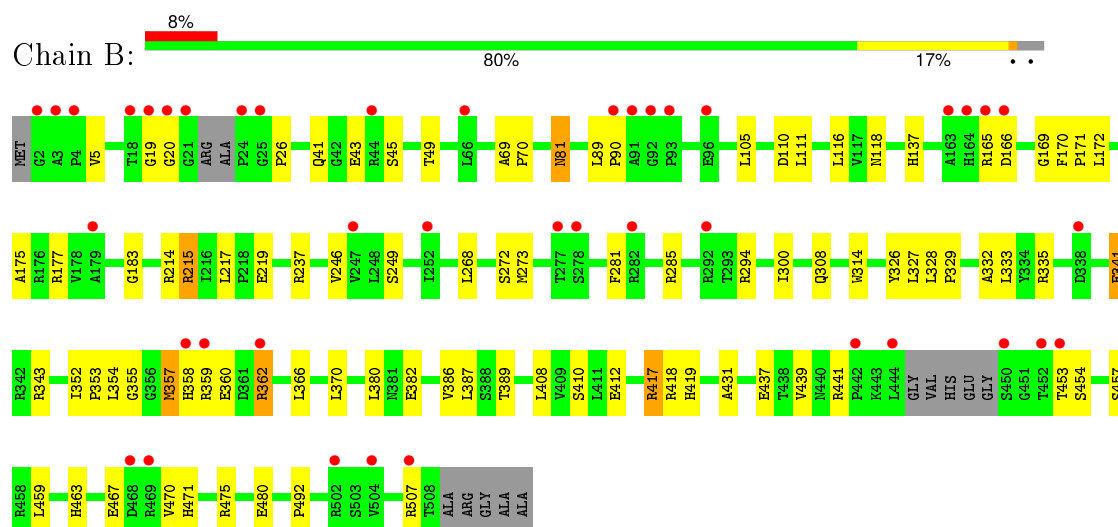
### 3 Residue-property plots

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: BETA-LACTAM SYNTHETASE



#### • Molecule 1: BETA-LACTAM SYNTHETASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.35Å 97.87Å 80.97Å 90.00° 90.78° 90.00°	Depositor
Resolution (Å)	19.89 – 1.95 19.97 – 1.95	Depositor EDS
% Data completeness (in resolution range)	95.0 (19.89-1.95) 95.0 (19.97-1.95)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.41 (at 1.94Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.195 , 0.228 0.195 , 0.228	Depositor DCC
$R_{free}$ test set	5838 reflections (8.83%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.0	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 57.6	EDS
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 69625 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8189	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, CMA, APC

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	0.31	0/3763	0.62	0/5131
1	B	0.33	0/3824	0.62	0/5216
All	All	0.32	0/7587	0.62	0/10347

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3690	0	3686	88	0
1	B	3749	0	3733	70	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	12	6	0
3	B	31	0	12	2	0
4	A	17	0	15	7	0
4	B	17	0	15	1	0
5	B	30	0	40	6	0
6	A	289	0	0	5	0
6	B	333	0	0	4	0
All	All	8189	0	7513	163	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 11.

All (163) 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)
3:A:801:APC:PA	4:A:803:CMA:O2	2.26	0.94
1:A:41:GLN:HB2	1:A:45:SER:HB3	1.48	0.92
1:A:17:ARG:HB3	1:A:151:GLU:HG2	1.54	0.88
1:B:358:HIS:HB2	1:B:366:LEU:HD13	1.57	0.85
4:A:803:CMA:O1	6:A:955:HOH:O	1.95	0.84
1:A:342:ARG:H	1:A:393:HIS:HD2	1.24	0.81
1:B:341:GLU:HG3	6:B:1233:HOH:O	1.80	0.80
1:B:215:ARG:HG3	5:B:712:GOL:H31	1.62	0.79
3:A:801:APC:H5'1	4:A:803:CMA:O2	1.84	0.78
1:B:81:ASN:H	1:B:81:ASN:HD22	1.32	0.77
1:A:41:GLN:HE21	1:A:45:SER:HB3	1.49	0.76
1:B:355:GLY:HA3	1:B:366:LEU:HD11	1.66	0.75
1:A:306:LEU:HD21	1:A:455:SER:HB3	1.69	0.74
1:B:41:GLN:OE1	1:B:45:SER:HB3	1.87	0.74
1:A:92:GLY:H	1:A:93:PRO:CD	2.01	0.74
1:A:167:PRO:HG2	1:A:168:LYS:HD3	1.72	0.71
1:A:92:GLY:H	1:A:93:PRO:HD2	1.55	0.71
1:A:41:GLN:HE21	1:A:45:SER:CB	2.07	0.68
3:A:801:APC:O2A	4:A:803:CMA:O2	2.12	0.68
1:A:17:ARG:CB	1:A:151:GLU:HG2	2.25	0.66
1:A:294:ARG:HD2	1:A:294:ARG:C	2.15	0.66
1:A:466:ALA:O	1:A:469:ARG:HB2	1.97	0.65
1:B:453:THR:HG23	1:B:457:SER:HB2	1.78	0.64
1:B:308:GLN:HE22	1:B:335:ARG:HH21	1.44	0.64
1:A:476:GLN:O	1:A:480:GLU:HG2	1.98	0.64
1:B:328:LEU:HB2	1:B:329:PRO:HD3	1.80	0.63
1:A:168:LYS:HD3	1:A:168:LYS:H	1.64	0.63
1:B:358:HIS:CB	1:B:366:LEU:HD13	2.27	0.62
1:A:491:HIS:HD2	1:A:493:SER:H	1.47	0.62
1:A:17:ARG:HG3	1:A:18:THR:H	1.66	0.61
1:A:92:GLY:N	1:A:93:PRO:HD2	2.15	0.61
1:B:69:ALA:HB1	1:B:70:PRO:HD2	1.82	0.61
1:A:460:LEU:HB3	1:A:465:VAL:HG11	1.82	0.60
1:A:466:ALA:HB3	1:A:469:ARG:HD2	1.83	0.60
1:A:321:PRO:HG3	1:A:475:ARG:HA	1.83	0.60
1:A:116:LEU:HD23	1:B:214:ARG:HB2	1.84	0.60
1:A:467:GLU:C	1:A:469:ARG:H	2.05	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:LEU:HD21	1:B:105:LEU:HD23	1.84	0.59
1:B:26:PRO:HG3	1:B:49:THR:HG21	1.85	0.58
1:B:170:PHE:HB3	1:B:171:PRO:HD2	1.85	0.58
1:B:410:SER:OG	5:B:713:GOL:H31	2.04	0.58
1:B:453:THR:HG22	1:B:454:SER:O	2.04	0.58
1:A:168:LYS:HD3	1:A:168:LYS:N	2.18	0.58
1:A:73:ALA:HB2	1:A:103:LEU:HD13	1.87	0.57
1:A:92:GLY:N	1:A:93:PRO:CD	2.68	0.57
1:A:60:ARG:HH21	1:A:60:ARG:HG3	1.69	0.57
1:A:342:ARG:N	1:A:393:HIS:HD2	2.01	0.56
1:B:386:VAL:HA	1:B:389:THR:OG1	2.05	0.56
3:A:801:APC:H5'1	4:A:803:CMA:C3	2.35	0.56
1:A:491:HIS:CD2	1:A:493:SER:H	2.24	0.56
1:B:471:HIS:HE1	1:B:475:ARG:NH1	2.04	0.55
3:A:801:APC:O2A	4:A:803:CMA:C3	2.55	0.55
1:A:167:PRO:HG2	1:A:168:LYS:CD	2.35	0.55
1:A:214:ARG:HB2	1:B:116:LEU:HD23	1.89	0.54
1:B:418:ARG:HG2	1:B:419:HIS:CD2	2.42	0.54
1:B:467:GLU:HA	1:B:470:VAL:HG23	1.89	0.54
1:A:497:THR:O	1:A:501:VAL:HG23	2.08	0.54
1:B:300:ILE:HG13	1:B:300:ILE:O	2.08	0.54
1:A:480:GLU:O	1:A:484:LEU:HG	2.08	0.53
1:B:437:GLU:O	1:B:441:ARG:HB2	2.08	0.53
1:B:110:ASP:CG	1:B:111:LEU:H	2.11	0.53
1:A:467:GLU:O	1:A:468:ASP:HB3	2.07	0.53
1:A:19:GLY:HA2	1:A:43:GLU:HB3	1.91	0.53
1:B:453:THR:CG2	1:B:457:SER:HB2	2.39	0.52
1:A:321:PRO:CG	1:A:475:ARG:HA	2.40	0.52
1:A:300:ILE:HD13	1:A:332:ALA:HB1	1.91	0.52
1:B:169:GLY:HA3	1:B:183:GLY:O	2.10	0.52
1:B:354:LEU:HD21	1:B:408:LEU:HD22	1.92	0.51
1:A:460:LEU:HD13	1:A:501:VAL:HG13	1.93	0.51
1:B:417:ARG:HH21	1:B:417:ARG:HB2	1.76	0.51
1:A:29:ALA:HA	1:A:314:TRP:CZ2	2.46	0.51
1:B:353:PRO:HA	1:B:370:LEU:HD13	1.91	0.51
1:A:13:LEU:C	1:A:13:LEU:HD13	2.31	0.51
1:A:292:ARG:HG2	1:A:292:ARG:HH11	1.76	0.51
1:B:215:ARG:HB3	5:B:713:GOL:O3	2.10	0.51
1:A:127:THR:HG23	1:A:127:THR:O	2.10	0.51
1:A:390:LEU:HD12	1:A:391:ALA:N	2.25	0.50
1:A:81:ASN:H	1:A:81:ASN:HD22	1.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ASN:N	1:B:81:ASN:HD22	2.00	0.50
1:B:172:LEU:HB2	1:B:175:ALA:HB3	1.93	0.50
1:B:326:TYR:CE1	4:B:804:CMA:HG1	2.47	0.50
1:A:390:LEU:HD12	1:A:390:LEU:C	2.32	0.49
1:B:353:PRO:HA	1:B:370:LEU:CD1	2.42	0.49
1:B:358:HIS:CE1	1:B:360:GLU:O	2.65	0.49
1:A:342:ARG:H	1:A:393:HIS:CD2	2.16	0.49
1:A:162:ALA:C	1:A:164:HIS:H	2.15	0.49
3:A:801:APC:H5'2	4:A:803:CMA:O2	2.07	0.49
1:B:358:HIS:CE1	1:B:362:ARG:O	2.66	0.48
1:B:418:ARG:HG2	1:B:419:HIS:CG	2.48	0.48
1:B:314:TRP:CE3	1:B:492:PRO:HG2	2.49	0.48
1:A:443:LYS:O	1:A:444:LEU:HB3	2.13	0.48
1:A:288:VAL:HG21	1:A:295:HIS:CG	2.48	0.48
1:A:467:GLU:C	1:A:469:ARG:N	2.67	0.48
1:B:137:HIS:HD2	6:B:1044:HOH:O	1.97	0.48
1:B:357:MET:CE	1:B:357:MET:HA	2.43	0.48
1:A:325:GLU:OE2	1:A:456:PHE:HB3	2.14	0.48
1:B:333:LEU:HD23	1:B:333:LEU:C	2.34	0.48
1:A:302:THR:O	1:A:306:LEU:HD23	2.14	0.47
1:A:147:VAL:HB	1:A:172:LEU:HD21	1.96	0.47
1:A:386:VAL:HA	1:A:389:THR:OG1	2.14	0.47
1:A:81:ASN:HD22	1:A:81:ASN:N	2.11	0.47
1:A:335:ARG:NH1	6:A:1185:HOH:O	2.47	0.47
1:B:281:PHE:O	1:B:285:ARG:HG3	2.14	0.47
1:B:217:LEU:HG	5:B:713:GOL:O3	2.14	0.47
1:B:382:GLU:HG2	6:B:1078:HOH:O	2.14	0.47
1:B:294:ARG:HG2	5:B:709:GOL:O1	2.15	0.46
1:A:73:ALA:CB	1:A:103:LEU:HD13	2.46	0.46
1:A:273:MET:HG2	1:A:274:GLY:N	2.31	0.46
1:B:81:ASN:ND2	1:B:118:ASN:H	2.14	0.46
1:A:475:ARG:HG2	1:A:475:ARG:HH11	1.81	0.46
1:A:73:ALA:HB2	1:A:103:LEU:CD1	2.45	0.46
1:B:418:ARG:HG2	1:B:419:HIS:N	2.30	0.46
1:B:246:VAL:HG23	1:B:268:LEU:HD11	1.97	0.46
1:A:335:ARG:NH2	6:A:1186:HOH:O	2.48	0.45
1:A:366:LEU:HD23	1:A:366:LEU:C	2.37	0.45
1:A:349:GLY:O	1:A:353:PRO:HD2	2.17	0.45
1:A:17:ARG:HD3	1:A:151:GLU:OE2	2.17	0.45
1:A:60:ARG:HG3	1:A:60:ARG:NH2	2.31	0.45
1:A:335:ARG:NE	6:A:1186:HOH:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:HIS:CG	1:A:435:PRO:HD3	2.52	0.45
1:B:165:ARG:HG3	1:B:166:ASP:OD2	2.16	0.45
1:B:177:ARG:HB3	1:B:177:ARG:NH1	2.32	0.44
1:A:301:PRO:HB2	1:A:303:THR:HG22	1.99	0.44
1:B:19:GLY:HA2	1:B:43:GLU:HG2	1.99	0.44
1:A:350:ALA:HB2	1:A:399:TYR:CD1	2.52	0.44
1:A:292:ARG:NH1	1:A:292:ARG:HG2	2.32	0.44
1:A:320:ASP:O	1:A:324:ILE:HG12	2.18	0.44
1:A:435:PRO:HG2	1:A:438:THR:OG1	2.17	0.44
1:A:496:ASP:O	1:A:500:VAL:HG23	2.18	0.44
1:A:406:ASP:OD1	5:B:712:GOL:H32	2.18	0.43
1:B:431:ALA:HA	1:B:439:VAL:HG21	2.00	0.43
1:A:456:PHE:O	1:A:460:LEU:HD23	2.17	0.43
1:A:223:VAL:HG13	1:A:429:ALA:HA	2.00	0.43
1:B:177:ARG:HH11	1:B:177:ARG:HB3	1.82	0.43
1:A:19:GLY:CA	1:A:43:GLU:HB3	2.48	0.43
1:B:237:ARG:O	1:B:343:ARG:HD3	2.18	0.43
1:B:359:ARG:HA	1:B:417:ARG:NH1	2.34	0.43
1:B:272:SER:HA	3:B:802:APC:H2	2.01	0.43
1:A:305:LEU:HD11	1:A:329:PRO:HA	2.00	0.43
1:A:29:ALA:HA	1:A:314:TRP:CH2	2.54	0.42
1:B:308:GLN:HG3	1:B:332:ALA:HB2	2.01	0.42
1:B:169:GLY:O	1:B:183:GLY:HA2	2.19	0.42
1:A:470:VAL:HG23	1:A:471:HIS:N	2.34	0.42
1:B:41:GLN:HG2	1:B:70:PRO:HB3	2.01	0.42
1:B:333:LEU:O	1:B:333:LEU:HD23	2.19	0.42
1:B:249:SER:HB3	3:B:802:APC:O1B	2.20	0.42
1:B:20:GLY:N	1:B:43:GLU:OE2	2.53	0.41
1:A:352:ILE:HB	1:A:353:PRO:CD	2.49	0.41
1:B:480:GLU:OE2	1:B:507:ARG:NH1	2.52	0.41
1:A:129:ASP:O	1:A:197:LEU:HB2	2.20	0.41
1:B:358:HIS:HD2	6:B:981:HOH:O	2.03	0.41
1:A:393:HIS:HE1	6:A:1055:HOH:O	2.02	0.41
1:B:352:ILE:HB	1:B:353:PRO:CD	2.49	0.41
1:A:335:ARG:HG2	1:A:335:ARG:HH11	1.85	0.41
1:B:308:GLN:HE22	1:B:335:ARG:HD3	1.84	0.41
1:A:316:SER:HB3	1:A:387:LEU:HD21	2.02	0.41
1:A:231:GLU:CD	1:A:263:ARG:HE	2.24	0.41
1:B:453:THR:HG23	1:B:457:SER:CB	2.48	0.41
1:A:328:LEU:N	1:A:329:PRO:HD2	2.35	0.41
1:B:327:LEU:HD13	1:B:387:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ARG:O	1:A:294:ARG:HD2	2.20	0.40
1:A:96:GLU:HG3	1:A:100:GLU:OE2	2.21	0.40
1:B:459:LEU:O	1:B:463:HIS:HD2	2.04	0.40

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	482/513 (94%)	458 (95%)	20 (4%)	4 (1%)	24	11
1	B	494/513 (96%)	482 (98%)	11 (2%)	1 (0%)	52	43
All	All	976/1026 (95%)	940 (96%)	31 (3%)	5 (0%)	34	21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	90	PRO
1	A	19	GLY
1	A	91	ALA
1	A	465	VAL
1	A	169	GLY

### 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	
1	A	383/395 (97%)	374 (98%)	9 (2%)	58	50
1	B	388/395 (98%)	377 (97%)	11 (3%)	51	39
All	All	771/790 (98%)	751 (97%)	20 (3%)	54	43

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	81	ASN
1	A	151	GLU
1	A	161	LEU
1	A	168	LYS
1	A	197	LEU
1	A	276	ASP
1	A	403	GLU
1	A	456	PHE
1	B	5	VAL
1	B	81	ASN
1	B	215	ARG
1	B	219	GLU
1	B	273	MET
1	B	341	GLU
1	B	357	MET
1	B	362	ARG
1	B	380	LEU
1	B	412	GLU
1	B	417	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	81	ASN
1	A	118	ASN
1	A	236	GLN
1	A	393	HIS
1	A	440	ASN
1	A	491	HIS
1	B	81	ASN
1	B	137	HIS
1	B	236	GLN

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Mol	Chain	Res	Type
1	B	295	HIS
1	B	308	GLN
1	B	358	HIS
1	B	372	HIS
1	B	419	HIS
1	B	463	HIS
1	B	471	HIS

### 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 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	APC	A	801	2,4	25,33,33	2.19	7 (28%)	30,52,52	2.36	6 (20%)
4	CMA	A	803	3	7,16,16	0.59	0	6,19,19	2.55	1 (16%)
5	GOL	B	709	-	5,5,5	0.92	0	5,5,5	0.37	0
5	GOL	B	710	-	5,5,5	1.00	0	5,5,5	0.34	0
5	GOL	B	711	-	5,5,5	0.99	0	5,5,5	0.33	0
5	GOL	B	712	-	5,5,5	0.97	0	5,5,5	0.32	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	B	713	-	5,5,5	0.90	0	5,5,5	0.34	0
3	APC	B	802	2	25,33,33	2.18	7 (28%)	30,52,52	2.38	6 (20%)
4	CMA	B	804	-	7,16,16	0.44	0	6,19,19	2.59	1 (16%)

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	APC	A	801	2,4	-	0/15/38/38	0/3/3/3
4	CMA	A	803	3	-	0/9/17/17	0/0/0/0
5	GOL	B	709	-	-	0/4/4/4	0/0/0/0
5	GOL	B	710	-	-	0/4/4/4	0/0/0/0
5	GOL	B	711	-	-	0/4/4/4	0/0/0/0
5	GOL	B	712	-	-	0/4/4/4	0/0/0/0
5	GOL	B	713	-	-	0/4/4/4	0/0/0/0
3	APC	B	802	2	-	0/15/38/38	0/3/3/3
4	CMA	B	804	-	-	0/9/17/17	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	APC	O5'-C5'	-6.93	1.16	1.44
3	A	801	APC	O5'-C5'	-6.71	1.17	1.44
3	A	801	APC	C6-N6	-3.92	1.22	1.34
3	B	802	APC	C6-N6	-3.85	1.23	1.34
3	A	801	APC	PB-O2B	-3.37	1.48	1.56
3	B	802	APC	PB-O2B	-3.03	1.49	1.56
3	A	801	APC	PA-O2A	-2.17	1.51	1.56
3	B	802	APC	PA-O2A	-2.02	1.51	1.56
3	B	802	APC	PA-O5'	2.62	1.60	1.57
3	A	801	APC	C4-N3	3.05	1.40	1.35
3	A	801	APC	PA-O5'	3.38	1.61	1.57
3	B	802	APC	C4-N3	3.42	1.40	1.35
3	A	801	APC	C2-N1	3.48	1.40	1.33
3	B	802	APC	C2-N1	3.52	1.40	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	APC	N3-C2-N1	-9.10	121.92	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	APC	N3-C2-N1	-9.10	121.93	128.89
3	B	802	APC	O5'-PA-O1A	-3.59	104.43	113.98
3	A	801	APC	O5'-PA-O1A	-3.55	104.54	113.98
3	B	802	APC	O1B-PB-C3A	-2.90	101.72	109.02
3	A	801	APC	O1B-PB-C3A	-2.73	102.14	109.02
3	B	802	APC	O5'-PA-C3A	2.94	112.64	104.42
3	A	801	APC	O5'-PA-C3A	3.11	113.12	104.42
3	A	801	APC	C4'-O4'-C1'	3.53	113.59	109.72
3	B	802	APC	C4'-O4'-C1'	3.73	113.81	109.72
3	A	801	APC	C2-N1-C6	4.74	127.24	118.77
3	B	802	APC	C2-N1-C6	4.78	127.30	118.77
4	A	803	CMA	C1-N-CA	6.18	123.28	113.91
4	B	804	CMA	C1-N-CA	6.20	123.30	113.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	APC	6	0
4	A	803	CMA	7	0
5	B	709	GOL	1	0
5	B	712	GOL	2	0
5	B	713	GOL	3	0
3	B	802	APC	2	0
4	B	804	CMA	1	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<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	490/513 (95%)	0.67	62 (12%) 5 8	16, 27, 63, 76	0
1	B	500/513 (97%)	0.53	41 (8%) 14 23	15, 25, 47, 68	0
All	All	990/1026 (96%)	0.60	103 (10%) 8 13	15, 26, 55, 76	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	91	ALA	11.2
1	B	2	GLY	8.2
1	A	19	GLY	8.0
1	A	164	HIS	7.5
1	A	167	PRO	7.2
1	A	20	GLY	6.9
1	A	468	ASP	6.8
1	B	20	GLY	6.7
1	B	444	LEU	6.2
1	A	18	THR	6.1
1	B	18	THR	6.0
1	A	444	LEU	5.9
1	B	21	GLY	5.8
1	A	467	GLU	5.6
1	A	163	ALA	5.5
1	B	165	ARG	5.3
1	B	164	HIS	5.3
1	A	504	VAL	4.8
1	A	507	ARG	4.7
1	A	469	ARG	4.7
1	A	92	GLY	4.6
1	B	24	PRO	4.6
1	B	93	PRO	4.6
1	A	169	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	470	VAL	4.6
1	A	170	PHE	4.6
1	A	182	THR	4.5
1	B	92	GLY	4.5
1	A	17	ARG	4.4
1	A	93	PRO	4.3
1	A	508	THR	4.3
1	B	166	ASP	4.2
1	A	326	TYR	4.2
1	A	180	GLY	4.1
1	B	25	GLY	4.1
1	A	292	ARG	3.9
1	B	452	THR	3.9
1	A	168	LYS	3.8
1	A	359	ARG	3.8
1	B	3	ALA	3.7
1	A	505	ALA	3.6
1	A	4	PRO	3.6
1	A	91	ALA	3.6
1	A	496	ASP	3.6
1	A	96	GLU	3.6
1	B	450	SER	3.6
1	A	501	VAL	3.6
1	B	359	ARG	3.5
1	A	472	GLU	3.5
1	B	44	ARG	3.5
1	B	19	GLY	3.4
1	A	506	ASP	3.4
1	A	240	PRO	3.4
1	B	282	ARG	3.4
1	A	40	PRO	3.4
1	A	44	ARG	3.2
1	B	338	ASP	3.1
1	A	43	GLU	3.1
1	A	241	GLY	3.1
1	A	502	ARG	3.0
1	A	498	ASP	3.0
1	A	458	ARG	2.9
1	A	461	LEU	2.9
1	B	442	PRO	2.9
1	A	173	ALA	2.9
1	B	4	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	468	ASP	2.9
1	A	466	ALA	2.9
1	A	500	VAL	2.9
1	A	94	ALA	2.8
1	A	338	ASP	2.8
1	A	282	ARG	2.7
1	B	469	ARG	2.7
1	A	42	GLY	2.6
1	B	179	ALA	2.6
1	A	25	GLY	2.5
1	A	475	ARG	2.5
1	B	453	THR	2.5
1	B	90	PRO	2.5
1	A	460	LEU	2.5
1	B	66	LEU	2.5
1	A	499	ASP	2.4
1	A	464	GLY	2.3
1	B	507	ARG	2.3
1	B	96	GLU	2.3
1	A	41	GLN	2.3
1	B	358	HIS	2.2
1	A	181	LEU	2.2
1	B	247	VAL	2.2
1	A	27	VAL	2.2
1	A	90	PRO	2.2
1	B	502	ARG	2.1
1	B	292	ARG	2.1
1	A	463	HIS	2.1
1	B	163	ALA	2.1
1	A	465	VAL	2.1
1	A	454	SER	2.1
1	B	362	ARG	2.0
1	B	278	SER	2.0
1	A	354	LEU	2.0
1	B	277	THR	2.0
1	B	504	VAL	2.0
1	B	252	ILE	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 [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<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
5	GOL	B	713	6/6	0.67	0.33	7.16	59,60,61,63	0
5	GOL	B	712	6/6	0.63	0.27	5.83	61,62,62,62	0
4	CMA	B	804	17/17	0.80	0.21	2.30	28,36,47,48	0
4	CMA	A	803	17/17	0.73	0.25	1.87	46,50,61,62	0
5	GOL	B	710	6/6	0.73	0.23	1.04	60,61,62,62	0
5	GOL	B	709	6/6	0.79	0.19	0.72	55,56,57,57	0
3	APC	A	801	31/31	0.91	0.15	0.51	27,37,40,41	0
3	APC	B	802	31/31	0.85	0.18	0.44	30,40,45,45	0
2	MG	A	902	1/1	0.86	0.13	-0.22	42,42,42,42	0
2	MG	B	901	1/1	0.92	0.09	-	39,39,39,39	0
5	GOL	B	711	6/6	0.65	0.47	-	64,64,65,65	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.