



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 10:48 PM UTC

PDB ID : 2HP2 / pdb\_00002hp2  
Title : Inter-subunit signaling in GSAM  
Authors : Stetefeld, J.  
Deposited on : 2006-07-17  
Resolution : 2.70 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
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

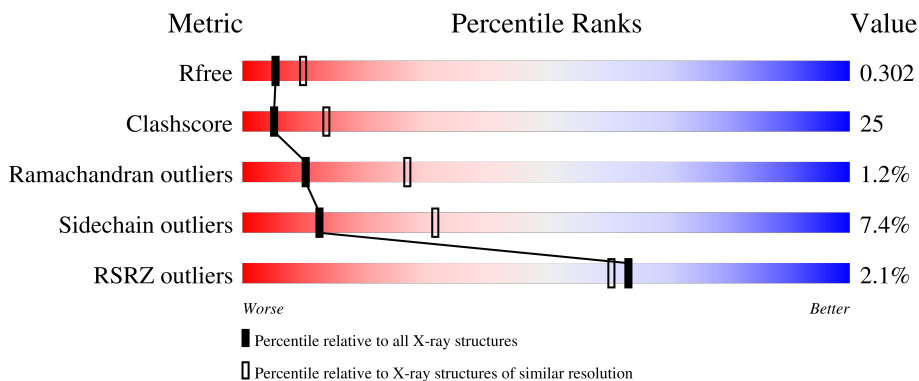
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	 2% 60% 34% 5%
1	B	432	 3% 55% 39% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	KE4	A	5000	X	-	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6814 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.

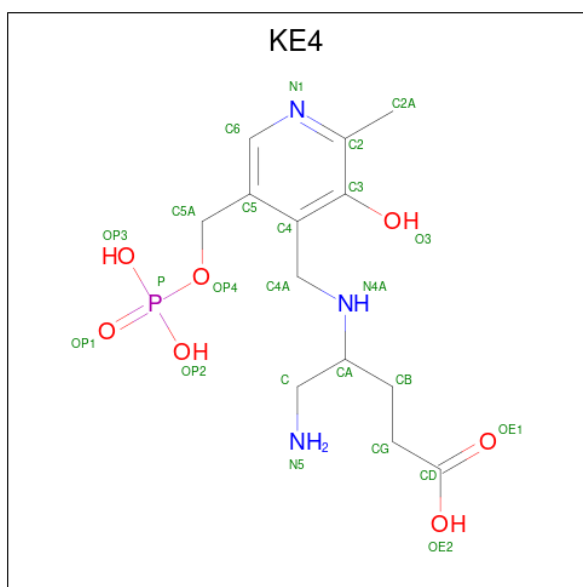
- Molecule 1 is a protein called Glutamate-1-semialdehyde 2,1-aminomutase (GSAM) hybrid-form.

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

There are 12 discrepancies between the modelled and reference sequences:

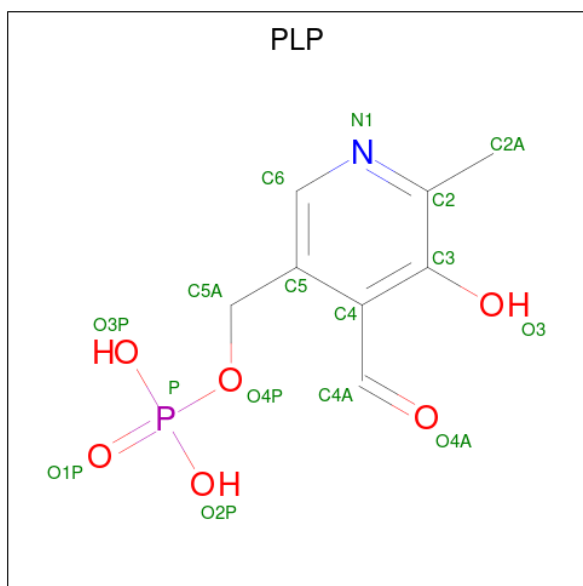
Chain	Residue	Modelled	Actual	Comment	Reference
A	1108	ASN	ILE	conflict	UNP P24630
A	1133	ILE	LEU	conflict	UNP P24630
A	1172	SER	ASP	conflict	UNP P24630
A	1179	LYS	SER	conflict	UNP P24630
A	1187	THR	ALA	conflict	UNP P24630
A	1327	GLY	ALA	conflict	UNP P24630
B	2108	ASN	ILE	conflict	UNP P24630
B	2133	ILE	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 (4R)-5-AMINO-4-[(3-HYDROXY-2-METHYL-5-[(PHOSPHONOOXY)METHYL]PYRIDIN-4-YL)METHYL)AMINO]PENTANOIC ACID (CCD ID: KE4) (formula: C<sub>13</sub>H<sub>22</sub>N<sub>3</sub>O<sub>7</sub>P).



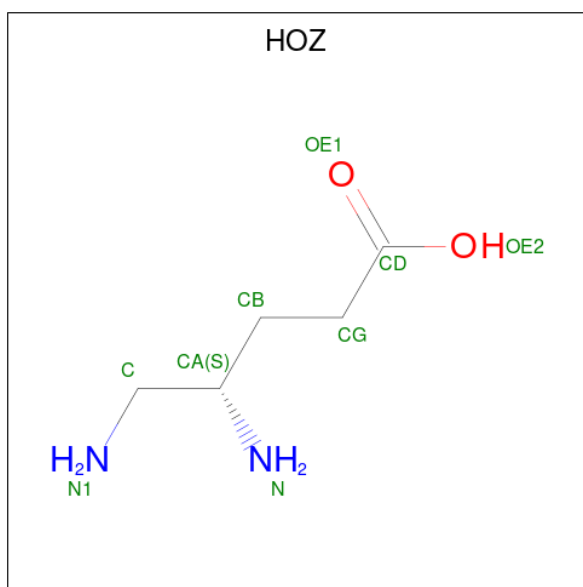
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	24	13	3	7	1	0	0

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



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

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



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

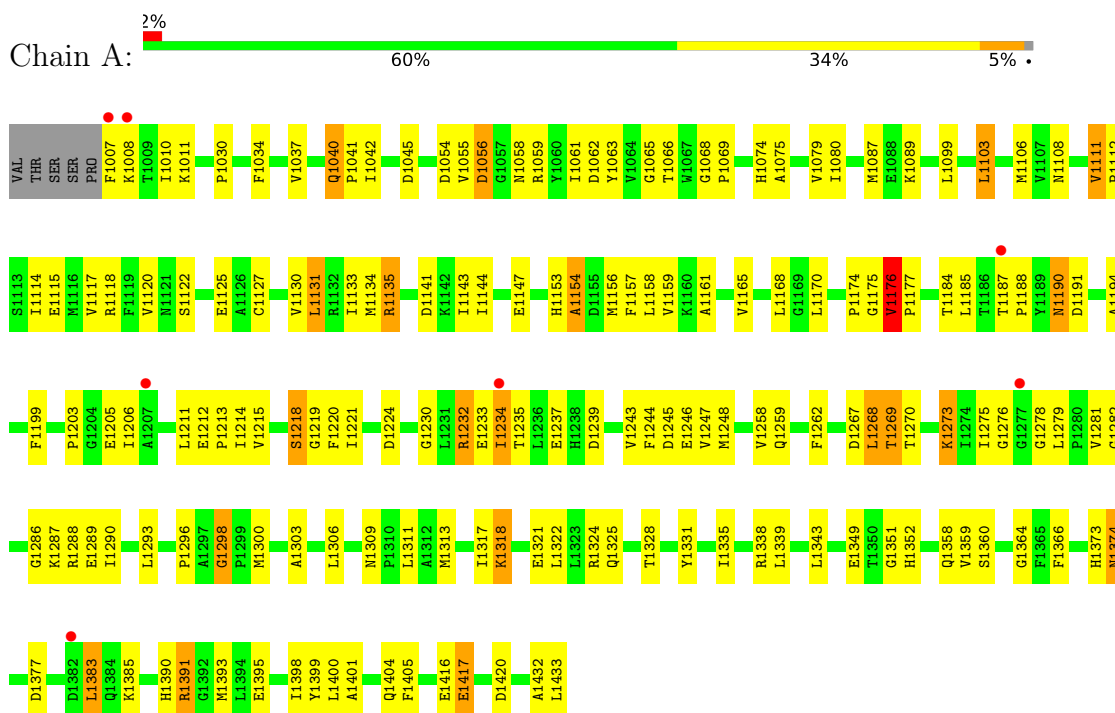
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	193	Total	O	0	0
			193	193		
5	B	169	Total	O	0	0
			169	169		

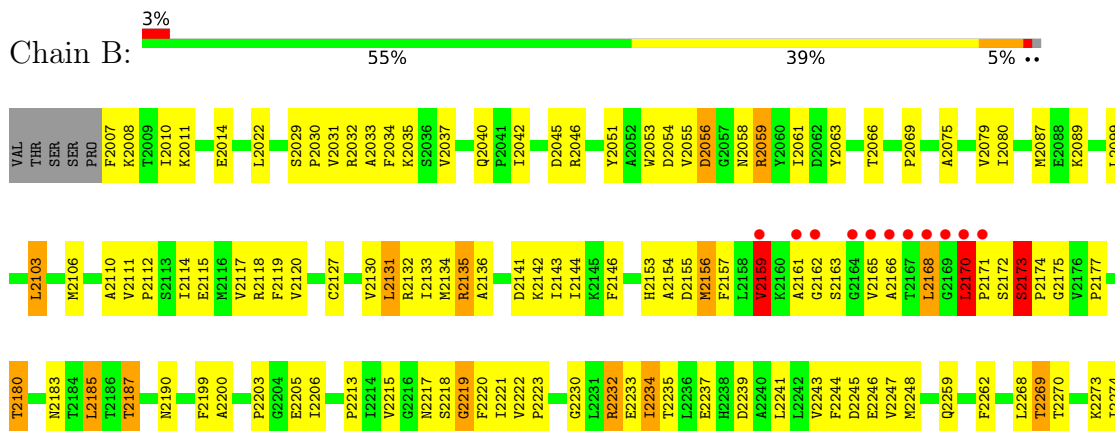
### 3 Residue-property plots [i](#)

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) hybrid-form



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



I2275	G2276	G2277	G2278	L2279	P2280	V2281	G2282	G2286	K2287	R2288	F2289	L2290	L2293	P2296	A2297	G2298	P2299	T2305	L2306	S2307	G2308	R2309	P2310	M2313	L2317	K2318	E2321	L2322	L2323	R2324	Q2325	T2328	Y2331	L2335	T2336	K2337	R2338	L2339	G2342	L2343	L2344	A2345	L2346	T2350	G2356	G2357
Q2368	V2369	S2360	G2361	M2362	F2363	F2366	F2367	P2371	V2372	H2373	M2374	D2377	S2381	D2382	L2383	Q2384	K2385	R2391	G2392	M2393	L2394	E2395	Q2396	G2397	I2398	Y2399	L2400	A2401	P2402	S2403	Q2404	F2405	E2406	A2407	G2408	F2409	E2416	E2417	D2420	S2431	A2432	L2433				

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.77Å 109.08Å 124.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.59 – 2.70 24.59 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.6 (24.59-2.70) 92.5 (24.59-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.95 (at 2.72Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.229 , 0.296 0.224 , 0.302	Depositor DCC
$R_{free}$ test set	2335 reflections (9.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.8	Xtrriage
Anisotropy	0.559	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6814	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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, KE4

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	0.48	0/3271	1.01	13/4430 (0.3%)
1	B	0.46	0/3271	0.98	13/4430 (0.3%)
All	All	0.47	0/6542	0.99	26/8860 (0.3%)

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1055	VAL	N-CA-C	-12.07	100.88	112.83
1	B	2055	VAL	N-CA-C	-11.03	101.91	112.83
1	A	1040	GLN	CA-C-N	10.46	130.56	120.31
1	A	1040	GLN	C-N-CA	10.46	130.56	120.31
1	A	1219	GLY	N-CA-C	-9.30	99.14	112.17

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	160	0
1	B	3202	0	3180	173	0
2	A	24	0	18	6	0
3	B	15	0	7	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	9	0	11	4	0
5	A	193	0	0	5	0
5	B	169	0	0	6	0
All	All	6814	0	6398	315	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 25.

The worst 5 of 315 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1144:ILE:HD11	1:A:1206:ILE:HD13	1.43	0.98
1:B:2217:ASN:HD21	4:B:2:HOZ:HN12	1.00	0.98
1:B:2144:ILE:HD11	1:B:2206:ILE:HD13	1.43	0.97
1:B:2131:LEU:HA	1:B:2134:MET:HE3	1.50	0.92
1:B:2217:ASN:ND2	4:B:2:HOZ:HN12	1.71	0.89

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	425/432 (98%)	394 (93%)	29 (7%)	2 (0%)	24	48
1	B	425/432 (98%)	378 (89%)	39 (9%)	8 (2%)	6	17
All	All	850/864 (98%)	772 (91%)	68 (8%)	10 (1%)	10	27

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2173	SER

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Mol	Chain	Res	Type
1	A	1273	LYS
1	B	2159	VAL
1	B	2273	LYS
1	B	2170	LEU

### 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	330/335 (98%)	309 (94%)	21 (6%)	16	38
1	B	330/335 (98%)	302 (92%)	28 (8%)	10	25
All	All	660/670 (98%)	611 (93%)	49 (7%)	13	32

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2159	VAL
1	B	2234	ILE
1	B	2168	LEU
1	B	2185	LEU
1	B	2239	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2190	ASN
1	B	2348	GLN
1	B	2292	GLN
1	B	2352	HIS
1	A	1352	HIS

### 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](#)

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	1.34	2 (13%)	21,22,23	1.11	3 (14%)
4	HOZ	B	2	-	8,8,8	1.35	1 (12%)	9,9,9	1.41	2 (22%)
2	KE4	A	5000	-	23,24,24	1.84	7 (30%)	29,33,33	2.27	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	-	3/6/6/8	0/1/1/1
4	HOZ	B	2	-	-	1/7/7/7	-
2	KE4	A	5000	-	1/1/3/4	8/18/18/18	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5000	KE4	CA-N4A	-4.62	1.35	1.48
2	A	5000	KE4	C2-N1	3.64	1.40	1.33
4	B	2	HOZ	CB-CA	2.71	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5000	KE4	C2A-C2	2.55	1.54	1.50
3	B	6000	PLP	C3-C2	-2.53	1.38	1.41

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5000	KE4	CB-CA-C	7.12	121.63	109.47
2	A	5000	KE4	C4A-N4A-CA	5.43	122.82	113.84
2	A	5000	KE4	OP3-P-OP2	-3.76	93.71	107.80
2	A	5000	KE4	OP3-P-OP1	3.31	123.72	110.83
2	A	5000	KE4	C6-C5-C4	3.30	120.56	118.06

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	5000	KE4	CA

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5000	KE4	C5-C4-C4A-N4A
2	A	5000	KE4	CB-CA-N4A-C4A
2	A	5000	KE4	C-CA-CB-CG
3	B	6000	PLP	C4-C5-C5A-O4P
4	B	2	HOZ	N-CA-CB-CG

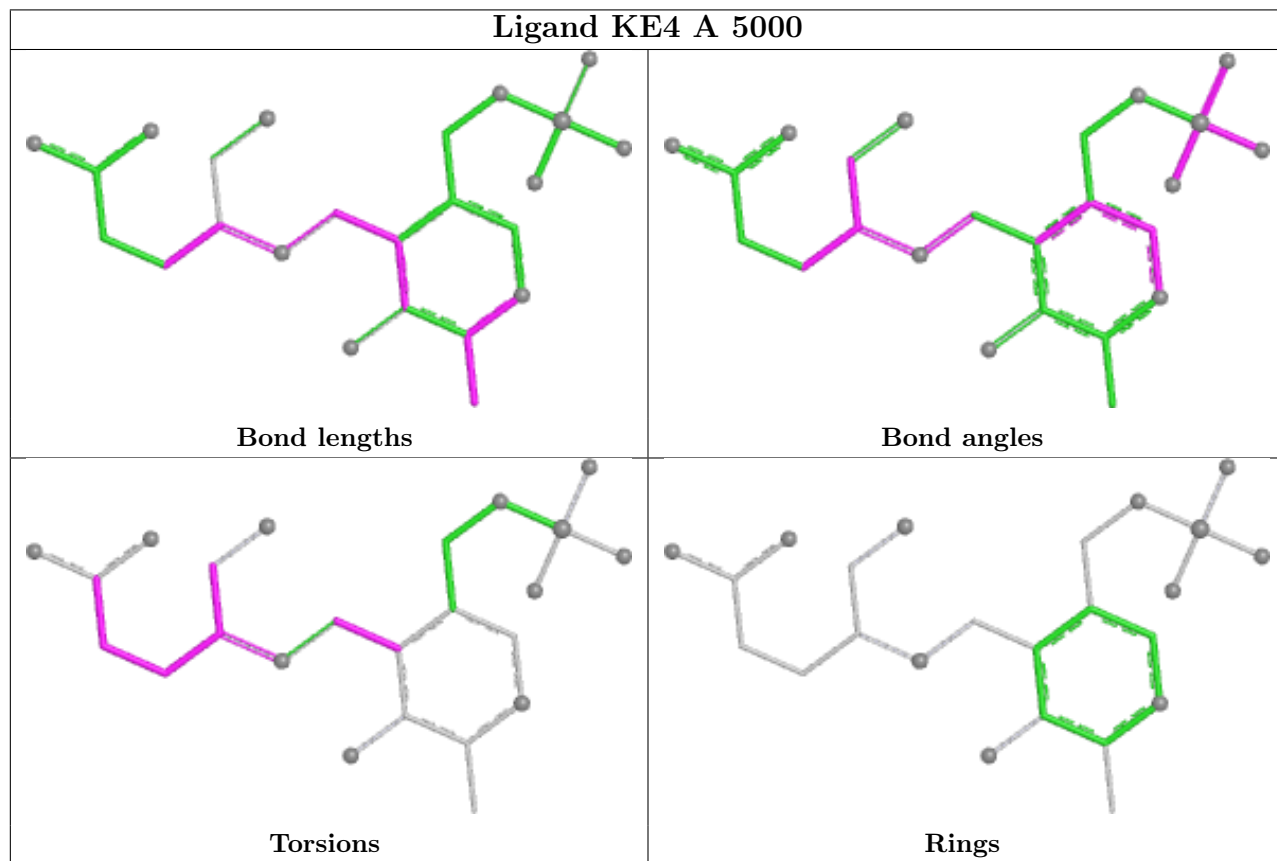
There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	6000	PLP	3	0
4	B	2	HOZ	4	0
2	A	5000	KE4	6	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	7 (1%) 70 68	11, 26, 40, 51	0
1	B	427/432 (98%)	0.24	11 (2%) 57 54	12, 26, 47, 78	0
All	All	854/864 (98%)	0.20	18 (2%) 63 61	11, 26, 42, 78	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2169	GLY	3.9
1	B	2164	GLY	3.8
1	B	2159	VAL	3.8
1	B	2165	VAL	3.6
1	B	2168	LEU	3.3

### 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](#)

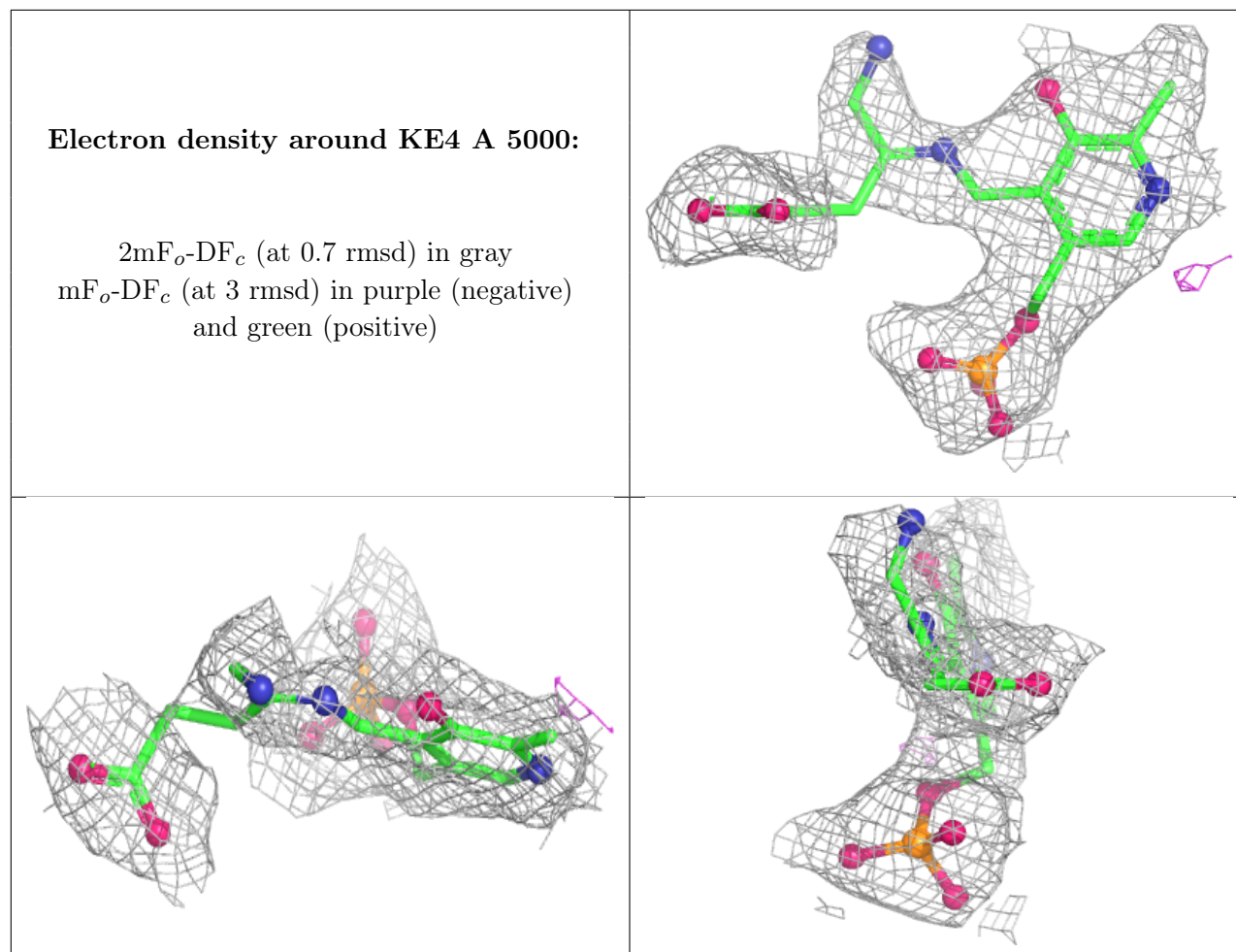
There are no oligosaccharides in this entry.

### 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, 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	0.82	0.24	67,69,70,70	0
2	KE4	A	5000	24/24	0.91	0.12	31,36,44,45	0
3	PLP	B	6000	15/16	0.93	0.09	17,20,24,27	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 [i](#)

There are no such residues in this entry.