



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 05:30 am GMT

PDB ID : 3FQA  
Title : Gabaculien complex of gabaculine resistant GSAM version  
Authors : Stetefeld, J.  
Deposited on : 2009-01-07  
Resolution : 2.35 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

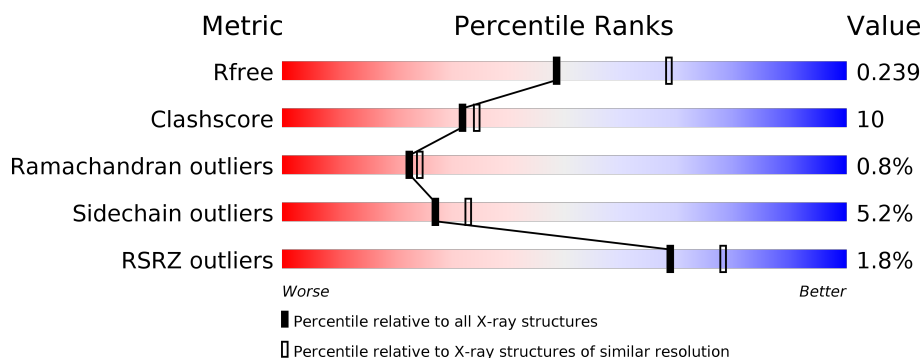
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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))
$R_{free}$	100719	1522 (2.38-2.34)
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

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	427	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>21%</div> <div>•</div> </div> </div>
1	B	427	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>18%</div> <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
3	GAB	A	2000	-	-	X	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6643 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.

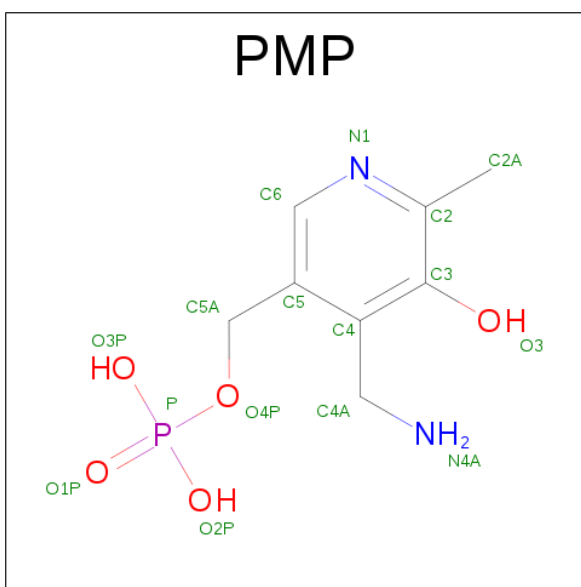
- Molecule 1 is a protein called Glutamate-1-semialdehyde 2,1-aminomutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	0	0
			3191	2035	534	604	18			
1	B	426	Total	C	N	O	S	200	0	0
			3191	2035	534	604	18			

There are 12 discrepancies between the modelled and reference sequences:

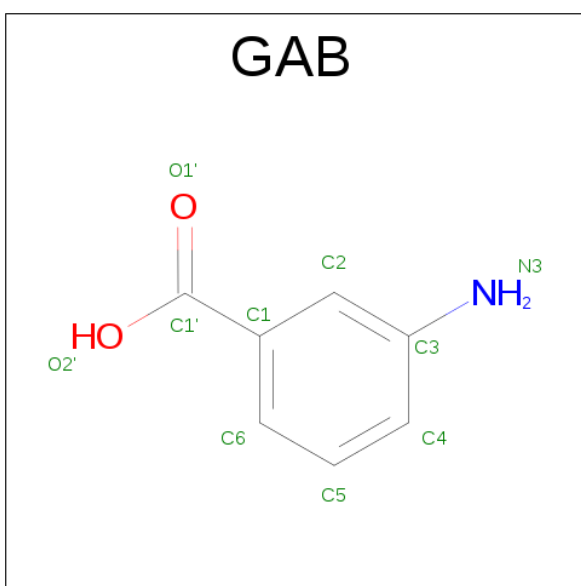
Chain	Residue	Modelled	Actual	Comment	Reference
A	1108	ASN	ILE	CONFLICT	UNP P24630
A	1172	SER	ASP	CONFLICT	UNP P24630
A	1179	LYS	SER	CONFLICT	UNP P24630
A	1187	THR	ALA	CONFLICT	UNP P24630
A	1248	ILE	MET	ENGINEERED	UNP P24630
A	1327	GLY	ALA	CONFLICT	UNP P24630
B	2108	ASN	ILE	CONFLICT	UNP P24630
B	2172	SER	ASP	CONFLICT	UNP P24630
B	2179	LYS	SER	CONFLICT	UNP P24630
B	2187	THR	ALA	CONFLICT	UNP P24630
B	2248	ILE	MET	ENGINEERED	UNP P24630
B	2327	GLY	ALA	CONFLICT	UNP P24630

- Molecule 2 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula: C<sub>8</sub>H<sub>13</sub>N<sub>2</sub>O<sub>5</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
2	B	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

- Molecule 3 is 3-AMINO BENZOIC ACID (three-letter code: GAB) (formula:  $C_7H_7NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	7	1	2		

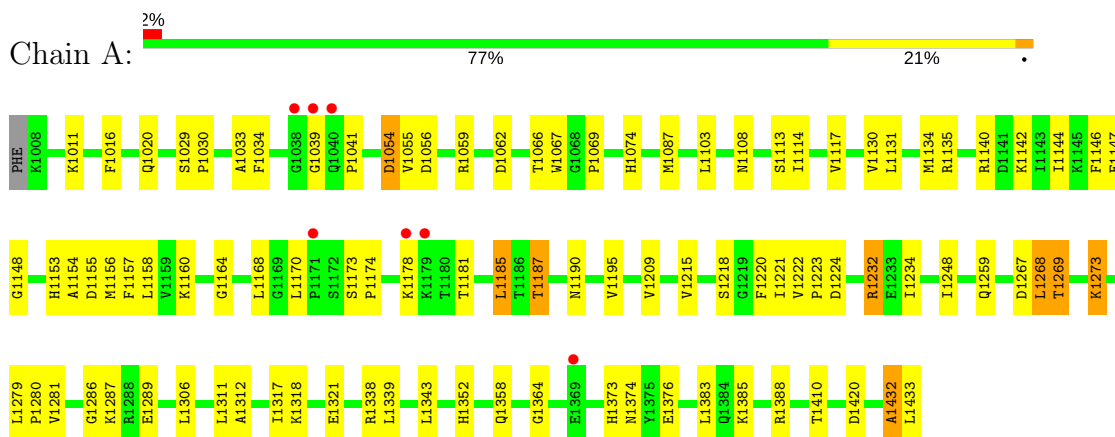
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	110	Total 110	O 110	0	0
4	B	109	Total 109	O 109	0	0

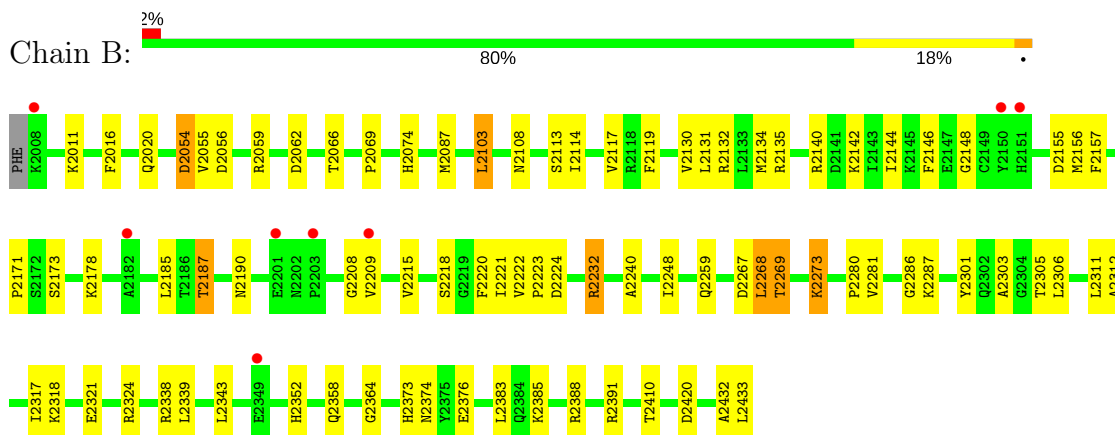
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Glutamate-1-semialdehyde 2,1-aminomutase



- Molecule 1: Glutamate-1-semialdehyde 2,1-aminomutase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.94Å 107.87Å 123.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.31 – 2.35 20.31 – 2.35	Depositor EDS
% Data completeness (in resolution range)	90.7 (20.31-2.35) 90.8 (20.31-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.98 (at 2.35Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.208 , 0.241 0.207 , 0.239	Depositor DCC
$R_{free}$ test set	3451 reflections (9.92%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.2	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 40.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6643	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: PMP, GAB

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	0.35	0/3259	0.62	0/4415
1	B	0.34	0/3259	0.61	0/4415
All	All	0.35	0/6518	0.62	0/8830

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	3191	0	3175	73	0
1	B	3191	0	3175	58	0
2	A	16	0	11	0	0
2	B	16	0	11	0	0
3	A	10	0	6	7	0
4	A	110	0	0	1	0
4	B	109	0	0	1	0
All	All	6643	0	6378	125	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (125) 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)
1:A:1131:LEU:HD23	1:A:1134:MET:HE3	1.47	0.97
1:A:1190:ASN:HD21	1:A:1224:ASP:H	1.15	0.92
1:B:2131:LEU:HD23	1:B:2134:MET:HE3	1.49	0.91
1:A:1190:ASN:ND2	1:A:1224:ASP:H	1.77	0.82
1:A:1135:ARG:NH1	1:A:1156:MET:SD	2.55	0.80
1:A:1374:ASN:HD21	1:A:1376:GLU:HB3	1.59	0.68
1:A:1259:GLN:HE22	1:A:1269:THR:HG21	1.61	0.66
1:A:1232:ARG:O	1:A:1232:ARG:HD3	1.96	0.66
1:B:2374:ASN:HD21	1:B:2376:GLU:HB3	1.61	0.66
1:A:1131:LEU:HD23	1:A:1134:MET:CE	2.24	0.65
1:A:1190:ASN:HD21	1:A:1224:ASP:N	1.93	0.65
1:B:2232:ARG:HD3	1:B:2232:ARG:O	1.96	0.64
1:B:2220:PHE:HB3	1:B:2364:GLY:HA3	1.78	0.64
1:A:1220:PHE:HB3	1:A:1364:GLY:HA3	1.80	0.64
1:B:2190:ASN:ND2	1:B:2224:ASP:H	1.95	0.64
1:B:2131:LEU:HD23	1:B:2134:MET:CE	2.24	0.64
1:A:1374:ASN:ND2	1:A:1376:GLU:HB3	2.12	0.63
1:B:2374:ASN:ND2	1:B:2376:GLU:HB3	2.13	0.63
1:A:1281:VAL:CG2	1:A:1312:ALA:HB1	2.29	0.63
1:B:2281:VAL:CG2	1:B:2312:ALA:HB1	2.29	0.62
1:B:2011:LYS:HB2	1:B:2055:VAL:HG13	1.82	0.61
1:B:2190:ASN:HD21	1:B:2224:ASP:H	1.47	0.61
1:A:1011:LYS:HB2	1:A:1055:VAL:HG13	1.81	0.61
1:A:1067:TRP:CG	3:A:2000:GAB:H6	2.36	0.61
1:A:1153:HIS:CD2	1:B:2132:ARG:HH12	2.19	0.60
1:B:2259:GLN:HE22	1:B:2269:THR:HG21	1.64	0.60
1:A:1135:ARG:HH22	1:A:1156:MET:CE	2.16	0.58
1:A:1374:ASN:HD22	1:A:1376:GLU:H	1.50	0.58
1:B:2317:ILE:O	1:B:2321:GLU:HG3	2.04	0.58
3:A:2000:GAB:HN31	1:B:2303:ALA:CB	2.17	0.57
1:A:1147:GLU:HG2	1:A:1160:LYS:HG2	1.87	0.57
1:A:1135:ARG:HH22	1:A:1156:MET:HE1	1.68	0.56
1:A:1142:LYS:HD3	1:A:1185:LEU:HD21	1.86	0.56
1:B:2267:ASP:OD2	1:B:2287:LYS:HE2	2.06	0.56
1:B:2281:VAL:HG22	1:B:2312:ALA:HB1	1.86	0.56
1:A:1267:ASP:OD2	1:A:1287:LYS:HE2	2.05	0.56
1:A:1281:VAL:HG22	1:A:1312:ALA:HB1	1.88	0.56
1:A:1029:SER:OG	3:A:2000:GAB:H2	2.06	0.55
1:B:2352:HIS:HD2	1:B:2385:LYS:NZ	2.04	0.55
1:A:1374:ASN:HD22	1:A:1376:GLU:N	2.03	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2190:ASN:HD21	1:B:2223:PRO:HA	1.70	0.55
1:A:1248:ILE:HG12	1:A:1273:LYS:HE3	1.89	0.54
1:B:2054:ASP:HB3	1:B:2056:ASP:H	1.73	0.54
1:B:2232:ARG:HD3	1:B:2232:ARG:C	2.27	0.54
1:A:1317:ILE:O	1:A:1321:GLU:HG3	2.08	0.54
1:A:1352:HIS:HD2	1:A:1385:LYS:NZ	2.06	0.54
1:B:2374:ASN:HD22	1:B:2376:GLU:H	1.55	0.53
1:B:2222:VAL:HG13	1:B:2223:PRO:HD2	1.91	0.53
1:A:1034:PHE:HB2	1:A:1041:PRO:HG3	1.89	0.53
1:A:1232:ARG:HD3	1:A:1232:ARG:C	2.28	0.53
1:B:2374:ASN:HD22	1:B:2376:GLU:N	2.06	0.52
1:A:1153:HIS:HD2	1:B:2132:ARG:HH12	1.55	0.52
1:A:1062:ASP:OD1	1:A:1074:HIS:HE1	1.92	0.52
1:A:1131:LEU:CD2	1:A:1134:MET:HE3	2.33	0.52
1:A:1222:VAL:HG13	1:A:1223:PRO:HD2	1.90	0.52
1:B:2062:ASP:OD1	1:B:2074:HIS:HE1	1.93	0.52
1:A:1039:GLY:O	1:A:1041:PRO:HD3	2.10	0.52
1:B:2338:ARG:NH1	1:B:2420:ASP:OD1	2.43	0.52
1:A:1168:LEU:HB3	1:A:1170:LEU:HD13	1.91	0.52
3:A:2000:GAB:HN31	1:B:2303:ALA:HB1	1.74	0.51
1:B:2248:ILE:HG12	1:B:2273:LYS:HE3	1.92	0.51
1:B:2108:ASN:OD1	1:B:2114:ILE:HG22	2.11	0.51
1:B:2215:VAL:HB	1:B:2221:ILE:HB	1.92	0.51
1:A:1054:ASP:HB3	1:A:1056:ASP:H	1.76	0.51
1:A:1108:ASN:OD1	1:A:1114:ILE:HG22	2.11	0.50
1:A:1338:ARG:NH1	1:A:1420:ASP:OD1	2.44	0.50
1:A:1215:VAL:HB	1:A:1221:ILE:HB	1.93	0.50
1:B:2268:LEU:HD12	1:B:2286:GLY:HA3	1.92	0.50
1:A:1168:LEU:CB	1:A:1170:LEU:HD13	2.42	0.50
1:A:1222:VAL:CG1	1:A:1223:PRO:HD2	2.43	0.49
1:B:2131:LEU:CD2	1:B:2134:MET:HE3	2.34	0.49
1:B:2222:VAL:CG1	1:B:2223:PRO:HD2	2.43	0.49
1:A:1029:SER:CB	3:A:2000:GAB:O1'	2.60	0.49
1:A:1135:ARG:NH2	1:A:1156:MET:SD	2.86	0.49
1:A:1135:ARG:CZ	1:A:1156:MET:SD	3.02	0.48
1:A:1144:ILE:HB	1:A:1209:VAL:HG22	1.96	0.48
3:A:2000:GAB:C1	1:B:2305:THR:HA	2.44	0.48
1:A:1154:ALA:O	1:A:1158:LEU:HD22	2.13	0.47
4:A:7036:HOH:O	1:B:2074:HIS:HD2	1.97	0.47
1:B:2144:ILE:HB	1:B:2209:VAL:HG22	1.98	0.46
1:B:2432:ALA:O	1:B:2433:LEU:OXT	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1268:LEU:HD12	1:A:1286:GLY:HA3	1.98	0.45
1:B:2113:SER:OG	1:B:2269:THR:CG2	2.65	0.45
1:B:2148:GLY:O	1:B:2218:SER:HB3	2.16	0.45
1:A:1432:ALA:O	1:A:1433:LEU:OXT	2.35	0.45
1:B:2016:PHE:O	1:B:2020:GLN:HG3	2.17	0.45
1:A:1131:LEU:HD11	1:A:1157:PHE:CZ	2.52	0.44
1:B:2066:THR:HG23	1:B:2069:PRO:HD2	1.99	0.44
1:A:1113:SER:OG	1:A:1269:THR:CG2	2.66	0.44
1:A:1146:PHE:CD1	1:A:1187:THR:HG23	2.53	0.44
1:A:1178:LYS:O	1:A:1181:THR:HG22	2.16	0.44
1:A:1148:GLY:O	1:A:1218:SER:HB3	2.18	0.44
1:A:1338:ARG:HH12	1:A:1420:ASP:CG	2.21	0.44
1:A:1074:HIS:HD2	4:B:7162:HOH:O	1.99	0.44
1:B:2146:PHE:CD1	1:B:2187:THR:HG23	2.53	0.44
1:A:1087:MET:HB3	1:A:1311:LEU:HD21	2.00	0.44
3:A:2000:GAB:C1'	1:B:2305:THR:HA	2.47	0.43
1:A:1033:ALA:O	1:A:1034:PHE:HB2	2.18	0.43
1:B:2224:ASP:OD1	1:B:2373:HIS:HD2	2.02	0.43
1:B:2338:ARG:HH12	1:B:2420:ASP:CG	2.21	0.43
1:A:1135:ARG:HG2	1:A:1140:ARG:O	2.18	0.42
1:B:2142:LYS:HB3	1:B:2185:LEU:CD2	2.49	0.42
1:A:1279:LEU:C	1:B:2306:LEU:HD22	2.40	0.42
1:A:1066:THR:HG23	1:A:1069:PRO:HD2	2.00	0.42
1:A:1016:PHE:O	1:A:1020:GLN:HG3	2.19	0.42
1:B:2220:PHE:CB	1:B:2364:GLY:HA3	2.49	0.42
1:B:2391:ARG:HA	1:B:2391:ARG:HD2	1.89	0.42
1:A:1164:GLY:HA3	1:B:2301:TYR:OH	2.20	0.42
1:A:1280:PRO:N	1:B:2306:LEU:HD22	2.35	0.42
1:B:2388:ARG:HG3	1:B:2388:ARG:HH21	1.84	0.42
1:A:1173:SER:HA	1:A:1174:PRO:HD3	1.77	0.41
1:A:1224:ASP:OD1	1:A:1373:HIS:HD2	2.03	0.41
1:A:1155:ASP:HA	1:A:1158:LEU:HD23	2.02	0.41
1:B:2190:ASN:HD22	1:B:2190:ASN:HA	1.73	0.41
1:B:2208:GLY:HA2	1:B:2240:ALA:HB1	2.02	0.41
1:A:1029:SER:HA	1:A:1030:PRO:HD3	1.87	0.41
1:A:1131:LEU:HG	1:A:1157:PHE:CZ	2.56	0.41
1:A:1306:LEU:HD22	1:B:2280:PRO:N	2.36	0.41
1:A:1388:ARG:HH21	1:A:1388:ARG:HG3	1.84	0.41
1:A:1289:GLU:H	1:A:1289:GLU:CD	2.24	0.41
1:A:1131:LEU:HA	1:A:1134:MET:HE2	2.03	0.41
1:B:2087:MET:HB3	1:B:2311:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2135:ARG:HG2	1:B:2140:ARG:O	2.20	0.40
1:B:2103:LEU:HD13	1:B:2119:PHE:CE2	2.56	0.40
1:A:1195:VAL:HG11	1:A:1234:ILE:HD11	2.03	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	424/427 (99%)	403 (95%)	19 (4%)	2 (0%)	32	37
1	B	424/427 (99%)	397 (94%)	22 (5%)	5 (1%)	15	14
All	All	848/854 (99%)	800 (94%)	41 (5%)	7 (1%)	22	24

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2155	ASP
1	B	2157	PHE
1	B	2171	PRO
1	B	2173	SER
1	A	1273	LYS
1	B	2273	LYS
1	A	1432	ALA

### 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	329/330 (100%)	313 (95%)	16 (5%)	29	36
1	B	329/330 (100%)	311 (94%)	18 (6%)	25	30
All	All	658/660 (100%)	624 (95%)	34 (5%)	27	33

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1054	ASP
1	A	1059	ARG
1	A	1103	LEU
1	A	1117	VAL
1	A	1130	VAL
1	A	1185	LEU
1	A	1187	THR
1	A	1232	ARG
1	A	1268	LEU
1	A	1269	THR
1	A	1318	LYS
1	A	1339	LEU
1	A	1343	LEU
1	A	1358	GLN
1	A	1383	LEU
1	A	1410	THR
1	B	2054	ASP
1	B	2059	ARG
1	B	2103	LEU
1	B	2117	VAL
1	B	2130	VAL
1	B	2156	MET
1	B	2178	LYS
1	B	2187	THR
1	B	2232	ARG
1	B	2268	LEU
1	B	2269	THR
1	B	2318	LYS
1	B	2324	ARG
1	B	2339	LEU
1	B	2343	LEU
1	B	2358	GLN
1	B	2383	LEU
1	B	2410	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1040	GLN
1	A	1058	ASN
1	A	1074	HIS
1	A	1153	HIS
1	A	1190	ASN
1	A	1259	GLN
1	A	1334	GLN
1	A	1352	HIS
1	A	1358	GLN
1	A	1373	HIS
1	A	1374	ASN
1	B	2040	GLN
1	B	2058	ASN
1	B	2074	HIS
1	B	2190	ASN
1	B	2217	ASN
1	B	2259	GLN
1	B	2334	GLN
1	B	2352	HIS
1	B	2358	GLN
1	B	2373	HIS
1	B	2374	ASN

### 5.3.3 RNA [i](#)

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](#)

3 ligands are modelled in this entry.

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	$\# Z  > 2$
2	PMP	A	1434	-	16,16,16	1.86	5 (31%)	20,23,23	1.57	4 (20%)
3	GAB	A	2000	-	7,10,10	4.63	4 (57%)	9,13,13	2.39	2 (22%)
2	PMP	B	2434	-	16,16,16	1.72	4 (25%)	20,23,23	1.53	4 (20%)

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
2	PMP	A	1434	-	-	0/8/8/8	0/1/1/1
3	GAB	A	2000	-	-	0/0/4/4	0/1/1/1
2	PMP	B	2434	-	-	0/8/8/8	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1434	PMP	C3-C2	-2.56	1.39	1.40
3	A	2000	GAB	C4-C3	2.31	1.45	1.39
2	B	2434	PMP	C2A-C2	2.31	1.54	1.50
2	B	2434	PMP	C6-N1	2.74	1.40	1.34
2	A	1434	PMP	C2A-C2	2.75	1.55	1.50
2	A	1434	PMP	C5-C4	2.89	1.44	1.40
2	A	1434	PMP	C6-N1	2.93	1.40	1.34
2	B	2434	PMP	C2-N1	3.03	1.40	1.33
2	B	2434	PMP	C5-C4	3.11	1.44	1.40
2	A	1434	PMP	C2-N1	3.37	1.40	1.33
3	A	2000	GAB	C5-C6	4.47	1.47	1.38
3	A	2000	GAB	C2-C3	7.02	1.50	1.39
3	A	2000	GAB	C2-C1	8.50	1.54	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2000	GAB	C1-C2-C3	-6.37	115.31	120.70
2	A	1434	PMP	C5-C6-N1	-2.53	119.59	123.87
2	B	2434	PMP	C5-C6-N1	-2.43	119.76	123.87
2	A	1434	PMP	O2P-P-O4P	-2.22	100.82	106.73
2	B	2434	PMP	O2P-P-O4P	-2.16	100.98	106.73
2	B	2434	PMP	O3P-P-O2P	2.04	115.82	107.61
2	A	1434	PMP	O3P-P-O2P	2.10	116.07	107.61
3	A	2000	GAB	C4-C3-C2	2.20	121.56	118.65
2	A	1434	PMP	O4P-P-O1P	2.96	114.77	106.47
2	B	2434	PMP	O4P-P-O1P	3.16	115.35	106.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2000	GAB	7	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	426/427 (99%)	-0.22	7 (1%) 72 81	7, 19, 35, 43	0
1	B	397/427 (92%)	-0.17	8 (2%) 65 75	7, 19, 35, 65	0
All	All	823/854 (96%)	-0.20	15 (1%) 69 78	7, 19, 35, 65	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1039	GLY	4.9
1	B	2150	TYR	3.8
1	B	2182	ALA	3.2
1	A	1038	GLY	3.0
1	B	2008	LYS	2.9
1	A	1040	GLN	2.8
1	A	1178	LYS	2.8
1	A	1171	PRO	2.5
1	B	2209	VAL	2.3
1	B	2349	GLU	2.2
1	B	2201	GLU	2.2
1	B	2151	HIS	2.2
1	A	1179	LYS	2.1
1	B	2203	PRO	2.0
1	A	1369	GLU	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, 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( $\text{\AA}^2$ )	Q<0.9
3	GAB	A	2000	10/10	0.80	0.41	6.44	61,62,63,64	0
2	PMP	B	2434	16/16	0.89	0.19	0.85	33,40,43,46	0
2	PMP	A	1434	16/16	0.97	0.11	0.17	15,19,20,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.