



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:29 PM GMT

PDB ID : 1FTA
Title : FRUCTOSE-1,6-BISPHOSPHATASE(D-FRUCTOSE-1,6-BISPHOSPHATE, 1-PHOSPHOHYDROLASE) (E.C.3.1.3.11) COMPLEXED WITH THE ALLOSTERIC INHIBITOR AMP
Authors : Zhang, Y.; Liang, J.-Y.; Huang, S.; Lipscomb, W.N.
Deposited on : 1993-09-27
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 ⓘ 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

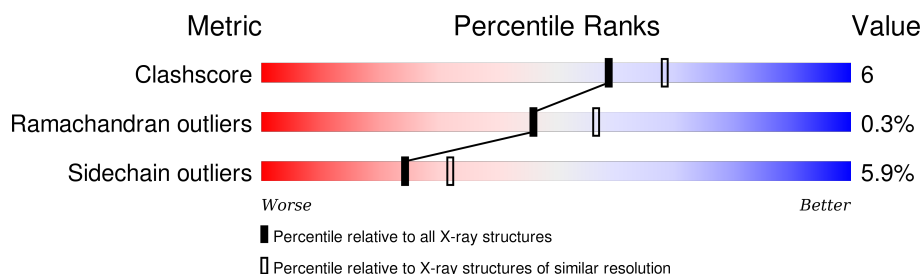
1 Overall quality at a glance

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))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (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 $\leq 5\%$. 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	337	 72% 20% •• 5%
1	B	337	 78% 15% • 6%
1	C	337	 73% 19% • 6%
1	D	337	 74% 18% •• 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12987 atoms, of which 2819 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.

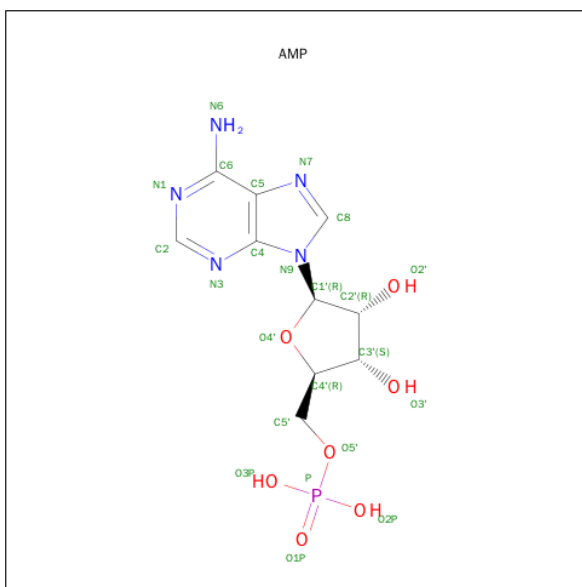
- Molecule 1 is a protein called FRUCTOSE-1,6-BISPHOSPHATASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	319	Total	C	H	N	O	S	0	0	0
			2976	1559	534	408	458	17			
1	B	317	Total	C	H	N	O	S	0	0	0
			2955	1548	529	405	456	17			
1	C	317	Total	C	H	N	O	S	0	0	0
			2955	1548	529	405	456	17			
1	D	318	Total	C	H	N	O	S	0	0	0
			2968	1554	533	407	457	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	VAL	ASN	CONFLICT	UNP P09467
A	214	ALA	GLY	CONFLICT	UNP P09467
A	316	ILE	VAL	CONFLICT	UNP P09467
B	11	VAL	ASN	CONFLICT	UNP P09467
B	214	ALA	GLY	CONFLICT	UNP P09467
B	316	ILE	VAL	CONFLICT	UNP P09467
C	11	VAL	ASN	CONFLICT	UNP P09467
C	214	ALA	GLY	CONFLICT	UNP P09467
C	316	ILE	VAL	CONFLICT	UNP P09467
D	11	VAL	ASN	CONFLICT	UNP P09467
D	214	ALA	GLY	CONFLICT	UNP P09467
D	316	ILE	VAL	CONFLICT	UNP P09467

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is water.

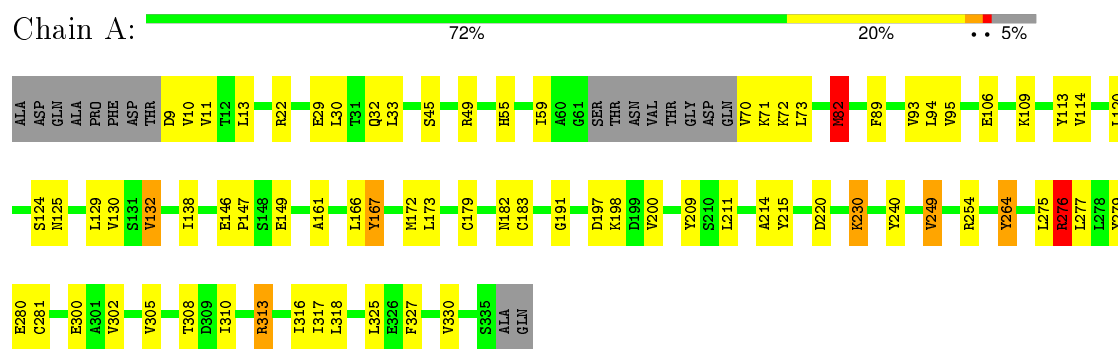
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	75	Total	H	O	0	0
			225	150	75		
3	B	89	Total	H	O	0	0
			267	178	89		
3	C	59	Total	H	O	0	0
			177	118	59		
3	D	124	Total	H	O	0	0
			372	248	124		

3 Residue-property plots

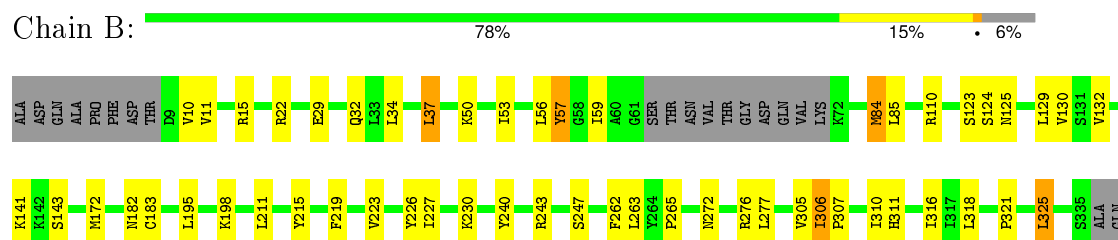
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

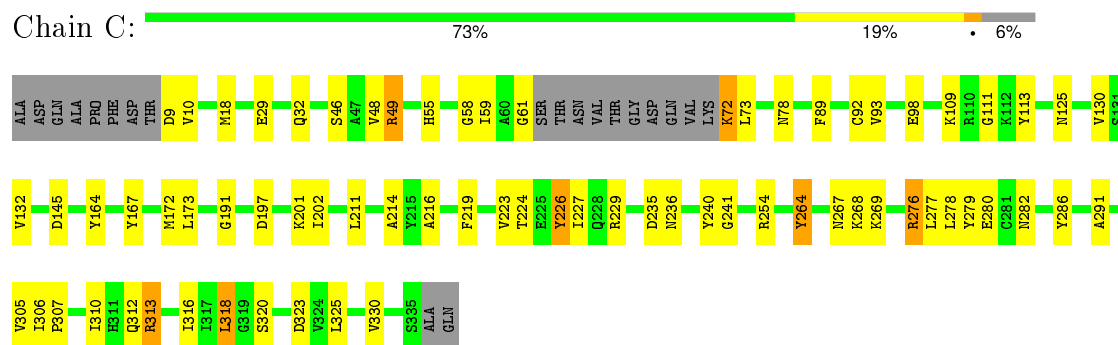
• Molecule 1: FRUCTOSE-1,6-BISPHOSPHATASE



• Molecule 1: FRUCTOSE-1,6-BISPHOSPHATASE

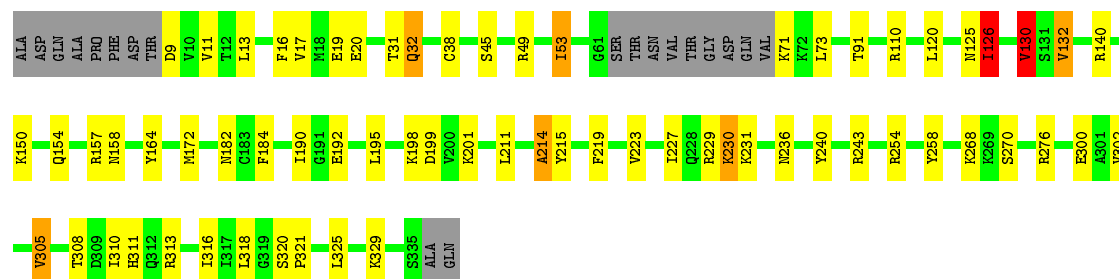


• Molecule 1: FRUCTOSE-1,6-BISPHOSPHATASE



• Molecule 1: FRUCTOSE-1,6-BISPHOSPHATASE

Chain D:



4 Data and refinement statistics

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	68.60Å 84.80Å 281.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.200 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12987	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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: AMP

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	0/2485	1.31	14/3356 (0.4%)
1	B	0.68	0/2469	1.32	11/3335 (0.3%)
1	C	0.70	0/2469	1.36	15/3335 (0.4%)
1	D	0.69	0/2478	1.36	17/3346 (0.5%)
All	All	0.69	0/9901	1.34	57/13372 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	2
1	C	0	2
1	D	0	1
All	All	0	9

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	254	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	D	229	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	D	254	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	C	279	TYR	CB-CG-CD2	-7.55	116.47	121.00
1	A	215	TYR	CB-CG-CD2	-7.21	116.67	121.00
1	B	215	TYR	CB-CG-CD2	-7.15	116.71	121.00
1	D	164	TYR	CB-CG-CD1	-7.13	116.72	121.00
1	D	214	ALA	CB-CA-C	-7.13	99.41	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	313	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	C	49	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	C	264	TYR	CB-CG-CD2	-6.59	117.05	121.00
1	C	49	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	A	276	ARG	CB-CG-CD	6.38	128.19	111.60
1	B	22	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	A	179	CYS	CA-CB-SG	6.19	125.15	114.00
1	C	240	TYR	CB-CG-CD2	-6.03	117.38	121.00
1	D	243	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	C	164	TYR	CB-CG-CD1	-5.98	117.41	121.00
1	A	49	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	A	82	MET	CA-CB-CG	-5.91	103.25	113.30
1	B	22	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	C	229	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	D	313	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	B	110	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	B	263	LEU	CA-CB-CG	5.72	128.46	115.30
1	D	130	VAL	CA-CB-CG1	-5.72	102.31	110.90
1	D	329	LYS	CB-CG-CD	-5.66	96.89	111.60
1	A	240	TYR	CB-CG-CD2	-5.62	117.62	121.00
1	B	132	VAL	N-CA-CB	-5.60	99.19	111.50
1	C	286	TYR	CB-CG-CD2	-5.60	117.64	121.00
1	C	72	LYS	N-CA-C	-5.58	95.94	111.00
1	D	140	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	243	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B	84	MET	CG-SD-CE	5.48	108.97	100.20
1	A	317	ILE	N-CA-C	-5.48	96.21	111.00
1	D	318	LEU	CA-CB-CG	5.47	127.88	115.30
1	A	313	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	D	132	VAL	N-CA-CB	-5.40	99.62	111.50
1	A	279	TYR	CB-CG-CD1	-5.36	117.78	121.00
1	C	254	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	22	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	132	VAL	CA-C-N	5.31	126.81	116.20
1	C	132	VAL	N-CA-CB	-5.28	99.88	111.50
1	A	132	VAL	N-CA-CB	-5.22	100.02	111.50
1	A	249	VAL	CG1-CB-CG2	-5.18	102.62	110.90
1	B	276	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	247	SER	N-CA-C	-5.15	97.10	111.00
1	C	93	VAL	CG1-CB-CG2	-5.14	102.67	110.90
1	D	53	ILE	CB-CA-C	-5.12	101.35	111.60
1	D	11	VAL	CG1-CB-CG2	-5.12	102.71	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	214	ALA	N-CA-CB	5.10	117.25	110.10
1	D	313	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	D	126	ILE	CA-CB-CG1	-5.08	101.35	111.00
1	C	113	TYR	CB-CG-CD1	-5.05	117.97	121.00
1	A	254	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	211	LEU	CA-CB-CG	5.02	126.84	115.30
1	C	132	VAL	CB-CA-C	5.01	120.91	111.40

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	TYR	Sidechain
1	A	209	TYR	Sidechain
1	A	264	TYR	Sidechain
1	A	276	ARG	Sidechain
1	B	226	TYR	Sidechain
1	B	57	TYR	Sidechain
1	C	167	TYR	Sidechain
1	C	226	TYR	Sidechain
1	D	258	TYR	Sidechain

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	2442	534	2498	35	0
1	B	2426	529	2476	28	0
1	C	2426	529	2476	26	0
1	D	2435	533	2489	35	0
2	A	23	0	12	1	0
2	B	23	0	12	0	0
2	C	23	0	12	1	0
2	D	23	0	12	0	0
3	A	75	150	0	0	0
3	B	89	178	0	1	0
3	C	59	118	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	124	248	0	3	0
All	All	10168	2819	9987	114	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 6.

All (114) 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:125:ASN:HB3	1:A:130:VAL:HB	1.66	0.78
1:A:302:VAL:O	1:A:305:VAL:HG12	1.92	0.70
1:C:241:GLY:HA2	1:D:214:ALA:HB2	1.74	0.70
1:D:211:LEU:HD11	1:D:227:ILE:HD11	1.74	0.67
1:B:211:LEU:HD11	1:B:227:ILE:HD11	1.77	0.67
1:D:182:ASN:HD22	1:D:198:LYS:HA	1.60	0.67
1:D:302:VAL:HG21	1:D:316:ILE:HD13	1.77	0.67
1:A:183:CYS:SG	1:A:200:VAL:HG21	2.36	0.65
1:B:84:MET:HE2	1:B:84:MET:HA	1.80	0.64
1:B:182:ASN:HD22	1:B:198:LYS:HA	1.61	0.64
1:B:32:GLN:HA	1:B:32:GLN:HE21	1.64	0.61
1:A:30:LEU:HD12	1:A:33:LEU:HD23	1.83	0.60
1:D:182:ASN:ND2	1:D:198:LYS:HA	2.16	0.60
1:B:37:LEU:HD23	1:B:85:LEU:HD21	1.83	0.59
1:D:302:VAL:HG21	1:D:316:ILE:CD1	2.34	0.57
1:A:129:LEU:HD11	1:B:172:MET:HB2	1.86	0.55
1:A:166:LEU:HD13	1:A:249:VAL:HG12	1.88	0.55
1:D:154:GLN:HE21	1:D:158:ASN:HD22	1.52	0.55
1:C:211:LEU:HD11	1:C:227:ILE:HD11	1.89	0.55
1:A:191:GLY:HA3	1:C:191:GLY:HA3	1.89	0.55
1:C:278:LEU:HD12	1:C:310:ILE:HA	1.89	0.54
1:D:230:LYS:HE2	1:D:230:LYS:HA	1.89	0.54
1:B:219:PHE:HB3	1:B:223:VAL:HG13	1.90	0.54
1:B:172:MET:SD	1:B:183:CYS:HB3	2.48	0.53
1:D:32:GLN:HA	1:D:32:GLN:HE21	1.73	0.53
1:D:73:LEU:HD23	1:D:126:ILE:HD13	1.90	0.53
1:A:89:PHE:CD2	1:A:109:LYS:HA	2.45	0.52
1:C:9:ASP:HA	3:D:416:HOH:O	2.09	0.51
1:D:195:LEU:HD21	1:D:198:LYS:HG2	1.91	0.51
1:D:45:SER:O	1:D:49:ARG:HD3	2.10	0.51
1:C:58:GLY:O	1:D:9:ASP:N	2.43	0.51
1:A:32:GLN:HE21	1:A:32:GLN:HA	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:GLN:HA	1:B:32:GLN:NE2	2.27	0.50
1:C:214:ALA:HB1	1:D:240:TYR:O	2.12	0.50
1:C:89:PHE:HD1	1:C:109:LYS:HA	1.78	0.49
1:B:125:ASN:HB3	1:B:130:VAL:HB	1.93	0.49
1:A:10:VAL:HG11	1:B:59:ILE:HA	1.93	0.49
1:A:138:ILE:HD12	1:A:161:ALA:HB3	1.95	0.48
1:A:277:LEU:HA	1:A:281:CYS:HB2	1.94	0.48
1:A:214:ALA:HB1	1:B:240:TYR:O	2.12	0.48
1:D:19:GLU:HG2	3:D:344:HOH:O	2.11	0.48
1:B:195:LEU:HD21	1:B:198:LYS:HG2	1.96	0.48
1:A:276:ARG:HD3	1:A:313:ARG:HG2	1.94	0.48
1:B:262:PHE:HB3	1:B:318:LEU:HD12	1.95	0.48
1:C:32:GLN:HE21	1:C:32:GLN:HA	1.78	0.48
1:D:126:ILE:HD12	1:D:132:VAL:HG21	1.96	0.47
1:C:316:ILE:HD11	1:C:318:LEU:HD23	1.95	0.47
1:C:216:ALA:HA	1:C:219:PHE:CD2	2.50	0.47
1:A:55:HIS:HA	1:A:59:ILE:HG22	1.96	0.47
1:A:95:VAL:HG13	1:A:310:ILE:HD12	1.97	0.46
1:A:32:GLN:HA	1:A:32:GLN:NE2	2.31	0.45
1:B:316:ILE:HD11	1:B:318:LEU:HD23	1.97	0.45
1:C:125:ASN:HB3	1:C:130:VAL:HB	1.97	0.45
1:C:55:HIS:HA	1:C:59:ILE:HG22	1.99	0.45
1:C:202:ILE:HG22	1:C:291:ALA:O	2.17	0.45
1:C:48:VAL:HA	1:C:73:LEU:HD21	1.99	0.45
1:A:120:LEU:HD12	1:A:120:LEU:HA	1.78	0.45
1:A:316:ILE:HD11	1:A:318:LEU:HD23	1.99	0.45
1:B:84:MET:HA	1:B:84:MET:CE	2.46	0.44
1:A:82:MET:HG3	1:A:94:LEU:HD13	2.00	0.44
1:D:172:MET:HG3	1:D:184:PHE:O	2.17	0.44
1:A:132:VAL:HG12	1:A:167:TYR:HD2	1.82	0.44
1:B:15:ARG:HA	1:D:32:GLN:HE22	1.83	0.44
1:A:13:LEU:HD22	1:A:173:LEU:HD22	1.99	0.44
1:C:29:GLU:HB2	2:C:338:AMP:O1P	2.17	0.44
1:D:302:VAL:O	1:D:305:VAL:HG12	2.18	0.43
1:C:226:TYR:HB2	1:C:330:VAL:HG21	2.00	0.43
1:A:113:TYR:OH	2:A:338:AMP:H3'	2.18	0.43
1:B:321:PRO:O	1:B:325:LEU:HB2	2.19	0.43
1:A:9:ASP:HA	3:C:396:HOH:O	2.18	0.43
1:D:182:ASN:ND2	1:D:199:ASP:H	2.17	0.43
1:B:182:ASN:ND2	1:B:198:LYS:HA	2.30	0.43
1:A:276:ARG:HA	1:A:313:ARG:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:LEU:HD12	1:A:316:ILE:HG21	2.01	0.43
1:C:92:CYS:HB3	1:C:111:GLY:O	2.18	0.43
1:D:227:ILE:HG22	1:D:231:LYS:HE3	2.00	0.43
1:A:183:CYS:HB2	1:A:197:ASP:HB3	2.01	0.43
1:D:154:GLN:NE2	1:D:158:ASN:HD22	2.15	0.43
1:D:73:LEU:HG	1:D:120:LEU:CD2	2.49	0.43
1:B:230:LYS:HE2	1:B:230:LYS:HA	2.02	0.42
1:D:157:ARG:HD3	1:D:157:ARG:HA	1.87	0.42
1:C:89:PHE:CD1	1:C:109:LYS:HA	2.54	0.42
1:D:215:TYR:HB2	1:D:219:PHE:CE1	2.54	0.42
1:D:190:ILE:HG13	1:D:192:GLU:HB2	2.00	0.42
1:D:71:LYS:N	3:D:445:HOH:O	2.52	0.42
1:D:17:VAL:HG12	1:D:31:THR:HG23	2.02	0.42
1:A:327:PHE:O	1:A:330:VAL:HG22	2.20	0.42
1:C:78:ASN:HB2	1:C:98:GLU:HG3	2.02	0.42
1:C:306:ILE:HA	1:C:307:PRO:HD3	1.88	0.42
1:B:306:ILE:HA	1:B:307:PRO:HD3	1.76	0.42
1:A:172:MET:HB2	1:B:129:LEU:HD11	2.02	0.42
1:A:146:GLU:HA	1:A:147:PRO:HD2	1.91	0.42
1:D:310:ILE:HG13	1:D:311:HIS:CD2	2.55	0.41
1:B:29:GLU:HG3	3:B:355:HOH:O	2.20	0.41
1:B:50:LYS:O	1:B:53:ILE:HG13	2.20	0.41
1:A:230:LYS:HD2	1:A:230:LYS:N	2.35	0.41
1:C:268:LYS:HA	1:C:268:LYS:HD2	1.91	0.41
1:B:310:ILE:HG13	1:B:311:HIS:CD2	2.55	0.41
1:C:320:SER:HB2	1:C:323:ASP:OD2	2.20	0.41
1:A:276:ARG:O	1:A:280:GLU:HB2	2.19	0.41
1:A:70:VAL:HG22	1:A:71:LYS:H	1.84	0.41
1:D:16:PHE:O	1:D:20:GLU:HB2	2.20	0.41
1:D:91:THR:O	1:D:110:ARG:HA	2.21	0.41
1:C:61:GLY:O	1:D:9:ASP:N	2.53	0.41
1:B:141:LYS:HZ1	1:B:143:SER:HB2	1.86	0.41
1:C:277:LEU:HD22	1:C:312:GLN:NE2	2.36	0.41
1:D:125:ASN:HB3	1:D:130:VAL:HG23	2.03	0.41
1:A:182:ASN:HD22	1:A:198:LYS:HA	1.85	0.41
1:D:13:LEU:HD23	1:D:38:CYS:SG	2.61	0.40
1:A:93:VAL:O	1:A:114:VAL:HA	2.21	0.40
1:C:276:ARG:O	1:C:280:GLU:HB2	2.21	0.40
1:D:320:SER:HA	1:D:321:PRO:HD3	1.88	0.40
1:B:53:ILE:HG22	1:B:56:LEU:HD12	2.02	0.40
1:B:277:LEU:HD11	1:B:305:VAL:HG13	2.04	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	315/337 (94%)	304 (96%)	11 (4%)	0	100	100
1	B	313/337 (93%)	296 (95%)	16 (5%)	1 (0%)	46	57
1	C	313/337 (93%)	299 (96%)	12 (4%)	2 (1%)	30	36
1	D	314/337 (93%)	300 (96%)	13 (4%)	1 (0%)	46	57
All	All	1255/1348 (93%)	1199 (96%)	52 (4%)	4 (0%)	46	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	235	ASP
1	C	269	LYS
1	D	270	SER
1	B	57	TYR

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	266/280 (95%)	250 (94%)	16 (6%)	24	31
1	B	264/280 (94%)	254 (96%)	10 (4%)	40	54
1	C	264/280 (94%)	243 (92%)	21 (8%)	15	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	265/280 (95%)	250 (94%)	15 (6%)	25	34
All	All	1059/1120 (95%)	997 (94%)	62 (6%)	24	32

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	VAL
1	A	29	GLU
1	A	45	SER
1	A	72	LYS
1	A	73	LEU
1	A	82	MET
1	A	106	GLU
1	A	124	SER
1	A	149	GLU
1	A	220	ASP
1	A	230	LYS
1	A	264	TYR
1	A	276	ARG
1	A	300	GLU
1	A	308	THR
1	A	325	LEU
1	B	10	VAL
1	B	11	VAL
1	B	34	LEU
1	B	37	LEU
1	B	123	SER
1	B	124	SER
1	B	265	PRO
1	B	272	ASN
1	B	306	ILE
1	B	325	LEU
1	C	10	VAL
1	C	18	MET
1	C	46	SER
1	C	49	ARG
1	C	72	LYS
1	C	145	ASP
1	C	172	MET
1	C	173	LEU
1	C	197	ASP
1	C	201	LYS

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Mol	Chain	Res	Type
1	C	223	VAL
1	C	224	THR
1	C	236	ASN
1	C	264	TYR
1	C	267	ASN
1	C	276	ARG
1	C	282	ASN
1	C	305	VAL
1	C	313	ARG
1	C	318	LEU
1	C	325	LEU
1	D	32	GLN
1	D	53	ILE
1	D	126	ILE
1	D	130	VAL
1	D	150	LYS
1	D	201	LYS
1	D	223	VAL
1	D	230	LYS
1	D	236	ASN
1	D	268	LYS
1	D	276	ARG
1	D	300	GLU
1	D	305	VAL
1	D	308	THR
1	D	325	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	154	GLN
1	A	182	ASN
1	B	32	GLN
1	B	154	GLN
1	B	182	ASN
1	B	228	GLN
1	B	282	ASN
1	C	32	GLN
1	C	35	ASN
1	C	154	GLN
1	C	267	ASN

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Mol	Chain	Res	Type
1	C	282	ASN
1	D	32	GLN
1	D	154	GLN
1	D	182	ASN
1	D	282	ASN

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](#)

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	AMP	A	338	-	20,25,25	1.10	3 (15%)	22,38,38	2.05	3 (13%)
2	AMP	B	338	-	20,25,25	1.05	2 (10%)	22,38,38	2.55	8 (36%)
2	AMP	C	338	-	20,25,25	1.09	2 (10%)	22,38,38	2.10	4 (18%)
2	AMP	D	338	-	20,25,25	1.09	2 (10%)	22,38,38	2.34	5 (22%)

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	AMP	A	338	-	-	0/6/26/26	0/3/3/3
2	AMP	B	338	-	-	0/6/26/26	0/3/3/3
2	AMP	C	338	-	-	0/6/26/26	0/3/3/3
2	AMP	D	338	-	-	0/6/26/26	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	338	AMP	C5'-C4'	-2.02	1.45	1.51
2	D	338	AMP	C2-N1	2.01	1.37	1.33
2	B	338	AMP	C2-N1	2.03	1.37	1.33
2	C	338	AMP	C2-N1	2.15	1.38	1.33
2	A	338	AMP	C2-N1	2.17	1.38	1.33
2	A	338	AMP	C2-N3	2.57	1.36	1.32
2	D	338	AMP	C2-N3	2.71	1.37	1.32
2	B	338	AMP	C2-N3	2.72	1.37	1.32
2	C	338	AMP	C2-N3	2.86	1.37	1.32

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	338	AMP	N3-C2-N1	-8.73	122.21	128.89
2	B	338	AMP	N3-C2-N1	-8.14	122.66	128.89
2	A	338	AMP	N3-C2-N1	-7.68	123.02	128.89
2	C	338	AMP	N3-C2-N1	-6.34	124.04	128.89
2	C	338	AMP	C2'-C1'-N9	-5.03	106.60	114.29
2	D	338	AMP	C2'-C1'-N9	-3.83	108.44	114.29
2	B	338	AMP	O3P-P-O1P	-3.31	99.94	110.58
2	B	338	AMP	C1'-N9-C4	-3.06	122.32	126.94
2	B	338	AMP	C2'-C1'-N9	-2.59	110.34	114.29
2	A	338	AMP	C1'-N9-C4	-2.35	123.40	126.94
2	D	338	AMP	O5'-P-O1P	2.00	112.24	107.14
2	D	338	AMP	O4'-C1'-N9	2.13	112.55	108.10
2	B	338	AMP	O3'-C3'-C4'	2.19	117.63	111.05
2	C	338	AMP	O2P-P-O5'	2.44	113.60	106.56
2	C	338	AMP	O5'-P-O1P	2.67	113.93	107.14
2	D	338	AMP	C4'-O4'-C1'	2.92	112.93	109.72
2	B	338	AMP	O2P-P-O5'	3.05	115.35	106.56
2	A	338	AMP	C4'-O4'-C1'	3.18	113.21	109.72
2	B	338	AMP	O5'-P-O1P	3.26	115.45	107.14
2	B	338	AMP	C4'-O4'-C1'	3.46	113.52	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	338	AMP	1	0
2	C	338	AMP	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.