Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 12:56 AM EDT

PDB ID	:	3D54
Title	:	Structure of PurLQS from Thermotoga maritima
Authors	:	Ealick, S.E.; Morar, M.
Deposited on	:	2008-05-15
Resolution	:	3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

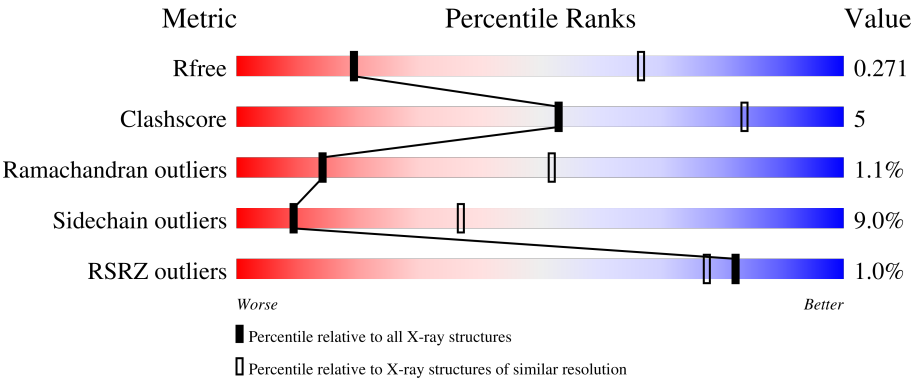
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	629	78% 14% • 7%
1	E	629	81% 12% 7%
1	I	629	4% 80% 12% 7%
2	B	82	73% 22% 5%
2	C	82	78% 18% •

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Mol	Chain	Length	Quality of chain
2	F	82	78% 17%
2	G	82	% 77% 21%
2	J	82	73% 22%
2	K	82	79% 17%
3	D	213	71% 23% 5%
3	H	213	72% 23% 5%
3	L	213	73% 23%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NA	A	3003	-	-	-	X
4	NA	I	3001	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 22584 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 Phosphoribosylformylglycinamidine synthase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	583	Total	C	N	O	S	0	0	0
			4493	2859	769	846	19			
1	E	583	Total	C	N	O	S	0	0	0
			4493	2859	769	846	19			
1	I	583	Total	C	N	O	S	0	0	0
			4493	2859	769	846	19			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	Expression Tag	UNP Q9X0X3
A	-24	GLY	-	Expression Tag	UNP Q9X0X3
A	-23	SER	-	Expression Tag	UNP Q9X0X3
A	-22	HIS	-	Expression Tag	UNP Q9X0X3
A	-21	HIS	-	Expression Tag	UNP Q9X0X3
A	-20	HIS	-	Expression Tag	UNP Q9X0X3
A	-19	HIS	-	Expression Tag	UNP Q9X0X3
A	-18	HIS	-	Expression Tag	UNP Q9X0X3
A	-17	HIS	-	Expression Tag	UNP Q9X0X3
A	-16	ASP	-	Expression Tag	UNP Q9X0X3
A	-15	ILE	-	Expression Tag	UNP Q9X0X3
A	-14	THR	-	Expression Tag	UNP Q9X0X3
A	-13	SER	-	Expression Tag	UNP Q9X0X3
A	-12	LEU	-	Expression Tag	UNP Q9X0X3
A	-11	TYR	-	Expression Tag	UNP Q9X0X3
A	-10	LYS	-	Expression Tag	UNP Q9X0X3
A	-9	LYS	-	Expression Tag	UNP Q9X0X3
A	-8	ALA	-	Expression Tag	UNP Q9X0X3
A	-7	GLY	-	Expression Tag	UNP Q9X0X3
A	-6	SER	-	Expression Tag	UNP Q9X0X3
A	-5	GLU	-	Expression Tag	UNP Q9X0X3
A	-4	ASN	-	Expression Tag	UNP Q9X0X3
A	-3	LEU	-	Expression Tag	UNP Q9X0X3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	TYR	-	Expression Tag	UNP Q9X0X3
A	-1	PHE	-	Expression Tag	UNP Q9X0X3
A	0	GLN	-	Expression Tag	UNP Q9X0X3
E	-25	MET	-	Expression Tag	UNP Q9X0X3
E	-24	GLY	-	Expression Tag	UNP Q9X0X3
E	-23	SER	-	Expression Tag	UNP Q9X0X3
E	-22	HIS	-	Expression Tag	UNP Q9X0X3
E	-21	HIS	-	Expression Tag	UNP Q9X0X3
E	-20	HIS	-	Expression Tag	UNP Q9X0X3
E	-19	HIS	-	Expression Tag	UNP Q9X0X3
E	-18	HIS	-	Expression Tag	UNP Q9X0X3
E	-17	HIS	-	Expression Tag	UNP Q9X0X3
E	-16	ASP	-	Expression Tag	UNP Q9X0X3
E	-15	ILE	-	Expression Tag	UNP Q9X0X3
E	-14	THR	-	Expression Tag	UNP Q9X0X3
E	-13	SER	-	Expression Tag	UNP Q9X0X3
E	-12	LEU	-	Expression Tag	UNP Q9X0X3
E	-11	TYR	-	Expression Tag	UNP Q9X0X3
E	-10	LYS	-	Expression Tag	UNP Q9X0X3
E	-9	LYS	-	Expression Tag	UNP Q9X0X3
E	-8	ALA	-	Expression Tag	UNP Q9X0X3
E	-7	GLY	-	Expression Tag	UNP Q9X0X3
E	-6	SER	-	Expression Tag	UNP Q9X0X3
E	-5	GLU	-	Expression Tag	UNP Q9X0X3
E	-4	ASN	-	Expression Tag	UNP Q9X0X3
E	-3	LEU	-	Expression Tag	UNP Q9X0X3
E	-2	TYR	-	Expression Tag	UNP Q9X0X3
E	-1	PHE	-	Expression Tag	UNP Q9X0X3
E	0	GLN	-	Expression Tag	UNP Q9X0X3
I	-25	MET	-	Expression Tag	UNP Q9X0X3
I	-24	GLY	-	Expression Tag	UNP Q9X0X3
I	-23	SER	-	Expression Tag	UNP Q9X0X3
I	-22	HIS	-	Expression Tag	UNP Q9X0X3
I	-21	HIS	-	Expression Tag	UNP Q9X0X3
I	-20	HIS	-	Expression Tag	UNP Q9X0X3
I	-19	HIS	-	Expression Tag	UNP Q9X0X3
I	-18	HIS	-	Expression Tag	UNP Q9X0X3
I	-17	HIS	-	Expression Tag	UNP Q9X0X3
I	-16	ASP	-	Expression Tag	UNP Q9X0X3
I	-15	ILE	-	Expression Tag	UNP Q9X0X3
I	-14	THR	-	Expression Tag	UNP Q9X0X3
I	-13	SER	-	Expression Tag	UNP Q9X0X3

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-12	LEU	-	Expression Tag	UNP Q9X0X3
I	-11	TYR	-	Expression Tag	UNP Q9X0X3
I	-10	LYS	-	Expression Tag	UNP Q9X0X3
I	-9	LYS	-	Expression Tag	UNP Q9X0X3
I	-8	ALA	-	Expression Tag	UNP Q9X0X3
I	-7	GLY	-	Expression Tag	UNP Q9X0X3
I	-6	SER	-	Expression Tag	UNP Q9X0X3
I	-5	GLU	-	Expression Tag	UNP Q9X0X3
I	-4	ASN	-	Expression Tag	UNP Q9X0X3
I	-3	LEU	-	Expression Tag	UNP Q9X0X3
I	-2	TYR	-	Expression Tag	UNP Q9X0X3
I	-1	PHE	-	Expression Tag	UNP Q9X0X3
I	0	GLN	-	Expression Tag	UNP Q9X0X3

- Molecule 2 is a protein called Formylglycinamide ribonucleotide amidotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	82	Total	C	N	O	S	0	0	0
			678	431	118	127	2			
2	C	82	Total	C	N	O	S	0	0	0
			678	431	118	127	2			
2	F	82	Total	C	N	O	S	0	0	0
			678	431	118	127	2			
2	G	82	Total	C	N	O	S	0	0	0
			678	431	118	127	2			
2	J	82	Total	C	N	O	S	0	0	0
			678	431	118	127	2			
2	K	82	Total	C	N	O	S	0	0	0
			678	431	118	127	2			

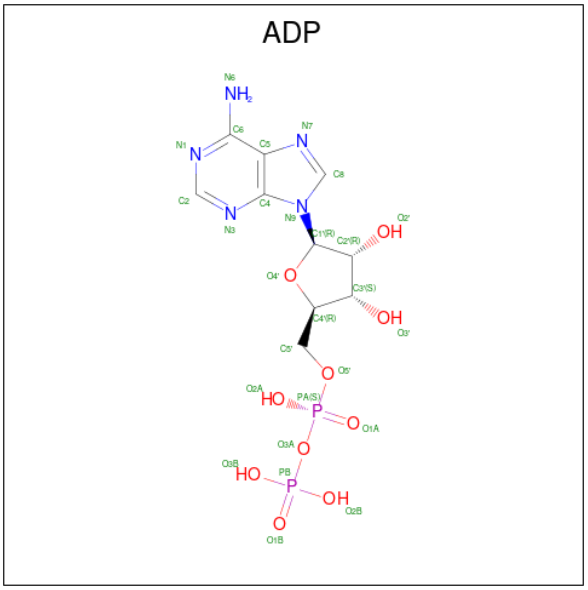
- Molecule 3 is a protein called Phosphoribosylformylglycinamidine synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	212	Total	C	N	O	S	0	0	0
			1651	1056	279	309	7			
3	H	212	Total	C	N	O	S	0	0	0
			1651	1056	279	309	7			
3	L	212	Total	C	N	O	S	0	0	0
			1651	1056	279	309	7			

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	E	1	Total Na 1 1	0	0
4	I	1	Total Na 1 1	0	0

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



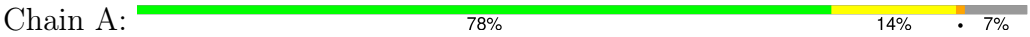
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 27 10 5 10 2	0	0
5	E	1	Total C N O P 27 10 5 10 2	0	0
5	I	1	Total C N O P 27 10 5 10 2	0	0

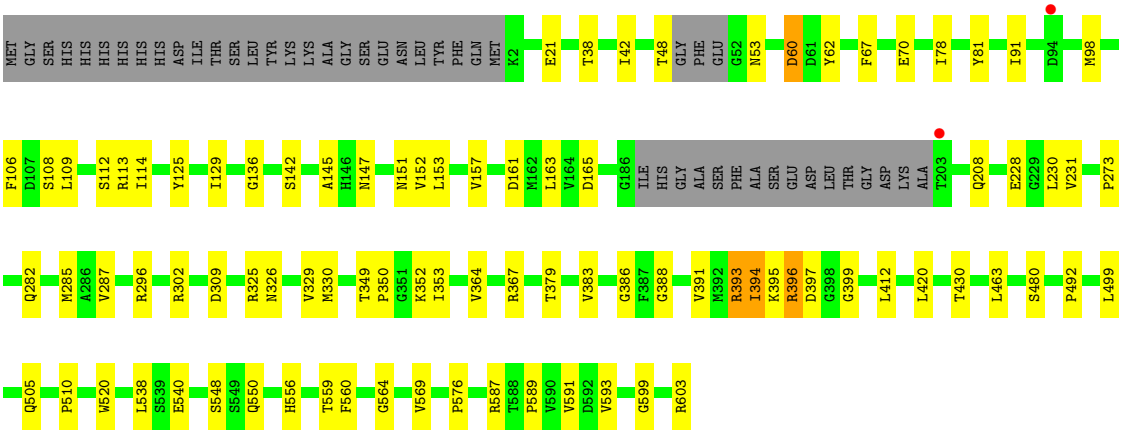
3 Residue-property plots (i)

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

• Molecule 1: Phosphoribosylformylglycinamidine synthase II

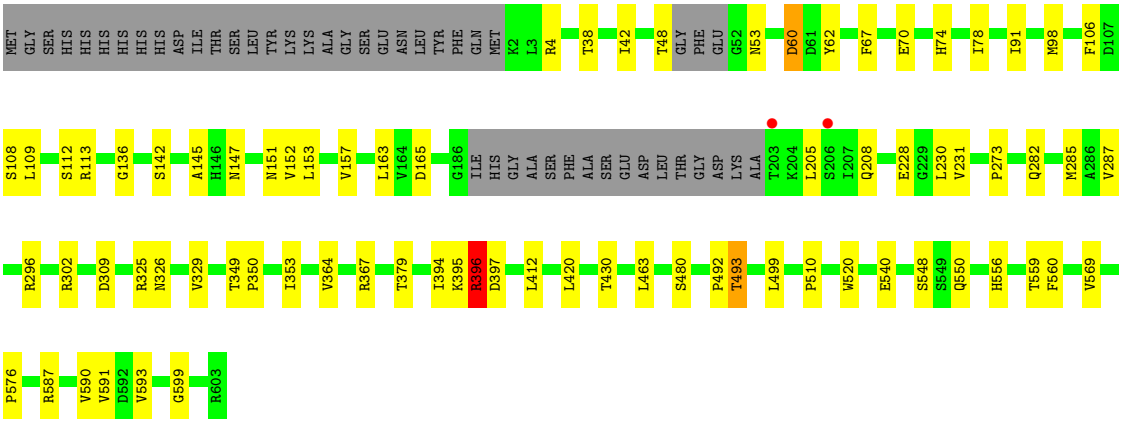
Chain A:





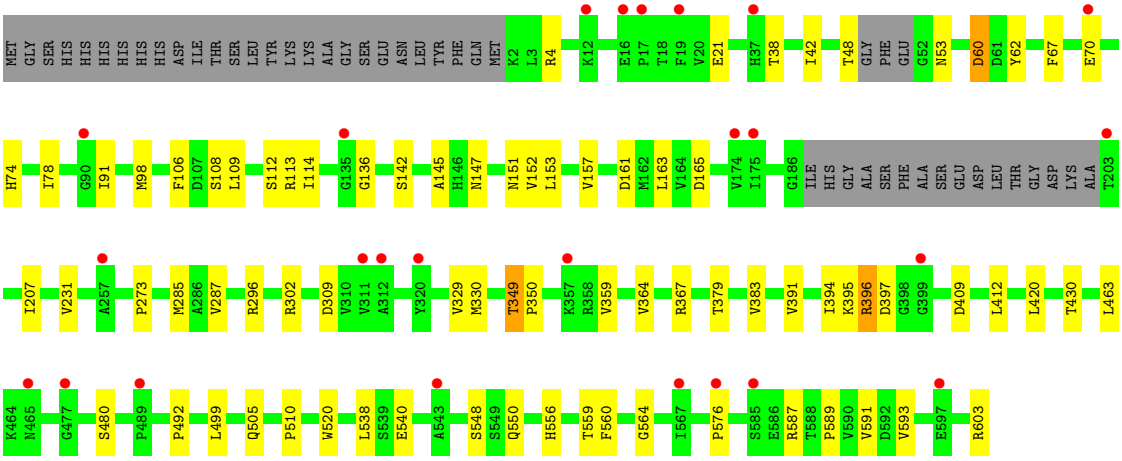
• Molecule 1: Phosphoribosylformylglycinamidine synthase II

Chain E:



• Molecule 1: Phosphoribosylformylglycinamidine synthase II

Chain I:

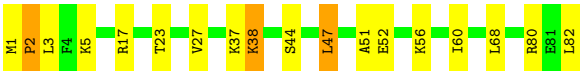


• Molecule 2: Formylglycinamide ribonucleotide amidotransferase

Chain B:

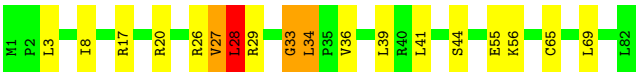
• Molecule 2: Formylglycinamide ribonucleotide amidotransferase

Chain C:



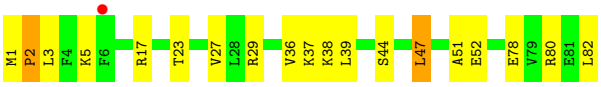
• Molecule 2: Formylglycinamide ribonucleotide amidotransferase

Chain F:



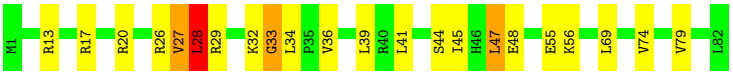
• Molecule 2: Formylglycinamide ribonucleotide amidotransferase

Chain G:



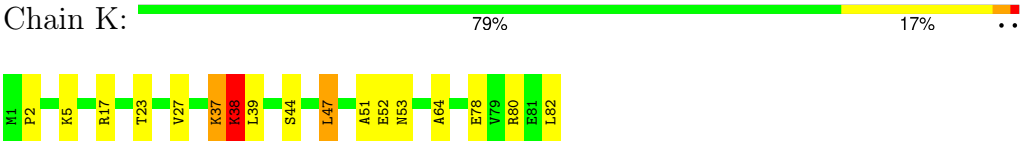
• Molecule 2: Formylglycinamide ribonucleotide amidotransferase

Chain J:



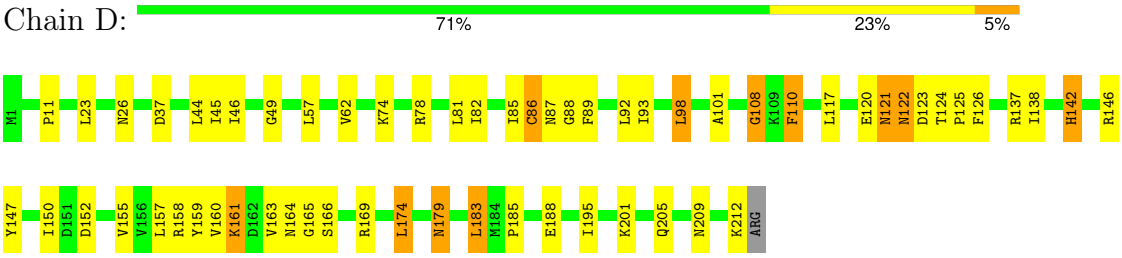
• Molecule 2: Formylglycinamide ribonucleotide amidotransferase

Chain K:



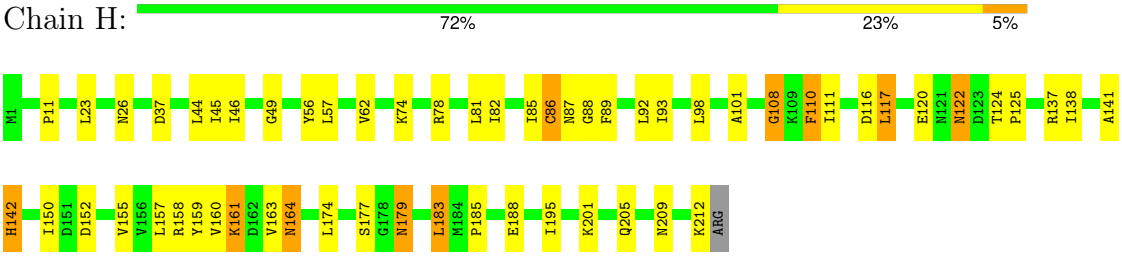
• Molecule 3: Phosphoribosylformylglycinamidine synthase 1

Chain D:



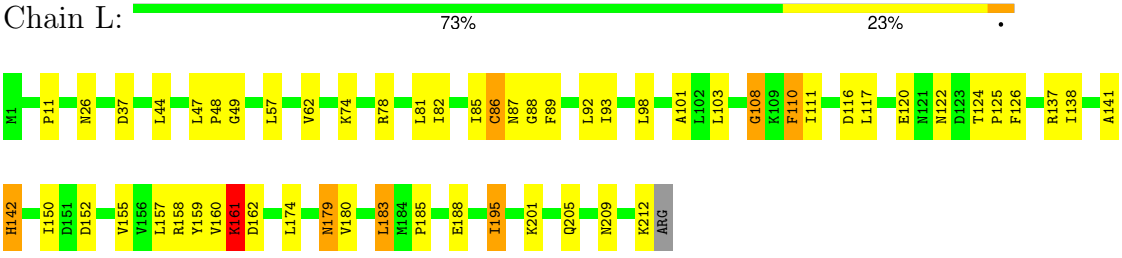
• Molecule 3: Phosphoribosylformylglycinamidine synthase 1

Chain H:



• Molecule 3: Phosphoribosylformylglycinamidine synthase 1

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	256.85Å 187.34Å 159.18Å 90.00° 99.12° 90.00°	Depositor
Resolution (Å)	45.70 – 3.50 48.10 – 3.50	Depositor EDS
% Data completeness (in resolution range)	83.8 (45.70-3.50) 83.8 (48.10-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 3.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.252 , 0.282 0.250 , 0.271	Depositor DCC
R_{free} test set	9327 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å^2)	88.4	Xtriage
Anisotropy	0.766	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 70.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	22584	wwPDB-VP
Average B, all atoms (Å^2)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CYG, ADP

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	0.67	0/4582	0.77	0/6217
1	E	0.67	0/4582	0.77	1/6217 (0.0%)
1	I	0.70	0/4582	0.76	0/6217
2	B	0.66	0/687	0.73	1/920 (0.1%)
2	C	0.64	0/687	0.75	0/920
2	F	0.66	0/687	0.79	2/920 (0.2%)
2	G	0.61	0/687	0.77	0/920
2	J	0.65	0/687	0.76	2/920 (0.2%)
2	K	0.68	0/687	0.80	0/920
3	D	0.71	0/1667	0.84	1/2249 (0.0%)
3	H	0.70	0/1667	0.85	2/2249 (0.1%)
3	L	0.72	0/1667	0.88	2/2249 (0.1%)
All	All	0.68	0/22869	0.79	11/30918 (0.0%)

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	3
1	E	0	2
1	I	0	2
2	C	0	1
2	K	0	1
3	D	0	3
3	H	0	2
3	L	0	2
All	All	0	16

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	161	LYS	CB-CA-C	5.99	122.38	110.40
1	E	205	LEU	CA-CB-CG	5.93	128.94	115.30
2	F	33	GLY	N-CA-C	5.72	127.41	113.10
2	J	33	GLY	N-CA-C	5.62	127.14	113.10
2	B	33	GLY	N-CA-C	5.36	126.50	113.10
3	H	108	GLY	N-CA-C	5.25	126.22	113.10
2	F	41	LEU	CA-CB-CG	5.14	127.13	115.30
3	L	108	GLY	N-CA-C	5.13	125.93	113.10
3	H	117	LEU	CA-CB-CG	5.10	127.04	115.30
2	J	41	LEU	CA-CB-CG	5.10	127.02	115.30
3	D	108	GLY	N-CA-C	5.02	125.64	113.10

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	394	ILE	Peptide
1	A	396	ARG	Peptide
1	A	397	ASP	Peptide
2	C	68	LEU	Peptide
3	D	121	ASN	Peptide
3	D	142	HIS	Peptide
3	D	161	LYS	Peptide
1	E	396	ARG	Peptide
1	E	397	ASP	Peptide
3	H	142	HIS	Peptide
3	H	161	LYS	Peptide
1	I	396	ARG	Peptide
1	I	397	ASP	Peptide
2	K	37	LYS	Peptide
3	L	142	HIS	Peptide
3	L	161	LYS	Peptide

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	4493	0	4532	27	0
1	E	4493	0	4532	17	0
1	I	4493	0	4532	16	0
2	B	678	0	707	22	0
2	C	678	0	707	12	0
2	F	678	0	707	16	0
2	G	678	0	707	10	0
2	J	678	0	707	19	0
2	K	678	0	707	13	0
3	D	1651	0	1642	41	0
3	H	1651	0	1642	32	0
3	L	1651	0	1642	34	0
4	A	1	0	0	0	0
4	E	1	0	0	0	0
4	I	1	0	0	0	0
5	A	27	0	12	4	0
5	E	27	0	12	2	0
5	I	27	0	12	2	0
All	All	22584	0	22800	243	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 5.

All (243) 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:395:LYS:O	1:A:396:ARG:HD2	1.43	1.19
2:B:26:ARG:HG2	2:B:26:ARG:HH11	1.06	1.14
2:J:28:LEU:O	2:J:28:LEU:HG	1.42	1.08
2:F:28:LEU:HD12	2:F:34:LEU:HD13	1.44	0.99
2:B:41:LEU:HD22	2:B:42:GLY:H	1.29	0.96
3:L:179:ASN:H	3:L:179:ASN:HD22	0.98	0.96
2:B:26:ARG:HG2	2:B:26:ARG:NH1	1.71	0.94
3:H:179:ASN:HD22	3:H:179:ASN:H	0.98	0.93
3:D:179:ASN:H	3:D:179:ASN:HD22	0.95	0.92
3:D:124:THR:HG23	3:D:125:PRO:HD2	1.54	0.88
2:B:26:ARG:HH11	2:B:26:ARG:CG	1.85	0.87
2:B:24:ILE:O	2:B:28:LEU:HD22	1.74	0.86
2:C:2:PRO:HD2	2:C:51:ALA:O	1.75	0.86
2:F:28:LEU:HD11	2:F:36:VAL:HG11	1.57	0.85
3:D:179:ASN:HD22	3:D:179:ASN:N	1.74	0.85
3:D:179:ASN:H	3:D:179:ASN:ND2	1.74	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:28:LEU:HD12	2:J:34:LEU:HD13	1.57	0.84
2:G:2:PRO:HD2	2:G:51:ALA:O	1.77	0.84
3:L:179:ASN:H	3:L:179:ASN:ND2	1.78	0.82
3:L:160:VAL:O	3:L:161:LYS:HG2	1.79	0.81
3:H:179:ASN:H	3:H:179:ASN:ND2	1.77	0.81
3:H:179:ASN:HD22	3:H:179:ASN:N	1.77	0.80
3:D:124:THR:CG2	3:D:125:PRO:HD2	2.12	0.80
3:D:121:ASN:OD1	3:D:122:ASN:O	1.99	0.79
3:D:160:VAL:C	3:D:161:LYS:HG2	2.01	0.79
1:I:395:LYS:O	1:I:396:ARG:HD2	1.83	0.78
3:H:160:VAL:O	3:H:161:LYS:HG2	1.84	0.77
1:A:157:VAL:HG11	1:A:394:ILE:HG21	1.65	0.76
2:B:41:LEU:HD22	2:B:42:GLY:N	2.00	0.76
3:H:110:PHE:HA	3:H:142:HIS:O	1.86	0.76
3:D:163:VAL:HG12	3:D:164:ASN:ND2	2.01	0.75
3:L:110:PHE:HA	3:L:142:HIS:O	1.87	0.74
1:A:395:LYS:O	1:A:396:ARG:CD	2.32	0.74
3:D:157:LEU:HD12	3:D:183:LEU:HD21	1.69	0.74
2:F:28:LEU:O	2:F:28:LEU:HG	1.88	0.74
3:L:160:VAL:C	3:L:161:LYS:HG2	2.10	0.72
3:L:157:LEU:HD12	3:L:183:LEU:HD21	1.71	0.72
3:D:110:PHE:HA	3:D:142:HIS:O	1.89	0.72
3:L:92:LEU:HB3	3:L:98:LEU:HD23	1.72	0.71
3:L:179:ASN:HD22	3:L:179:ASN:N	1.77	0.71
3:D:124:THR:HG23	3:D:174:LEU:HD11	1.71	0.71
3:H:81:LEU:HD12	3:H:81:LEU:H	1.57	0.69
3:H:157:LEU:HD12	3:H:183:LEU:HD21	1.74	0.69
3:D:81:LEU:HD12	3:D:81:LEU:H	1.58	0.68
3:H:183:LEU:HD22	3:H:185:PRO:HD2	1.75	0.68
3:D:92:LEU:HB3	3:D:98:LEU:HD23	1.76	0.67
2:F:28:LEU:CD1	2:F:34:LEU:HD13	2.23	0.67
3:L:81:LEU:HD12	3:L:81:LEU:H	1.59	0.67
2:F:28:LEU:O	2:F:28:LEU:CG	2.44	0.66
3:D:124:THR:CG2	3:D:174:LEU:HD11	2.25	0.66
3:D:183:LEU:HD22	3:D:185:PRO:HD2	1.78	0.65
2:B:24:ILE:O	2:B:28:LEU:CD2	2.45	0.65
3:H:92:LEU:HB3	3:H:98:LEU:HD23	1.78	0.65
3:H:163:VAL:HG12	3:H:164:ASN:ND2	2.12	0.64
3:L:183:LEU:HD22	3:L:185:PRO:HD2	1.79	0.64
2:K:37:LYS:O	2:K:38:LYS:HB2	1.98	0.64
3:L:160:VAL:HG12	3:L:161:LYS:HG2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:160:VAL:HG12	3:D:161:LYS:HE2	1.83	0.61
3:D:159:TYR:O	3:D:169:ARG:NH1	2.32	0.60
2:B:44:SER:HB2	2:C:44:SER:HB3	1.82	0.60
1:A:157:VAL:HG11	1:A:394:ILE:CG2	2.32	0.60
3:H:160:VAL:C	3:H:161:LYS:HG2	2.22	0.59
3:H:160:VAL:HG12	3:H:161:LYS:HG2	1.85	0.59
1:I:106:PHE:HB2	1:I:153:LEU:HB3	1.85	0.58
2:J:39:LEU:HD12	2:K:47:LEU:HB3	1.85	0.58
2:B:39:LEU:HD12	2:C:47:LEU:HB3	1.85	0.58
1:I:108:SER:HB3	1:I:151:ASN:HB2	1.84	0.58
2:J:28:LEU:O	2:J:28:LEU:CG	2.29	0.58
3:D:160:VAL:O	3:D:161:LYS:HG2	2.04	0.57
2:B:41:LEU:C	2:B:41:LEU:HD13	2.25	0.57
2:F:39:LEU:HD12	2:G:47:LEU:HB3	1.85	0.56
2:F:44:SER:HB2	2:G:44:SER:HB3	1.86	0.56
1:A:106:PHE:HB2	1:A:153:LEU:HB3	1.85	0.56
1:A:112:SER:HB3	1:A:145:ALA:HA	1.87	0.56
2:J:44:SER:HB2	2:K:44:SER:HB3	1.86	0.56
2:J:27:VAL:O	2:J:29:ARG:N	2.39	0.56
3:D:160:VAL:HG12	3:D:161:LYS:HG2	1.87	0.56
1:I:60:ASP:C	1:I:62:TYR:H	2.08	0.56
3:D:117:LEU:HD11	3:D:185:PRO:HG2	1.88	0.55
1:A:108:SER:HB3	1:A:151:ASN:HB2	1.89	0.55
1:A:564:GLY:O	1:A:603:ARG:OXT	2.25	0.55
3:D:124:THR:O	3:D:126:PHE:N	2.40	0.55
1:E:395:LYS:O	1:E:396:ARG:HD2	2.06	0.55
3:H:111:ILE:O	3:H:141:ALA:HA	2.07	0.54
3:L:93:ILE:HD13	3:L:101:ALA:HA	1.87	0.54
2:B:28:LEU:HG	2:B:28:LEU:O	2.07	0.54
2:F:27:VAL:O	2:F:29:ARG:N	2.40	0.54
3:D:93:ILE:HD13	3:D:101:ALA:HA	1.90	0.54
3:H:117:LEU:HD11	3:H:185:PRO:HG2	1.89	0.54
3:D:85:ILE:O	3:D:88:GLY:N	2.41	0.54
3:L:116:ASP:O	3:L:160:VAL:HG23	2.08	0.53
1:E:106:PHE:HB2	1:E:153:LEU:HB3	1.89	0.53
1:E:112:SER:HB3	1:E:145:ALA:HA	1.90	0.53
2:F:3:LEU:HD21	2:G:37:LYS:NZ	2.24	0.53
1:A:60:ASP:C	1:A:62:TYR:H	2.11	0.52
1:I:112:SER:HB3	1:I:145:ALA:HA	1.90	0.52
1:E:60:ASP:C	1:E:62:TYR:H	2.12	0.52
2:J:28:LEU:HD13	2:K:64:ALA:HB1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:SER:HB3	1:E:151:ASN:HB2	1.91	0.52
3:L:74:LYS:HE2	3:L:78:ARG:NH2	2.26	0.51
3:H:93:ILE:HD13	3:H:101:ALA:HA	1.92	0.50
2:B:27:VAL:HG12	2:B:28:LEU:N	2.25	0.50
2:J:69:LEU:HD23	3:L:57:LEU:HD11	1.93	0.50
2:B:69:LEU:HD23	3:D:57:LEU:HD11	1.92	0.50
3:L:117:LEU:HD11	3:L:185:PRO:HG2	1.94	0.50
1:A:393:ARG:HA	1:A:399:GLY:HA2	1.94	0.50
3:L:85:ILE:O	3:L:88:GLY:N	2.45	0.50
1:E:493:THR:HG22	1:E:493:THR:O	2.10	0.50
5:E:2006:ADP:H5'1	5:E:2006:ADP:O3B	2.12	0.50
1:E:367:ARG:NH1	1:E:559:THR:HG23	2.27	0.50
3:L:111:ILE:O	3:L:141:ALA:HA	2.11	0.50
1:A:231:VAL:HG13	1:A:287:VAL:HG13	1.93	0.49
1:I:70:GLU:HB2	1:I:91:ILE:HD13	1.95	0.49
1:A:136:GLY:O	5:A:2004:ADP:C8	2.66	0.49
1:A:569:VAL:HG12	1:A:599:GLY:HA3	1.95	0.49
3:H:74:LYS:HE2	3:H:78:ARG:NH2	2.28	0.49
1:E:70:GLU:HB2	1:E:91:ILE:HD13	1.95	0.48
3:D:124:THR:C	3:D:126:PHE:H	2.15	0.48
1:A:367:ARG:NH1	1:A:559:THR:HG23	2.28	0.48
5:A:2004:ADP:O3B	5:A:2004:ADP:H5'1	2.13	0.48
1:I:231:VAL:HG13	1:I:287:VAL:HG13	1.95	0.48
1:E:136:GLY:O	5:E:2006:ADP:C8	2.66	0.48
2:F:28:LEU:CD1	2:F:36:VAL:HG11	2.35	0.48
5:I:2005:ADP:H5'1	5:I:2005:ADP:O3B	2.13	0.48
3:L:26:ASN:HD21	3:L:201:LYS:HB2	1.78	0.48
1:E:394:ILE:O	1:E:395:LYS:HB2	2.14	0.48
2:J:36:VAL:HG21	2:K:47:LEU:HD12	1.94	0.48
1:I:564:GLY:O	1:I:603:ARG:OXT	2.32	0.48
2:F:3:LEU:HD21	2:G:37:LYS:HZ1	1.77	0.47
1:E:231:VAL:HG13	1:E:287:VAL:HG13	1.96	0.47
2:J:28:LEU:HA	2:J:32:LYS:HB2	1.97	0.47
1:A:70:GLU:HB2	1:A:91:ILE:HD13	1.96	0.47
2:C:5:LYS:HB3	2:C:82:LEU:HB2	1.96	0.47
2:K:5:LYS:HB3	2:K:82:LEU:HB2	1.97	0.47
3:H:122:ASN:C	3:H:124:THR:H	2.18	0.47
3:D:205:GLN:O	3:D:209:ASN:ND2	2.48	0.47
2:J:48:GLU:HB2	2:K:37:LYS:O	2.14	0.47
2:J:27:VAL:C	2:J:29:ARG:H	2.18	0.46
3:D:45:ILE:HB	3:D:82:ILE:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:367:ARG:NH1	1:I:559:THR:HG23	2.31	0.46
3:D:74:LYS:HE2	3:D:78:ARG:NH2	2.30	0.46
1:I:394:ILE:O	1:I:395:LYS:HB2	2.14	0.46
3:D:26:ASN:HD21	3:D:201:LYS:HB2	1.81	0.46
3:H:155:VAL:HG21	3:H:158:ARG:HH22	1.81	0.46
2:F:27:VAL:C	2:F:29:ARG:H	2.19	0.46
3:H:49:GLY:HA2	3:H:87:ASN:HB3	1.97	0.46
3:H:85:ILE:O	3:H:88:GLY:N	2.49	0.46
1:I:349:THR:HA	1:I:350:PRO:HD3	1.58	0.46
3:D:146:ARG:HG3	3:D:165:GLY:O	2.16	0.46
3:L:49:GLY:HA2	3:L:87:ASN:HB3	1.98	0.45
2:B:23:THR:O	2:B:27:VAL:HG23	2.17	0.45
1:E:569:VAL:HG12	1:E:599:GLY:HA3	1.98	0.45
3:L:155:VAL:HG21	3:L:158:ARG:HH22	1.81	0.45
2:B:3:LEU:HD21	2:C:37:LYS:NZ	2.31	0.45
3:H:183:LEU:HD13	3:H:185:PRO:O	2.17	0.45
1:A:208:GLN:NE2	1:A:282:GLN:HG3	2.31	0.44
3:D:123:ASP:O	3:D:123:ASP:OD2	2.35	0.44
2:K:2:PRO:HD2	2:K:51:ALA:O	2.16	0.44
2:J:74:VAL:HG21	3:L:103:LEU:HD21	1.99	0.44
3:D:49:GLY:HA2	3:D:87:ASN:HB3	2.00	0.44
2:C:1:MET:HA	2:C:2:PRO:HA	1.51	0.44
3:L:205:GLN:O	3:L:209:ASN:ND2	2.51	0.44
2:G:5:LYS:HB3	2:G:82:LEU:HB2	1.98	0.44
3:L:116:ASP:HB3	3:L:160:VAL:HG21	2.00	0.43
3:D:160:VAL:O	3:D:161:LYS:CG	2.66	0.43
3:L:124:THR:HG22	3:L:126:PHE:H	1.83	0.43
2:B:28:LEU:O	2:B:28:LEU:CG	2.66	0.43
2:B:36:VAL:HG21	2:C:47:LEU:HD12	2.00	0.43
2:J:45:ILE:HD13	2:J:69:LEU:HD22	2.00	0.43
1:A:538:LEU:HD21	1:A:589:PRO:HB3	2.00	0.43
2:B:45:ILE:HD13	2:B:69:LEU:HD22	2.00	0.43
1:I:21:GLU:HG2	1:I:330:MET:HG3	2.01	0.43
1:I:538:LEU:HD21	1:I:589:PRO:HB3	1.99	0.43
2:F:29:ARG:O	2:F:33:GLY:HA2	2.19	0.43
3:D:155:VAL:HG21	3:D:158:ARG:HH22	1.82	0.43
2:F:36:VAL:O	2:F:36:VAL:HG13	2.18	0.43
3:H:120:GLU:HG2	3:H:158:ARG:HH21	1.83	0.43
2:B:65:CYS:HA	2:B:69:LEU:HB2	2.00	0.43
3:D:23:LEU:HD11	3:D:46:ILE:HG13	2.01	0.43
3:H:26:ASN:HD21	3:H:201:LYS:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:LEU:HD13	2:B:42:GLY:N	2.34	0.42
3:D:86:CYG:HB13	3:D:87:ASN:HB2	2.01	0.42
3:L:47:LEU:HA	3:L:48:PRO:HD2	1.90	0.42
1:A:349:THR:HA	1:A:350:PRO:HD3	1.54	0.42
2:C:1:MET:O	2:C:1:MET:HG3	2.19	0.42
2:G:1:MET:HA	2:G:2:PRO:HA	1.51	0.42
1:I:136:GLY:O	5:I:2005:ADP:C8	2.72	0.42
2:J:47:LEU:HB3	2:K:39:LEU:HD12	2.01	0.42
2:B:13:ARG:HG3	2:B:13:ARG:HH11	1.85	0.42
3:D:160:VAL:C	3:D:161:LYS:CG	2.81	0.42
2:J:28:LEU:CD1	2:J:34:LEU:HD13	2.40	0.42
2:F:69:LEU:HD23	3:H:57:LEU:HD11	2.00	0.42
1:A:325:ARG:HB3	1:A:326:ASN:H	1.62	0.42
1:E:208:GLN:NE2	1:E:282:GLN:HG3	2.35	0.42
1:A:383:VAL:HB	1:A:391:VAL:H	1.85	0.42
1:E:325:ARG:HB3	1:E:326:ASN:H	1.61	0.42
3:H:85:ILE:O	3:H:86:CYG:C	2.67	0.42
1:I:359:VAL:HB	1:I:409:ASP:HB2	2.01	0.42
2:K:23:THR:O	2:K:27:VAL:HG23	2.19	0.42
1:E:353:ILE:H	1:E:353:ILE:HG13	1.66	0.42
2:F:8:ILE:HD13	2:F:65:CYS:SG	2.60	0.42
2:B:29:ARG:O	2:B:33:GLY:HA2	2.20	0.42
2:C:56:LYS:O	2:C:60:ILE:HG12	2.20	0.42
2:G:23:THR:O	2:G:27:VAL:HG23	2.20	0.42
1:A:125:TYR:O	1:A:129:ILE:HG12	2.19	0.42
1:E:349:THR:HA	1:E:350:PRO:HD3	1.55	0.41
2:C:38:LYS:HD3	2:C:38:LYS:HA	1.82	0.41
3:L:86:CYG:HB13	3:L:87:ASN:HB2	2.02	0.41
2:G:1:MET:O	2:G:1:MET:HG3	2.20	0.41
3:H:116:ASP:O	3:H:160:VAL:HG23	2.21	0.41
2:J:28:LEU:CD1	2:K:64:ALA:HB1	2.50	0.41
1:A:228:GLU:HB3	1:A:230:LEU:HG	2.02	0.41
3:D:85:ILE:O	3:D:86:CYG:C	2.67	0.41
3:H:45:ILE:HB	3:H:82:ILE:HG12	2.02	0.41
3:H:122:ASN:C	3:H:124:THR:N	2.74	0.41
3:H:142:HIS:HE1	3:H:159:TYR:OH	2.04	0.41
2:J:29:ARG:O	2:J:33:GLY:HA2	2.20	0.41
1:A:21:GLU:HG2	1:A:330:MET:HG3	2.03	0.41
1:A:352:LYS:H	1:A:352:LYS:HG3	1.69	0.41
1:E:228:GLU:HB3	1:E:230:LEU:HG	2.02	0.41
1:A:353:ILE:H	1:A:353:ILE:HG13	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:124:THR:HG22	3:D:125:PRO:HD2	2.01	0.41
3:H:23:LEU:HD11	3:H:46:ILE:HG13	2.02	0.41
2:K:52:GLU:HB2	2:K:53:ASN:H	1.77	0.41
3:L:142:HIS:HE1	3:L:159:TYR:OH	2.03	0.41
3:D:120:GLU:HG2	3:D:158:ARG:HH21	1.85	0.41
3:H:205:GLN:O	3:H:209:ASN:ND2	2.54	0.41
3:L:195:ILE:H	3:L:195:ILE:HG13	1.66	0.41
1:A:388:GLY:HA2	5:A:2004:ADP:H3'	2.03	0.40
3:L:85:ILE:O	3:L:86:CYG:C	2.68	0.40
2:C:23:THR:O	2:C:27:VAL:HG23	2.21	0.40
1:I:383:VAL:HB	1:I:391:VAL:H	1.87	0.40
2:J:13:ARG:HG3	2:J:13:ARG:HH11	1.85	0.40
2:K:37:LYS:HB3	2:K:37:LYS:HE2	1.87	0.40
3:L:82:ILE:HB	3:L:180:VAL:HG13	2.03	0.40
3:L:120:GLU:HG2	3:L:158:ARG:HH21	1.84	0.40
1:A:386:GLY:O	5:A:2004:ADP:H4'	2.21	0.40
2:G:29:ARG:HD3	2:G:36:VAL:O	2.22	0.40
3:L:155:VAL:HG21	3:L:158:ARG:NH2	2.35	0.40
3:H:56:TYR:HD1	3:H:56:TYR:HA	1.61	0.40
2:C:3:LEU:HD23	2:C:3:LEU:H	1.87	0.40
3:D:147:TYR:HB3	3:D:166:SER:HB3	2.03	0.40
3:L:160:VAL:HG12	3:L:161:LYS:CG	2.51	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	577/629 (92%)	520 (90%)	53 (9%)	4 (1%)	22	61
1	E	577/629 (92%)	519 (90%)	56 (10%)	2 (0%)	41	75
1	I	577/629 (92%)	519 (90%)	55 (10%)	3 (0%)	29	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	80/82 (98%)	69 (86%)	10 (12%)	1 (1%)	12 48
2	C	80/82 (98%)	75 (94%)	4 (5%)	1 (1%)	12 48
2	F	80/82 (98%)	69 (86%)	9 (11%)	2 (2%)	5 34
2	G	80/82 (98%)	74 (92%)	5 (6%)	1 (1%)	12 48
2	J	80/82 (98%)	68 (85%)	10 (12%)	2 (2%)	5 34
2	K	80/82 (98%)	73 (91%)	6 (8%)	1 (1%)	12 48
3	D	209/213 (98%)	184 (88%)	21 (10%)	4 (2%)	8 40
3	H	209/213 (98%)	186 (89%)	18 (9%)	5 (2%)	6 35
3	L	209/213 (98%)	186 (89%)	18 (9%)	5 (2%)	6 35
All	All	2838/3018 (94%)	2542 (90%)	265 (9%)	31 (1%)	14 52

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	108	GLY
3	H	108	GLY
2	J	27	VAL
2	K	38	LYS
3	L	108	GLY
2	F	27	VAL
3	D	110	PHE
3	D	152	ASP
2	G	2	PRO
3	H	110	PHE
2	J	28	LEU
3	L	152	ASP
2	B	27	VAL
2	C	2	PRO
2	F	28	LEU
3	H	152	ASP
3	L	110	PHE
1	E	492	PRO
1	A	81	TYR
1	A	492	PRO
1	I	492	PRO
3	L	11	PRO
1	A	510	PRO
3	D	11	PRO
3	L	125	PRO

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Mol	Chain	Res	Type
1	E	510	PRO
3	H	11	PRO
3	H	125	PRO
1	I	114	ILE
1	I	510	PRO
1	A	114	ILE

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	487/525 (93%)	445 (91%)	42 (9%)	10 38
1	E	487/525 (93%)	442 (91%)	45 (9%)	9 36
1	I	487/525 (93%)	441 (91%)	46 (9%)	8 35
2	B	75/75 (100%)	68 (91%)	7 (9%)	9 35
2	C	75/75 (100%)	70 (93%)	5 (7%)	16 48
2	F	75/75 (100%)	68 (91%)	7 (9%)	9 35
2	G	75/75 (100%)	67 (89%)	8 (11%)	6 30
2	J	75/75 (100%)	67 (89%)	8 (11%)	6 30
2	K	75/75 (100%)	70 (93%)	5 (7%)	16 48
3	D	171/174 (98%)	156 (91%)	15 (9%)	10 38
3	H	171/174 (98%)	155 (91%)	16 (9%)	8 35
3	L	171/174 (98%)	156 (91%)	15 (9%)	10 38
All	All	2424/2547 (95%)	2205 (91%)	219 (9%)	9 37

All (219) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	THR
1	A	42	ILE
1	A	48	THR
1	A	53	ASN

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Mol	Chain	Res	Type
1	A	60	ASP
1	A	67	PHE
1	A	78	ILE
1	A	98	MET
1	A	109	LEU
1	A	113	ARG
1	A	142	SER
1	A	147	ASN
1	A	152	VAL
1	A	161	ASP
1	A	163	LEU
1	A	165	ASP
1	A	273	PRO
1	A	285	MET
1	A	296	ARG
1	A	302	ARG
1	A	309	ASP
1	A	329	VAL
1	A	364	VAL
1	A	379	THR
1	A	393	ARG
1	A	412	LEU
1	A	420	LEU
1	A	430	THR
1	A	463	LEU
1	A	480	SER
1	A	499	LEU
1	A	505	GLN
1	A	520	TRP
1	A	540	GLU
1	A	548	SER
1	A	550	GLN
1	A	556	HIS
1	A	560	PHE
1	A	576	PRO
1	A	587	ARG
1	A	591	VAL
1	A	593	VAL
2	B	17	ARG
2	B	20	ARG
2	B	26	ARG
2	B	28	LEU

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Mol	Chain	Res	Type
2	B	47	LEU
2	B	55	GLU
2	B	56	LYS
2	C	17	ARG
2	C	38	LYS
2	C	47	LEU
2	C	52	GLU
2	C	80	ARG
3	D	37	ASP
3	D	44	LEU
3	D	62	VAL
3	D	89	PHE
3	D	98	LEU
3	D	122	ASN
3	D	137	ARG
3	D	138	ILE
3	D	150	ILE
3	D	174	LEU
3	D	179	ASN
3	D	183	LEU
3	D	188	GLU
3	D	195	ILE
3	D	212	LYS
1	E	4	ARG
1	E	38	THR
1	E	42	ILE
1	E	48	THR
1	E	53	ASN
1	E	60	ASP
1	E	67	PHE
1	E	74	HIS
1	E	78	ILE
1	E	98	MET
1	E	109	LEU
1	E	113	ARG
1	E	142	SER
1	E	147	ASN
1	E	152	VAL
1	E	157	VAL
1	E	163	LEU
1	E	165	ASP
1	E	273	PRO

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Mol	Chain	Res	Type
1	E	285	MET
1	E	296	ARG
1	E	302	ARG
1	E	309	ASP
1	E	329	VAL
1	E	364	VAL
1	E	379	THR
1	E	396	ARG
1	E	412	LEU
1	E	420	LEU
1	E	430	THR
1	E	463	LEU
1	E	480	SER
1	E	493	THR
1	E	499	LEU
1	E	520	TRP
1	E	540	GLU
1	E	548	SER
1	E	550	GLN
1	E	556	HIS
1	E	560	PHE
1	E	576	PRO
1	E	587	ARG
1	E	590	VAL
1	E	591	VAL
1	E	593	VAL
2	F	17	ARG
2	F	20	ARG
2	F	26	ARG
2	F	28	LEU
2	F	34	LEU
2	F	55	GLU
2	F	56	LYS
2	G	3	LEU
2	G	17	ARG
2	G	38	LYS
2	G	39	LEU
2	G	47	LEU
2	G	52	GLU
2	G	78	GLU
2	G	80	ARG
3	H	37	ASP

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Mol	Chain	Res	Type
3	H	44	LEU
3	H	62	VAL
3	H	89	PHE
3	H	122	ASN
3	H	137	ARG
3	H	138	ILE
3	H	150	ILE
3	H	164	ASN
3	H	174	LEU
3	H	177	SER
3	H	179	ASN
3	H	183	LEU
3	H	188	GLU
3	H	195	ILE
3	H	212	LYS
1	I	4	ARG
1	I	38	THR
1	I	42	ILE
1	I	48	THR
1	I	53	ASN
1	I	60	ASP
1	I	67	PHE
1	I	74	HIS
1	I	78	ILE
1	I	98	MET
1	I	109	LEU
1	I	113	ARG
1	I	142	SER
1	I	147	ASN
1	I	152	VAL
1	I	157	VAL
1	I	161	ASP
1	I	163	LEU
1	I	165	ASP
1	I	207	ILE
1	I	273	PRO
1	I	285	MET
1	I	296	ARG
1	I	302	ARG
1	I	309	ASP
1	I	329	VAL
1	I	349	THR

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Mol	Chain	Res	Type
1	I	364	VAL
1	I	379	THR
1	I	412	LEU
1	I	420	LEU
1	I	430	THR
1	I	463	LEU
1	I	480	SER
1	I	499	LEU
1	I	505	GLN
1	I	520	TRP
1	I	540	GLU
1	I	548	SER
1	I	550	GLN
1	I	556	HIS
1	I	560	PHE
1	I	576	PRO
1	I	587	ARG
1	I	591	VAL
1	I	593	VAL
2	J	17	ARG
2	J	20	ARG
2	J	26	ARG
2	J	28	LEU
2	J	47	LEU
2	J	55	GLU
2	J	56	LYS
2	J	79	VAL
2	K	17	ARG
2	K	38	LYS
2	K	47	LEU
2	K	78	GLU
2	K	80	ARG
3	L	37	ASP
3	L	44	LEU
3	L	62	VAL
3	L	89	PHE
3	L	122	ASN
3	L	137	ARG
3	L	138	ILE
3	L	150	ILE
3	L	162	ASP
3	L	174	LEU

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Mol	Chain	Res	Type
3	L	179	ASN
3	L	183	LEU
3	L	188	GLU
3	L	195	ILE
3	L	212	LYS

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

Mol	Chain	Res	Type
1	A	151	ASN
1	A	208	GLN
1	A	235	GLN
1	A	442	ASN
1	A	465	ASN
1	A	478	ASN
1	A	503	ASN
2	C	11	GLN
3	D	14	ASN
3	D	26	ASN
3	D	154	ASN
3	D	175	ASN
3	D	179	ASN
3	D	209	ASN
1	E	151	ASN
1	E	208	GLN
1	E	235	GLN
1	E	442	ASN
1	E	465	ASN
1	E	478	ASN
1	E	503	ASN
2	G	11	GLN
3	H	14	ASN
3	H	26	ASN
3	H	142	HIS
3	H	154	ASN
3	H	164	ASN
3	H	175	ASN
3	H	179	ASN
3	H	209	ASN
1	I	53	ASN
1	I	151	ASN
1	I	208	GLN

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Mol	Chain	Res	Type
1	I	235	GLN
1	I	442	ASN
1	I	465	ASN
1	I	478	ASN
1	I	503	ASN
2	K	11	GLN
3	L	14	ASN
3	L	26	ASN
3	L	142	HIS
3	L	154	ASN
3	L	164	ASN
3	L	175	ASN
3	L	179	ASN
3	L	209	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)

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	CYG	H	86	3	12,14,15	1.11	1 (8%)	10,17,19	2.31	3 (30%)
3	CYG	D	86	3	12,14,15	1.10	1 (8%)	10,17,19	2.33	3 (30%)
3	CYG	L	86	3	12,14,15	1.12	1 (8%)	10,17,19	2.37	3 (30%)

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
3	CYG	H	86	3	-	4/14/16/18	-
3	CYG	D	86	3	-	4/14/16/18	-
3	CYG	L	86	3	-	4/14/16/18	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	86	CYG	CG1-CD1	2.58	1.53	1.50
3	H	86	CYG	CG1-CD1	2.56	1.53	1.50
3	D	86	CYG	CG1-CD1	2.55	1.53	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	86	CYG	CG1-CD1-SG	6.00	120.55	113.40
3	D	86	CYG	CG1-CD1-SG	5.86	120.38	113.40
3	H	86	CYG	CG1-CD1-SG	5.85	120.37	113.40
3	L	86	CYG	OE2-CD1-CG1	-3.21	120.28	123.98
3	D	86	CYG	OE2-CD1-CG1	-3.15	120.35	123.98
3	H	86	CYG	OE2-CD1-CG1	-3.12	120.38	123.98
3	L	86	CYG	OE2-CD1-SG	-2.76	119.17	122.68
3	H	86	CYG	OE2-CD1-SG	-2.70	119.25	122.68
3	D	86	CYG	OE2-CD1-SG	-2.68	119.27	122.68

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	86	CYG	OE2-CD1-SG-CB
3	H	86	CYG	OE2-CD1-SG-CB
3	L	86	CYG	OE2-CD1-SG-CB
3	D	86	CYG	CG1-CD1-SG-CB
3	H	86	CYG	CG1-CD1-SG-CB
3	L	86	CYG	CG1-CD1-SG-CB
3	H	86	CYG	O2-C1-CA1-CB1
3	D	86	CYG	O2-C1-CA1-CB1
3	H	86	CYG	O1-C1-CA1-CB1
3	L	86	CYG	O2-C1-CA1-CB1
3	D	86	CYG	O1-C1-CA1-CB1
3	L	86	CYG	O1-C1-CA1-CB1

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	86	CYG	1	0
3	D	86	CYG	2	0
3	L	86	CYG	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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	$\#\|Z\| > 2$
5	ADP	A	2004	-	24,29,29	1.25	2 (8%)	29,45,45	1.52	6 (20%)
5	ADP	I	2005	-	24,29,29	1.26	2 (8%)	29,45,45	1.52	6 (20%)
5	ADP	E	2006	-	24,29,29	1.25	2 (8%)	29,45,45	1.52	5 (17%)

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
5	ADP	A	2004	-	-	1/12/32/32	0/3/3/3
5	ADP	I	2005	-	-	1/12/32/32	0/3/3/3
5	ADP	E	2006	-	-	1/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	2005	ADP	PB-O1B	3.53	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	2006	ADP	PB-O1B	3.49	1.61	1.50
5	A	2004	ADP	PB-O1B	3.48	1.61	1.50
5	I	2005	ADP	O4'-C1'	2.59	1.44	1.40
5	A	2004	ADP	O4'-C1'	2.48	1.44	1.40
5	E	2006	ADP	O4'-C1'	2.47	1.44	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	2006	ADP	N3-C2-N1	-5.06	121.80	128.67
5	I	2005	ADP	N3-C2-N1	-5.01	121.87	128.67
5	A	2004	ADP	N3-C2-N1	-4.98	121.91	128.67
5	I	2005	ADP	C4'-O4'-C1'	-2.71	107.44	109.92
5	A	2004	ADP	O2B-PB-O3A	2.57	113.24	104.64
5	E	2006	ADP	C4'-O4'-C1'	-2.53	107.61	109.92
5	A	2004	ADP	C4'-O4'-C1'	-2.52	107.62	109.92
5	I	2005	ADP	O2B-PB-O3A	2.50	113.03	104.64
5	E	2006	ADP	O2B-PB-O3A	2.50	113.03	104.64
5	A	2004	ADP	O4'-C1'-N9	2.26	111.75	108.75
5	A	2004	ADP	C2'-C3'-C4'	-2.24	98.28	102.61
5	E	2006	ADP	C2'-C3'-C4'	-2.24	98.28	102.61
5	I	2005	ADP	C2'-C3'-C4'	-2.22	98.31	102.61
5	E	2006	ADP	O4'-C1'-N9	2.19	111.65	108.75
5	I	2005	ADP	O4'-C1'-N9	2.14	111.59	108.75
5	A	2004	ADP	C5'-C4'-C3'	-2.05	107.84	115.21
5	I	2005	ADP	C5'-C4'-C3'	-2.03	107.91	115.21

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2004	ADP	PA-O3A-PB-O1B
5	E	2006	ADP	PA-O3A-PB-O1B
5	I	2005	ADP	PA-O3A-PB-O1B

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2004	ADP	4	0
5	I	2005	ADP	2	0

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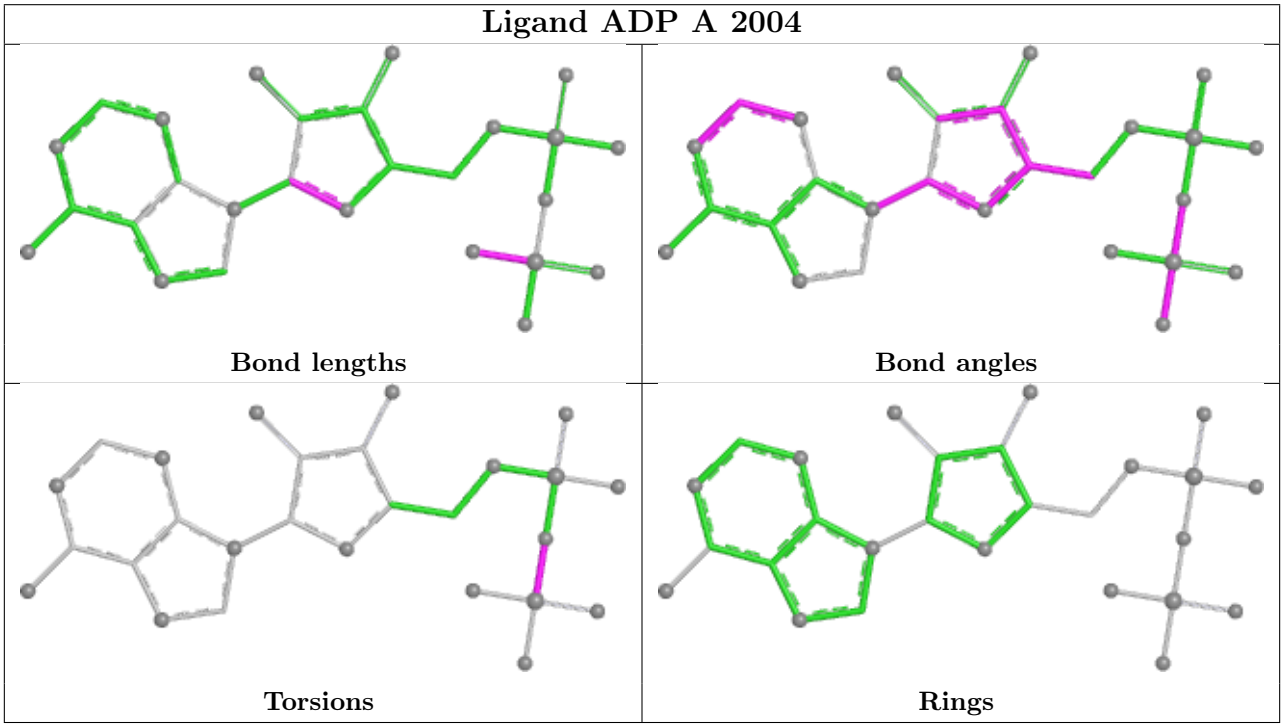
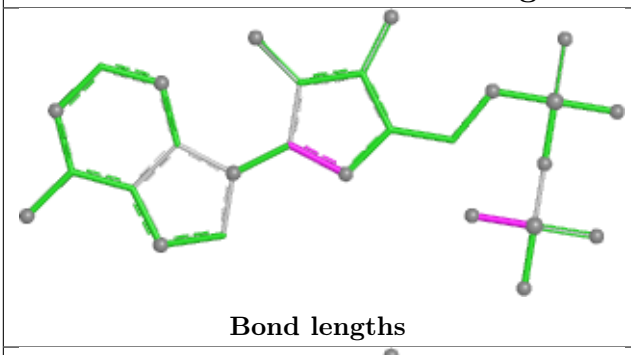
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	2006	ADP	2	0

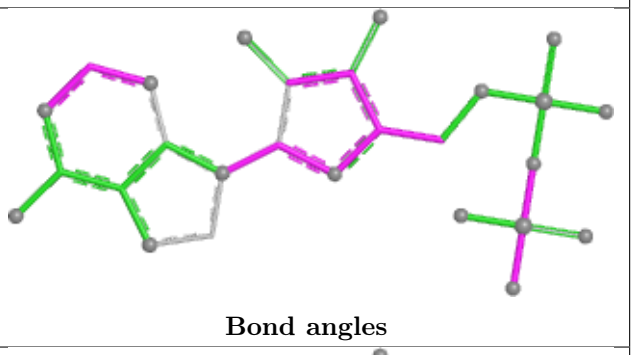
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



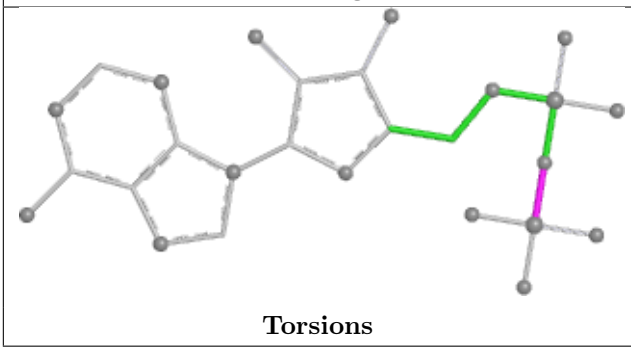
Ligand ADP I 2005



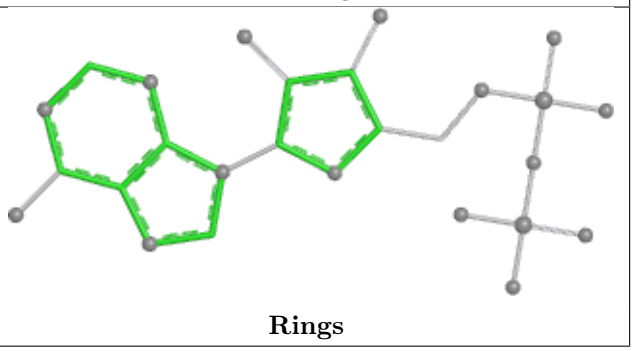
Bond lengths



Bond angles

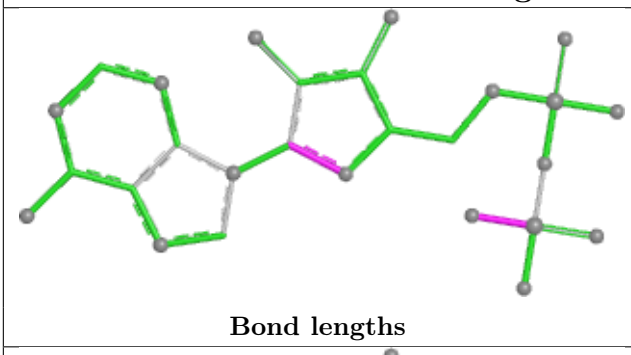


Torsions

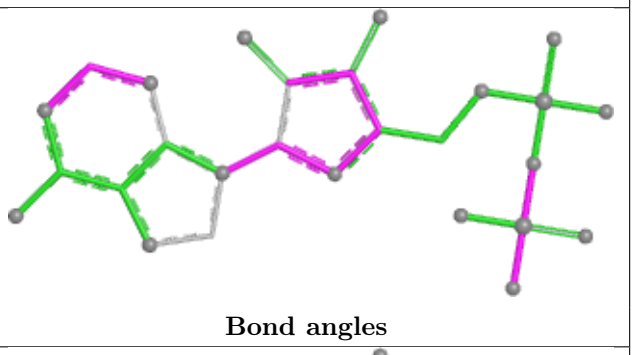


Rings

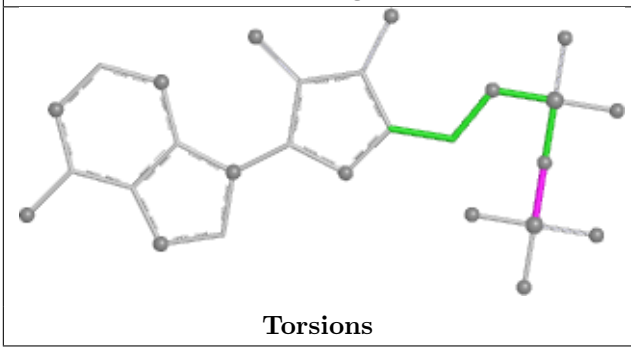
Ligand ADP E 2006



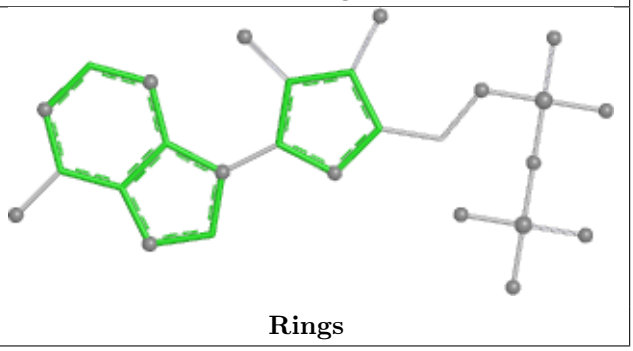
Bond lengths



Bond angles



Torsions



Rings

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

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	583/629 (92%)	-0.25	2 (0%) 94 91	71, 126, 177, 203	0
1	E	583/629 (92%)	-0.19	2 (0%) 94 91	83, 139, 183, 205	0
1	I	583/629 (92%)	0.41	25 (4%) 35 31	111, 185, 205, 205	0
2	B	82/82 (100%)	-0.43	0 100 100	72, 114, 152, 160	0
2	C	82/82 (100%)	-0.38	0 100 100	77, 128, 163, 183	0
2	F	82/82 (100%)	0.10	0 100 100	93, 151, 193, 202	0
2	G	82/82 (100%)	0.09	1 (1%) 79 73	114, 165, 197, 204	0
2	J	82/82 (100%)	-0.26	0 100 100	83, 126, 169, 192	0
2	K	82/82 (100%)	-0.20	0 100 100	95, 141, 172, 187	0
3	D	211/213 (99%)	-0.39	0 100 100	72, 117, 162, 203	0
3	H	211/213 (99%)	-0.22	0 100 100	90, 141, 182, 205	0
3	L	211/213 (99%)	-0.23	0 100 100	95, 141, 177, 205	0
All	All	2874/3018 (95%)	-0.10	30 (1%) 82 77	71, 143, 201, 205	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	203	THR	4.3
1	I	17	PRO	3.7
1	I	312	ALA	3.4
1	I	19	PHE	3.2
1	A	203	THR	3.1
1	I	135	GLY	3.1
1	E	203	THR	2.9
1	I	175	ILE	2.7
1	I	12	LYS	2.7
1	I	399	GLY	2.7
1	I	585	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	174	VAL	2.6
2	G	6	PHE	2.6
1	I	576	PRO	2.5
1	I	357	LYS	2.5
1	A	94	ASP	2.4
1	I	320	TYR	2.4
1	I	70	GLU	2.3
1	I	311	VAL	2.3
1	I	16	GLU	2.2
1	I	90	GLY	2.2
1	E	206	SER	2.1
1	I	257	ALA	2.1
1	I	567	ILE	2.1
1	I	37	HIS	2.1
1	I	543	ALA	2.0
1	I	477	GLY	2.0
1	I	465	ASN	2.0
1	I	489	PRO	2.0
1	I	597	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å^2)	Q<0.9
3	CYG	L	86	15/16	0.87	0.35	165,167,168,170	0
3	CYG	H	86	15/16	0.89	0.33	165,167,168,170	0
3	CYG	D	86	15/16	0.93	0.36	165,167,168,170	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

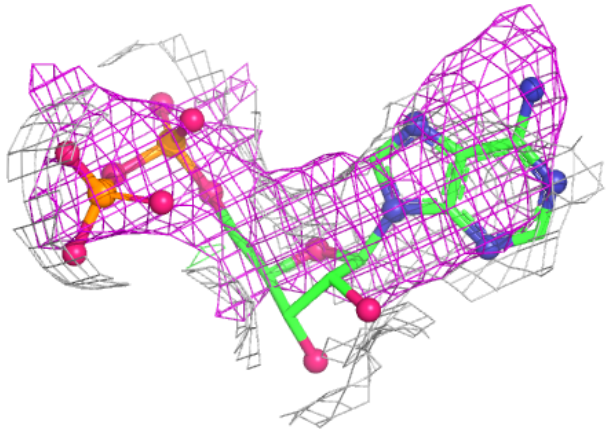
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

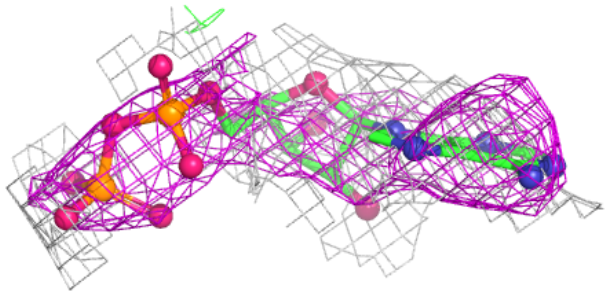
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NA	I	3001	1/1	0.50	0.93	145,145,145,145	0
4	NA	A	3003	1/1	0.76	1.95	145,145,145,145	0
5	ADP	I	2005	27/27	0.82	0.24	161,167,186,306	0
5	ADP	E	2006	27/27	0.84	0.29	161,167,186,306	0
4	NA	E	3002	1/1	0.88	1.62	145,145,145,145	0
5	ADP	A	2004	27/27	0.89	0.32	161,167,186,306	0

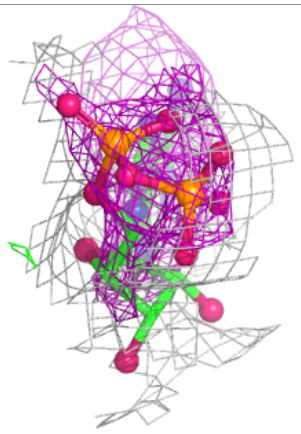
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP I 2005:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

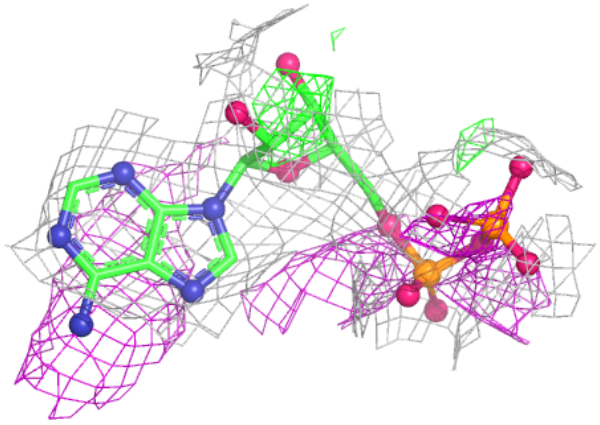


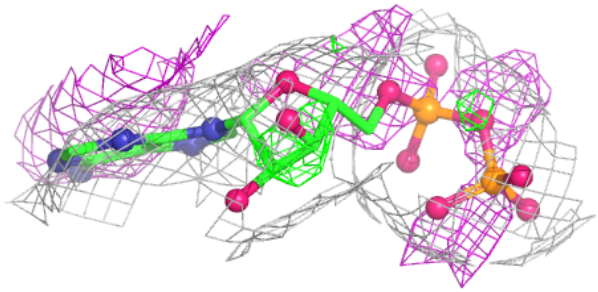


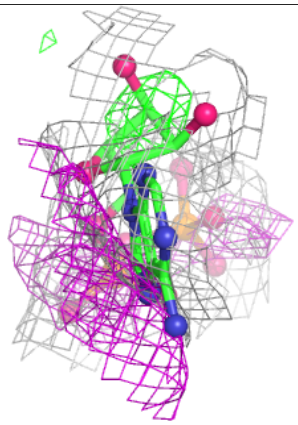


Electron density around ADP E 2006:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

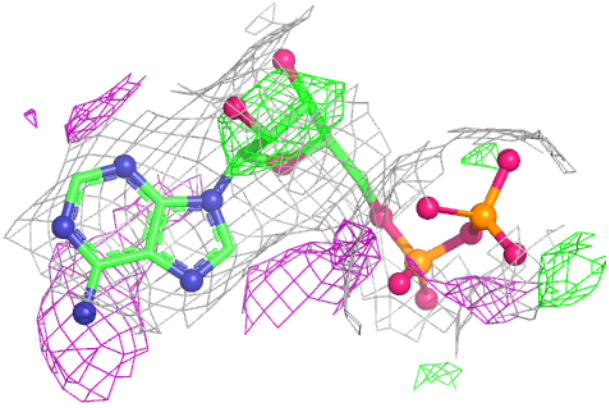


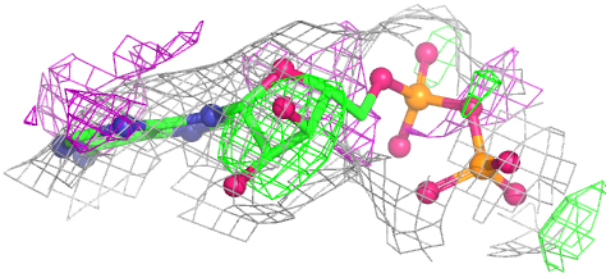


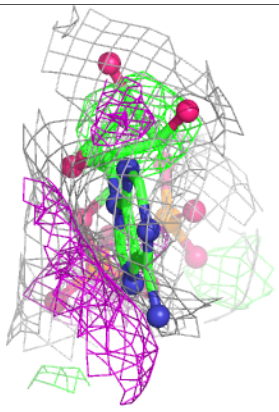


Electron density around ADP A 2004:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.