Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:42 AM GMT

PDB ID	:	3FQ8
Title	:	M248I mutant of GSAM
Authors	:	Stetefeld, J.
Deposited on	:	2009-01-07
Resolution	:	2.00 Å(reported)

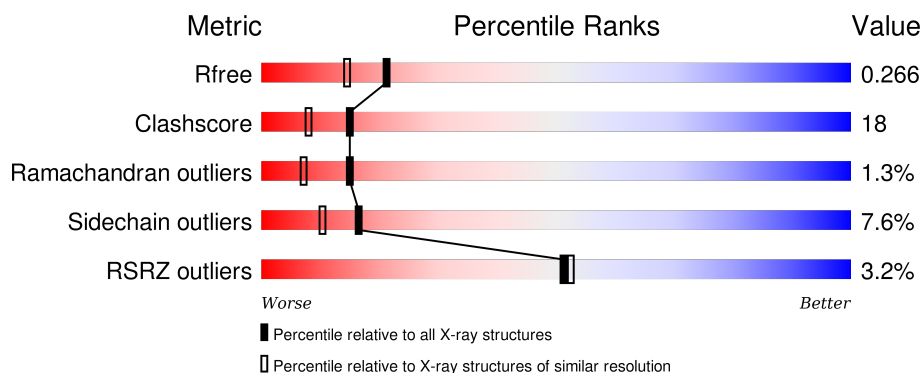# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 <=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	
1	B	427	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7129 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	427	Total 3202	C 2044	N 535	O 605	S 18	0	0	0
1	B	427	Total 3202	C 2044	N 535	O 605	S 18	200	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1108	ASN	ILE	CONFLICT	UNP P24630
A	1133	ILE	LEU	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	2133	ILE	LEU	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: $C_8H_{13}N_2O_5P$).
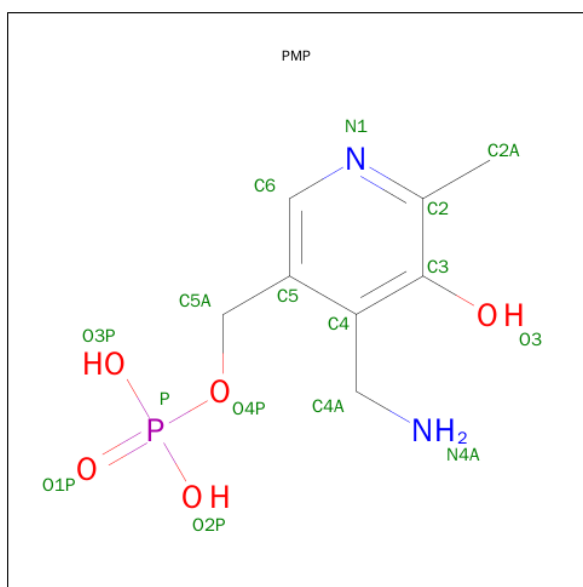
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
2	B	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

• Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	365	Total	O	0	0
			365	365		
3	B	328	Total	O	0	0
			328	328		

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: Glutamate-1-semialdehyde 2,1-aminomutase
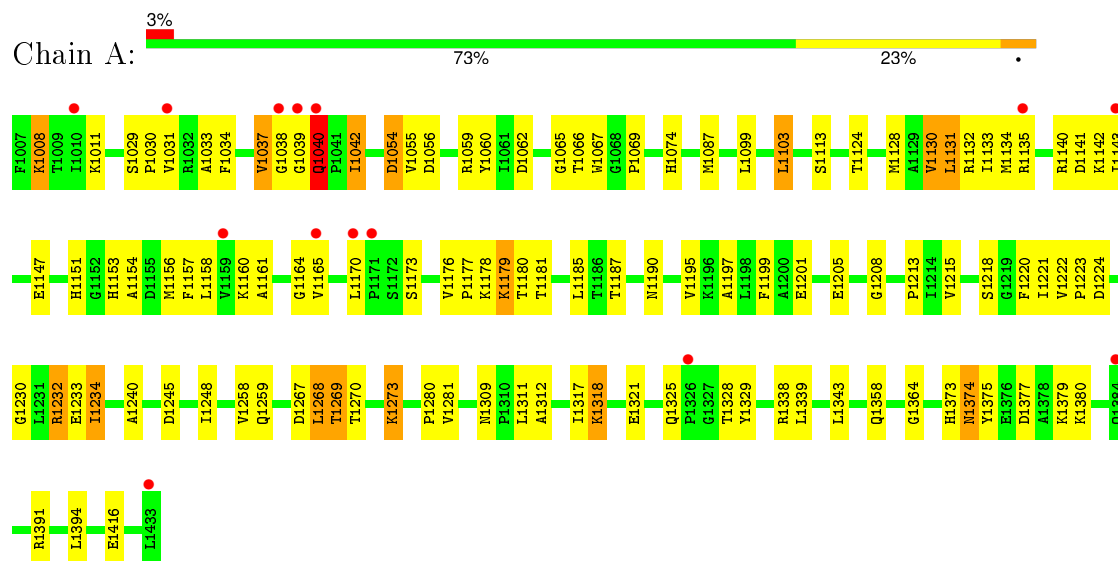
- Molecule 1: Glutamate-1-semialdehyde 2,1-aminomutase
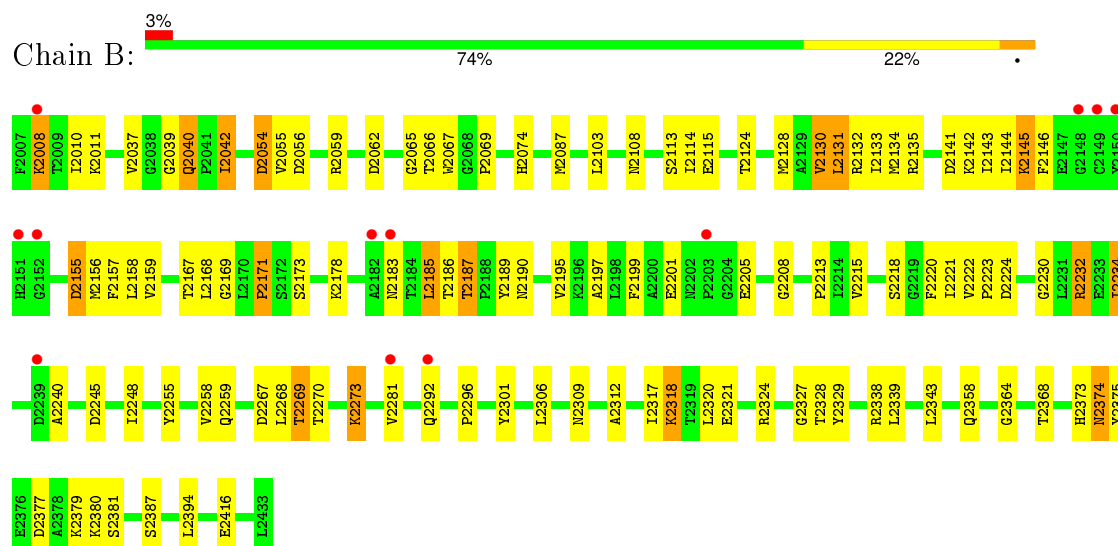
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.68Å 106.95Å 122.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.90 – 2.00 27.90 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.0 (27.90-2.00) 94.2 (27.90-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.61 (at 1.99Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.208 , 0.245 0.227 , 0.266	Depositor DCC
R_{free} test set	5750 reflections (10.17%)	DCC
Wilson B-factor (Å^2)	16.6	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	1 of 56587 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7129	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PMP

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	0.33	0/3271	0.62	1/4431 (0.0%)
1	B	0.33	0/3271	0.61	0/4431
All	All	0.33	0/6542	0.62	1/8862 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1268	LEU	CA-CB-CG	5.30	127.48	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	3202	0	3184	130	0
1	B	3202	0	3184	105	0
2	A	16	0	11	0	0
2	B	16	0	11	0	0
3	A	365	0	0	10	0
3	B	328	0	0	7	0
All	All	7129	0	6390	218	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 18.

All (218) 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:B:2131:LEU:HA	1:B:2134:MET:HE2	1.47	0.95
1:A:1131:LEU:HD22	1:A:1134:MET:HE1	1.50	0.93
1:A:1233:GLU:HB2	3:A:7435:HOH:O	1.68	0.92
1:A:1039:GLY:O	1:A:1040:GLN:HB2	1.71	0.89
1:A:1190:ASN:HD21	1:A:1224:ASP:H	1.20	0.88
1:A:1325:GLN:HG3	3:A:7197:HOH:O	1.77	0.84
1:A:1131:LEU:HD12	1:A:1135:ARG:NH1	1.94	0.82
1:A:1259:GLN:HE22	1:A:1269:THR:HG21	1.43	0.81
1:A:1190:ASN:ND2	1:A:1224:ASP:H	1.78	0.80
1:A:1179:LYS:HD2	1:A:1180:THR:N	1.97	0.79
1:B:2259:GLN:HE22	1:B:2269:THR:HG21	1.46	0.79
1:A:1131:LEU:HD23	1:A:1157:PHE:CZ	2.18	0.79
1:A:1131:LEU:HA	1:A:1134:MET:HE2	1.65	0.77
1:A:1135:ARG:NH2	1:A:1143:ILE:HD13	2.00	0.76
1:B:2197:ALA:O	1:B:2201:GLU:HG3	1.86	0.76
1:A:1135:ARG:HH22	1:A:1156:MET:CE	1.97	0.76
1:A:1281:VAL:CG2	1:A:1312:ALA:HB1	2.16	0.75
1:A:1135:ARG:NH1	1:A:1156:MET:SD	2.59	0.75
1:B:2135:ARG:NH2	1:B:2143:ILE:HD13	2.01	0.74
1:B:2131:LEU:HD12	1:B:2135:ARG:NH1	2.04	0.72
1:A:1197:ALA:O	1:A:1201:GLU:HG3	1.89	0.72
1:B:2248:ILE:HG12	1:B:2273:LYS:HE3	1.71	0.72
1:B:2130:VAL:O	1:B:2134:MET:HG3	1.89	0.72
1:A:1222:VAL:HG13	1:A:1223:PRO:HD2	1.72	0.72
1:B:2281:VAL:CG2	1:B:2312:ALA:HB1	2.20	0.71
1:A:1130:VAL:HA	1:A:1133:ILE:HG22	1.71	0.71
1:B:2130:VAL:HA	1:B:2133:ILE:HG22	1.73	0.70
1:B:2131:LEU:HD22	1:B:2134:MET:HE1	1.72	0.70
1:A:1130:VAL:O	1:A:1134:MET:HG3	1.90	0.70
1:B:2213:PRO:HB2	1:B:2258:VAL:HG11	1.73	0.70
1:A:1031:VAL:HG23	3:A:7358:HOH:O	1.92	0.69
1:A:1128:MET:SD	1:B:2128:MET:SD	2.90	0.69
1:B:2130:VAL:O	1:B:2133:ILE:HG22	1.93	0.68
1:A:1248:ILE:HG12	1:A:1273:LYS:HE3	1.74	0.68
1:B:2190:ASN:HD21	1:B:2224:ASP:H	1.42	0.68
1:A:1179:LYS:HD2	1:A:1180:THR:HG23	1.74	0.68
1:B:2281:VAL:HG22	1:B:2312:ALA:HB1	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1151:HIS:HD2	1:A:1245:ASP:OD2	1.78	0.67
1:B:2230:GLY:O	1:B:2234:ILE:HG23	1.95	0.67
1:B:2318:LYS:HE3	1:B:2318:LYS:HA	1.77	0.66
1:A:1153:HIS:CD2	1:B:2132:ARG:HH12	2.13	0.66
1:B:2222:VAL:HG13	1:B:2223:PRO:HD2	1.76	0.65
1:A:1374:ASN:ND2	1:A:1377:ASP:H	1.93	0.65
1:A:1135:ARG:HH22	1:A:1156:MET:HE1	1.61	0.65
1:B:2218:SER:HB2	1:B:2375:TYR:CD1	2.32	0.64
1:A:1008:LYS:HD2	3:A:7234:HOH:O	1.97	0.64
3:A:7057:HOH:O	1:B:2074:HIS:HD2	1.81	0.64
1:A:1318:LYS:HA	1:A:1318:LYS:HE3	1.79	0.64
1:A:1213:PRO:HB2	1:A:1258:VAL:HG11	1.80	0.63
1:B:2011:LYS:HB2	1:B:2055:VAL:HG23	1.78	0.63
1:A:1230:GLY:O	1:A:1234:ILE:HG23	2.00	0.62
1:A:1179:LYS:CD	1:A:1180:THR:HG23	2.29	0.62
1:A:1281:VAL:HG22	1:A:1312:ALA:HB1	1.81	0.62
1:B:2190:ASN:ND2	1:B:2224:ASP:H	1.97	0.61
1:A:1135:ARG:HH21	1:A:1143:ILE:HD13	1.66	0.61
1:B:2317:ILE:O	1:B:2321:GLU:HG3	2.00	0.61
1:A:1130:VAL:O	1:A:1133:ILE:HG22	2.00	0.61
1:A:1179:LYS:HE3	1:A:1180:THR:HG23	1.83	0.61
1:A:1222:VAL:HG11	3:A:7429:HOH:O	2.01	0.61
1:B:2135:ARG:HH21	1:B:2143:ILE:HD13	1.66	0.60
1:B:2374:ASN:ND2	1:B:2377:ASP:H	1.99	0.60
1:A:1377:ASP:HA	1:A:1380:LYS:NZ	2.17	0.60
1:B:2309:ASN:ND2	1:B:2312:ALA:H	1.99	0.60
1:B:2037:VAL:O	1:B:2037:VAL:HG22	2.01	0.60
1:A:1190:ASN:HD21	1:A:1224:ASP:N	1.97	0.59
1:A:1177:PRO:HB2	1:A:1179:LYS:HE2	1.84	0.59
1:A:1131:LEU:HD22	1:A:1134:MET:CE	2.28	0.59
1:A:1179:LYS:CE	1:A:1180:THR:HG23	2.33	0.59
1:A:1222:VAL:CG1	1:A:1223:PRO:HD2	2.33	0.58
1:A:1011:LYS:HB2	1:A:1055:VAL:HG23	1.85	0.58
1:A:1153:HIS:HD2	1:B:2132:ARG:HH12	1.50	0.58
1:A:1317:ILE:O	1:A:1321:GLU:HG3	2.02	0.58
1:A:1131:LEU:HD23	1:A:1157:PHE:HZ	1.68	0.58
1:A:1039:GLY:O	1:A:1040:GLN:CB	2.48	0.57
1:A:1147:GLU:HG3	1:A:1160:LYS:HB3	1.87	0.57
1:A:1135:ARG:NH2	1:A:1156:MET:SD	2.79	0.56
1:B:2195:VAL:HG12	1:B:2234:ILE:HD11	1.85	0.56
1:A:1066:THR:HG23	1:A:1069:PRO:HD2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2142:LYS:HB2	1:B:2205:GLU:O	2.06	0.56
1:A:1179:LYS:NZ	1:B:2183:ASN:ND2	2.54	0.56
1:B:2054:ASP:HB3	1:B:2056:ASP:H	1.71	0.56
1:B:2142:LYS:C	1:B:2143:ILE:HD12	2.26	0.55
1:A:1131:LEU:CD2	1:A:1134:MET:HE1	2.32	0.55
1:B:2377:ASP:HA	1:B:2380:LYS:NZ	2.22	0.55
1:B:2141:ASP:O	1:B:2183:ASN:HB3	2.06	0.55
1:A:1130:VAL:HA	1:A:1133:ILE:CG2	2.37	0.55
1:B:2131:LEU:HD22	1:B:2134:MET:CE	2.36	0.55
1:A:1128:MET:HG2	1:A:1154:ALA:HB2	1.89	0.55
1:A:1195:VAL:HG12	1:A:1234:ILE:HD11	1.90	0.54
1:A:1135:ARG:NH2	1:A:1156:MET:HE1	2.23	0.54
1:B:2338:ARG:HH21	1:B:2416:GLU:HG3	1.71	0.54
1:B:2130:VAL:CA	1:B:2133:ILE:HG22	2.38	0.54
1:B:2374:ASN:C	1:B:2374:ASN:HD22	2.11	0.54
1:A:1142:LYS:C	1:A:1143:ILE:HD12	2.28	0.53
1:B:2066:THR:HG23	1:B:2069:PRO:HD2	1.89	0.53
1:A:1179:LYS:HD2	1:A:1180:THR:H	1.73	0.53
1:B:2375:TYR:CE2	1:B:2379:LYS:HD2	2.43	0.53
1:A:1280:PRO:HG3	1:B:2306:LEU:HB3	1.90	0.53
1:B:2130:VAL:HA	1:B:2133:ILE:CG2	2.39	0.53
1:A:1031:VAL:HG21	1:A:1067:TRP:CH2	2.43	0.53
1:A:1130:VAL:CA	1:A:1133:ILE:HG22	2.37	0.52
1:B:2062:ASP:OD1	1:B:2074:HIS:HE1	1.93	0.52
1:A:1220:PHE:HB3	1:A:1364:GLY:HA3	1.92	0.52
1:B:2037:VAL:HG23	1:B:2387:SER:HA	1.91	0.52
1:A:1131:LEU:HA	1:A:1134:MET:CE	2.35	0.52
1:A:1135:ARG:CZ	1:A:1156:MET:SD	2.98	0.52
1:B:2145:LYS:O	1:B:2186:THR:HA	2.09	0.52
1:A:1374:ASN:HD22	1:A:1374:ASN:C	2.14	0.51
1:B:2213:PRO:HB2	1:B:2258:VAL:CG1	2.38	0.51
1:B:2113:SER:OG	1:B:2269:THR:CG2	2.59	0.51
1:A:1131:LEU:HD12	1:A:1135:ARG:CZ	2.40	0.51
1:B:2220:PHE:HB3	1:B:2364:GLY:HA3	1.93	0.50
1:B:2368:THR:HB	1:B:2381:SER:HA	1.94	0.50
1:B:2222:VAL:CG1	1:B:2223:PRO:HD2	2.41	0.50
1:B:2255:TYR:OH	1:B:2324:ARG:HD3	2.11	0.50
1:A:1245:ASP:HA	1:A:1270:THR:OG1	2.11	0.50
1:A:1065:GLY:O	1:A:1066:THR:HG22	2.12	0.50
1:A:1113:SER:OG	1:A:1269:THR:CG2	2.60	0.50
1:B:2248:ILE:CG1	1:B:2273:LYS:HE3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2187:THR:HG21	1:B:2195:VAL:HG22	1.94	0.50
1:A:1153:HIS:HA	1:A:1158:LEU:HD11	1.94	0.50
1:B:2215:VAL:HB	1:B:2221:ILE:HB	1.93	0.50
1:B:2309:ASN:HD21	1:B:2312:ALA:H	1.58	0.50
1:B:2218:SER:HB2	1:B:2375:TYR:HD1	1.73	0.50
1:A:1074:HIS:HD2	3:B:7077:HOH:O	1.94	0.49
1:A:1008:LYS:HD3	1:A:1056:ASP:HB3	1.93	0.49
1:A:1375:TYR:CZ	1:A:1379:LYS:HD2	2.48	0.49
1:A:1131:LEU:HD23	1:A:1157:PHE:CE2	2.47	0.48
1:B:2011:LYS:HG2	1:B:2056:ASP:OD1	2.13	0.48
1:A:1224:ASP:OD1	1:A:1373:HIS:HD2	1.96	0.48
1:A:1124:THR:O	1:A:1128:MET:HG3	2.13	0.48
1:A:1185:LEU:N	1:A:1185:LEU:HD22	2.29	0.48
1:B:2130:VAL:C	1:B:2133:ILE:HG22	2.32	0.48
1:A:1179:LYS:HZ3	1:B:2183:ASN:ND2	2.12	0.48
1:A:1054:ASP:HB3	1:A:1056:ASP:H	1.77	0.48
1:B:2011:LYS:HE3	3:B:7691:HOH:O	2.14	0.48
1:A:1215:VAL:HB	1:A:1221:ILE:HB	1.96	0.48
1:B:2146:PHE:CD1	1:B:2187:THR:HG23	2.49	0.47
1:A:1377:ASP:HA	1:A:1380:LYS:HZ3	1.79	0.47
1:A:1033:ALA:HB2	1:B:2296:PRO:HG3	1.95	0.47
1:B:2232:ARG:HA	1:B:2232:ARG:HD3	1.56	0.47
1:B:2232:ARG:HH12	1:B:2267:ASP:CG	2.16	0.47
1:A:1179:LYS:NZ	1:B:2183:ASN:HD22	2.13	0.47
1:A:1232:ARG:HH12	1:A:1267:ASP:CG	2.17	0.47
1:B:2245:ASP:HA	1:B:2270:THR:OG1	2.15	0.47
1:A:1130:VAL:C	1:A:1133:ILE:HG22	2.34	0.47
1:A:1338:ARG:HH21	1:A:1416:GLU:HG3	1.80	0.47
1:A:1087:MET:HE1	1:B:2087:MET:HE3	1.97	0.47
1:A:1011:LYS:HG2	1:A:1056:ASP:OD1	2.16	0.46
1:A:1087:MET:HE1	1:B:2087:MET:CE	2.45	0.46
1:B:2189:TYR:O	1:B:2190:ASN:HB2	2.14	0.46
1:B:2065:GLY:O	1:B:2066:THR:HG22	2.16	0.46
1:A:1213:PRO:HB2	1:A:1258:VAL:CG1	2.46	0.46
1:B:2131:LEU:HD12	1:B:2135:ARG:CZ	2.46	0.46
1:A:1232:ARG:HA	1:A:1232:ARG:HD3	1.60	0.46
1:A:1176:VAL:HG22	1:A:1181:THR:HG23	1.97	0.46
1:B:2224:ASP:OD1	1:B:2373:HIS:HD2	1.99	0.45
1:B:2042:ILE:HD12	1:B:2054:ASP:OD1	2.17	0.45
1:B:2142:LYS:HA	1:B:2183:ASN:O	2.16	0.45
1:A:1042:ILE:CD1	1:A:1060:TYR:CE1	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1280:PRO:HA	1:B:2306:LEU:HG	1.99	0.45
1:A:1179:LYS:HE2	1:B:2183:ASN:HD22	1.81	0.45
1:B:2292:GLN:HG3	3:B:7577:HOH:O	2.17	0.45
1:A:1135:ARG:HG2	1:A:1140:ARG:O	2.17	0.45
1:B:2124:THR:O	1:B:2128:MET:HG3	2.17	0.44
1:A:1153:HIS:HE1	3:B:7038:HOH:O	1.99	0.44
1:B:2320:LEU:O	1:B:2324:ARG:HG3	2.17	0.44
1:A:1309:ASN:ND2	1:A:1312:ALA:H	2.15	0.44
1:A:1038:GLY:HA2	3:A:7692:HOH:O	2.16	0.44
1:A:1161:ALA:HB3	1:A:1165:VAL:HG21	2.00	0.44
1:B:2195:VAL:HG12	1:B:2234:ILE:CD1	2.47	0.43
1:B:2199:PHE:CE1	1:B:2234:ILE:HD11	2.53	0.43
1:B:2328:THR:HG22	1:B:2329:TYR:N	2.34	0.43
1:A:1218:SER:HB2	1:A:1375:TYR:CD1	2.53	0.43
1:B:2008:LYS:HD3	1:B:2056:ASP:HB3	1.99	0.43
1:A:1062:ASP:OD1	1:A:1074:HIS:HE1	2.01	0.43
1:B:2039:GLY:C	1:B:2040:GLN:OE1	2.58	0.43
1:A:1142:LYS:O	1:A:1143:ILE:HD12	2.19	0.42
1:A:1040:GLN:HA	3:A:7629:HOH:O	2.20	0.42
1:B:2146:PHE:CE1	1:B:2187:THR:HG23	2.53	0.42
1:A:1087:MET:CE	1:B:2087:MET:HE1	2.49	0.42
1:A:1281:VAL:HG21	1:A:1312:ALA:HB1	1.99	0.42
1:A:1033:ALA:O	1:A:1034:PHE:HB2	2.18	0.42
1:B:2108:ASN:OD1	1:B:2114:ILE:HG22	2.19	0.42
1:A:1177:PRO:CB	1:A:1179:LYS:HE2	2.47	0.42
1:A:1037:VAL:HG13	1:A:1037:VAL:O	2.19	0.42
1:A:1135:ARG:HD3	1:A:1141:ASP:O	2.19	0.42
1:A:1135:ARG:NH2	1:A:1156:MET:CE	2.74	0.42
1:B:2190:ASN:HD21	1:B:2223:PRO:HA	1.84	0.42
1:B:2208:GLY:HA2	1:B:2240:ALA:HB1	2.02	0.42
1:A:1208:GLY:HA2	1:A:1240:ALA:HB1	2.02	0.42
1:B:2142:LYS:HE2	1:B:2185:LEU:HD21	2.01	0.42
1:B:2377:ASP:HA	1:B:2380:LYS:HZ2	1.85	0.42
1:A:1164:GLY:HA3	1:B:2301:TYR:OH	2.19	0.42
1:A:1179:LYS:CE	1:B:2183:ASN:HD22	2.32	0.42
1:A:1103:LEU:HG	1:A:1317:ILE:HG13	2.02	0.41
1:A:1132:ARG:NH1	3:A:7397:HOH:O	2.52	0.41
1:B:2067:TRP:O	1:B:2273:LYS:HD3	2.21	0.41
1:A:1179:LYS:HZ1	1:B:2183:ASN:HB2	1.86	0.41
1:A:1158:LEU:HD23	1:A:1173:SER:HB3	2.01	0.41
1:A:1377:ASP:HA	1:A:1380:LYS:HZ2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1375:TYR:CE2	1:A:1379:LYS:HD2	2.55	0.41
1:A:1042:ILE:HD12	1:A:1054:ASP:OD1	2.21	0.41
1:B:2327:GLY:N	3:B:7134:HOH:O	2.53	0.41
1:A:1328:THR:HG22	1:A:1329:TYR:N	2.35	0.41
1:B:2010:ILE:HD11	3:B:7690:HOH:O	2.21	0.41
1:A:1199:PHE:CE1	1:A:1234:ILE:HD11	2.56	0.41
1:A:1029:SER:HA	1:A:1030:PRO:HD3	1.89	0.41
1:A:1030:PRO:HA	1:B:2296:PRO:HD3	2.02	0.41
1:A:1087:MET:HB3	1:A:1311:LEU:HD21	2.02	0.40
1:B:2131:LEU:HA	1:B:2134:MET:CE	2.35	0.40
1:A:1133:ILE:HG23	1:A:1134:MET:N	2.35	0.40
1:A:1142:LYS:HB2	1:A:1205:GLU:O	2.21	0.40
1:A:1099:LEU:HD23	3:A:7135:HOH:O	2.20	0.40
1:B:2115:GLU:HG2	3:B:7167:HOH:O	2.21	0.40
1:B:2144:ILE:HA	1:B:2185:LEU:O	2.21	0.40
1:B:2281:VAL:HG21	1:B:2312:ALA:HB1	2.01	0.40
1:B:2145:LYS:HB2	1:B:2145:LYS:HE2	1.91	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	425/427 (100%)	407 (96%)	16 (4%)	2 (0%)	34	26
1	B	425/427 (100%)	389 (92%)	27 (6%)	9 (2%)	9	3
All	All	850/854 (100%)	796 (94%)	43 (5%)	11 (1%)	15	7

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2155	ASP

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Mol	Chain	Res	Type
1	B	2156	MET
1	B	2168	LEU
1	B	2159	VAL
1	B	2171	PRO
1	A	1040	GLN
1	A	1273	LYS
1	B	2273	LYS
1	B	2158	LEU
1	B	2173	SER
1	B	2169	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	330/330 (100%)	306 (93%)	24 (7%)	17	11
1	B	330/330 (100%)	304 (92%)	26 (8%)	15	9
All	All	660/660 (100%)	610 (92%)	50 (8%)	16	10

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1008	LYS
1	A	1037	VAL
1	A	1040	GLN
1	A	1042	ILE
1	A	1054	ASP
1	A	1059	ARG
1	A	1103	LEU
1	A	1130	VAL
1	A	1131	LEU
1	A	1170	LEU
1	A	1178	LYS
1	A	1179	LYS
1	A	1187	THR

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Mol	Chain	Res	Type
1	A	1232	ARG
1	A	1234	ILE
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	1374	ASN
1	A	1391	ARG
1	A	1394	LEU
1	B	2008	LYS
1	B	2040	GLN
1	B	2042	ILE
1	B	2054	ASP
1	B	2059	ARG
1	B	2103	LEU
1	B	2130	VAL
1	B	2131	LEU
1	B	2145	LYS
1	B	2155	ASP
1	B	2157	PHE
1	B	2167	THR
1	B	2171	PRO
1	B	2178	LYS
1	B	2185	LEU
1	B	2187	THR
1	B	2232	ARG
1	B	2234	ILE
1	B	2268	LEU
1	B	2269	THR
1	B	2318	LYS
1	B	2339	LEU
1	B	2343	LEU
1	B	2358	GLN
1	B	2374	ASN
1	B	2394	LEU

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	1074	HIS

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Mol	Chain	Res	Type
1	A	1121	ASN
1	A	1151	HIS
1	A	1153	HIS
1	A	1190	ASN
1	A	1259	GLN
1	A	1292	GLN
1	A	1309	ASN
1	A	1352	HIS
1	A	1358	GLN
1	A	1373	HIS
1	A	1374	ASN
1	B	2074	HIS
1	B	2121	ASN
1	B	2151	HIS
1	B	2183	ASN
1	B	2190	ASN
1	B	2259	GLN
1	B	2292	GLN
1	B	2309	ASN
1	B	2352	HIS
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)

2 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	5000	-	16,16,16	1.62	6 (37%)	20,23,23	1.47	4 (20%)
2	PMP	B	6000	-	16,16,16	1.63	5 (31%)	20,23,23	1.58	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	5000	-	-	0/8/8/8	0/1/1/1
2	PMP	B	6000	-	-	0/8/8/8	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5000	PMP	P-O2P	-2.15	1.47	1.54
2	B	6000	PMP	P-O2P	-2.13	1.47	1.54
2	A	5000	PMP	P-O1P	-2.05	1.44	1.51
2	A	5000	PMP	C5-C4	2.11	1.43	1.40
2	A	5000	PMP	C2A-C2	2.20	1.54	1.50
2	B	6000	PMP	C2A-C2	2.23	1.54	1.50
2	B	6000	PMP	C5-C4	2.47	1.43	1.40
2	B	6000	PMP	C2-N1	2.73	1.39	1.34
2	A	5000	PMP	C2-N1	2.81	1.40	1.34
2	A	5000	PMP	C6-N1	2.85	1.40	1.34
2	B	6000	PMP	C6-N1	2.90	1.40	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5000	PMP	C5-C6-N1	-2.49	119.55	123.86
2	B	6000	PMP	C5-C6-N1	-2.35	119.78	123.86
2	B	6000	PMP	O2P-P-O4P	-2.09	100.56	106.56
2	A	5000	PMP	O3-C3-C2	2.09	121.30	117.66
2	A	5000	PMP	O4P-P-O1P	2.20	112.73	107.14
2	A	5000	PMP	O3P-P-O2P	2.23	115.87	107.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	6000	PMP	O3P-P-O2P	2.32	116.21	107.38
2	B	6000	PMP	O4P-P-O1P	3.51	116.08	107.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	427/427 (100%)	0.20	14 (3%)	50	51	8, 16, 28, 36	0
1	B	398/427 (93%)	0.22	12 (3%)	54	55	7, 16, 29, 52	0
All	All	825/854 (96%)	0.21	26 (3%)	51	52	7, 16, 28, 52	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1038	GLY	5.3
1	B	2182	ALA	5.1
1	B	2150	TYR	3.8
1	A	1039	GLY	3.6
1	A	1031	VAL	3.2
1	A	1165	VAL	3.0
1	B	2203	PRO	3.0
1	A	1384	GLN	2.9
1	B	2239	ASP	2.7
1	A	1171	PRO	2.7
1	B	2008	LYS	2.6
1	A	1170	LEU	2.5
1	B	2151	HIS	2.4
1	B	2183	ASN	2.4
1	B	2152	GLY	2.4
1	A	1010	ILE	2.4
1	B	2148	GLY	2.4
1	A	1143	ILE	2.3
1	A	1040	GLN	2.3
1	B	2292	GLN	2.3
1	A	1159	VAL	2.3
1	A	1433	LEU	2.2
1	B	2281	VAL	2.2
1	B	2149	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1135	ARG	2.1
1	A	1326	PRO	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
2	PMP	A	5000	16/16	0.94	0.14	1.23	15,17,20,20	0
2	PMP	B	6000	16/16	0.85	0.21	1.19	30,33,34,37	0

6.5 Other polymers (i)

There are no such residues in this entry.