Full wwPDB X-ray Structure Validation Report (i)

Aug 3, 2023 – 03:21 AM EDT

PDB ID	:	1IBJ
Title	:	Crystal structure of cystathionine beta-lyase from Arabidopsis thaliana
Authors	:	Breitinger, U.; Clausen, T.; Messerschmidt, A.
Deposited on	:	2001-03-28
Resolution	:	2.30 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

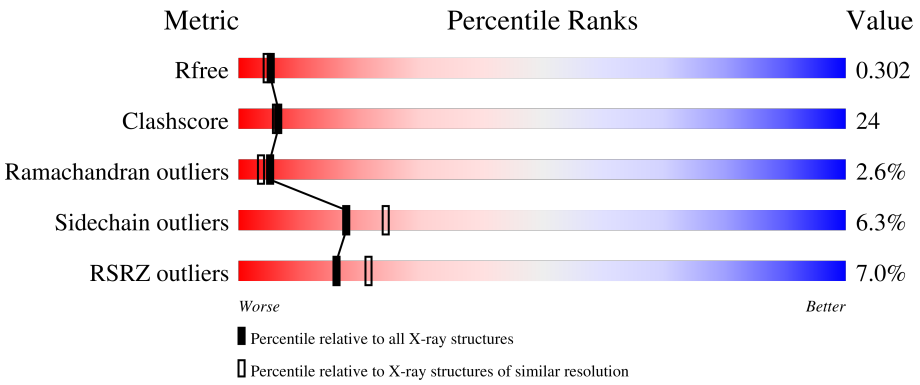
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 >=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 <=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	464	5% 50% 28% • 18%
1	C	464	6% 48% 31% • 18%

2 Entry composition (i)

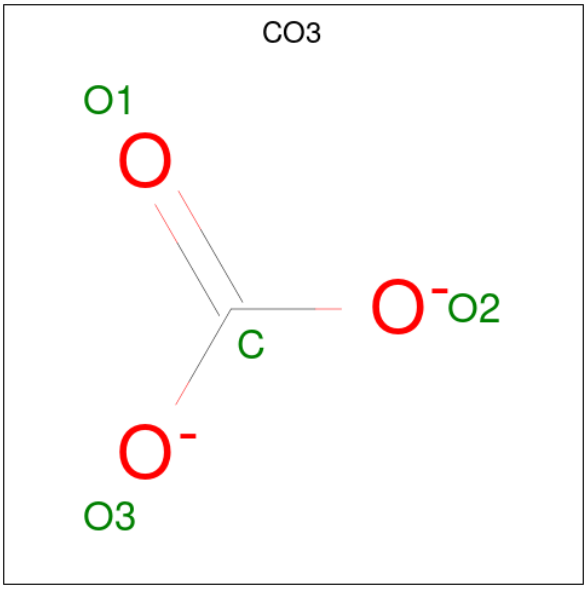
There are 5 unique types of molecules in this entry. The entry contains 5965 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CYSTATHIONINE BETA-LYASE.

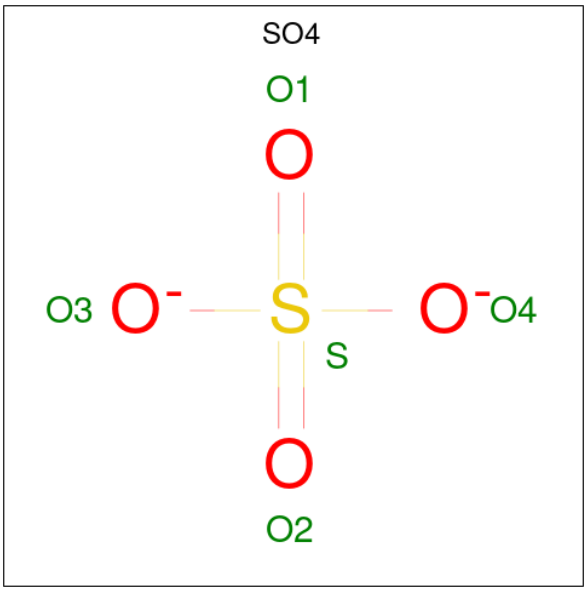
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	380	2834	1798	483	541	12	0	0	0
1	C	380	2835	1798	483	541	13	0	0	0

- Molecule 2 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).



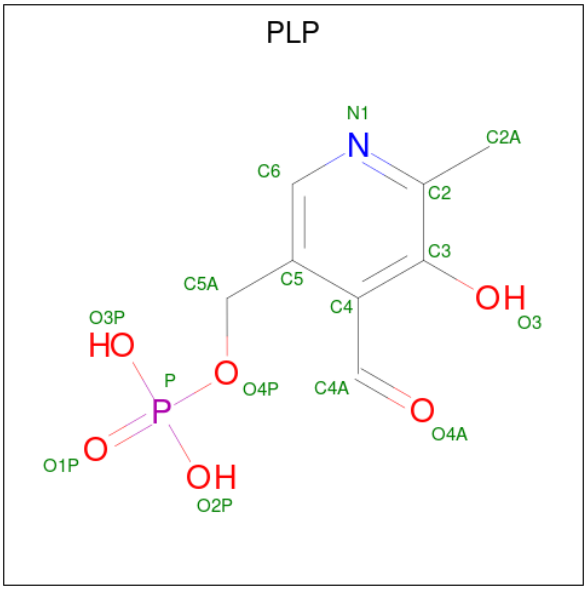
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	4	1	3	0	0
2	C	1	4	1	3	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



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

- Molecule 5 is water.

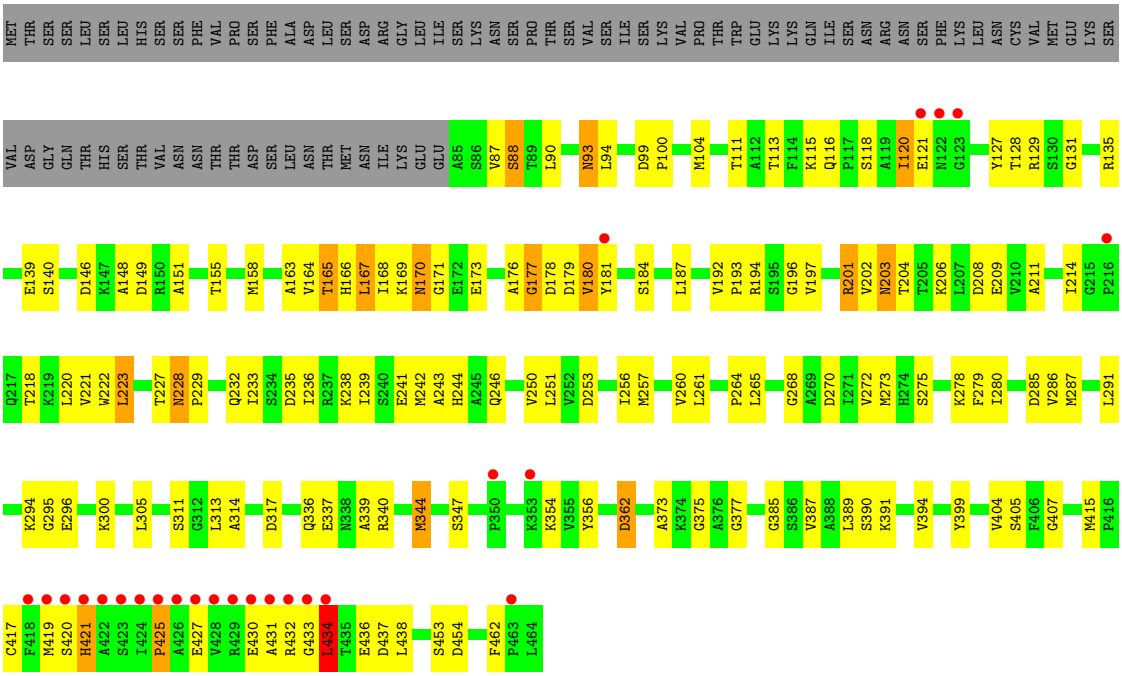
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	132	132	132	0	0
			Total	O		
5	C	121	121	121	0	0

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.

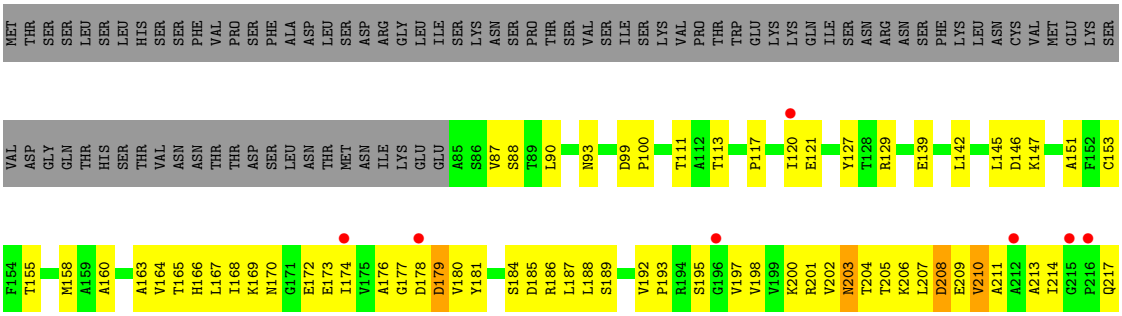
- Molecule 1: CYSTATHIONINE BETA-LYASE

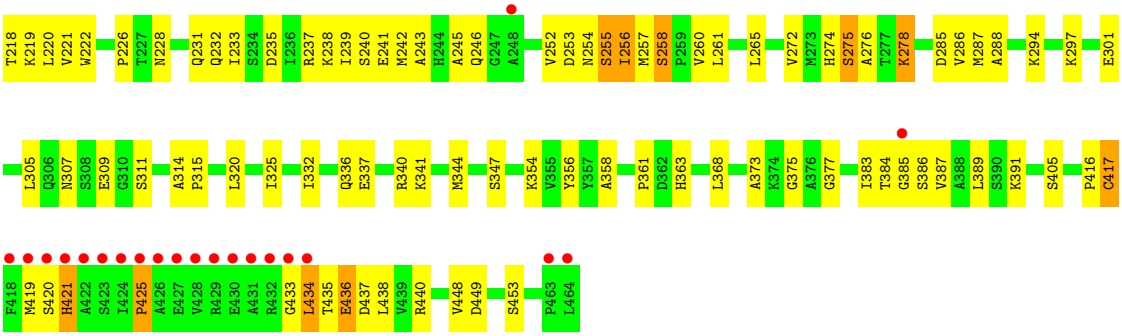
Chain A:



- Molecule 1: CYSTATHIONINE BETA-LYASE

Chain C:




T218 K219 L220 V221 W222 P226 T227 N228 Q231 Q232 I233 S234 D235 I236 R237 K238 I239 S240 E241 M242 A243 H244 A245 Q246 G247 A248 V252 D253 N254 S255 I256 M257 S258 P259 V260 L261 L265 V272 M273 H274 S275 A276 T277 K278 D285 V286 M287 A288 K294 K297 E301
L305 Q306 N307 S308 E309 G310 S311 A314 P315 L320 I325 I332 Q336 E337 R340 K341 M344 S347 K354 V355 Y356 Y357 A358 P361 D362 H363 L368 A373 K374 G375 A376 G377 I383 T384 G385 S386 V387 A388 L389 S390 K391 S405 P416 C417
F418 M419 S420 H421 A422 S423 I424 P425 A426 E427 V428 R429 E430 A431 R432 G433 L434 T435 E436 D437 L438 V439 R440 V448 D449 S453 P463 L464

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	107.75Å 154.33Å 118.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.30 19.79 – 2.30	Depositor EDS
% Data completeness (in resolution range)	87.5 (6.00-2.30) 88.5 (19.79-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.30Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.249 , 0.309 0.246 , 0.302	Depositor DCC
R_{free} test set	1959 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	32.6	Xtriage
Anisotropy	0.655	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 71.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5965	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.40 % 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 2.7531e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, CO3, 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	0.68	0/2888	0.87	3/3920 (0.1%)
1	C	0.66	0/2889	0.87	3/3921 (0.1%)
All	All	0.67	0/5777	0.87	6/7841 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	434	LEU	CA-CB-CG	8.08	133.88	115.30
1	C	434	LEU	CA-CB-CG	7.18	131.82	115.30
1	C	275	SER	N-CA-C	-6.26	94.10	111.00
1	A	275	SER	N-CA-C	-5.31	96.67	111.00
1	C	425	PRO	N-CA-CB	5.31	109.67	103.30
1	A	425	PRO	N-CA-CB	5.11	109.43	103.30

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	2834	0	2806	123	0
1	C	2835	0	2809	154	0
2	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	4	0	0	0	0
3	A	5	0	0	0	0
4	A	15	0	7	0	0
4	C	15	0	7	2	0
5	A	132	0	0	8	0
5	C	121	0	0	19	1
All	All	5965	0	5629	270	1

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 24.

All (270) 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:C:90:LEU:HD12	1:C:93:ASN:HD21	1.23	1.01
1:C:305:LEU:O	1:C:309:GLU:HG2	1.60	0.98
1:A:87:VAL:HG23	5:A:1434:HOH:O	1.70	0.91
1:C:178:ASP:HA	1:C:201:ARG:HH11	1.38	0.86
1:C:294:LYS:HG2	5:C:2414:HOH:O	1.74	0.85
1:A:314:ALA:HB3	5:C:2485:HOH:O	1.75	0.84
1:C:168:ILE:HG23	1:C:172:GLU:HB2	1.62	0.80
1:A:168:ILE:HD11	1:A:220:LEU:HB2	1.64	0.79
1:A:336:GLN:HE21	1:A:377:GLY:H	1.29	0.79
1:C:173:GLU:HG2	1:C:198:VAL:HB	1.63	0.79
1:A:336:GLN:HE21	1:A:377:GLY:N	1.81	0.77
1:C:214:ILE:CG2	1:C:246:GLN:HG3	2.14	0.76
1:C:235:ASP:O	1:C:239:ILE:HG13	1.85	0.76
1:C:203:ASN:ND2	1:C:205:THR:H	1.84	0.76
1:C:200:LYS:HZ3	1:C:213:ALA:HA	1.50	0.75
1:C:361:PRO:HG3	5:C:2423:HOH:O	1.86	0.75
1:C:200:LYS:NZ	1:C:213:ALA:HA	2.01	0.75
1:C:258:SER:OG	1:C:260:VAL:HG22	1.87	0.75
1:A:362:ASP:HB2	5:A:1509:HOH:O	1.87	0.74
1:A:229:PRO:CG	1:A:438:LEU:HD21	2.16	0.74
1:A:336:GLN:NE2	1:A:377:GLY:H	1.86	0.72
1:C:358:ALA:HA	1:C:363:HIS:CD2	2.25	0.71
1:A:203:ASN:C	1:A:203:ASN:HD22	1.93	0.71
1:C:419:MET:C	1:C:421:HIS:H	1.93	0.71
1:A:164:VAL:O	1:A:167:LEU:HB2	1.90	0.71
1:C:177:GLY:O	1:C:180:VAL:HG23	1.90	0.71
1:C:90:LEU:HD12	1:C:93:ASN:ND2	2.01	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LEU:O	1:A:192:VAL:HG23	1.91	0.70
1:C:278:LYS:HE2	1:C:405:SER:HB2	1.72	0.70
1:A:257:MET:HE2	1:A:373:ALA:HB1	1.73	0.70
1:A:434:LEU:HD13	1:A:438:LEU:HD23	1.73	0.69
1:A:221:VAL:HG21	1:A:243:ALA:HB2	1.74	0.69
1:C:139:GLU:O	1:C:151:ALA:HB3	1.93	0.69
1:A:404:VAL:HG22	5:C:2474:HOH:O	1.92	0.68
1:C:435:THR:O	1:C:437:ASP:N	2.26	0.68
1:C:207:LEU:HB3	1:C:242:MET:HE1	1.77	0.67
1:C:176:ALA:CB	1:C:188:LEU:HD13	2.25	0.66
1:C:241:GLU:HA	5:C:2437:HOH:O	1.95	0.66
1:C:238:LYS:HE3	5:C:2487:HOH:O	1.95	0.66
1:A:221:VAL:HB	1:A:250:VAL:HG22	1.77	0.66
1:C:203:ASN:C	1:C:203:ASN:HD22	1.99	0.66
1:C:242:MET:O	1:C:245:ALA:HB3	1.96	0.65
1:C:214:ILE:HG22	1:C:246:GLN:HG3	1.77	0.65
1:C:187:LEU:O	1:C:192:VAL:HG23	1.96	0.65
1:A:206:LYS:HD2	1:A:209:GLU:OE2	1.96	0.65
1:A:111:THR:HA	1:C:285:ASP:HA	1.78	0.64
1:A:229:PRO:HG2	1:A:438:LEU:HD21	1.79	0.64
1:A:294:LYS:HG2	5:A:1502:HOH:O	1.96	0.64
1:A:202:VAL:CG1	1:A:209:GLU:HB3	2.27	0.64
1:C:164:VAL:O	1:C:167:LEU:HB2	1.98	0.63
1:A:180:VAL:HG12	1:A:184:SER:HB2	1.81	0.63
1:C:178:ASP:HA	1:C:201:ARG:NH1	2.14	0.62
1:C:297:LYS:O	1:C:301:GLU:HG2	1.99	0.62
1:A:256:ILE:O	1:A:256:ILE:HG12	1.98	0.62
1:A:229:PRO:HG3	1:A:438:LEU:HD21	1.81	0.61
1:C:178:ASP:HB2	1:C:201:ARG:HB3	1.82	0.61
1:A:229:PRO:HG3	1:A:438:LEU:CD2	2.31	0.60
1:A:87:VAL:HG11	1:A:260:VAL:HG12	1.82	0.60
1:C:256:ILE:O	1:C:256:ILE:HD13	2.00	0.60
1:A:417:CYS:CB	1:A:436:GLU:HA	2.32	0.59
1:C:340:ARG:O	1:C:344:MET:HG3	2.03	0.59
1:A:419:MET:C	1:A:421:HIS:H	2.05	0.59
1:C:257:MET:HE2	1:C:373:ALA:HB1	1.85	0.59
1:C:417:CYS:HB3	1:C:434:LEU:HG	1.84	0.58
1:A:344:MET:CE	1:A:344:MET:HA	2.33	0.58
1:C:265:LEU:HG	1:C:272:VAL:CG2	2.34	0.58
1:C:160:ALA:O	1:C:164:VAL:HG23	2.05	0.57
1:C:168:ILE:HG22	1:C:197:VAL:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:GLY:HA2	1:A:196:GLY:O	2.05	0.56
1:A:314:ALA:CB	5:C:2485:HOH:O	2.45	0.56
1:A:264:PRO:HB2	1:A:272:VAL:HG22	1.87	0.56
1:A:296:GLU:O	1:A:300:LYS:HG2	2.04	0.56
1:C:203:ASN:O	1:C:205:THR:N	2.38	0.56
1:A:280:ILE:HG13	5:A:1433:HOH:O	2.06	0.56
1:A:387:VAL:HG21	1:A:436:GLU:CG	2.37	0.55
1:C:285:ASP:OD1	1:C:286:VAL:HG23	2.05	0.55
1:A:427:GLU:O	1:A:431:ALA:HB2	2.06	0.55
1:A:238:LYS:O	1:A:242:MET:HG3	2.06	0.55
1:C:168:ILE:HG22	1:C:197:VAL:CG2	2.36	0.55
1:C:203:ASN:ND2	1:C:203:ASN:C	2.60	0.55
1:C:207:LEU:HA	1:C:210:VAL:CG1	2.37	0.54
1:C:169:LYS:O	1:C:172:GLU:HG3	2.07	0.54
1:C:254:ASN:ND2	5:C:2427:HOH:O	2.41	0.54
1:A:257:MET:CE	1:A:373:ALA:HB1	2.36	0.54
1:C:252:VAL:O	1:C:272:VAL:HA	2.07	0.54
1:A:177:GLY:HA2	1:A:202:VAL:O	2.08	0.54
1:A:287:MET:HE1	1:C:127:TYR:CE2	2.42	0.54
1:A:337:GLU:HA	1:A:337:GLU:OE1	2.06	0.54
1:A:223:LEU:HD11	1:A:239:ILE:HG21	1.90	0.54
1:A:168:ILE:CD1	1:A:220:LEU:HB2	2.35	0.54
1:C:87:VAL:HG23	5:C:2435:HOH:O	2.08	0.54
1:A:90:LEU:HD12	1:A:90:LEU:O	2.08	0.53
1:C:169:LYS:O	1:C:197:VAL:HG22	2.09	0.53
1:A:149:ASP:OD2	1:A:295:GLY:N	2.35	0.53
1:A:387:VAL:CG2	1:A:436:GLU:HG2	2.38	0.53
1:A:118:SER:OG	1:A:120:ILE:HD12	2.09	0.53
1:C:166:HIS:O	1:C:305:LEU:HD11	2.09	0.53
1:A:168:ILE:HD11	1:A:220:LEU:CB	2.37	0.52
1:C:203:ASN:HD22	1:C:205:THR:H	1.56	0.52
1:A:116:GLN:HE21	1:A:116:GLN:N	2.08	0.52
1:A:203:ASN:C	1:A:203:ASN:ND2	2.63	0.52
1:A:257:MET:HE2	1:A:373:ALA:CB	2.40	0.52
1:A:391:LYS:HD3	1:C:120:ILE:HD11	1.92	0.52
1:C:139:GLU:HG2	1:C:153:CYS:SG	2.49	0.52
1:C:207:LEU:O	1:C:211:ALA:HB2	2.10	0.52
1:C:258:SER:HG	1:C:260:VAL:HG22	1.73	0.52
1:A:115:LYS:C	1:A:116:GLN:HE21	2.13	0.52
1:C:221:VAL:HG21	1:C:243:ALA:HB2	1.92	0.52
1:C:203:ASN:HD21	1:C:205:THR:HG23	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:LYS:O	1:C:241:GLU:HG2	2.10	0.51
1:C:237:ARG:O	1:C:240:SER:HB2	2.10	0.51
1:C:253:ASP:OD1	4:C:2400:PLP:H2A2	2.11	0.51
1:A:354:LYS:HD3	1:A:356:TYR:CZ	2.46	0.50
1:C:368:LEU:HD12	1:C:368:LEU:O	2.11	0.50
1:A:184:SER:HB3	1:A:222:TRP:CZ2	2.47	0.50
1:C:185:ASP:OD2	1:C:201:ARG:NH2	2.45	0.50
1:A:87:VAL:O	1:A:88:SER:C	2.49	0.50
1:C:257:MET:CE	1:C:373:ALA:HB1	2.41	0.50
1:A:354:LYS:HD3	1:A:356:TYR:CE2	2.47	0.50
1:C:180:VAL:HG12	1:C:184:SER:CB	2.41	0.50
1:C:176:ALA:HB1	1:C:188:LEU:HD13	1.92	0.50
1:A:238:LYS:O	1:A:241:GLU:HG3	2.12	0.50
1:A:176:ALA:O	1:A:201:ARG:HD2	2.12	0.50
1:A:206:LYS:CD	1:A:209:GLU:OE2	2.59	0.49
1:A:120:ILE:HD12	1:A:120:ILE:H	1.77	0.49
1:C:186:ARG:NH2	5:C:2455:HOH:O	2.19	0.49
1:A:148:ALA:HB2	1:A:265:LEU:CD1	2.42	0.49
1:C:419:MET:C	1:C:421:HIS:N	2.63	0.49
1:A:264:PRO:HB2	1:A:272:VAL:CG2	2.43	0.48
1:C:206:LYS:HG3	1:C:209:GLU:OE2	2.13	0.48
1:A:394:VAL:HG21	1:A:415:MET:HG3	1.94	0.48
1:C:265:LEU:HG	1:C:272:VAL:HG23	1.95	0.48
1:C:127:TYR:HE2	1:C:129:ARG:NH2	2.11	0.48
1:C:253:ASP:CG	4:C:2400:PLP:H2A2	2.32	0.48
1:C:383:ILE:HG23	1:C:437:ASP:OD2	2.13	0.48
1:C:260:VAL:HG21	1:C:332:ILE:HD12	1.95	0.48
1:A:127:TYR:CE2	1:C:287:MET:HE1	2.48	0.48
1:A:168:ILE:HD11	1:A:220:LEU:HD22	1.95	0.48
1:A:313:LEU:HD11	1:A:317:ASP:HB3	1.96	0.48
1:A:285:ASP:HA	1:C:111:THR:HA	1.96	0.48
1:A:208:ASP:O	1:A:211:ALA:HB3	2.13	0.48
1:C:260:VAL:HG21	1:C:332:ILE:CD1	2.44	0.48
1:A:387:VAL:CG2	1:A:436:GLU:CG	2.92	0.47
1:C:203:ASN:C	1:C:205:THR:H	2.18	0.47
1:C:222:TRP:CD1	1:C:222:TRP:C	2.87	0.47
1:C:314:ALA:CB	5:C:2485:HOH:O	2.62	0.47
1:C:337:GLU:HG3	1:C:341:LYS:HE3	1.95	0.47
1:C:385:GLY:N	1:C:437:ASP:OD2	2.46	0.47
1:C:387:VAL:HG12	1:C:391:LYS:HE3	1.96	0.47
1:A:389:LEU:HD13	1:A:462:PHE:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:TYR:CD1	1:A:454:ASP:HB2	2.50	0.47
1:A:90:LEU:O	1:A:93:ASN:HB3	2.14	0.47
1:A:128:THR:O	1:A:135:ARG:NH2	2.41	0.47
1:C:228:ASN:HD21	1:C:440:ARG:NH1	2.13	0.47
1:A:170:ASN:ND2	5:A:1429:HOH:O	2.48	0.47
1:C:174:ILE:HD12	1:C:192:VAL:HG11	1.95	0.47
1:C:384:THR:C	1:C:386:SER:H	2.17	0.47
1:A:279:PHE:CE2	1:A:407:GLY:HA2	2.50	0.47
1:C:147:LYS:NZ	5:C:2461:HOH:O	2.39	0.47
1:C:226:PRO:HB3	1:C:231:GLN:HA	1.96	0.47
1:C:286:VAL:HG22	1:C:320:LEU:HD13	1.97	0.47
1:A:223:LEU:HD23	1:A:236:ILE:HG12	1.97	0.46
1:C:257:MET:HE2	1:C:373:ALA:CB	2.44	0.46
1:C:117:PRO:HD2	1:C:121:GLU:O	2.14	0.46
1:C:207:LEU:HA	1:C:210:VAL:HG13	1.96	0.46
1:C:219:LYS:HA	1:C:219:LYS:HD2	1.73	0.46
1:C:260:VAL:HG23	1:C:261:LEU:HG	1.97	0.46
1:C:139:GLU:OE1	1:C:153:CYS:N	2.42	0.46
1:C:158:MET:HE1	1:C:187:LEU:HD22	1.97	0.46
1:C:189:SER:O	1:C:193:PRO:HG2	2.15	0.46
1:C:210:VAL:O	1:C:214:ILE:HG13	2.16	0.46
1:A:158:MET:CE	1:A:187:LEU:HD22	2.46	0.46
1:C:163:ALA:O	1:C:164:VAL:C	2.54	0.46
1:A:238:LYS:HA	1:A:241:GLU:HG2	1.98	0.46
1:A:270:ASP:HB3	5:A:1462:HOH:O	2.15	0.46
1:A:257:MET:HE1	1:A:375:GLY:O	2.16	0.46
1:A:260:VAL:O	1:A:261:LEU:HD23	2.16	0.46
1:C:200:LYS:HE2	1:C:200:LYS:HB3	1.76	0.46
1:A:432:ARG:O	1:A:434:LEU:N	2.49	0.45
1:A:265:LEU:CD2	1:A:272:VAL:HG23	2.46	0.45
1:C:203:ASN:ND2	1:C:205:THR:OG1	2.49	0.45
1:C:205:THR:HG22	1:C:233:ILE:O	2.16	0.45
1:A:430:GLU:C	1:A:432:ARG:H	2.17	0.45
1:C:192:VAL:HB	1:C:193:PRO:HD3	1.98	0.45
1:C:417:CYS:SG	1:C:438:LEU:O	2.74	0.45
1:A:164:VAL:HG23	1:A:291:LEU:HD11	1.99	0.45
1:C:232:GLN:HE21	1:C:232:GLN:HB3	1.54	0.45
1:A:94:LEU:HD13	1:A:104:MET:O	2.17	0.45
1:A:387:VAL:HG21	1:A:436:GLU:HG2	1.99	0.44
1:C:192:VAL:N	1:C:193:PRO:CD	2.79	0.44
1:C:203:ASN:C	1:C:205:THR:N	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:LYS:HD2	1:C:448:VAL:HG11	2.00	0.44
1:A:99:ASP:HA	1:A:100:PRO:HD3	1.67	0.44
1:A:278:LYS:HE2	1:A:405:SER:CB	2.47	0.44
1:C:180:VAL:HG12	1:C:184:SER:HB2	1.99	0.44
1:C:188:LEU:HD23	1:C:192:VAL:HG21	1.99	0.44
1:A:273:MET:SD	1:A:273:MET:C	2.95	0.44
1:A:291:LEU:HD23	1:A:291:LEU:HA	1.50	0.44
1:C:265:LEU:HD22	1:C:294:LYS:HB2	1.98	0.44
1:C:449:ASP:O	1:C:453:SER:HB3	2.17	0.44
1:A:417:CYS:N	1:A:434:LEU:HD11	2.33	0.44
1:C:419:MET:O	1:C:421:HIS:N	2.50	0.44
1:A:129:ARG:HB2	1:C:287:MET:HE1	1.99	0.44
1:A:201:ARG:HH11	1:A:201:ARG:CG	2.30	0.44
1:A:227:THR:HG23	1:A:232:GLN:HB2	1.99	0.44
1:A:434:LEU:HD13	1:A:438:LEU:CD2	2.44	0.44
1:C:158:MET:CE	1:C:187:LEU:HD22	2.48	0.44
1:A:169:LYS:O	1:A:197:VAL:HG22	2.18	0.43
1:A:244:HIS:HE1	1:A:268:GLY:O	2.01	0.43
1:C:387:VAL:HG21	1:C:436:GLU:HG2	2.00	0.43
1:A:390:SER:O	1:A:394:VAL:HG23	2.18	0.43
1:C:278:LYS:CE	1:C:405:SER:HB2	2.45	0.43
1:A:192:VAL:N	1:A:193:PRO:CD	2.82	0.43
1:C:142:LEU:HD22	5:C:2402:HOH:O	2.17	0.43
1:C:90:LEU:O	1:C:93:ASN:ND2	2.51	0.43
1:C:438:LEU:C	1:C:438:LEU:HD23	2.39	0.43
1:A:385:GLY:N	1:A:437:ASP:OD2	2.52	0.43
1:A:253:ASP:C	1:A:253:ASP:OD1	2.58	0.43
1:C:315:PRO:HD2	5:C:2409:HOH:O	2.19	0.43
1:A:178:ASP:HA	1:A:201:ARG:NH1	2.35	0.42
1:C:168:ILE:HG21	1:C:197:VAL:HG13	2.02	0.42
1:A:164:VAL:HG11	1:A:251:LEU:HD22	2.01	0.42
1:C:173:GLU:HB2	1:C:217:GLN:O	2.19	0.42
1:A:163:ALA:O	1:A:164:VAL:C	2.56	0.42
1:C:176:ALA:HB1	1:C:188:LEU:CD1	2.50	0.42
1:C:207:LEU:HD22	1:C:242:MET:CE	2.50	0.42
1:C:254:ASN:O	1:C:255:SER:C	2.58	0.42
1:C:375:GLY:HA2	5:C:2521:HOH:O	2.19	0.42
1:A:233:ILE:HD12	1:A:233:ILE:HG23	1.88	0.42
1:C:208:ASP:HB2	5:C:2447:HOH:O	2.20	0.42
1:A:173:GLU:OE2	1:A:218:THR:OG1	2.38	0.42
1:A:228:ASN:HA	1:A:229:PRO:HA	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:ILE:HG12	1:C:220:LEU:HD23	2.02	0.42
1:C:188:LEU:HA	1:C:192:VAL:HG21	2.01	0.42
1:C:336:GLN:HG3	1:C:377:GLY:O	2.19	0.42
1:A:167:LEU:HD13	1:A:305:LEU:HD12	2.02	0.42
1:C:168:ILE:HD11	1:C:220:LEU:HB2	2.01	0.42
1:A:131:GLY:HA2	5:A:1494:HOH:O	2.20	0.41
1:A:294:LYS:HE3	5:A:1502:HOH:O	2.20	0.41
1:A:339:ALA:O	1:A:340:ARG:C	2.58	0.41
1:A:116:GLN:NE2	1:A:116:GLN:CA	2.84	0.41
1:A:165:THR:HG22	1:A:166:HIS:CD2	2.55	0.41
1:A:235:ASP:O	1:A:239:ILE:HG13	2.20	0.41
1:C:256:ILE:O	1:C:256:ILE:CD1	2.67	0.41
1:A:139:GLU:O	1:A:151:ALA:HB3	2.20	0.41
1:C:99:ASP:HA	1:C:100:PRO:HD2	1.90	0.41
1:C:188:LEU:HA	1:C:192:VAL:CG2	2.51	0.41
1:C:276:ALA:HB3	1:C:288:ALA:HB3	2.01	0.41
1:A:178:ASP:N	1:A:202:VAL:O	2.54	0.41
1:C:193:PRO:C	1:C:195:SER:H	2.24	0.41
1:C:193:PRO:C	1:C:195:SER:N	2.74	0.41
1:C:307:ASN:O	1:C:307:ASN:CG	2.57	0.41
1:C:179:ASP:OD1	1:C:179:ASP:C	2.59	0.41
1:C:314:ALA:HB3	5:C:2485:HOH:O	2.21	0.41
1:C:384:THR:C	1:C:386:SER:N	2.75	0.41
1:C:416:PRO:HD2	1:C:438:LEU:CD2	2.50	0.41
1:A:179:ASP:HB2	1:A:227:THR:HB	2.03	0.41
1:C:168:ILE:CG2	1:C:172:GLU:HB2	2.43	0.41
1:C:241:GLU:CA	5:C:2437:HOH:O	2.61	0.41
1:C:265:LEU:HG	1:C:272:VAL:HG21	2.03	0.41
1:A:168:ILE:CD1	1:A:220:LEU:CB	2.99	0.40
1:C:203:ASN:HD21	1:C:205:THR:CG2	2.33	0.40
1:C:237:ARG:HD2	5:C:2499:HOH:O	2.21	0.40
1:A:129:ARG:HB2	1:C:287:MET:CE	2.51	0.40
1:A:148:ALA:HB2	1:A:265:LEU:HD11	2.03	0.40
1:A:214:ILE:CG2	1:A:246:GLN:HG3	2.51	0.40
1:C:145:LEU:CD1	1:C:325:ILE:HD11	2.51	0.40
1:C:254:ASN:HB3	1:C:274:HIS:CE1	2.57	0.40
1:C:354:LYS:HD3	1:C:356:TYR:CZ	2.56	0.40
1:C:384:THR:HB	1:C:389:LEU:HD23	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:2516:HOH:O	5:C:2516:HOH:O[3_655]	1.18	1.02

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	378/464 (82%)	345 (91%)	24 (6%)	9 (2%)	6 4
1	C	378/464 (82%)	343 (91%)	24 (6%)	11 (3%)	4 3
All	All	756/928 (82%)	688 (91%)	48 (6%)	20 (3%)	5 4

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	421	HIS
1	C	436	GLU
1	A	177	GLY
1	A	180	VAL
1	A	204	THR
1	A	425	PRO
1	A	433	GLY
1	C	179	ASP
1	C	181	TYR
1	C	204	THR
1	A	420	SER
1	C	420	SER
1	C	421	HIS
1	C	425	PRO
1	C	433	GLY
1	A	181	TYR
1	A	194	ARG
1	C	255	SER
1	C	278	LYS
1	C	202	VAL

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	300/398 (75%)	278 (93%)	22 (7%)	14	18
1	C	301/398 (76%)	285 (95%)	16 (5%)	22	31
All	All	601/796 (76%)	563 (94%)	38 (6%)	18	24

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	SER
1	A	93	ASN
1	A	113	THR
1	A	120	ILE
1	A	121	GLU
1	A	140	SER
1	A	146	ASP
1	A	155	THR
1	A	165	THR
1	A	167	LEU
1	A	170	ASN
1	A	201	ARG
1	A	203	ASN
1	A	223	LEU
1	A	228	ASN
1	A	286	VAL
1	A	311	SER
1	A	344	MET
1	A	347	SER
1	A	362	ASP
1	A	434	LEU
1	A	453	SER
1	C	88	SER
1	C	113	THR
1	C	146	ASP
1	C	155	THR
1	C	165	THR

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Mol	Chain	Res	Type
1	C	170	ASN
1	C	203	ASN
1	C	208	ASP
1	C	210	VAL
1	C	218	THR
1	C	256	ILE
1	C	258	SER
1	C	275	SER
1	C	311	SER
1	C	347	SER
1	C	417	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	203	ASN
1	A	228	ASN
1	A	244	HIS
1	A	246	GLN
1	A	336	GLN
1	A	363	HIS
1	C	93	ASN
1	C	166	HIS
1	C	203	ASN
1	C	232	GLN
1	C	246	GLN
1	C	254	ASN
1	C	307	ASN
1	C	372	GLN
1	C	392	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	SO4	A	500	-	4,4,4	0.31	0	6,6,6	0.35	0
4	PLP	C	2400	1	15,15,16	3.83	4 (26%)	20,22,23	2.80	11 (55%)
4	PLP	A	1400	1	15,15,16	4.60	5 (33%)	20,22,23	2.47	10 (50%)
2	CO3	C	2401	-	2,3,3	0.34	0	2,3,3	0.10	0
2	CO3	A	1401	-	2,3,3	0.25	0	2,3,3	0.26	0

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
4	PLP	A	1400	1	-	2/6/6/8	0/1/1/1
4	PLP	C	2400	1	-	0/6/6/8	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2400	PLP	C5-C4	13.69	1.55	1.40
4	A	1400	PLP	C5-C4	13.65	1.55	1.40
4	A	1400	PLP	C3-C2	9.72	1.50	1.40
4	A	1400	PLP	C2-N1	4.08	1.41	1.33
4	C	2400	PLP	C2-N1	3.56	1.40	1.33
4	A	1400	PLP	C2A-C2	2.50	1.54	1.50
4	C	2400	PLP	C3-C4	2.37	1.45	1.40
4	A	1400	PLP	C6-N1	2.32	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2400	PLP	C5A-C5	2.15	1.56	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1400	PLP	C2A-C2-C3	5.23	127.35	120.89
4	C	2400	PLP	O3-C3-C4	4.72	130.52	118.10
4	C	2400	PLP	C6-N1-C2	4.53	127.56	119.17
4	C	2400	PLP	C2A-C2-C3	4.36	126.28	120.89
4	C	2400	PLP	O2P-P-O4P	4.29	118.14	106.73
4	C	2400	PLP	O4P-P-O1P	-4.11	94.93	106.47
4	A	1400	PLP	C6-N1-C2	4.06	126.70	119.17
4	C	2400	PLP	O3-C3-C2	-3.56	109.75	117.49
4	A	1400	PLP	O3-C3-C4	3.55	127.46	118.10
4	A	1400	PLP	C3-C2-N1	-3.42	116.35	120.77
4	C	2400	PLP	C5-C6-N1	-3.41	118.14	123.82
4	A	1400	PLP	C6-C5-C4	3.03	120.54	118.16
4	A	1400	PLP	C5-C6-N1	-2.97	118.87	123.82
4	C	2400	PLP	O3P-P-O1P	2.83	121.75	110.68
4	A	1400	PLP	O3P-P-O1P	2.80	121.65	110.68
4	A	1400	PLP	C4A-C4-C5	2.80	123.82	120.94
4	C	2400	PLP	O4P-C5A-C5	2.71	114.51	109.35
4	C	2400	PLP	C3-C2-N1	-2.27	117.83	120.77
4	A	1400	PLP	O4P-C5A-C5	2.22	113.58	109.35
4	A	1400	PLP	O3-C3-C2	-2.18	112.74	117.49
4	C	2400	PLP	C6-C5-C4	2.18	119.87	118.16

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1400	PLP	C4-C5-C5A-O4P
4	A	1400	PLP	C6-C5-C5A-O4P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2400	PLP	2	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, 95th 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^2)	Q<0.9
1	A	380/464 (81%)	0.22	25 (6%)	18	23	23, 39, 79, 134	0
1	C	380/464 (81%)	0.25	28 (7%)	14	19	21, 40, 83, 137	0
All	All	760/928 (81%)	0.24	53 (6%)	16	21	21, 40, 82, 137	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	423	SER	13.9
1	A	426	ALA	12.9
1	C	426	ALA	12.3
1	C	429	ARG	11.7
1	C	431	ALA	11.2
1	A	421	HIS	10.7
1	C	430	GLU	10.6
1	A	424	ILE	10.1
1	C	424	ILE	9.2
1	C	427	GLU	8.9
1	A	430	GLU	8.7
1	A	418	PHE	8.7
1	A	429	ARG	7.7
1	A	422	ALA	7.2
1	A	428	VAL	7.2
1	A	423	SER	7.0
1	A	427	GLU	7.0
1	C	421	HIS	7.0
1	A	425	PRO	6.4
1	C	422	ALA	6.1
1	C	425	PRO	6.0
1	C	432	ARG	5.9
1	C	418	PHE	5.7
1	C	464	LEU	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	431	ALA	5.6
1	A	420	SER	5.3
1	C	428	VAL	5.3
1	A	216	PRO	4.9
1	C	433	GLY	4.5
1	A	433	GLY	4.4
1	C	419	MET	3.9
1	A	434	LEU	3.5
1	C	463	PRO	3.5
1	A	432	ARG	3.5
1	C	216	PRO	3.3
1	C	212	ALA	3.1
1	C	420	SER	3.1
1	C	385	GLY	3.1
1	A	121	GLU	3.1
1	A	350	PRO	3.0
1	C	196	GLY	2.9
1	A	463	PRO	2.9
1	A	419	MET	2.5
1	C	120	ILE	2.5
1	C	248	ALA	2.3
1	C	434	LEU	2.3
1	C	178	ASP	2.3
1	C	215	GLY	2.2
1	A	353	LYS	2.2
1	C	174	ILE	2.2
1	A	123	GLY	2.2
1	A	181	TYR	2.2
1	A	122	ASN	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, 95th 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(Å^2)	Q<0.9
2	CO3	A	1401	4/4	0.89	0.15	49,51,52,53	0
2	CO3	C	2401	4/4	0.95	0.08	44,46,47,49	0
4	PLP	C	2400	15/16	0.96	0.13	28,47,56,56	0
4	PLP	A	1400	15/16	0.97	0.12	21,38,47,52	0
3	SO4	A	500	5/5	0.98	0.10	47,47,55,56	0

6.5 Other polymers (i)

There are no such residues in this entry.