



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:50 PM GMT

PDB ID : 1MC1
Title : BETA-LACTAM SYNTHETASE WITH PRODUCT (DGPC), AMP AND PPI
Authors : Miller, M.T.; Bachmann, B.O.; Townsend, C.A.; Rosenzweig, A.C.
Deposited on : 2002-08-04
Resolution : 2.16 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

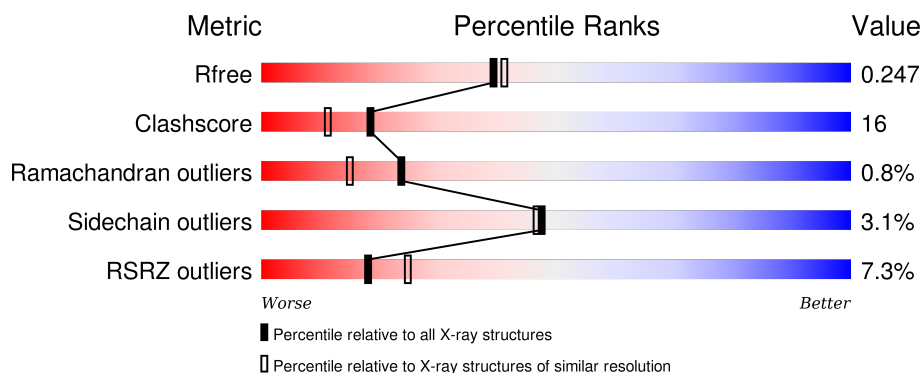
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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 ≥ 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>8%</div> <div>68%</div> <div>24%</div> <div>• • •</div> </div>
1	B	513	<div> <div>6%</div> <div>72%</div> <div>23%</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	PCX	B	706	-	-	X	-
5	AMP	A	702	-	-	X	-
5	AMP	B	705	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7946 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.

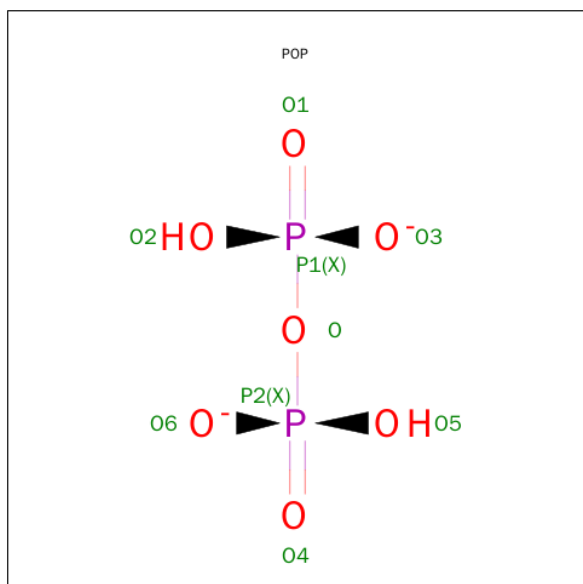
- Molecule 1 is a protein called BETA-LACTAM SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	0
			3693	2305	678	702	8			
1	B	498	Total	C	N	O	S	0	0	0
			3748	2339	692	709	8			

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

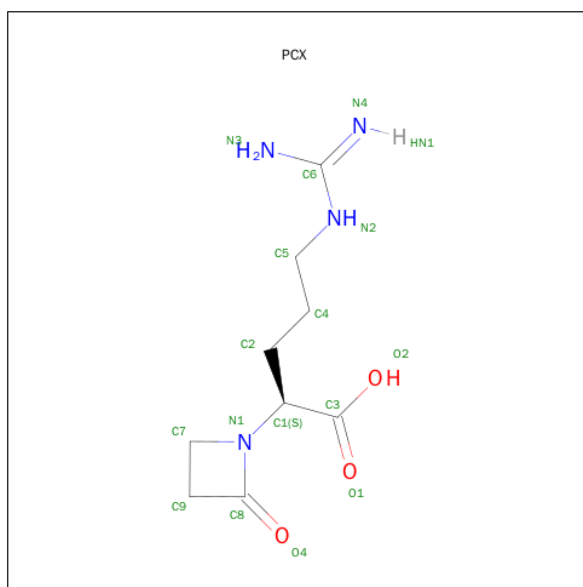
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: H₂O₇P₂).



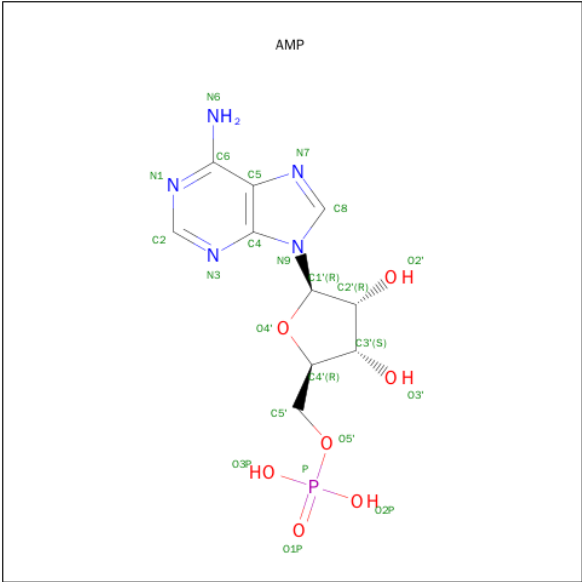
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			9	7	2		
3	B	1	Total	O	P	0	0
			9	7	2		

- Molecule 4 is DEOXYGUANIDINOPROCLAVAMINIC ACID (three-letter code: PCX) (formula: $C_9H_{16}N_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			16	9	4	3		
4	A	1	Total	C	N	O	0	0
			16	9	4	3		

- Molecule 5 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
5	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	175	Total	O	0	0
			175	175		
6	B	230	Total	O	0	0
			230	230		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.04Å 96.57Å 80.91Å 90.00° 90.54° 90.00°	Depositor
Resolution (Å)	29.10 – 2.16 29.10 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.7 (29.10-2.16) 94.6 (29.10-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.208 , 0.247 0.208 , 0.247	Depositor DCC
R_{free} test set	4350 reflections (9.11%)	DCC
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 54.5	EDS
Estimated twinning fraction	0.053 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 63373 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7946	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: AMP, PCX, MG, POP

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	4/3765 (0.1%)	0.87	19/5136 (0.4%)
1	B	0.41	1/3824 (0.0%)	0.74	8/5219 (0.2%)
All	All	0.46	5/7589 (0.1%)	0.81	27/10355 (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
1	A	0	9
1	B	1	5
All	All	1	14

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	169	GLY	CA-C	-6.76	1.41	1.51
1	A	169	GLY	N-CA	-6.73	1.35	1.46
1	A	468	ASP	N-CA	6.52	1.59	1.46
1	A	445	GLY	C-O	6.07	1.33	1.23
1	B	23	ALA	N-CA	5.26	1.56	1.46

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	PHE	C-N-CD	12.67	155.00	128.40
1	A	169	GLY	N-CA-C	11.90	142.85	113.10
1	A	69	ALA	C-N-CD	11.84	153.26	128.40
1	B	23	ALA	O-C-N	-11.46	99.32	121.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	469	ARG	O-C-N	-10.71	105.57	122.70
1	B	22	ARG	NE-CZ-NH1	9.77	125.18	120.30
1	A	174	ASP	CB-CG-OD2	-9.32	109.91	118.30
1	A	171	PRO	CA-N-CD	-9.22	98.59	111.50
1	B	174	ASP	CB-CG-OD2	9.14	126.53	118.30
1	A	70	PRO	CA-N-CD	-8.20	100.03	111.50
1	A	445	GLY	O-C-N	-8.10	109.75	122.70
1	A	467	GLU	CA-C-N	7.98	134.75	117.20
1	A	446	VAL	C-N-CA	7.46	140.36	121.70
1	B	22	ARG	CA-C-N	7.26	133.18	117.20
1	A	170	PHE	CB-CG-CD1	7.08	125.75	120.80
1	A	169	GLY	O-C-N	-6.61	112.12	122.70
1	A	169	GLY	CA-C-N	6.05	130.51	117.20
1	B	21	GLY	O-C-N	-6.03	113.06	122.70
1	B	20	GLY	C-N-CA	-6.02	109.65	122.30
1	A	467	GLU	O-C-N	-5.97	113.14	122.70
1	A	174	ASP	CB-CG-OD1	-5.85	113.03	118.30
1	B	22	ARG	CD-NE-CZ	5.72	131.61	123.60
1	A	467	GLU	N-CA-C	5.60	126.11	111.00
1	A	41	GLN	C-N-CA	5.50	133.84	122.30
1	A	468	ASP	N-CA-CB	-5.47	100.76	110.60
1	A	467	GLU	CA-C-O	-5.37	108.83	120.10
1	B	22	ARG	C-N-CA	5.34	135.05	121.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	22	ARG	CA

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	174	ASP	Sidechain
1	A	42	GLY	Mainchain,Peptide
1	A	44	ARG	Mainchain
1	A	445	GLY	Mainchain
1	A	446	VAL	Mainchain
1	A	467	GLU	Mainchain
1	A	469	ARG	Mainchain
1	A	70	PRO	Mainchain
1	B	21	GLY	Mainchain,Peptide
1	B	22	ARG	Mainchain,Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	23	ALA	Mainchain

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	3693	0	3680	128	2
1	B	3748	0	3742	102	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	9	0	0	0	0
3	B	9	0	0	1	0
4	A	16	0	14	5	0
4	B	16	0	14	8	0
5	A	23	0	12	13	0
5	B	23	0	12	3	0
6	A	175	0	0	3	0
6	B	230	0	0	7	0
All	All	7946	0	7474	233	2

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 16.

All (233) 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:A:702:AMP:O3P	4:A:703:PCX:H9C1	1.14	1.32
1:A:149:PRO:CD	1:A:170:PHE:CZ	2.20	1.23
1:A:149:PRO:CD	1:A:170:PHE:CE1	2.30	1.15
1:A:149:PRO:HD3	1:A:170:PHE:CE1	1.80	1.15
1:A:326:TYR:CE2	1:A:447:HIS:CE1	2.44	1.05
5:A:702:AMP:O3P	4:A:703:PCX:C9	2.06	1.03
1:A:149:PRO:HD3	1:A:170:PHE:CZ	1.86	1.02
1:A:446:VAL:HG21	5:A:702:AMP:C8	1.97	1.00
1:A:446:VAL:CG2	5:A:702:AMP:C8	2.46	0.99
1:A:149:PRO:HD2	1:A:170:PHE:CE1	1.97	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:LEU:HD12	1:B:26:PRO:HB3	1.48	0.94
1:B:357:MET:CE	4:B:706:PCX:O4	2.15	0.94
1:A:149:PRO:HD2	1:A:170:PHE:CZ	2.02	0.94
1:A:41:GLN:O	1:A:43:GLU:N	2.01	0.93
4:B:706:PCX:H7C2	5:B:705:AMP:O3P	1.70	0.91
1:A:326:TYR:CE2	1:A:447:HIS:ND1	2.42	0.87
1:A:13:LEU:HD23	1:A:26:PRO:HG3	1.58	0.85
1:A:326:TYR:HE2	1:A:447:HIS:CE1	1.92	0.83
1:A:444:LEU:HD12	1:A:448:GLU:HB2	1.60	0.82
1:B:357:MET:HE3	4:B:706:PCX:O4	1.79	0.81
1:B:459:LEU:HD11	1:B:501:VAL:HG11	1.62	0.81
1:A:446:VAL:HG22	5:A:702:AMP:N7	1.96	0.81
1:A:446:VAL:HG22	5:A:702:AMP:C8	2.16	0.80
1:A:444:LEU:CD1	1:A:448:GLU:HB2	2.13	0.79
1:A:446:VAL:CG2	5:A:702:AMP:H8	1.95	0.77
1:B:174:ASP:O	1:B:188:PRO:HG3	1.83	0.77
1:A:112:HIS:HD2	1:A:115:ARG:HE	1.31	0.76
1:B:17:ARG:HG2	1:B:19:GLY:H	1.52	0.74
1:A:149:PRO:CG	1:A:170:PHE:CZ	2.72	0.72
1:A:273:MET:HB2	1:A:333:LEU:HD13	1.72	0.71
1:B:22:ARG:CG	1:B:23:ALA:HB3	2.18	0.71
1:A:352:ILE:HB	1:A:353:PRO:HD3	1.73	0.70
1:A:300:ILE:HG13	1:A:300:ILE:O	1.91	0.70
1:B:22:ARG:HG2	1:B:23:ALA:HB3	1.72	0.69
1:B:328:LEU:HB2	1:B:329:PRO:HD3	1.73	0.69
1:B:174:ASP:O	1:B:188:PRO:CG	2.41	0.69
1:A:326:TYR:CD2	1:A:447:HIS:ND1	2.61	0.68
1:A:321:PRO:HG2	1:A:475:ARG:HG2	1.75	0.68
1:B:327:LEU:O	1:B:331:THR:HG23	1.93	0.68
1:B:153:ARG:HG2	1:B:153:ARG:HH21	1.61	0.66
1:A:446:VAL:HG21	5:A:702:AMP:H8	1.53	0.66
1:B:459:LEU:CD1	1:B:501:VAL:HG11	2.26	0.65
1:A:176:ARG:HH11	1:A:176:ARG:HG2	1.62	0.65
1:A:41:GLN:HG2	1:A:45:SER:HB2	1.79	0.65
1:A:446:VAL:CG2	5:A:702:AMP:N7	2.59	0.64
1:B:357:MET:HE1	4:B:706:PCX:O4	1.97	0.64
1:A:44:ARG:O	1:A:126:ARG:CZ	2.46	0.64
1:A:327:LEU:HD22	1:A:387:LEU:HD21	1.79	0.63
1:A:444:LEU:HD12	1:A:448:GLU:OE2	1.99	0.62
1:B:437:GLU:HG2	1:B:441:ARG:NH2	2.15	0.62
1:B:357:MET:CE	4:B:706:PCX:C8	2.77	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:GLU:OE2	1:A:444:LEU:HD23	2.00	0.61
1:A:300:ILE:HD11	1:A:305:LEU:HG	1.83	0.61
1:B:360:GLU:CG	1:B:362:ARG:HG3	2.30	0.61
1:A:148:ALA:HA	1:A:170:PHE:CD1	2.35	0.61
1:A:443:LYS:HD3	1:A:444:LEU:N	2.15	0.60
1:A:73:ALA:HB2	1:A:103:LEU:HD13	1.83	0.60
1:B:41:GLN:HG2	1:B:45:SER:OG	2.01	0.60
1:A:360:GLU:HB2	6:A:820:HOH:O	2.01	0.60
1:B:357:MET:HE1	4:B:706:PCX:C8	2.31	0.60
1:B:132:LEU:HD23	1:B:194:ASP:HA	1.83	0.60
1:B:170:PHE:HB3	1:B:171:PRO:HD2	1.84	0.60
1:A:193:MET:HE2	1:A:195:ILE:HD11	1.84	0.60
1:B:153:ARG:HH22	1:B:164:HIS:CD2	2.19	0.60
1:A:92:GLY:N	1:A:93:PRO:HD2	2.17	0.60
1:B:308:GLN:HG3	1:B:332:ALA:HB2	1.83	0.59
4:B:706:PCX:C7	5:B:705:AMP:O3P	2.47	0.59
1:A:133:LEU:HD12	1:A:193:MET:HE2	1.84	0.59
1:B:3:ALA:HB3	1:B:4:PRO:HD3	1.85	0.59
1:B:386:VAL:HA	1:B:389:THR:OG1	2.03	0.59
1:A:314:TRP:CD1	1:A:485:THR:HB	2.38	0.58
1:B:359:ARG:HD3	6:B:927:HOH:O	2.03	0.58
1:A:280:GLU:CD	1:A:444:LEU:HD23	2.23	0.58
1:B:85:LEU:HG	1:B:105:LEU:HD11	1.84	0.58
1:B:358:HIS:CE1	1:B:360:GLU:HB3	2.39	0.57
1:B:215:ARG:HH11	1:B:215:ARG:HG3	1.68	0.57
1:B:491:HIS:O	1:B:494:GLU:HG2	2.04	0.57
1:A:41:GLN:C	1:A:43:GLU:H	1.96	0.57
1:B:308:GLN:HE22	1:B:335:ARG:HH21	1.50	0.57
1:A:296:ARG:HH12	1:A:338:ASP:H	1.52	0.57
1:B:360:GLU:HG3	1:B:362:ARG:HG3	1.87	0.57
1:B:85:LEU:O	1:B:88:VAL:HG22	2.05	0.57
1:A:345:LEU:HD13	1:A:396:THR:HG23	1.84	0.57
1:B:355:GLY:HA3	6:B:849:HOH:O	2.04	0.57
1:B:314:TRP:CD1	1:B:485:THR:HB	2.40	0.57
1:A:176:ARG:NH1	1:A:176:ARG:HG2	2.20	0.56
1:A:354:LEU:HB3	1:A:423:LYS:HG2	1.88	0.56
1:B:169:GLY:HA3	1:B:183:GLY:O	2.06	0.56
1:B:418:ARG:HG2	1:B:419:HIS:CD2	2.40	0.56
1:B:360:GLU:HG3	1:B:362:ARG:H	1.70	0.56
1:B:71:THR:OG1	1:B:127:THR:HG23	2.06	0.56
1:B:65:SER:HB3	1:B:71:THR:HB	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ALA:HA	1:A:314:TRP:CH2	2.41	0.55
1:A:306:LEU:HD21	1:A:455:SER:HB3	1.87	0.55
1:A:193:MET:CE	1:A:195:ILE:HD11	2.36	0.55
1:A:284:ALA:O	1:A:288:VAL:HG13	2.07	0.55
1:B:461:LEU:HD13	1:B:470:VAL:HG21	1.88	0.55
1:B:122:ALA:HB1	1:B:143:LEU:HG	1.89	0.54
1:B:351:ASP:OD2	1:B:356:GLY:HA2	2.07	0.54
1:A:52:HIS:CE1	1:A:58:PRO:HG3	2.43	0.54
1:A:313:VAL:HG21	1:A:481:LEU:HB3	1.89	0.54
1:A:112:HIS:CD2	1:A:115:ARG:HE	2.21	0.54
1:A:437:GLU:HG2	1:A:441:ARG:NH1	2.23	0.53
1:B:172:LEU:HB2	1:B:175:ALA:HB3	1.91	0.53
1:B:437:GLU:HG2	1:B:441:ARG:HH22	1.72	0.53
1:B:459:LEU:HD12	1:B:460:LEU:HD22	1.91	0.52
1:A:282:ARG:C	1:A:282:ARG:HD3	2.29	0.52
1:A:472:GLU:OE2	1:A:475:ARG:HD2	2.10	0.52
1:A:52:HIS:NE2	1:A:58:PRO:HG3	2.25	0.52
1:B:357:MET:HE3	4:B:706:PCX:C8	2.40	0.52
1:A:149:PRO:HG2	1:A:170:PHE:CZ	2.45	0.52
1:A:285:ARG:O	1:A:288:VAL:HG22	2.10	0.52
1:A:507:ARG:N	1:A:507:ARG:HD3	2.25	0.51
1:A:148:ALA:HA	1:A:170:PHE:CE1	2.46	0.51
1:B:89:LEU:HD11	1:B:105:LEU:HD23	1.93	0.51
1:A:344:ILE:HB	1:A:395:THR:HG22	1.93	0.51
1:A:497:THR:O	1:A:501:VAL:HG23	2.10	0.51
1:B:247:VAL:HG23	5:B:705:AMP:O2'	2.10	0.51
1:B:153:ARG:HG2	1:B:153:ARG:NH2	2.26	0.51
1:A:247:VAL:O	1:A:247:VAL:HG23	2.11	0.51
1:B:125:VAL:CG1	1:B:132:LEU:HB2	2.41	0.51
1:B:111:LEU:HD12	1:B:112:HIS:N	2.26	0.51
1:B:22:ARG:HG3	1:B:23:ALA:HB3	1.91	0.50
1:B:327:LEU:HD13	1:B:387:LEU:HD21	1.92	0.50
1:B:253:ASP:HB2	3:B:704:POP:P1	2.51	0.50
1:A:435:PRO:HG2	1:A:438:THR:OG1	2.12	0.50
1:B:275:THR:OG1	1:B:277:THR:HG22	2.12	0.50
1:A:300:ILE:HD13	1:A:332:ALA:HB1	1.94	0.49
1:A:321:PRO:HG2	1:A:475:ARG:CG	2.40	0.49
1:A:358:HIS:HB3	6:A:776:HOH:O	2.11	0.49
1:B:85:LEU:O	1:B:89:LEU:HD13	2.13	0.49
1:A:446:VAL:CG2	5:A:702:AMP:H5'1	2.43	0.49
1:A:111:LEU:HD12	1:A:112:HIS:N	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:PRO:HG3	1:A:475:ARG:HA	1.95	0.48
1:B:176:ARG:NH1	6:B:853:HOH:O	2.43	0.48
1:A:85:LEU:O	1:A:88:VAL:HG22	2.14	0.48
1:A:147:VAL:HB	1:A:172:LEU:HD21	1.95	0.48
1:B:370:LEU:HD13	1:B:370:LEU:C	2.34	0.48
1:B:349:GLY:O	1:B:353:PRO:HD2	2.14	0.48
1:A:31:ARG:NH2	1:A:392:GLY:HA3	2.29	0.48
1:B:421:ARG:HD2	6:B:761:HOH:O	2.14	0.48
1:A:39:THR:O	1:A:42:GLY:HA2	2.13	0.48
1:A:275:THR:HG21	1:A:305:LEU:HD12	1.96	0.47
1:A:285:ARG:HA	1:A:288:VAL:HG22	1.96	0.47
1:A:268:LEU:O	1:A:293:THR:HB	2.14	0.47
1:A:323:ILE:O	1:A:327:LEU:HG	2.14	0.47
1:B:195:ILE:HG12	1:B:202:ALA:HB2	1.97	0.47
1:B:30:THR:HG23	1:B:389:THR:HB	1.97	0.47
1:B:215:ARG:NH1	1:B:215:ARG:HG3	2.30	0.47
1:A:444:LEU:CD1	1:A:448:GLU:CB	2.89	0.47
1:A:302:THR:O	1:A:306:LEU:HD23	2.15	0.47
1:A:491:HIS:HD2	1:A:493:SER:OG	1.96	0.47
1:B:281:PHE:O	1:B:285:ARG:HG3	2.15	0.47
1:A:314:TRP:HD1	1:A:485:THR:HB	1.80	0.47
1:A:444:LEU:HD11	1:A:448:GLU:HB2	1.91	0.46
1:B:237:ARG:O	1:B:343:ARG:HD3	2.15	0.46
1:B:473:ALA:O	1:B:477:VAL:HG23	2.15	0.46
1:A:92:GLY:H	1:A:93:PRO:HD2	1.80	0.46
1:B:237:ARG:HD3	1:B:396:THR:HG23	1.97	0.46
1:A:86:LEU:HD11	1:A:95:PRO:HD2	1.98	0.46
1:A:362:ARG:NH2	1:B:107:GLU:O	2.49	0.46
1:B:22:ARG:HG2	1:B:23:ALA:O	2.16	0.45
1:B:40:PRO:HG2	1:B:41:GLN:NE2	2.31	0.45
1:A:15:SER:HA	1:A:152:VAL:O	2.16	0.45
1:B:422:ASP:OD2	1:B:423:LYS:HE2	2.16	0.45
1:B:247:VAL:HG23	1:B:247:VAL:O	2.17	0.45
1:B:366:LEU:HD23	1:B:366:LEU:C	2.37	0.45
1:B:26:PRO:HG3	1:B:49:THR:HG21	1.99	0.45
1:A:178:VAL:HB	1:A:181:LEU:HD12	1.98	0.45
1:A:288:VAL:HG11	1:A:295:HIS:CG	2.52	0.45
1:B:370:LEU:HD13	1:B:371:ALA:N	2.32	0.45
1:A:43:GLU:C	1:A:45:SER:H	2.19	0.45
1:A:73:ALA:HB2	1:A:103:LEU:CD1	2.45	0.45
1:A:285:ARG:HD3	1:A:288:VAL:CG2	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:ASP:O	1:B:339:GLY:O	2.35	0.45
1:A:363:LEU:N	1:A:364:PRO:CD	2.80	0.45
1:A:460:LEU:HD13	1:A:473:ALA:HB3	1.99	0.44
1:B:125:VAL:HG13	1:B:132:LEU:HB2	2.00	0.44
1:A:274:GLY:O	1:A:299:THR:HA	2.17	0.44
1:A:6:LEU:HD11	1:A:341:GLU:HG3	1.98	0.44
1:B:71:THR:HA	1:B:126:ARG:O	2.18	0.44
1:B:89:LEU:HD11	1:B:105:LEU:CD2	2.48	0.44
1:A:85:LEU:HD13	1:A:105:LEU:HD11	2.00	0.44
1:A:382:GLU:OE1	4:A:703:PCX:H5C2	2.17	0.44
1:B:284:ALA:O	1:B:288:VAL:HG23	2.18	0.44
1:B:124:VAL:HG22	1:B:133:LEU:CD2	2.48	0.43
1:A:359:ARG:HH21	1:A:359:ARG:HG3	1.83	0.43
1:A:8:ALA:HB3	1:A:61:ALA:HB2	2.00	0.43
1:B:352:ILE:HB	1:B:353:PRO:CD	2.49	0.43
1:B:33:SER:O	1:B:51:VAL:HA	2.17	0.43
1:B:308:GLN:NE2	1:B:335:ARG:HH21	2.14	0.43
1:B:461:LEU:HA	1:B:461:LEU:HD12	1.95	0.43
1:A:96:GLU:HG2	1:A:100:GLU:OE2	2.19	0.43
1:B:407:LEU:O	1:B:411:LEU:HG	2.19	0.43
1:A:116:LEU:HD23	1:B:214:ARG:HB2	2.01	0.43
1:A:461:LEU:HD23	1:A:465:VAL:O	2.20	0.42
1:A:444:LEU:HD12	1:A:448:GLU:CB	2.41	0.42
1:B:441:ARG:HG3	1:B:441:ARG:HH11	1.84	0.42
1:B:41:GLN:HE21	1:B:45:SER:HB3	1.85	0.42
1:B:174:ASP:O	1:B:188:PRO:HG2	2.16	0.42
1:B:217:LEU:HD11	6:B:875:HOH:O	2.19	0.42
1:A:11:GLY:HA2	1:A:156:THR:HG21	2.01	0.42
1:A:382:GLU:HG2	6:A:751:HOH:O	2.19	0.42
1:B:110:ASP:O	1:B:112:HIS:N	2.53	0.42
1:A:460:LEU:HD22	1:A:465:VAL:HG21	2.01	0.42
1:A:9:ALA:HA	1:A:52:HIS:HB3	2.01	0.42
5:A:702:AMP:H5'1	5:A:702:AMP:H8	1.85	0.42
1:A:290:HIS:CG	1:A:435:PRO:HD3	2.54	0.42
1:A:291:LEU:HD12	1:A:291:LEU:N	2.35	0.42
1:A:149:PRO:HD3	1:A:170:PHE:CD1	2.46	0.42
1:B:320:ASP:O	1:B:324:ILE:HG12	2.19	0.42
1:A:397:HIS:HA	1:A:398:PRO:HD2	1.95	0.42
1:B:357:MET:SD	1:B:357:MET:N	2.93	0.41
1:A:247:VAL:HB	5:A:702:AMP:N3	2.35	0.41
1:A:473:ALA:O	1:A:477:VAL:HG23	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:LEU:HD21	1:B:408:LEU:HD22	2.03	0.41
1:B:24:PRO:HG2	1:B:164:HIS:CE1	2.55	0.41
1:B:206:ARG:NH2	6:B:802:HOH:O	2.53	0.41
1:A:446:VAL:HG21	5:A:702:AMP:H5'1	2.03	0.41
1:B:313:VAL:HG22	1:B:478:VAL:HG13	2.02	0.41
1:A:149:PRO:HD2	1:A:170:PHE:HE1	1.72	0.41
1:A:305:LEU:CD2	1:A:328:LEU:HB3	2.50	0.41
1:A:469:ARG:O	1:A:470:VAL:C	2.59	0.41
1:A:103:LEU:HA	1:A:103:LEU:HD12	1.81	0.41
1:A:238:VAL:HG23	1:A:238:VAL:O	2.21	0.41
1:A:352:ILE:HD11	4:A:703:PCX:H5C1	2.03	0.41
1:B:43:GLU:H	1:B:43:GLU:HG2	1.54	0.41
1:B:325:GLU:OE1	1:B:456:PHE:HB3	2.21	0.41
1:B:476:GLN:HB3	6:B:835:HOH:O	2.20	0.41
1:A:352:ILE:HG13	4:A:703:PCX:O1	2.21	0.40
1:A:31:ARG:HH11	1:A:31:ARG:HG2	1.85	0.40
1:A:118:ASN:HD21	1:A:402:ARG:H	1.68	0.40
1:A:89:LEU:HA	1:A:90:PRO:HD3	1.84	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:GLY:O	1:B:359:ARG:NE[1_655]	2.10	0.10
1:A:44:ARG:NE	1:A:276:ASP:OD1[1_455]	2.10	0.10

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	485/513 (94%)	461 (95%)	18 (4%)	6 (1%)	16 9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	494/513 (96%)	474 (96%)	18 (4%)	2 (0%)	39	34
All	All	979/1026 (95%)	935 (96%)	36 (4%)	8 (1%)	24	15

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	GLY
1	A	90	PRO
1	A	111	LEU
1	B	111	LEU
1	B	339	GLY
1	A	469	ARG
1	A	40	PRO
1	A	93	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	383/395 (97%)	373 (97%)	10 (3%)	54	55
1	B	388/395 (98%)	374 (96%)	14 (4%)	42	40
All	All	771/790 (98%)	747 (97%)	24 (3%)	47	47

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LEU
1	A	161	LEU
1	A	282	ARG
1	A	305	LEU
1	A	308	GLN
1	A	354	LEU
1	A	362	ARG
1	A	387	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	403	GLU
1	A	412	GLU
1	B	13	LEU
1	B	85	LEU
1	B	101	LEU
1	B	143	LEU
1	B	153	ARG
1	B	291	LEU
1	B	294	ARG
1	B	330	LEU
1	B	341	GLU
1	B	357	MET
1	B	370	LEU
1	B	412	GLU
1	B	426	LEU
1	B	467	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	HIS
1	A	118	ASN
1	A	236	GLN
1	A	491	HIS
1	B	41	GLN
1	B	164	HIS
1	B	186	GLN
1	B	236	GLN
1	B	308	GLN
1	B	358	HIS
1	B	381	ASN
1	B	440	ASN
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 [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 10 ligands modelled in this entry, 4 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$
3	POP	A	701	2	8,8,8	1.25	0	13,13,13	0.87	0
5	AMP	A	702	2	20,25,25	2.03	5 (25%)	22,38,38	1.99	6 (27%)
4	PCX	A	703	-	7,16,16	11.60	3 (42%)	5,21,21	10.53	2 (40%)
3	POP	B	704	2	8,8,8	1.25	1 (12%)	13,13,13	0.62	0
5	AMP	B	705	2	20,25,25	2.03	5 (25%)	22,38,38	1.92	5 (22%)
4	PCX	B	706	-	7,16,16	7.62	2 (28%)	5,21,21	6.60	2 (40%)

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	POP	A	701	2	-	0/6/6/6	0/0/0/0
5	AMP	A	702	2	-	0/6/26/26	0/3/3/3
4	PCX	A	703	-	-	0/7/24/24	0/1/1/1
3	POP	B	704	2	-	0/6/6/6	0/0/0/0
5	AMP	B	705	2	-	0/6/26/26	0/3/3/3
4	PCX	B	706	-	-	0/7/24/24	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	PCX	C1-N1	-29.44	1.02	1.47
4	B	706	PCX	C1-N1	-18.76	1.18	1.47
4	A	703	PCX	C7-C9	-7.40	1.42	1.54
4	B	706	PCX	C7-C9	-7.02	1.42	1.54
4	A	703	PCX	O4-C8	-4.24	1.13	1.23
3	B	704	POP	P2-O	-2.02	1.56	1.61
5	B	705	AMP	C2-N3	2.28	1.36	1.32
5	A	702	AMP	C2-N3	2.40	1.36	1.32
5	A	702	AMP	C2'-C3'	2.53	1.60	1.53
5	B	705	AMP	C2'-C3'	2.74	1.60	1.53
5	A	702	AMP	O3'-C3'	3.17	1.50	1.43
5	B	705	AMP	O3'-C3'	3.39	1.51	1.43
5	A	702	AMP	O4'-C1'	3.48	1.45	1.41
5	B	705	AMP	O4'-C1'	3.51	1.45	1.41
5	A	702	AMP	C3'-C4'	5.66	1.68	1.53
5	B	705	AMP	C3'-C4'	5.71	1.68	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	PCX	C2-C1-N1	-21.55	95.32	112.85
4	B	706	PCX	C7-N1-C8	-10.89	87.61	95.75
4	B	706	PCX	C2-C1-N1	-9.94	104.76	112.85
4	A	703	PCX	C7-N1-C8	-9.48	88.66	95.75
5	A	702	AMP	N3-C2-N1	-5.14	124.95	128.89
5	B	705	AMP	N3-C2-N1	-4.86	125.17	128.89
5	A	702	AMP	C2'-C1'-N9	-2.17	110.98	114.29
5	B	705	AMP	C4'-O4'-C1'	2.15	112.08	109.72
5	A	702	AMP	C4'-O4'-C1'	2.20	112.13	109.72
5	B	705	AMP	C2-N1-C6	2.37	123.00	118.77
5	A	702	AMP	C2-N1-C6	2.41	123.08	118.77
5	B	705	AMP	N6-C6-N1	2.77	125.14	119.20
5	A	702	AMP	N6-C6-N1	2.95	125.53	119.20
5	B	705	AMP	C4-C5-N7	4.74	113.84	109.48
5	A	702	AMP	C4-C5-N7	4.96	114.04	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	702	AMP	13	0
4	A	703	PCX	5	0
3	B	704	POP	1	0
5	B	705	AMP	3	0
4	B	706	PCX	8	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

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, 95th 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	A	491/513 (95%)	0.42	42 (8%)	13 19	10, 25, 46, 59	0
1	B	498/513 (97%)	0.30	30 (6%)	25 34	13, 23, 42, 60	0
All	All	989/1026 (96%)	0.36	72 (7%)	18 25	10, 24, 45, 60	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	22	ARG	9.7
1	B	93	PRO	7.3
1	A	91	ALA	7.0
1	A	170	PHE	7.0
1	B	23	ALA	6.6
1	A	359	ARG	6.1
1	A	44	ARG	5.9
1	B	91	ALA	5.9
1	B	25	GLY	5.7
1	B	92	GLY	5.5
1	B	94	ALA	5.2
1	A	92	GLY	5.2
1	B	165	ARG	5.1
1	A	447	HIS	4.9
1	B	21	GLY	4.8
1	A	163	ALA	4.7
1	A	490	ARG	4.6
1	B	359	ARG	4.4
1	B	24	PRO	4.4
1	A	358	HIS	4.4
1	B	338	ASP	4.2
1	A	446	VAL	4.1
1	A	42	GLY	3.8
1	A	506	ASP	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	18	THR	3.6
1	A	467	GLU	3.4
1	A	469	ARG	3.4
1	B	360	GLU	3.3
1	B	20	GLY	3.3
1	A	326	TYR	3.3
1	A	43	GLU	3.3
1	A	338	ASP	3.2
1	A	468	ASP	3.2
1	A	169	GLY	3.2
1	A	94	ALA	3.2
1	A	41	GLN	3.1
1	A	93	PRO	3.0
1	A	340	PRO	2.9
1	A	96	GLU	2.9
1	A	17	ARG	2.8
1	A	448	GLU	2.7
1	B	96	GLU	2.7
1	A	444	LEU	2.6
1	A	241	GLY	2.6
1	A	445	GLY	2.6
1	A	496	ASP	2.6
1	B	164	HIS	2.6
1	B	3	ALA	2.6
1	B	19	GLY	2.5
1	B	358	HIS	2.5
1	B	339	GLY	2.5
1	B	355	GLY	2.5
1	A	240	PRO	2.5
1	B	282	ARG	2.4
1	B	362	ARG	2.4
1	A	360	GLU	2.4
1	A	25	GLY	2.4
1	A	507	ARG	2.3
1	B	475	ARG	2.3
1	A	294	ARG	2.3
1	A	450	SER	2.3
1	B	326	TYR	2.2
1	A	173	ALA	2.2
1	B	420	GLY	2.2
1	B	469	ARG	2.2
1	A	277	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	498	ASP	2.2
1	A	60	ARG	2.1
1	B	174	ASP	2.1
1	A	40	PRO	2.1
1	A	357	MET	2.0
1	A	454	SER	2.0

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 [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, 95th 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	AMP	B	705	23/23	0.59	0.32	7.74	41,46,60,61	0
4	PCX	B	706	16/16	0.81	0.19	1.45	23,31,37,39	0
5	AMP	A	702	23/23	0.84	0.19	0.55	26,39,49,50	0
4	PCX	A	703	16/16	0.80	0.20	0.24	39,46,49,51	0
2	MG	A	601	1/1	0.93	0.14	-0.05	32,32,32,32	0
3	POP	A	701	9/9	0.95	0.10	-1.10	23,27,30,31	0
2	MG	A	603	1/1	0.89	0.13	-1.16	35,35,35,35	0
3	POP	B	704	9/9	0.97	0.09	-1.75	19,20,22,23	0
2	MG	B	602	1/1	0.91	0.06	-	38,38,38,38	0
2	MG	B	605	1/1	0.89	0.07	-	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.