



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2025 – 06:12 PM EDT

PDB ID : 2HP1  
Title : Inter-subunit signaling in GSAM  
Authors : Stetefeld, J.  
Deposited on : 2006-07-17  
Resolution : 2.08 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

<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>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

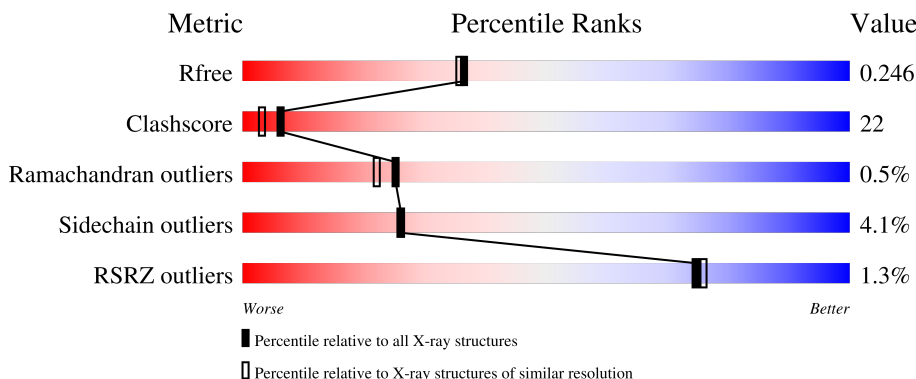
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.08 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))
$R_{free}$	164625	7574 (2.10-2.06)
Clashscore	180529	8325 (2.10-2.06)
Ramachandran outliers	177936	8271 (2.10-2.06)
Sidechain outliers	177891	8272 (2.10-2.06)
RSRZ outliers	164620	7574 (2.10-2.06)

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  $\geq 3$ , 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	432	<div> <div>0%</div> <div>71%</div> <div>25%</div> <div>• •</div> </div>
1	B	432	<div> <div>2%</div> <div>59%</div> <div>31%</div> <div>• 8%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6820 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.

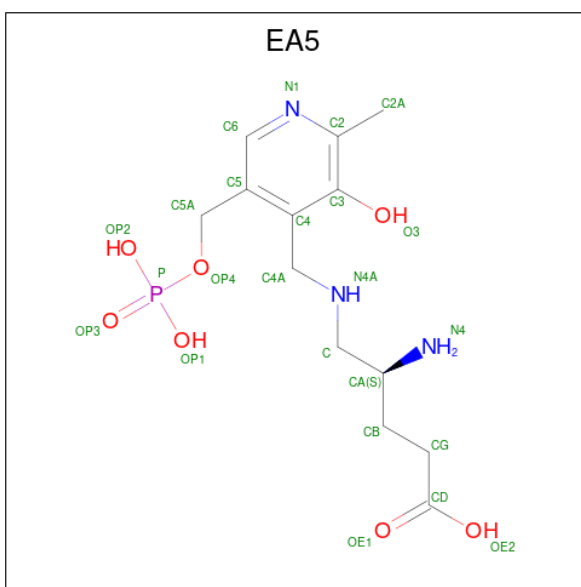
- Molecule 1 is a protein called Glutamate-1-semialdehyde 2,1-aminomutase (GSAM) plp-form.

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	398	Total	C	N	O	S	0	0	0
			3007	1918	503	568	18			

There are 12 discrepancies between the modelled and reference sequences:

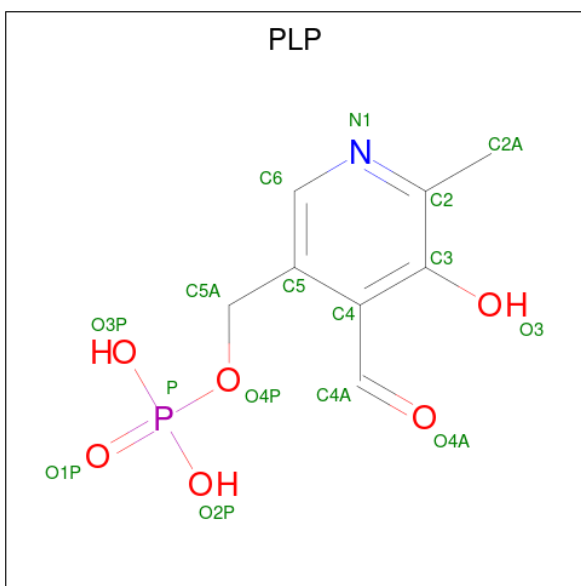
Chain	Residue	Modelled	Actual	Comment	Reference
A	1108	ASN	ILE	conflict	UNP P24630
A	1133	ILE	LEU	conflict	UNP P24630
A	1172	SER	ASP	conflict	UNP P24630
A	1179	LYS	SER	conflict	UNP P24630
A	1187	THR	ALA	conflict	UNP P24630
A	1327	GLY	ALA	conflict	UNP P24630
B	2108	ASN	ILE	conflict	UNP P24630
B	2133	ILE	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 (4S)-4-AMINO-5-[(3-HYDROXY-2-METHYL-5-[(PHOSPHONOOXY)METHYL]PYRIDIN-4-YL}METHYL)AMINO]PENTANOIC ACID (three-letter code: EA5) (formula: C<sub>13</sub>H<sub>22</sub>N<sub>3</sub>O<sub>7</sub>P).



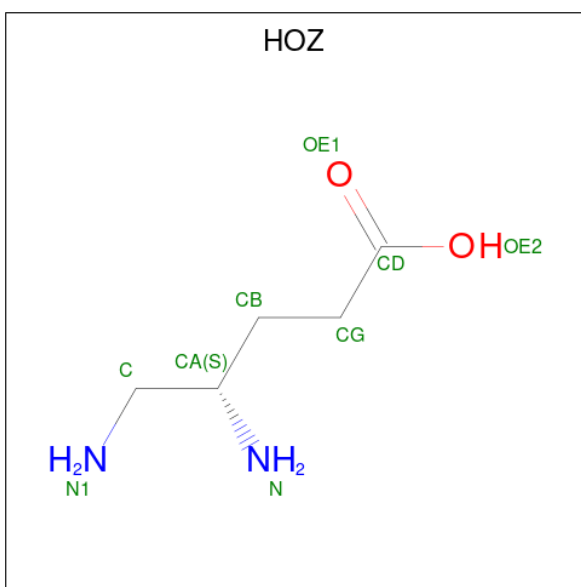
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			24	13	3	7	1		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is (4S)-4,5-DIAMINOPENTANOIC ACID (three-letter code: HOZ) (formula:  $C_5H_{12}N_2O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	305	Total	O	0	0
			305	305		
5	B	258	Total	O	0	0
			258	258		

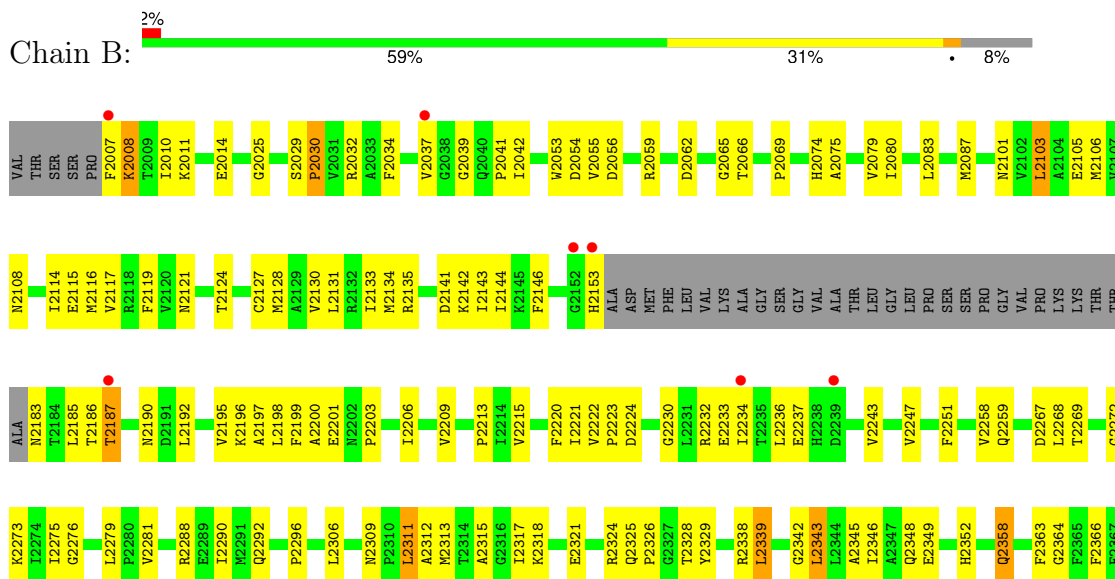
### 3 Residue-property plots

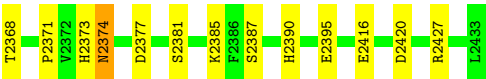
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 (GSAM) plp-form



- Molecule 1: Glutamate-1-semialdehyde 2,1-aminomutase (GSAM) plp-form





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.48Å 106.98Å 119.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.52 – 2.08 22.52 – 2.08	Depositor EDS
% Data completeness (in resolution range)	90.7 (22.52-2.08) 90.7 (22.52-2.08)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.08Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.201 , 0.254 0.196 , 0.246	Depositor DCC
$R_{free}$ test set	4730 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.7	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 51.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6820	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PLP, HOZ, EA5

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	0.32	0/3071	0.61	0/4156
All	All	0.32	0/6342	0.61	1/8586 (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	-5.17	97.05	111.00

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	3182	130	0
1	B	3007	0	2969	145	0
2	A	24	0	19	7	0
3	B	15	0	7	0	0
4	B	9	0	11	3	0
5	A	305	0	0	4	0
5	B	258	0	0	3	0
All	All	6820	0	6188	273	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 22.

All (273) 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)
2:A:5000:EA5:HA	5:A:7266:HOH:O	1.16	1.26
1:A:1131:LEU:HA	1:A:1134:MET:HE2	1.37	1.06
1:B:2131:LEU:HA	1:B:2134:MET:HE3	1.45	0.98
1:B:2131:LEU:HD12	1:B:2143:ILE:HD13	1.44	0.97
1:B:2259:GLN:HE22	1:B:2269:THR:HG21	1.29	0.97
1:A:1008:LYS:H	1:A:1008:LYS:HD3	1.41	0.84
1:A:1338:ARG:HH21	1:A:1416:GLU:HG3	1.42	0.84
1:A:1273:LYS:HZ1	2:A:5000:EA5:H2	1.42	0.84
1:B:2190:ASN:HD21	1:B:2224:ASP:H	1.20	0.83
1:A:1273:LYS:NZ	2:A:5000:EA5:H2	1.96	0.81
1:A:1213:PRO:HB2	1:A:1258:VAL:HG11	1.60	0.81
1:B:2190:ASN:ND2	1:B:2224:ASP:H	1.78	0.80
1:A:1259:GLN:HE22	1:A:1269:THR:HG21	1.47	0.78
1:A:1067:TRP:HZ3	1:A:1406:GLU:HG3	1.48	0.78
1:A:1281:VAL:CG2	1:A:1312:ALA:HB1	2.16	0.75
1:A:1130:VAL:HA	1:A:1133:ILE:HG22	1.68	0.74
1:B:2197:ALA:O	1:B:2201:GLU:HG3	1.86	0.74
1:B:2374:ASN:ND2	1:B:2377:ASP:H	1.83	0.74
1:B:2053:TRP:CE2	1:B:2059:ARG:HG3	2.23	0.74
1:B:2008:LYS:H	1:B:2008:LYS:HD3	1.54	0.73
1:B:2114:ILE:HG21	1:B:2117:VAL:HG22	1.70	0.73
1:A:1114:ILE:CG2	1:A:1117:VAL:HG13	2.18	0.73
1:B:2106:MET:CE	1:B:2324:ARG:HH22	2.02	0.73
1:B:2037:VAL:HG13	1:B:2387:SER:HA	1.70	0.72
1:B:2144:ILE:HB	1:B:2209:VAL:HG22	1.73	0.71
1:B:2114:ILE:CG2	1:B:2117:VAL:HG22	2.21	0.71
1:B:2131:LEU:HD13	1:B:2134:MET:HE1	1.73	0.70
1:A:1281:VAL:HG22	1:A:1312:ALA:HB1	1.72	0.70
1:A:1114:ILE:HG21	1:A:1117:VAL:HG13	1.74	0.69
1:A:1338:ARG:NH2	1:A:1416:GLU:HG3	2.07	0.69
1:B:2131:LEU:HD13	1:B:2134:MET:CE	2.22	0.69
1:A:1034:PHE:HB2	1:A:1041:PRO:HG3	1.74	0.68
1:A:1379:LYS:NZ	1:A:1379:LYS:HB3	2.07	0.68
1:A:1040:GLN:HE21	1:A:1040:GLN:HA	1.60	0.67
1:B:2037:VAL:HG12	1:B:2037:VAL:O	1.94	0.67
1:A:1374:ASN:ND2	1:A:1377:ASP:H	1.93	0.67
1:B:2275:ILE:HD13	1:B:2281:VAL:HG12	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1232:ARG:O	1:A:1232:ARG:HD3	1.95	0.66
1:B:2131:LEU:HD12	1:B:2143:ILE:CD1	2.24	0.66
1:B:2131:LEU:CD1	1:B:2143:ILE:HD13	2.24	0.66
1:B:2115:GLU:HB3	1:B:2288:ARG:HH22	1.59	0.66
1:B:2338:ARG:NH2	1:B:2416:GLU:HG3	2.12	0.65
1:B:2101:ASN:O	1:B:2105:GLU:HG3	1.97	0.65
1:A:1190:ASN:HD21	1:A:1224:ASP:H	1.43	0.64
1:B:2213:PRO:HB2	1:B:2258:VAL:HG11	1.79	0.64
1:B:2272:GLY:HA2	1:B:2275:ILE:HD11	1.79	0.64
1:B:2130:VAL:O	1:B:2133:ILE:HG22	1.97	0.64
1:B:2374:ASN:C	1:B:2374:ASN:HD22	2.00	0.64
1:B:2127:CYS:O	1:B:2131:LEU:HD23	1.97	0.64
1:A:1140:ARG:HD2	1:A:1206:ILE:O	1.98	0.63
1:B:2037:VAL:HG11	1:B:2390:HIS:HB3	1.81	0.63
1:A:1318:LYS:HA	1:A:1318:LYS:HE3	1.80	0.63
1:A:1213:PRO:HB2	1:A:1258:VAL:CG1	2.28	0.63
1:A:1374:ASN:C	1:A:1374:ASN:HD22	2.03	0.62
1:B:2281:VAL:CG2	1:B:2312:ALA:HB1	2.28	0.62
1:B:2281:VAL:HG22	1:B:2312:ALA:HB1	1.81	0.62
1:B:2195:VAL:HG12	1:B:2234:ILE:HD13	1.81	0.62
1:B:2079:VAL:HA	1:B:2318:LYS:HG2	1.81	0.62
1:A:1339:LEU:HD23	1:A:1343:LEU:HD13	1.82	0.62
1:B:2288:ARG:NH2	1:B:2288:ARG:HB2	2.15	0.62
1:A:1040:GLN:HA	1:A:1040:GLN:NE2	2.15	0.61
1:A:1079:VAL:HA	1:A:1318:LYS:HG2	1.81	0.61
1:B:2268:LEU:HD11	1:B:2290:ILE:HG21	1.82	0.61
1:A:1031:VAL:HG22	1:A:1067:TRP:CH2	2.36	0.61
1:A:1130:VAL:O	1:A:1134:MET:HG3	2.00	0.61
1:B:2309:ASN:ND2	1:B:2312:ALA:H	1.99	0.61
1:A:1083:LEU:HD22	1:A:1311:LEU:HD22	1.83	0.61
1:A:1190:ASN:ND2	1:A:1224:ASP:H	1.99	0.61
1:A:1008:LYS:H	1:A:1008:LYS:CD	2.11	0.60
1:B:2288:ARG:O	1:B:2292:GLN:HG2	2.00	0.60
1:A:1103:LEU:HD13	1:A:1119:PHE:CE2	2.36	0.60
1:A:1230:GLY:O	1:A:1234:ILE:HG23	2.01	0.60
1:A:1375:TYR:O	1:A:1379:LYS:HG3	2.02	0.59
1:A:1130:VAL:O	1:A:1133:ILE:HG22	2.03	0.59
1:B:2190:ASN:HD21	1:B:2224:ASP:N	1.95	0.59
1:B:2317:ILE:O	1:B:2321:GLU:HG3	2.02	0.59
1:B:2338:ARG:NH1	1:B:2420:ASP:OD1	2.34	0.59
1:B:2106:MET:HE3	1:B:2324:ARG:HH22	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1197:ALA:O	1:A:1201:GLU:HG3	2.04	0.58
1:B:2222:VAL:CG1	1:B:2223:PRO:HD2	2.34	0.58
1:A:1272:GLY:HA2	1:A:1275:ILE:HD11	1.86	0.58
1:B:2279:LEU:HD21	1:B:2311:LEU:HD13	1.84	0.58
1:A:1309:ASN:ND2	1:A:1312:ALA:H	2.01	0.57
1:A:1042:ILE:HD11	1:A:1399:TYR:CE1	2.38	0.57
1:A:1033:ALA:O	1:A:1034:PHE:HB2	2.03	0.57
1:A:1130:VAL:HA	1:A:1133:ILE:CG2	2.35	0.57
1:A:1222:VAL:HG13	1:A:1223:PRO:HD2	1.85	0.57
1:A:1158:LEU:HD13	1:A:1173:SER:HB3	1.86	0.57
1:B:2130:VAL:HA	1:B:2133:ILE:HG22	1.85	0.57
1:B:2232:ARG:O	1:B:2232:ARG:HD3	2.03	0.57
1:A:1130:VAL:CA	1:A:1133:ILE:HG22	2.33	0.56
1:A:1039:GLY:O	1:A:1040:GLN:HB2	2.06	0.56
1:A:1379:LYS:HB3	1:A:1379:LYS:HZ2	1.68	0.56
1:A:1037:VAL:HG21	1:A:1390:HIS:CG	2.40	0.56
1:A:1296:PRO:HD3	1:B:2030:PRO:HA	1.88	0.56
1:B:2318:LYS:HA	1:B:2318:LYS:HE3	1.88	0.55
1:B:2230:GLY:O	1:B:2234:ILE:HG22	2.06	0.55
1:B:2259:GLN:NE2	1:B:2269:THR:HG21	2.12	0.55
1:A:1127:CYS:O	1:A:1130:VAL:HG12	2.06	0.55
1:B:2054:ASP:HB3	1:B:2056:ASP:H	1.71	0.55
1:B:2232:ARG:HH12	1:B:2267:ASP:CG	2.09	0.55
1:B:2368:THR:HB	1:B:2381:SER:HA	1.88	0.55
1:A:1185:LEU:HD12	1:A:1185:LEU:N	2.21	0.54
1:B:2288:ARG:HD3	5:B:7350:HOH:O	2.06	0.54
1:B:2371:PRO:HG2	1:B:2373:HIS:HE1	1.72	0.54
1:A:1114:ILE:HG21	1:A:1117:VAL:CG1	2.37	0.54
1:B:2011:LYS:HE2	1:B:2011:LYS:HA	1.88	0.54
1:B:2324:ARG:HH21	1:B:2324:ARG:HG3	1.73	0.54
1:B:2124:THR:O	1:B:2128:MET:HG3	2.08	0.53
1:B:2259:GLN:HE22	1:B:2269:THR:CG2	2.12	0.53
1:A:1037:VAL:HG21	1:A:1390:HIS:ND1	2.23	0.53
1:B:2325:GLN:HB3	1:B:2326:PRO:HD2	1.91	0.53
1:B:2083:LEU:O	1:B:2087:MET:HG2	2.08	0.53
1:B:2066:THR:HG23	1:B:2069:PRO:HD2	1.90	0.53
1:A:1011:LYS:HE2	1:A:1011:LYS:HA	1.89	0.53
1:B:2267:ASP:O	1:B:2268:LEU:HD12	2.08	0.53
1:A:1031:VAL:HG23	5:A:7122:HOH:O	2.08	0.52
1:A:1179:LYS:HD2	1:B:2183:ASN:ND2	2.23	0.52
1:A:1195:VAL:HG12	1:A:1234:ILE:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1011:LYS:HB2	1:A:1055:VAL:HG23	1.91	0.52
1:A:1391:ARG:HG2	1:A:1391:ARG:HH11	1.75	0.52
1:A:1275:ILE:HD12	1:A:1276:GLY:N	2.26	0.51
1:B:2029:SER:HB3	4:B:2:HOZ:OE1	2.11	0.51
1:B:2213:PRO:HB2	1:B:2258:VAL:CG1	2.40	0.51
1:B:2215:VAL:HB	1:B:2221:ILE:HB	1.91	0.51
1:B:2146:PHE:CD1	1:B:2187:THR:HG23	2.46	0.51
1:A:1328:THR:HG23	1:A:1412:LEU:HD21	1.91	0.51
1:A:1195:VAL:CG1	1:A:1234:ILE:HD11	2.41	0.51
1:B:2075:ALA:HB1	1:B:2080:ILE:HD11	1.91	0.51
1:A:1042:ILE:HD11	1:A:1399:TYR:CD1	2.46	0.50
1:A:1113:SER:OG	1:A:1269:THR:CG2	2.58	0.50
5:A:7134:HOH:O	1:B:2074:HIS:HD2	1.93	0.50
1:A:1074:HIS:HD2	5:B:7050:HOH:O	1.95	0.50
1:B:2062:ASP:OD1	1:B:2074:HIS:HE1	1.94	0.50
1:B:2032:ARG:HE	4:B:2:HOZ:CD	2.25	0.50
1:A:1251:PHE:CE1	1:A:1275:ILE:HG23	2.47	0.50
1:A:1145:LYS:HE2	1:A:1146:PHE:O	2.13	0.49
1:B:2251:PHE:CE1	1:B:2275:ILE:HG23	2.47	0.49
1:A:1075:ALA:HB1	1:A:1080:ILE:HD11	1.94	0.49
1:B:2192:LEU:O	1:B:2196:LYS:HG2	2.12	0.49
1:A:1222:VAL:CG1	1:A:1223:PRO:HD2	2.42	0.49
1:A:1232:ARG:NH1	1:A:1242:LEU:HB3	2.26	0.49
1:A:1339:LEU:HD23	1:A:1339:LEU:O	2.12	0.49
1:A:1349:GLU:OE2	1:A:1427:ARG:NH1	2.45	0.49
1:B:2083:LEU:HD22	1:B:2311:LEU:HD22	1.94	0.49
1:B:2131:LEU:HD13	1:B:2134:MET:HE3	1.95	0.49
1:B:2247:VAL:HG13	1:B:2272:GLY:HA3	1.95	0.49
1:B:2366:PHE:HB3	1:B:2368:THR:HG22	1.95	0.49
1:A:1232:ARG:HH12	1:A:1267:ASP:CG	2.16	0.49
1:B:2034:PHE:HB2	1:B:2041:PRO:HG3	1.95	0.49
1:B:2103:LEU:HB3	1:B:2119:PHE:CZ	2.48	0.48
1:A:1275:ILE:HD13	1:A:1281:VAL:HG12	1.94	0.48
1:A:1345:ALA:O	1:A:1349:GLU:HG3	2.14	0.48
1:B:2135:ARG:HD3	1:B:2141:ASP:O	2.13	0.48
1:B:2325:GLN:HG3	5:B:7334:HOH:O	2.13	0.48
1:B:2374:ASN:HD22	1:B:2377:ASP:H	1.59	0.48
1:A:1067:TRP:CE3	2:A:5000:EA5:HB1	2.48	0.48
1:A:1130:VAL:C	1:A:1133:ILE:HG22	2.33	0.48
1:A:1189:TYR:O	1:A:1190:ASN:HB2	2.14	0.48
1:A:1339:LEU:O	1:A:1343:LEU:HD13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1037:VAL:HG23	1:A:1390:HIS:HB3	1.95	0.48
1:A:1037:VAL:O	1:A:1037:VAL:HG22	2.13	0.48
1:A:1065:GLY:O	1:A:1066:THR:HG22	2.13	0.48
1:A:1273:LYS:HZ1	2:A:5000:EA5:C	2.18	0.48
1:A:1339:LEU:HD23	1:A:1339:LEU:C	2.34	0.48
1:A:1031:VAL:HG11	2:A:5000:EA5:HG2	1.95	0.47
1:A:1134:MET:SD	1:A:1243:VAL:HG21	2.54	0.47
1:A:1187:THR:HG21	1:A:1195:VAL:HG22	1.95	0.47
1:A:1030:PRO:HA	1:B:2296:PRO:HD3	1.96	0.47
1:B:2065:GLY:O	1:B:2066:THR:HG22	2.15	0.47
1:A:1190:ASN:HD21	1:A:1223:PRO:HA	1.79	0.47
1:B:2313:MET:O	1:B:2317:ILE:HG13	2.14	0.47
1:A:1064:VAL:HG12	1:A:1067:TRP:H	1.79	0.47
1:B:2339:LEU:HD22	1:B:2343:LEU:HD22	1.96	0.47
1:B:2352:HIS:HD2	1:B:2385:LYS:NZ	2.12	0.47
1:B:2338:ARG:HH22	1:B:2416:GLU:HG3	1.80	0.47
1:A:1309:ASN:HD21	1:A:1312:ALA:H	1.61	0.47
1:B:2010:ILE:O	1:B:2014:GLU:HG3	2.14	0.47
1:A:1146:PHE:CD1	1:A:1187:THR:HG23	2.50	0.47
1:B:2130:VAL:C	1:B:2133:ILE:HG22	2.36	0.46
1:B:2232:ARG:HD3	1:B:2232:ARG:C	2.35	0.46
1:B:2349:GLU:OE2	1:B:2427:ARG:NH1	2.48	0.46
1:B:2222:VAL:HG13	1:B:2223:PRO:HD2	1.97	0.46
1:B:2358:GLN:HB3	1:B:2363:PHE:HB3	1.98	0.46
1:A:1177:PRO:HB2	1:A:1180:THR:HG23	1.97	0.46
1:A:1391:ARG:HG2	1:A:1391:ARG:NH1	2.30	0.46
1:A:1296:PRO:HG2	1:B:2025:GLY:HA3	1.97	0.46
1:A:1368:THR:HB	1:A:1381:SER:HA	1.97	0.46
1:B:2134:MET:SD	1:B:2243:VAL:HG21	2.55	0.46
1:A:1142:LYS:HD3	1:A:1185:LEU:HD11	1.97	0.46
1:B:2053:TRP:NE1	1:B:2059:ARG:HG3	2.30	0.46
1:B:2275:ILE:HD11	1:B:2281:VAL:O	2.16	0.46
1:A:1037:VAL:CG2	1:A:1390:HIS:HB3	2.45	0.45
1:A:1083:LEU:HD22	1:A:1311:LEU:CD2	2.46	0.45
1:A:1215:VAL:HB	1:A:1221:ILE:HB	1.98	0.45
1:B:2371:PRO:HG2	1:B:2373:HIS:CE1	2.51	0.45
1:B:2374:ASN:HD21	1:B:2377:ASP:H	1.61	0.45
1:A:1224:ASP:OD1	1:A:1373:HIS:HD2	1.99	0.45
1:A:1374:ASN:HD22	1:A:1377:ASP:H	1.63	0.45
1:B:2220:PHE:HB3	1:B:2364:GLY:HA3	1.99	0.45
1:B:2275:ILE:HD12	1:B:2276:GLY:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2108:ASN:OD1	1:B:2114:ILE:HG22	2.16	0.45
1:A:1062:ASP:OD1	1:A:1074:HIS:HE1	1.99	0.44
1:B:2039:GLY:O	1:B:2041:PRO:HD3	2.18	0.44
1:B:2222:VAL:HG12	1:B:2223:PRO:HD2	1.99	0.44
1:B:2103:LEU:HD13	1:B:2119:PHE:CE2	2.53	0.44
1:B:2309:ASN:O	1:B:2313:MET:HG2	2.18	0.44
1:A:1114:ILE:HG23	1:A:1117:VAL:HG13	1.98	0.44
1:A:1232:ARG:HD3	1:A:1232:ARG:C	2.33	0.44
1:A:1131:LEU:HD23	1:A:1134:MET:CE	2.47	0.44
1:A:1143:ILE:CG2	1:A:1144:ILE:N	2.79	0.44
1:B:2130:VAL:HA	1:B:2133:ILE:CG2	2.48	0.44
1:A:1131:LEU:HA	1:A:1134:MET:CE	2.27	0.44
1:A:1425:ALA:O	1:A:1429:VAL:HG23	2.17	0.44
1:B:2233:GLU:O	1:B:2237:GLU:HB2	2.18	0.44
1:B:2127:CYS:O	1:B:2131:LEU:CD2	2.63	0.43
1:A:1042:ILE:HB	1:A:1054:ASP:OD1	2.18	0.43
1:B:2008:LYS:H	1:B:2008:LYS:CD	2.29	0.43
1:A:1008:LYS:HD3	1:A:1008:LYS:N	2.20	0.43
1:A:1190:ASN:HD22	1:A:1190:ASN:HA	1.67	0.43
2:A:5000:EA5:CA	5:A:7266:HOH:O	2.02	0.43
1:A:1029:SER:HA	1:A:1030:PRO:HD3	1.83	0.43
1:B:2142:LYS:HD2	1:B:2185:LEU:HD21	1.99	0.43
1:B:2232:ARG:HD2	1:B:2236:LEU:HG	2.00	0.43
1:B:2288:ARG:HB2	1:B:2288:ARG:CZ	2.48	0.43
1:B:2324:ARG:HG3	1:B:2324:ARG:NH2	2.32	0.43
1:B:2358:GLN:HB3	1:B:2363:PHE:CB	2.49	0.43
1:A:1232:ARG:HH11	1:A:1266:PRO:HA	1.84	0.43
1:B:2115:GLU:HB3	1:B:2288:ARG:NH2	2.31	0.43
1:B:2133:ILE:HG23	1:B:2134:MET:N	2.33	0.43
1:A:1054:ASP:HB3	1:A:1056:ASP:H	1.84	0.43
1:A:1281:VAL:HG12	1:A:1282:GLY:N	2.34	0.43
1:A:1309:ASN:O	1:A:1313:MET:HG2	2.18	0.43
1:B:2042:ILE:O	1:B:2042:ILE:HG13	2.19	0.43
1:A:1220:PHE:HB3	1:A:1364:GLY:HA3	2.00	0.42
1:A:1404:GLN:O	1:A:1404:GLN:HG3	2.18	0.42
1:A:1195:VAL:HG12	1:A:1234:ILE:CD1	2.49	0.42
1:B:2116:MET:CE	1:B:2292:GLN:HE22	2.33	0.42
1:B:2142:LYS:HB2	1:B:2206:ILE:HD13	2.00	0.42
1:B:2195:VAL:HG12	1:B:2234:ILE:CD1	2.49	0.42
1:B:2196:LYS:HD3	1:B:2234:ILE:HD12	2.01	0.42
1:B:2328:THR:HG22	1:B:2329:TYR:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2345:ALA:O	1:B:2349:GLU:HG3	2.19	0.42
1:B:2011:LYS:HB2	1:B:2055:VAL:HG23	2.00	0.42
1:A:1185:LEU:N	1:A:1185:LEU:CD1	2.82	0.42
1:A:1343:LEU:HB3	1:A:1365:PHE:CE1	2.55	0.42
1:B:2121:ASN:HD21	1:B:2306:LEU:C	2.23	0.42
1:B:2130:VAL:CA	1:B:2133:ILE:HG22	2.48	0.42
1:B:2186:THR:O	1:B:2198:LEU:HD11	2.19	0.42
1:B:2083:LEU:HD21	1:B:2315:ALA:HB2	2.02	0.41
1:B:2345:ALA:O	1:B:2348:GLN:HB3	2.20	0.41
1:B:2007:PHE:CD2	1:B:2395:GLU:HG2	2.56	0.41
1:B:2037:VAL:HG11	1:B:2390:HIS:CB	2.48	0.41
1:B:2106:MET:HE2	1:B:2324:ARG:HH22	1.83	0.41
1:B:2309:ASN:HD21	1:B:2312:ALA:H	1.68	0.41
1:A:1042:ILE:CD1	1:A:1394:LEU:HD11	2.50	0.41
1:B:2127:CYS:HA	1:B:2130:VAL:HG12	2.03	0.41
1:B:2232:ARG:HD2	1:B:2236:LEU:CD1	2.51	0.41
1:B:2032:ARG:HG3	4:B:2:HOZ:OE1	2.21	0.41
1:B:2342:GLY:O	1:B:2346:ILE:HG13	2.20	0.41
1:A:1159:VAL:HG12	1:A:1186:THR:HG21	2.02	0.41
1:A:1067:TRP:CZ3	1:A:1406:GLU:HG3	2.39	0.41
1:B:2037:VAL:CG1	1:B:2390:HIS:HB3	2.48	0.41
1:B:2374:ASN:ND2	1:B:2374:ASN:C	2.70	0.41
1:A:1244:PHE:O	1:A:1269:THR:HA	2.20	0.40
1:A:1251:PHE:CE1	1:A:1275:ILE:CG2	3.04	0.40
1:B:2037:VAL:HG11	1:B:2390:HIS:CG	2.56	0.40
1:B:2213:PRO:HB2	1:B:2258:VAL:CB	2.51	0.40
1:A:1039:GLY:O	1:A:1040:GLN:CB	2.66	0.40
1:A:1213:PRO:HG2	1:A:1258:VAL:HG21	2.03	0.40
1:A:1131:LEU:HD11	1:A:1156:MET:HB2	2.02	0.40
1:B:2199:PHE:CD1	1:B:2234:ILE:HD11	2.56	0.40
1:B:2200:ALA:O	1:B:2203:PRO:HD3	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%)	404 (95%)	19 (4%)	2 (0%)	25	22
1	B	394/432 (91%)	373 (95%)	19 (5%)	2 (0%)	25	22
All	All	819/864 (95%)	777 (95%)	38 (5%)	4 (0%)	25	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2273	LYS
1	A	1273	LYS
1	A	1040	GLN
1	B	2030	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%)	313 (95%)	17 (5%)	19	17
1	B	309/335 (92%)	300 (97%)	9 (3%)	37	40
All	All	639/670 (95%)	613 (96%)	26 (4%)	26	26

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1008	LYS
1	A	1059	ARG
1	A	1103	LEU
1	A	1117	VAL
1	A	1131	LEU
1	A	1141	ASP
1	A	1170	LEU
1	A	1179	LYS
1	A	1187	THR

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Mol	Chain	Res	Type
1	A	1190	ASN
1	A	1234	ILE
1	A	1268	LEU
1	A	1269	THR
1	A	1311	LEU
1	A	1358	GLN
1	A	1374	ASN
1	A	1391	ARG
1	B	2008	LYS
1	B	2103	LEU
1	B	2153	HIS
1	B	2187	THR
1	B	2311	LEU
1	B	2339	LEU
1	B	2343	LEU
1	B	2358	GLN
1	B	2374	ASN

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	1040	GLN
1	A	1058	ASN
1	A	1074	HIS
1	A	1121	ASN
1	A	1190	ASN
1	A	1309	ASN
1	A	1352	HIS
1	A	1358	GLN
1	A	1373	HIS
1	A	1374	ASN
1	B	2058	ASN
1	B	2074	HIS
1	B	2121	ASN
1	B	2183	ASN
1	B	2190	ASN
1	B	2217	ASN
1	B	2259	GLN
1	B	2292	GLN
1	B	2309	ASN
1	B	2352	HIS
1	B	2373	HIS

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Mol	Chain	Res	Type
1	B	2374	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides 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	PLP	B	6000	1	15,15,16	1.32	2 (13%)	21,22,23	1.17	3 (14%)
4	HOZ	B	2	-	8,8,8	1.16	0	9,9,9	1.34	2 (22%)
2	EA5	A	5000	-	24,24,24	1.57	5 (20%)	30,33,33	1.98	6 (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
3	PLP	B	6000	1	-	0/6/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HOZ	B	2	-	-	4/7/7/7	-
2	EA5	A	5000	-	-	7/17/17/17	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5000	EA5	C2-N1	3.35	1.39	1.33
3	B	6000	PLP	C3-C2	-2.70	1.38	1.41
2	A	5000	EA5	CB-CA	2.69	1.57	1.53
2	A	5000	EA5	C2A-C2	2.48	1.54	1.50
2	A	5000	EA5	C-CA	2.23	1.55	1.53
2	A	5000	EA5	C4A-N4A	-2.12	1.36	1.45
3	B	6000	PLP	C2-N1	2.07	1.37	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5000	EA5	C4-C4A-N4A	6.37	123.26	111.50
2	A	5000	EA5	OP2-P-OP3	-4.11	94.83	110.83
2	A	5000	EA5	C6-C5-C4	3.17	120.46	118.06
2	A	5000	EA5	OP1-P-OP3	2.91	122.17	110.83
2	A	5000	EA5	C5-C6-N1	-2.84	119.20	123.83
2	A	5000	EA5	CG-CB-CA	2.68	118.60	112.87
4	B	2	HOZ	CG-CB-CA	2.44	118.07	112.87
3	B	6000	PLP	O3P-P-O1P	2.38	120.11	110.83
4	B	2	HOZ	CB-CA-C	2.20	113.35	109.50
3	B	6000	PLP	C5-C6-N1	-2.18	120.29	123.83
3	B	6000	PLP	C6-C5-C4	2.01	119.74	118.10

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5000	EA5	C5-C4-C4A-N4A
2	A	5000	EA5	C-CA-CB-CG
2	A	5000	EA5	N4A-C-CA-N4
2	A	5000	EA5	N4A-C-CA-CB
2	A	5000	EA5	CA-CB-CG-CD
2	A	5000	EA5	C3-C4-C4A-N4A
4	B	2	HOZ	OE2-CD-CG-CB
4	B	2	HOZ	OE1-CD-CG-CB

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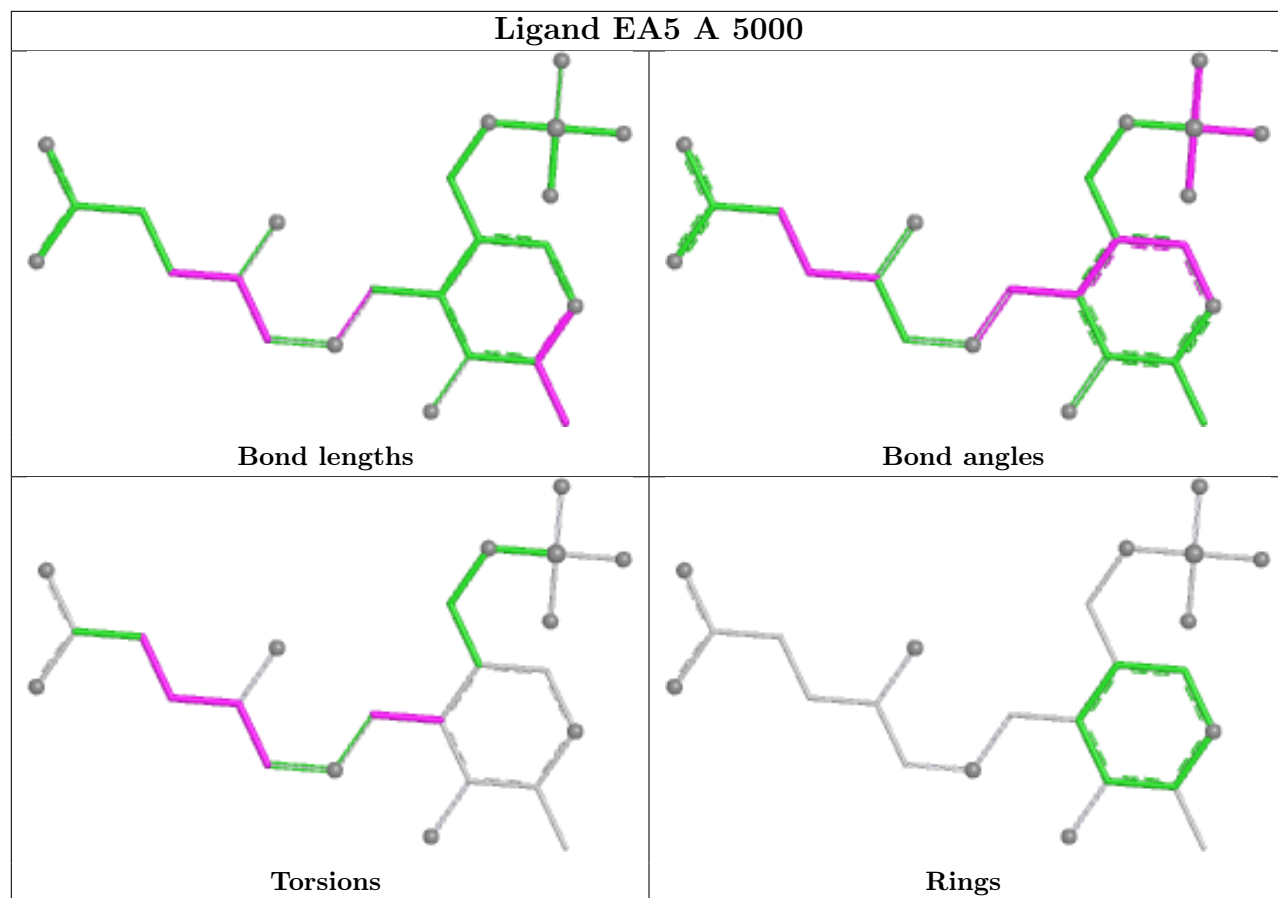
Mol	Chain	Res	Type	Atoms
4	B	2	HOZ	C-CA-CB-CG
2	A	5000	EA5	N4-CA-CB-CG
4	B	2	HOZ	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2	HOZ	3	0
2	A	5000	EA5	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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	427/432 (98%)	-0.16	4 (0%) 81 82	14, 26, 40, 49	0
1	B	398/432 (92%)	-0.17	7 (1%) 67 69	14, 26, 42, 54	0
All	All	825/864 (95%)	-0.16	11 (1%) 74 76	14, 26, 41, 54	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2153	HIS	3.8
1	A	1038	GLY	3.5
1	A	1187	THR	3.3
1	B	2187	THR	3.2
1	B	2152	GLY	2.5
1	B	2239	ASP	2.4
1	B	2234	ILE	2.4
1	B	2037	VAL	2.3
1	A	1037	VAL	2.2
1	A	1054	ASP	2.1
1	B	2007	PHE	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](#)

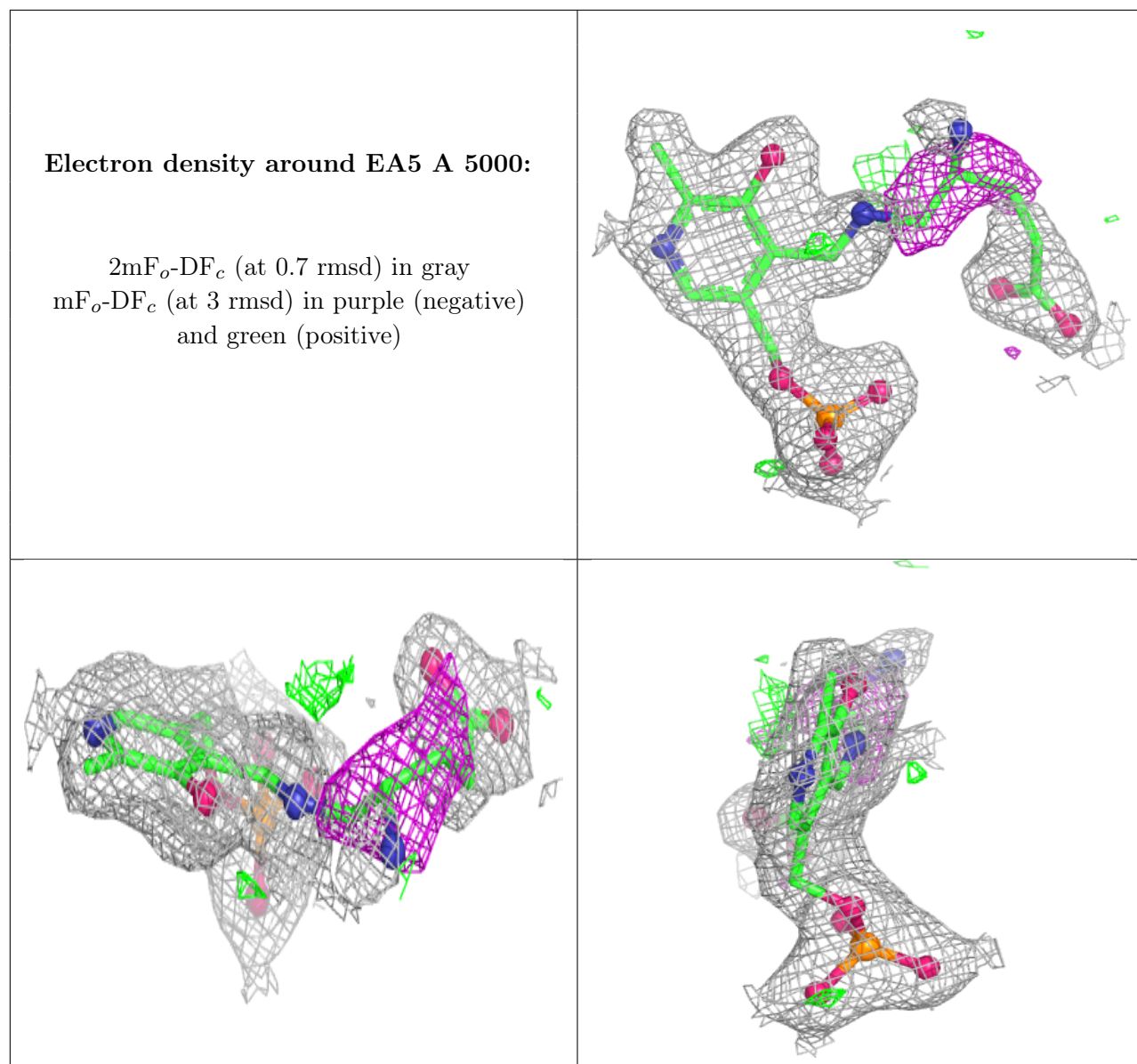
There are no monosaccharides in this entry.

## 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
4	HOZ	B	2	9/9	0.76	0.24	66,68,69,70	0
2	EA5	A	5000	24/24	0.94	0.10	15,22,37,38	0
3	PLP	B	6000	15/16	0.98	0.05	15,18,22,22	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers ⓘ

There are no such residues in this entry.