



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2025 – 04:05 PM EDT

PDB ID : 1IAX  
Title : CRYSTAL STRUCTURE OF ACC SYNTHASE COMPLEXED WITH PLP  
Authors : Huai, Q.; Xia, Y.; Chen, Y.; Callahan, B.; Li, N.; Ke, H.  
Deposited on : 2001-03-24  
Resolution : 2.80 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  
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

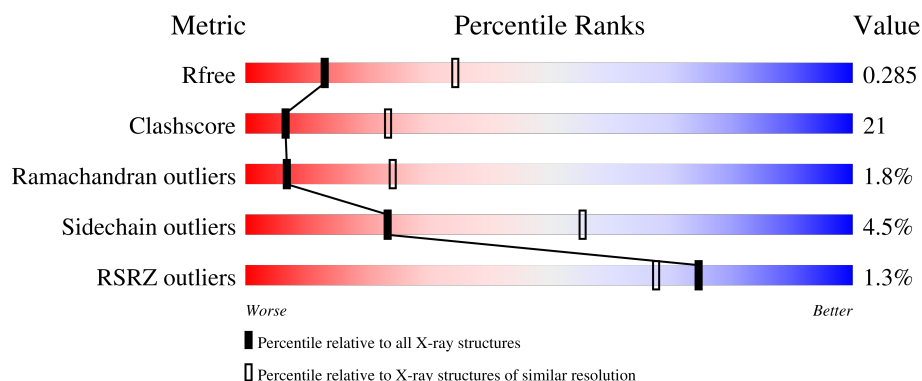
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


The reported resolution of this entry is 2.80 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	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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	428	
1	B	428	

## 2 Entry composition [i](#)

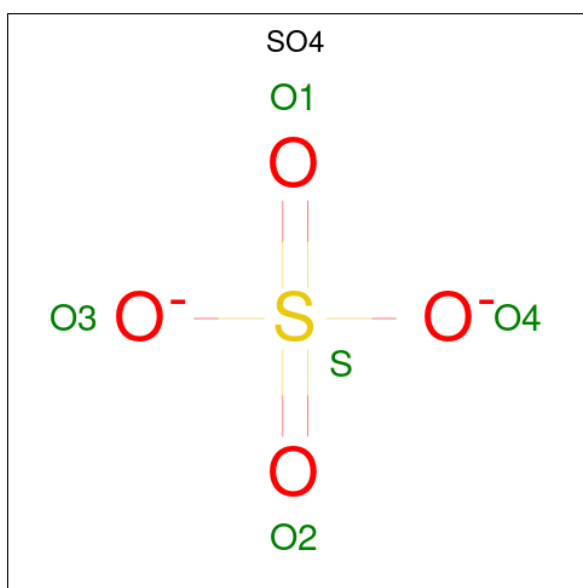
There are 4 unique types of molecules in this entry. The entry contains 6679 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 1-AMINOCYCLOPROPANE-1-CARBOXYLATE SYNTHASE 2.

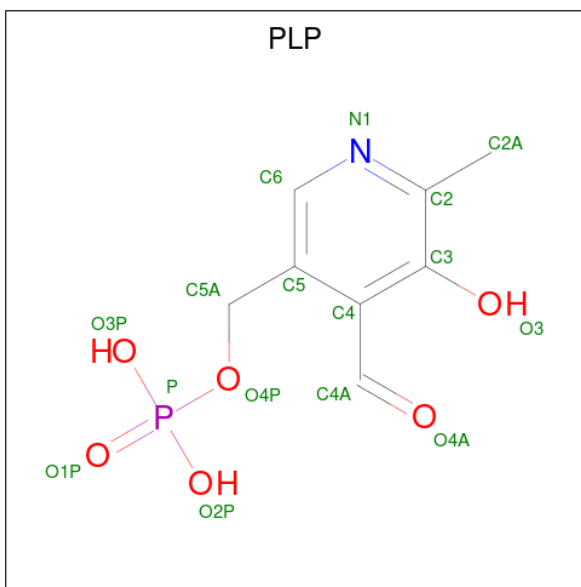
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3310	2112	566	611	21			
1	B	417	Total	C	N	O	S	0	0	0
			3310	2112	566	611	21			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



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

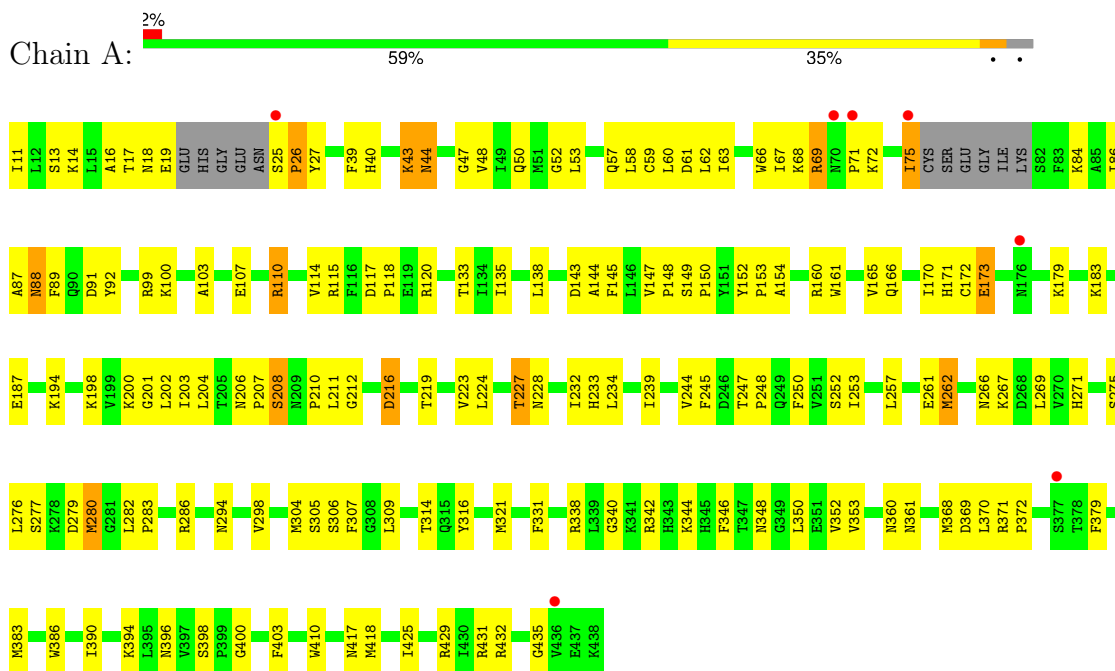
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	11	Total	O	0	0
			11	11		
4	B	8	Total	O	0	0
			8	8		

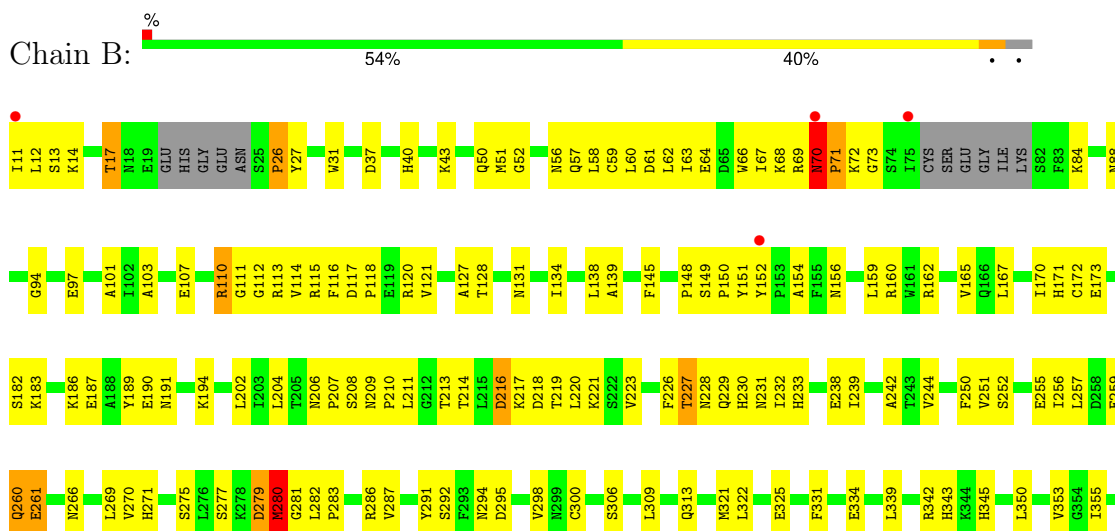
### 3 Residue-property plots

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: 1-AMINOCYCLOPROPANE-1-CARBOXYLATE SYNTHASE 2



#### • Molecule 1: 1-AMINOCYCLOPROPANE-1-CARBOXYLATE SYNTHASE 2



N360	N361	A362	G363	L364
N368	D369	L370	R371	P372
L373	L374			
T378	F379			
E382				
R387	V388	I389		
V393				
N396				
P399				
S402				
C405	Q406	E407	P408	
N417	M418	D419		
T422	V423	D424	T425	A426
I430	R431	R432	F433	V434
G435	V436	E437	K438	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.20Å 123.20Å 212.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.80) 95.9 (50.00-2.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.65 (at 2.80Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.218 , 0.293 0.215 , 0.285	Depositor DCC
$R_{free}$ test set	2366 reflections (9.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.7	Xtrriage
Anisotropy	0.168	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 40.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6679	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1071e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: PLP, SO4

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	0.41	0/3384	0.63	0/4573
1	B	0.41	0/3384	0.64	0/4573
All	All	0.41	0/6768	0.64	0/9146

There are no bond length outliers.

There are no bond angle outliers.

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	3310	0	3274	126	0
1	B	3310	0	3274	169	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	15	0	7	1	0
3	B	15	0	7	0	0
4	A	11	0	0	1	0
4	B	8	0	0	1	0
All	All	6679	0	6562	281	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 21.

All (281) 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:110:ARG:HG2	1:A:252:SER:HB2	1.45	0.96
1:B:40:HIS:HD2	1:B:43:LYS:H	1.05	0.96
1:B:50:GLN:HE22	1:B:396:ASN:HD22	1.20	0.89
1:B:110:ARG:HG2	1:B:252:SER:HB2	1.56	0.88
1:A:194:LYS:HE2	1:A:194:LYS:HA	1.55	0.87
1:B:40:HIS:CD2	1:B:43:LYS:H	1.92	0.87
1:B:69:ARG:O	1:B:71:PRO:HA	1.78	0.83
1:B:228:ASN:HD21	1:B:266:ASN:H	1.26	0.83
1:B:437:GLU:O	1:B:438:LYS:HB2	1.76	0.83
1:A:57:GLN:NE2	1:A:417:ASN:HB2	1.96	0.81
1:B:40:HIS:HD2	1:B:43:LYS:N	1.80	0.80
1:B:242:ALA:HB3	1:B:279:ASP:CB	2.13	0.78
1:A:152:TYR:CE2	1:A:154:ALA:HB3	2.19	0.77
1:A:309:LEU:HB2	1:B:286:ARG:HD2	1.66	0.77
1:A:48:VAL:HA	1:A:394:LYS:O	1.86	0.76
1:A:228:ASN:ND2	1:A:266:ASN:H	1.84	0.75
1:B:13:SER:O	1:B:17:THR:HB	1.86	0.75
1:B:57:GLN:HE21	1:B:417:ASN:HB2	1.52	0.74
1:B:50:GLN:HE22	1:B:396:ASN:ND2	1.84	0.74
1:B:227:THR:HG23	1:B:232:ILE:O	1.88	0.73
1:A:60:LEU:HD13	1:B:84:LYS:HG2	1.71	0.73
1:B:72:LYS:HG3	1:B:73:GLY:N	2.04	0.71
1:B:50:GLN:NE2	1:B:396:ASN:HD22	1.89	0.70
1:B:171:HIS:NE2	1:B:173:GLU:HG3	2.05	0.70
1:B:228:ASN:HD21	1:B:266:ASN:N	1.88	0.69
1:A:198:LYS:HD3	1:A:200:LYS:HE2	1.75	0.69
1:B:242:ALA:HB3	1:B:279:ASP:HB2	1.73	0.69
1:A:369:ASP:HB2	1:A:410:TRP:CZ3	2.27	0.69
1:A:348:ASN:O	1:A:352:VAL:HG23	1.92	0.68
1:B:194:LYS:HA	1:B:194:LYS:HE2	1.77	0.67
1:A:314:THR:HA	1:B:313:GLN:HE22	1.59	0.67
1:A:183:LYS:O	1:A:187:GLU:HG3	1.95	0.67
1:A:63:ILE:O	1:A:67:ILE:HG13	1.95	0.67
1:A:171:HIS:NE2	1:A:173:GLU:HG2	2.09	0.67
1:A:294:ASN:O	1:A:298:VAL:HG23	1.94	0.67
1:B:50:GLN:NE2	1:B:52:GLY:H	1.94	0.66
1:B:355:ILE:HD11	1:B:434:VAL:HG21	1.78	0.66
1:B:368:MET:HE3	1:B:370:LEU:HD11	1.79	0.65
1:B:40:HIS:CD2	1:B:43:LYS:HG3	2.32	0.65
1:A:212:GLY:O	1:A:360:ASN:HB2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:TRP:O	1:A:390:ILE:HG23	1.98	0.64
1:B:233:HIS:HD2	1:B:271:HIS:NE2	1.95	0.64
1:B:72:LYS:HG3	1:B:73:GLY:H	1.62	0.64
1:A:286:ARG:HD2	1:B:309:LEU:HB2	1.78	0.63
1:A:305:SER:O	1:A:309:LEU:HG	1.99	0.63
1:B:257:LEU:HD11	1:B:270:VAL:HG11	1.79	0.63
1:B:233:HIS:CD2	1:B:271:HIS:NE2	2.66	0.63
1:A:138:LEU:HD22	1:A:233:HIS:CD2	2.34	0.63
1:B:118:PRO:HA	1:B:121:VAL:HG23	1.81	0.63
1:A:144:ALA:HB2	1:A:166:GLN:HG3	1.80	0.63
1:A:149:SER:O	1:A:172:CYS:HB2	1.99	0.63
1:A:208:SER:OG	1:A:211:LEU:HB2	1.98	0.63
1:A:353:VAL:CG1	1:A:431:ARG:HG3	2.29	0.62
1:A:40:HIS:CD2	1:A:43:LYS:HE3	2.34	0.62
1:A:179:LYS:HZ1	1:A:216:ASP:HB2	1.65	0.61
1:B:399:PRO:O	1:B:402:SER:HB3	1.99	0.61
1:A:89:PHE:CE1	1:A:91:ASP:HB3	2.36	0.61
1:A:92:TYR:CZ	1:A:306:SER:HB3	2.35	0.61
1:A:228:ASN:HD21	1:A:266:ASN:H	1.47	0.61
1:A:110:ARG:HG2	1:A:252:SER:CB	2.24	0.60
1:B:152:TYR:CE2	1:B:154:ALA:HB3	2.36	0.60
1:B:59:CYS:SG	1:B:62:LEU:HD12	2.41	0.60
1:B:350:LEU:HB3	1:B:355:ILE:HB	1.83	0.60
1:B:244:VAL:HG21	1:B:250:PHE:HB2	1.84	0.59
1:A:280:MET:HE1	1:A:331:PHE:CD2	2.38	0.59
1:A:371:ARG:N	1:A:372:PRO:HD2	2.18	0.58
1:B:219:THR:O	1:B:223:VAL:HG23	2.04	0.58
1:A:58:LEU:HD21	1:A:342:ARG:HH21	1.68	0.58
1:A:103:ALA:O	1:A:107:GLU:HG3	2.03	0.58
1:A:369:ASP:HB2	1:A:410:TRP:CH2	2.38	0.58
1:B:50:GLN:HE21	1:B:52:GLY:H	1.51	0.58
1:B:182:SER:O	1:B:186:LYS:HG3	2.04	0.58
1:A:244:VAL:HG21	1:A:250:PHE:HB2	1.86	0.58
1:A:257:LEU:HD13	1:A:267:LYS:HG2	1.86	0.58
1:B:111:GLY:C	1:B:113:ARG:H	2.07	0.58
1:B:183:LYS:O	1:B:187:GLU:HG3	2.03	0.57
1:B:426:ALA:O	1:B:430:ILE:HG13	2.02	0.57
1:A:279:ASP:O	1:A:280:MET:HG2	2.05	0.57
1:A:276:LEU:HD22	1:A:280:MET:HG3	1.86	0.57
1:B:63:ILE:O	1:B:67:ILE:HG13	2.05	0.57
1:A:194:LYS:HE2	1:A:194:LYS:CA	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:THR:HA	1:A:248:PRO:O	2.06	0.56
1:A:227:THR:HG21	1:A:234:LEU:HB2	1.87	0.56
1:A:84:LYS:HE3	1:B:64:GLU:CD	2.26	0.56
1:A:400:GLY:HA3	4:A:602:HOH:O	2.05	0.55
1:B:418:MET:HG3	1:B:422:THR:HB	1.88	0.55
1:A:58:LEU:HD21	1:A:342:ARG:NH2	2.21	0.55
1:A:368:MET:CE	1:A:370:LEU:HD11	2.36	0.55
1:A:39:PHE:HB2	1:A:47:GLY:O	2.06	0.55
1:A:286:ARG:HH22	3:A:500:PLP:P	2.29	0.55
1:B:418:MET:SD	1:B:423:VAL:HG22	2.46	0.55
1:A:257:LEU:HD13	1:A:267:LYS:HE2	1.89	0.55
1:A:353:VAL:HG11	1:A:431:ARG:HG3	1.87	0.55
1:A:144:ALA:CB	1:A:166:GLN:HG3	2.37	0.55
1:B:353:VAL:HG12	1:B:431:ARG:HG3	1.89	0.54
1:A:16:ALA:HA	1:B:300:CYS:SG	2.48	0.54
1:A:100:LYS:HA	1:A:118:PRO:HB3	1.90	0.54
1:B:202:LEU:HD23	1:B:202:LEU:C	2.28	0.54
1:B:353:VAL:CG1	1:B:431:ARG:HG3	2.38	0.54
1:A:216:ASP:OD1	1:A:219:THR:N	2.40	0.54
1:A:304:MET:CE	1:B:162:ARG:HD3	2.37	0.54
1:A:143:ASP:OD2	1:A:200:LYS:HE3	2.09	0.53
1:A:340:GLY:O	1:A:344:LYS:HD3	2.08	0.53
1:B:97:GLU:CD	1:B:97:GLU:H	2.11	0.53
1:B:152:TYR:CZ	1:B:154:ALA:HB3	2.44	0.53
1:B:419:ASP:O	1:B:423:VAL:HG23	2.08	0.53
1:A:144:ALA:HB2	1:A:166:GLN:CG	2.38	0.53
1:B:221:LYS:HE2	1:B:259:GLU:OE1	2.08	0.53
1:A:342:ARG:NH2	1:A:418:MET:O	2.41	0.53
1:B:279:ASP:O	1:B:280:MET:CG	2.57	0.53
1:A:84:LYS:HG2	1:B:60:LEU:HB3	1.91	0.53
1:B:213:THR:HG22	1:B:360:ASN:HA	1.90	0.53
1:A:59:CYS:HB3	1:A:62:LEU:HD12	1.91	0.53
1:A:88:ASN:O	1:A:88:ASN:ND2	2.42	0.53
1:B:110:ARG:CG	1:B:252:SER:HB2	2.32	0.52
1:A:40:HIS:NE2	1:A:43:LYS:HE3	2.24	0.52
1:B:50:GLN:HE21	1:B:51:MET:N	2.06	0.52
1:A:120:ARG:NH1	1:A:298:VAL:HG21	2.24	0.52
1:B:120:ARG:NH1	1:B:292:SER:O	2.40	0.51
1:A:307:PHE:CD1	1:B:128:THR:HG22	2.46	0.51
1:B:107:GLU:OE2	1:B:115:ARG:HG2	2.10	0.51
1:A:239:ILE:HG13	1:A:275:SER:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:THR:HG23	1:A:304:MET:SD	2.50	0.51
1:A:261:GLU:C	1:A:262:MET:HG2	2.31	0.51
1:B:343:HIS:CD2	1:B:360:ASN:HD21	2.28	0.51
1:B:110:ARG:HG2	1:B:252:SER:CB	2.36	0.51
1:B:148:PRO:HA	1:B:170:ILE:HB	1.92	0.51
1:B:110:ARG:NH1	1:B:238:GLU:OE1	2.44	0.51
1:A:50:GLN:HE21	1:A:52:GLY:H	1.58	0.50
1:B:279:ASP:O	1:B:280:MET:HG2	2.11	0.50
1:B:353:VAL:HG23	1:B:355:ILE:HG13	1.93	0.50
1:A:179:LYS:NZ	1:A:216:ASP:HB2	2.26	0.50
1:A:280:MET:HE1	1:A:331:PHE:CE2	2.47	0.50
1:B:280:MET:O	1:B:282:LEU:HG	2.12	0.50
1:A:26:PRO:HG2	1:A:27:TYR:H	1.76	0.50
1:B:294:ASN:O	1:B:298:VAL:HG23	2.12	0.50
1:B:66:TRP:CH2	1:B:321:MET:HA	2.47	0.49
1:B:275:SER:HA	1:B:287:VAL:O	2.12	0.49
1:B:14:LYS:HA	1:B:17:THR:HG22	1.94	0.49
1:A:223:VAL:O	1:A:227:THR:HB	2.12	0.49
1:B:217:LYS:HG2	1:B:221:LYS:HE3	1.94	0.49
1:B:228:ASN:ND2	1:B:266:ASN:H	2.05	0.49
1:A:233:HIS:HD2	1:A:271:HIS:NE2	2.11	0.49
1:A:206:ASN:HA	1:A:207:PRO:C	2.33	0.49
1:B:389:ILE:HA	1:B:393:VAL:CG2	2.42	0.49
1:A:11:ILE:HG13	1:B:231:ASN:HD21	1.78	0.48
1:A:432:ARG:O	1:A:435:GLY:N	2.47	0.48
1:B:256:ILE:O	1:B:256:ILE:HG22	2.12	0.48
1:B:379:PHE:HZ	1:B:405:CYS:O	1.95	0.48
1:B:379:PHE:CZ	1:B:405:CYS:O	2.66	0.48
1:A:171:HIS:NE2	1:A:173:GLU:CG	2.75	0.48
1:B:280:MET:HG2	1:B:331:PHE:CE2	2.48	0.48
1:A:14:LYS:HA	1:A:17:THR:HG22	1.95	0.48
1:B:208:SER:OG	1:B:211:LEU:HB2	2.13	0.48
1:B:233:HIS:HA	1:B:269:LEU:HB3	1.94	0.48
1:B:389:ILE:HA	1:B:393:VAL:HB	1.95	0.48
1:B:127:ALA:HB2	1:B:239:ILE:CD1	2.43	0.48
1:B:183:LYS:HG2	1:B:187:GLU:OE1	2.14	0.48
1:B:239:ILE:HD11	1:B:275:SER:HB3	1.95	0.48
1:A:86:ILE:HG13	1:A:87:ALA:N	2.29	0.47
1:A:67:ILE:O	1:A:67:ILE:HG22	2.13	0.47
1:A:143:ASP:O	1:A:166:GLN:HG2	2.14	0.47
1:B:156:ASN:O	1:B:160:ARG:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:GLN:HE21	1:B:417:ASN:CB	2.22	0.47
1:A:276:LEU:O	1:A:280:MET:HB2	2.14	0.47
1:B:111:GLY:C	1:B:113:ARG:N	2.68	0.47
1:A:135:ILE:CG2	1:A:165:VAL:HG21	2.45	0.47
1:B:59:CYS:HB3	1:B:331:PHE:HE1	1.80	0.47
1:B:58:LEU:HD12	1:B:339:LEU:HD23	1.97	0.47
1:B:111:GLY:O	1:B:113:ARG:N	2.49	0.46
1:B:139:ALA:HB3	1:B:165:VAL:HG21	1.97	0.46
1:B:306:SER:HA	1:B:309:LEU:HG	1.97	0.46
1:B:436:VAL:HG12	1:B:436:VAL:O	2.14	0.46
1:A:84:LYS:HE3	1:B:64:GLU:OE1	2.15	0.46
1:B:26:PRO:HG2	1:B:27:TYR:H	1.80	0.46
1:A:245:PHE:CE1	1:A:361:ASN:HA	2.50	0.46
1:B:94:GLY:HA2	4:B:607:HOH:O	2.14	0.46
1:B:433:PHE:O	1:B:437:GLU:HG2	2.15	0.46
1:B:57:GLN:NE2	1:B:417:ASN:HB2	2.25	0.46
1:B:116:PHE:HD2	1:B:291:TYR:CZ	2.34	0.46
1:B:220:LEU:HB3	1:B:256:ILE:HD12	1.98	0.46
1:B:101:ALA:HB1	1:B:322:LEU:HB2	1.97	0.46
1:B:114:VAL:CG1	1:B:255:GLU:HA	2.46	0.46
1:B:244:VAL:HA	1:B:362:ALA:HB2	1.97	0.46
1:A:17:THR:C	1:A:19:GLU:H	2.19	0.46
1:A:202:LEU:C	1:A:202:LEU:HD23	2.35	0.46
1:B:371:ARG:N	1:B:372:PRO:HD2	2.30	0.46
1:A:368:MET:HE2	1:A:370:LEU:HD11	1.97	0.46
1:B:186:LYS:O	1:B:190:GLU:HG3	2.15	0.46
1:B:206:ASN:O	1:B:238:GLU:HA	2.15	0.46
1:A:280:MET:O	1:A:282:LEU:HG	2.16	0.46
1:B:114:VAL:HG13	1:B:255:GLU:HG2	1.98	0.45
1:B:138:LEU:HD11	1:B:271:HIS:CD2	2.51	0.45
1:B:374:LEU:HD21	1:B:382:GLU:HA	1.98	0.45
1:A:227:THR:HG22	1:A:228:ASN:N	2.30	0.45
1:B:14:LYS:O	1:B:17:THR:HG22	2.16	0.45
1:A:239:ILE:HG12	1:A:239:ILE:O	2.16	0.45
1:A:148:PRO:HA	1:A:170:ILE:HB	1.99	0.45
1:A:149:SER:HA	1:A:150:PRO:C	2.37	0.45
1:B:66:TRP:NE1	1:B:70:ASN:O	2.50	0.45
1:B:368:MET:CE	1:B:370:LEU:HD11	2.44	0.45
1:A:84:LYS:HB3	1:B:60:LEU:HD13	1.99	0.45
1:B:399:PRO:HG2	1:B:402:SER:HB2	1.97	0.45
1:A:201:GLY:HA2	1:A:232:ILE:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:PRO:HG2	1:A:204:LEU:HD23	1.99	0.44
1:A:13:SER:O	1:A:17:THR:HG22	2.18	0.44
1:B:66:TRP:CZ2	1:B:321:MET:HA	2.52	0.44
1:B:117:ASP:HA	1:B:118:PRO:HD2	1.84	0.44
1:A:66:TRP:CZ2	1:A:321:MET:HA	2.52	0.44
1:B:216:ASP:OD1	1:B:218:ASP:N	2.51	0.44
1:B:148:PRO:HG2	1:B:204:LEU:CD2	2.48	0.44
1:B:382:GLU:OE1	1:B:408:PRO:HA	2.17	0.44
1:A:277:SER:OG	1:A:283:PRO:HA	2.18	0.43
1:A:398:SER:HB3	1:A:403:PHE:HE1	1.83	0.43
1:B:353:VAL:HG11	1:B:431:ARG:HA	2.00	0.43
1:A:179:LYS:NZ	1:A:216:ASP:CB	2.82	0.43
1:A:72:LYS:HD2	1:A:72:LYS:HA	1.84	0.43
1:A:53:LEU:HD23	1:A:53:LEU:HA	1.81	0.43
1:B:131:ASN:O	1:B:134:ILE:HG22	2.17	0.43
1:B:260:GLN:CG	1:B:261:GLU:N	2.82	0.43
1:B:229:GLN:HB3	1:B:230:HIS:HD2	1.83	0.43
1:A:224:LEU:HD22	1:A:253:ILE:HD11	2.01	0.43
1:B:231:ASN:O	1:B:231:ASN:CG	2.57	0.43
1:B:277:SER:O	1:B:281:GLY:HA2	2.19	0.43
1:A:68:LYS:O	1:A:69:ARG:CG	2.67	0.43
1:A:72:LYS:HB3	1:A:316:TYR:OH	2.19	0.43
1:B:148:PRO:O	1:B:151:TYR:HB3	2.18	0.43
1:B:103:ALA:O	1:B:107:GLU:HG3	2.19	0.43
1:B:120:ARG:NH2	1:B:295:ASP:OD1	2.52	0.43
1:B:206:ASN:HA	1:B:207:PRO:C	2.38	0.43
1:B:207:PRO:HG3	1:B:214:THR:HG22	2.01	0.43
1:B:260:GLN:HG2	1:B:261:GLU:N	2.33	0.42
1:A:198:LYS:CD	1:A:200:LYS:HE2	2.48	0.42
1:A:202:LEU:HD23	1:A:203:ILE:N	2.34	0.42
1:B:131:ASN:HB3	1:B:159:LEU:CD2	2.49	0.42
1:A:43:LYS:O	1:A:44:ASN:HB2	2.19	0.42
1:B:345:HIS:CE1	1:B:424:ASP:OD1	2.72	0.42
1:B:71:PRO:HG2	1:B:72:LYS:N	2.34	0.42
1:B:127:ALA:HB2	1:B:239:ILE:HD12	2.01	0.42
1:A:60:LEU:HD23	1:A:60:LEU:HA	1.80	0.42
1:B:220:LEU:HD23	1:B:220:LEU:HA	1.84	0.42
1:A:371:ARG:N	1:A:372:PRO:CD	2.81	0.41
1:B:271:HIS:HD1	1:B:292:SER:HG	1.68	0.41
1:A:160:ARG:HE	1:A:160:ARG:HB2	1.70	0.41
1:A:346:PHE:CE2	1:A:350:LEU:HD11	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:PHE:O	1:A:383:MET:HG2	2.20	0.41
1:B:14:LYS:HA	1:B:17:THR:CG2	2.50	0.41
1:B:97:GLU:CD	1:B:97:GLU:N	2.74	0.41
1:B:149:SER:HA	1:B:150:PRO:C	2.40	0.41
1:B:160:ARG:HD2	1:B:167:LEU:HG	2.01	0.41
1:B:56:ASN:HB2	1:B:364:LEU:HD13	2.01	0.41
1:B:189:TYR:CD2	1:B:226:PHE:HZ	2.38	0.41
1:B:231:ASN:HA	1:B:269:LEU:HD11	2.03	0.41
1:A:61:ASP:OD1	1:A:338:ARG:NH1	2.51	0.41
1:B:64:GLU:O	1:B:68:LYS:HG3	2.20	0.41
1:A:50:GLN:HE22	1:A:396:ASN:HD22	1.68	0.41
1:B:114:VAL:HG11	1:B:255:GLU:HA	2.03	0.41
1:A:84:LYS:CB	1:B:60:LEU:HD13	2.51	0.41
1:A:99:ARG:HD2	1:A:118:PRO:O	2.20	0.41
1:B:127:ALA:CB	1:B:239:ILE:HD12	2.51	0.41
1:A:114:VAL:HG22	1:A:115:ARG:N	2.36	0.41
1:A:117:ASP:HA	1:A:118:PRO:HD2	1.98	0.41
1:A:152:TYR:HA	1:A:153:PRO:HD2	1.93	0.41
1:A:233:HIS:HE1	1:B:11:ILE:O	2.04	0.41
1:B:12:LEU:HD23	1:B:12:LEU:HA	1.91	0.41
1:B:342:ARG:NH2	1:B:418:MET:O	2.54	0.41
1:B:233:HIS:CD2	1:B:269:LEU:HA	2.56	0.41
1:B:374:LEU:HD23	1:B:374:LEU:HA	1.89	0.41
1:B:61:ASP:HA	1:B:64:GLU:OE1	2.21	0.40
1:B:387:ARG:HH11	1:B:387:ARG:HB3	1.86	0.40
1:B:434:VAL:O	1:B:437:GLU:HB2	2.20	0.40
1:B:31:TRP:CE3	1:B:31:TRP:HA	2.56	0.40
1:B:40:HIS:CD2	1:B:43:LYS:CG	3.04	0.40
1:B:56:ASN:HD22	1:B:364:LEU:HD21	1.86	0.40
1:B:149:SER:O	1:B:172:CYS:HB2	2.21	0.40
1:B:282:LEU:N	1:B:283:PRO:CD	2.84	0.40
1:B:152:TYR:HB2	1:B:209:ASN:HD22	1.87	0.40
1:B:171:HIS:CE1	1:B:173:GLU:HG3	2.56	0.40
1:A:72:LYS:HE2	1:A:75:ILE:HG13	2.03	0.40
1:A:425:ILE:O	1:A:429:ARG:HG3	2.22	0.40
1:B:407:GLU:HA	1:B:408:PRO:HD3	1.89	0.40

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	411/428 (96%)	381 (93%)	23 (6%)	7 (2%)	7	26
1	B	411/428 (96%)	375 (91%)	28 (7%)	8 (2%)	6	23
All	All	822/856 (96%)	756 (92%)	51 (6%)	15 (2%)	7	24

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	PRO
1	A	161	TRP
1	A	280	MET
1	B	26	PRO
1	B	70	ASN
1	B	71	PRO
1	B	280	MET
1	B	261	GLU
1	A	18	ASN
1	A	26	PRO
1	A	69	ARG
1	B	112	GLY
1	B	436	VAL
1	B	37	ASP
1	A	44	ASN

### 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	364/373 (98%)	350 (96%)	14 (4%)	28	62
1	B	364/373 (98%)	345 (95%)	19 (5%)	19	50
All	All	728/746 (98%)	695 (96%)	33 (4%)	23	55

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

Mol	Chain	Res	Type
1	A	25	SER
1	A	43	LYS
1	A	75	ILE
1	A	88	ASN
1	A	110	ARG
1	A	145	PHE
1	A	147	VAL
1	A	173	GLU
1	A	208	SER
1	A	210	PRO
1	A	216	ASP
1	A	227	THR
1	A	262	MET
1	A	269	LEU
1	B	17	THR
1	B	70	ASN
1	B	88	ASN
1	B	110	ARG
1	B	145	PHE
1	B	191	ASN
1	B	210	PRO
1	B	216	ASP
1	B	227	THR
1	B	251	VAL
1	B	260	GLN
1	B	279	ASP
1	B	280	MET
1	B	325	GLU
1	B	334	GLU
1	B	360	ASN
1	B	378	THR
1	B	387	ARG
1	B	418	MET

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

Mol	Chain	Res	Type
1	A	46	ASN
1	A	50	GLN
1	A	57	GLN
1	A	88	ASN
1	A	90	GLN
1	A	228	ASN
1	A	233	HIS
1	A	313	GLN
1	A	345	HIS
1	B	40	HIS
1	B	50	GLN
1	B	57	GLN
1	B	70	ASN
1	B	88	ASN
1	B	228	ASN
1	B	231	ASN
1	B	233	HIS
1	B	313	GLN
1	B	360	ASN
1	B	391	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 ⓘ

4 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	A	500	1	15,15,16	1.42	1 (6%)	21,22,23	0.89	0
2	SO4	A	600	-	4,4,4	0.26	0	6,6,6	0.30	0
2	SO4	B	601	-	4,4,4	0.23	0	6,6,6	0.32	0
3	PLP	B	501	1	15,15,16	1.44	3 (20%)	21,22,23	0.93	1 (4%)

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	A	500	1	-	2/6/6/8	0/1/1/1
3	PLP	B	501	1	-	0/6/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	PLP	C6-C5	2.29	1.42	1.37
3	B	501	PLP	C5-C4	2.15	1.43	1.40
3	B	501	PLP	C6-C5	2.13	1.41	1.37
3	B	501	PLP	C2-N1	2.10	1.37	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	PLP	C5-C6-N1	-2.00	120.57	123.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	500	PLP	C4-C5-C5A-O4P
3	A	500	PLP	C6-C5-C5A-O4P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	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	417/428 (97%)	-0.16	7 (1%) 69 61	30, 52, 85, 101	0
1	B	417/428 (97%)	-0.14	4 (0%) 79 73	32, 53, 82, 101	0
All	All	834/856 (97%)	-0.15	11 (1%) 74 67	30, 53, 83, 101	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	ASN	5.2
1	B	75	ILE	4.2
1	A	75	ILE	3.7
1	B	11	ILE	2.5
1	A	25	SER	2.4
1	A	71	PRO	2.3
1	A	377	SER	2.1
1	A	176	ASN	2.0
1	B	152	TYR	2.0
1	B	70	ASN	2.0
1	A	436	VAL	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 [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
3	PLP	B	501	15/16	0.63	0.31	78,85,90,90	1
3	PLP	A	500	15/16	0.64	0.30	86,90,92,92	1
2	SO4	A	600	5/5	0.90	0.11	47,47,49,51	1
2	SO4	B	601	5/5	0.92	0.12	53,54,55,56	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.