Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:00 PM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

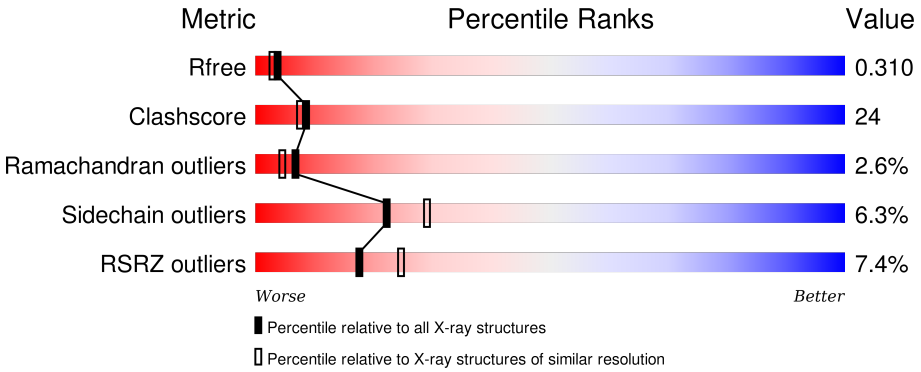
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	6%, 50%, 28%, •, 18%
1	C	464	6%, 48%, 31%, •, 18%

2 Entry composition

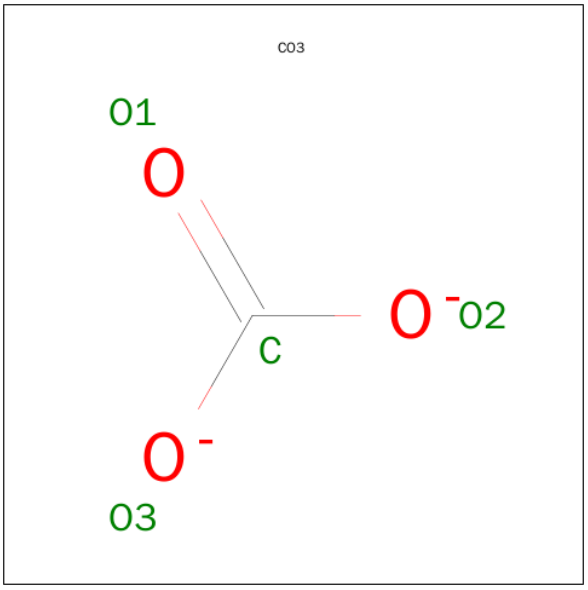
There are 5 unique types of molecules in this entry. The entry contains 5965 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

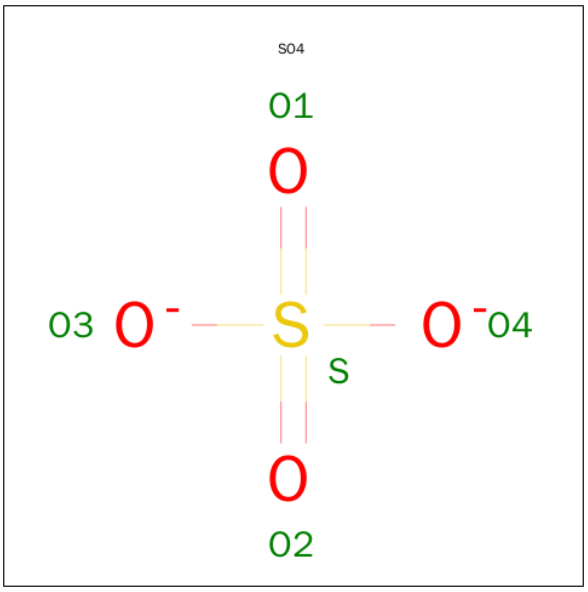
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	0	0
			2834	1798	483	541	12			
1	C	380	Total	C	N	O	S	0	0	0
			2835	1798	483	541	13			

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



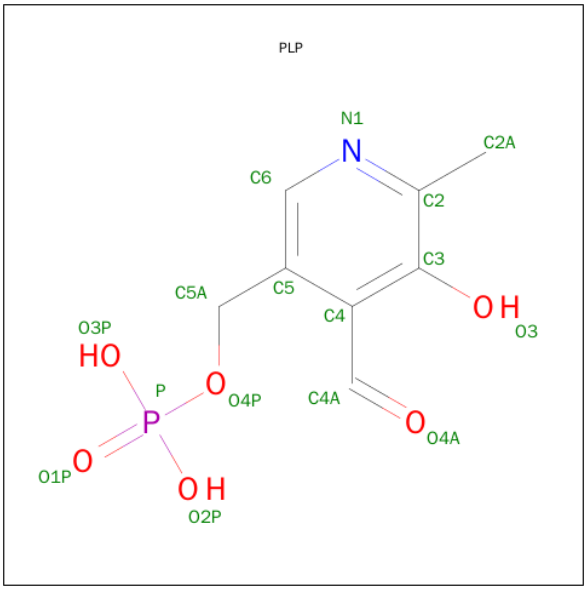
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	1	3		
2	C	1	Total	C	O	0	0
			4	1	3		

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



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

- Molecule 5 is water.

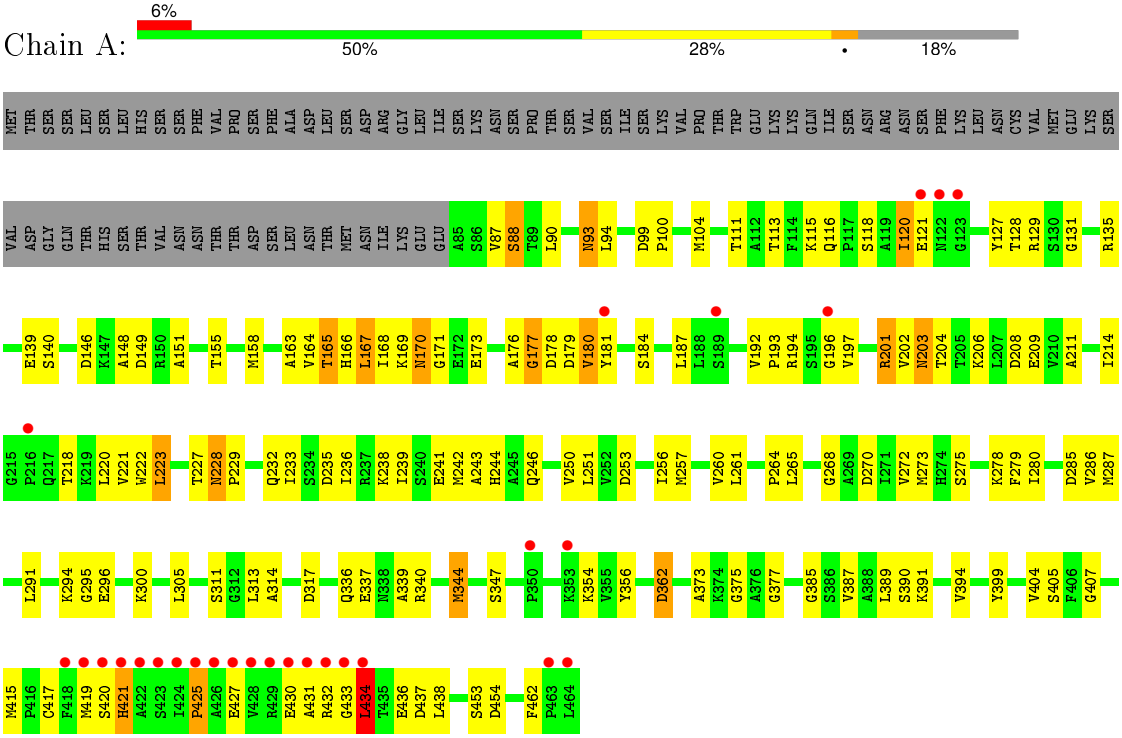
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	132	Total O 132 132	0	0
5	C	121	Total O 121 121	0	0

3 Residue-property plots (i)

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

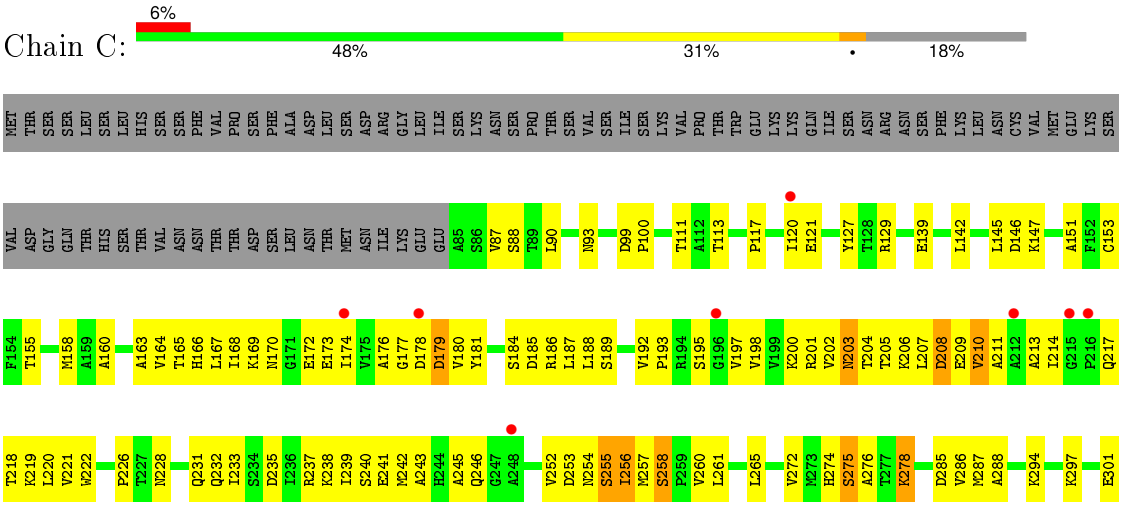
- Molecule 1: CYSTATHIONINE BETA-LYASE

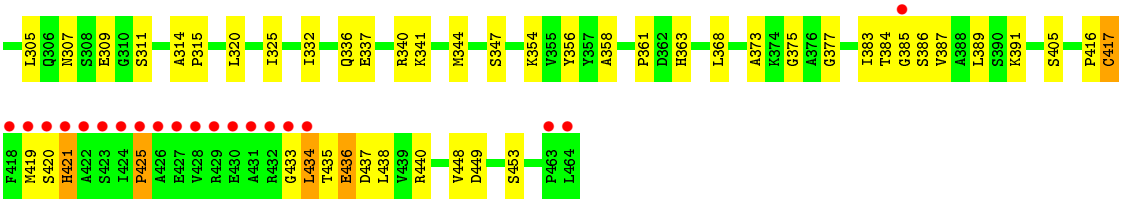
Chain A:



- Molecule 1: CYSTATHIONINE BETA-LYASE

Chain C:




L305
Q306
N307
S308
E309
G310
S311
A314
P315
L320
I325
I332
Q336
E337
R340
K341
M344
S347
K354
Y355
Y356
Y357
A358
P361
D362
H363
L368
A373
K374
G375
A376
G377
I383
T384
G385
S386
V387
A388
L389
S390
K391
S405
P416
G417
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
S463
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 0.253 , 0.310	Depositor DCC
R_{free} test set	1855 reflections (5.05%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	1 of 39111 reflections (0.003%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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: CO3, SO4, 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

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

Continued on next page...

Continued from previous page...

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:HD22	1:A:203:ASN:C	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:LYS:HE2	1:C:405:SER:HB2	1.72	0.70
1:A:187:LEU:O	1:A:192:VAL:HG23	1.91	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:C:203:ASN:HD22	1:C:203:ASN:C	1.99	0.66
1:A:221:VAL:HB	1:A:250:VAL:HG22	1.77	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:HD13	1:C:256:ILE:O	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:C:265:LEU:HG	1:C:272:VAL:CG2	2.34	0.58
1:A:344:MET:CE	1:A:344:MET:HA	2.33	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ALA:CB	5:C:2485:HOH:O	2.45	0.56
1:A:171:GLY:HA2	1:A:196:GLY:O	2.05	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:C:252:VAL:O	1:C:272:VAL:HA	2.07	0.54
1:A:257:MET:CE	1:A:373:ALA:HB1	2.36	0.54
1:A:177:GLY:HA2	1:A:202:VAL:O	2.08	0.54
1:A:337:GLU:HA	1:A:337:GLU:OE1	2.06	0.54
1:A:287:MET:HE1	1:C:127:TYR:CE2	2.42	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:C:169:LYS:O	1:C:197:VAL:HG22	2.09	0.53
1:A:90:LEU:HD12	1:A:90:LEU:O	2.08	0.53
1:A:387:VAL:CG2	1:A:436:GLU:HG2	2.38	0.53
1:A:149:ASP:OD2	1:A:295:GLY:N	2.35	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:203:ASN:ND2	1:A:203:ASN:C	2.63	0.52
1:A:257:MET:HE2	1:A:373:ALA:CB	2.40	0.52
1:C:139:GLU:HG2	1:C:153:CYS:SG	2.49	0.52
1:A:116:GLN:N	1:A:116:GLN:HE21	2.08	0.52
1:A:391:LYS:HD3	1:C:120:ILE:HD11	1.92	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

Continued on next page...

Continued from previous page...

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:O	1:C:368:LEU:HD12	2.11	0.50
1:C:185:ASP:OD2	1:C:201:ARG:NH2	2.45	0.50
1:A:184:SER:HB3	1:A:222:TRP:CZ2	2.47	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:C:180:VAL:HG12	1:C:184:SER:CB	2.41	0.50
1:A:354:LYS:HD3	1:A:356:TYR:CE2	2.47	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:C:265:LEU:HG	1:C:272:VAL:HG23	1.95	0.48
1:A:394:VAL:HG21	1:A:415:MET:HG3	1.94	0.48
1:C:383:ILE:HG23	1:C:437:ASP:OD2	2.13	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:260:VAL:HG21	1:C:332:ILE:HD12	1.95	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:127:TYR:CE2	1:C:287:MET:HE1	2.48	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:C:314:ALA:CB	5:C:2485:HOH:O	2.62	0.47
1:C:203:ASN:C	1:C:205:THR:H	2.18	0.47
1:A:387:VAL:CG2	1:A:436:GLU:CG	2.92	0.47
1:C:385:GLY:N	1:C:437:ASP:OD2	2.46	0.47
1:C:222:TRP:CD1	1:C:222:TRP:C	2.87	0.47
1:C:337:GLU:HG3	1:C:341:LYS:HE3	1.95	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

Continued on next page...

Continued from previous page...

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:C:174:ILE:HD12	1:C:192:VAL:HG11	1.95	0.47
1:A:170:ASN:ND2	5:A:1429:HOH:O	2.48	0.47
1:C:384:THR:C	1:C:386:SER:H	2.17	0.47
1:C:286:VAL:HG22	1:C:320:LEU:HD13	1.97	0.47
1:A:279:PHE:CE2	1:A:407:GLY:HA2	2.50	0.47
1:C:226:PRO:HB3	1:C:231:GLN:HA	1.96	0.47
1:C:147:LYS:NZ	5:C:2461:HOH:O	2.39	0.47
1:C:257:MET:HE2	1:C:373:ALA:CB	2.44	0.46
1:A:223:LEU:HD23	1:A:236:ILE:HG12	1.97	0.46
1:C:207:LEU:HA	1:C:210:VAL:HG13	1.96	0.46
1:C:117:PRO:HD2	1:C:121:GLU:O	2.14	0.46
1:C:219:LYS:HD2	1:C:219:LYS:HA	1.73	0.46
1:C:260:VAL:HG23	1:C:261:LEU:HG	1.97	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:C:139:GLU:OE1	1:C:153:CYS:N	2.42	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:260:VAL:O	1:A:261:LEU:HD23	2.16	0.46
1:C:200:LYS:HB3	1:C:200:LYS:HE2	1.76	0.46
1:A:257:MET:HE1	1:A:375:GLY:O	2.16	0.46
1:A:432:ARG:O	1:A:434:LEU:N	2.49	0.45
1:C:205:THR:HG22	1:C:233:ILE:O	2.16	0.45
1:C:203:ASN:ND2	1:C:205:THR:OG1	2.49	0.45
1:A:265:LEU:CD2	1:A:272:VAL:HG23	2.46	0.45
1:C:192:VAL:HB	1:C:193:PRO:HD3	1.98	0.45
1:A:430:GLU:C	1:A:432:ARG:H	2.17	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: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
1:A:387:VAL:HG21	1:A:436:GLU:HG2	1.99	0.44

Continued on next page...

Continued from previous page...

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:C:188:LEU:HD23	1:C:192:VAL:HG21	1.99	0.44
1:C:180:VAL:HG12	1:C:184:SER:HB2	1.99	0.44
1:A:278:LYS:HE2	1:A:405:SER:CB	2.47	0.44
1:A:99:ASP:HA	1:A:100:PRO:HD3	1.67	0.44
1:C:265:LEU:HD22	1:C:294:LYS:HB2	1.98	0.44
1:A:291:LEU:HD23	1:A:291:LEU:HA	1.50	0.44
1:A:273:MET:SD	1:A:273:MET:C	2.95	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:C:158:MET:CE	1:C:187:LEU:HD22	2.48	0.44
1:A:434:LEU:HD13	1:A:438:LEU:CD2	2.44	0.44
1:C:387:VAL:HG21	1:C:436:GLU:HG2	2.00	0.43
1:A:244:HIS:HE1	1:A:268:GLY:O	2.01	0.43
1:A:169:LYS:O	1:A:197:VAL:HG22	2.18	0.43
1:C:278:LYS:CE	1:C:405:SER:HB2	2.45	0.43
1:A:390:SER:O	1:A:394:VAL:HG23	2.18	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:C:173:GLU:HB2	1:C:217:GLN:O	2.19	0.42
1:A:164:VAL:HG11	1:A:251:LEU:HD22	2.01	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:A:163:ALA:O	1:A:164:VAL:C	2.56	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:HG23	1:A:233:ILE:HD12	1.88	0.42
1:C:208:ASP:HB2	5:C:2447:HOH:O	2.20	0.42
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ASN:HA	1:A:229:PRO:HA	1.78	0.42
1:A:173:GLU:OE2	1:A:218:THR:OG1	2.38	0.42
1:C:336:GLN:HG3	1:C:377:GLY:O	2.19	0.42
1:C:168:ILE:HD11	1:C:220:LEU:HB2	2.01	0.42
1:A:167:LEU:HD13	1:A:305:LEU:HD12	2.02	0.42
1:A:294:LYS:HE3	5:A:1502:HOH:O	2.20	0.41
1:A:131:GLY:HA2	5:A:1494:HOH:O	2.20	0.41
1:A:339:ALA:O	1:A:340:ARG:C	2.58	0.41
1:A:116:GLN:CA	1:A:116:GLN:NE2	2.84	0.41
1:A:165:THR:HG22	1:A:166:HIS:CD2	2.55	0.41
1:C:256:ILE:O	1:C:256:ILE:CD1	2.67	0.41
1:A:235:ASP:O	1:A:239:ILE:HG13	2.20	0.41
1:C:188:LEU:HA	1:C:192:VAL:CG2	2.51	0.41
1:C:99:ASP:HA	1:C:100:PRO:HD2	1.90	0.41
1:A:139:GLU:O	1:A:151:ALA:HB3	2.20	0.41
1:C:276:ALA:HB3	1:C:288:ALA:HB3	2.01	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:A:178:ASP:N	1:A:202:VAL:O	2.54	0.41
1:C:307:ASN:O	1:C:307:ASN:CG	2.57	0.41
1:C:314:ALA:HB3	5:C:2485:HOH:O	2.21	0.41
1:C:416:PRO:HD2	1:C:438:LEU:CD2	2.50	0.41
1:C:384:THR:C	1:C:386:SER:N	2.75	0.41
1:C:179:ASP:OD1	1:C:179:ASP:C	2.59	0.41
1:C:265:LEU:HG	1:C:272:VAL:HG21	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:A:179:ASP:HB2	1:A:227:THR:HB	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:C:254:ASN:HB3	1:C:274:HIS:CE1	2.57	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: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%)	7 5
1	C	378/464 (82%)	343 (91%)	24 (6%)	11 (3%)	6 3
All	All	756/928 (82%)	688 (91%)	48 (6%)	20 (3%)	7 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%)	17 22
1	C	301/398 (76%)	285 (95%)	16 (5%)	28 37
All	All	601/796 (76%)	563 (94%)	38 (6%)	22 29

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

Continued on next page...

Continued from previous page...

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

Some 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 carbohydrates 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	$\#\|Z\|>2$
4	PLP	A	1400	1	15,15,16	5.18	5 (33%)	21,22,23	2.49	12 (57%)
2	CO3	A	1401	-	0,3,3	0.00	-	0,3,3	0.00	-
3	SO4	A	500	-	4,4,4	0.38	0	6,6,6	0.23	0
4	PLP	C	2400	1	15,15,16	3.66	5 (33%)	21,22,23	2.84	12 (57%)
2	CO3	C	2401	-	0,3,3	0.00	-	0,3,3	0.00	-

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	-	0/6/6/8	0/1/1/1
2	CO3	A	1401	-	-	0/0/0/0	0/0/0/0
3	SO4	A	500	-	-	0/0/0/0	0/0/0/0
4	PLP	C	2400	1	-	0/6/6/8	0/1/1/1
2	CO3	C	2401	-	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2400	PLP	C3-C4	2.01	1.45	1.40
4	C	2400	PLP	C5A-C5	2.03	1.56	1.50
4	A	1400	PLP	C2A-C2	2.14	1.54	1.50
4	A	1400	PLP	C6-N1	2.27	1.39	1.34
4	C	2400	PLP	C3-C2	2.65	1.42	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2400	PLP	C2-N1	3.06	1.40	1.34
4	A	1400	PLP	C2-N1	3.51	1.41	1.34
4	A	1400	PLP	C5-C4	13.00	1.55	1.40
4	C	2400	PLP	C5-C4	13.04	1.55	1.40
4	A	1400	PLP	C3-C2	14.25	1.50	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	2400	PLP	O4P-P-O1P	-4.80	94.93	107.14
4	C	2400	PLP	O3-C3-C2	-4.55	109.75	117.66
4	C	2400	PLP	C5-C6-N1	-3.29	118.14	123.86
4	A	1400	PLP	C3-C2-N1	-3.09	116.35	120.61
4	A	1400	PLP	C5-C6-N1	-2.87	118.87	123.86
4	A	1400	PLP	O3-C3-C2	-2.83	112.74	117.66
4	C	2400	PLP	O2P-P-O1P	-2.16	103.64	110.58
4	A	1400	PLP	C5A-C5-C4	-2.02	118.97	121.65
4	C	2400	PLP	C3-C2-N1	-2.01	117.83	120.61
4	A	1400	PLP	O2P-P-O1P	-2.01	104.11	110.58
4	C	2400	PLP	C6-C5-C4	2.03	119.87	118.15
4	A	1400	PLP	O4P-C5A-C5	2.78	113.58	108.99
4	A	1400	PLP	C4A-C4-C5	2.82	123.82	120.88
4	A	1400	PLP	C6-C5-C4	2.83	120.54	118.15
4	A	1400	PLP	O3-C3-C4	3.32	127.46	118.12
4	C	2400	PLP	O4P-C5A-C5	3.34	114.51	108.99
4	A	1400	PLP	O3P-P-O1P	3.44	121.65	110.58
4	C	2400	PLP	O3P-P-O1P	3.47	121.75	110.58
4	A	1400	PLP	C6-N1-C2	3.64	126.70	119.28
4	C	2400	PLP	O2P-P-O4P	4.02	118.14	106.56
4	C	2400	PLP	C6-N1-C2	4.06	127.56	119.28
4	C	2400	PLP	C2A-C2-C3	4.34	126.28	121.04
4	C	2400	PLP	O3-C3-C4	4.41	130.52	118.12
4	A	1400	PLP	C2A-C2-C3	5.24	127.35	121.04

There are no chirality outliers.

There are no torsion outliers.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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^{th} 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%)	0.29	28 (7%)	17	25	23, 39, 79, 134	0
1	C	380/464 (81%)	0.32	28 (7%)	17	25	21, 40, 83, 137	0
All	All	760/928 (81%)	0.31	56 (7%)	17	25	21, 40, 82, 137	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	423	SER	14.2
1	A	426	ALA	13.3
1	C	426	ALA	12.6
1	C	429	ARG	12.1
1	C	431	ALA	11.8
1	A	421	HIS	11.2
1	C	430	GLU	10.7
1	A	424	ILE	10.4
1	C	424	ILE	9.6
1	A	418	PHE	9.2
1	C	427	GLU	9.1
1	A	430	GLU	8.9
1	A	429	ARG	7.8
1	A	428	VAL	7.6
1	A	422	ALA	7.3
1	C	421	HIS	7.3
1	A	427	GLU	7.1
1	A	423	SER	7.0
1	A	425	PRO	6.6
1	C	422	ALA	6.4
1	C	432	ARG	6.3
1	C	425	PRO	6.2
1	C	418	PHE	6.1
1	C	464	LEU	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	431	ALA	5.9
1	A	420	SER	5.6
1	C	428	VAL	5.5
1	A	216	PRO	5.1
1	C	433	GLY	4.8
1	A	433	GLY	4.7
1	C	419	MET	4.0
1	A	434	LEU	3.7
1	C	463	PRO	3.6
1	A	432	ARG	3.6
1	C	216	PRO	3.4
1	C	212	ALA	3.4
1	C	385	GLY	3.3
1	C	420	SER	3.2
1	C	196	GLY	3.2
1	A	121	GLU	3.1
1	A	350	PRO	3.1
1	A	463	PRO	3.1
1	C	120	ILE	2.7
1	A	419	MET	2.7
1	C	248	ALA	2.6
1	C	434	LEU	2.5
1	C	178	ASP	2.4
1	C	174	ILE	2.4
1	A	181	TYR	2.3
1	A	353	LYS	2.3
1	A	123	GLY	2.3
1	C	215	GLY	2.3
1	A	122	ASN	2.1
1	A	464	LEU	2.1
1	A	196	GLY	2.1
1	A	189	SER	2.1

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

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^{th} 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^2)	Q<0.9
4	PLP	C	2400	15/16	0.96	0.13	0.45	28,47,56,56	0
4	PLP	A	1400	15/16	0.97	0.12	0.04	21,38,47,52	0
2	CO3	A	1401	4/4	0.89	0.15	-0.04	49,51,52,53	0
3	SO4	A	500	5/5	0.98	0.10	-0.91	47,47,55,56	0
2	CO3	C	2401	4/4	0.95	0.08	-1.79	44,46,47,49	0

6.5 Other polymers

There are no such residues in this entry.