



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:02 am GMT

PDB ID : 2HP2  
Title : Inter-subunit signaling in GSAM  
Authors : Stetefeld, J.  
Deposited on : 2006-07-17  
Resolution : 2.70 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

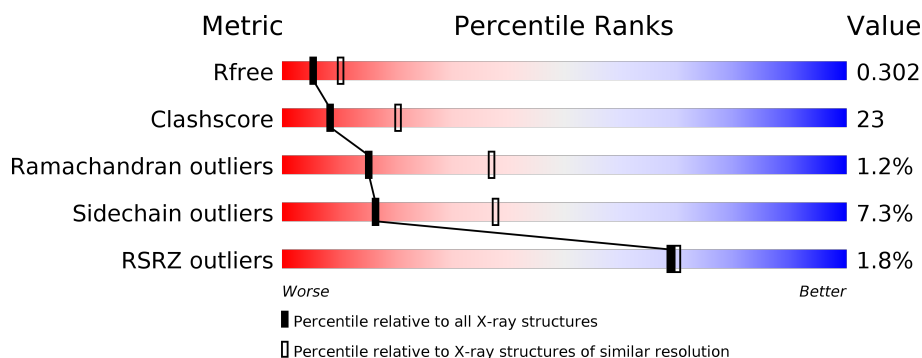
# 1 Overall quality at a glance

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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	 63% 33% 3% 1%
1	B	432	 58% 36% 5% 1%

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	-	-	X
4	HOZ	B	2	-	-	-	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.

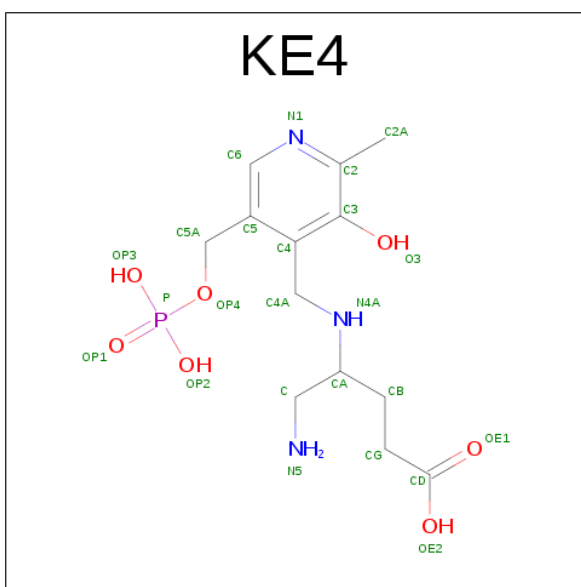
- Molecule 1 is a protein called Glutamate-1-semialdehyde 2,1-aminomutase (GSAM) hybrid-form.

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

There are 12 discrepancies between the modelled and reference sequences:

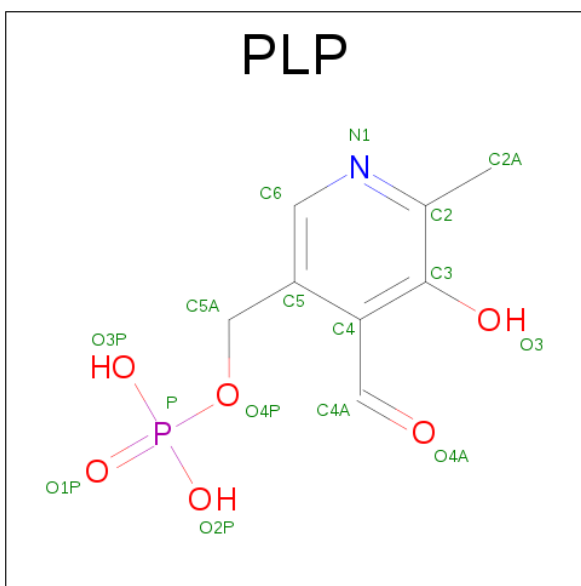
Chain	Residue	Modelled	Actual	Comment	Reference
A	1108	ASN	ILE	CONFLICT	UNP P24630
A	1133	ILE	LEU	CONFLICT	UNP P24630
A	1172	SER	ASP	CONFLICT	UNP P24630
A	1179	LYS	SER	CONFLICT	UNP P24630
A	1187	THR	ALA	CONFLICT	UNP P24630
A	1327	GLY	ALA	CONFLICT	UNP P24630
B	2108	ASN	ILE	CONFLICT	UNP P24630
B	2133	ILE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



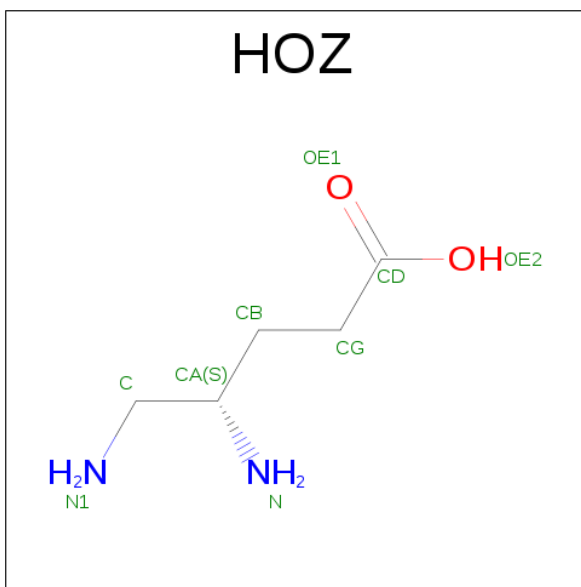
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			24	13	3	7	1		

- 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		

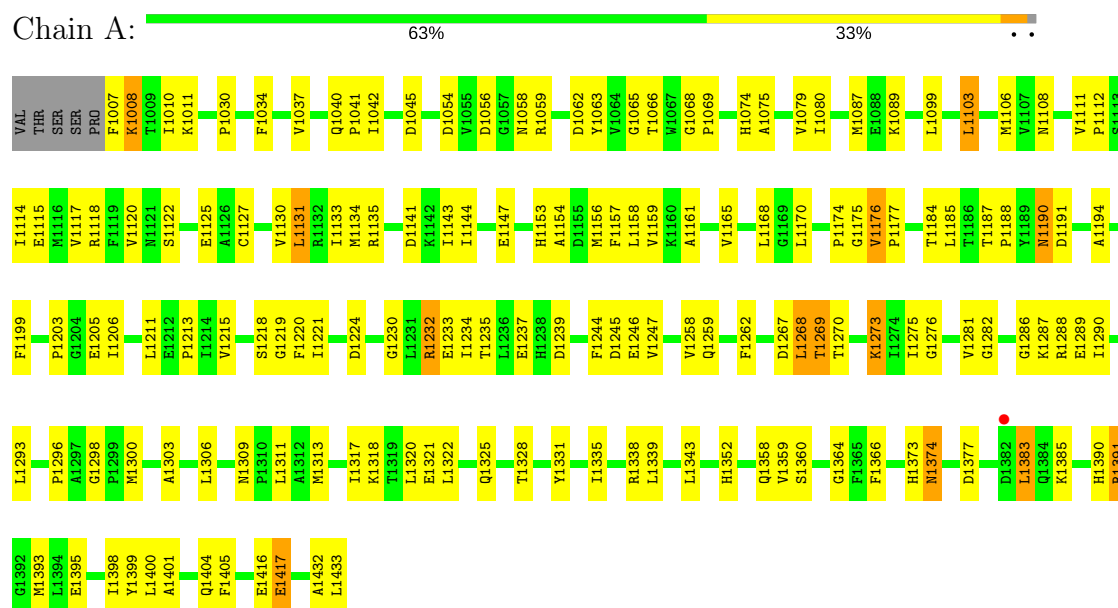
- Molecule 5 is water.

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

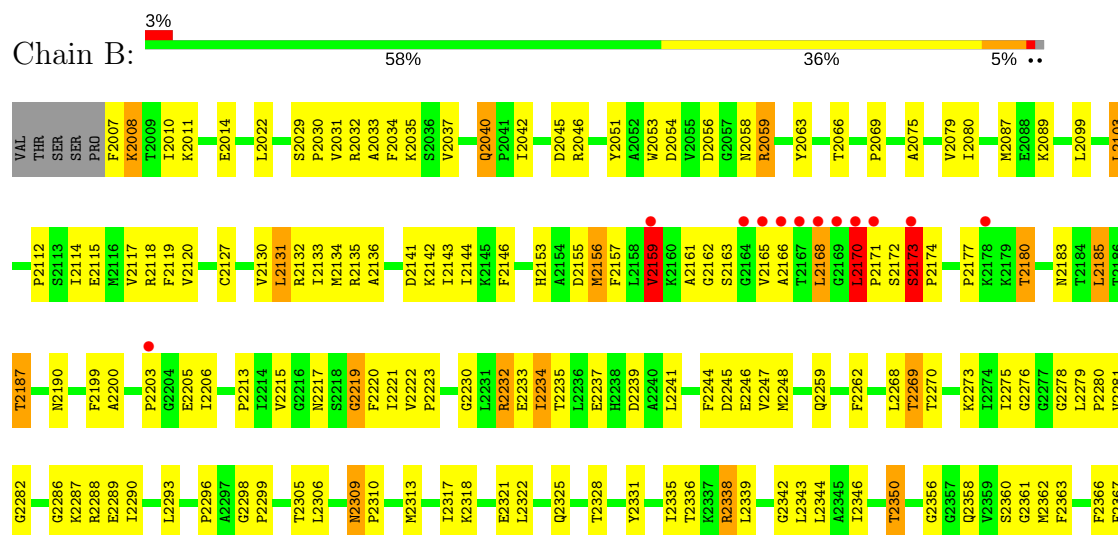
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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







## 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) 92.7 (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)	Xtriage
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%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.8	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 43.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	6814	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage'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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KE4, HOZ, PLP

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	0.38	0/3271	0.64	3/4430 (0.1%)
1	B	0.38	0/3271	0.64	3/4430 (0.1%)
All	All	0.38	0/6542	0.64	6/8860 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2338	ARG	NE-CZ-NH1	-7.20	116.70	120.30
1	A	1338	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	A	1338	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	B	2338	ARG	NE-CZ-NH2	6.50	123.55	120.30
1	A	1219	GLY	N-CA-C	-5.58	99.14	113.10
1	B	2219	GLY	N-CA-C	-5.51	99.32	113.10

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	3182	152	0
1	B	3202	0	3180	163	0
2	A	24	0	18	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	15	0	7	1	0
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	296	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 23.

All (296) 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:2131:LEU:HA	1:B:2134:MET:HE3	1.43	0.97
1:B:2144:ILE:HD11	1:B:2206:ILE:HD13	1.43	0.97
1:A:1131:LEU:HA	1:A:1134:MET:HE3	1.52	0.91
1:B:2217:ASN:ND2	4:B:2:HOZ:HN12	1.71	0.89
1:A:1066:THR:HG23	1:A:1069:PRO:HD2	1.55	0.87
1:B:2168:LEU:HD23	1:B:2168:LEU:H	1.39	0.87
1:A:1114:ILE:HA	1:A:1286:GLY:HA2	1.56	0.87
1:B:2114:ILE:HA	1:B:2286:GLY:HA2	1.58	0.86
1:A:1296:PRO:HG3	1:B:2030:PRO:HA	1.56	0.86
1:B:2066:THR:HG23	1:B:2069:PRO:HD2	1.57	0.84
1:A:1190:ASN:HD21	1:A:1224:ASP:H	1.26	0.83
1:A:1187:THR:OG1	1:A:1188:PRO:HD2	1.81	0.81
1:A:1030:PRO:HA	1:B:2296:PRO:HG3	1.62	0.79
1:A:1054:ASP:HB3	1:A:1056:ASP:H	1.47	0.79
1:A:1318:LYS:HE3	1:A:1318:LYS:HA	1.65	0.77
1:B:2374:ASN:ND2	1:B:2377:ASP:H	1.83	0.76
1:A:1203:PRO:HA	5:A:7047:HOH:O	1.85	0.76
1:B:2161:ALA:HB3	1:B:2165:VAL:HG11	1.67	0.76
1:B:2054:ASP:HB3	1:B:2056:ASP:H	1.49	0.76
1:A:1374:ASN:HD21	1:A:1377:ASP:H	1.34	0.75
1:A:1374:ASN:ND2	1:A:1377:ASP:H	1.83	0.75
1:B:2318:LYS:HE3	1:B:2318:LYS:HA	1.68	0.75
1:A:1190:ASN:ND2	1:A:1224:ASP:H	1.85	0.73
1:B:2173:SER:CB	1:B:2174:PRO:HA	2.19	0.73
1:A:1153:HIS:ND1	1:B:2132:ARG:NH1	2.36	0.72
1:A:1296:PRO:CG	1:B:2030:PRO:HA	2.20	0.71
1:B:2215:VAL:HB	1:B:2221:ILE:HB	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2054:ASP:HB2	1:B:2058:ASN:H	1.56	0.71
1:A:1147:GLU:HG3	1:A:1161:ALA:CB	2.21	0.71
1:A:1232:ARG:O	1:A:1232:ARG:HD3	1.90	0.71
1:A:1220:PHE:HZ	1:A:1359:VAL:HG23	1.56	0.70
1:B:2162:GLY:HA2	1:B:2166:ALA:HB2	1.74	0.70
1:B:2190:ASN:HD21	1:B:2223:PRO:HA	1.57	0.69
1:B:2230:GLY:O	1:B:2234:ILE:HG22	1.93	0.69
1:A:1054:ASP:OD2	1:A:1058:ASN:HB2	1.93	0.68
1:A:1220:PHE:CZ	1:A:1359:VAL:HG23	2.28	0.68
1:A:1352:HIS:HD2	1:A:1385:LYS:NZ	1.92	0.68
1:A:1159:VAL:HG11	1:A:1184:THR:HG21	1.76	0.67
1:B:2366:PHE:HA	1:B:2404:GLN:NE2	2.09	0.67
1:B:2391:ARG:HG2	1:B:2391:ARG:HH11	1.59	0.67
1:A:1153:HIS:HA	1:A:1158:LEU:HD11	1.76	0.66
1:B:2232:ARG:HD3	1:B:2232:ARG:O	1.94	0.66
1:A:1165:VAL:HG12	1:A:1168:LEU:HD23	1.77	0.66
1:B:2173:SER:OG	1:B:2174:PRO:HA	1.96	0.66
1:B:2233:GLU:O	1:B:2237:GLU:HG3	1.96	0.66
1:A:1159:VAL:HG11	1:A:1184:THR:CG2	2.26	0.65
1:B:2155:ASP:HB3	1:B:2180:THR:HG21	1.77	0.65
1:B:2075:ALA:HB1	1:B:2080:ILE:HD11	1.77	0.65
1:B:2054:ASP:OD2	1:B:2058:ASN:HB2	1.96	0.65
1:B:2040:GLN:HA	1:B:2040:GLN:HE21	1.61	0.65
1:A:1037:VAL:HG12	1:A:1037:VAL:O	1.98	0.64
1:B:2338:ARG:NH1	1:B:2420:ASP:OD1	2.20	0.64
1:A:1296:PRO:HG3	1:B:2030:PRO:CA	2.28	0.64
1:B:2054:ASP:HB2	1:B:2058:ASN:N	2.13	0.64
1:A:1099:LEU:HD22	1:A:1317:ILE:HD12	1.79	0.64
1:A:1075:ALA:HB1	1:A:1080:ILE:HD11	1.79	0.63
1:A:1187:THR:OG1	1:A:1194:ALA:HB1	1.99	0.63
1:A:1215:VAL:HB	1:A:1221:ILE:HB	1.80	0.62
1:B:2417:GLU:OE1	1:B:2417:GLU:N	2.31	0.62
1:A:1030:PRO:HA	1:B:2296:PRO:CG	2.29	0.62
1:A:1230:GLY:O	1:A:1234:ILE:HG22	1.99	0.62
1:A:1199:PHE:CD1	1:A:1234:ILE:HD11	2.35	0.62
1:B:2144:ILE:HA	1:B:2185:LEU:O	1.98	0.62
1:A:1011:LYS:HB2	1:A:1056:ASP:OD1	1.99	0.61
1:B:2366:PHE:HA	1:B:2404:GLN:HE22	1.64	0.61
1:B:2011:LYS:HB2	1:B:2056:ASP:OD1	2.00	0.61
1:A:1144:ILE:CD1	1:A:1206:ILE:HD13	2.27	0.60
1:B:2219:GLY:HA3	1:B:2366:PHE:CZ	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1054:ASP:HB2	1:A:1058:ASN:H	1.64	0.60
1:B:2317:ILE:O	1:B:2321:GLU:HG3	2.01	0.60
1:A:1391:ARG:HG2	1:A:1391:ARG:HH11	1.65	0.60
1:A:1300:MET:HA	1:B:2174:PRO:HD2	1.83	0.60
1:A:1147:GLU:HG3	1:A:1161:ALA:HB1	1.82	0.60
1:B:2374:ASN:C	1:B:2374:ASN:HD22	2.04	0.60
1:B:2199:PHE:CD1	1:B:2234:ILE:HD11	2.37	0.60
1:B:2162:GLY:HA2	1:B:2166:ALA:CB	2.32	0.60
1:A:1147:GLU:HG3	1:A:1161:ALA:HB3	1.84	0.59
1:B:2350:THR:HG21	1:B:2431:SER:HA	1.85	0.58
1:A:1054:ASP:HB2	1:A:1058:ASN:N	2.17	0.58
1:A:1205:GLU:HB3	5:A:7245:HOH:O	2.03	0.58
1:B:2168:LEU:CD2	1:B:2168:LEU:H	2.16	0.58
1:B:2117:VAL:HG22	1:B:2118:ARG:N	2.17	0.58
1:A:1374:ASN:HD22	1:A:1374:ASN:C	2.06	0.58
1:A:1115:GLU:CG	1:A:1288:ARG:H	2.17	0.58
1:B:2374:ASN:HD21	1:B:2377:ASP:H	1.51	0.58
1:B:2275:ILE:HG13	1:B:2281:VAL:CG1	2.34	0.57
1:A:1273:LYS:NZ	2:A:5000:KE4:N4A	2.51	0.57
2:A:5000:KE4:HB2	1:B:2305:THR:OG1	2.03	0.57
1:B:2165:VAL:HA	1:B:2170:LEU:HB3	1.86	0.57
1:B:2008:LYS:HD3	1:B:2010:ILE:HG12	1.86	0.57
1:B:2344:LEU:HD11	1:B:2356:GLY:H	1.68	0.57
1:A:1117:VAL:HG22	1:A:1118:ARG:N	2.20	0.56
1:B:2173:SER:HB3	1:B:2174:PRO:HA	1.87	0.56
1:B:2245:ASP:OD1	1:B:2247:VAL:HG23	2.04	0.56
1:A:1417:GLU:OE1	1:A:1417:GLU:N	2.37	0.56
1:B:2344:LEU:HD11	1:B:2356:GLY:N	2.21	0.56
1:A:1154:ALA:O	1:A:1158:LEU:HD13	2.06	0.56
1:A:1115:GLU:HG3	1:A:1288:ARG:HB2	1.86	0.56
1:B:2115:GLU:HG3	1:B:2288:ARG:HB2	1.87	0.56
1:A:1339:LEU:O	1:A:1343:LEU:HB2	2.06	0.56
1:B:2248:MET:HB2	3:B:6000:PLP:O3	2.06	0.56
1:B:2156:MET:CE	1:B:2156:MET:H	2.20	0.55
1:A:1303:ALA:HB2	1:B:2030:PRO:HD2	1.89	0.55
1:A:1233:GLU:O	1:A:1237:GLU:HG3	2.06	0.55
1:A:1120:VAL:HG23	1:A:1282:GLY:HA3	1.89	0.55
1:B:2115:GLU:CG	1:B:2288:ARG:H	2.20	0.55
1:B:2099:LEU:HD22	1:B:2317:ILE:HD12	1.88	0.55
1:B:2391:ARG:HG2	1:B:2391:ARG:NH1	2.22	0.55
1:B:2103:LEU:HD12	1:B:2313:MET:SD	2.47	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2205:GLU:HB3	5:B:7339:HOH:O	2.07	0.54
1:A:1154:ALA:HB3	1:A:1157:PHE:CD1	2.43	0.54
1:A:1130:VAL:HA	1:A:1133:ILE:HG22	1.89	0.54
1:A:1317:ILE:O	1:A:1321:GLU:HG3	2.08	0.54
1:B:2159:VAL:HA	1:B:2172:SER:OG	2.07	0.54
1:B:2163:SER:OG	1:B:2217:ASN:ND2	2.41	0.54
1:A:1087:MET:HE1	1:B:2087:MET:HE3	1.90	0.53
1:B:2130:VAL:HA	1:B:2133:ILE:HG22	1.90	0.53
1:B:2156:MET:HG2	1:B:2157:PHE:N	2.24	0.53
1:B:2114:ILE:HA	1:B:2286:GLY:CA	2.35	0.53
1:B:2162:GLY:O	1:B:2165:VAL:HG12	2.08	0.53
1:B:2275:ILE:HG13	1:B:2281:VAL:HG11	1.91	0.53
1:B:2393:MET:HB3	1:B:2398:ILE:HB	1.90	0.53
1:A:1114:ILE:HA	1:A:1286:GLY:CA	2.35	0.53
1:B:2385:LYS:HD2	1:B:2433:LEU:HD13	1.90	0.53
1:A:1008:LYS:HD3	1:A:1010:ILE:HG12	1.91	0.53
1:A:1103:LEU:HD12	1:A:1313:MET:SD	2.48	0.53
1:B:2120:VAL:HG23	1:B:2282:GLY:HA3	1.90	0.53
1:B:2289:GLU:H	1:B:2289:GLU:CD	2.10	0.52
1:B:2259:GLN:HE22	1:B:2269:THR:HG21	1.74	0.52
1:B:2144:ILE:CD1	1:B:2206:ILE:HD13	2.31	0.52
1:A:1289:GLU:H	1:A:1289:GLU:CD	2.13	0.52
1:B:2063:TYR:HB2	1:B:2400:LEU:HD23	1.92	0.52
1:A:1275:ILE:HG13	1:A:1281:VAL:CG1	2.40	0.51
1:A:1391:ARG:NH1	1:A:1391:ARG:HG2	2.26	0.51
1:A:1188:PRO:HG2	1:A:1191:ASP:CB	2.40	0.51
1:A:1079:VAL:HA	1:A:1318:LYS:HG2	1.92	0.51
1:A:1168:LEU:HD23	1:A:1170:LEU:HD11	1.92	0.51
1:B:2350:THR:CG2	1:B:2431:SER:HA	2.40	0.51
1:B:2079:VAL:HA	1:B:2318:LYS:HG2	1.93	0.51
1:A:1366:PHE:HA	1:A:1404:GLN:NE2	2.26	0.51
1:A:1175:GLY:HA2	1:B:2136:ALA:N	2.25	0.50
1:A:1331:TYR:CE2	1:A:1335:ILE:HD13	2.46	0.50
1:A:1416:GLU:HB3	1:A:1417:GLU:OE1	2.11	0.50
1:A:1275:ILE:HG13	1:A:1281:VAL:HG11	1.94	0.50
1:A:1276:GLY:N	1:A:1281:VAL:HG11	2.27	0.50
1:A:1385:LYS:HD2	1:A:1433:LEU:HD13	1.94	0.50
1:B:2276:GLY:N	1:B:2281:VAL:HG11	2.27	0.50
1:B:2035:LYS:HB2	1:B:2168:LEU:HD13	1.92	0.49
1:B:2173:SER:CB	1:B:2174:PRO:CA	2.88	0.49
1:A:1030:PRO:CA	1:B:2296:PRO:HG3	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2146:PHE:CD1	1:B:2187:THR:HG22	2.46	0.49
1:A:1007:PHE:CD2	1:A:1395:GLU:HG2	2.47	0.49
1:A:1366:PHE:HA	1:A:1404:GLN:HE22	1.76	0.49
1:B:2344:LEU:HD11	1:B:2356:GLY:CA	2.43	0.49
1:B:2142:LYS:HB3	1:B:2185:LEU:HD22	1.94	0.49
1:B:2033:ALA:O	1:B:2034:PHE:HB2	2.10	0.49
1:B:2153:HIS:ND1	1:B:2153:HIS:O	2.46	0.49
1:B:2336:THR:HG21	1:B:2360:SER:O	2.13	0.49
1:B:2007:PHE:CD2	1:B:2395:GLU:HG2	2.46	0.49
1:A:1259:GLN:HE22	1:A:1269:THR:HG21	1.78	0.49
1:A:1393:MET:HB3	1:A:1398:ILE:HB	1.94	0.49
1:B:2287:LYS:HB3	1:B:2290:ILE:HD12	1.94	0.49
1:B:2339:LEU:O	1:B:2343:LEU:HB2	2.12	0.49
1:A:1245:ASP:OD1	1:A:1247:VAL:HG23	2.13	0.49
1:A:1220:PHE:HZ	1:A:1359:VAL:CG2	2.26	0.49
1:B:2245:ASP:HA	1:B:2270:THR:OG1	2.13	0.49
1:A:1306:LEU:HG	1:B:2280:PRO:HA	1.95	0.49
1:B:2213:PRO:HG3	1:B:2244:PHE:CG	2.48	0.49
1:A:1130:VAL:O	1:A:1134:MET:HB2	2.14	0.48
1:B:2416:GLU:HB3	1:B:2417:GLU:OE1	2.13	0.48
1:B:2130:VAL:O	1:B:2134:MET:HB2	2.14	0.48
1:B:2115:GLU:HG2	1:B:2286:GLY:O	2.13	0.48
1:B:2373:HIS:HA	5:B:7288:HOH:O	2.14	0.48
1:A:1089:LYS:HA	5:B:7236:HOH:O	2.14	0.48
1:A:1127:CYS:O	1:A:1130:VAL:HG12	2.14	0.47
1:B:2293:LEU:HA	1:B:2298:GLY:HA3	1.96	0.47
1:A:1190:ASN:HD21	1:A:1224:ASP:N	2.03	0.47
1:B:2367:PHE:O	1:B:2381:SER:HA	2.14	0.47
1:A:1065:GLY:O	1:A:1066:THR:HG22	2.14	0.47
1:B:2344:LEU:HD21	1:B:2356:GLY:N	2.30	0.47
1:A:1213:PRO:HB2	1:A:1258:VAL:HG21	1.96	0.47
1:A:1087:MET:HE1	1:B:2087:MET:CE	2.44	0.47
1:A:1174:PRO:HG3	1:B:2299:PRO:HG2	1.96	0.47
1:A:1293:LEU:HA	1:A:1298:GLY:HA3	1.97	0.47
1:A:1131:LEU:O	1:A:1135:ARG:HG3	2.15	0.47
1:B:2309:ASN:HB2	1:B:2310:PRO:HD2	1.97	0.47
1:A:1220:PHE:CB	1:A:1364:GLY:HA3	2.45	0.47
1:A:1063:TYR:HB2	1:A:1400:LEU:HD23	1.98	0.46
1:B:2287:LYS:HB3	1:B:2290:ILE:CD1	2.45	0.46
1:B:2342:GLY:O	1:B:2346:ILE:HG13	2.14	0.46
1:B:2336:THR:OG1	1:B:2361:GLY:HA2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1287:LYS:HB3	1:A:1290:ILE:HD12	1.98	0.46
1:A:1352:HIS:HD2	1:A:1385:LYS:HZ2	1.62	0.46
1:A:1213:PRO:HG3	1:A:1244:PHE:CG	2.51	0.46
1:A:1273:LYS:HZ3	2:A:5000:KE4:HN4A	1.64	0.46
1:A:1432:ALA:HA	5:A:7353:HOH:O	2.16	0.46
1:B:2397:GLY:O	1:B:2398:ILE:HD13	2.16	0.46
1:A:1108:ASN:HD22	1:B:2022:LEU:HD22	1.81	0.46
1:A:1245:ASP:HA	1:A:1270:THR:OG1	2.16	0.46
1:A:1273:LYS:NZ	2:A:5000:KE4:HN4A	2.12	0.46
1:B:2165:VAL:HG23	1:B:2170:LEU:HD12	1.97	0.45
1:A:1276:GLY:CA	1:A:1281:VAL:HG11	2.46	0.45
1:A:1352:HIS:HD2	1:A:1385:LYS:HZ3	1.61	0.45
1:B:2278:GLY:C	1:B:2279:LEU:HD12	2.37	0.45
1:A:1220:PHE:HB3	1:A:1364:GLY:HA3	1.98	0.45
1:B:2042:ILE:HD11	1:B:2399:TYR:CE1	2.52	0.45
1:B:2163:SER:HA	1:B:2406:GLU:OE1	2.16	0.45
1:B:2117:VAL:CG2	1:B:2118:ARG:N	2.80	0.45
1:B:2135:ARG:HD3	1:B:2141:ASP:O	2.17	0.45
1:A:1154:ALA:HB3	1:A:1157:PHE:HD1	1.82	0.45
1:A:1416:GLU:HB2	5:A:7175:HOH:O	2.16	0.45
1:B:2146:PHE:HA	1:B:2187:THR:O	2.16	0.45
1:A:1232:ARG:NH1	1:A:1267:ASP:OD1	2.47	0.45
1:B:2051:TYR:HB3	1:B:2059:ARG:HD3	1.99	0.45
1:A:1262:PHE:N	1:A:1262:PHE:CD2	2.83	0.45
1:A:1106:MET:HE2	1:A:1320:LEU:HB3	1.98	0.45
1:B:2142:LYS:HA	1:B:2183:ASN:O	2.16	0.45
1:A:1045:ASP:O	1:B:2089:LYS:HE2	2.17	0.45
1:B:2417:GLU:H	1:B:2417:GLU:CD	2.20	0.44
1:A:1224:ASP:OD2	1:A:1373:HIS:HD2	2.00	0.44
1:B:2219:GLY:HA3	1:B:2366:PHE:CE2	2.52	0.44
1:B:2131:LEU:HD23	1:B:2157:PHE:CZ	2.52	0.44
1:B:2401:ALA:O	1:B:2403:SER:N	2.44	0.44
1:B:2131:LEU:O	1:B:2135:ARG:HG3	2.18	0.44
1:A:1359:VAL:O	1:A:1360:SER:C	2.56	0.44
1:A:1099:LEU:HD22	1:A:1317:ILE:CD1	2.48	0.44
1:A:1267:ASP:O	1:A:1268:LEU:HD12	2.18	0.44
1:B:2010:ILE:N	1:B:2010:ILE:HD13	2.33	0.44
1:B:2262:PHE:N	1:B:2262:PHE:CD2	2.86	0.44
1:A:1042:ILE:HD11	1:A:1399:TYR:CE1	2.53	0.43
1:B:2131:LEU:HD23	1:B:2157:PHE:CE1	2.53	0.43
1:A:1034:PHE:CD2	1:A:1041:PRO:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1313:MET:O	1:A:1317:ILE:HG13	2.17	0.43
1:B:2159:VAL:HG23	5:B:7083:HOH:O	2.17	0.43
1:B:2200:ALA:O	1:B:2203:PRO:HD3	2.18	0.43
1:B:2103:LEU:HD13	1:B:2119:PHE:CE2	2.54	0.43
1:A:1037:VAL:HG11	1:A:1390:HIS:ND1	2.33	0.43
1:B:2177:PRO:O	1:B:2180:THR:HB	2.19	0.43
1:B:2046:ARG:HB2	5:B:7236:HOH:O	2.19	0.43
1:B:2220:PHE:CE1	1:B:2362:MET:HG2	2.54	0.43
1:B:2276:GLY:CA	1:B:2281:VAL:HG11	2.48	0.43
1:A:1042:ILE:HG13	1:A:1042:ILE:O	2.18	0.43
1:A:1054:ASP:CG	1:A:1058:ASN:HB2	2.39	0.42
1:A:1135:ARG:HD3	1:A:1141:ASP:O	2.20	0.42
1:B:2275:ILE:HG13	1:B:2281:VAL:HG13	2.01	0.42
1:A:1040:GLN:HA	1:A:1040:GLN:NE2	2.34	0.42
1:A:1218:SER:HA	1:A:1405:PHE:HB3	2.01	0.42
1:A:1066:THR:HG23	1:A:1069:PRO:CD	2.36	0.42
1:A:1089:LYS:HE2	1:B:2045:ASP:O	2.20	0.42
1:A:1211:LEU:HD23	1:A:1211:LEU:N	2.35	0.42
1:A:1246:GLU:OE2	1:A:1259:GLN:HG2	2.19	0.42
1:B:2331:TYR:CE2	1:B:2335:ILE:HD13	2.55	0.42
1:A:1062:ASP:OD1	1:A:1074:HIS:HE1	2.03	0.42
1:A:1393:MET:HE3	1:A:1398:ILE:HG21	2.01	0.42
1:B:2131:LEU:HG	1:B:2156:MET:SD	2.59	0.42
1:B:2173:SER:HB3	1:B:2174:PRO:CA	2.48	0.42
1:B:2363:PHE:CZ	1:B:2408:GLY:HA3	2.55	0.42
1:A:1322:LEU:O	1:A:1325:GLN:HG2	2.19	0.42
1:A:1417:GLU:CD	1:A:1417:GLU:H	2.22	0.42
1:B:2222:VAL:HG22	5:B:7095:HOH:O	2.20	0.42
1:B:2031:VAL:HG13	1:B:2032:ARG:N	2.34	0.42
1:B:2246:GLU:OE2	1:B:2259:GLN:HG2	2.19	0.42
1:B:2248:MET:CE	4:B:2:HOZ:HN11	2.33	0.41
1:A:1087:MET:HE3	1:B:2087:MET:HE1	2.02	0.41
1:B:2053:TRP:NE1	1:B:2059:ARG:HG2	2.35	0.41
1:A:1111:VAL:HA	1:A:1112:PRO:HD2	1.90	0.41
1:A:1144:ILE:HD11	1:A:1206:ILE:CD1	2.30	0.41
1:B:2134:MET:HA	1:B:2241:LEU:HD12	2.03	0.41
1:B:2322:LEU:O	1:B:2325:GLN:HG2	2.20	0.41
1:A:1318:LYS:CA	1:A:1318:LYS:HE3	2.44	0.41
1:B:2217:ASN:ND2	4:B:2:HOZ:N1	2.52	0.41
1:B:2309:ASN:CB	1:B:2310:PRO:HD2	2.49	0.41
1:A:1158:LEU:N	1:A:1158:LEU:HD12	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1176:VAL:HA	1:A:1177:PRO:HD3	1.86	0.41
1:B:2371:PRO:HB2	1:B:2373:HIS:CE1	2.56	0.41
1:A:1232:ARG:C	1:A:1232:ARG:HD3	2.40	0.41
1:A:1068:GLY:N	1:A:1069:PRO:CD	2.84	0.41
1:A:1352:HIS:CD2	1:A:1385:LYS:HZ2	2.39	0.41
2:A:5000:KE4:HG2	2:A:5000:KE4:H1	1.91	0.41
1:A:1287:LYS:HB3	1:A:1290:ILE:CD1	2.51	0.41
1:A:1287:LYS:HE3	1:A:1287:LYS:HB2	1.94	0.41
1:B:2362:MET:HE3	1:B:2409:PHE:HE2	1.86	0.41
1:A:1087:MET:CE	1:B:2087:MET:HE1	2.52	0.41
1:A:1303:ALA:HB1	1:B:2029:SER:OG	2.20	0.41
1:A:1087:MET:HB3	1:A:1311:LEU:HD21	2.03	0.40
1:B:2127:CYS:O	1:B:2130:VAL:HG12	2.21	0.40
1:A:1117:VAL:CG2	1:A:1118:ARG:N	2.82	0.40
1:A:1401:ALA:HB2	5:A:7346:HOH:O	2.20	0.40
1:B:2010:ILE:O	1:B:2014:GLU:HG3	2.21	0.40
1:A:1122:SER:OG	1:A:1125:GLU:HG3	2.20	0.40
1:A:1383:LEU:HA	1:A:1383:LEU:HD12	1.85	0.40
1:A:1153:HIS:CA	1:A:1158:LEU:HD11	2.47	0.40
1:B:2156:MET:HE2	1:B:2156:MET:H	1.86	0.40
1:B:2232:ARG:HD3	1:B:2232:ARG:C	2.41	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%)	394 (93%)	29 (7%)	2 (0%)	32	60
1	B	425/432 (98%)	378 (89%)	39 (9%)	8 (2%)	9	23
All	All	850/864 (98%)	772 (91%)	68 (8%)	10 (1%)	15	37

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2173	SER
1	A	1273	LYS
1	B	2159	VAL
1	B	2273	LYS
1	B	2170	LEU
1	B	2180	THR
1	A	1328	THR
1	B	2328	THR
1	B	2171	PRO
1	B	2112	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%)	310 (94%)	20 (6%)	22	47
1	B	330/335 (98%)	302 (92%)	28 (8%)	12	28
All	All	660/670 (98%)	612 (93%)	48 (7%)	16	38

All (48) 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	1131	LEU
1	A	1143	ILE
1	A	1156	MET
1	A	1176	VAL
1	A	1185	LEU
1	A	1190	ASN
1	A	1232	ARG
1	A	1235	THR
1	A	1239	ASP
1	A	1268	LEU

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Mol	Chain	Res	Type
1	A	1269	THR
1	A	1309	ASN
1	A	1358	GLN
1	A	1374	ASN
1	A	1383	LEU
1	A	1391	ARG
1	A	1417	GLU
1	B	2008	LYS
1	B	2037	VAL
1	B	2040	GLN
1	B	2059	ARG
1	B	2103	LEU
1	B	2131	LEU
1	B	2143	ILE
1	B	2156	MET
1	B	2159	VAL
1	B	2168	LEU
1	B	2170	LEU
1	B	2173	SER
1	B	2185	LEU
1	B	2187	THR
1	B	2232	ARG
1	B	2234	ILE
1	B	2235	THR
1	B	2239	ASP
1	B	2268	LEU
1	B	2269	THR
1	B	2306	LEU
1	B	2309	ASN
1	B	2350	THR
1	B	2358	GLN
1	B	2374	ASN
1	B	2383	LEU
1	B	2391	ARG
1	B	2417	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1040	GLN
1	A	1058	ASN
1	A	1074	HIS

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Mol	Chain	Res	Type
1	A	1190	ASN
1	A	1292	GLN
1	A	1348	GLN
1	A	1352	HIS
1	A	1373	HIS
1	A	1374	ASN
1	B	2040	GLN
1	B	2058	ASN
1	B	2074	HIS
1	B	2190	ASN
1	B	2217	ASN
1	B	2292	GLN
1	B	2348	GLN
1	B	2352	HIS
1	B	2358	GLN
1	B	2373	HIS
1	B	2374	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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
2	KE4	A	5000	-	20,24,24	1.87	6 (30%)	24,33,33	2.68	7 (29%)
4	HOZ	B	2	-	5,8,8	1.24	1 (20%)	2,9,9	1.79	1 (50%)
3	PLP	B	6000	1	15,15,16	1.39	1 (6%)	20,22,23	1.08	1 (5%)

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	KE4	A	5000	-	1/1/3/4	0/16/18/18	0/1/1/1
4	HOZ	B	2	-	-	0/5/7/7	0/0/0/0
3	PLP	B	6000	1	-	0/6/6/8	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5000	KE4	CA-N4A	-4.88	1.35	1.48
3	B	6000	PLP	C3-C2	-3.45	1.38	1.40
2	A	5000	KE4	C4A-N4A	-2.32	1.39	1.46
2	A	5000	KE4	C2A-C2	2.21	1.54	1.50
2	A	5000	KE4	CB-CA	2.22	1.57	1.53
4	B	2	HOZ	CB-CA	2.61	1.57	1.53
2	A	5000	KE4	C4A-C4	2.80	1.55	1.51
2	A	5000	KE4	C2-N1	3.11	1.40	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5000	KE4	OP3-P-OP2	-3.45	93.71	107.61
2	A	5000	KE4	C5-C6-N1	-2.52	119.60	123.87
3	B	6000	PLP	O3P-P-O1P	2.49	120.26	110.50
4	B	2	HOZ	CB-CA-C	2.52	114.17	109.71
2	A	5000	KE4	C6-C5-C4	3.27	120.56	118.13
2	A	5000	KE4	OP3-P-OP1	3.38	123.72	110.50
2	A	5000	KE4	C4-C4A-N4A	5.25	126.23	111.78
2	A	5000	KE4	C4A-N4A-CA	5.79	122.82	114.11
2	A	5000	KE4	CB-CA-C	7.22	121.63	109.64

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	5000	KE4	CA

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5000	KE4	5	0
4	B	2	HOZ	4	0
3	B	6000	PLP	1	0

## 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%)	-0.19	1 (0%) 94 96	11, 26, 40, 51	0
1	B	427/432 (98%)	-0.04	14 (3%) 47 46	12, 26, 47, 78	0
All	All	854/864 (98%)	-0.11	15 (1%) 69 70	11, 26, 42, 78	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2166	ALA	4.8
1	B	2169	GLY	4.1
1	B	2167	THR	4.0
1	B	2165	VAL	3.7
1	B	2159	VAL	3.6
1	B	2170	LEU	3.6
1	B	2168	LEU	3.4
1	B	2171	PRO	2.9
1	B	2415	THR	2.8
1	B	2178	LYS	2.7
1	B	2173	SER	2.6
1	A	1382	ASP	2.3
1	B	2164	GLY	2.2
1	B	2432	ALA	2.0
1	B	2203	PRO	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.



## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	HOZ	B	2	9/9	0.77	0.37	4.56	67,69,70,70	0
2	KE4	A	5000	24/24	0.92	0.19	2.01	31,36,44,45	0
3	PLP	B	6000	15/16	0.96	0.12	-0.81	17,20,24,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.