Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:41 PM GMT

PDB ID	:	1YAA
Title	:	ASPARTATE AMINOTRANSFERASE FROM SACCHAROMYCES CEREVISIAE CYTOPLASM
Authors	:	Jeffery, C.J.
Deposited on	:	1998-01-27
Resolution	:	2.05 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 ⓘ symbol.

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

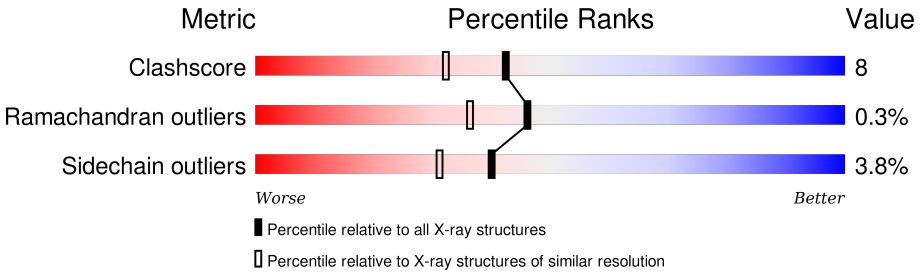
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.05 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))
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	412	77% 22%
1	B	412	78% 20%
1	C	412	79% 20%
1	D	412	81% 17%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13596 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.

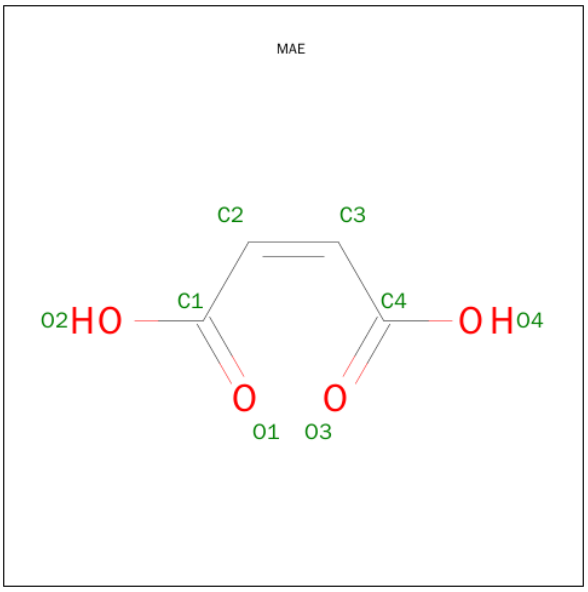
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	S	0	0	0
			3197	2039	550	597	11			
1	B	412	Total	C	N	O	S	0	0	0
			3197	2039	550	597	11			
1	C	412	Total	C	N	O	S	0	0	0
			3197	2039	550	597	11			
1	D	412	Total	C	N	O	S	0	0	0
			3197	2039	550	597	11			

There are 4 discrepancies between the modelled and reference sequences:

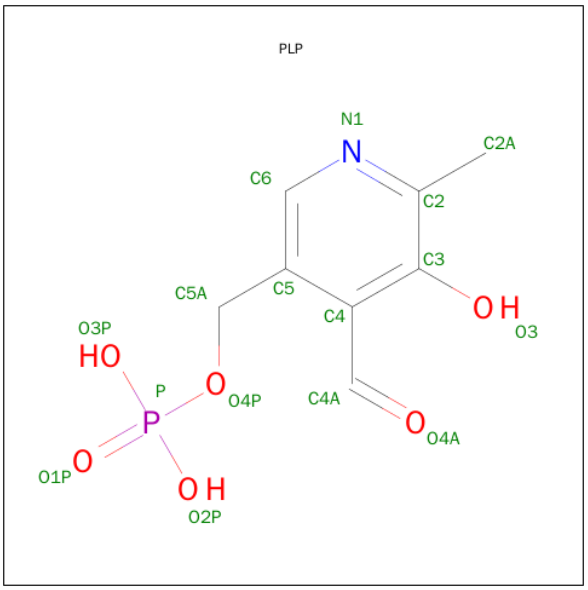
Chain	Residue	Modelled	Actual	Comment	Reference
A	95	LEU	PHE	CONFLICT	UNP P23542
B	95	LEU	PHE	CONFLICT	UNP P23542
C	95	LEU	PHE	CONFLICT	UNP P23542
D	95	LEU	PHE	CONFLICT	UNP P23542

- Molecule 2 is MALEIC ACID (three-letter code: MAE) (formula: $C_4H_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 8 4 4	0	0
2	B	1	Total C O 8 4 4	0	0
2	C	1	Total C O 8 4 4	0	0
2	D	1	Total C O 8 4 4	0	0

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



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		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	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	163	Total	O	0	0
			163	163		
4	B	183	Total	O	0	0
			183	183		
4	C	190	Total	O	0	0
			190	190		
4	D	180	Total	O	0	0
			180	180		

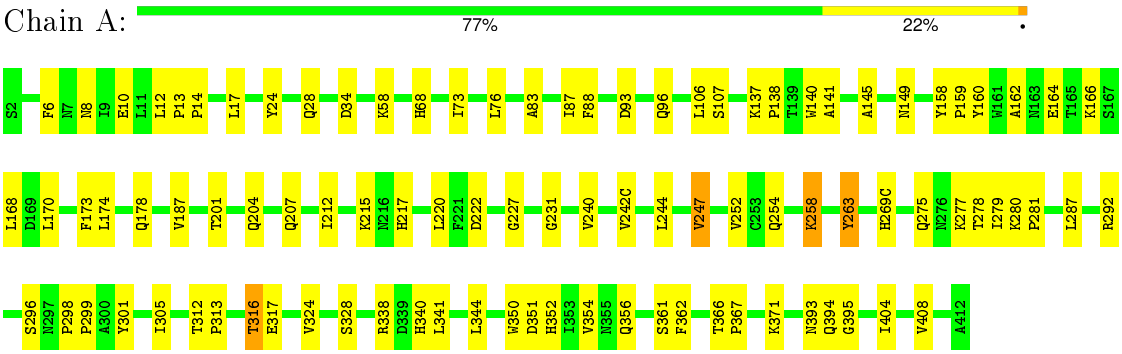
3 Residue-property plots (i)

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.

Note EDS was not executed.

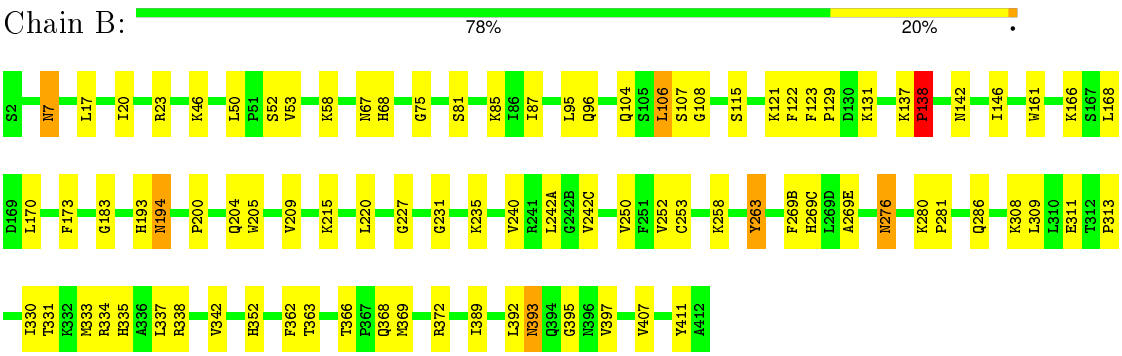
• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain A:



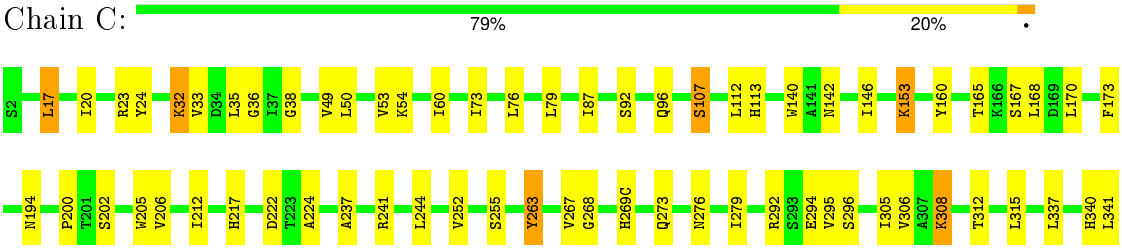
• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain B:



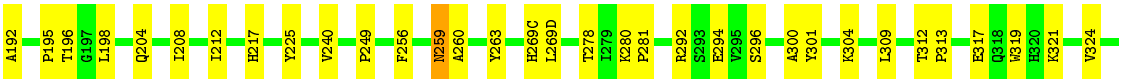
• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain C:



• Molecule 1: ASPARTATE AMINOTRANSFERASE

Chain D:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	130.31Å 134.63Å 98.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.05	Depositor
% Data completeness (in resolution range)	93.0 (10.00-2.05)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.231 , 0.299	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13596	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAE, 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	0.37	1/3271 (0.0%)	0.59	0/4439
1	B	0.32	0/3271	0.72	7/4439 (0.2%)
1	C	0.33	0/3271	0.62	3/4439 (0.1%)
1	D	0.32	0/3271	0.61	0/4439
All	All	0.34	1/13084 (0.0%)	0.64	10/17756 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	258	LYS	CD-CE	10.23	1.76	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	137	LYS	C-N-CD	-20.74	74.98	120.60
1	B	137	LYS	C-N-CA	9.14	160.38	122.00
1	B	137	LYS	N-CA-C	-9.04	86.61	111.00
1	B	194	ASN	N-CA-C	-7.57	90.55	111.00
1	C	194	ASN	C-N-CD	-7.31	104.51	120.60
1	B	194	ASN	C-N-CD	-7.07	105.05	120.60
1	C	194	ASN	N-CA-C	-5.88	95.14	111.00
1	B	138	PRO	CA-N-CD	-5.83	103.33	111.50
1	C	194	ASN	C-N-CA	5.67	145.81	122.00
1	B	194	ASN	C-N-CA	5.62	145.61	122.00

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	3197	0	3182	60	0
1	B	3197	0	3182	60	0
1	C	3197	0	3182	54	0
1	D	3197	0	3181	48	0
2	A	8	0	2	0	0
2	B	8	0	2	0	0
2	C	8	0	2	0	0
2	D	8	0	2	0	0
3	A	15	0	6	2	0
3	B	15	0	6	3	0
3	C	15	0	6	3	0
3	D	15	0	6	1	0
4	A	163	0	0	1	0
4	B	183	0	0	3	0
4	C	190	0	0	2	0
4	D	180	0	0	4	0
All	All	13596	0	12759	213	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 8.

All (213) 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:258:LYS:CE	1:A:258:LYS:CD	1.76	1.61
1:A:280:LYS:HB3	1:A:281:PRO:HD3	1.69	0.74
1:B:20:ILE:HG22	1:B:23:ARG:HH22	1.51	0.73
1:B:393:ASN:O	1:B:397:VAL:HG23	1.89	0.72
1:A:244:LEU:HA	1:A:247:VAL:HG13	1.71	0.72
1:A:201:THR:HG22	1:A:204:GLN:HG3	1.71	0.72
1:C:393:ASN:O	1:C:397:VAL:HG23	1.90	0.71
1:A:212:ILE:HG23	1:A:217:HIS:HB2	1.71	0.71
1:A:393:ASN:HD22	1:A:395:GLY:H	1.35	0.70
1:A:252:VAL:HB	1:A:269(C):HIS:HB2	1.73	0.69
1:C:308:LYS:HA	1:C:308:LYS:HE3	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:HIS:HD2	1:C:398:GLU:HG2	1.59	0.67
1:D:212:ILE:HG23	1:D:217:HIS:HB2	1.77	0.66
1:B:393:ASN:HD22	1:B:395:GLY:H	1.45	0.64
1:A:263:TYR:HB2	1:B:68:HIS:O	1.98	0.64
1:C:340:HIS:CD2	1:C:398:GLU:HG2	2.33	0.64
1:C:33:VAL:HG12	1:C:35:LEU:HD13	1.79	0.64
1:D:367:PRO:HG2	1:D:368:GLN:NE2	2.15	0.62
1:D:256:PHE:HA	1:D:259:ASN:HD21	1.65	0.61
1:D:360:PHE:CD1	1:D:386:ARG:HD3	2.36	0.61
1:C:346:THR:HA	1:C:409:ARG:HH12	1.66	0.60
1:C:53:VAL:HG21	4:C:946:HOH:O	2.01	0.60
1:C:92:SER:O	1:C:96:GLN:HG2	2.01	0.60
1:D:300:ALA:O	1:D:304:LYS:HG2	2.01	0.60
1:C:224:ALA:HA	1:C:255:SER:HB3	1.84	0.60
1:A:170:LEU:HD22	1:A:204:GLN:HE21	1.68	0.59
1:A:258:LYS:NZ	1:A:258:LYS:CD	2.61	0.59
1:C:17:LEU:O	1:C:20:ILE:HG12	2.02	0.58
1:C:340:HIS:HA	1:C:343:LYS:HG2	1.85	0.58
1:D:313:PRO:HG2	4:D:1056:HOH:O	2.02	0.58
1:D:108:GLY:O	1:D:112:LEU:HD23	2.04	0.58
1:B:81:SER:O	1:B:85:LYS:HD3	2.04	0.57
1:C:50:LEU:O	1:C:53:VAL:HG22	2.04	0.57
1:B:17:LEU:O	1:B:20:ILE:HG12	2.05	0.57
1:C:140:TRP:HB2	3:C:907:PLP:H2A3	1.86	0.57
1:C:24:TYR:CE1	1:C:32:LYS:HD3	2.40	0.56
1:C:60:ILE:HD11	1:C:305:ILE:HA	1.87	0.56
1:B:20:ILE:HG22	1:B:23:ARG:NH2	2.19	0.56
1:A:352:HIS:HA	4:A:1028:HOH:O	2.06	0.56
1:A:275:GLN:O	1:A:279:ILE:HG12	2.06	0.56
1:B:7:ASN:HD22	1:B:7:ASN:N	2.03	0.56
1:B:252:VAL:HB	1:B:269(C):HIS:HB2	1.88	0.55
1:A:17:LEU:HD21	1:A:141:ALA:HB3	1.88	0.55
1:C:87:ILE:HD13	1:C:252:VAL:HG11	1.89	0.54
1:D:164:GLU:HG2	1:D:165:THR:HG23	1.88	0.54
1:B:138:PRO:HG3	1:B:161:TRP:HB3	1.89	0.54
1:C:212:ILE:HG23	1:C:217:HIS:HB2	1.88	0.54
1:B:115:SER:HG	1:B:269(B):PHE:HE1	1.54	0.54
1:B:240:VAL:O	1:B:242(C):VAL:HG23	2.08	0.53
1:D:73:ILE:HD13	1:D:292:ARG:HB2	1.91	0.52
1:A:324:VAL:O	1:A:328:SER:HB2	2.09	0.52
1:A:24:TYR:CZ	1:A:34:ASP:HB2	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:GLN:NE2	1:C:361:SER:HA	2.25	0.52
1:D:367:PRO:HG2	1:D:368:GLN:HE22	1.74	0.52
1:A:240:VAL:O	1:A:242(C):VAL:HG13	2.10	0.52
1:D:280:LYS:HB3	1:D:281:PRO:HD3	1.92	0.51
1:D:40:TYR:OH	1:D:329:ARG:HD2	2.10	0.51
1:B:368:GLN:HG2	1:B:411:TYR:CZ	2.45	0.51
1:A:93:ASP:HA	1:A:96:GLN:HG2	1.91	0.51
1:B:194:ASN:CB	3:B:906:PLP:H2A1	2.40	0.51
1:D:153:LYS:N	1:D:153:LYS:HE3	2.25	0.51
1:D:4:THR:HA	1:D:7:ASN:ND2	2.25	0.51
1:A:170:LEU:O	1:A:174:LEU:HD23	2.11	0.51
1:A:204:GLN:HA	1:A:207:GLN:HE21	1.76	0.50
1:D:149:ASN:HD22	1:D:150:GLN:HE21	1.59	0.50
1:B:52:SER:HB2	1:B:309:LEU:HD11	1.94	0.50
1:D:394:GLN:HA	1:D:394:GLN:HE21	1.77	0.50
1:D:192:ALA:HB3	1:D:225:TYR:HB2	1.92	0.50
1:C:202:SER:O	1:C:206:VAL:HG23	2.12	0.50
1:D:196:THR:HA	1:D:362:PHE:HB2	1.93	0.50
1:C:153:LYS:HB2	1:C:153:LYS:NZ	2.28	0.49
1:D:278:THR:O	1:D:281:PRO:HD2	2.12	0.49
1:A:12:LEU:HD13	1:B:286:GLN:NE2	2.27	0.49
1:A:10:GLU:CD	1:A:10:GLU:H	2.16	0.49
1:A:292:ARG:HA	1:A:296:SER:HA	1.94	0.49
1:D:24:TYR:CE1	1:D:34:ASP:HB2	2.47	0.49
1:B:209:VAL:HG21	1:B:242(A):LEU:HD12	1.94	0.49
1:A:68:HIS:O	1:B:263:TYR:HB2	2.13	0.49
1:B:121:LYS:HB3	1:B:121:LYS:NZ	2.28	0.49
1:A:87:ILE:HD12	1:A:252:VAL:HG11	1.94	0.49
1:D:259:ASN:HD22	1:D:260:ALA:N	2.10	0.49
1:A:244:LEU:HA	1:A:247:VAL:CG1	2.42	0.48
1:D:113:HIS:HD2	4:D:910:HOH:O	1.95	0.48
1:D:292:ARG:NH1	1:D:296:SER:OG	2.47	0.48
1:B:87:ILE:HG21	1:B:252:VAL:HG11	1.95	0.48
1:D:204:GLN:O	1:D:208:ILE:HG13	2.13	0.48
1:A:258:LYS:CE	1:A:258:LYS:CG	2.83	0.48
1:A:160:TYR:O	1:A:168:LEU:HD12	2.13	0.47
1:B:337:LEU:HD22	1:B:392:LEU:HD11	1.96	0.47
1:A:350:TRP:HA	1:A:352:HIS:CE1	2.50	0.47
1:C:366:THR:HB	1:C:367:PRO:HD2	1.95	0.47
1:D:48:TRP:CZ3	1:D:50:LEU:HD22	2.50	0.47
1:B:115:SER:OG	1:B:269(B):PHE:HE1	1.98	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:ILE:O	1:B:334:ARG:HG3	2.15	0.47
1:B:220:LEU:HD21	1:B:253:CYS:SG	2.55	0.47
1:C:142:ASN:O	1:C:146:ILE:HG13	2.14	0.47
1:D:249:PRO:HB2	1:D:269(D):LEU:HD11	1.97	0.47
1:C:38:GLY:HA3	1:C:360:PHE:CZ	2.50	0.47
1:A:404:ILE:O	1:A:408:VAL:HG23	2.15	0.47
1:A:393:ASN:ND2	1:A:395:GLY:H	2.08	0.47
1:A:73:ILE:HD12	1:A:292:ARG:HD3	1.96	0.46
1:A:222:ASP:OD2	3:A:905:PLP:N1	2.49	0.46
1:D:43:ASP:HA	1:D:329:ARG:NH2	2.31	0.46
1:B:308:LYS:HB2	1:B:308:LYS:NZ	2.30	0.46
1:C:113:HIS:HD2	4:D:961:HOH:O	1.98	0.46
1:A:356:GLN:OE1	1:A:361:SER:HA	2.16	0.46
1:B:161:TRP:CH2	1:B:166:LYS:HG3	2.50	0.46
1:A:277:LYS:HG3	1:A:278:THR:HG23	1.97	0.46
1:C:49:VAL:HB	1:C:54:LYS:NZ	2.31	0.46
1:D:61:HIS:HE1	1:D:301:TYR:OH	1.99	0.46
1:B:194:ASN:HD22	3:B:906:PLP:H2A1	1.81	0.46
1:A:145:ALA:O	1:A:149:ASN:HB2	2.16	0.46
1:C:222:ASP:OD2	3:C:907:PLP:N1	2.49	0.46
1:A:58:LYS:HB3	1:A:58:LYS:NZ	2.31	0.46
1:D:167:SER:HA	1:D:198:LEU:HD21	1.96	0.46
1:C:273:GLN:NE2	1:D:4:THR:HG22	2.31	0.46
1:B:352:HIS:HE1	1:B:363:THR:O	1.98	0.46
1:C:337:LEU:HD22	1:C:392:LEU:HD11	1.97	0.46
1:B:50:LEU:O	1:B:53:VAL:HG22	2.16	0.45
1:A:279:ILE:CD1	1:B:7:ASN:HA	2.45	0.45
1:C:73:ILE:HD12	1:C:292:ARG:HD3	1.97	0.45
1:A:351:ASP:O	1:A:354:VAL:HG22	2.16	0.45
1:B:67:ASN:HB2	4:B:983:HOH:O	2.16	0.45
1:D:309:LEU:HD21	1:D:319:TRP:CG	2.51	0.45
1:C:252:VAL:HB	1:C:269(C):HIS:HB2	1.97	0.45
1:B:138:PRO:O	1:B:193:HIS:HE1	1.98	0.45
1:B:168:LEU:HD11	1:B:200:PRO:HG3	1.98	0.45
1:B:311:GLU:O	1:B:313:PRO:HD3	2.17	0.45
1:D:110:GLY:O	1:D:114:ILE:HG13	2.16	0.45
1:B:170:LEU:HG	1:B:204:GLN:HE21	1.82	0.45
1:A:106:LEU:HD21	1:B:106:LEU:HD21	1.99	0.45
1:C:276:ASN:HA	1:C:279:ILE:HB	1.98	0.45
1:A:227:GLY:O	1:A:231:GLY:HA2	2.17	0.45
1:D:67:ASN:HD22	1:D:69:GLU:H	1.63	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:MET:HB3	1:C:407:VAL:HG11	1.98	0.45
1:C:292:ARG:HG2	4:D:1069:HOH:O	2.17	0.45
1:B:372:ARG:HD3	1:B:407:VAL:HG13	1.98	0.45
1:C:165:THR:HG23	1:C:167:SER:OG	2.16	0.45
1:C:32:LYS:HA	1:C:378:ALA:O	2.17	0.45
1:D:51:PRO:HA	1:D:54:LYS:HD3	1.99	0.45
1:C:347:PRO:HD3	1:C:409:ARG:NH1	2.31	0.44
1:B:366:THR:OG1	1:B:369:MET:HG3	2.17	0.44
1:B:131:LYS:HD2	1:B:183:GLY:O	2.17	0.44
1:B:331:THR:O	1:B:335:HIS:HD2	2.00	0.44
1:B:123:PHE:N	1:B:129:PRO:HD3	2.32	0.44
1:C:237:ALA:O	1:C:241:ARG:HG3	2.18	0.44
1:D:321:LYS:O	1:D:324:VAL:HG22	2.17	0.44
1:A:170:LEU:HD21	1:A:207:GLN:NE2	2.32	0.44
1:D:113:HIS:HE1	1:D:294:GLU:OE1	2.00	0.44
1:C:263:TYR:HB2	1:D:68:HIS:O	2.17	0.44
1:D:101:ILE:O	1:D:269(C):HIS:HA	2.18	0.44
1:A:312:THR:O	1:A:316:THR:HG22	2.18	0.44
1:B:58:LYS:HE3	4:B:1064:HOH:O	2.18	0.44
1:B:227:GLY:O	1:B:231:GLY:HA2	2.18	0.44
1:A:73:ILE:CD1	1:A:292:ARG:HD3	2.48	0.43
1:C:267:VAL:HG11	1:C:306:VAL:HG21	1.99	0.43
1:A:215:LYS:HB3	1:A:215:LYS:HE3	1.83	0.43
1:C:73:ILE:CD1	1:C:292:ARG:HD3	2.47	0.43
1:D:309:LEU:HD21	1:D:319:TRP:CD2	2.53	0.43
1:B:338:ARG:O	1:B:342:VAL:HG23	2.18	0.43
1:C:113:HIS:HE1	1:C:294:GLU:OE1	2.01	0.43
1:B:250:VAL:HB	1:B:269(E):ALA:HB3	1.99	0.43
1:A:6:PHE:HE1	1:B:123:PHE:HE2	1.67	0.43
1:D:334:ARG:HD3	1:D:353:ILE:O	2.18	0.43
1:D:87:ILE:HD12	1:D:240:VAL:HG11	1.99	0.43
1:A:394:GLN:NE2	1:A:394:GLN:HA	2.33	0.43
1:C:368:GLN:NE2	4:C:1072:HOH:O	2.52	0.43
1:C:20:ILE:HG22	1:C:23:ARG:HH22	1.84	0.43
1:C:273:GLN:HE22	1:D:4:THR:HG22	1.83	0.43
1:A:312:THR:HA	1:A:313:PRO:HD2	1.76	0.43
1:B:75:GLY:HA3	1:B:104:GLN:HB3	2.01	0.43
1:A:301:TYR:O	1:A:305:ILE:HG12	2.18	0.42
1:C:160:TYR:O	1:C:168:LEU:HD12	2.19	0.42
1:B:276:ASN:HA	1:B:276:ASN:HD22	1.55	0.42
1:A:137:LYS:HA	1:A:138:PRO:HA	1.91	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:ILE:HD11	1:C:36:GLY:HA3	2.00	0.42
1:A:158:TYR:HA	1:A:159:PRO:HD3	1.94	0.42
1:C:140:TRP:CB	3:C:907:PLP:H2A3	2.49	0.42
1:D:76:LEU:H	1:D:104:GLN:NE2	2.18	0.42
1:C:312:THR:HB	1:C:315:LEU:HB2	2.01	0.42
1:A:83:ALA:HB1	1:A:254:GLN:OE1	2.20	0.42
1:B:85:LYS:N	1:B:85:LYS:HD3	2.35	0.42
1:C:292:ARG:HA	1:C:296:SER:HA	2.02	0.41
1:B:85:LYS:HD2	1:B:95:LEU:HD13	2.03	0.41
1:A:87:ILE:HG13	1:A:88:PHE:N	2.36	0.41
1:A:298:PRO:HA	1:A:299:PRO:HD3	1.90	0.41
1:C:404:ILE:O	1:C:408:VAL:HG23	2.21	0.41
1:D:411:TYR:O	1:D:412:ALA:HB3	2.20	0.41
1:B:333:MET:SD	1:B:397:VAL:HG21	2.60	0.41
1:D:312:THR:HA	1:D:313:PRO:HD2	1.84	0.41
1:B:280:LYS:HB3	1:B:281:PRO:CD	2.50	0.41
1:D:108:GLY:HA3	3:D:908:PLP:H5A2	2.03	0.41
1:C:295:VAL:O	1:C:296:SER:HB3	2.21	0.41
1:A:162:ALA:O	1:A:166:LYS:N	2.54	0.41
1:C:405:ASP:OD1	1:C:409:ARG:NH1	2.54	0.41
1:A:140:TRP:HB2	3:A:905:PLP:H2A3	2.03	0.41
1:C:107:SER:HA	1:C:268:GLY:HA3	2.03	0.41
1:B:142:ASN:O	1:B:146:ILE:HG13	2.20	0.41
1:A:340:HIS:O	1:A:344:LEU:HG	2.21	0.41
1:B:108:GLY:N	3:B:906:PLP:O1P	2.46	0.40
1:B:122:PHE:C	1:B:129:PRO:HD3	2.40	0.40
1:A:313:PRO:O	1:A:317:GLU:HG3	2.22	0.40
1:B:96:GLN:HB2	4:B:1067:HOH:O	2.20	0.40
1:A:366:THR:HB	1:A:367:PRO:HD2	2.01	0.40
1:D:149:ASN:HD22	1:D:150:GLN:NE2	2.20	0.40
1:B:330:ILE:HG23	1:B:389:ILE:HB	2.01	0.40
1:B:215:LYS:HB3	1:B:215:LYS:HE3	1.90	0.40
1:B:46:LYS:HE3	1:B:46:LYS:HB2	1.88	0.40
1:C:200:PRO:HG2	1:C:205:TRP:CE2	2.57	0.40
1:A:13:PRO:HA	1:A:14:PRO:HD3	1.93	0.40
1:D:195:PRO:HB2	1:D:386:ARG:HG3	2.02	0.40
1:A:187:VAL:HG13	1:A:220:LEU:HD22	2.03	0.40
1:B:205:TRP:O	1:B:209:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	410/412 (100%)	393 (96%)	16 (4%)	1 (0%)	52	43
1	B	410/412 (100%)	393 (96%)	15 (4%)	2 (0%)	34	22
1	C	410/412 (100%)	393 (96%)	16 (4%)	1 (0%)	52	43
1	D	410/412 (100%)	403 (98%)	6 (2%)	1 (0%)	52	43
All	All	1640/1648 (100%)	1582 (96%)	53 (3%)	5 (0%)	46	36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	TYR
1	B	138	PRO
1	C	263	TYR
1	D	263	TYR
1	B	263	TYR

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	342/342 (100%)	328 (96%)	14 (4%)	37	28
1	B	342/342 (100%)	333 (97%)	9 (3%)	54	47
1	C	342/342 (100%)	327 (96%)	15 (4%)	35	26
1	D	342/342 (100%)	328 (96%)	14 (4%)	37	28
All	All	1368/1368 (100%)	1316 (96%)	52 (4%)	40	31

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	28	GLN
1	A	76	LEU
1	A	107	SER
1	A	164	GLU
1	A	173	PHE
1	A	178	GLN
1	A	247	VAL
1	A	287	LEU
1	A	316	THR
1	A	338	ARG
1	A	341	LEU
1	A	362	PHE
1	A	371	LYS
1	B	7	ASN
1	B	106	LEU
1	B	107	SER
1	B	173	PHE
1	B	235	LYS
1	B	258	LYS
1	B	276	ASN
1	B	362	PHE
1	B	393	ASN
1	C	17	LEU
1	C	32	LYS
1	C	76	LEU
1	C	79	LEU
1	C	107	SER
1	C	112	LEU
1	C	153	LYS
1	C	170	LEU
1	C	173	PHE
1	C	244	LEU
1	C	308	LYS
1	C	341	LEU
1	C	362	PHE
1	C	394	GLN
1	C	398	GLU
1	D	54	LYS
1	D	67	ASN
1	D	87	ILE
1	D	91	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	107	SER
1	D	153	LYS
1	D	164	GLU
1	D	173	PHE
1	D	259	ASN
1	D	317	GLU
1	D	329	ARG
1	D	341	LEU
1	D	362	PHE
1	D	374	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	61	HIS
1	A	193	HIS
1	A	204	GLN
1	A	207	GLN
1	A	216	ASN
1	A	273	GLN
1	A	335	HIS
1	A	340	HIS
1	A	393	ASN
1	A	394	GLN
1	B	7	ASN
1	B	22	GLN
1	B	62	ASN
1	B	149	ASN
1	B	217	HIS
1	B	276	ASN
1	B	297	ASN
1	B	335	HIS
1	B	340	HIS
1	B	352	HIS
1	B	368	GLN
1	B	393	ASN
1	C	22	GLN
1	C	28	GLN
1	C	61	HIS
1	C	113	HIS
1	C	142	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	149	ASN
1	C	276	ASN
1	C	335	HIS
1	C	340	HIS
1	C	356	GLN
1	C	368	GLN
1	C	377	HIS
1	D	61	HIS
1	D	67	ASN
1	D	82	ASN
1	D	104	GLN
1	D	113	HIS
1	D	150	GLN
1	D	259	ASN
1	D	273	GLN
1	D	349	ASN
1	D	355	ASN
1	D	368	GLN
1	D	394	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MAE	A	901	-	1,7,7	0.23	0	0,8,8	0.00	-
3	PLP	A	905	1	15,15,16	2.49	2 (13%)	21,22,23	2.05	5 (23%)
2	MAE	B	902	-	1,7,7	0.47	0	0,8,8	0.00	-
3	PLP	B	906	1	15,15,16	2.84	2 (13%)	21,22,23	2.30	7 (33%)
2	MAE	C	903	-	1,7,7	0.26	0	0,8,8	0.00	-
3	PLP	C	907	1	15,15,16	2.63	2 (13%)	21,22,23	1.80	4 (19%)
2	MAE	D	904	-	1,7,7	0.49	0	0,8,8	0.00	-
3	PLP	D	908	1	15,15,16	2.03	3 (20%)	21,22,23	2.07	5 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAE	A	901	-	-	0/0/5/5	0/0/0/0
3	PLP	A	905	1	-	0/6/6/8	0/1/1/1
2	MAE	B	902	-	-	0/0/5/5	0/0/0/0
3	PLP	B	906	1	-	0/6/6/8	0/1/1/1
2	MAE	C	903	-	-	0/0/5/5	0/0/0/0
3	PLP	C	907	1	-	0/6/6/8	0/1/1/1
2	MAE	D	904	-	-	0/0/5/5	0/0/0/0
3	PLP	D	908	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)
3	B	906	PLP	C3-C2	-9.97	1.33	1.40
3	C	907	PLP	C3-C2	-8.96	1.34	1.40
3	A	905	PLP	C4A-C4	-8.40	1.34	1.51
3	D	908	PLP	C3-C2	-5.34	1.37	1.40
3	B	906	PLP	P-O3P	-2.33	1.46	1.54
3	A	905	PLP	P-O3P	-2.22	1.46	1.54
3	D	908	PLP	P-O3P	-2.12	1.47	1.54
3	C	907	PLP	P-O3P	-2.10	1.47	1.54
3	D	908	PLP	C4A-C4	2.85	1.57	1.51

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	905	PLP	C3-C4-C5	-2.64	115.90	118.78
3	C	907	PLP	C5-C6-N1	-2.59	119.36	123.86
3	B	906	PLP	C4A-C4-C3	-2.58	115.69	120.36
3	C	907	PLP	O2P-P-O4P	-2.24	100.11	106.56
3	B	906	PLP	O2P-P-O4P	-2.16	100.33	106.56
3	B	906	PLP	C5-C6-N1	-2.15	120.13	123.86
3	A	905	PLP	C5-C6-N1	-2.09	120.24	123.86
3	D	908	PLP	C5-C6-N1	-2.08	120.25	123.86
3	B	906	PLP	C5A-C5-C4	2.06	124.38	121.65
3	A	905	PLP	O3P-P-O1P	2.47	118.52	110.58
3	D	908	PLP	O3P-P-O1P	2.49	118.59	110.58
3	D	908	PLP	C4A-C4-C5	2.50	123.49	120.88
3	D	908	PLP	C6-C5-C4	2.62	120.36	118.15
3	B	906	PLP	O3P-P-O1P	2.70	119.28	110.58
3	C	907	PLP	O3P-P-O1P	2.72	119.33	110.58
3	B	906	PLP	C4A-C4-C5	4.36	125.43	120.88
3	A	905	PLP	C6-C5-C4	4.55	122.01	118.15
3	C	907	PLP	O4P-C5A-C5	5.49	118.07	108.99
3	A	905	PLP	O4P-C5A-C5	5.85	118.66	108.99
3	D	908	PLP	O4P-C5A-C5	7.07	120.68	108.99
3	B	906	PLP	O4P-C5A-C5	7.25	120.97	108.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	905	PLP	2	0
3	B	906	PLP	3	0
3	C	907	PLP	3	0
3	D	908	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.