



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:07 AM GMT

PDB ID : 2HOZ  
Title : Inter-subunit signaling in GSAM  
Authors : Stetefeld, J.  
Deposited on : 2006-07-17  
Resolution : 2.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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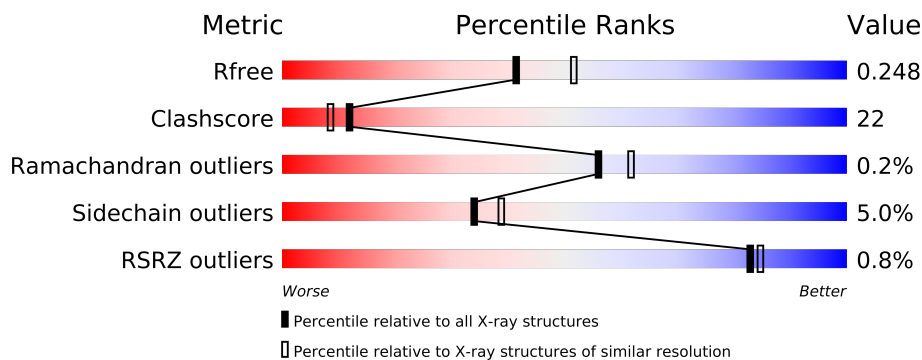
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.20 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))
$R_{free}$	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	432	
1	B	432	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	HOZ	A	1	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7001 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

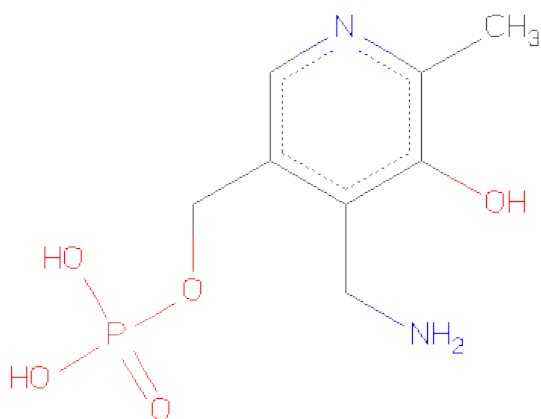
- Molecule 1 is a protein called Glutamate-1-semialdehyde2,1-aminomutase (GSAM) pmp-form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3202	2043	535	605	19			
1	B	420	Total	C	N	O	S	0	0	0
			3161	2018	528	596	19			

There are 12 discrepancies between the modelled and reference sequences:

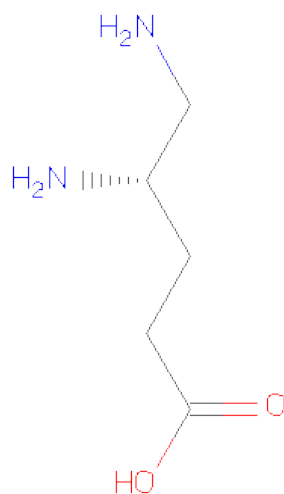
Chain	Residue	Modelled	Actual	Comment	Reference
A	1108	ASN	ILE	CONFLICT	UNP P24630
A	1133	ILE	LEU	CONFLICT	UNP P24630
A	1172	SER	ASP	CONFLICT	UNP P24630
A	1179	LYS	SER	CONFLICT	UNP P24630
A	1187	THR	ALA	CONFLICT	UNP P24630
A	1327	GLY	ALA	CONFLICT	UNP P24630
B	2108	ASN	ILE	CONFLICT	UNP P24630
B	2133	ILE	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	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 (4S)-4,5-DIAMINOPENTANOICACID (three-letter code: HOZ) (formula: C<sub>5</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 4 is water.

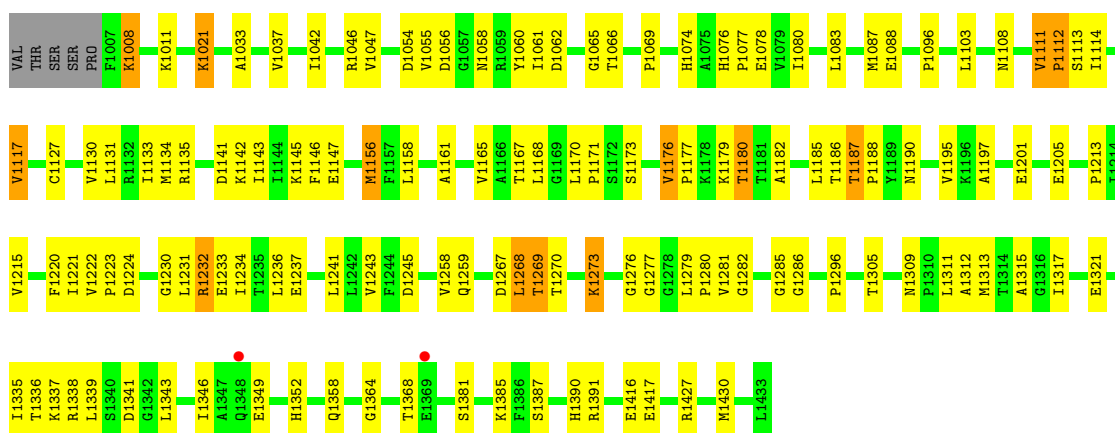
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	301	Total 301	O 301	0	0
4	B	296	Total 296	O 296	0	0

### 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.

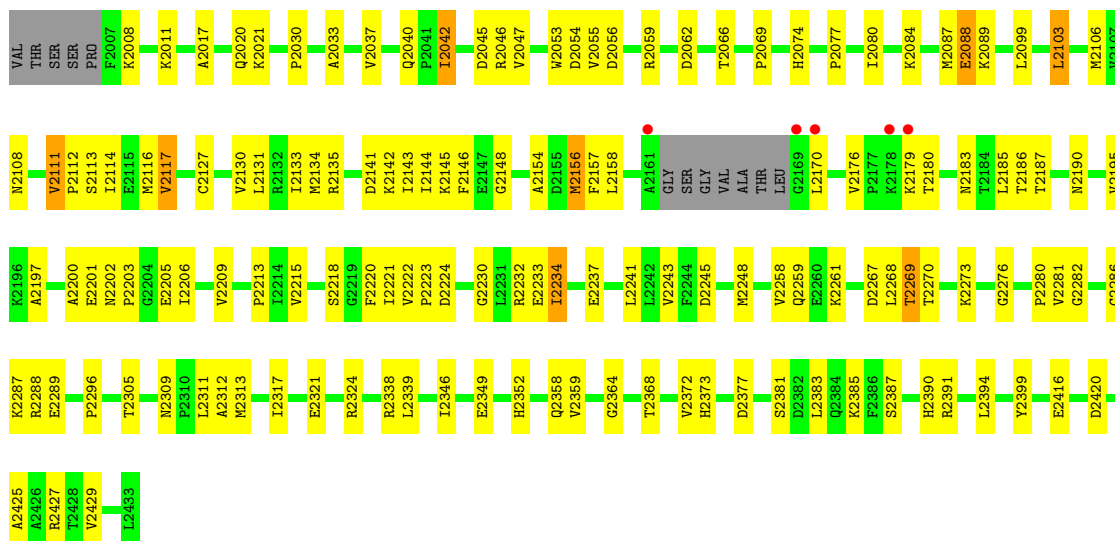
- Molecule 1: Glutamate-1-semialdehyde2,1-aminomutase (GSAM) pmp-form

Chain A:



- Molecule 1: Glutamate-1-semialdehyde2,1-aminomutase (GSAM) pmp-form

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.42Å 107.78Å 121.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.98 – 2.20 22.98 – 2.17	Depositor EDS
% Data completeness (in resolution range)	94.4 (22.98-2.20) 94.5 (22.98-2.17)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.54 (at 2.17Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.197 , 0.250 0.194 , 0.248	Depositor DCC
$R_{free}$ test set	2091 reflections (4.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.6	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 45.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 43477 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7001	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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: HOZ, 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	0.61	1/4430 (0.0%)
1	B	0.33	0/3229	0.61	0/4371
All	All	0.33	0/6500	0.61	1/8801 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1061	ILE	N-CA-C	-5.69	95.63	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3202	0	3182	153	0
1	B	3161	0	3138	144	0
2	A	16	0	11	0	0
2	B	16	0	11	0	0
3	A	9	0	11	4	0
4	A	301	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	296	0	0	6	0
All	All	7001	0	6353	275	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 22.

All (275) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2131:LEU:HD12	1:B:2134:MET:HE3	1.36	1.03
1:A:1131:LEU:HA	1:A:1134:MET:HE2	1.43	0.98
1:A:1309:ASN:HD22	1:A:1312:ALA:H	1.12	0.95
1:B:2037:VAL:HG23	1:B:2387:SER:HA	1.51	0.91
1:A:1259:GLN:HE22	1:A:1269:THR:HG21	1.39	0.86
1:A:1083:LEU:O	1:A:1087:MET:HG2	1.77	0.85
1:B:2055:VAL:HB	4:B:7219:HOH:O	1.77	0.85
1:A:1190:ASN:HD21	1:A:1224:ASP:H	1.25	0.84
1:A:1037:VAL:HG21	1:A:1390:HIS:HB3	1.59	0.83
1:A:1190:ASN:ND2	1:A:1224:ASP:H	1.77	0.82
1:B:2190:ASN:HD21	1:B:2224:ASP:H	1.25	0.82
1:A:1134:MET:HE3	1:A:1143:ILE:HD12	1.60	0.81
1:B:2106:MET:CE	1:B:2324:ARG:HH22	1.92	0.81
1:A:1130:VAL:O	1:A:1134:MET:HG3	1.81	0.80
1:B:2259:GLN:HE22	1:B:2269:THR:HG21	1.44	0.80
1:B:2106:MET:HE2	1:B:2324:ARG:HH22	1.44	0.80
1:A:1179:LYS:HA	1:B:2179:LYS:HE3	1.64	0.80
1:A:1188:PRO:HB3	3:A:1:HOZ:HN11	1.47	0.80
1:A:1180:THR:HA	1:B:2180:THR:HG22	1.65	0.79
1:B:2190:ASN:ND2	1:B:2224:ASP:H	1.81	0.78
1:A:1037:VAL:HG23	1:A:1387:SER:HA	1.69	0.73
1:A:1273:LYS:HE3	1:B:2305:THR:HG21	1.69	0.73
1:A:1309:ASN:HD21	1:A:1311:LEU:HB2	1.54	0.73
1:B:2309:ASN:HD22	1:B:2312:ALA:H	1.36	0.73
1:B:2042:ILE:HD11	1:B:2399:TYR:HE1	1.53	0.72
1:B:2338:ARG:NH1	1:B:2420:ASP:OD1	2.22	0.72
1:B:2011:LYS:HB2	1:B:2055:VAL:HG13	1.72	0.72
1:A:1338:ARG:NH2	1:A:1416:GLU:HG3	2.05	0.71
1:B:2267:ASP:HA	1:B:2287:LYS:HE3	1.70	0.71
1:A:1083:LEU:HB3	1:B:2087:MET:HE1	1.71	0.71
1:A:1130:VAL:O	1:A:1133:ILE:HG22	1.91	0.71
1:A:1008:LYS:HD3	4:A:7270:HOH:O	1.91	0.70
1:B:2154:ALA:HB1	1:B:2156:MET:HE3	1.73	0.70
1:A:1131:LEU:HD11	1:A:1143:ILE:HG21	1.73	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2338:ARG:NH2	1:B:2416:GLU:HG3	2.07	0.70
1:B:2037:VAL:HG21	1:B:2390:HIS:HB3	1.74	0.69
1:B:2232:ARG:HH12	1:B:2267:ASP:CG	1.95	0.69
1:B:2131:LEU:HA	1:B:2134:MET:HE2	1.73	0.69
1:A:1131:LEU:HD12	1:A:1134:MET:HE1	1.77	0.67
1:A:1268:LEU:HD12	1:A:1286:GLY:HA3	1.77	0.66
1:A:1173:SER:O	1:A:1176:VAL:HG13	1.96	0.66
1:A:1114:ILE:CG2	1:A:1117:VAL:HG13	2.25	0.66
1:A:1281:VAL:HG12	1:A:1282:GLY:H	1.61	0.66
1:B:2232:ARG:HD3	1:B:2232:ARG:O	1.96	0.65
1:B:2213:PRO:HB2	1:B:2258:VAL:HG11	1.79	0.65
1:A:1309:ASN:ND2	1:A:1312:ALA:H	1.90	0.65
1:A:1279:LEU:O	1:A:1281:VAL:HG23	1.97	0.64
1:B:2317:ILE:O	1:B:2321:GLU:HG3	1.97	0.64
1:A:1185:LEU:N	1:A:1185:LEU:HD12	2.12	0.63
1:B:2066:THR:HG23	1:B:2069:PRO:HD2	1.80	0.63
1:A:1168:LEU:HB3	1:A:1170:LEU:HG	1.81	0.62
1:A:1021:LYS:HB3	1:A:1021:LYS:NZ	2.15	0.62
1:A:1188:PRO:HG3	3:A:1:HOZ:HA	1.81	0.62
1:A:1296:PRO:HD3	1:B:2030:PRO:HA	1.81	0.62
1:B:2054:ASP:HB3	1:B:2056:ASP:H	1.65	0.61
1:A:1134:MET:CE	1:A:1143:ILE:HD12	2.31	0.60
1:B:2338:ARG:HH22	1:B:2416:GLU:HG3	1.66	0.60
1:B:2190:ASN:HD21	1:B:2224:ASP:N	1.98	0.60
1:A:1281:VAL:HG12	1:A:1282:GLY:N	2.15	0.60
1:B:2017:ALA:HA	1:B:2020:GLN:HE21	1.64	0.60
1:B:2131:LEU:HA	1:B:2134:MET:CE	2.32	0.60
1:B:2230:GLY:O	1:B:2234:ILE:HG23	2.01	0.60
1:A:1232:ARG:O	1:A:1232:ARG:HD3	2.00	0.60
1:B:2135:ARG:HD3	1:B:2141:ASP:O	2.01	0.60
1:A:1062:ASP:OD1	1:A:1074:HIS:HE1	1.85	0.60
1:A:1346:ILE:HA	1:A:1349:GLU:HG2	1.84	0.60
1:A:1080:ILE:HD12	1:B:2088:GLU:OE1	2.01	0.60
1:B:2106:MET:HE2	1:B:2324:ARG:NH2	2.16	0.59
1:B:2131:LEU:HD11	1:B:2143:ILE:HG21	1.82	0.59
1:A:1179:LYS:HB3	1:B:2179:LYS:O	2.03	0.59
1:A:1114:ILE:HG23	1:A:1117:VAL:HG13	1.83	0.59
1:B:2040:GLN:HA	1:B:2040:GLN:NE2	2.18	0.59
1:A:1222:VAL:HG13	1:A:1223:PRO:HD2	1.84	0.59
1:A:1037:VAL:HG22	1:A:1037:VAL:O	2.03	0.59
1:B:2042:ILE:HD11	1:B:2399:TYR:CE1	2.36	0.59
1:A:1190:ASN:HD21	1:A:1224:ASP:N	1.97	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2346:ILE:HA	1:B:2349:GLU:HG2	1.84	0.58
4:A:7325:HOH:O	1:B:2074:HIS:HD2	1.85	0.58
1:B:2220:PHE:HB3	1:B:2364:GLY:HA3	1.86	0.58
1:B:2352:HIS:HD2	1:B:2385:LYS:NZ	2.01	0.58
1:A:1190:ASN:HD21	1:A:1223:PRO:HA	1.69	0.57
1:B:2011:LYS:HD2	1:B:2055:VAL:O	2.03	0.57
1:B:2368:THR:HB	1:B:2381:SER:HA	1.85	0.57
1:A:1309:ASN:O	1:A:1313:MET:HG2	2.05	0.57
1:A:1042:ILE:CG2	1:A:1054:ASP:OD1	2.52	0.57
1:B:2130:VAL:HA	1:B:2133:ILE:HG22	1.85	0.57
1:B:2309:ASN:HD21	1:B:2311:LEU:HB2	1.69	0.57
1:A:1171:PRO:HB3	1:A:1176:VAL:HG22	1.86	0.57
1:A:1066:THR:HG23	1:A:1069:PRO:HD2	1.86	0.57
1:A:1054:ASP:OD1	1:A:1060:TYR:HE1	1.88	0.57
1:A:1131:LEU:HD12	1:A:1134:MET:CE	2.35	0.56
1:A:1281:VAL:HG22	1:A:1312:ALA:HB1	1.88	0.56
1:A:1335:ILE:HG13	1:A:1336:THR:N	2.21	0.56
1:A:1368:THR:HB	1:A:1381:SER:HA	1.87	0.56
1:B:2195:VAL:HG12	1:B:2234:ILE:HD11	1.87	0.56
1:A:1276:GLY:CA	1:A:1281:VAL:HG21	2.36	0.56
1:A:1215:VAL:HB	1:A:1221:ILE:HB	1.88	0.56
1:A:1179:LYS:HG3	1:B:2183:ASN:HD21	1.71	0.55
1:A:1352:HIS:HD2	1:A:1385:LYS:NZ	2.04	0.55
1:A:1276:GLY:HA3	1:A:1281:VAL:HG21	1.88	0.55
1:B:2233:GLU:O	1:B:2237:GLU:HG3	2.05	0.55
1:B:2130:VAL:O	1:B:2133:ILE:HG22	2.07	0.55
1:B:2248:MET:HE3	4:B:7410:HOH:O	2.06	0.55
1:B:2215:VAL:HB	1:B:2221:ILE:HB	1.87	0.55
1:A:1179:LYS:HB3	1:B:2179:LYS:HG2	1.88	0.55
1:A:1220:PHE:HB3	1:A:1364:GLY:HA3	1.87	0.55
1:B:2131:LEU:HD22	1:B:2156:MET:SD	2.47	0.55
1:B:2154:ALA:HB1	1:B:2156:MET:CE	2.35	0.54
1:A:1338:ARG:HH22	1:A:1416:GLU:HG3	1.72	0.54
1:A:1232:ARG:HH12	1:A:1267:ASP:CG	2.11	0.54
1:A:1349:GLU:OE2	1:A:1427:ARG:HD3	2.07	0.54
1:A:1146:PHE:CD1	1:A:1187:THR:HG23	2.41	0.54
1:B:2106:MET:HE3	1:B:2324:ARG:HH22	1.71	0.54
1:A:1165:VAL:HG12	1:A:1168:LEU:HD22	1.90	0.54
1:B:2381:SER:O	1:B:2383:LEU:HD12	2.08	0.54
1:A:1037:VAL:HG21	1:A:1390:HIS:CB	2.35	0.53
1:A:1142:LYS:HE2	1:A:1205:GLU:OE1	2.07	0.53
1:A:1130:VAL:HA	1:A:1133:ILE:HG22	1.91	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2349:GLU:CD	1:B:2427:ARG:HH11	2.12	0.53
1:B:2372:VAL:HA	1:B:2377:ASP:HB3	1.90	0.53
1:B:2111:VAL:HG11	1:B:2114:ILE:HD12	1.89	0.53
1:B:2037:VAL:HG23	1:B:2387:SER:CA	2.34	0.53
1:A:1134:MET:SD	1:A:1243:VAL:HG21	2.48	0.53
1:A:1054:ASP:HB3	1:A:1056:ASP:H	1.74	0.53
1:A:1117:VAL:HG12	1:A:1285:GLY:HA3	1.91	0.53
1:B:2108:ASN:OD1	1:B:2114:ILE:HG22	2.08	0.53
1:A:1167:THR:O	1:A:1167:THR:HG22	2.08	0.53
1:B:2222:VAL:HG13	1:B:2223:PRO:HD2	1.91	0.52
1:B:2008:LYS:HE3	1:B:2056:ASP:O	2.09	0.52
1:B:2190:ASN:HD21	1:B:2223:PRO:HA	1.73	0.52
1:B:2114:ILE:HG21	1:B:2117:VAL:HG13	1.92	0.52
1:B:2180:THR:HG21	4:B:7470:HOH:O	2.08	0.52
1:B:2040:GLN:HA	1:B:2040:GLN:HE21	1.73	0.52
1:A:1108:ASN:OD1	1:A:1114:ILE:HG22	2.10	0.51
1:B:2021:LYS:NZ	1:B:2021:LYS:HB3	2.25	0.51
1:A:1188:PRO:HB3	3:A:1:HOZ:N1	2.22	0.51
1:B:2146:PHE:CD1	1:B:2187:THR:HG23	2.45	0.51
1:B:2213:PRO:HB2	1:B:2258:VAL:CG1	2.40	0.51
1:B:2037:VAL:O	1:B:2037:VAL:HG22	2.11	0.51
1:A:1222:VAL:CG1	1:A:1223:PRO:HD2	2.40	0.51
1:B:2111:VAL:CG1	1:B:2114:ILE:HD12	2.41	0.51
1:B:2267:ASP:O	1:B:2268:LEU:HD12	2.10	0.51
1:A:1232:ARG:C	1:A:1232:ARG:HD3	2.31	0.50
1:B:2170:LEU:N	1:B:2170:LEU:HD22	2.27	0.50
1:B:2037:VAL:HG21	1:B:2390:HIS:CB	2.41	0.50
1:B:2383:LEU:N	1:B:2383:LEU:HD12	2.26	0.50
1:B:2042:ILE:H	1:B:2042:ILE:HD13	1.75	0.50
1:B:2338:ARG:NH1	1:B:2420:ASP:CG	2.65	0.50
1:A:1245:ASP:HA	1:A:1270:THR:OG1	2.11	0.50
1:B:2042:ILE:N	1:B:2042:ILE:HD13	2.27	0.49
1:B:2197:ALA:O	1:B:2201:GLU:HG3	2.11	0.49
1:A:1127:CYS:O	1:A:1130:VAL:HG12	2.12	0.49
1:A:1130:VAL:C	1:A:1133:ILE:HG22	2.33	0.49
1:A:1317:ILE:O	1:A:1321:GLU:HG3	2.12	0.49
1:A:1277:GLY:HA3	1:A:1315:ALA:HB1	1.93	0.49
1:B:2309:ASN:ND2	1:B:2311:LEU:HB2	2.28	0.49
1:B:2042:ILE:HD12	1:B:2394:LEU:HD21	1.93	0.49
1:B:2113:SER:OG	1:B:2269:THR:CG2	2.61	0.48
1:B:2185:LEU:HD12	1:B:2185:LEU:N	2.29	0.48
1:A:1179:LYS:HG3	1:B:2183:ASN:ND2	2.27	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1195:VAL:CG1	1:A:1234:ILE:HD12	2.44	0.48
1:A:1309:ASN:ND2	1:A:1311:LEU:HB2	2.24	0.48
1:B:2037:VAL:CG2	1:B:2390:HIS:HB3	2.43	0.48
1:A:1077:PRO:HA	1:A:1080:ILE:HG12	1.96	0.48
1:A:1054:ASP:OD1	1:A:1060:TYR:CE1	2.66	0.48
1:B:2372:VAL:HA	1:B:2377:ASP:CB	2.44	0.48
1:B:2145:LYS:O	1:B:2186:THR:HA	2.13	0.48
1:A:1309:ASN:HD21	1:A:1311:LEU:CB	2.25	0.48
1:A:1114:ILE:HG21	1:A:1117:VAL:HG13	1.96	0.48
1:A:1021:LYS:HB3	1:A:1021:LYS:HZ3	1.76	0.48
1:B:2127:CYS:O	1:B:2130:VAL:HG12	2.14	0.48
1:A:1309:ASN:ND2	1:A:1311:LEU:H	2.12	0.47
1:A:1074:HIS:HD2	4:B:7174:HOH:O	1.97	0.47
1:B:2195:VAL:HG12	1:B:2234:ILE:CD1	2.44	0.47
1:A:1296:PRO:HG3	1:B:2033:ALA:HB2	1.96	0.47
1:A:1145:LYS:O	1:A:1186:THR:HA	2.14	0.47
1:A:1113:SER:OG	1:A:1269:THR:CG2	2.63	0.47
1:A:1179:LYS:HG2	4:A:7358:HOH:O	2.15	0.47
1:A:1338:ARG:NH2	1:A:1416:GLU:CG	2.76	0.47
1:B:2195:VAL:CG1	1:B:2234:ILE:HD11	2.44	0.46
1:A:1352:HIS:HE1	1:A:1430:MET:O	1.99	0.46
1:B:2008:LYS:O	1:B:2008:LYS:HG3	2.16	0.46
1:B:2261:LYS:HE2	1:B:2359:VAL:HG13	1.98	0.46
1:B:2309:ASN:O	1:B:2313:MET:HG2	2.15	0.46
1:A:1349:GLU:CD	1:A:1427:ARG:HH11	2.19	0.46
1:B:2116:MET:HE3	1:B:2288:ARG:HD3	1.98	0.46
1:B:2134:MET:SD	1:B:2243:VAL:HG21	2.55	0.46
1:A:1230:GLY:O	1:A:1234:ILE:HG23	2.16	0.46
1:B:2077:PRO:HA	1:B:2080:ILE:HD11	1.98	0.46
1:A:1185:LEU:N	1:A:1185:LEU:CD1	2.79	0.46
1:A:1135:ARG:HD3	1:A:1141:ASP:O	2.16	0.46
1:A:1147:GLU:HG3	1:A:1161:ALA:HB3	1.97	0.46
1:A:1280:PRO:HB2	1:B:2280:PRO:HB2	1.98	0.46
1:A:1145:LYS:HG3	1:A:1186:THR:HG22	1.98	0.45
1:A:1267:ASP:O	1:A:1268:LEU:HD13	2.16	0.45
1:B:2114:ILE:CG2	1:B:2117:VAL:HG13	2.46	0.45
1:A:1054:ASP:CG	1:A:1058:ASN:HB2	2.37	0.45
1:B:2080:ILE:O	1:B:2084:LYS:HG3	2.17	0.45
1:B:2245:ASP:HA	1:B:2270:THR:OG1	2.17	0.45
1:B:2113:SER:O	1:B:2286:GLY:HA2	2.16	0.45
1:A:1167:THR:CG2	1:A:1167:THR:O	2.64	0.45
1:B:2224:ASP:OD1	1:B:2373:HIS:HD2	1.97	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1011:LYS:HB2	1:A:1055:VAL:HG13	1.99	0.45
1:A:1273:LYS:HE3	1:B:2305:THR:CG2	2.44	0.45
1:B:2200:ALA:O	1:B:2203:PRO:HD3	2.17	0.45
1:A:1197:ALA:O	1:A:1201:GLU:HG3	2.17	0.45
1:B:2011:LYS:CB	1:B:2055:VAL:HG13	2.45	0.45
1:A:1231:LEU:HA	1:A:1234:ILE:CD1	2.47	0.45
1:B:2103:LEU:HG	1:B:2317:ILE:HG13	1.99	0.44
1:B:2281:VAL:HG22	1:B:2282:GLY:N	2.32	0.44
1:A:1276:GLY:HA3	1:A:1281:VAL:CG2	2.47	0.44
1:A:1337:LYS:HG2	1:A:1341:ASP:OD2	2.18	0.44
1:B:2130:VAL:O	1:B:2133:ILE:CG2	2.65	0.44
1:B:2202:ASN:HB2	1:B:2206:ILE:HD11	2.00	0.44
1:A:1130:VAL:CA	1:A:1133:ILE:HG22	2.48	0.44
1:B:2130:VAL:CA	1:B:2133:ILE:HG22	2.47	0.44
1:B:2144:ILE:HB	1:B:2209:VAL:HG22	1.99	0.44
1:B:2131:LEU:HD13	1:B:2157:PHE:CZ	2.52	0.44
1:A:1177:PRO:O	1:A:1180:THR:HG23	2.17	0.44
1:A:1281:VAL:CG2	1:A:1312:ALA:HB1	2.47	0.44
1:A:1259:GLN:HE22	1:A:1269:THR:CG2	2.21	0.44
1:A:1305:THR:HG21	1:B:2273:LYS:NZ	2.33	0.44
1:A:1037:VAL:CG2	1:A:1390:HIS:HB3	2.39	0.44
1:B:2045:ASP:OD1	1:B:2046:ARG:NH1	2.51	0.43
1:A:1232:ARG:HD2	1:A:1236:LEU:CD1	2.49	0.43
1:A:1145:LYS:CG	1:A:1186:THR:HG22	2.48	0.43
1:A:1156:MET:H	1:A:1156:MET:CE	2.32	0.43
1:A:1391:ARG:HA	1:A:1391:ARG:HD2	1.86	0.43
1:B:2142:LYS:HB2	1:B:2205:GLU:O	2.17	0.43
1:A:1046:ARG:HB3	1:B:2089:LYS:HB3	2.01	0.43
1:A:1182:ALA:HB3	1:B:2179:LYS:HD3	2.01	0.43
1:B:2062:ASP:OD1	1:B:2074:HIS:HE1	2.01	0.43
1:B:2383:LEU:H	1:B:2383:LEU:HD12	1.83	0.43
1:A:1047:VAL:HG23	1:A:1074:HIS:HB3	2.00	0.43
1:A:1111:VAL:HA	1:A:1112:PRO:HD3	1.84	0.43
1:A:1033:ALA:HB2	1:B:2296:PRO:HG3	2.00	0.42
1:A:1276:GLY:HA2	1:A:1281:VAL:HG21	2.02	0.42
1:B:2111:VAL:HA	1:B:2112:PRO:HD3	1.74	0.42
1:A:1309:ASN:ND2	1:A:1311:LEU:N	2.67	0.42
1:B:2148:GLY:O	1:B:2218:SER:HB3	2.20	0.42
1:A:1213:PRO:HB2	1:A:1258:VAL:HG11	2.01	0.42
1:B:2037:VAL:HG21	1:B:2390:HIS:CG	2.53	0.42
1:B:2130:VAL:HA	1:B:2133:ILE:CG2	2.49	0.42
1:A:1179:LYS:HD3	1:B:2179:LYS:NZ	2.34	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1008:LYS:O	1:A:1008:LYS:HD2	2.20	0.42
1:B:2142:LYS:HD2	1:B:2205:GLU:HB3	2.00	0.42
1:A:1127:CYS:HA	1:A:1130:VAL:HG12	2.01	0.42
1:A:1042:ILE:HG21	1:A:1054:ASP:OD1	2.19	0.42
1:A:1054:ASP:HB2	1:A:1058:ASN:HB2	2.02	0.42
1:B:2391:ARG:HD2	1:B:2391:ARG:HA	1.69	0.42
1:A:1176:VAL:HG22	1:A:1176:VAL:O	2.20	0.42
1:B:2287:LYS:HB2	1:B:2289:GLU:HG2	2.02	0.42
1:A:1179:LYS:CB	1:B:2179:LYS:HG2	2.50	0.41
1:A:1279:LEU:HD21	1:A:1311:LEU:HB3	2.03	0.41
1:A:1220:PHE:CB	1:A:1364:GLY:HA3	2.49	0.41
1:A:1231:LEU:O	1:A:1234:ILE:HG12	2.20	0.41
1:A:1076:HIS:CE1	1:A:1078:GLU:HB2	2.54	0.41
1:B:2185:LEU:N	1:B:2185:LEU:CD1	2.84	0.41
1:B:2220:PHE:CB	1:B:2364:GLY:HA3	2.50	0.41
1:A:1179:LYS:CA	1:B:2179:LYS:HG2	2.50	0.41
1:A:1011:LYS:CB	1:A:1055:VAL:HG13	2.51	0.41
1:B:2276:GLY:HA3	1:B:2281:VAL:HG11	2.03	0.41
1:B:2425:ALA:O	1:B:2429:VAL:HG23	2.21	0.41
1:A:1417:GLU:OE2	1:A:1417:GLU:N	2.46	0.41
1:B:2232:ARG:NH1	1:B:2267:ASP:OD2	2.54	0.41
1:A:1065:GLY:O	1:A:1066:THR:HG22	2.20	0.41
1:A:1087:MET:HE3	1:B:2087:MET:HE1	2.03	0.40
1:A:1037:VAL:HG21	1:A:1390:HIS:CG	2.56	0.40
1:B:2047:VAL:HB	1:B:2074:HIS:CG	2.56	0.40
1:A:1233:GLU:O	1:A:1237:GLU:HG3	2.20	0.40
1:A:1188:PRO:CG	3:A:1:HOZ:HA	2.50	0.40
1:A:1083:LEU:HD13	1:B:2087:MET:HE2	2.03	0.40
1:A:1096:PRO:HD3	4:B:7102:HOH:O	2.21	0.40
1:A:1147:GLU:HG3	1:A:1161:ALA:CB	2.51	0.40
1:B:2099:LEU:HG	4:B:7167:HOH:O	2.21	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	425/432 (98%)	401 (94%)	22 (5%)	2 (0%)	38	38
1	B	416/432 (96%)	395 (95%)	21 (5%)	0	100	100
All	All	841/864 (97%)	796 (95%)	43 (5%)	2 (0%)	56	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1273	LYS
1	A	1112	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	330/335 (98%)	312 (94%)	18 (6%)	30	34
1	B	326/335 (97%)	311 (95%)	15 (5%)	37	43
All	All	656/670 (98%)	623 (95%)	33 (5%)	34	39

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1008	LYS
1	A	1021	LYS
1	A	1088	GLU
1	A	1103	LEU
1	A	1111	VAL
1	A	1117	VAL
1	A	1156	MET
1	A	1158	LEU
1	A	1176	VAL
1	A	1180	THR
1	A	1187	THR
1	A	1232	ARG
1	A	1241	LEU
1	A	1268	LEU
1	A	1269	THR

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Mol	Chain	Res	Type
1	A	1339	LEU
1	A	1343	LEU
1	A	1358	GLN
1	B	2042	ILE
1	B	2053	TRP
1	B	2059	ARG
1	B	2088	GLU
1	B	2103	LEU
1	B	2111	VAL
1	B	2117	VAL
1	B	2156	MET
1	B	2158	LEU
1	B	2176	VAL
1	B	2234	ILE
1	B	2241	LEU
1	B	2269	THR
1	B	2339	LEU
1	B	2358	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1058	ASN
1	A	1074	HIS
1	A	1190	ASN
1	A	1309	ASN
1	A	1352	HIS
1	A	1358	GLN
1	A	1373	HIS
1	B	2020	GLN
1	B	2040	GLN
1	B	2058	ASN
1	B	2074	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	2384	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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$
3	HOZ	A	1	-	8,8,8	1.32	1 (12%)	9,9,9	1.64	2 (22%)
2	PMP	A	5000	-	16,16,16	2.75	5 (31%)	23,23,23	1.49	5 (21%)
2	PMP	B	6000	-	16,16,16	2.69	5 (31%)	23,23,23	1.57	5 (21%)

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	HOZ	A	1	-	-	0/7/7/7	0/0/0/0
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	B	6000	PMP	C2-N1	8.70	1.50	1.33
2	A	5000	PMP	C2-N1	8.61	1.49	1.33
2	A	5000	PMP	C5-C4	3.42	1.45	1.40
2	A	5000	PMP	C3-C2	-3.11	1.38	1.40
2	B	6000	PMP	C5-C4	3.04	1.45	1.40
2	A	5000	PMP	P-O3P	-2.79	1.44	1.54
2	B	6000	PMP	C3-C2	-2.77	1.38	1.40
3	A	1	HOZ	CB-CA	2.76	1.57	1.53
2	B	6000	PMP	P-O3P	-2.59	1.45	1.54
2	A	5000	PMP	C2A-C2	2.19	1.54	1.50
2	B	6000	PMP	C2A-C2	2.10	1.54	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	HOZ	CG-CB-CA	3.48	119.56	112.93
2	B	6000	PMP	O3P-P-O4P	3.22	115.52	106.65
2	A	5000	PMP	O3P-P-O4P	2.80	114.36	106.65
3	A	1	HOZ	C-CA-N	2.66	118.85	111.70
2	A	5000	PMP	C3-C4-C5	2.33	121.22	118.74
2	A	5000	PMP	O4P-P-O1P	-2.32	99.91	106.71
2	B	6000	PMP	O4P-P-O1P	-2.30	99.96	106.71
2	B	6000	PMP	C3-C4-C5	2.26	121.14	118.74
2	A	5000	PMP	C5-C6-N1	-2.19	119.91	123.86
2	B	6000	PMP	C6-C5-C4	2.13	119.72	118.10
2	A	5000	PMP	C6-C5-C4	2.11	119.70	118.10
2	B	6000	PMP	C5-C6-N1	-2.07	120.13	123.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	427/432 (98%)	-0.40	2 (0%) 88 90	9, 16, 29, 37	0
1	B	420/432 (97%)	-0.33	5 (1%) 75 76	9, 16, 32, 49	0
All	All	847/864 (98%)	-0.37	7 (0%) 83 85	9, 16, 30, 49	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2161	ALA	3.6
1	B	2169	GLY	3.3
1	B	2170	LEU	3.3
1	B	2178	LYS	2.5
1	A	1369	GLU	2.1
1	A	1348	GLN	2.1
1	B	2179	LYS	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	HOZ	A	1	9/9	0.31	4.33	29,30,34,35	0
2	PMP	B	6000	16/16	0.13	1.93	13,18,26,28	0
2	PMP	A	5000	16/16	0.11	0.76	12,14,17,27	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.