Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2024 – 09:22 PM EDT

PDB ID	:	1S4E
Title	:	Pyrococcus furiosus galactokinase in complex with galactose, ADP and magnesium
Authors	:	Hartley, A.; Glynn, S.E.; Barynin, V.; Baker, P.J.; Sedelnikova, S.E.; Verhees, C.; de Geus, D.; van der Oost, J.; Timson, D.J.; Reece, R.J.; Rice, D.W.
Deposited on	:	2004-01-16
Resolution	:	2.90 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

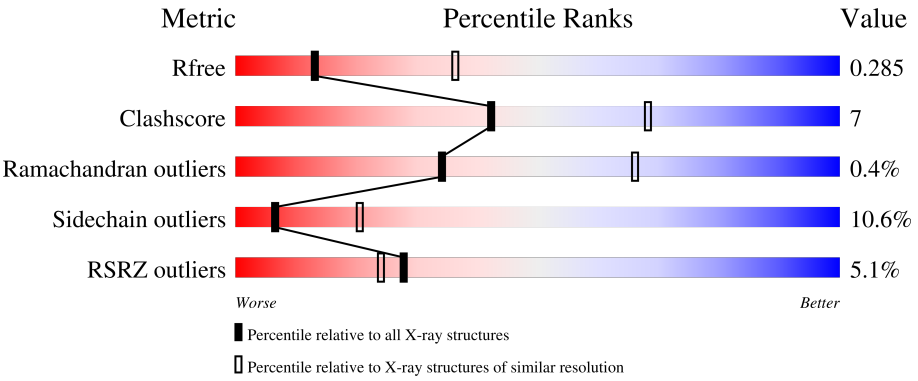
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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 2.90 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))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 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	352	2% 74% 20%
1	B	352	5% 69% 16% 12%
1	C	352	4% 79% 15%
1	D	352	3% 77% 19%

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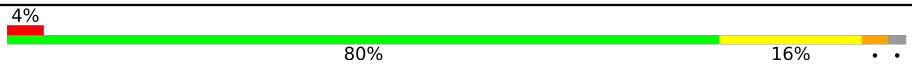
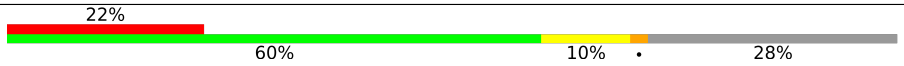
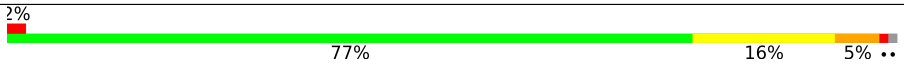
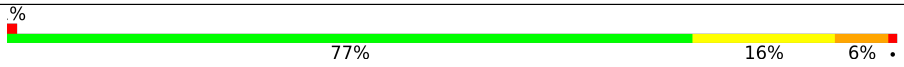
Mol	Chain	Length	Quality of chain
1	E	352	
1	F	352	
1	G	352	
1	H	352	
1	I	352	

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
2	GLA	E	4500	X	-	-	-
4	ADP	G	6400	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 22711 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 Galactokinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	Se	0	0	0
			2554	1660	410	479	2	3			
1	B	310	Total	C	N	O	S	Se	0	0	0
			2266	1463	368	430	2	3			
1	C	337	Total	C	N	O	S	Se	0	0	0
			2419	1564	396	454	2	3			
1	D	349	Total	C	N	O	S	Se	0	0	0
			2643	1715	420	503	2	3			
1	E	346	Total	C	N	O	S	Se	0	0	0
			2616	1703	414	494	2	3			
1	F	351	Total	C	N	O	S	Se	0	0	0
			2722	1769	433	515	2	3			
1	G	255	Total	C	N	O	S	Se	0	0	0
			1811	1157	303	346	2	3			
1	H	347	Total	C	N	O	S	Se	0	0	0
			2652	1728	422	497	2	3			
1	I	351	Total	C	N	O	S	Se	0	0	0
			2668	1741	416	506	2	3			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q9HHB6
A	27	MSE	MET	modified residue	UNP Q9HHB6
A	29	MSE	MET	modified residue	UNP Q9HHB6
A	293	MSE	MET	modified residue	UNP Q9HHB6
B	1	MSE	MET	modified residue	UNP Q9HHB6
B	27	MSE	MET	modified residue	UNP Q9HHB6
B	29	MSE	MET	modified residue	UNP Q9HHB6
B	293	MSE	MET	modified residue	UNP Q9HHB6
C	1	MSE	MET	modified residue	UNP Q9HHB6
C	27	MSE	MET	modified residue	UNP Q9HHB6
C	29	MSE	MET	modified residue	UNP Q9HHB6

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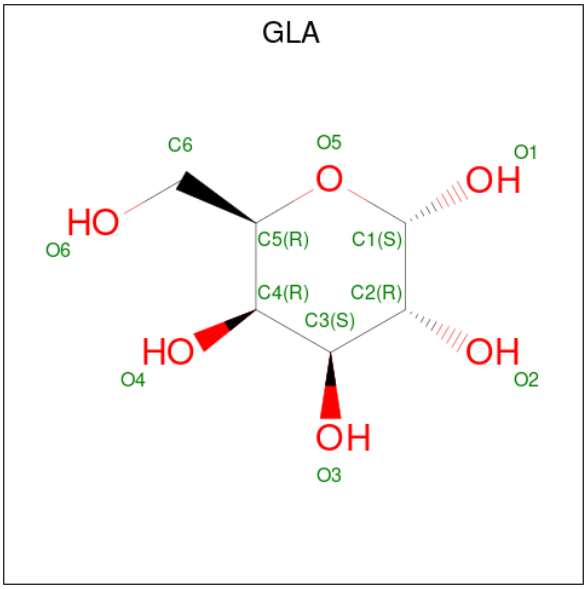
Chain	Residue	Modelled	Actual	Comment	Reference
C	293	MSE	MET	modified residue	UNP Q9HHB6
D	1	MSE	MET	modified residue	UNP Q9HHB6
D	27	MSE	MET	modified residue	UNP Q9HHB6
D	29	MSE	MET	modified residue	UNP Q9HHB6
D	293	MSE	MET	modified residue	UNP Q9HHB6
E	1	MSE	MET	modified residue	UNP Q9HHB6
E	27	MSE	MET	modified residue	UNP Q9HHB6
E	29	MSE	MET	modified residue	UNP Q9HHB6
E	293	MSE	MET	modified residue	UNP Q9HHB6
F	1	MSE	MET	modified residue	UNP Q9HHB6
F	27	MSE	MET	modified residue	UNP Q9HHB6
F	29	MSE	MET	modified residue	UNP Q9HHB6
F	293	MSE	MET	modified residue	UNP Q9HHB6
G	1	MSE	MET	modified residue	UNP Q9HHB6
G	27	MSE	MET	modified residue	UNP Q9HHB6
G	29	MSE	MET	modified residue	UNP Q9HHB6
G	293	MSE	MET	modified residue	UNP Q9HHB6
H	1	MSE	MET	modified residue	UNP Q9HHB6
H	27	MSE	MET	modified residue	UNP Q9HHB6
H	29	MSE	MET	modified residue	UNP Q9HHB6
H	293	MSE	MET	modified residue	UNP Q9HHB6
I	1	MSE	MET	modified residue	UNP Q9HHB6
I	27	MSE	MET	modified residue	UNP Q9HHB6
I	29	MSE	MET	modified residue	UNP Q9HHB6
I	293	MSE	MET	modified residue	UNP Q9HHB6

- Molecule 2 is alpha-D-galactopyranose (three-letter code: GLA) (formula: $C_6H_{12}O_6$).

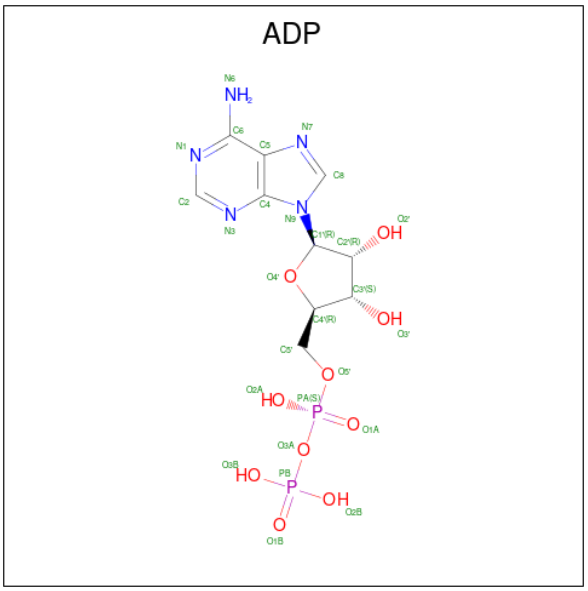


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 12 6 6	0	0
2	B	1	Total C O 12 6 6	0	0
2	C	1	Total C O 12 6 6	0	0
2	D	1	Total C O 12 6 6	0	0
2	E	1	Total C O 12 6 6	0	0
2	F	1	Total C O 12 6 6	0	0
2	G	1	Total C O 12 6 6	0	0
2	H	1	Total C O 12 6 6	0	0
2	I	1	Total C O 12 6 6	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0
3	G	1	Total Mg 1 1	0	0
3	H	1	Total Mg 1 1	0	0
3	I	1	Total Mg 1 1	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



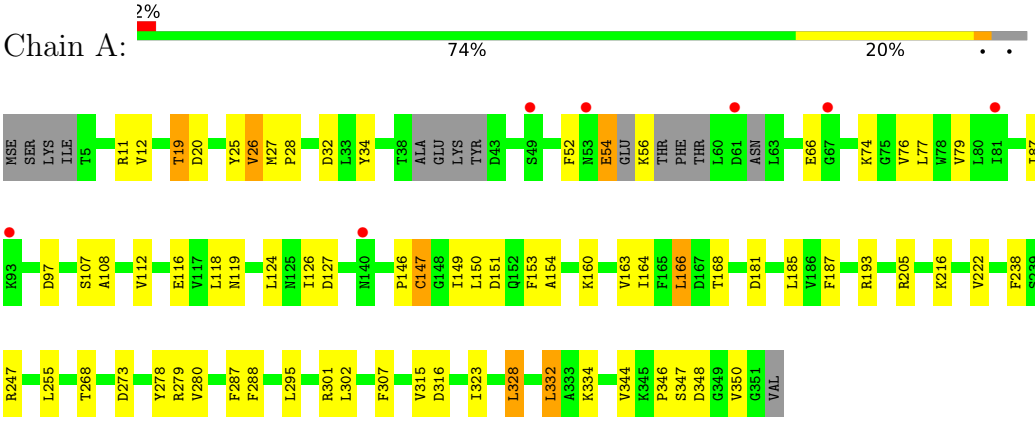
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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.

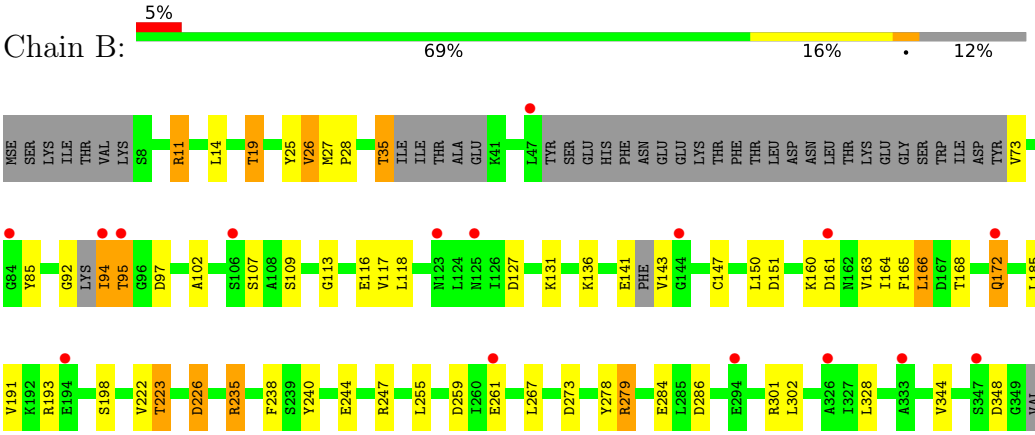
• Molecule 1: Galactokinase

Chain A:



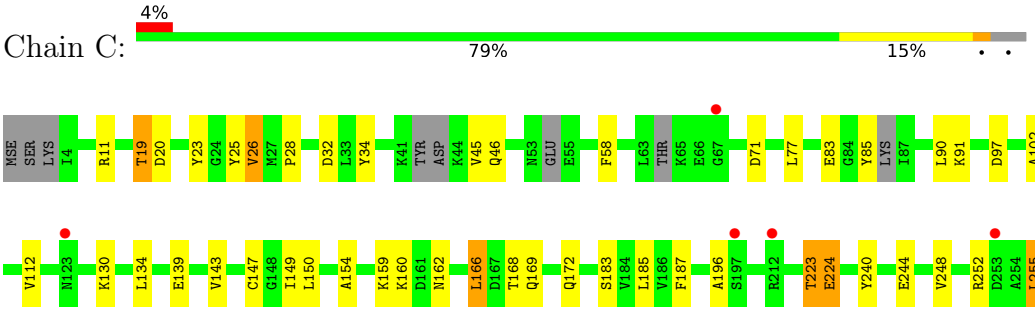
• Molecule 1: Galactokinase

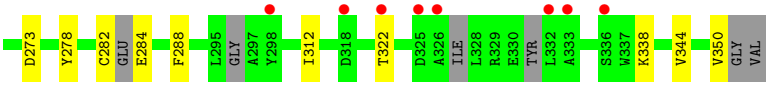
Chain B:



• Molecule 1: Galactokinase

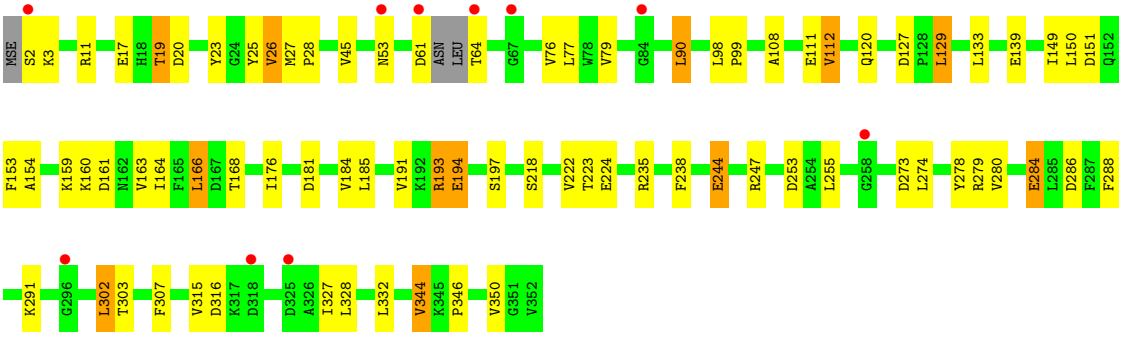
Chain C:





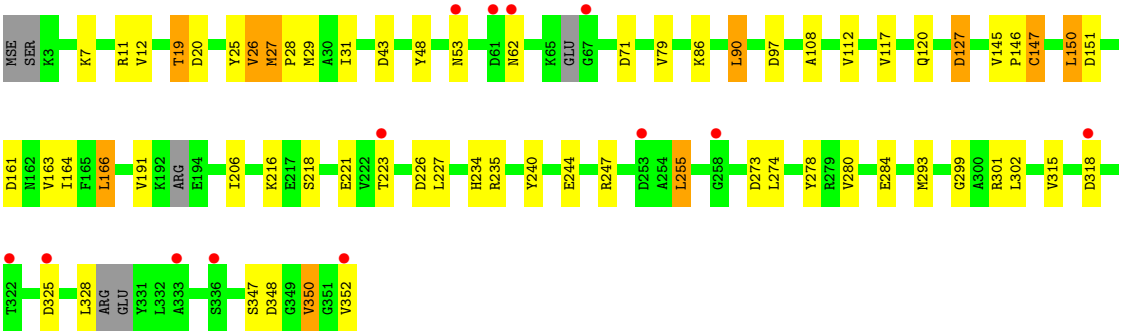
• Molecule 1: Galactokinase

Chain D:



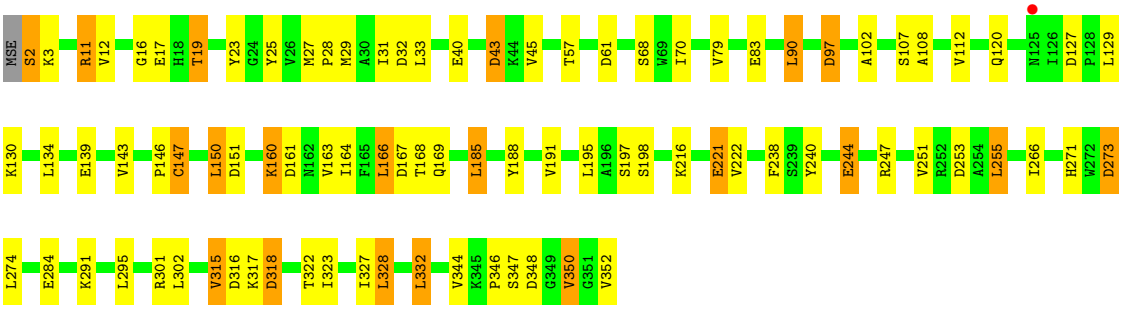
• Molecule 1: Galactokinase

Chain E:



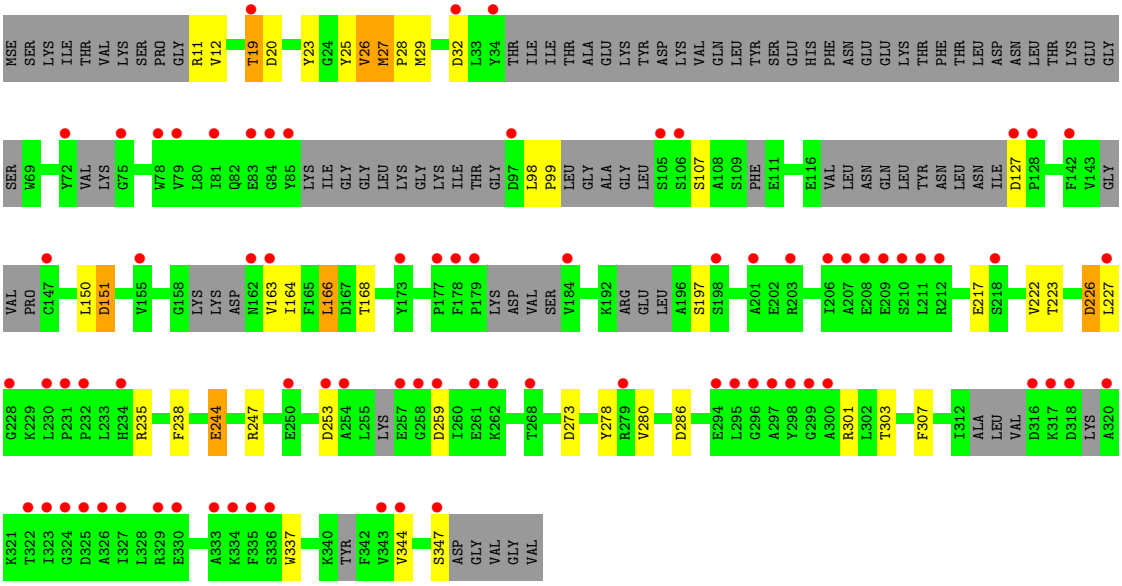
• Molecule 1: Galactokinase

Chain F:



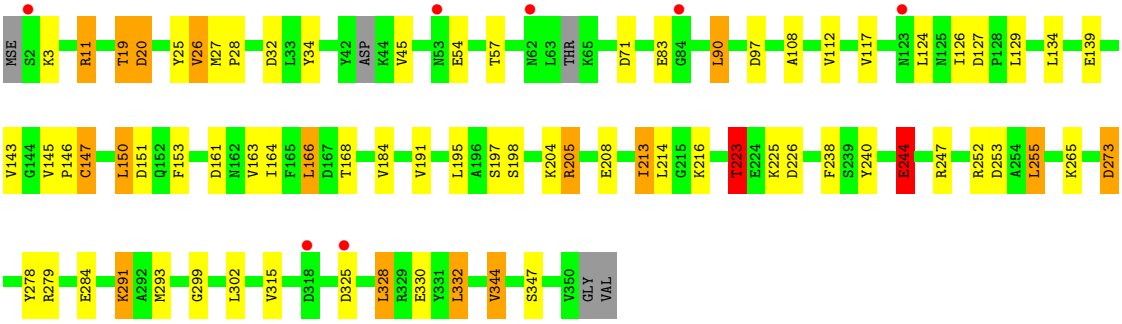
• Molecule 1: Galactokinase

Chain G:



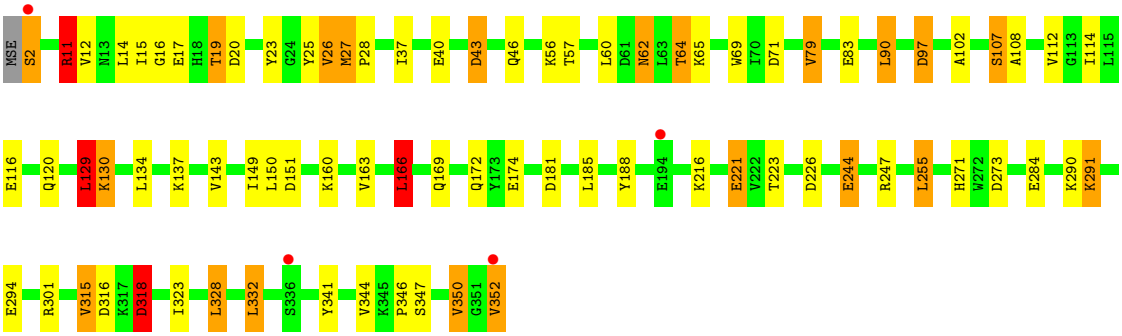
• Molecule 1: Galactokinase

Chain H:



• Molecule 1: Galactokinase

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	211.97Å 355.67Å 165.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90 10.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (10.00-2.90) 100.0 (10.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	4.47 (at 2.89Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.230 , 0.270 0.257 , 0.285	Depositor DCC
R_{free} test set	6821 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	61.5	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.007 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	22711	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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: GLA, MG, 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	0/2599	0.89	7/3513 (0.2%)
1	B	0.67	1/2301 (0.0%)	0.86	9/3116 (0.3%)
1	C	0.53	0/2457	0.76	5/3336 (0.1%)
1	D	0.60	0/2694	0.85	11/3659 (0.3%)
1	E	0.55	0/2665	0.82	10/3616 (0.3%)
1	F	0.80	1/2774 (0.0%)	1.00	16/3752 (0.4%)
1	G	0.54	0/1828	0.78	9/2464 (0.4%)
1	H	0.78	0/2701	0.96	15/3656 (0.4%)
1	I	0.88	2/2720 (0.1%)	1.03	21/3689 (0.6%)
All	All	0.69	4/22739 (0.0%)	0.89	103/30801 (0.3%)

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	F	0	1
1	I	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	97	ASP	CB-CG	-8.05	1.34	1.51
1	I	221	GLU	CG-CD	5.92	1.60	1.51
1	B	92	GLY	CA-C	5.67	1.60	1.51
1	I	2	SER	CA-CB	5.14	1.60	1.52

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	97	ASP	CB-CG-OD1	-11.48	107.97	118.30
1	I	316	ASP	CB-CG-OD2	9.94	127.24	118.30
1	F	97	ASP	CB-CG-OD2	9.76	127.08	118.30
1	A	193	ARG	NE-CZ-NH1	8.95	124.77	120.30
1	A	273	ASP	CB-CG-OD2	8.75	126.18	118.30
1	I	318	ASP	CB-CG-OD2	8.67	126.11	118.30
1	I	350	VAL	CB-CA-C	-8.60	95.05	111.40
1	B	151	ASP	CB-CG-OD2	7.74	125.27	118.30
1	F	316	ASP	CB-CG-OD2	7.74	125.27	118.30
1	I	226	ASP	CB-CG-OD2	7.48	125.04	118.30
1	F	273	ASP	CB-CG-OD2	7.47	125.02	118.30
1	I	97	ASP	CB-CG-OD2	7.44	125.00	118.30
1	B	286	ASP	CB-CG-OD2	7.39	124.95	118.30
1	B	127	ASP	CB-CG-OD2	7.34	124.90	118.30
1	H	273	ASP	CB-CG-OD2	7.27	124.84	118.30
1	H	20	ASP	CB-CG-OD2	7.17	124.75	118.30
1	F	151	ASP	CB-CG-OD2	7.15	124.73	118.30
1	I	97	ASP	CB-CG-OD1	-7.13	111.88	118.30
1	H	11	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	B	226	ASP	CB-CG-OD2	6.80	124.42	118.30
1	B	161	ASP	CB-CG-OD2	6.66	124.29	118.30
1	D	151	ASP	CB-CG-OD2	6.63	124.27	118.30
1	I	129	LEU	CB-CG-CD2	-6.63	99.73	111.00
1	F	253	ASP	CB-CG-OD2	6.54	124.19	118.30
1	A	32	ASP	CB-CG-OD2	6.47	124.13	118.30
1	I	143	VAL	C-N-CA	-6.45	108.75	122.30
1	E	348	ASP	CB-CG-OD2	6.45	124.10	118.30
1	I	221	GLU	OE1-CD-OE2	-6.43	115.58	123.30
1	F	43	ASP	CB-CG-OD2	6.38	124.05	118.30
1	E	151	ASP	CB-CG-OD2	6.34	124.01	118.30
1	G	226	ASP	CB-CG-OD2	6.31	123.98	118.30
1	I	181	ASP	CB-CG-OD2	6.26	123.93	118.30
1	G	20	ASP	CB-CG-OD2	6.18	123.86	118.30
1	F	348	ASP	CB-CG-OD1	6.17	123.85	118.30
1	E	71	ASP	CB-CG-OD2	6.12	123.81	118.30
1	E	273	ASP	CB-CG-OD2	6.06	123.76	118.30
1	H	127	ASP	CB-CG-OD2	6.04	123.74	118.30
1	F	160	LYS	C-N-CA	-6.03	106.62	121.70
1	C	20	ASP	CB-CG-OD2	6.02	123.72	118.30
1	D	161	ASP	CB-CG-OD2	5.99	123.69	118.30
1	F	161	ASP	CB-CG-OD2	5.97	123.68	118.30
1	E	20	ASP	CB-CG-OD2	5.93	123.64	118.30
1	G	259	ASP	CB-CG-OD2	5.92	123.63	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	350	VAL	CB-CA-C	-5.92	100.16	111.40
1	D	20	ASP	CB-CG-OD2	5.89	123.60	118.30
1	H	325	ASP	CB-CG-OD2	5.86	123.58	118.30
1	G	32	ASP	CB-CG-OD2	5.84	123.56	118.30
1	F	185	LEU	CA-CB-CG	5.75	128.53	115.30
1	B	348	ASP	CB-CG-OD2	5.73	123.46	118.30
1	D	273	ASP	CB-CG-OD2	5.70	123.43	118.30
1	H	223	THR	N-CA-CB	-5.65	99.56	110.30
1	E	226	ASP	CB-CG-OD2	5.65	123.38	118.30
1	G	286	ASP	CB-CG-OD2	5.64	123.38	118.30
1	G	127	ASP	CB-CG-OD2	5.64	123.37	118.30
1	E	318	ASP	CB-CG-OD2	5.63	123.36	118.30
1	G	151	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	20	ASP	CB-CG-OD2	5.57	123.31	118.30
1	H	32	ASP	CB-CG-OD2	5.56	123.31	118.30
1	G	273	ASP	CB-CG-OD2	5.55	123.30	118.30
1	E	161	ASP	CB-CG-OD2	5.53	123.28	118.30
1	D	127	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	151	ASP	CB-CG-OD2	5.51	123.26	118.30
1	I	143	VAL	CA-C-N	5.50	127.21	116.20
1	H	151	ASP	CB-CG-OD2	5.48	123.23	118.30
1	I	71	ASP	CB-CG-OD2	5.46	123.22	118.30
1	D	286	ASP	CB-CG-OD2	5.43	123.18	118.30
1	C	71	ASP	CB-CG-OD2	5.42	123.18	118.30
1	D	129	LEU	CA-CB-CG	5.34	127.57	115.30
1	I	11	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	I	60	LEU	CB-CG-CD2	-5.30	101.99	111.00
1	I	43	ASP	CB-CG-OD2	5.29	123.06	118.30
1	F	167	ASP	CB-CG-OD1	5.29	123.06	118.30
1	D	253	ASP	CB-CG-OD2	5.27	123.04	118.30
1	D	316	ASP	CB-CG-OD2	5.26	123.03	118.30
1	E	127	ASP	CB-CG-OD2	5.26	123.03	118.30
1	F	32	ASP	CB-CG-OD2	5.24	123.01	118.30
1	B	279	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	H	11	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	181	ASP	CB-CG-OD1	5.20	122.98	118.30
1	I	273	ASP	CB-CG-OD2	5.19	122.97	118.30
1	I	20	ASP	CB-CG-OD2	5.18	122.97	118.30
1	F	61	ASP	CB-CG-OD1	5.18	122.96	118.30
1	H	161	ASP	CB-CG-OD2	5.17	122.95	118.30
1	H	71	ASP	CB-CG-OD2	5.15	122.94	118.30
1	D	181	ASP	CB-CG-OD2	5.14	122.93	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	259	ASP	CB-CG-OD2	5.14	122.92	118.30
1	A	316	ASP	CB-CG-OD2	5.13	122.92	118.30
1	I	166	LEU	CA-CB-CG	5.13	127.10	115.30
1	B	259	ASP	CB-CG-OD2	5.13	122.92	118.30
1	G	253	ASP	CB-CG-OD2	5.12	122.91	118.30
1	I	90	LEU	CA-CB-CG	5.11	127.06	115.30
1	C	273	ASP	CB-CG-OD2	5.09	122.88	118.30
1	F	11	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	H	244	GLU	CA-CB-CG	-5.07	102.26	113.40
1	D	61	ASP	CB-CG-OD2	5.05	122.85	118.30
1	H	195	LEU	CA-CB-CG	5.05	126.92	115.30
1	H	253	ASP	CB-CG-OD2	5.04	122.84	118.30
1	E	350	VAL	CB-CA-C	-5.04	101.83	111.40
1	H	279	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	I	151	ASP	CB-CG-OD2	5.03	122.83	118.30
1	C	32	ASP	CB-CG-OD2	5.02	122.82	118.30
1	I	143	VAL	O-C-N	-5.01	114.69	123.20
1	B	235	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	221	GLU	Peptide
1	I	221	GLU	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	2554	0	2465	37	0
1	B	2266	0	2131	35	0
1	C	2419	0	2187	26	0
1	D	2643	0	2524	33	0
1	E	2616	0	2499	28	0
1	F	2722	0	2687	51	0
1	G	1811	0	1608	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	2652	0	2592	38	0
1	I	2668	0	2578	44	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0
2	C	12	0	12	0	0
2	D	12	0	12	1	0
2	E	12	0	12	1	0
2	F	12	0	12	1	0
2	G	12	0	12	0	0
2	H	12	0	12	0	0
2	I	12	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
4	A	27	0	12	0	0
4	B	27	0	12	1	0
4	C	27	0	12	1	0
4	D	27	0	12	0	0
4	E	27	0	12	0	0
4	F	27	0	12	0	0
4	G	27	0	12	1	0
4	H	27	0	12	0	0
4	I	27	0	12	1	0
All	All	22711	0	21487	305	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 7.

All (305) 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:F:19:THR:HG21	1:F:25:TYR:O	1.56	1.04
1:A:19:THR:HG21	1:A:25:TYR:O	1.59	1.02
1:C:19:THR:HG21	1:C:25:TYR:O	1.66	0.95
1:B:172:GLN:HA	1:B:172:GLN:NE2	1.82	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:244:GLU:HG2	1:F:247:ARG:NH1	1.83	0.92
1:F:146:PRO:O	1:F:147:CYS:HB3	1.65	0.92
1:C:26:VAL:HG13	1:C:28:PRO:HD3	1.56	0.88
1:I:19:THR:HG21	1:I:25:TYR:O	1.73	0.87
1:I:244:GLU:HG3	1:I:247:ARG:NH1	1.90	0.86
1:E:19:THR:HG21	1:E:25:TYR:O	1.78	0.83
1:H:244:GLU:HG2	1:H:247:ARG:NH1	1.92	0.83
1:H:19:THR:HG21	1:H:25:TYR:O	1.79	0.81
1:B:19:THR:HG21	1:B:25:TYR:O	1.81	0.80
1:G:244:GLU:HG2	1:G:247:ARG:NH1	1.95	0.80
1:B:26:VAL:HG13	1:B:28:PRO:HD3	1.65	0.78
1:B:223:THR:HG22	1:B:226:ASP:H	1.49	0.77
1:H:223:THR:HG22	1:H:226:ASP:H	1.47	0.77
1:B:240:TYR:CZ	1:B:244:GLU:HG3	2.18	0.77
1:I:27:MSE:HE1	1:I:255:LEU:HD12	1.65	0.77
1:E:108:ALA:O	1:E:112:VAL:HG13	1.85	0.76
1:H:291:LYS:HE3	1:H:330:GLU:OE2	1.85	0.76
1:G:19:THR:HG21	1:G:25:TYR:O	1.86	0.76
1:E:26:VAL:HG13	1:E:28:PRO:HD3	1.68	0.76
1:I:160:LYS:O	1:I:346:PRO:O	2.06	0.74
1:A:26:VAL:HG13	1:A:28:PRO:HD3	1.68	0.74
1:F:146:PRO:O	1:F:147:CYS:CB	2.36	0.74
1:F:244:GLU:HG2	1:F:247:ARG:HH11	1.53	0.73
1:D:19:THR:HG21	1:D:25:TYR:O	1.90	0.71
1:H:26:VAL:HG13	1:H:28:PRO:HD3	1.72	0.71
1:F:191:VAL:HG21	1:F:284:GLU:HG3	1.72	0.71
1:I:27:MSE:HE3	1:I:163:VAL:HG21	1.72	0.71
1:A:160:LYS:O	1:A:346:PRO:O	2.07	0.70
1:H:244:GLU:CG	1:H:247:ARG:NH1	2.56	0.69
1:B:244:GLU:HG2	1:B:247:ARG:NH1	2.08	0.69
1:I:26:VAL:HG13	1:I:28:PRO:HD3	1.76	0.68
1:B:240:TYR:OH	1:B:244:GLU:HG3	1.94	0.68
1:E:146:PRO:O	1:E:147:CYS:HB3	1.94	0.68
1:A:27:MSE:CE	1:A:163:VAL:HG21	2.25	0.67
1:F:315:VAL:HG22	1:F:323:ILE:HD13	1.77	0.67
1:F:216:LYS:NZ	1:F:221:GLU:HB3	2.11	0.66
1:I:244:GLU:HG3	1:I:247:ARG:HH11	1.60	0.66
1:G:26:VAL:HG12	1:G:166:LEU:HB3	1.79	0.64
1:D:26:VAL:HG13	1:D:28:PRO:HD3	1.79	0.64
1:A:108:ALA:O	1:A:112:VAL:HG13	1.97	0.64
1:I:328:LEU:HD22	1:I:332:LEU:HD22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:244:GLU:CG	1:G:247:ARG:NH1	2.61	0.63
1:A:328:LEU:HD22	1:A:332:LEU:HD22	1.81	0.62
1:H:139:GLU:O	1:H:143:VAL:O	2.18	0.62
1:B:172:GLN:HA	1:B:172:GLN:HE21	1.62	0.62
1:H:153:PHE:HE2	1:H:164:ILE:HG21	1.64	0.62
1:A:240:TYR:CZ	1:A:244:GLU:HG3	2.35	0.61
1:I:11:ARG:C	1:I:11:ARG:HD2	2.20	0.61
1:D:27:MSE:HE2	1:D:163:VAL:HG21	1.81	0.61
1:H:244:GLU:HG2	1:H:247:ARG:HH11	1.63	0.61
1:B:35:THR:HB	1:B:109:SER:OG	2.01	0.60
1:A:27:MSE:HE3	1:A:163:VAL:HG21	1.84	0.60
1:F:23:TYR:HB3	1:F:169:GLN:HB2	1.82	0.60
1:B:27:MSE:HE3	1:B:163:VAL:HG21	1.84	0.59
1:D:191:VAL:HG21	1:D:284:GLU:HG3	1.83	0.59
1:D:302:LEU:C	1:D:302:LEU:HD12	2.22	0.59
1:I:62:ASN:C	1:I:62:ASN:HD22	2.06	0.59
1:D:108:ALA:O	1:D:112:VAL:HG13	2.03	0.59
1:B:80:LEU:HD12	1:B:118:LEU:HD13	1.82	0.59
1:A:27:MSE:HE3	1:A:163:VAL:CG2	2.32	0.59
1:F:83:GLU:HG3	1:F:134:LEU:HD21	1.84	0.59
1:H:83:GLU:HG3	1:H:134:LEU:HD21	1.84	0.59
1:F:29:MSE:HE3	1:F:31:ILE:HG22	1.85	0.58
1:C:240:TYR:CZ	1:C:244:GLU:HG3	2.38	0.58
1:B:26:VAL:HG12	1:B:166:LEU:HB3	1.84	0.58
1:I:318:ASP:OD2	1:I:318:ASP:N	2.34	0.58
1:D:193:ARG:HG2	1:D:307:PHE:O	2.02	0.58
1:B:191:VAL:HG21	1:B:284:GLU:HG3	1.86	0.58
1:F:302:LEU:C	1:F:302:LEU:HD12	2.24	0.58
1:H:146:PRO:O	1:H:147:CYS:HB3	2.03	0.58
1:I:2:SER:HB3	1:I:40:GLU:HB2	1.86	0.57
1:G:227:LEU:O	1:G:235:ARG:HG3	2.04	0.57
1:A:205:ARG:CZ	1:C:172:GLN:HB2	2.35	0.57
1:D:26:VAL:HG12	1:D:166:LEU:HB3	1.86	0.57
1:E:191:VAL:HG21	1:E:284:GLU:HG3	1.86	0.57
1:I:244:GLU:CG	1:I:247:ARG:HH11	2.19	0.56
1:A:244:GLU:HG2	1:A:247:ARG:HH12	1.70	0.56
1:E:146:PRO:O	1:E:147:CYS:CB	2.53	0.56
1:F:27:MSE:HE1	1:F:255:LEU:HD12	1.86	0.56
1:C:19:THR:CG2	1:C:25:TYR:O	2.47	0.56
1:A:77:LEU:HD11	1:A:118:LEU:HD11	1.88	0.55
1:I:107:SER:OG	4:I:8400:ADP:O2A	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:244:GLU:HG3	1:I:247:ARG:HH12	1.71	0.55
1:D:222:VAL:HG21	1:D:238:PHE:CE2	2.41	0.55
1:B:244:GLU:HG2	1:B:247:ARG:HH12	1.72	0.54
1:G:27:MSE:HE3	1:G:163:VAL:HG21	1.89	0.54
1:H:108:ALA:O	1:H:112:VAL:HG13	2.06	0.54
1:E:302:LEU:HD12	1:E:302:LEU:C	2.28	0.54
1:F:28:PRO:HG3	1:F:150:LEU:HD23	1.89	0.54
1:I:244:GLU:CG	1:I:247:ARG:NH1	2.69	0.54
1:A:153:PHE:HE2	1:A:164:ILE:HG21	1.72	0.54
1:H:191:VAL:HG21	1:H:284:GLU:HG3	1.90	0.53
1:F:27:MSE:CE	1:F:163:VAL:HG21	2.39	0.53
1:A:244:GLU:HG2	1:A:247:ARG:NH1	2.24	0.53
1:C:83:GLU:HG3	1:C:134:LEU:HD21	1.89	0.53
1:D:17:GLU:OE1	2:D:3500:GLA:O6	2.25	0.53
1:C:108:ALA:O	1:C:112:VAL:HG13	2.09	0.53
1:A:76:VAL:O	1:A:79:VAL:HG12	2.09	0.53
1:F:16:GLY:HA2	1:F:244:GLU:OE2	2.08	0.53
1:E:120:GLN:OE1	1:E:352:VAL:HG21	2.08	0.53
1:F:31:ILE:HD12	1:F:33:LEU:HD12	1.91	0.53
1:E:145:VAL:HG12	1:E:146:PRO:O	2.09	0.52
1:G:222:VAL:HG21	1:G:238:PHE:CE2	2.44	0.52
1:H:26:VAL:HG12	1:H:166:LEU:HB3	1.91	0.52
1:F:2:SER:HB2	1:F:40:GLU:HA	1.90	0.52
1:H:27:MSE:CE	1:H:163:VAL:HG21	2.40	0.52
1:E:26:VAL:HG12	1:E:166:LEU:HB3	1.90	0.52
1:F:28:PRO:HB3	1:F:150:LEU:HD21	1.90	0.52
1:B:301:ARG:HG2	1:B:302:LEU:O	2.09	0.52
1:H:293:MSE:SE	1:H:299:GLY:HA2	2.59	0.52
1:I:108:ALA:O	1:I:112:VAL:HG13	2.09	0.52
1:A:27:MSE:HE1	1:A:163:VAL:HG21	1.91	0.51
1:H:328:LEU:HD22	1:H:332:LEU:HD22	1.92	0.51
1:B:113:GLY:O	1:B:117:VAL:HG23	2.11	0.51
1:G:98:LEU:HD12	1:G:99:PRO:HD2	1.93	0.51
1:H:124:LEU:HB3	1:H:126:ILE:HG13	1.92	0.51
1:F:216:LYS:HZ3	1:F:221:GLU:HB3	1.75	0.51
1:I:56:LYS:HG3	1:I:69:TRP:CZ2	2.46	0.51
1:A:19:THR:CG2	1:A:25:TYR:O	2.46	0.51
1:H:143:VAL:HG12	1:H:145:VAL:HG23	1.92	0.51
1:I:17:GLU:N	1:I:244:GLU:OE2	2.42	0.51
1:I:27:MSE:CE	1:I:163:VAL:HG21	2.39	0.51
1:A:240:TYR:OH	1:A:244:GLU:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:90:LEU:N	1:F:90:LEU:HD12	2.27	0.50
1:F:139:GLU:O	1:F:143:VAL:O	2.29	0.50
1:C:102:ALA:O	4:C:2400:ADP:O2B	2.29	0.50
1:C:28:PRO:HB2	1:C:154:ALA:HB2	1.92	0.50
1:G:222:VAL:HG21	1:G:238:PHE:HE2	1.77	0.50
1:B:11:ARG:HD2	1:B:11:ARG:C	2.32	0.50
1:F:102:ALA:HB1	1:F:188:TYR:CD1	2.46	0.50
1:F:108:ALA:O	1:F:112:VAL:HG13	2.11	0.50
1:A:347:SER:OG	1:A:348:ASP:N	2.45	0.49
1:H:291:LYS:HE3	1:H:330:GLU:CD	2.33	0.49
1:F:244:GLU:CG	1:F:247:ARG:NH1	2.67	0.49
1:C:46:GLN:O	1:C:91:LYS:HA	2.13	0.49
1:C:45:VAL:HG21	1:C:58:PHE:CE1	2.47	0.49
1:I:16:GLY:CA	1:I:244:GLU:OE2	2.61	0.49
1:F:16:GLY:CA	1:F:244:GLU:OE2	2.61	0.49
1:H:213:ILE:CG1	1:I:129:LEU:HD21	2.43	0.48
1:D:274:LEU:HD22	1:D:280:VAL:CG2	2.42	0.48
1:E:27:MSE:HA	1:E:164:ILE:O	2.13	0.48
1:F:216:LYS:HZ2	1:F:221:GLU:HB3	1.78	0.48
1:I:16:GLY:N	1:I:244:GLU:OE2	2.46	0.48
1:A:116:GLU:OE1	1:A:119:ASN:ND2	2.36	0.48
1:I:46:GLN:HG3	1:I:57:THR:HG22	1.95	0.48
1:B:27:MSE:HA	1:B:164:ILE:O	2.14	0.48
1:F:271:HIS:HB2	1:F:301:ARG:HA	1.96	0.48
1:I:23:TYR:HB3	1:I:169:GLN:HB2	1.95	0.48
1:G:223:THR:HG22	1:G:226:ASP:OD2	2.13	0.47
1:B:172:GLN:HE21	1:B:172:GLN:CA	2.21	0.47
1:D:45:VAL:HG13	1:D:90:LEU:CD1	2.44	0.47
1:I:83:GLU:CG	1:I:134:LEU:HD21	2.44	0.47
1:E:227:LEU:O	1:E:235:ARG:HG3	2.15	0.47
1:E:301:ARG:HG2	1:E:302:LEU:O	2.14	0.47
1:I:83:GLU:HG3	1:I:134:LEU:HD21	1.97	0.47
1:E:28:PRO:HB3	1:E:150:LEU:HD21	1.97	0.47
1:F:328:LEU:HD22	1:F:332:LEU:HD22	1.97	0.47
1:B:116:GLU:OE2	1:B:131:LYS:NZ	2.46	0.47
1:C:139:GLU:O	1:C:143:VAL:O	2.33	0.47
1:I:102:ALA:HB1	1:I:188:TYR:CD1	2.49	0.47
1:B:94:ILE:O	1:B:95:THR:HG23	2.15	0.46
1:H:166:LEU:HD13	1:H:168:THR:HG22	1.97	0.46
1:H:213:ILE:HD13	1:H:213:ILE:HG21	1.53	0.46
1:E:29:MSE:HB3	1:E:163:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:28:PRO:HD2	1:G:164:ILE:O	2.16	0.46
1:B:136:LYS:HE2	1:B:147:CYS:O	2.15	0.46
1:B:222:VAL:HG21	1:B:238:PHE:CE2	2.51	0.46
1:F:150:LEU:C	1:F:150:LEU:CD2	2.84	0.46
1:B:107:SER:HB3	4:B:1400:ADP:O2A	2.14	0.46
1:E:244:GLU:OE1	1:E:247:ARG:NH1	2.49	0.46
1:D:27:MSE:CE	1:D:163:VAL:HG21	2.46	0.46
1:F:274:LEU:HD13	1:F:302:LEU:HD11	1.98	0.46
1:F:315:VAL:HG22	1:F:323:ILE:CD1	2.45	0.46
1:H:45:VAL:O	1:H:57:THR:HA	2.16	0.46
1:I:129:LEU:HD23	1:I:130:LYS:N	2.31	0.46
1:A:295:LEU:HD21	1:F:322:THR:HG22	1.96	0.46
1:B:166:LEU:HD13	1:B:168:THR:HG22	1.97	0.46
1:C:45:VAL:HG21	1:C:58:PHE:CZ	2.50	0.46
1:D:160:LYS:O	1:D:346:PRO:O	2.34	0.46
1:I:129:LEU:HD23	1:I:129:LEU:C	2.35	0.46
1:B:247:ARG:NH2	1:B:273:ASP:OD2	2.48	0.46
1:H:247:ARG:NH2	1:H:273:ASP:OD2	2.49	0.46
1:E:240:TYR:CZ	1:E:244:GLU:HG3	2.51	0.45
1:F:323:ILE:HG22	1:F:327:ILE:HD12	1.97	0.45
1:H:205:ARG:NH2	1:I:172:GLN:CB	2.79	0.45
1:A:77:LEU:CD1	1:A:118:LEU:HD11	2.46	0.45
1:A:315:VAL:HG22	1:A:323:ILE:HD13	1.97	0.45
1:F:45:VAL:O	1:F:57:THR:HA	2.16	0.45
1:H:27:MSE:HE1	1:H:255:LEU:HD12	1.98	0.45
1:E:244:GLU:HG2	1:E:247:ARG:HH12	1.80	0.45
1:A:287:PHE:CE1	1:A:334:LYS:HD2	2.51	0.45
1:I:26:VAL:HG12	1:I:166:LEU:HB3	1.99	0.45
1:C:23:TYR:HB3	1:C:169:GLN:HB2	1.99	0.45
1:E:206:ILE:HG23	1:E:234:HIS:CD2	2.52	0.45
1:E:216:LYS:HD3	1:E:221:GLU:HB2	1.98	0.45
1:C:85:TYR:OH	1:C:130:LYS:NZ	2.50	0.44
1:H:302:LEU:C	1:H:302:LEU:HD12	2.38	0.44
1:B:11:ARG:C	1:B:11:ARG:CD	2.86	0.44
1:B:27:MSE:HG3	1:B:165:PHE:HA	1.99	0.44
1:F:150:LEU:C	1:F:150:LEU:HD22	2.38	0.44
1:A:166:LEU:HD13	1:A:168:THR:HG22	1.98	0.44
1:F:274:LEU:CD1	1:F:302:LEU:HD11	2.47	0.44
1:G:23:TYR:HA	1:G:168:THR:OG1	2.18	0.44
1:D:184:VAL:HB	1:D:344:VAL:HG12	2.00	0.44
1:F:240:TYR:CZ	1:F:244:GLU:HG3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:PHE:HB2	1:C:288:PHE:CE1	2.53	0.44
1:H:27:MSE:HE3	1:H:163:VAL:CG2	2.47	0.44
1:I:27:MSE:CE	1:I:255:LEU:HD12	2.42	0.44
1:D:244:GLU:CG	1:D:247:ARG:HH11	2.31	0.43
4:G:6400:ADP:H8	4:G:6400:ADP:H5'1	1.83	0.43
1:H:204:LYS:NZ	1:H:208:GLU:OE2	2.45	0.43
1:D:244:GLU:HG3	1:D:247:ARG:NH1	2.32	0.43
1:F:318:ASP:OD2	1:F:318:ASP:N	2.51	0.43
1:A:301:ARG:HG2	1:A:302:LEU:O	2.18	0.43
1:E:274:LEU:HD22	1:E:280:VAL:CG2	2.49	0.43
1:F:2:SER:HB2	1:F:3:LYS:H	1.59	0.43
1:I:37:ILE:HD13	1:I:114:ILE:HD13	1.99	0.43
1:D:27:MSE:HE3	1:D:176:ILE:HD12	2.00	0.43
1:D:302:LEU:HD12	1:D:303:THR:N	2.34	0.43
1:E:90:LEU:HD23	1:E:117:VAL:HG11	2.00	0.43
1:A:28:PRO:HB2	1:A:154:ALA:HB2	2.00	0.43
1:D:166:LEU:HD13	1:D:168:THR:HG22	2.01	0.43
1:I:271:HIS:HB2	1:I:301:ARG:HG3	2.01	0.43
1:I:291:LYS:NZ	1:I:294:GLU:OE1	2.38	0.43
1:B:141:GLU:O	1:B:143:VAL:N	2.52	0.42
1:D:288:PHE:CD1	1:D:327:ILE:HG21	2.53	0.42
1:G:27:MSE:HE3	1:G:163:VAL:CG2	2.49	0.42
1:G:244:GLU:CG	1:G:247:ARG:HH12	2.32	0.42
1:C:26:VAL:CG1	1:C:28:PRO:HD3	2.39	0.42
1:F:247:ARG:NH2	1:F:273:ASP:OD2	2.52	0.42
1:H:214:LEU:HD13	1:H:226:ASP:HB3	2.01	0.42
1:I:15:ILE:HD12	1:I:15:ILE:HA	1.89	0.42
1:I:315:VAL:HG22	1:I:323:ILE:HD13	2.00	0.42
1:D:2:SER:OG	1:D:3:LYS:N	2.51	0.42
1:H:20:ASP:OD1	1:H:150:LEU:HB2	2.19	0.42
1:I:120:GLN:OE1	1:I:352:VAL:HG23	2.18	0.42
1:A:279:ARG:HG2	1:A:279:ARG:HH11	1.83	0.42
1:E:29:MSE:HE2	1:E:31:ILE:HG22	2.01	0.42
1:F:45:VAL:HG22	1:F:90:LEU:HD12	2.01	0.42
1:F:160:LYS:O	1:F:346:PRO:O	2.37	0.42
1:A:52:PHE:HB3	1:A:54:GLU:OE1	2.19	0.42
1:C:23:TYR:HA	1:C:168:THR:OG1	2.20	0.42
1:C:223:THR:HG22	1:C:224:GLU:H	1.84	0.42
1:E:293:MSE:SE	1:E:299:GLY:HA2	2.70	0.42
1:F:222:VAL:HG21	1:F:238:PHE:HE2	1.85	0.42
1:B:188:TYR:CE2	1:B:190:GLY:HA2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:LEU:HA	1:D:99:PRO:HD3	1.92	0.42
1:D:111:GLU:OE2	1:D:139:GLU:HB2	2.20	0.42
1:F:27:MSE:HA	1:F:164:ILE:O	2.20	0.42
1:H:34:TYR:H	1:H:97:ASP:HB2	1.84	0.42
1:A:34:TYR:H	1:A:97:ASP:HB2	1.84	0.42
1:C:166:LEU:HD13	1:C:168:THR:HG22	2.01	0.42
1:D:153:PHE:HE2	1:D:164:ILE:HG21	1.84	0.42
1:I:79:VAL:HG21	1:I:137:LYS:HB3	2.02	0.42
1:D:223:THR:HG22	1:D:224:GLU:N	2.35	0.42
1:I:290:LYS:O	1:I:294:GLU:HG3	2.20	0.42
1:A:146:PRO:O	1:A:147:CYS:HB3	2.19	0.41
1:B:14:LEU:HD23	1:B:27:MSE:HE2	2.02	0.41
1:C:282:CYS:O	1:C:284:GLU:N	2.53	0.41
1:D:23:TYR:HA	1:D:168:THR:OG1	2.20	0.41
1:B:240:TYR:CD2	1:B:240:TYR:C	2.93	0.41
1:D:159:LYS:O	1:D:160:LYS:C	2.58	0.41
1:F:17:GLU:OE1	2:F:5500:GLA:O6	2.27	0.41
1:A:66:GLU:OE2	1:A:74:LYS:NZ	2.53	0.41
1:I:116:GLU:O	1:I:120:GLN:HG3	2.20	0.41
1:C:185:LEU:O	1:C:312:ILE:HA	2.19	0.41
1:G:280:VAL:HG12	1:G:307:PHE:CE1	2.55	0.41
1:H:240:TYR:CD2	1:H:240:TYR:C	2.94	0.41
1:D:133:LEU:HD23	1:D:149:ILE:HD13	2.03	0.41
1:E:255:LEU:HD23	1:E:255:LEU:HA	1.90	0.41
1:F:191:VAL:HG21	1:F:284:GLU:CG	2.46	0.41
1:B:14:LEU:HD23	1:B:27:MSE:CE	2.50	0.41
1:B:255:LEU:HD23	1:B:255:LEU:HA	1.87	0.41
1:F:166:LEU:HD13	1:F:168:THR:HG22	2.01	0.41
1:F:295:LEU:HD12	1:F:327:ILE:HG13	2.03	0.41
1:I:14:LEU:HD23	1:I:27:MSE:HE2	2.03	0.41
1:A:27:MSE:HE2	1:A:27:MSE:HB3	1.83	0.41
1:A:280:VAL:HG12	1:A:307:PHE:CZ	2.56	0.41
1:B:102:ALA:HA	1:B:188:TYR:CE1	2.56	0.41
1:C:34:TYR:H	1:C:97:ASP:HB2	1.86	0.41
1:C:159:LYS:HB3	1:C:162:ASN:HB2	2.03	0.41
1:D:28:PRO:HB2	1:D:154:ALA:HB2	2.03	0.41
1:D:76:VAL:O	1:D:79:VAL:HG12	2.21	0.41
1:I:62:ASN:ND2	1:I:64:THR:HB	2.35	0.41
1:H:28:PRO:HD2	1:H:164:ILE:O	2.21	0.41
1:H:147:CYS:O	1:H:147:CYS:SG	2.78	0.41
1:H:90:LEU:HD23	1:H:117:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:PRO:HB3	1:E:150:LEU:CD2	2.50	0.40
1:G:27:MSE:CE	1:G:163:VAL:HG21	2.51	0.40
1:H:184:VAL:HB	1:H:344:VAL:HG12	2.02	0.40
1:A:187:PHE:HB2	1:A:288:PHE:CE1	2.56	0.40
1:C:255:LEU:HD23	1:C:255:LEU:HA	1.95	0.40
1:D:193:ARG:HB2	1:D:194:GLU:OE1	2.22	0.40
1:F:70:ILE:HD12	1:F:70:ILE:HA	1.89	0.40
1:F:251:VAL:HG23	1:F:266:ILE:HG21	2.03	0.40
1:C:244:GLU:O	1:C:248:VAL:HG23	2.21	0.40
1:D:27:MSE:HA	1:D:164:ILE:O	2.21	0.40
1:E:48:TYR:OH	1:E:53:ASN:OD1	2.33	0.40
1:A:124:LEU:HD13	1:A:126:ILE:HD11	2.03	0.40
1:A:222:VAL:HG21	1:A:238:PHE:CE2	2.57	0.40
1:E:147:CYS:HB2	2:E:4500:GLA:O2	2.22	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	326/352 (93%)	311 (95%)	14 (4%)	1 (0%)	41 71
1	B	300/352 (85%)	282 (94%)	16 (5%)	2 (1%)	22 54
1	C	317/352 (90%)	292 (92%)	22 (7%)	3 (1%)	17 48
1	D	345/352 (98%)	336 (97%)	8 (2%)	1 (0%)	41 71
1	E	338/352 (96%)	316 (94%)	21 (6%)	1 (0%)	41 71
1	F	349/352 (99%)	329 (94%)	18 (5%)	2 (1%)	25 58
1	G	225/352 (64%)	210 (93%)	13 (6%)	2 (1%)	17 48
1	H	341/352 (97%)	328 (96%)	12 (4%)	1 (0%)	41 71
1	I	349/352 (99%)	332 (95%)	17 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2890/3168 (91%)	2736 (95%)	141 (5%)	13 (0%)	34 66

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	85	TYR
1	D	194	GLU
1	E	147	CYS
1	F	147	CYS
1	B	160	LYS
1	C	160	LYS
1	C	196	ALA
1	C	338	LYS
1	G	337	TRP
1	H	147	CYS
1	F	195	LEU
1	G	301	ARG
1	A	147	CYS

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	251/293 (86%)	229 (91%)	22 (9%)	10 30
1	B	210/293 (72%)	187 (89%)	23 (11%)	6 19
1	C	212/293 (72%)	193 (91%)	19 (9%)	9 29
1	D	260/293 (89%)	231 (89%)	29 (11%)	6 18
1	E	254/293 (87%)	230 (91%)	24 (9%)	8 26
1	F	278/293 (95%)	247 (89%)	31 (11%)	6 18
1	G	157/293 (54%)	140 (89%)	17 (11%)	6 20
1	H	264/293 (90%)	236 (89%)	28 (11%)	6 20
1	I	262/293 (89%)	227 (87%)	35 (13%)	4 11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2148/2637 (82%)	1920 (89%)	228 (11%)	6 20

All (228) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	12	VAL
1	A	19	THR
1	A	26	VAL
1	A	54	GLU
1	A	56	LYS
1	A	87	ILE
1	A	90	LEU
1	A	107	SER
1	A	127	ASP
1	A	149	ILE
1	A	150	LEU
1	A	166	LEU
1	A	185	LEU
1	A	216	LYS
1	A	255	LEU
1	A	268	THR
1	A	278	TYR
1	A	328	LEU
1	A	332	LEU
1	A	344	VAL
1	A	350	VAL
1	B	11	ARG
1	B	19	THR
1	B	26	VAL
1	B	35	THR
1	B	73	VAL
1	B	79	VAL
1	B	94	ILE
1	B	95	THR
1	B	97	ASP
1	B	150	LEU
1	B	166	LEU
1	B	172	GLN
1	B	185	LEU
1	B	193	ARG
1	B	198	SER

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Mol	Chain	Res	Type
1	B	223	THR
1	B	235	ARG
1	B	261	GLU
1	B	267	LEU
1	B	278	TYR
1	B	279	ARG
1	B	328	LEU
1	B	344	VAL
1	C	11	ARG
1	C	19	THR
1	C	26	VAL
1	C	77	LEU
1	C	90	LEU
1	C	106	SER
1	C	147	CYS
1	C	149	ILE
1	C	150	LEU
1	C	166	LEU
1	C	183	SER
1	C	223	THR
1	C	224	GLU
1	C	252	ARG
1	C	255	LEU
1	C	278	TYR
1	C	322	THR
1	C	344	VAL
1	C	350	VAL
1	D	11	ARG
1	D	19	THR
1	D	26	VAL
1	D	53	ASN
1	D	64	THR
1	D	77	LEU
1	D	90	LEU
1	D	112	VAL
1	D	120	GLN
1	D	129	LEU
1	D	150	LEU
1	D	166	LEU
1	D	185	LEU
1	D	193	ARG
1	D	197	SER

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Mol	Chain	Res	Type
1	D	218	SER
1	D	235	ARG
1	D	244	GLU
1	D	255	LEU
1	D	278	TYR
1	D	279	ARG
1	D	284	GLU
1	D	291	LYS
1	D	302	LEU
1	D	315	VAL
1	D	328	LEU
1	D	332	LEU
1	D	344	VAL
1	D	350	VAL
1	E	7	LYS
1	E	11	ARG
1	E	12	VAL
1	E	19	THR
1	E	26	VAL
1	E	27	MSE
1	E	43	ASP
1	E	62	ASN
1	E	79	VAL
1	E	86	LYS
1	E	90	LEU
1	E	97	ASP
1	E	127	ASP
1	E	150	LEU
1	E	166	LEU
1	E	218	SER
1	E	223	THR
1	E	255	LEU
1	E	278	TYR
1	E	315	VAL
1	E	325	ASP
1	E	328	LEU
1	E	347	SER
1	E	350	VAL
1	F	2	SER
1	F	11	ARG
1	F	12	VAL
1	F	19	THR

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Mol	Chain	Res	Type
1	F	43	ASP
1	F	68	SER
1	F	79	VAL
1	F	90	LEU
1	F	97	ASP
1	F	107	SER
1	F	120	GLN
1	F	127	ASP
1	F	129	LEU
1	F	130	LYS
1	F	150	LEU
1	F	166	LEU
1	F	185	LEU
1	F	197	SER
1	F	198	SER
1	F	244	GLU
1	F	255	LEU
1	F	291	LYS
1	F	315	VAL
1	F	317	LYS
1	F	318	ASP
1	F	328	LEU
1	F	332	LEU
1	F	344	VAL
1	F	347	SER
1	F	350	VAL
1	F	352	VAL
1	G	11	ARG
1	G	12	VAL
1	G	19	THR
1	G	26	VAL
1	G	27	MSE
1	G	29	MSE
1	G	107	SER
1	G	150	LEU
1	G	151	ASP
1	G	166	LEU
1	G	197	SER
1	G	217	GLU
1	G	244	GLU
1	G	278	TYR
1	G	303	THR

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Mol	Chain	Res	Type
1	G	344	VAL
1	G	347	SER
1	H	3	LYS
1	H	11	ARG
1	H	19	THR
1	H	26	VAL
1	H	54	GLU
1	H	90	LEU
1	H	129	LEU
1	H	150	LEU
1	H	166	LEU
1	H	197	SER
1	H	198	SER
1	H	205	ARG
1	H	213	ILE
1	H	216	LYS
1	H	223	THR
1	H	225	LYS
1	H	238	PHE
1	H	244	GLU
1	H	252	ARG
1	H	255	LEU
1	H	265	LYS
1	H	278	TYR
1	H	291	LYS
1	H	315	VAL
1	H	328	LEU
1	H	332	LEU
1	H	344	VAL
1	H	347	SER
1	I	11	ARG
1	I	12	VAL
1	I	19	THR
1	I	26	VAL
1	I	27	MSE
1	I	43	ASP
1	I	62	ASN
1	I	64	THR
1	I	65	LYS
1	I	79	VAL
1	I	90	LEU
1	I	97	ASP

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Mol	Chain	Res	Type
1	I	107	SER
1	I	129	LEU
1	I	130	LYS
1	I	149	ILE
1	I	150	LEU
1	I	166	LEU
1	I	174	GLU
1	I	185	LEU
1	I	216	LYS
1	I	223	THR
1	I	244	GLU
1	I	255	LEU
1	I	284	GLU
1	I	291	LYS
1	I	315	VAL
1	I	318	ASP
1	I	328	LEU
1	I	332	LEU
1	I	341	TYR
1	I	344	VAL
1	I	347	SER
1	I	350	VAL
1	I	352	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	ASN
1	B	172	GLN
1	C	53	ASN
1	C	162	ASN
1	E	62	ASN
1	F	51	HIS
1	F	62	ASN
1	F	162	ASN
1	I	51	HIS
1	I	62	ASN
1	I	123	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 27 ligands modelled in this entry, 9 are monoatomic - leaving 18 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	$\#\|Z\| > 2$
2	GLA	D	3500	-	12,12,12	0.52	0	17,17,17	1.19	2 (11%)
4	ADP	H	7400	3	24,29,29	1.35	2 (8%)	29,45,45	1.70	5 (17%)
2	GLA	I	8500	-	12,12,12	0.66	0	17,17,17	1.18	1 (5%)
4	ADP	A	400	3	24,29,29	1.32	2 (8%)	29,45,45	1.72	4 (13%)
2	GLA	G	6500	-	12,12,12	0.79	0	17,17,17	2.00	3 (17%)
2	GLA	B	1500	1	12,12,12	0.55	0	17,17,17	1.91	5 (29%)
2	GLA	A	500	-	12,12,12	0.39	0	17,17,17	1.08	1 (5%)
4	ADP	E	4400	3	24,29,29	1.10	2 (8%)	29,45,45	1.67	3 (10%)
4	ADP	I	8400	3	24,29,29	1.38	2 (8%)	29,45,45	1.87	11 (37%)
4	ADP	F	5400	3	24,29,29	1.33	2 (8%)	29,45,45	1.66	6 (20%)
2	GLA	F	5500	-	12,12,12	0.98	0	17,17,17	1.47	3 (17%)
4	ADP	B	1400	3	24,29,29	1.43	3 (12%)	29,45,45	1.79	5 (17%)
4	ADP	G	6400	3	24,29,29	1.69	3 (12%)	29,45,45	1.70	5 (17%)
2	GLA	E	4500	-	12,12,12	0.75	0	17,17,17	2.54	10 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GLA	H	7500	-	12,12,12	0.60	0	17,17,17	2.19	6 (35%)
4	ADP	D	3400	3	24,29,29	1.35	2 (8%)	29,45,45	1.77	4 (13%)
2	GLA	C	2500	-	12,12,12	0.83	1 (8%)	17,17,17	2.50	4 (23%)
4	ADP	C	2400	3	24,29,29	1.36	2 (8%)	29,45,45	1.83	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
2	GLA	D	3500	-	-	2/2/22/22	0/1/1/1
4	ADP	H	7400	3	-	1/12/32/32	0/3/3/3
2	GLA	I	8500	-	-	2/2/22/22	0/1/1/1
4	ADP	A	400	3	-	4/12/32/32	0/3/3/3
2	GLA	G	6500	-	-	1/2/22/22	0/1/1/1
2	GLA	B	1500	1	-	2/2/22/22	0/1/1/1
2	GLA	A	500	-	-	1/2/22/22	0/1/1/1
4	ADP	E	4400	3	-	7/12/32/32	0/3/3/3
4	ADP	I	8400	3	-	7/12/32/32	0/3/3/3
4	ADP	F	5400	3	-	7/12/32/32	0/3/3/3
2	GLA	F	5500	-	-	2/2/22/22	0/1/1/1
4	ADP	B	1400	3	-	5/12/32/32	0/3/3/3
4	ADP	G	6400	3	-	4/12/32/32	0/3/3/3
2	GLA	E	4500	-	1/1/5/5	1/2/22/22	0/1/1/1
2	GLA	H	7500	-	-	2/2/22/22	0/1/1/1
4	ADP	D	3400	3	-	7/12/32/32	0/3/3/3
2	GLA	C	2500	-	-	2/2/22/22	0/1/1/1
4	ADP	C	2400	3	-	4/12/32/32	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	6400	ADP	C2-N3	5.50	1.41	1.32
4	H	7400	ADP	C2-N3	4.79	1.39	1.32
4	B	1400	ADP	C2-N3	4.78	1.39	1.32
4	A	400	ADP	C2-N3	4.51	1.39	1.32
4	C	2400	ADP	C2-N3	4.43	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3400	ADP	C2-N3	4.37	1.39	1.32
4	I	8400	ADP	C2-N3	3.94	1.38	1.32
4	G	6400	ADP	C2-N1	3.55	1.40	1.33
4	E	4400	ADP	C2-N3	3.51	1.37	1.32
4	G	6400	ADP	O4'-C1'	3.45	1.45	1.41
4	B	1400	ADP	C2-N1	3.43	1.40	1.33
4	D	3400	ADP	C2-N1	3.18	1.39	1.33
4	A	400	ADP	C2-N1	3.14	1.39	1.33
4	C	2400	ADP	C2-N1	3.09	1.39	1.33
4	F	5400	ADP	C2-N3	3.08	1.37	1.32
4	I	8400	ADP	O4'-C4'	-2.83	1.38	1.45
4	H	7400	ADP	C2-N1	2.60	1.38	1.33
4	E	4400	ADP	C2-N1	2.50	1.38	1.33
4	F	5400	ADP	C2-N1	2.14	1.37	1.33
2	C	2500	GLA	C4-C5	2.13	1.57	1.53
4	B	1400	ADP	C4-N3	2.04	1.38	1.35

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2500	GLA	O5-C1-C2	8.69	125.78	110.28
4	H	7400	ADP	N3-C2-N1	-6.03	119.26	128.68
4	I	8400	ADP	N3-C2-N1	-5.82	119.58	128.68
4	C	2400	ADP	N3-C2-N1	-5.64	119.86	128.68
4	A	400	ADP	N3-C2-N1	-5.57	119.97	128.68
4	G	6400	ADP	N3-C2-N1	-5.31	120.38	128.68
4	E	4400	ADP	N3-C2-N1	-5.23	120.51	128.68
4	F	5400	ADP	N3-C2-N1	-5.20	120.55	128.68
4	B	1400	ADP	PA-O3A-PB	-5.16	115.13	132.83
4	C	2400	ADP	PA-O3A-PB	-5.06	115.45	132.83
4	D	3400	ADP	N3-C2-N1	-5.02	120.83	128.68
4	D	3400	ADP	PA-O3A-PB	-5.01	115.65	132.83
2	H	7500	GLA	O1-C1-O5	4.54	124.00	110.38
2	E	4500	GLA	C1-O5-C5	-4.53	105.11	113.66
2	G	6500	GLA	O1-C1-C2	4.53	121.78	109.03
2	B	1500	GLA	O5-C1-C2	4.50	118.31	110.28
4	B	1400	ADP	N3-C2-N1	-4.47	121.69	128.68
4	E	4400	ADP	PA-O3A-PB	-4.31	118.03	132.83
2	G	6500	GLA	O1-C1-O5	4.30	123.30	110.38
2	H	7500	GLA	C1-O5-C5	-4.13	105.87	113.66
2	E	4500	GLA	O1-C1-C2	4.03	120.39	109.03
4	G	6400	ADP	PA-O3A-PB	-4.01	119.06	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	400	ADP	PA-O3A-PB	-3.88	119.53	132.83
2	C	2500	GLA	C1-C2-C3	-3.68	102.68	110.31
2	E	4500	GLA	O1-C1-O5	3.64	121.32	110.38
4	D	3400	ADP	O2B-PB-O3A	3.56	116.58	104.64
4	B	1400	ADP	O2B-PB-O3A	3.52	116.45	104.64
4	B	1400	ADP	O4'-C1'-C2'	-3.42	101.93	106.93
2	H	7500	GLA	O5-C1-C2	3.39	116.33	110.28
2	E	4500	GLA	O5-C1-C2	3.38	116.31	110.28
4	A	400	ADP	O2B-PB-O3A	3.33	115.81	104.64
2	B	1500	GLA	O1-C1-O5	3.27	120.21	110.38
4	C	2400	ADP	O5'-C5'-C4'	-3.26	97.75	108.99
2	F	5500	GLA	C1-O5-C5	3.12	119.55	113.66
2	H	7500	GLA	C1-C2-C3	-3.04	104.00	110.31
2	E	4500	GLA	C1-C2-C3	-2.96	104.17	110.31
2	E	4500	GLA	O5-C5-C4	2.93	115.01	109.69
4	D	3400	ADP	C1'-N9-C4	-2.92	121.51	126.64
4	F	5400	ADP	O5'-C5'-C4'	-2.91	98.97	108.99
2	F	5500	GLA	O4-C4-C3	2.89	117.04	110.35
2	D	3500	GLA	O2-C2-C1	-2.88	102.48	109.16
4	H	7400	ADP	O2B-PB-O3A	2.86	114.22	104.64
2	E	4500	GLA	O3-C3-C4	2.71	116.62	110.35
2	B	1500	GLA	C1-O5-C5	-2.70	108.58	113.66
4	F	5400	ADP	C3'-C2'-C1'	2.67	105.00	100.98
4	C	2400	ADP	O2B-PB-O3A	2.65	113.51	104.64
2	A	500	GLA	C3-C4-C5	-2.64	105.53	110.24
2	B	1500	GLA	O1-C1-C2	2.61	116.37	109.03
4	I	8400	ADP	O2B-PB-O1B	2.58	120.76	110.68
4	I	8400	ADP	O2A-PA-O5'	2.56	119.62	107.75
4	I	8400	ADP	C4-C5-N7	-2.49	106.80	109.40
4	B	1400	ADP	C3'-C2'-C1'	2.48	104.71	100.98
4	H	7400	ADP	O3B-PB-O3A	2.47	112.93	104.64
4	E	4400	ADP	O3B-PB-O1B	-2.46	101.05	110.68
2	G	6500	GLA	O4-C4-C3	2.46	116.04	110.35
2	C	2500	GLA	C3-C4-C5	2.42	114.56	110.24
4	F	5400	ADP	O2B-PB-O1B	2.40	120.08	110.68
4	C	2400	ADP	N6-C6-N1	2.37	123.49	118.57
2	E	4500	GLA	O2-C2-C3	2.35	115.79	110.35
4	G	6400	ADP	O3B-PB-O2B	2.34	116.57	107.64
2	C	2500	GLA	O5-C5-C4	2.33	113.93	109.69
4	G	6400	ADP	C3'-C2'-C1'	2.33	104.49	100.98
2	H	7500	GLA	O2-C2-C3	2.33	115.73	110.35
2	E	4500	GLA	O4-C4-C3	2.31	115.70	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1500	GLA	O5-C5-C6	2.30	112.16	106.44
4	H	7400	ADP	PA-O3A-PB	-2.27	125.02	132.83
4	I	8400	ADP	C1'-N9-C4	-2.27	122.66	126.64
4	G	6400	ADP	C5-C6-N6	-2.23	116.96	120.35
4	F	5400	ADP	PA-O5'-C5'	2.19	134.53	121.68
4	I	8400	ADP	O5'-PA-O1A	-2.19	100.52	109.07
4	H	7400	ADP	C3'-C2'-C1'	2.18	104.26	100.98
2	D	3500	GLA	O2-C2-C3	2.17	115.36	110.35
4	I	8400	ADP	O4'-C1'-C2'	-2.15	103.79	106.93
2	F	5500	GLA	C6-C5-C4	-2.13	108.01	113.00
2	H	7500	GLA	O1-C1-C2	2.12	115.01	109.03
4	A	400	ADP	O5'-C5'-C4'	-2.12	101.70	108.99
4	F	5400	ADP	PA-O3A-PB	-2.11	125.60	132.83
4	I	8400	ADP	PA-O3A-PB	-2.09	125.64	132.83
4	I	8400	ADP	O3B-PB-O3A	2.09	111.65	104.64
4	I	8400	ADP	O5'-C5'-C4'	-2.07	101.87	108.99
2	E	4500	GLA	C3-C4-C5	2.04	113.88	110.24
2	I	8500	GLA	O4-C4-C5	2.04	114.35	109.30
4	I	8400	ADP	O3B-PB-O2B	-2.03	99.88	107.64

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	4500	GLA	C1

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	400	ADP	PA-O3A-PB-O2B
4	B	1400	ADP	C5'-O5'-PA-O1A
4	B	1400	ADP	C5'-O5'-PA-O2A
4	C	2400	ADP	O4'-C4'-C5'-O5'
4	C	2400	ADP	C3'-C4'-C5'-O5'
4	D	3400	ADP	C5'-O5'-PA-O1A
4	D	3400	ADP	C5'-O5'-PA-O2A
4	D	3400	ADP	C5'-O5'-PA-O3A
4	D	3400	ADP	C3'-C4'-C5'-O5'
4	E	4400	ADP	C5'-O5'-PA-O1A
4	E	4400	ADP	C5'-O5'-PA-O2A
4	E	4400	ADP	C5'-O5'-PA-O3A
4	E	4400	ADP	C3'-C4'-C5'-O5'
4	F	5400	ADP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
4	F	5400	ADP	C5'-O5'-PA-O3A
4	F	5400	ADP	O4'-C4'-C5'-O5'
4	F	5400	ADP	C3'-C4'-C5'-O5'
4	I	8400	ADP	PA-O3A-PB-O2B
2	H	7500	GLA	O5-C5-C6-O6
2	B	1500	GLA	C4-C5-C6-O6
4	A	400	ADP	O4'-C4'-C5'-O5'
4	A	400	ADP	C3'-C4'-C5'-O5'
4	I	8400	ADP	O4'-C4'-C5'-O5'
4	I	8400	ADP	C3'-C4'-C5'-O5'
2	B	1500	GLA	O5-C5-C6-O6
2	D	3500	GLA	O5-C5-C6-O6
2	F	5500	GLA	O5-C5-C6-O6
2	C	2500	GLA	O5-C5-C6-O6
2	I	8500	GLA	O5-C5-C6-O6
2	F	5500	GLA	C4-C5-C6-O6
2	D	3500	GLA	C4-C5-C6-O6
4	E	4400	ADP	O4'-C4'-C5'-O5'
2	H	7500	GLA	C4-C5-C6-O6
2	A	500	GLA	O5-C5-C6-O6
4	D	3400	ADP	O4'-C4'-C5'-O5'
4	G	6400	ADP	C4'-C5'-O5'-PA
2	G	6500	GLA	O5-C5-C6-O6
2	E	4500	GLA	O5-C5-C6-O6
2	I	8500	GLA	C4-C5-C6-O6
4	G	6400	ADP	PB-O3A-PA-O5'
4	A	400	ADP	PA-O3A-PB-O3B
4	B	1400	ADP	PA-O3A-PB-O2B
4	D	3400	ADP	PB-O3A-PA-O2A
4	F	5400	ADP	PB-O3A-PA-O1A
4	F	5400	ADP	C5'-O5'-PA-O1A
2	C	2500	GLA	C4-C5-C6-O6
4	C	2400	ADP	PB-O3A-PA-O2A
4	E	4400	ADP	PB-O3A-PA-O1A
4	F	5400	ADP	PB-O3A-PA-O2A
4	I	8400	ADP	PB-O3A-PA-O1A
4	B	1400	ADP	O4'-C4'-C5'-O5'
4	C	2400	ADP	PB-O3A-PA-O1A
4	G	6400	ADP	O4'-C4'-C5'-O5'
4	H	7400	ADP	PA-O3A-PB-O2B
4	B	1400	ADP	C5'-O5'-PA-O3A
4	I	8400	ADP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
4	D	3400	ADP	PB-O3A-PA-O1A
4	E	4400	ADP	PB-O3A-PA-O2A
4	I	8400	ADP	PB-O3A-PA-O2A
4	G	6400	ADP	C5'-O5'-PA-O1A
4	I	8400	ADP	C5'-O5'-PA-O1A

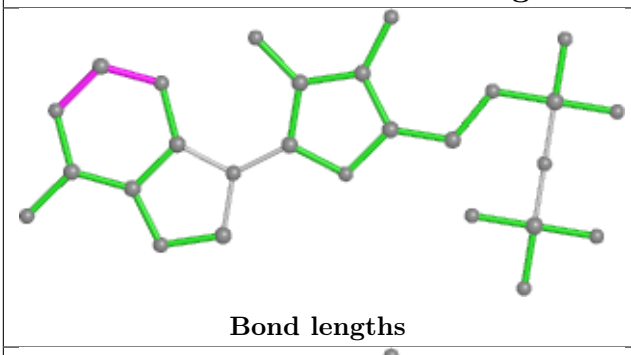
There are no ring outliers.

7 monomers are involved in 7 short contacts:

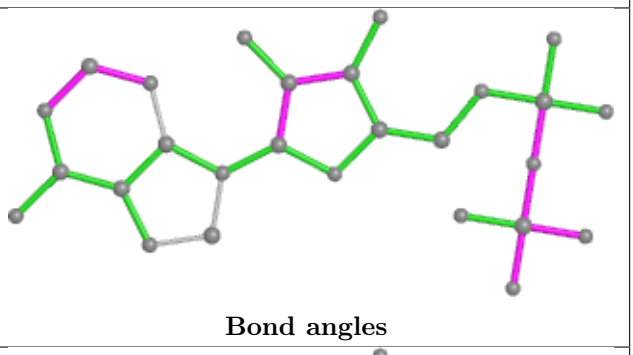
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3500	GLA	1	0
4	I	8400	ADP	1	0
2	F	5500	GLA	1	0
4	B	1400	ADP	1	0
4	G	6400	ADP	1	0
2	E	4500	GLA	1	0
4	C	2400	ADP	1	0

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.

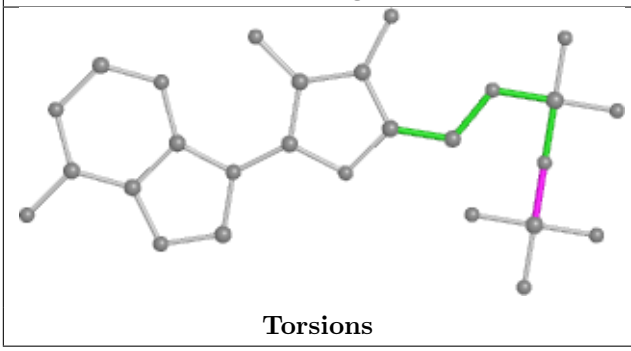
Ligand ADP H 7400



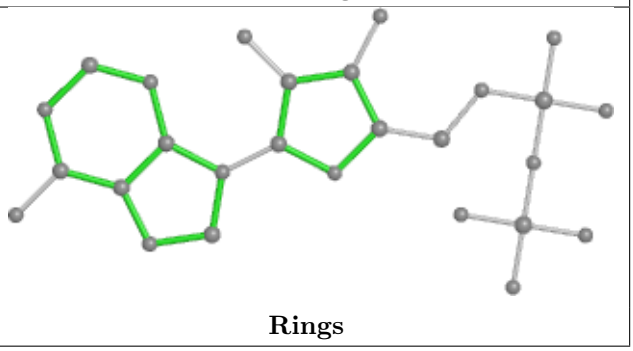
Bond lengths



Bond angles

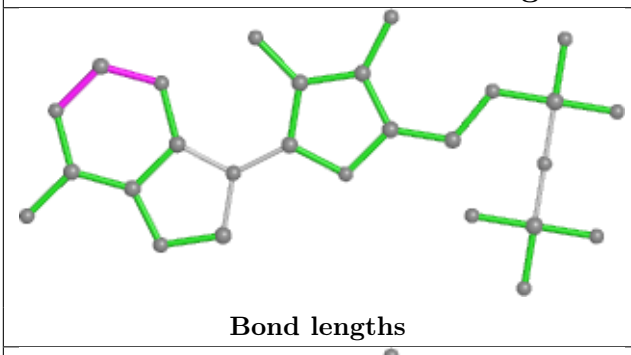


Torsions

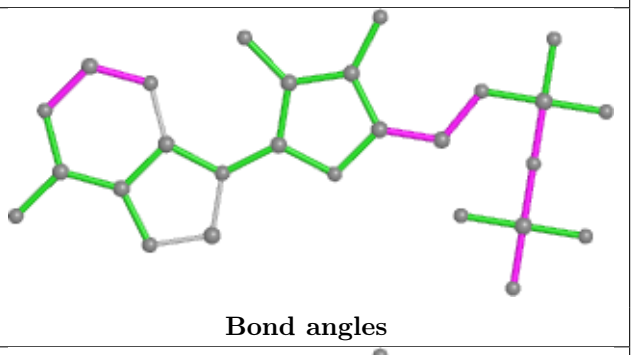


Rings

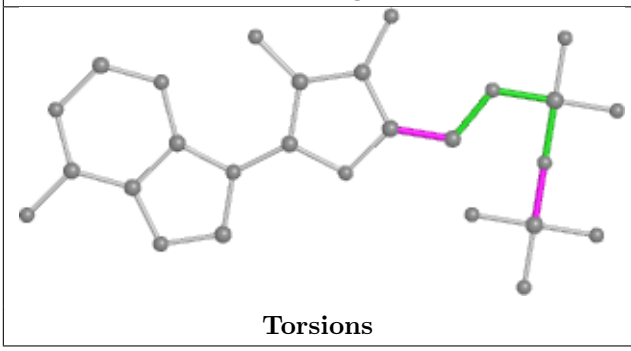
Ligand ADP A 400



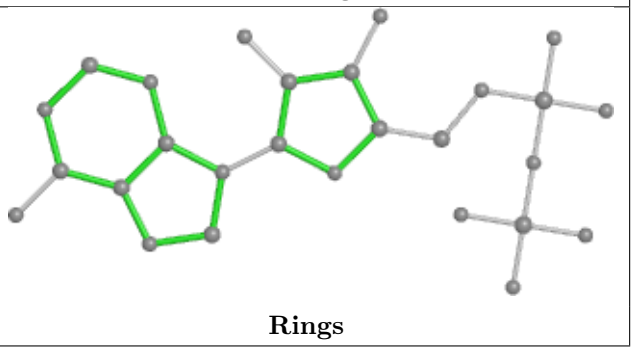
Bond lengths



Bond angles

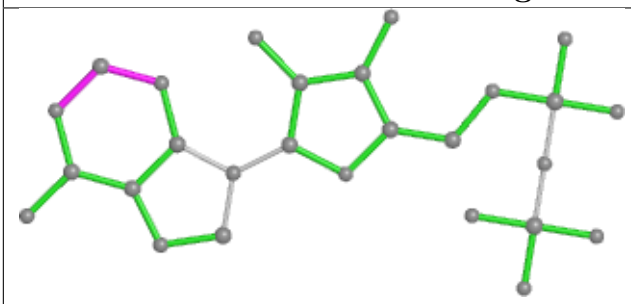


Torsions

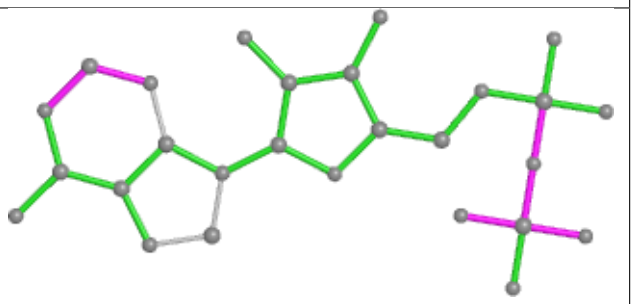


Rings

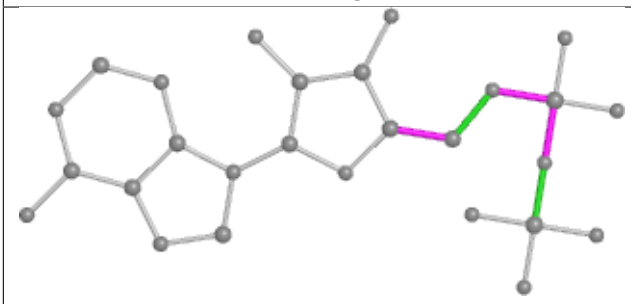
Ligand ADP E 4400



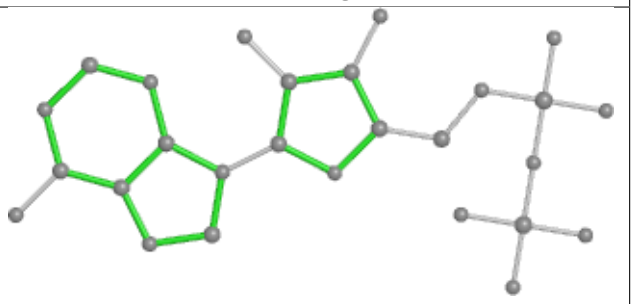
Bond lengths



Bond angles

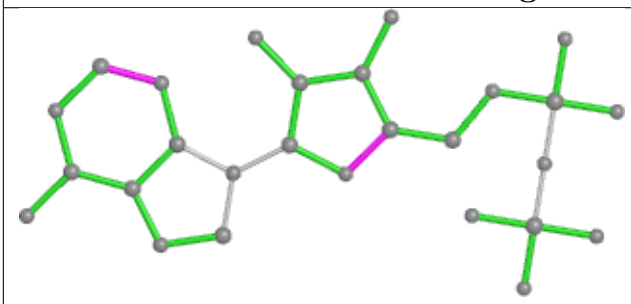


Torsions

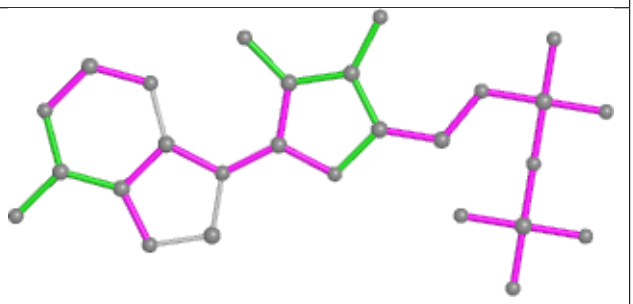


Rings

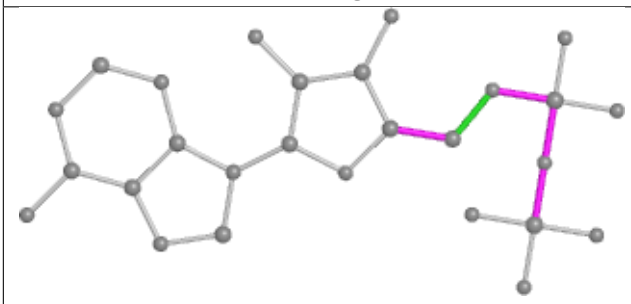
Ligand ADP I 8400



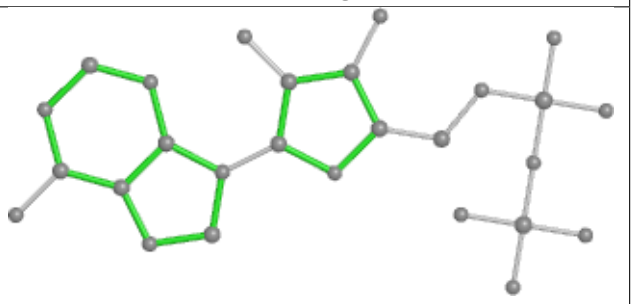
Bond lengths



Bond angles

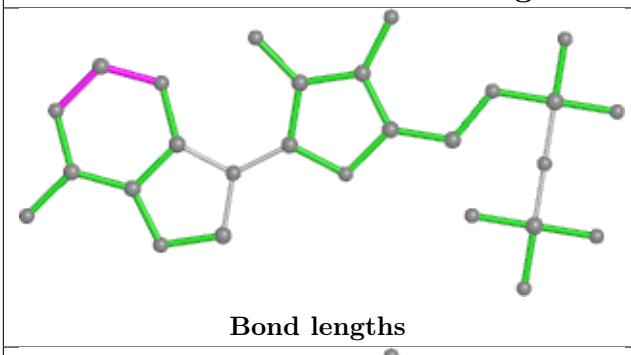


Torsions

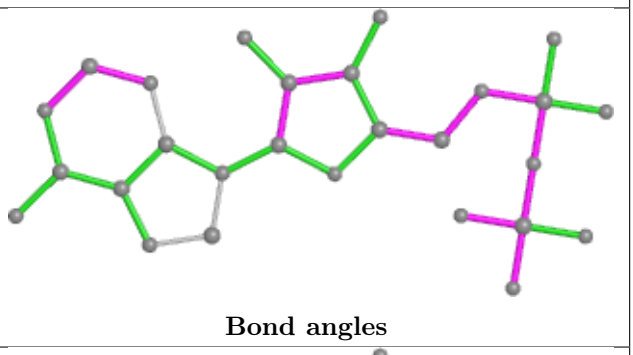


Rings

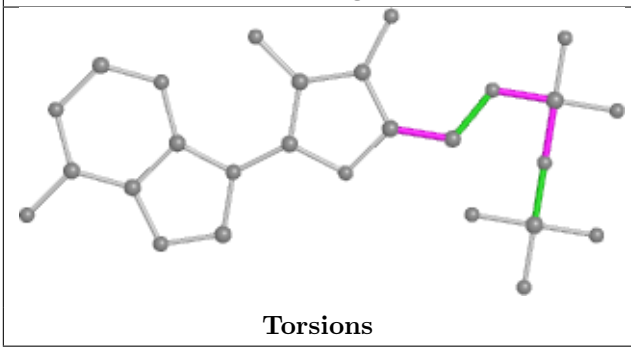
Ligand ADP F 5400



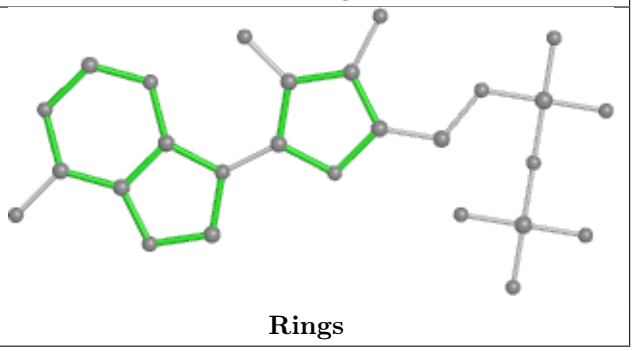
Bond lengths



Bond angles

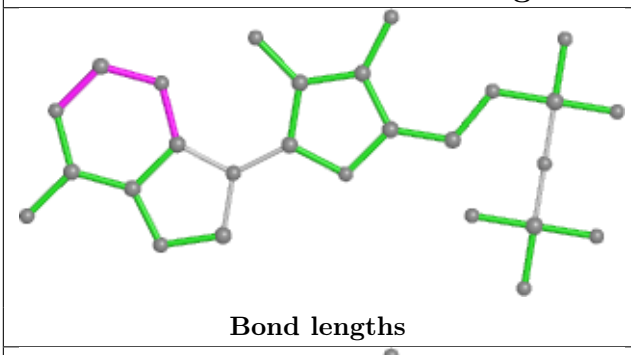


Torsions

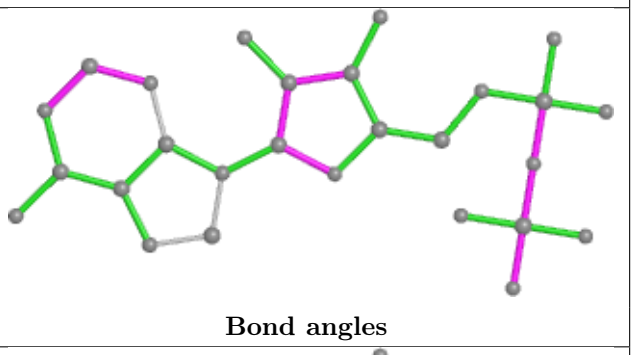


Rings

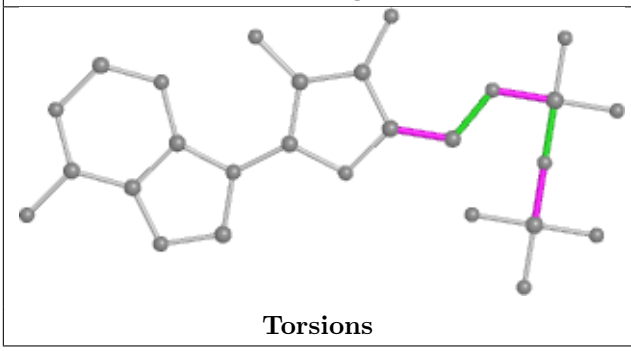
Ligand ADP B 1400



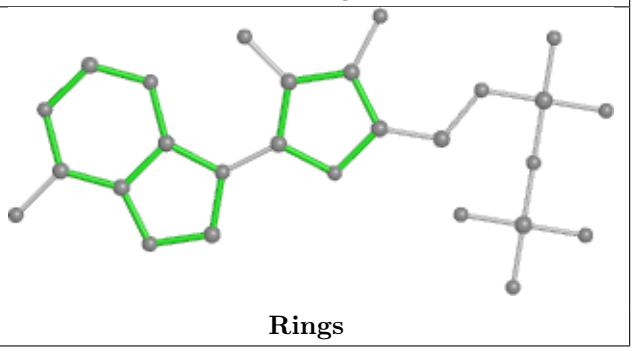
Bond lengths



Bond angles

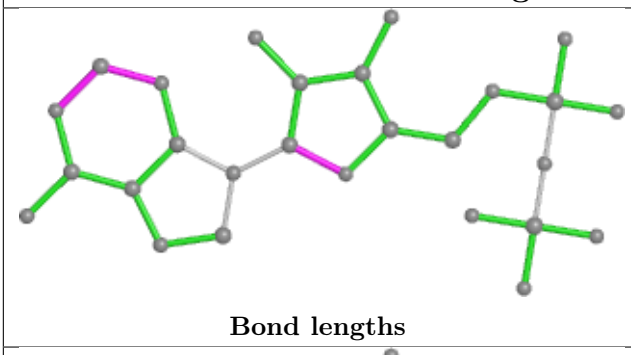


Torsions

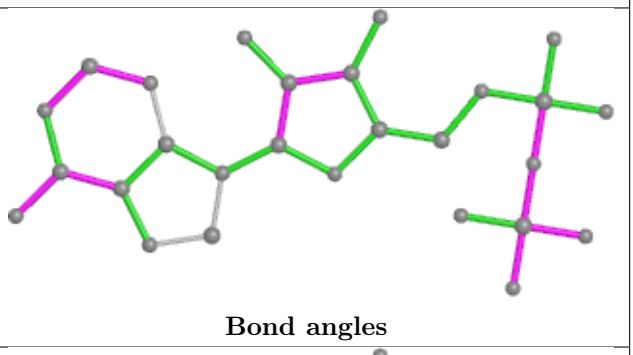


Rings

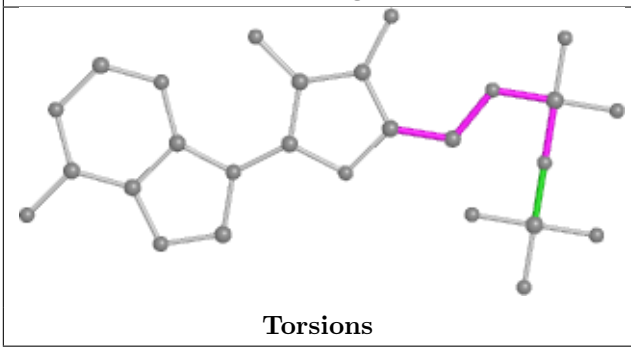
Ligand ADP G 6400



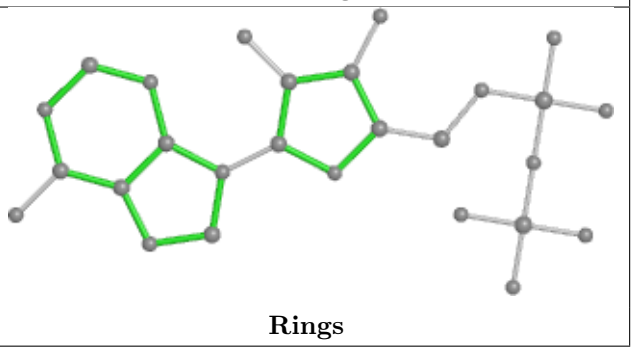
Bond lengths



Bond angles

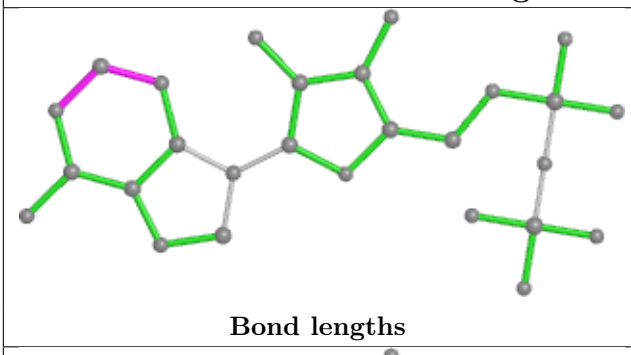


Torsions

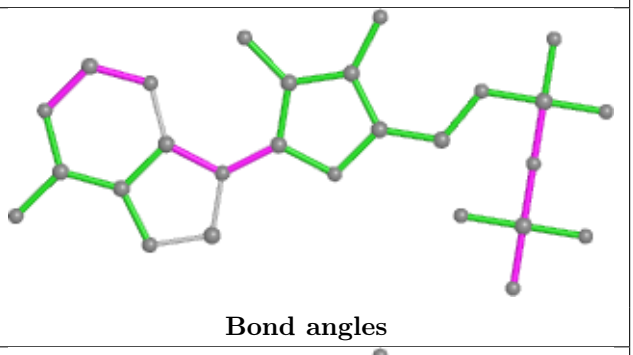


Rings

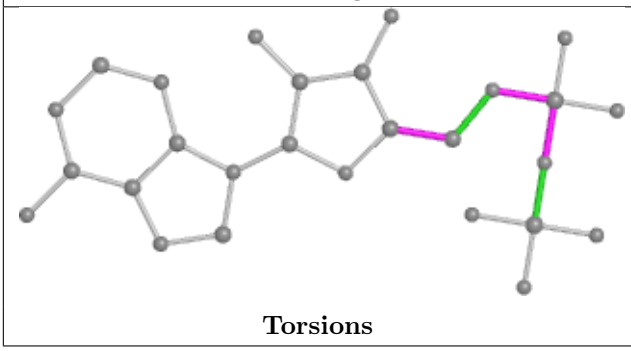
Ligand ADP D 3400



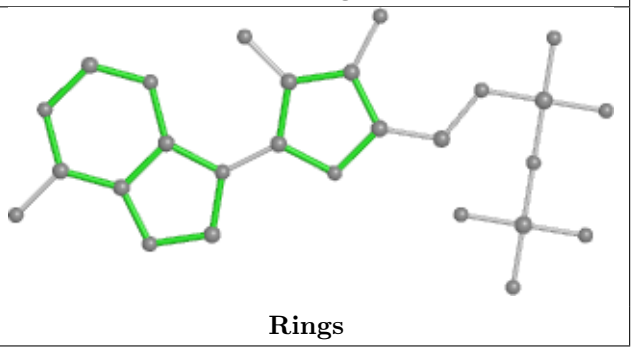
Bond lengths



Bond angles

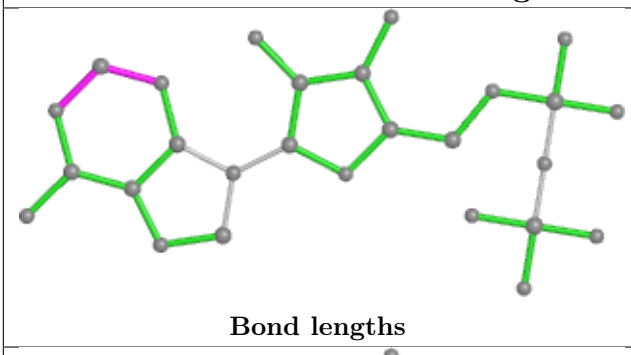


Torsions

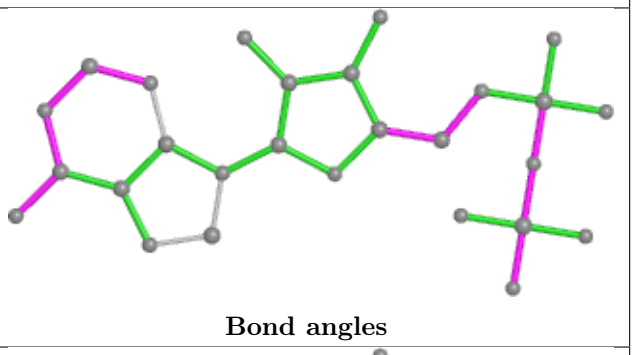


Rings

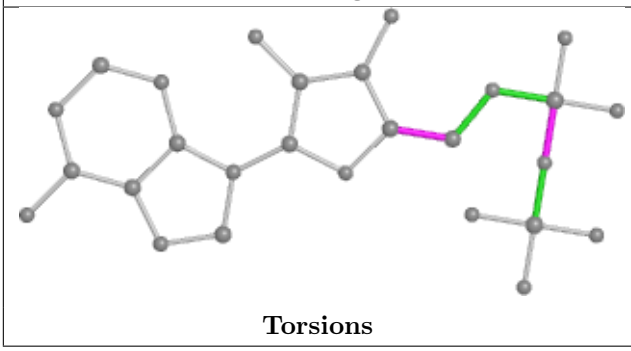
Ligand ADP C 2400



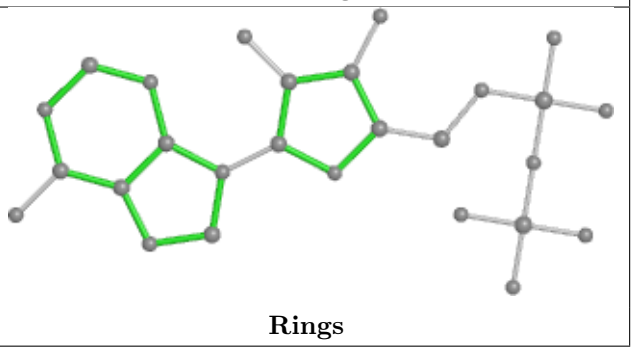
Bond lengths



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	334/352 (94%)	-0.33	7 (2%) 63 61	33, 54, 108, 137	0
1	B	307/352 (87%)	-0.01	17 (5%) 25 21	31, 78, 137, 173	0
1	C	334/352 (94%)	0.01	13 (3%) 39 35	50, 78, 126, 151	0
1	D	346/352 (98%)	-0.20	10 (2%) 51 47	46, 65, 93, 105	0
1	E	343/352 (97%)	0.06	13 (3%) 40 36	47, 66, 95, 108	0
1	F	348/352 (98%)	-0.34	1 (0%) 94 94	26, 42, 55, 70	0
1	G	252/352 (71%)	1.45	79 (31%) 0 0	45, 94, 148, 201	0
1	H	344/352 (97%)	-0.09	7 (2%) 65 63	24, 46, 73, 103	0
1	I	348/352 (98%)	-0.41	4 (1%) 80 80	23, 36, 56, 69	0
All	All	2956/3168 (93%)	-0.03	151 (5%) 28 24	23, 58, 116, 201	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	105	SER	5.5
1	G	294	GLU	5.1
1	G	162	ASN	4.9
1	G	336	SER	4.8
1	G	84	GLY	4.6
1	G	211	LEU	4.5
1	C	318	ASP	4.3
1	G	316	ASP	4.2
1	B	144	GLY	4.1
1	G	72	TYR	4.1
1	B	194	GLU	4.1
1	G	333	ALA	4.1
1	G	127	ASP	4.1
1	G	177	PRO	3.9
1	G	218	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	336	SER	3.7
1	A	49	SER	3.7
1	G	227	LEU	3.6
1	G	253	ASP	3.6
1	G	234	HIS	3.6
1	G	147	CYS	3.6
1	G	85	TYR	3.5
1	G	326	ALA	3.5
1	G	318	ASP	3.5
1	G	258	GLY	3.5
1	G	83	GLU	3.5
1	B	106	SER	3.4
1	D	2	SER	3.4
1	C	333	ALA	3.4
1	G	179	PRO	3.4
1	E	258	GLY	3.4
1	G	347	SER	3.4
1	B	123	ASN	3.4
1	A	67	GLY	3.3
1	H	53	ASN	3.3
1	D	296	GLY	3.3
1	D	325	ASP	3.3
1	G	173	TYR	3.2
1	G	230	LEU	3.2
1	G	299	GLY	3.2
1	C	123	ASN	3.2
1	G	210	SER	3.2
1	G	198	SER	3.2
1	G	343	VAL	3.2
1	G	335	PHE	3.2
1	G	334	LYS	3.2
1	G	297	ALA	3.1
1	G	324	GLY	3.1
1	G	106	SER	3.1
1	G	128	PRO	3.1
1	G	261	GLU	3.0
1	E	322	THR	3.0
1	E	352	VAL	3.0
1	B	326	ALA	3.0
1	G	97	ASP	3.0
1	G	231	PRO	2.9
1	G	322	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	I	352	VAL	2.9
1	G	79	VAL	2.9
1	G	75	GLY	2.9
1	G	257	GLU	2.9
1	E	62	ASN	2.9
1	G	325	ASP	2.9
1	H	2	SER	2.9
1	B	125	ASN	2.9
1	E	336	SER	2.8
1	E	333	ALA	2.8
1	G	184	VAL	2.8
1	I	336	SER	2.8
1	D	84	GLY	2.8
1	D	67	GLY	2.8
1	G	268	THR	2.8
1	B	95	THR	2.7
1	I	2	SER	2.7
1	E	53	ASN	2.7
1	G	320	ALA	2.7
1	G	201	ALA	2.6
1	C	332	LEU	2.6
1	G	209	GLU	2.6
1	G	32	ASP	2.6
1	G	327	ILE	2.5
1	G	259	ASP	2.5
1	D	64	THR	2.5
1	C	253	ASP	2.5
1	G	300	ALA	2.5
1	D	318	ASP	2.5
1	C	322	THR	2.5
1	D	53	ASN	2.5
1	B	172	GLN	2.5
1	C	298	TYR	2.5
1	C	197	SER	2.5
1	H	123	ASN	2.5
1	E	325	ASP	2.4
1	C	67	GLY	2.4
1	B	81	ILE	2.4
1	D	258	GLY	2.4
1	G	262	LYS	2.4
1	A	53	ASN	2.4
1	G	155	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	81	ILE	2.4
1	G	323	ILE	2.3
1	G	163	VAL	2.3
1	G	232	PRO	2.3
1	I	194	GLU	2.3
1	C	212	ARG	2.3
1	B	294	GLU	2.3
1	C	325	ASP	2.3
1	G	34	TYR	2.3
1	G	206	ILE	2.3
1	A	61	ASP	2.3
1	G	298	TYR	2.3
1	B	47	LEU	2.3
1	G	330	GLU	2.3
1	G	296	GLY	2.3
1	B	333	ALA	2.2
1	H	318	ASP	2.2
1	B	161	ASP	2.2
1	B	261	GLU	2.2
1	G	228	GLY	2.2
1	G	207	ALA	2.2
1	E	318	ASP	2.2
1	F	125	ASN	2.2
1	G	178	PHE	2.2
1	H	325	ASP	2.2
1	E	223	THR	2.2
1	G	208	GLU	2.2
1	G	317	LYS	2.2
1	G	344	VAL	2.2
1	E	253	ASP	2.1
1	G	142	PHE	2.1
1	G	212	ARG	2.1
1	H	84	GLY	2.1
1	D	61	ASP	2.1
1	B	84	GLY	2.1
1	A	81	ILE	2.1
1	B	347	SER	2.1
1	G	19	THR	2.1
1	G	203	ARG	2.1
1	H	62	ASN	2.1
1	G	78	TRP	2.1
1	E	67	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	295	LEU	2.1
1	E	61	ASP	2.1
1	C	326	ALA	2.1
1	B	94	ILE	2.0
1	G	254	ALA	2.0
1	G	279	ARG	2.0
1	A	140	ASN	2.0
1	G	329	ARG	2.0
1	G	250	GLU	2.0
1	A	93	LYS	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no 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
3	MG	G	6600	1/1	0.22	0.39	60,60,60,60	0
3	MG	H	7600	1/1	0.63	0.34	44,44,44,44	0
3	MG	A	600	1/1	0.71	0.24	46,46,46,46	0
3	MG	I	8600	1/1	0.71	0.25	35,35,35,35	0
4	ADP	G	6400	27/27	0.74	0.45	67,71,73,76	0
3	MG	B	1600	1/1	0.76	0.35	55,55,55,55	0
2	GLA	F	5500	12/12	0.79	0.27	51,54,56,56	0
3	MG	D	3600	1/1	0.79	0.16	44,44,44,44	0
3	MG	E	4600	1/1	0.81	0.22	47,47,47,47	0
2	GLA	G	6500	12/12	0.82	0.34	54,59,61,62	0
3	MG	F	5600	1/1	0.82	0.18	32,32,32,32	0
3	MG	C	2600	1/1	0.83	0.16	51,51,51,51	0
2	GLA	E	4500	12/12	0.88	0.22	52,55,55,55	0

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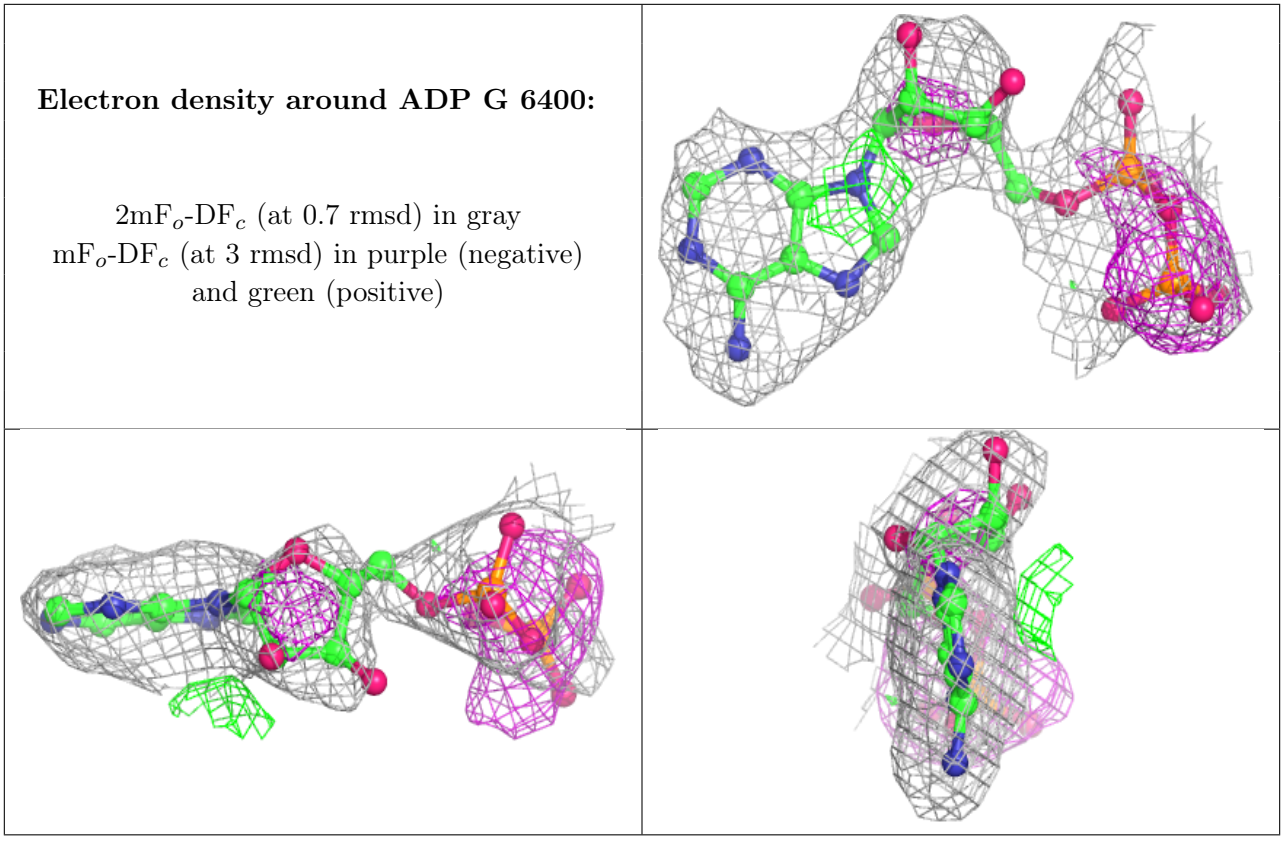
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLA	B	1500	12/12	0.90	0.20	53,56,57,58	0
4	ADP	B	1400	27/27	0.90	0.29	63,68,70,70	0
2	GLA	H	7500	12/12	0.90	0.19	36,39,41,42	0
2	GLA	D	3500	12/12	0.91	0.20	43,49,51,52	0
2	GLA	I	8500	12/12	0.92	0.18	33,34,36,37	0
2	GLA	A	500	12/12	0.92	0.17	42,46,49,50	0
4	ADP	E	4400	27/27	0.94	0.14	48,49,55,56	0
4	ADP	A	400	27/27	0.94	0.16	50,54,58,59	0
4	ADP	C	2400	27/27	0.95	0.19	58,60,61,63	0
4	ADP	D	3400	27/27	0.95	0.16	48,50,53,54	0
4	ADP	H	7400	27/27	0.95	0.16	40,50,53,54	0
4	ADP	I	8400	27/27	0.95	0.13	31,37,39,42	0
2	GLA	C	2500	12/12	0.96	0.11	45,49,50,51	0
4	ADP	F	5400	27/27	0.97	0.12	30,38,44,44	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.

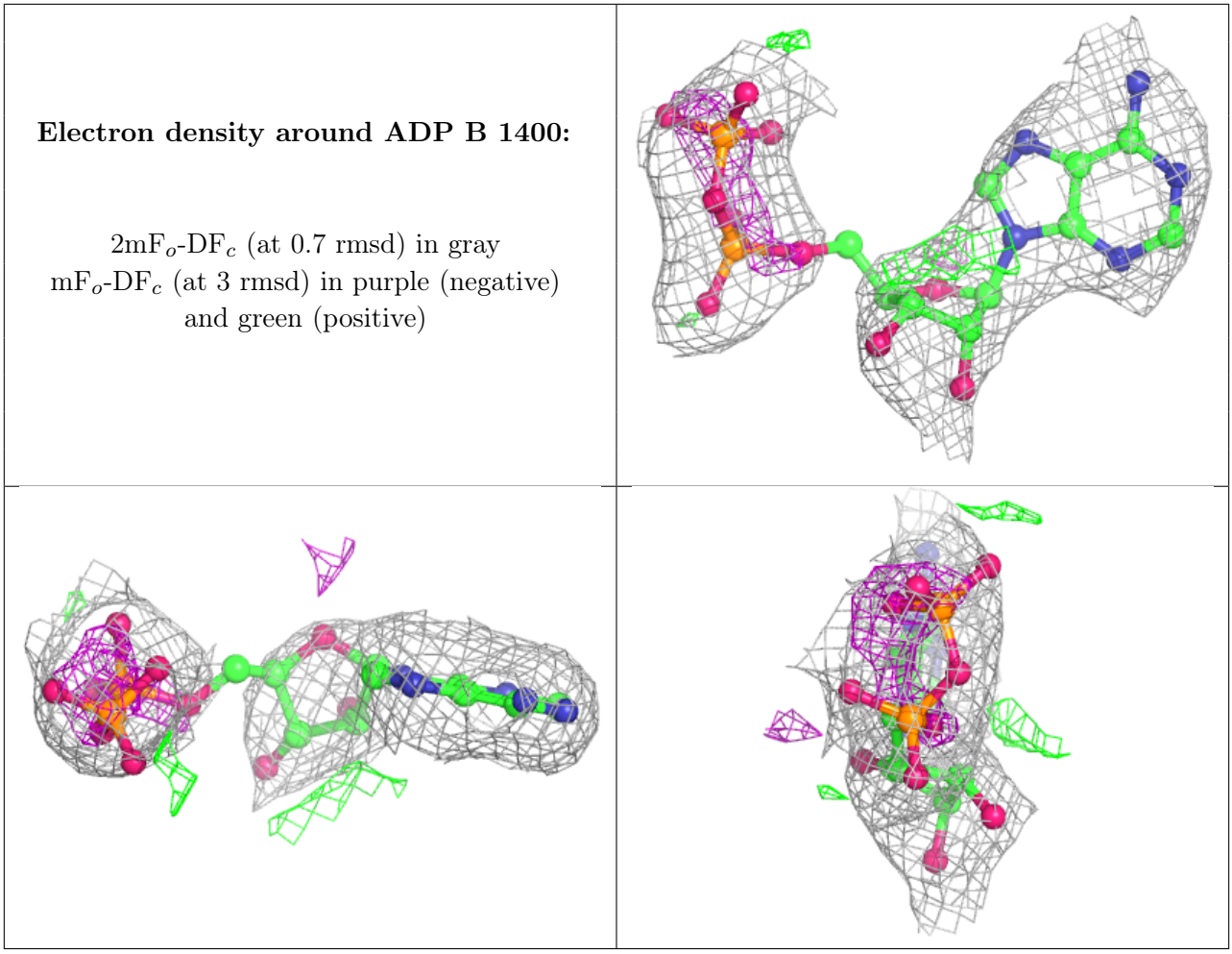
Electron density around ADP G 6400:

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



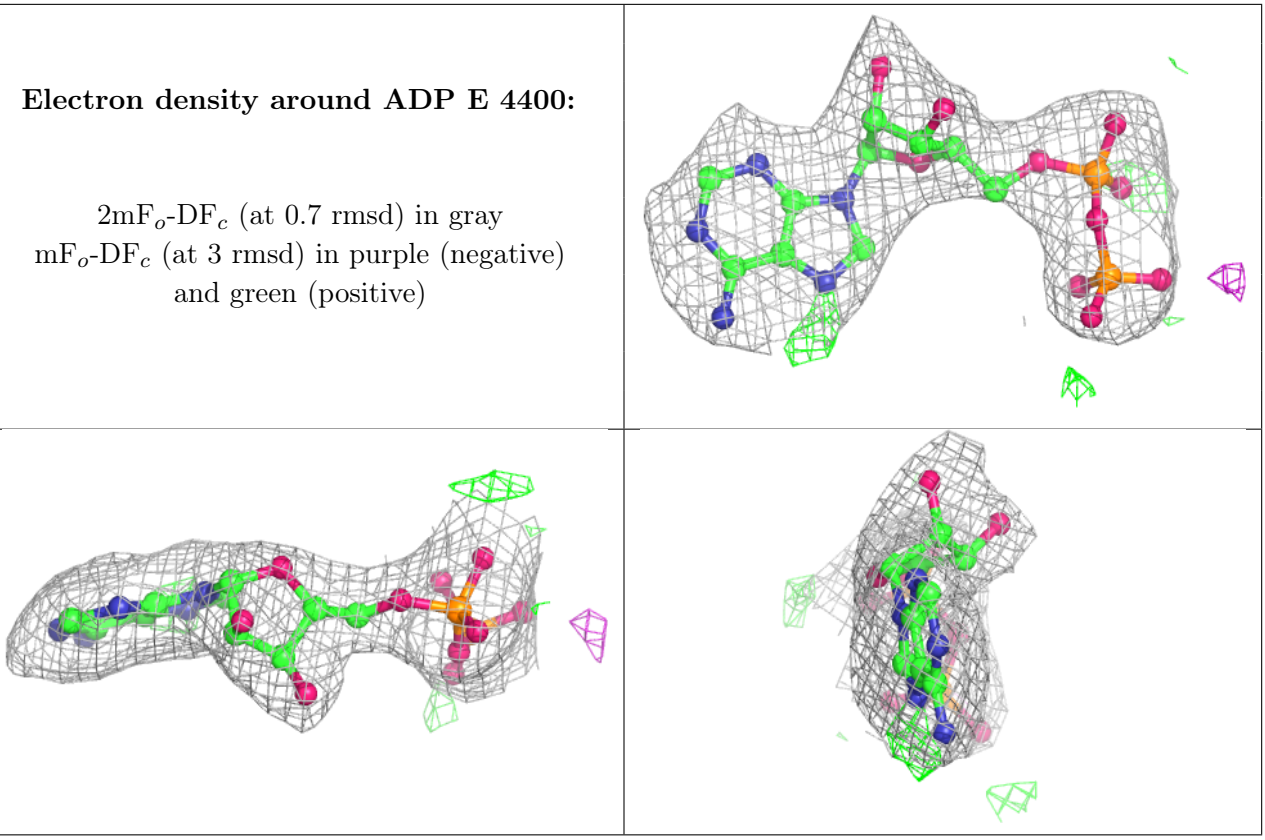
Electron density around ADP B 1400:

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



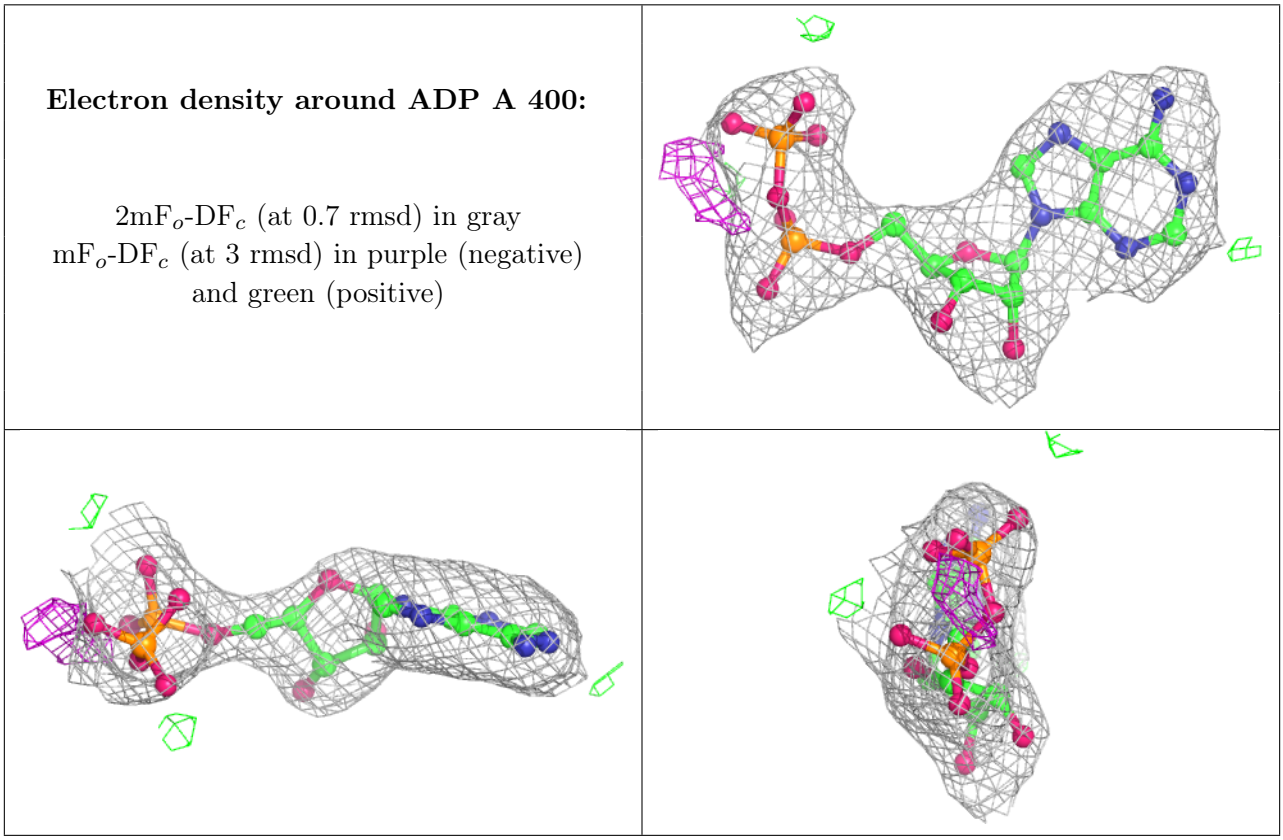
Electron density around ADP E 4400:

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



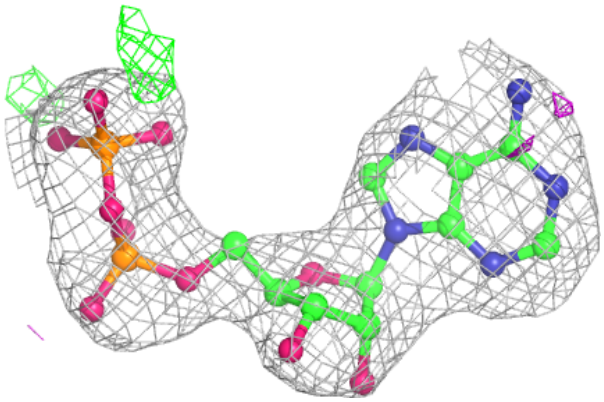
Electron density around ADP A 400:

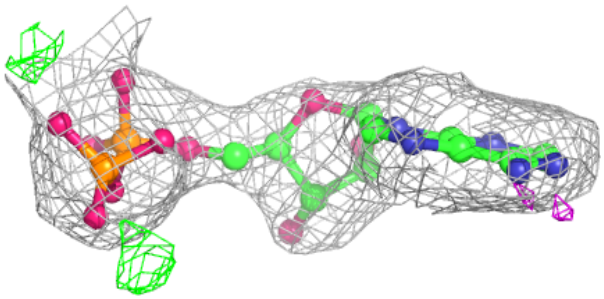
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

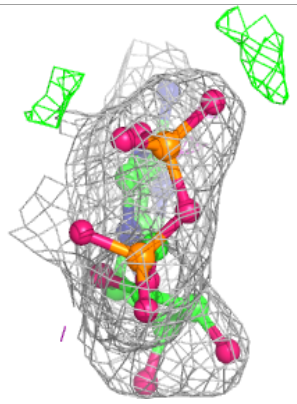


Electron density around ADP C 2400:

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

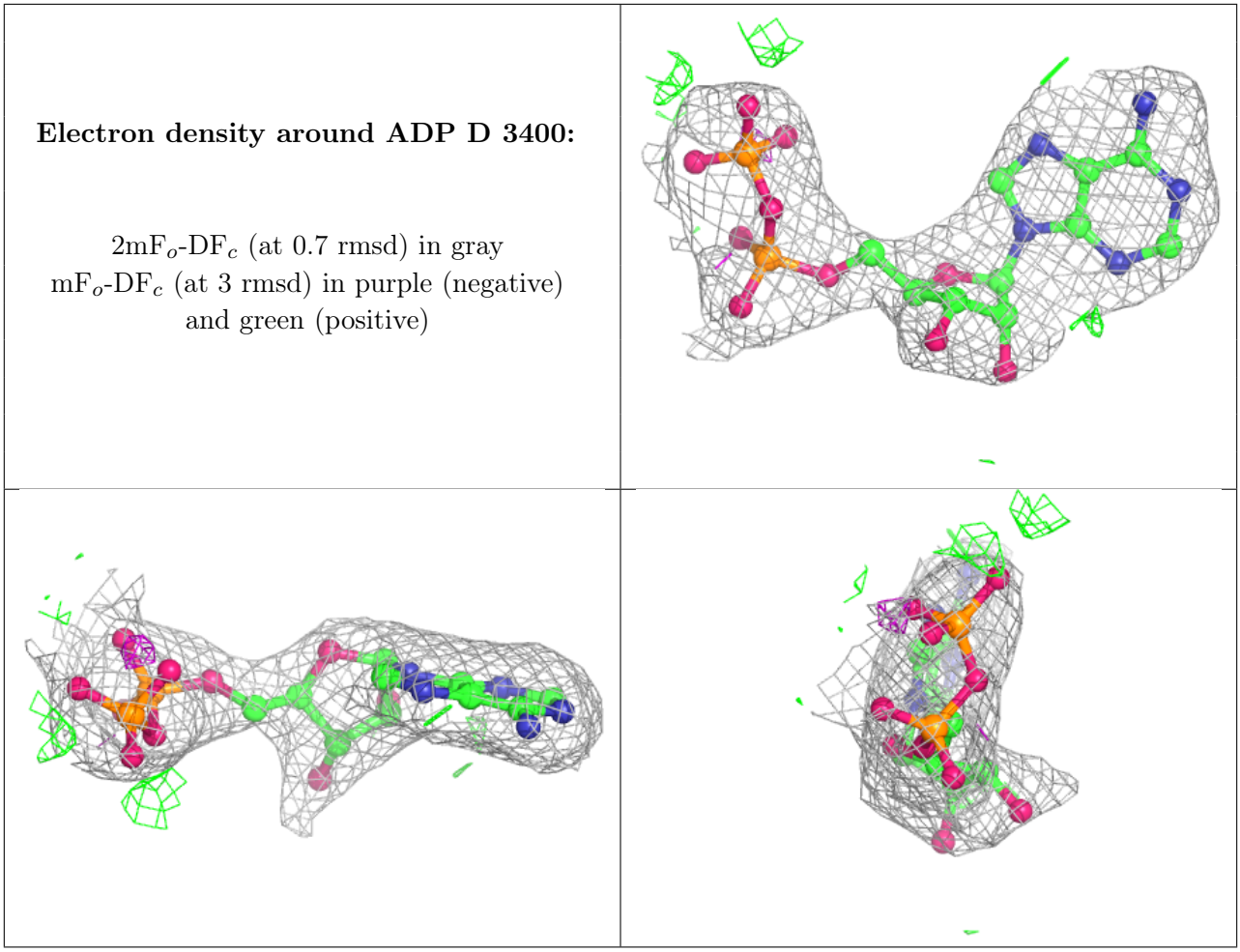






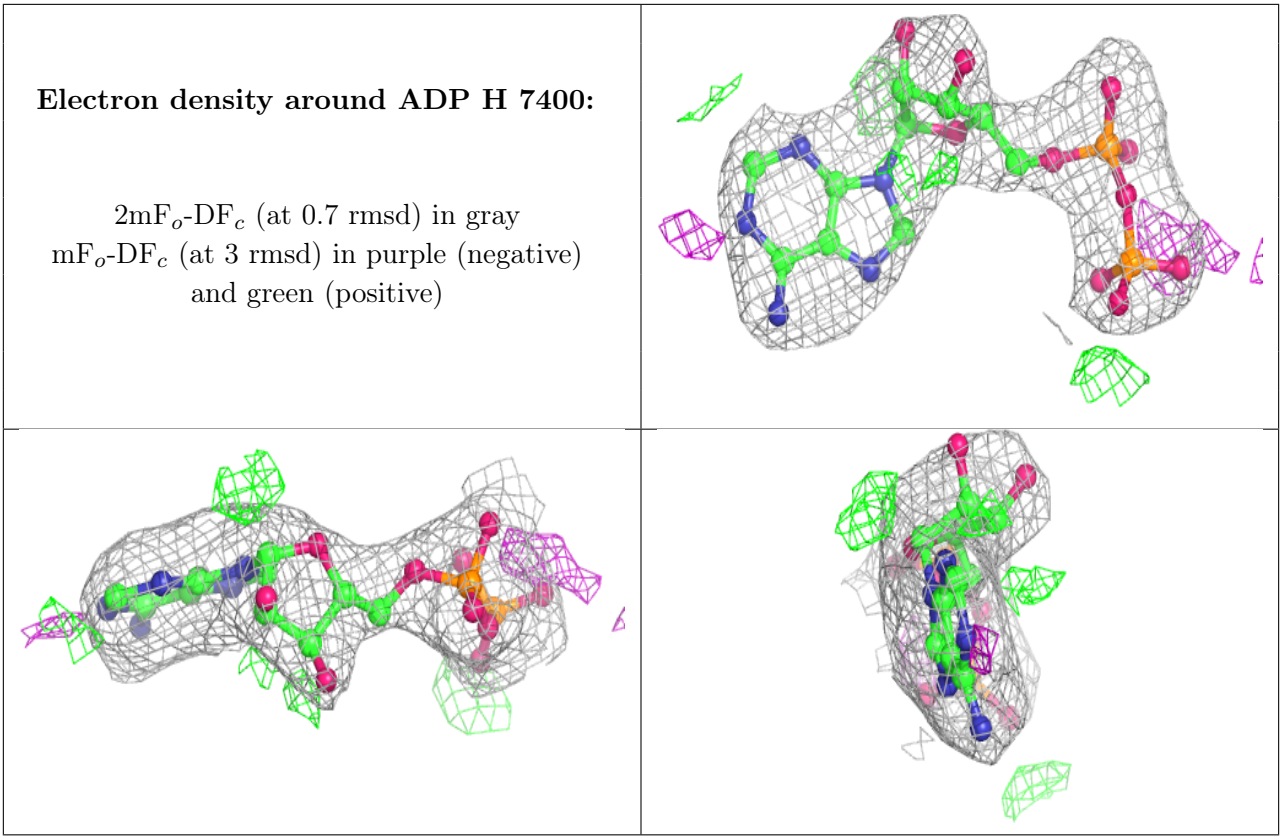
Electron density around ADP D 3400:

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



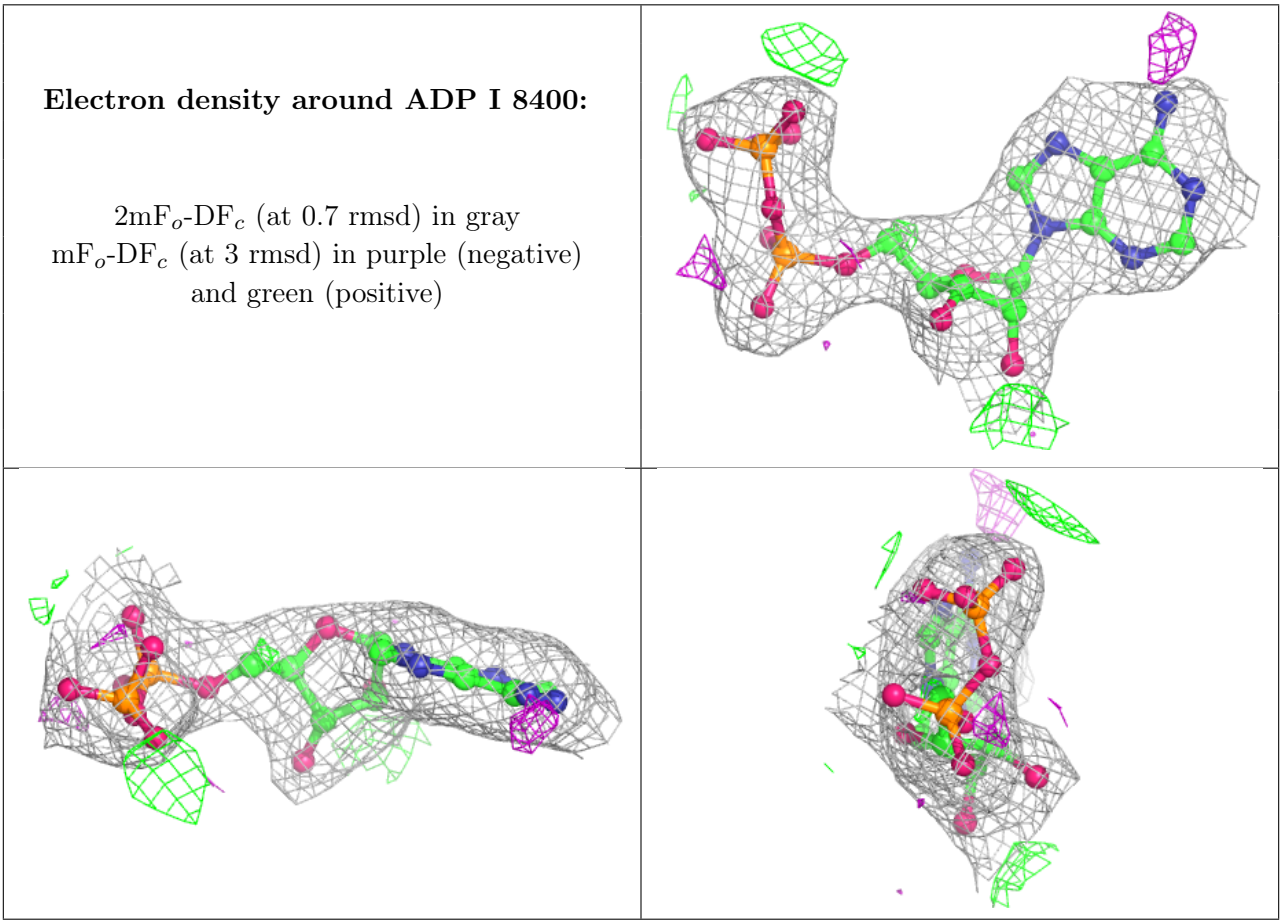
Electron density around ADP H 7400:

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



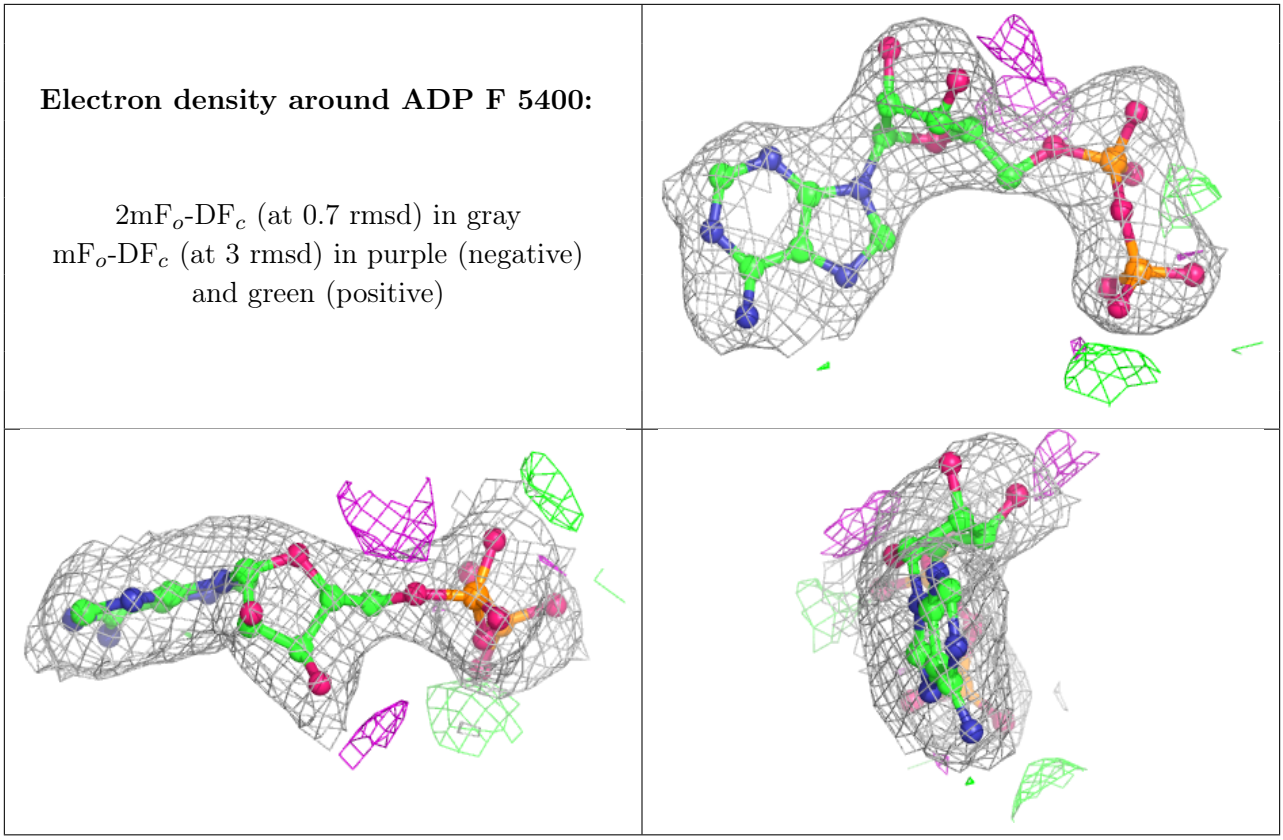
Electron density around ADP I 8400:

$2mF_o$-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 F 5400:

$2mF_o$-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.