



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2018 – 04:42 pm GMT

PDB ID : 2CST
Title : CRYSTAL STRUCTURE OF THE CLOSED FORM OF CHICKEN CYTOSOLIC ASPARTATE AMINOTRANSFERASE AT 1.9 ANGSTROMS RESOLUTION
Authors : Malashkevich, V.N.; Strokopytov, B.V.; Borisov, V.V.
Deposited on : 1994-09-06
Resolution : 1.90 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

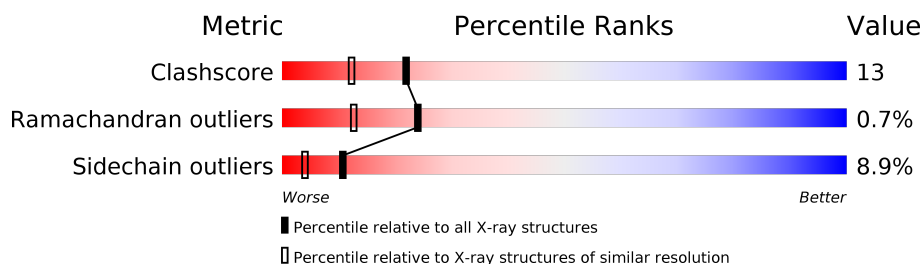
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	122078	6112 (1.90-1.90)
Ramachandran outliers	120005	6045 (1.90-1.90)
Sidechain outliers	119972	6045 (1.90-1.90)

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 $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	411	
1	B	411	

2 Entry composition [i](#)

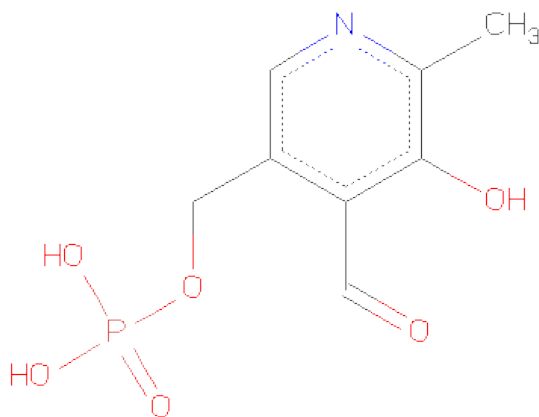
There are 4 unique types of molecules in this entry. The entry contains 7274 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

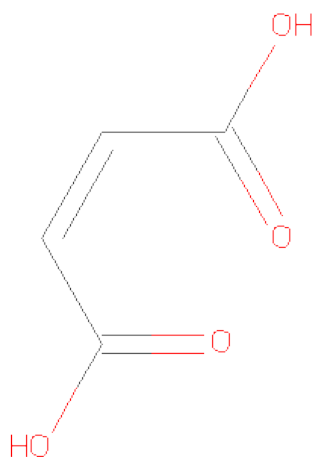
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3230	2049	568	599	14			
1	B	411	Total	C	N	O	S	0	0	0
			3230	2049	568	599	14			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



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

- Molecule 3 is MALEIC ACID (three-letter code: MAE) (formula: C₄H₄O₄).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	406	Total	O	0	0
			406	406		
4	B	362	Total	O	0	0
			362	362		

3 Residue-property plots

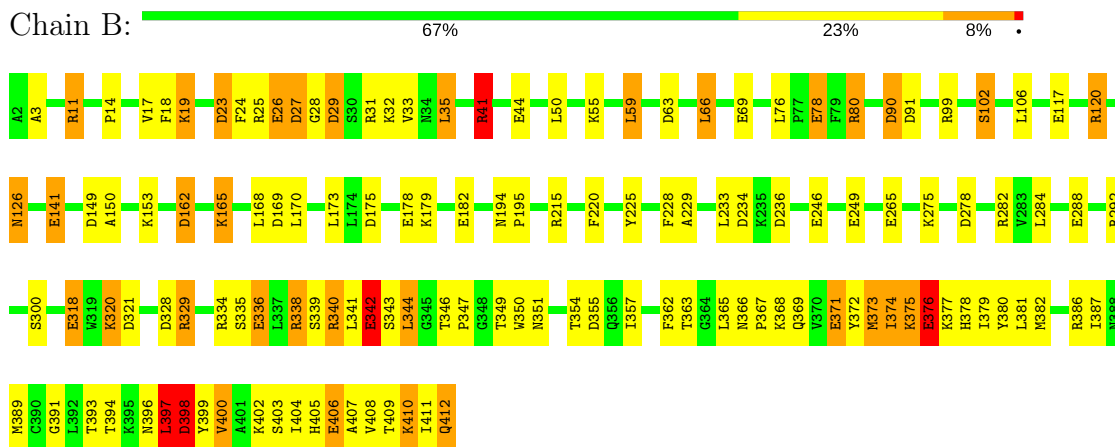
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: ASPARTATE AMINOTRANSFERASE



• Molecule 1: ASPARTATE AMINOTRANSFERASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.40 Å 126.00 Å 124.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.175 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7274	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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	0.83	17/3307 (0.5%)	1.15	43/4482 (1.0%)
1	B	0.83	18/3307 (0.5%)	1.20	43/4482 (1.0%)
All	All	0.83	35/6614 (0.5%)	1.18	86/8964 (1.0%)

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	141	GLU	CD-OE1	7.71	1.34	1.25
1	A	44	GLU	CD-OE1	6.80	1.33	1.25
1	B	78	GLU	CD-OE2	6.71	1.33	1.25
1	B	26	GLU	CD-OE1	6.54	1.32	1.25
1	A	265	GLU	CD-OE1	-6.36	1.18	1.25
1	A	141	GLU	CD-OE1	6.34	1.32	1.25
1	A	376	GLU	CD-OE1	6.33	1.32	1.25
1	A	288	GLU	CD-OE1	6.22	1.32	1.25
1	B	376	GLU	CD-OE2	6.21	1.32	1.25
1	A	371	GLU	CD-OE2	6.19	1.32	1.25
1	A	342	GLU	CD-OE2	6.15	1.32	1.25
1	B	44	GLU	CD-OE2	6.13	1.32	1.25
1	B	288	GLU	CD-OE1	6.01	1.32	1.25
1	B	371	GLU	CD-OE1	5.92	1.32	1.25
1	A	57	GLU	CD-OE1	5.91	1.32	1.25
1	B	117	GLU	CD-OE1	5.88	1.32	1.25
1	A	246	GLU	CD-OE1	5.87	1.32	1.25
1	B	182	GLU	CD-OE1	5.86	1.32	1.25
1	B	249	GLU	CD-OE2	-5.77	1.19	1.25
1	B	265	GLU	CD-OE2	5.70	1.31	1.25
1	A	318	GLU	CD-OE2	5.69	1.31	1.25
1	B	318	GLU	CD-OE2	5.64	1.31	1.25
1	A	78	GLU	CD-OE2	5.58	1.31	1.25
1	B	342	GLU	CD-OE2	5.58	1.31	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	GLU	CD-OE2	5.56	1.31	1.25
1	A	26	GLU	CD-OE2	5.55	1.31	1.25
1	B	178	GLU	CD-OE2	5.53	1.31	1.25
1	A	117	GLU	CD-OE1	5.42	1.31	1.25
1	B	69	GLU	CD-OE2	5.42	1.31	1.25
1	A	69	GLU	CD-OE2	5.38	1.31	1.25
1	A	182	GLU	CD-OE2	5.37	1.31	1.25
1	B	336	GLU	CD-OE1	5.25	1.31	1.25
1	A	277	GLU	CD-OE2	5.12	1.31	1.25
1	B	246	GLU	CD-OE1	5.10	1.31	1.25
1	B	406	GLU	CD-OE1	5.09	1.31	1.25

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	ARG	NE-CZ-NH1	12.13	126.36	120.30
1	B	80	ARG	NE-CZ-NH2	-10.45	115.08	120.30
1	B	99	ARG	NE-CZ-NH2	-9.59	115.50	120.30
1	B	99	ARG	NE-CZ-NH1	9.42	125.01	120.30
1	A	99	ARG	NE-CZ-NH1	9.15	124.87	120.30
1	B	120	ARG	NE-CZ-NH1	8.55	124.58	120.30
1	A	120	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	A	29	ASP	CB-CG-OD1	-7.77	111.31	118.30
1	B	355	ASP	CB-CG-OD2	-7.65	111.41	118.30
1	B	236	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	B	41	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	A	120	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	B	149	ASP	CB-CG-OD2	6.84	124.46	118.30
1	B	328	ASP	CB-CG-OD2	6.81	124.43	118.30
1	A	203	ASP	CB-CG-OD2	-6.77	112.21	118.30
1	B	234	ASP	CB-CG-OD2	-6.73	112.25	118.30
1	B	169	ASP	CB-CG-OD1	6.61	124.25	118.30
1	A	278	ASP	CB-CG-OD1	-6.61	112.36	118.30
1	A	176	ASP	CB-CG-OD1	-6.57	112.38	118.30
1	B	63	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	B	29	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	A	91	ASP	CB-CG-OD1	6.49	124.14	118.30
1	A	41	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	B	27	ASP	CB-CG-OD2	-6.42	112.53	118.30
1	B	149	ASP	CB-CG-OD1	-6.39	112.55	118.30
1	A	99	ARG	N-CA-CB	-6.33	99.20	110.60
1	B	355	ASP	CB-CG-OD1	6.32	123.99	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	ASP	CB-CG-OD2	6.31	123.98	118.30
1	B	328	ASP	CB-CG-OD1	-6.15	112.76	118.30
1	B	169	ASP	CB-CG-OD2	-6.14	112.78	118.30
1	B	321	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	B	234	ASP	CB-CG-OD1	6.09	123.79	118.30
1	A	41	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	B	90	ASP	CB-CG-OD1	-6.03	112.88	118.30
1	B	23	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	A	176	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	169	ASP	CB-CG-OD2	-5.97	112.92	118.30
1	A	321	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	B	225	TYR	CB-CG-CD1	-5.97	117.42	121.00
1	A	328	ASP	CB-CG-OD2	5.95	123.66	118.30
1	B	91	ASP	CB-CG-OD2	-5.92	112.98	118.30
1	B	398	ASP	CB-CA-C	5.89	122.18	110.40
1	A	355	ASP	CB-CG-OD2	-5.88	113.00	118.30
1	B	282	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	B	292	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	B	29	ASP	CB-CG-OD1	5.81	123.53	118.30
1	B	11	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	203	ASP	CB-CG-OD1	5.73	123.46	118.30
1	A	222	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	90	ASP	CB-CG-OD1	-5.70	113.17	118.30
1	B	120	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	B	162	ASP	CB-CG-OD1	-5.68	113.19	118.30
1	A	334	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	398	ASP	CB-CG-OD2	-5.65	113.22	118.30
1	A	175	ASP	CB-CG-OD1	-5.64	113.23	118.30
1	A	278	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	154	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	A	90	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	199	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	91	ASP	CB-CG-OD2	-5.56	113.29	118.30
1	A	169	ASP	CB-CG-OD1	5.54	123.29	118.30
1	A	175	ASP	CB-CG-OD2	5.53	123.28	118.30
1	B	282	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	154	ASP	CB-CG-OD1	5.51	123.25	118.30
1	A	23	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	B	175	ASP	CB-CG-OD1	-5.46	113.39	118.30
1	B	23	ASP	CB-CG-OD1	5.45	123.20	118.30
1	A	31	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	A	31	ARG	NE-CZ-NH2	-5.40	117.60	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	236	ASP	CB-CG-OD1	5.34	123.10	118.30
1	A	156	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	B	386	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	99	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	27	ASP	CB-CG-OD1	5.21	122.98	118.30
1	A	27	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	A	63	ASP	CB-CG-OD1	-5.16	113.65	118.30
1	A	398	ASP	CB-CG-OD1	5.16	122.94	118.30
1	B	90	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	54	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	328	ASP	CB-CG-OD1	-5.11	113.70	118.30
1	B	340	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	236	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	199	ASP	CB-CG-OD1	-5.07	113.74	118.30
1	B	278	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	B	215	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	91	ASP	CB-CG-OD1	5.02	122.82	118.30

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	3230	0	3177	46	0
1	B	3230	0	3177	121	0
2	A	15	0	6	0	0
2	B	15	0	6	0	0
3	A	8	0	2	0	0
3	B	8	0	2	0	0
4	A	406	0	0	6	0
4	B	362	0	0	12	0
All	All	7274	0	6370	164	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 13.

All (164) 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:B:233:LEU:HD12	1:B:320:LYS:HE3	1.40	1.02
1:A:54:ARG:HG2	1:A:54:ARG:HH11	1.29	0.97
1:B:407:ALA:HA	1:B:411:ILE:HG22	1.55	0.88
1:B:387:ILE:HD12	1:B:389:MET:HE1	1.55	0.87
1:B:233:LEU:CD1	1:B:320:LYS:HE3	2.08	0.84
1:B:389:MET:HA	1:B:389:MET:HE2	1.62	0.80
1:B:366:ASN:HB2	1:B:367:PRO:HD2	1.66	0.78
1:B:29:ASP:OD1	1:B:31:ARG:HD3	1.84	0.77
1:B:59:LEU:HD21	4:B:759:HOH:O	1.85	0.76
1:B:340:ARG:HD2	1:B:398:ASP:OD1	1.86	0.76
1:B:379:ILE:HD13	1:B:400:VAL:HG12	1.70	0.73
1:B:25:ARG:HH11	1:B:25:ARG:HG2	1.55	0.72
1:B:410:LYS:HB3	4:B:476:HOH:O	1.88	0.72
1:B:396:ASN:O	1:B:400:VAL:HG22	1.91	0.71
1:B:33:VAL:HG12	1:B:35:LEU:HD13	1.72	0.71
1:A:54:ARG:HG2	1:A:54:ARG:NH1	2.04	0.69
1:A:119:LEU:HD13	1:A:185:ILE:HD13	1.74	0.69
1:B:372:TYR:CB	1:B:411:ILE:HG21	2.22	0.69
1:B:120:ARG:HD3	1:B:150:ALA:O	1.92	0.69
1:B:389:MET:CE	1:B:389:MET:HA	2.23	0.69
1:B:334:ARG:HH11	1:B:334:ARG:HG2	1.57	0.68
1:A:99:ARG:HG2	1:A:274:GLY:O	1.94	0.67
1:B:19:LYS:HD3	1:B:19:LYS:C	2.14	0.67
1:B:31:ARG:HB3	1:B:399:TYR:CE2	2.30	0.67
1:B:162:ASP:CB	1:B:165:LYS:HD2	2.25	0.66
1:A:393:THR:H	1:A:396:ASN:ND2	1.94	0.66
1:B:377:LYS:HA	1:B:377:LYS:HE2	1.78	0.66
1:B:387:ILE:CD1	1:B:389:MET:HE1	2.24	0.65
1:A:120:ARG:HD3	1:A:150:ALA:O	1.97	0.65
1:B:349:THR:HG22	1:B:351:ASN:OD1	1.96	0.65
1:B:23:ASP:O	1:B:26:GLU:HG3	1.96	0.65
1:A:275:LYS:NZ	4:A:770:HOH:O	2.30	0.65
1:A:214:ARG:HG2	1:A:214:ARG:HH11	1.60	0.64
1:B:329:ARG:HG2	1:B:329:ARG:HH11	1.62	0.64
1:B:340:ARG:O	1:B:344:LEU:HD23	1.99	0.63
1:B:329:ARG:NH1	1:B:329:ARG:HG2	2.14	0.63
1:B:19:LYS:HD3	1:B:19:LYS:O	1.99	0.62
1:A:393:THR:H	1:A:396:ASN:HD21	1.46	0.62
1:B:340:ARG:NH1	1:B:398:ASP:OD1	2.29	0.62
1:B:29:ASP:O	1:B:32:LYS:HG3	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:MET:HE3	1:B:404:ILE:HG13	1.79	0.61
1:B:233:LEU:H	1:B:320:LYS:HZ2	1.48	0.61
1:B:162:ASP:HB3	1:B:165:LYS:HD2	1.81	0.61
1:B:25:ARG:HG2	1:B:25:ARG:NH1	2.14	0.61
1:B:35:LEU:HD12	1:B:391:GLY:HA3	1.82	0.61
1:B:17:VAL:HG12	1:B:382:MET:SD	2.41	0.60
1:A:2:ALA:HA	4:A:631:HOH:O	2.01	0.60
1:A:372:TYR:CD1	1:A:411:ILE:HD11	2.37	0.60
1:B:338:ARG:HH11	1:B:342:GLU:CD	2.05	0.60
1:B:409:THR:HA	4:B:680:HOH:O	2.00	0.60
1:A:171:GLN:CD	1:A:171:GLN:H	2.02	0.59
1:B:372:TYR:HE2	1:B:406:GLU:HB2	1.67	0.59
1:B:29:ASP:OD2	1:B:31:ARG:NH1	2.35	0.59
1:B:339:SER:HA	4:B:676:HOH:O	2.02	0.59
1:B:341:LEU:HD22	1:B:346:THR:HG21	1.85	0.58
1:B:78:GLU:HB2	4:B:681:HOH:O	2.01	0.58
1:B:402:LYS:O	1:B:405:HIS:HB3	2.03	0.58
1:B:366:ASN:ND2	1:B:369:GLN:OE1	2.36	0.58
1:B:372:TYR:CG	1:B:411:ILE:HG21	2.39	0.58
1:B:408:VAL:O	1:B:412:GLN:HG2	2.05	0.57
1:B:229:ALA:HB1	1:B:357:ILE:CG2	2.34	0.57
1:B:411:ILE:HG13	1:B:411:ILE:O	2.05	0.56
1:B:372:TYR:HD2	1:B:407:ALA:HB2	1.71	0.56
1:B:369:GLN:NE2	1:B:412:GLN:HB3	2.21	0.56
1:B:24:PHE:CE1	1:B:32:LYS:HB3	2.42	0.55
1:B:233:LEU:H	1:B:320:LYS:NZ	2.03	0.55
1:B:366:ASN:HB2	1:B:367:PRO:CD	2.35	0.55
1:B:55:LYS:HE3	1:B:318:GLU:OE1	2.07	0.55
1:B:14:PRO:HG2	1:B:19:LYS:HG2	1.88	0.54
1:A:396:ASN:HD22	1:A:396:ASN:C	2.11	0.54
1:B:338:ARG:NH1	1:B:342:GLU:OE2	2.38	0.54
1:B:377:LYS:CE	1:B:377:LYS:HA	2.37	0.54
1:B:229:ALA:HB1	1:B:357:ILE:HG21	1.89	0.53
1:B:375:LYS:HE3	1:B:376:GLU:OE2	2.09	0.52
1:B:50:LEU:N	1:B:50:LEU:HD23	2.24	0.52
1:A:54:ARG:HH11	1:A:54:ARG:CG	2.10	0.52
1:B:27:ASP:HB3	1:B:32:LYS:HD2	1.91	0.52
1:A:214:ARG:NH1	1:A:214:ARG:HG2	2.25	0.52
1:A:235:LYS:HD3	4:A:798:HOH:O	2.09	0.52
1:A:55:LYS:HB2	1:A:55:LYS:NZ	2.25	0.52
1:A:368:LYS:H	1:A:368:LYS:HE2	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ASP:OD1	1:B:28:GLY:N	2.43	0.51
1:B:398:ASP:O	1:B:402:LYS:HG3	2.10	0.51
1:B:162:ASP:CG	1:B:165:LYS:HD2	2.31	0.51
1:B:334:ARG:NH1	1:B:334:ARG:HG2	2.25	0.51
1:B:344:LEU:O	1:B:344:LEU:HD12	2.10	0.51
1:B:373:MET:CE	1:B:404:ILE:HG13	2.40	0.50
1:B:233:LEU:CG	1:B:320:LYS:HE3	2.41	0.50
1:B:368:LYS:HA	1:B:371:GLU:HG3	1.93	0.49
1:A:73:ILE:HD11	1:B:18:PHE:CD2	2.47	0.49
1:B:369:GLN:HB3	1:B:407:ALA:HB1	1.94	0.49
1:B:126:ASN:ND2	4:B:600:HOH:O	2.44	0.49
1:B:26:GLU:HB3	4:B:741:HOH:O	2.13	0.49
1:B:372:TYR:HB2	1:B:411:ILE:HG21	1.94	0.49
1:B:374:ILE:HD11	1:B:380:TYR:CE2	2.48	0.49
1:B:80:ARG:HD2	1:B:102:SER:O	2.12	0.48
1:B:402:LYS:O	1:B:405:HIS:N	2.47	0.48
1:B:338:ARG:NH2	1:B:351:ASN:HB3	2.29	0.48
1:B:372:TYR:CD1	1:B:376:GLU:HG3	2.48	0.48
1:A:344:LEU:HD21	1:A:402:LYS:HG3	1.96	0.48
1:B:346:THR:HG23	1:B:347:PRO:HD2	1.96	0.48
1:A:102:SER:OG	1:A:269:ASN:OD1	2.32	0.47
1:B:394:THR:HA	1:B:397:LEU:HD12	1.96	0.47
1:B:173:LEU:HD23	1:B:173:LEU:C	2.34	0.47
1:B:23:ASP:HA	1:B:26:GLU:CG	2.44	0.47
1:B:387:ILE:HD12	1:B:389:MET:CE	2.36	0.47
1:A:332:LEU:O	1:A:336:GLU:HG2	2.15	0.47
1:B:41:ARG:HD3	4:B:558:HOH:O	2.14	0.47
1:B:374:ILE:HG23	1:B:375:LYS:N	2.29	0.46
1:B:375:LYS:HG2	1:B:376:GLU:N	2.30	0.46
1:B:408:VAL:C	1:B:412:GLN:HG2	2.35	0.46
1:A:73:ILE:HD11	1:B:18:PHE:HD2	1.81	0.46
1:A:357:ILE:HD13	4:A:545:HOH:O	2.16	0.46
1:B:406:GLU:O	1:B:410:LYS:N	2.46	0.46
1:B:194:ASN:HA	1:B:195:PRO:HA	1.77	0.45
1:B:372:TYR:HD1	1:B:376:GLU:OE2	1.99	0.45
1:A:106:LEU:HD11	1:B:106:LEU:HD11	1.98	0.45
1:B:23:ASP:HA	1:B:26:GLU:HG2	1.98	0.45
1:A:368:LYS:CE	1:A:368:LYS:H	2.29	0.45
1:A:176:ASP:HA	1:A:179:LYS:HZ2	1.81	0.45
1:A:372:TYR:CG	1:A:411:ILE:CD1	3.00	0.45
1:B:29:ASP:CG	1:B:31:ARG:HH11	2.20	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:VAL:HG11	4:B:464:HOH:O	2.16	0.45
1:A:229:ALA:HB3	1:A:236:ASP:CG	2.37	0.45
1:A:168:LEU:HD22	1:A:169:ASP:N	2.32	0.45
1:B:393:THR:O	1:B:397:LEU:HD12	2.17	0.44
1:A:99:ARG:HD2	1:A:275:LYS:O	2.18	0.44
1:B:365:LEU:N	1:B:365:LEU:CD1	2.80	0.44
1:B:372:TYR:HB2	1:B:411:ILE:HG12	2.00	0.44
1:B:369:GLN:HE21	1:B:412:GLN:HB3	1.83	0.44
1:A:98:LYS:HA	4:A:628:HOH:O	2.17	0.44
1:B:367:PRO:O	1:B:371:GLU:HG3	2.18	0.44
1:B:341:LEU:HD23	1:B:341:LEU:HA	1.76	0.43
1:A:250:LEU:C	1:A:250:LEU:HD12	2.39	0.43
1:A:277:GLU:O	1:A:280:VAL:HG22	2.18	0.43
1:B:381:LEU:HD23	1:B:381:LEU:N	2.32	0.43
1:B:397:LEU:O	1:B:400:VAL:HG23	2.18	0.43
1:B:31:ARG:HB3	1:B:399:TYR:CZ	2.53	0.43
1:A:202:PRO:O	1:A:206:LYS:HG3	2.19	0.43
1:A:173:LEU:C	1:A:173:LEU:HD23	2.39	0.42
1:B:320:LYS:HE2	4:B:545:HOH:O	2.19	0.42
1:B:343:SER:HB3	4:B:676:HOH:O	2.18	0.42
1:B:31:ARG:O	1:B:33:VAL:HG23	2.18	0.42
1:A:229:ALA:HB3	1:A:236:ASP:OD2	2.19	0.42
1:B:338:ARG:O	1:B:342:GLU:HB2	2.19	0.42
1:B:403:SER:HA	1:B:406:GLU:HG3	2.00	0.42
1:B:374:ILE:CG2	1:B:375:LYS:N	2.82	0.42
1:A:74:LEU:O	1:A:80:ARG:HD2	2.20	0.42
1:B:336:GLU:OE1	1:B:336:GLU:HA	2.20	0.42
1:A:341:LEU:HA	1:A:341:LEU:HD23	1.80	0.41
1:A:194:ASN:HA	1:A:195:PRO:HA	1.85	0.41
1:B:410:LYS:HB2	1:B:411:ILE:H	1.64	0.41
1:A:275:LYS:NZ	4:A:755:HOH:O	2.53	0.41
1:A:22:ALA:O	1:A:26:GLU:HG2	2.21	0.41
1:B:341:LEU:CD1	1:B:350:TRP:CE3	3.04	0.41
1:A:368:LYS:H	1:A:368:LYS:CD	2.35	0.40
1:B:17:VAL:HG13	1:B:382:MET:CE	2.51	0.40
1:B:329:ARG:CG	1:B:329:ARG:HH11	2.29	0.40
1:A:140:TRP:CZ3	1:A:142:ASN:HB3	2.55	0.40
1:A:73:ILE:HG21	1:A:288:GLU:HG3	2.02	0.40
1:A:344:LEU:HA	1:A:344:LEU:HD12	1.80	0.40
1:B:412:GLN:NE2	4:B:678:HOH:O	2.54	0.40
1:B:66:LEU:HA	1:B:66:LEU:HD12	1.85	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:MET:HE1	1:B:404:ILE:HG12	2.03	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	409/411 (100%)	400 (98%)	9 (2%)	0	100	100
1	B	409/411 (100%)	378 (92%)	25 (6%)	6 (2%)	11	3
All	All	818/822 (100%)	778 (95%)	34 (4%)	6 (1%)	24	13

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	397	LEU
1	B	410	LYS
1	B	363	THR
1	B	378	HIS
1	B	342	GLU
1	B	3	ALA

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	342/342 (100%)	317 (93%)	25 (7%)	15	6
1	B	342/342 (100%)	306 (90%)	36 (10%)	7	3
All	All	684/684 (100%)	623 (91%)	61 (9%)	11	4

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ARG
1	A	65	SER
1	A	71	LEU
1	A	99	ARG
1	A	126	ASN
1	A	141	GLU
1	A	168	LEU
1	A	171	GLN
1	A	179	LYS
1	A	188	LEU
1	A	215	ARG
1	A	220	PHE
1	A	228	PHE
1	A	233	LEU
1	A	235	LYS
1	A	275	LYS
1	A	284	LEU
1	A	321	ASP
1	A	340	ARG
1	A	361	SER
1	A	362	PHE
1	A	368	LYS
1	A	376	GLU
1	A	396	ASN
1	A	410	LYS
1	B	11	ARG
1	B	19	LYS
1	B	35	LEU
1	B	41	ARG
1	B	59	LEU
1	B	66	LEU
1	B	76	LEU
1	B	90	ASP
1	B	102	SER
1	B	126	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	141	GLU
1	B	153	LYS
1	B	165	LYS
1	B	168	LEU
1	B	170	LEU
1	B	179	LYS
1	B	220	PHE
1	B	228	PHE
1	B	275	LYS
1	B	284	LEU
1	B	300	SER
1	B	320	LYS
1	B	329	ARG
1	B	335	SER
1	B	338	ARG
1	B	344	LEU
1	B	354	THR
1	B	362	PHE
1	B	373	MET
1	B	374	ILE
1	B	375	LYS
1	B	376	GLU
1	B	397	LEU
1	B	398	ASP
1	B	400	VAL
1	B	412	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	269	ASN
1	A	322	ASN
1	A	396	ASN
1	B	126	ASN
1	B	281	GLN
1	B	412	GLN

5.3.3 RNA ⓘ

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](#)

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	$\# Z > 2$
2	PLP	A	413	1	15,15,16	1.29	1 (6%)	20,22,23	1.85	7 (35%)
3	MAE	A	414	-	1,7,7	0.30	0	0,8,8	0.00	-
2	PLP	B	413	1	15,15,16	1.34	2 (13%)	20,22,23	2.04	9 (45%)
3	MAE	B	414	-	1,7,7	0.39	0	0,8,8	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
2	PLP	A	413	1	-	0/6/6/8	0/1/1/1
3	MAE	A	414	-	-	0/0/5/5	0/0/0/0
2	PLP	B	413	1	-	0/6/6/8	0/1/1/1
3	MAE	B	414	-	-	0/0/5/5	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	413	PLP	C4A-C4	-3.72	1.44	1.51
2	B	413	PLP	C4A-C4	-2.91	1.45	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	413	PLP	C5A-C5	2.16	1.56	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	413	PLP	C3-C2-N1	-3.13	116.64	120.75
2	A	413	PLP	C5-C6-N1	-2.79	119.11	123.83
2	A	413	PLP	C3-C2-N1	-2.62	117.31	120.75
2	B	413	PLP	C5-C6-N1	-2.56	119.50	123.83
2	B	413	PLP	C3-C4-C5	-2.42	115.93	118.66
2	B	413	PLP	C5A-C5-C6	-2.34	115.41	119.34
2	A	413	PLP	C3-C4-C5	-2.17	116.21	118.66
2	A	413	PLP	C2A-C2-C3	2.02	123.38	120.96
2	B	413	PLP	O3-C3-C4	2.11	123.89	118.14
2	A	413	PLP	C6-N1-C2	2.22	123.47	119.19
2	B	413	PLP	O4P-C5A-C5	2.38	113.97	109.39
2	A	413	PLP	C4A-C4-C5	2.57	123.44	120.85
2	B	413	PLP	C6-N1-C2	3.04	125.05	119.19
2	B	413	PLP	C2A-C2-C3	3.24	124.82	120.96
2	B	413	PLP	C6-C5-C4	3.69	121.18	118.19
2	A	413	PLP	C6-C5-C4	4.46	121.81	118.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.