



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:48 PM UTC

PDB ID : 3FQ8 / pdb_00003fq8
Title : M248I mutant of GSAM
Authors : Stetefeld, J.
Deposited on : 2009-01-07
Resolution : 2.00 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

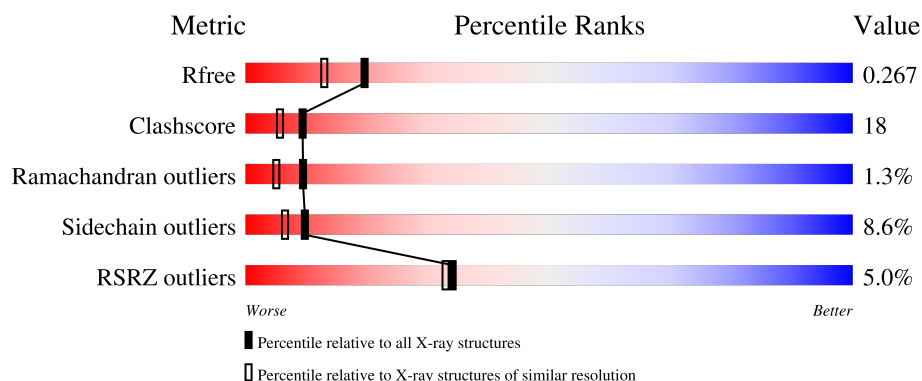
1 Overall quality at a glance

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	5% 70% 25% 5%
1	B	427	5% 70% 25% 5%

2 Entry composition

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.

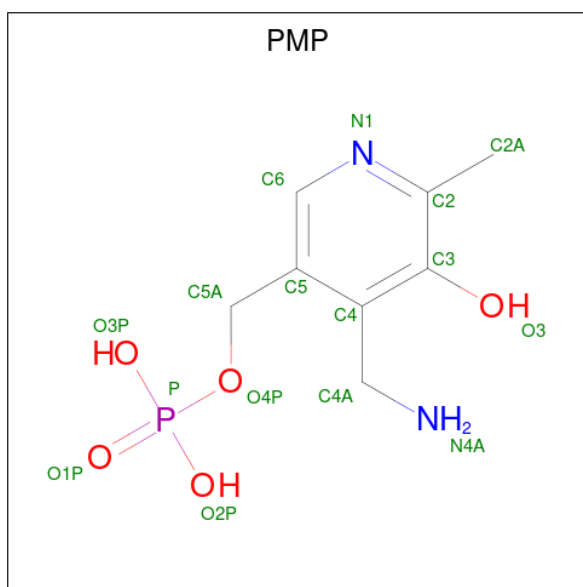
- Molecule 1 is a protein called Glutamate-1-semialdehyde 2,1-aminomutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3202	2044	535	605	18			
1	B	427	Total	C	N	O	S	200	0	0
			3202	2044	535	605	18			

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 mutation	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 mutation	UNP P24630
B	2327	GLY	ALA	conflict	UNP P24630

- Molecule 2 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (CCD ID: PMP) (formula: C₈H₁₃N₂O₅P).



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		

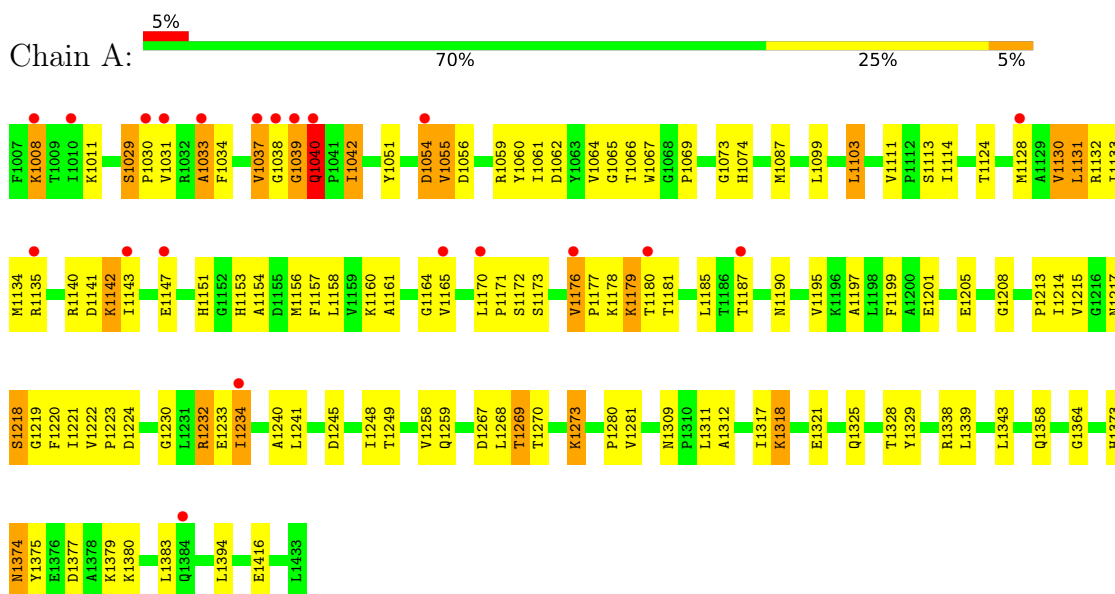
- Molecule 3 is water.

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

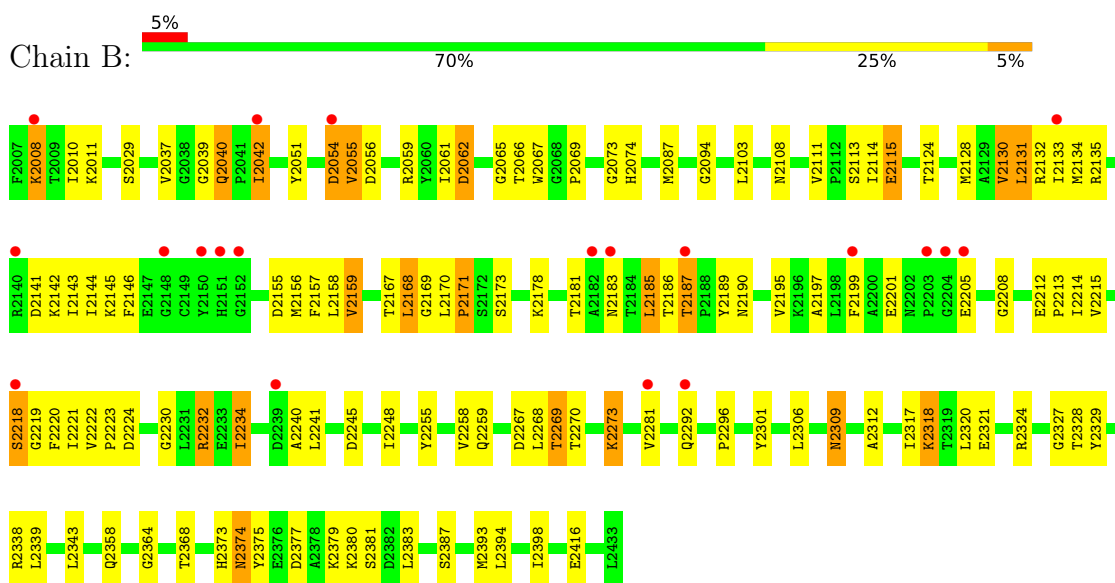
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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



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4 Data and refinement statistics

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) 94.1 (27.90-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.61 (at 1.99Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.208 , 0.245 0.228 , 0.267	Depositor DCC
R_{free} test set	5754 reflections (10.17%)	wwPDB-VP
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0.40	0/3271	0.95	16/4431 (0.4%)
1	B	0.39	0/3271	0.93	16/4431 (0.4%)
All	All	0.40	0/6542	0.94	32/8862 (0.4%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1039	GLY	N-CA-C	-9.22	103.19	111.95
1	A	1218	SER	N-CA-C	-8.69	99.75	110.61
1	A	1033	ALA	N-CA-C	8.66	121.67	111.71
1	B	2218	SER	N-CA-C	-7.92	100.64	111.56
1	A	1055	VAL	N-CA-C	-6.79	103.84	113.07
1	B	2212	GLU	N-CA-C	-6.59	100.08	109.24
1	A	1214	ILE	N-CA-C	-6.48	98.71	108.17
1	B	2055	VAL	N-CA-C	-6.39	104.38	113.07
1	A	1061	ILE	N-CA-C	-6.38	97.77	107.73
1	B	2309	ASN	CA-C-N	6.36	125.85	119.24
1	B	2309	ASN	C-N-CA	6.36	125.85	119.24
1	B	2219	GLY	N-CA-C	-6.10	102.47	112.83
1	A	1029	SER	CA-C-N	6.09	127.46	119.84
1	A	1029	SER	C-N-CA	6.09	127.46	119.84
1	B	2111	VAL	N-CA-C	6.06	114.56	107.77
1	B	2061	ILE	N-CA-C	-5.90	98.53	107.73
1	A	1073	GLY	N-CA-C	-5.65	105.96	112.29
1	B	2073	GLY	N-CA-C	-5.65	106.58	111.95
1	A	1051	TYR	N-CA-C	5.60	118.70	109.85
1	B	2115	GLU	N-CA-C	-5.52	107.19	114.04
1	B	2051	TYR	N-CA-C	5.49	118.53	109.85
1	B	2214	ILE	N-CA-C	-5.46	100.19	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1219	GLY	N-CA-C	-5.44	103.58	112.83
1	B	2029	SER	CA-C-N	5.39	126.58	119.84
1	B	2029	SER	C-N-CA	5.39	126.58	119.84
1	A	1111	VAL	N-CA-C	5.33	113.74	107.77
1	A	1217	ASN	N-CA-C	5.26	119.80	113.17
1	B	2094	GLY	N-CA-C	-5.20	107.62	115.32
1	A	1249	THR	N-CA-C	5.18	117.83	111.82
1	A	1064	VAL	N-CA-C	-5.11	107.85	112.96
1	A	1114	ILE	N-CA-C	5.04	115.94	108.23
1	B	2062	ASP	N-CA-C	5.03	116.96	108.96

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	3202	0	3184	132	0
1	B	3202	0	3184	107	0
2	A	16	0	11	0	0
2	B	16	0	11	0	0
3	A	365	0	0	11	0
3	B	328	0	0	7	0
All	All	7129	0	6390	224	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 (224) 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	1.39	1.02
1:A:1131:LEU:HA	1:A:1134:MET:HE2	1.43	0.97
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1190:ASN:HD21	1:A:1224:ASP:H	1.20	0.88
1:A:1135:ARG:HH22	1:A:1156:MET:HE1	1.39	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: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:A:1197:ALA:O	1:A:1201:GLU:HG3	1.89	0.72
1:B:2131:LEU:HD12	1:B:2135:ARG:NH1	2.04	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: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:1179:LYS:HZ3	1:B:2183:ASN:ND2	1.91	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:A:1135:ARG:NH2	1:A:1156:MET:HE1	2.08	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
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:HA	1:B:2318:LYS:HE3	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:B:2218:SER:HB2	1:B:2375:TYR:CD1	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1008:LYS:HD2	3:A:7234:HOH:O	1.97	0.64
1:A:1318:LYS:HA	1:A:1318:LYS:HE3	1.79	0.64
3:A:7057:HOH:O	1:B:2074:HIS:HD2	1.81	0.64
1:A:1131:LEU:HD22	1:A:1134:MET:CE	2.28	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:1131:LEU:HD22	1:A:1134:MET:HE1	1.82	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:2142:LYS:C	1:B:2143:ILE:HD12	2.26	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:1179:LYS:CE	1:A:1180:THR:HG23	2.33	0.59
1:A:1011:LYS:HB2	1:A:1055:VAL:HG23	1.85	0.58
1:A:1222:VAL:CG1	1:A:1223:PRO:HD2	2.33	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:B:2374:ASN:C	1:B:2374:ASN:HD22	2.11	0.58
1:A:1131:LEU:HD23	1:A:1157:PHE:HZ	1.68	0.58
1:A:1142:LYS:C	1:A:1143:ILE:HD12	2.28	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:1066:THR:HG23	1:A:1069:PRO:HD2	1.86	0.56
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:1374:ASN:C	1:A:1374:ASN:HD22	2.14	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1134:MET:HE1	1:A:1143:ILE:HG12	1.89	0.55
1:B:2377:ASP:HA	1:B:2380:LYS:NZ	2.22	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:B:2141:ASP:O	1:B:2183:ASN:HB3	2.06	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: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: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:A:1280:PRO:HG3	1:B:2306:LEU:HB3	1.90	0.53
1:B:2130:VAL:C	1:B:2133:ILE:HG22	2.32	0.53
1:B:2375:TYR:CE2	1:B:2379:LYS:HD2	2.43	0.53
1:A:1031:VAL:HG21	1:A:1067:TRP:CH2	2.43	0.53
1:B:2130:VAL:HA	1:B:2133:ILE:CG2	2.39	0.53
1:B:2377:ASP:HA	1:B:2380:LYS:HZ2	1.74	0.53
1:A:1130:VAL:CA	1:A:1133:ILE:HG22	2.37	0.52
1:A:1220:PHE:HB3	1:A:1364:GLY:HA3	1.92	0.52
1:B:2062:ASP:OD1	1:B:2074:HIS:HE1	1.93	0.52
1:B:2232:ARG:HH12	1:B:2267:ASP:CG	2.16	0.52
1:B:2037:VAL:HG23	1:B:2387:SER:HA	1.91	0.52
1:A:1135:ARG:CZ	1:A:1156:MET:SD	2.98	0.52
1:A:1232:ARG:HH12	1:A:1267:ASP:CG	2.17	0.52
1:B:2145:LYS:O	1:B:2186:THR:HA	2.09	0.52
1:A:1130:VAL:C	1:A:1133:ILE:HG22	2.34	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:1065:GLY:O	1:A:1066:THR:HG22	2.12	0.50
1:A:1245:ASP:HA	1:A:1270:THR:OG1	2.11	0.50
1:A:1113:SER:OG	1:A:1269:THR:CG2	2.60	0.50
1:A:1153:HIS:HA	1:A:1158:LEU:HD11	1.94	0.50
1:B:2187:THR:HG21	1:B:2195:VAL:HG22	1.94	0.50
1:B:2215:VAL:HB	1:B:2221:ILE:HB	1.93	0.50
1:B:2248:ILE:CG1	1:B:2273:LYS:HE3	2.41	0.50
1:B:2218:SER:HB2	1:B:2375:TYR:HD1	1.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2309:ASN:HD21	1:B:2312:ALA:H	1.58	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:B:2131:LEU:HD22	1:B:2134:MET:HE1	1.94	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: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:2039:GLY:C	1:B:2040:GLN:OE1	2.58	0.47
1:B:2232:ARG:HA	1:B:2232:ARG:HD3	1.56	0.47
1:A:1179:LYS:NZ	1:B:2183:ASN:HD22	2.13	0.47
1:B:2245:ASP:HA	1:B:2270:THR:OG1	2.15	0.47
1:B:2393:MET:HE3	1:B:2398:ILE:HG21	1.96	0.47
1:A:1338:ARG:HH21	1:A:1416:GLU:HG3	1.80	0.47
1:A:1011:LYS:HG2	1:A:1056:ASP:OD1	2.16	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:A:1176:VAL:HG22	1:A:1181:THR:HG23	1.97	0.46
1:A:1232:ARG:HD3	1:A:1232:ARG:HA	1.60	0.46
1:B:2131:LEU:HD12	1:B:2135:ARG:CZ	2.46	0.46
1:A:1087:MET:HE3	1:B:2087:MET:HE1	1.98	0.45
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:A:1042:ILE:CD1	1:A:1060:TYR:CE1	3.00	0.45
1:A:1280:PRO:HA	1:B:2306:LEU:HG	1.99	0.45
1:B:2142:LYS:HA	1:B:2183:ASN:O	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1038:GLY:HA2	3:A:7692:HOH:O	2.16	0.44
1:A:1309:ASN:ND2	1:A:1312:ALA:H	2.15	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:2134:MET:HE1	1:B:2143:ILE:HG12	2.00	0.43
1:B:2199:PHE:CE1	1:B:2234:ILE:HD11	2.53	0.43
1:B:2042:ILE:HD12	1:B:2054:ASP:CG	2.44	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:1087:MET:HE1	1:B:2087:MET:HE3	2.01	0.43
1:A:1062:ASP:OD1	1:A:1074:HIS:HE1	2.01	0.43
1:A:1171:PRO:O	1:A:1172:SER:C	2.62	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:1134:MET:HE1	1:A:1143:ILE:CG1	2.50	0.42
1:A:1281:VAL:HG21	1:A:1312:ALA:HB1	1.99	0.42
1:B:2108:ASN:OD1	1:B:2114:ILE:HG22	2.19	0.42
1:A:1033:ALA:O	1:A:1034:PHE:HB2	2.18	0.42
1:A:1037:VAL:O	1:A:1037:VAL:HG13	2.19	0.42
1:A:1177:PRO:CB	1:A:1179:LYS:HE2	2.47	0.42
1:A:1135:ARG:NH2	1:A:1156:MET:CE	2.74	0.42
1:A:1135:ARG:HD3	1:A:1141:ASP:O	2.19	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:1031:VAL:C	1:A:1033:ALA:H	2.28	0.42
1:A:1208:GLY:HA2	1:A:1240:ALA:HB1	2.02	0.42
1:A:1164:GLY:HA3	1:B:2301:TYR:OH	2.19	0.42
1:B:2142:LYS:HE2	1:B:2185:LEU:HD21	2.01	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:1042:ILE:HD12	1:A:1054:ASP:CG	2.46	0.41
1:A:1158:LEU:HD23	1:A:1173:SER:HB3	2.01	0.41
1:A:1375:TYR:CE2	1:A:1379:LYS:HD2	2.55	0.41
1:A:1377:ASP:HA	1:A:1380:LYS:HZ2	1.84	0.41
1:B:2131:LEU:HD22	1:B:2134:MET:HE2	2.02	0.41
1:A:1042:ILE:HD12	1:A:1054:ASP:OD1	2.21	0.41
1:B:2374:ASN:ND2	1:B:2374:ASN:C	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:2327:GLY:N	3:B:7134:HOH:O	2.53	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:1199:PHE:CE1	1:A:1234:ILE:HD11	2.56	0.41
1:A:1011:LYS:NZ	3:A:7239:HOH:O	2.53	0.41
1:A:1087:MET:HB3	1:A:1311:LEU:HD21	2.02	0.40
1:A:1099:LEU:HD23	3:A:7135:HOH:O	2.20	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: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:2145:LYS:HB2	1:B:2145:LYS:HE2	1.91	0.40
1:B:2281:VAL:HG21	1:B:2312:ALA:HB1	2.01	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	425/427 (100%)	407 (96%)	16 (4%)	2 (0%)	24	21
1	B	425/427 (100%)	389 (92%)	27 (6%)	9 (2%)	5	2
All	All	850/854 (100%)	796 (94%)	43 (5%)	11 (1%)	9	5

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2155	ASP
1	B	2156	MET
1	B	2168	LEU

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Mol	Chain	Res	Type
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 ⓘ

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%)	303 (92%)	27 (8%)	10	7
1	B	330/330 (100%)	300 (91%)	30 (9%)	9	6
All	All	660/660 (100%)	603 (91%)	57 (9%)	10	6

All (57) 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	1142	LYS
1	A	1170	LEU
1	A	1176	VAL
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	1241	LEU
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	1383	LEU
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	2157	PHE
1	B	2159	VAL
1	B	2167	THR
1	B	2168	LEU
1	B	2170	LEU
1	B	2171	PRO
1	B	2178	LYS
1	B	2181	THR
1	B	2185	LEU
1	B	2187	THR
1	B	2232	ARG
1	B	2234	ILE
1	B	2241	LEU
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	2383	LEU
1	B	2394	LEU

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

Mol	Chain	Res	Type
1	A	1074	HIS
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	2151	HIS
1	B	2183	ASN
1	B	2190	ASN
1	B	2259	GLN
1	B	2292	GLN
1	B	2309	ASN
1	B	2325	GLN
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 oligosaccharides 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	1.75	5 (31%)	22,23,23	1.52	4 (18%)
2	PMP	B	6000	-	16,16,16	1.77	5 (31%)	22,23,23	1.61	5 (22%)

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	-	-	3/8/8/8	0/1/1/1
2	PMP	B	6000	-	-	3/8/8/8	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5000	PMP	C2-N1	3.48	1.40	1.33
2	B	6000	PMP	C2-N1	3.38	1.39	1.33
2	B	6000	PMP	C6-N1	3.07	1.40	1.34
2	A	5000	PMP	C6-N1	3.02	1.40	1.34
2	B	6000	PMP	C2A-C2	2.79	1.54	1.50
2	A	5000	PMP	C2A-C2	2.74	1.54	1.50
2	B	6000	PMP	C5-C4	2.49	1.43	1.40
2	A	5000	PMP	C5-C4	2.12	1.43	1.40
2	A	5000	PMP	P-O2P	-2.11	1.47	1.54
2	B	6000	PMP	P-O2P	-2.08	1.47	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6000	PMP	O4P-P-O1P	3.57	116.08	106.44
2	A	5000	PMP	C5-C6-N1	-2.64	119.55	123.83
2	B	6000	PMP	C5-C6-N1	-2.49	119.78	123.83
2	A	5000	PMP	C3-C4-C5	2.38	120.89	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6000	PMP	O2P-P-O4P	-2.34	100.56	106.67
2	A	5000	PMP	O4P-P-O1P	2.33	112.73	106.44
2	B	6000	PMP	O3P-P-O2P	2.24	116.21	107.80
2	A	5000	PMP	O3P-P-O2P	2.15	115.87	107.80
2	B	6000	PMP	C3-C4-C5	2.08	120.62	118.73

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5000	PMP	C5A-O4P-P-O1P
2	A	5000	PMP	C5A-O4P-P-O2P
2	B	6000	PMP	C5A-O4P-P-O1P
2	B	6000	PMP	C5A-O4P-P-O2P
2	B	6000	PMP	C5A-O4P-P-O3P
2	A	5000	PMP	C5A-O4P-P-O3P

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%)	0.30	21 (4%) 35 34	8, 16, 28, 36	0
1	B	398/427 (93%)	0.32	20 (5%) 34 33	7, 16, 29, 52	0
All	All	825/854 (96%)	0.31	41 (4%) 34 33	7, 16, 28, 52	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1038	GLY	5.6
1	B	2182	ALA	5.3
1	B	2152	GLY	5.0
1	B	2150	TYR	4.8
1	A	1031	VAL	4.1
1	B	2183	ASN	3.8
1	A	1039	GLY	3.6
1	A	1170	LEU	3.3
1	B	2151	HIS	3.2
1	A	1135	ARG	3.2
1	B	2292	GLN	3.2
1	A	1384	GLN	3.1
1	B	2187	THR	3.1
1	A	1054	ASP	3.0
1	A	1037	VAL	2.9
1	A	1143	ILE	2.8
1	A	1165	VAL	2.8
1	A	1008	LYS	2.6
1	B	2281	VAL	2.6
1	A	1128	MET	2.6
1	B	2239	ASP	2.6
1	A	1033	ALA	2.5
1	A	1176	VAL	2.4
1	B	2204	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	2054	ASP	2.3
1	A	1030	PRO	2.3
1	B	2205	GLU	2.3
1	B	2218	SER	2.3
1	A	1040	GLN	2.2
1	B	2199	PHE	2.2
1	B	2148	GLY	2.2
1	B	2008	LYS	2.1
1	A	1180	THR	2.1
1	A	1187	THR	2.1
1	A	1010	ILE	2.1
1	A	1147	GLU	2.1
1	B	2203	PRO	2.1
1	A	1234	ILE	2.1
1	B	2042	ILE	2.1
1	B	2140	ARG	2.0
1	B	2133	ILE	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 oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	PMP	B	6000	16/16	0.82	0.17	30,33,34,37	0
2	PMP	A	5000	16/16	0.92	0.09	15,17,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.