Full wwPDB X-ray Structure Validation Report (i)

Sep 8, 2016 – 08:57 AM EDT

PDB ID	:	5L6S
Title	:	Crystal structure of E. coli ADP-glucose pyrophosphorylase (AGPase) in complex with a positive allosteric regulator beta-fructose-1,6-diphosphate (FBP) - AGPase*FBP
Authors	:	Cifuente, J.O.; Albesa-Jove, D.; Comino, N.; Madariaga-Marcos, J.; Agirre, J.; Lopez-Fernandez, S.; Garcia-Alija, M.; Guerin, M.E.
Deposited on	:	2016-05-31
Resolution	:	3.04 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

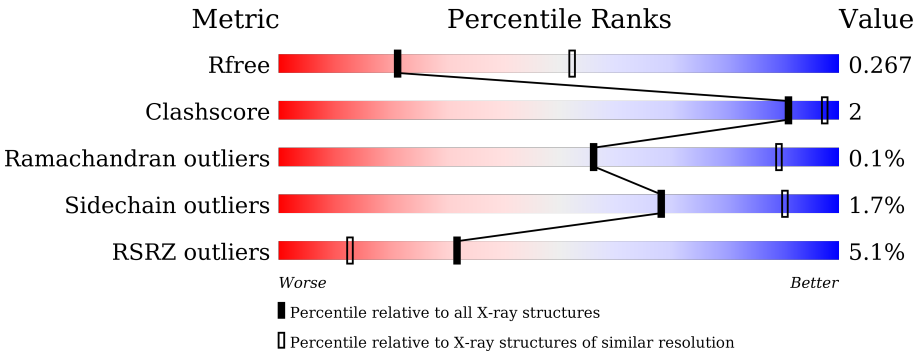
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 3.04 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}	91344	1995 (3.08-3.00)
Clashscore	102246	2351 (3.08-3.00)
Ramachandran outliers	100387	2272 (3.08-3.00)
Sidechain outliers	100360	2275 (3.08-3.00)
RSRZ outliers	91569	2013 (3.08-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	431	3% 90% · 5%
1	B	431	89% 7% · ·
1	C	431	88% 8% ·
1	D	431	3% 87% 6% 7%
1	E	431	3% 88% 7% 5%
1	F	431	3% 87% 6% 7%

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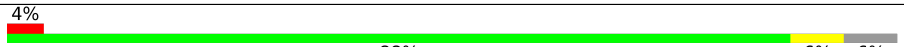
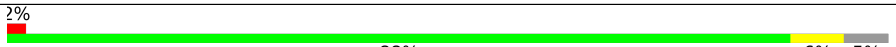
Mol	Chain	Length	Quality of chain
1	G	431	
1	H	431	
1	I	431	
1	J	431	
1	K	431	
1	L	431	
1	M	431	
1	N	431	
1	O	431	
1	P	431	

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	SO4	E	501	-	-	X	-
2	SO4	F	501	-	-	X	-
2	SO4	I	501	-	-	X	-
2	SO4	J	501	-	-	X	-
2	SO4	K	503	-	-	X	-

2 Entry composition

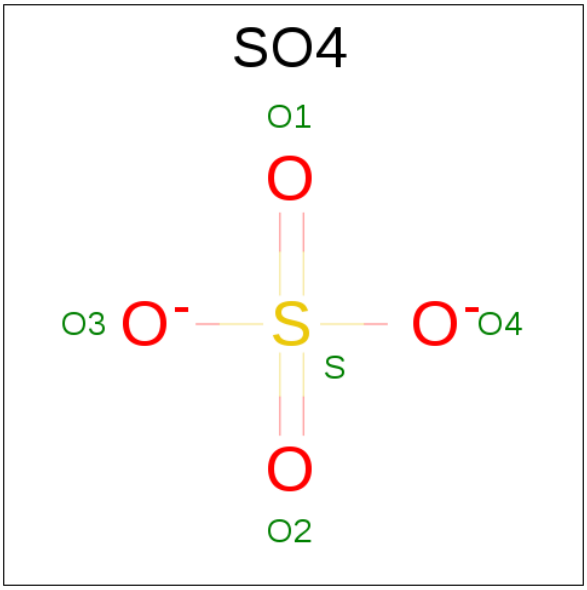
There are 3 unique types of molecules in this entry. The entry contains 45056 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glucose-1-phosphate adenylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	0
			3016	1913	518	567	18			
1	B	417	Total	C	N	O	S	0	0	0
			3194	2023	563	588	20			
1	C	418	Total	C	N	O	S	0	0	0
			3283	2071	580	611	21			
1	D	402	Total	C	N	O	S	0	0	0
			2938	1849	521	550	18			
1	E	408	Total	C	N	O	S	0	0	0
			3108	1969	544	575	20			
1	F	402	Total	C	N	O	S	0	0	0
			3059	1929	541	570	19			
1	G	409	Total	C	N	O	S	0	0	0
			3144	1988	551	585	20			
1	H	408	Total	C	N	O	S	0	0	0
			3076	1955	536	565	20			
1	I	409	Total	C	N	O	S	0	0	0
			3138	1983	551	585	19			
1	J	407	Total	C	N	O	S	0	0	0
			3074	1942	536	577	19			
1	K	409	Total	C	N	O	S	0	0	0
			3115	1966	546	583	20			
1	L	415	Total	C	N	O	S	0	0	0
			3196	2020	558	598	20			
1	M	229	Total	C	N	O		0	0	0
			1185	703	242	240				
1	N	369	Total	C	N	O	S	0	0	0
			2278	1416	407	443	12			
1	O	364	Total	C	N	O	S	0	0	0
			2145	1348	385	407	5			
1	P	339	Total	C	N	O	S	0	0	0
			1832	1096	367	361	8			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	I	1	Total O S 5 4 1	0	0
2	I	1	Total O S 5 4 1	0	0
2	I	1	Total O S 5 4 1	0	0
2	J	1	Total O S 5 4 1	0	0
2	J	1	Total O S 5 4 1	0	0
2	J	1	Total O S 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0

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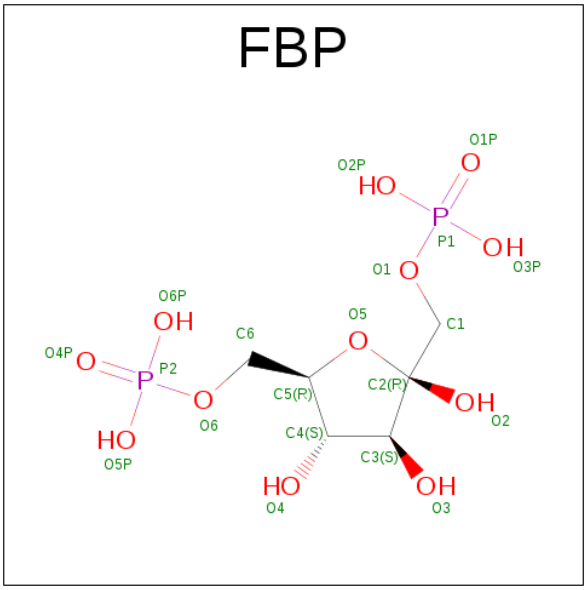
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	L	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0
2	P	1	Total O S 5 4 1	0	0
2	P	1	Total O S 5 4 1	0	0

- Molecule 3 is BETA-FRUCTOSE-1,6-DIPHOSPHATE (three-letter code: FBP) (formula: $C_6H_{14}O_{12}P_2$).



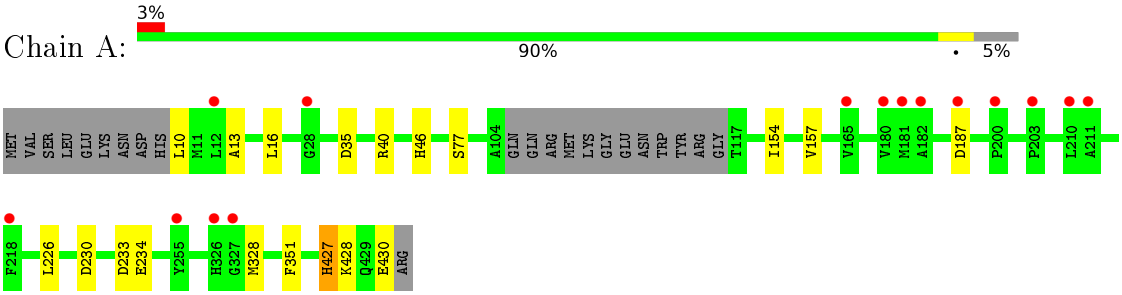
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O P 20 6 12 2	0	0
3	G	1	Total C O P 20 6 12 2	0	0
3	I	1	Total C O P 20 6 12 2	0	0
3	L	1	Total C O P 20 6 12 2	0	0

3 Residue-property plots (i)

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

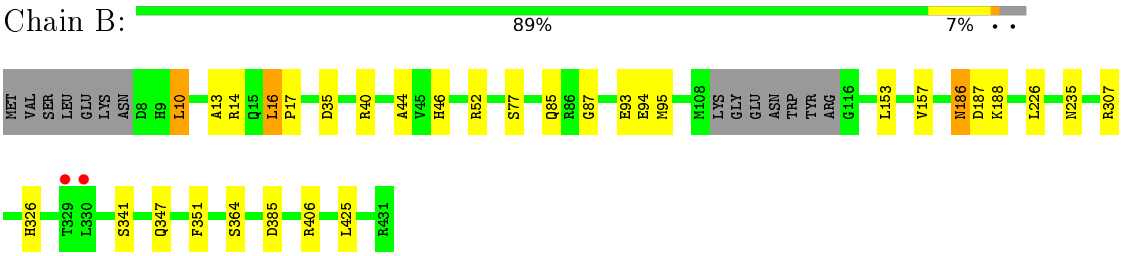
- Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain A:



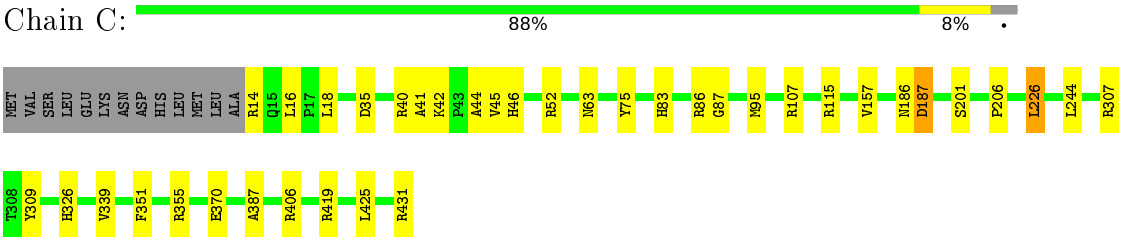
- Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain B:



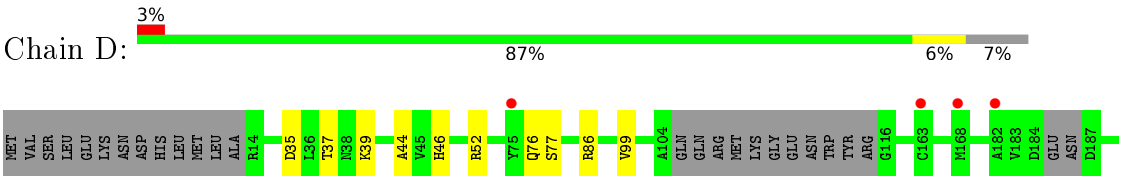
- Molecule 1: Glucose-1-phosphate adenylyltransferase

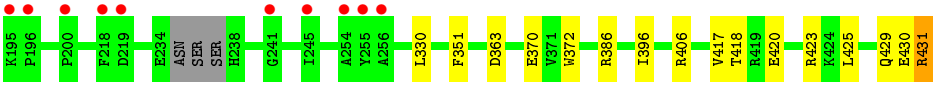
Chain C:



- Molecule 1: Glucose-1-phosphate adenylyltransferase

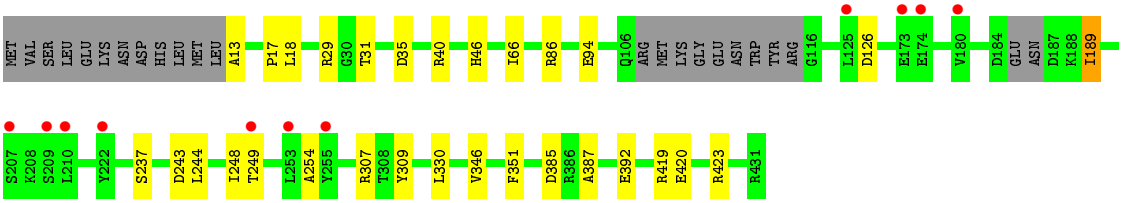
Chain D:





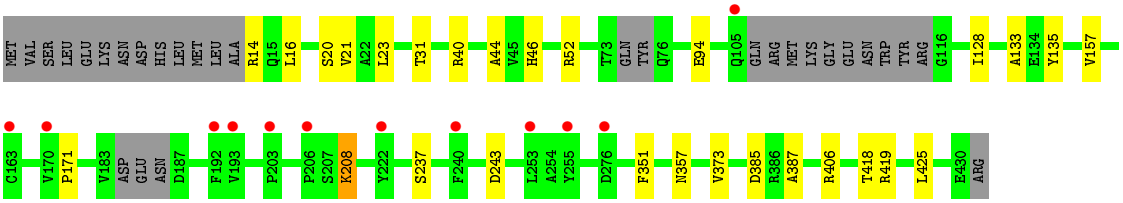
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain E:



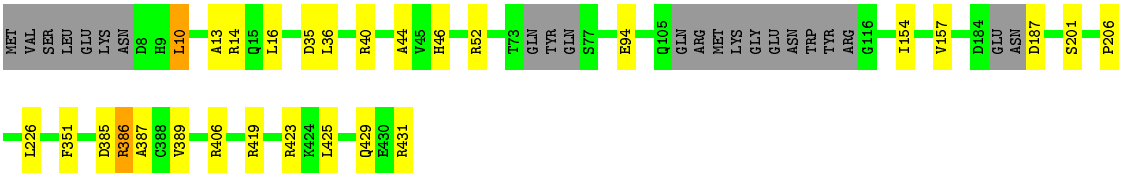
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain F:



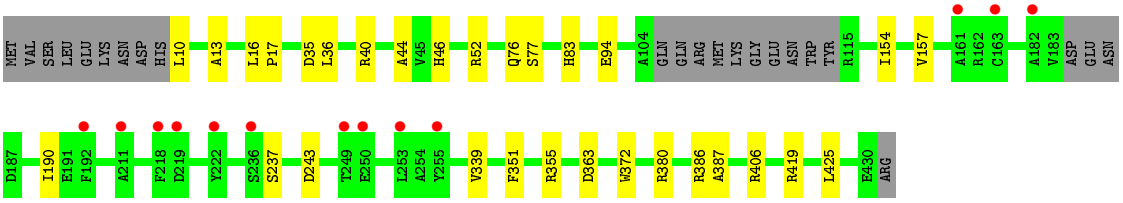
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain G:



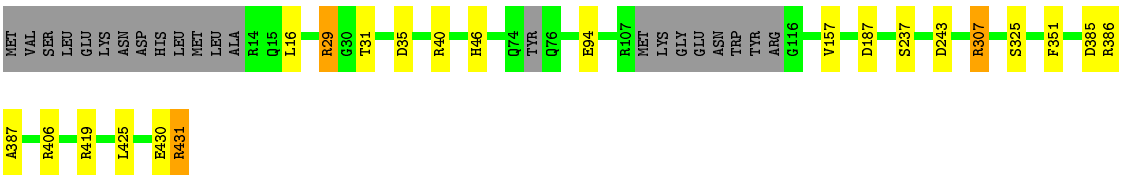
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain H:



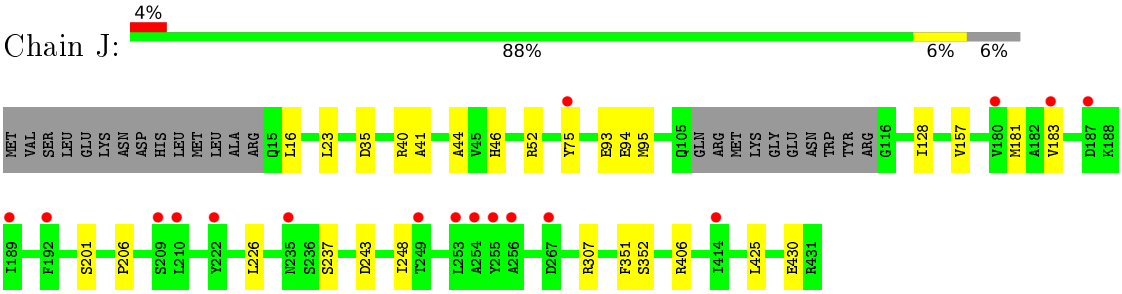
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain I:



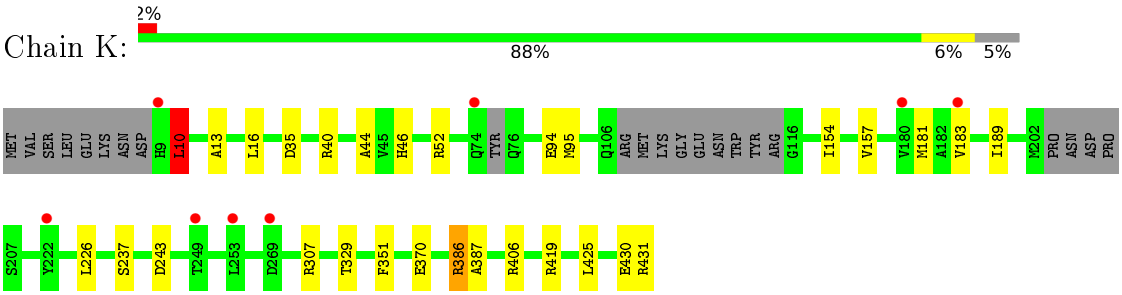
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain J:



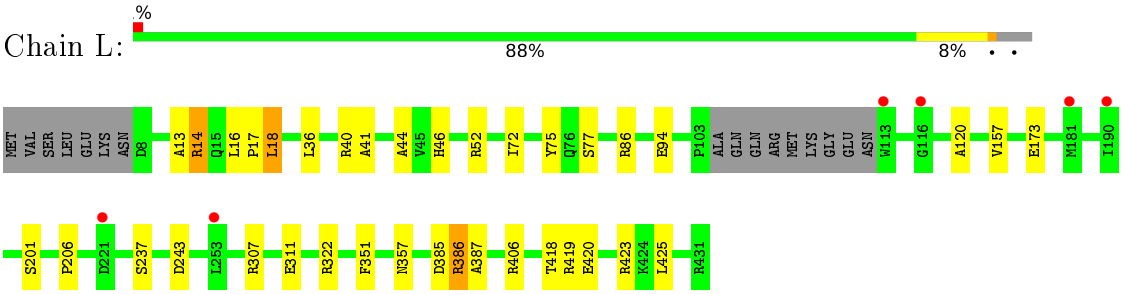
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain K:



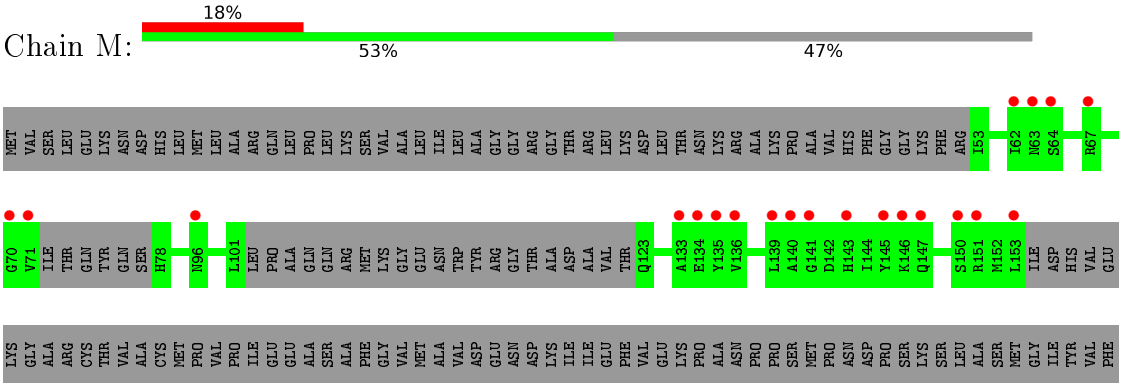
• Molecule 1: Glucose-1-phosphate adenylyltransferase

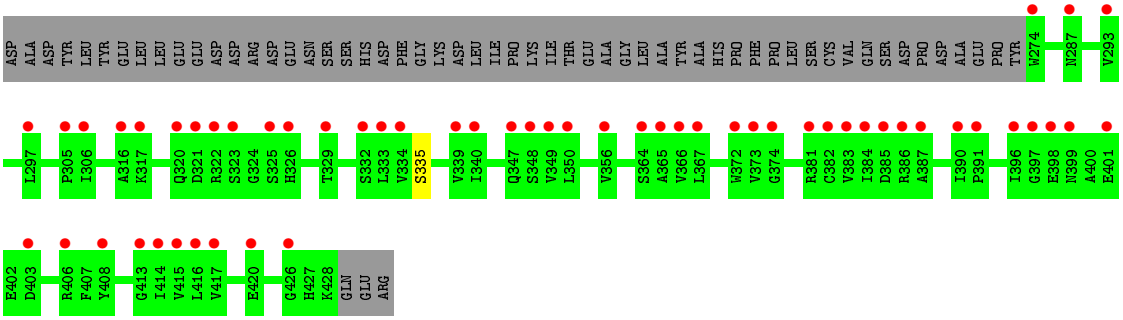
Chain L:



• Molecule 1: Glucose-1-phosphate adenylyltransferase

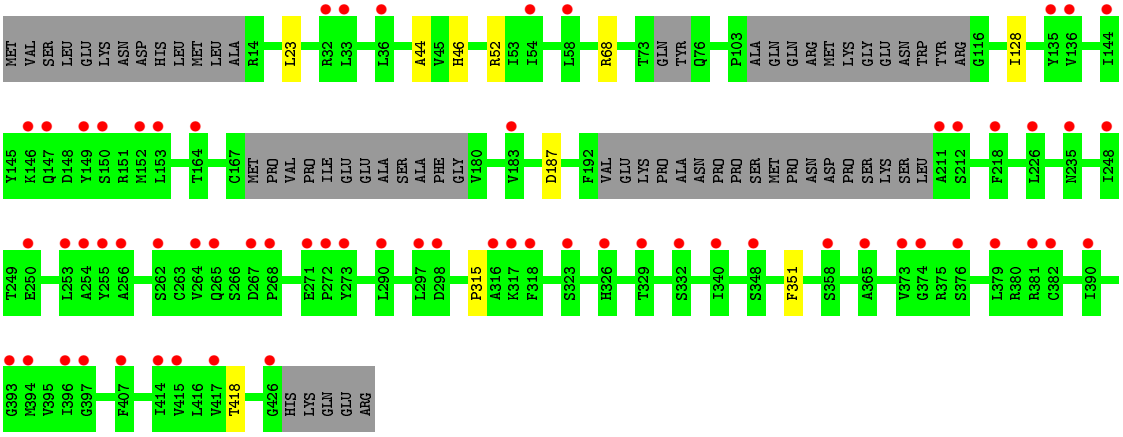
Chain M:





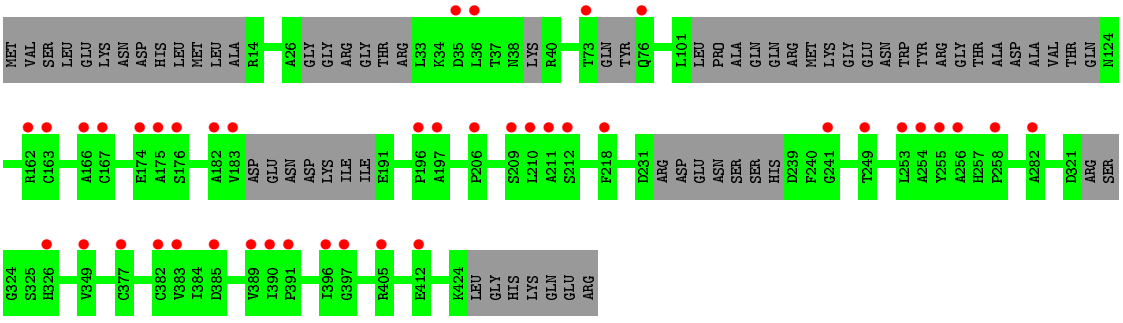
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain N:



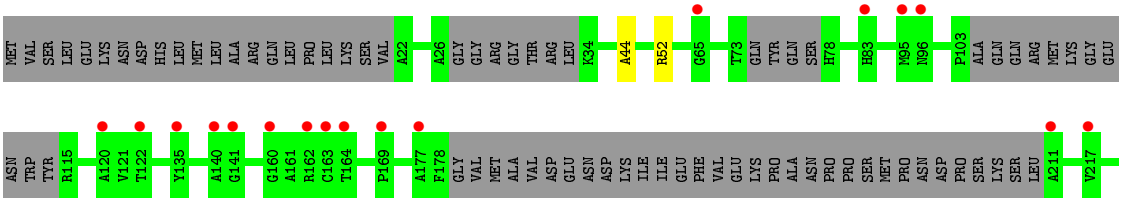
• Molecule 1: Glucose-1-phosphate adenylyltransferase

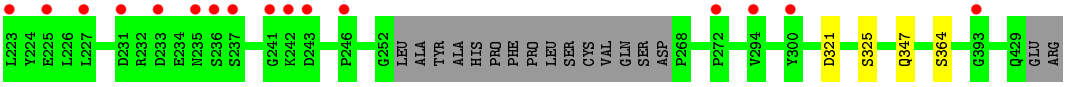
Chain O:



• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain P:




L223
Y224
E225
L226
L227
D231
R232
D233
E234
N235
S236
S237
G241
K242
D243
P246
G252
LEU
ALA
TYR
ALA
HIS
PRO
PHE
PRO
LEU
SER
CYS
VAL
GLN
SER
ASP
P268
P272
V294
Y300
D321
S325
Q347
S364
G393
Q429
GLU
ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	161.16Å 148.90Å 177.49Å 90.00° 113.10° 90.00°	Depositor
Resolution (Å)	70.75 – 3.04 70.75 – 3.04	Depositor EDS
% Data completeness (in resolution range)	98.7 (70.75-3.04) 98.6 (70.75-3.04)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 3.01Å)	Xtriage
Refinement program	PHENIX (dev_2219: ???)	Depositor
R, R_{free}	0.234 , 0.272 0.229 , 0.267	Depositor DCC
R_{free} test set	7261 reflections (4.97%)	DCC
Wilson B-factor (Å^2)	81.6	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 79.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	45056	wwPDB-VP
Average B, all atoms (Å^2)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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: FBP, SO4

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	0.24	0/3083	0.42	0/4212
1	B	0.24	0/3261	0.42	0/4428
1	C	0.25	0/3354	0.42	0/4546
1	D	0.25	0/2997	0.43	0/4083
1	E	0.25	0/3174	0.42	0/4311
1	F	0.24	0/3121	0.42	0/4240
1	G	0.25	0/3208	0.43	1/4353 (0.0%)
1	H	0.24	0/3142	0.42	0/4276
1	I	0.25	0/3203	0.43	0/4349
1	J	0.24	0/3140	0.42	0/4277
1	K	0.25	0/3176	0.44	1/4314 (0.0%)
1	L	0.25	0/3263	0.42	0/4431
1	M	0.23	0/1186	0.43	0/1642
1	N	0.24	0/2312	0.43	0/3186
1	O	0.25	0/2186	0.42	0/3030
1	P	0.24	0/1841	0.43	0/2542
All	All	0.24	0/45647	0.43	2/62220 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	10	LEU	CA-CB-CG	7.33	132.16	115.30
1	G	10	LEU	CA-CB-CG	5.11	127.05	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3016	0	2779	9	0
1	B	3194	0	3112	20	0
1	C	3283	0	3215	23	0
1	D	2938	0	2718	16	0
1	E	3108	0	2996	17	1
1	F	3059	0	2944	18	0
1	G	3144	0	3050	17	0
1	H	3076	0	2942	13	0
1	I	3138	0	3038	12	1
1	J	3074	0	2918	15	0
1	K	3115	0	2991	15	0
1	L	3196	0	3093	21	0
1	M	1185	0	606	1	0
1	N	2278	0	1714	4	0
1	O	2145	0	1418	0	0
1	P	1832	0	1096	3	0
2	A	15	0	0	1	0
2	B	15	0	0	1	0
2	C	15	0	0	1	0
2	D	20	0	0	1	0
2	E	15	0	0	3	0
2	F	10	0	0	3	0
2	G	15	0	0	1	0
2	H	20	0	0	0	0
2	I	15	0	0	2	0
2	J	15	0	0	2	0
2	K	15	0	0	2	0
2	L	15	0	0	2	0
2	P	10	0	0	0	0
3	C	20	0	10	0	0
3	G	20	0	10	1	0
3	I	20	0	10	0	0
3	L	20	0	10	1	0
All	All	45056	0	40670	186	1

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 2.

All (186) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:GLY:O	1:B:307:ARG:NH1	2.18	0.75
1:B:186:ASN:O	1:B:188:LYS:N	2.20	0.74
1:C:87:GLY:O	1:C:307:ARG:NH2	2.21	0.74
1:B:307:ARG:HB3	1:C:95:MET:HE3	1.70	0.73
1:G:36:LEU:O	1:G:40:ARG:NH1	2.21	0.73
1:E:40:ARG:NH1	2:E:501:SO4:S	2.64	0.71
1:B:16:LEU:HD12	1:B:153:LEU:HB3	1.74	0.69
1:B:40:ARG:NH2	1:B:385:ASP:OD1	2.26	0.69
1:G:13:ALA:HB2	1:G:154:ILE:HD11	1.73	0.69
1:E:40:ARG:NH1	2:E:501:SO4:O3	2.26	0.69
1:F:40:ARG:NH1	2:F:501:SO4:O4	2.26	0.69
1:L:36:LEU:O	1:L:40:ARG:NH1	2.27	0.66
1:F:40:ARG:NH1	2:F:501:SO4:S	2.69	0.66
1:D:370:GLU:O	1:D:431:ARG:NH2	2.28	0.66
1:J:95:MET:HE3	1:K:307:ARG:HB3	1.78	0.64
1:I:46:HIS:NE2	2:I:501:SO4:O4	2.30	0.63
1:B:40:ARG:NH1	2:B:503:SO4:O1	2.31	0.63
1:I:29:ARG:HG3	1:I:31:THR:HG23	1.81	0.62
1:E:13:ALA:O	1:E:17:PRO:HD2	2.00	0.62
1:E:40:ARG:NH1	2:E:501:SO4:O4	2.32	0.61
1:J:40:ARG:NH1	2:J:501:SO4:S	2.74	0.60
1:J:40:ARG:NH1	2:J:501:SO4:O3	2.35	0.60
1:G:40:ARG:NH2	1:G:385:ASP:OD1	2.34	0.60
1:L:13:ALA:O	1:L:17:PRO:HD2	2.03	0.59
1:F:14:ARG:HG3	1:G:14:ARG:HG3	1.86	0.58
1:C:406:ARG:HB3	1:C:425:LEU:HD21	1.86	0.58
1:L:44:ALA:O	1:L:52:ARG:NH1	2.35	0.58
1:F:21:VAL:HG23	1:F:133:ALA:HB2	1.85	0.57
1:I:16:LEU:HD21	1:I:157:VAL:HG21	1.86	0.57
1:E:17:PRO:HB3	1:E:66:ILE:HG12	1.86	0.57
1:G:16:LEU:HD21	1:G:157:VAL:HG21	1.87	0.57
1:J:16:LEU:HD21	1:J:157:VAL:HG21	1.87	0.57
1:B:85:GLN:NE2	1:D:99:VAL:O	2.39	0.56
1:H:387:ALA:O	1:H:419:ARG:NH1	2.38	0.56
1:E:420:GLU:OE2	1:E:423:ARG:NH2	2.39	0.55
1:H:406:ARG:HB3	1:H:425:LEU:HD21	1.89	0.55
1:I:387:ALA:O	1:I:419:ARG:NH1	2.38	0.55
1:E:189:ILE:HG13	1:E:254:ALA:HB3	1.89	0.55
1:H:13:ALA:HB2	1:H:154:ILE:HD11	1.89	0.55
1:F:406:ARG:HB3	1:F:425:LEU:HD21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:387:ALA:O	1:C:419:ARG:NH1	2.37	0.55
1:G:406:ARG:HB3	1:G:425:LEU:HD21	1.89	0.54
1:K:406:ARG:HB3	1:K:425:LEU:HD21	1.89	0.54
1:I:406:ARG:HB3	1:I:425:LEU:HD11	1.89	0.54
1:D:44:ALA:O	1:D:52:ARG:NH1	2.41	0.54
1:J:237:SER:OG	1:J:243:ASP:OD2	2.22	0.54
1:A:16:LEU:HD21	1:A:157:VAL:HG21	1.90	0.54
1:A:13:ALA:HB2	1:A:154:ILE:HD11	1.90	0.53
1:F:16:LEU:HD21	1:F:157:VAL:HG21	1.89	0.53
1:G:386:ARG:NH2	2:G:501:SO4:O1	2.41	0.53
1:K:13:ALA:HB2	1:K:154:ILE:HD11	1.90	0.53
1:E:189:ILE:HB	1:E:249:THR:HG23	1.91	0.53
1:F:237:SER:OG	1:F:243:ASP:OD2	2.20	0.53
1:G:387:ALA:O	1:G:419:ARG:NH1	2.39	0.52
1:D:430:GLU:HA	1:D:431:ARG:CB	2.39	0.52
1:D:39:LYS:HA	1:D:76:GLN:HG2	1.91	0.52
1:B:406:ARG:HB3	1:B:425:LEU:HD21	1.92	0.52
1:D:430:GLU:HA	1:D:431:ARG:HB3	1.92	0.52
1:L:406:ARG:HB3	1:L:425:LEU:HD21	1.91	0.51
1:B:235:ASN:HD21	1:G:423:ARG:HD2	1.74	0.51
1:H:13:ALA:O	1:H:17:PRO:HD2	2.10	0.51
1:H:36:LEU:O	1:H:40:ARG:NH1	2.43	0.51
1:J:23:LEU:HD21	1:J:128:ILE:HD13	1.92	0.51
1:K:44:ALA:O	1:K:52:ARG:NH1	2.38	0.51
1:K:237:SER:OG	1:K:243:ASP:OD2	2.26	0.51
1:I:237:SER:OG	1:I:243:ASP:OD2	2.24	0.51
1:J:406:ARG:HB3	1:J:425:LEU:HD21	1.92	0.50
1:I:40:ARG:NH1	2:I:501:SO4:S	2.84	0.50
1:F:23:LEU:HD21	1:F:128:ILE:HD13	1.93	0.50
1:J:44:ALA:O	1:J:52:ARG:NH1	2.44	0.50
1:K:16:LEU:HD21	1:K:157:VAL:HG21	1.94	0.50
1:L:387:ALA:O	1:L:419:ARG:NH2	2.43	0.50
1:B:95:MET:HE3	1:C:307:ARG:HB3	1.94	0.50
1:L:423:ARG:HE	3:L:504:FBP:H12	1.77	0.49
1:C:370:GLU:O	1:C:431:ARG:NH2	2.42	0.49
1:C:46:HIS:NE2	2:C:502:SO4:O1	2.42	0.49
1:J:93:GLU:HG2	1:L:86:ARG:NE	2.27	0.49
1:K:387:ALA:O	1:K:419:ARG:NH1	2.40	0.49
1:B:13:ALA:O	1:B:17:PRO:HD2	2.13	0.49
1:F:171:PRO:HA	1:F:208:LYS:HE2	1.94	0.49
1:D:372:TRP:HB2	1:D:431:ARG:HH12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:16:LEU:HD21	1:H:157:VAL:HG21	1.94	0.49
1:F:40:ARG:NH1	2:F:501:SO4:O2	2.46	0.48
1:I:431:ARG:OXT	1:I:431:ARG:HG3	2.13	0.48
1:I:46:HIS:HB3	1:I:351:PHE:CE2	2.49	0.48
1:G:419:ARG:NE	3:G:504:FBP:O4P	2.46	0.48
1:L:386:ARG:NH2	2:L:501:SO4:O4	2.46	0.48
1:B:44:ALA:O	1:B:52:ARG:NH1	2.45	0.48
1:P:44:ALA:O	1:P:52:ARG:NH1	2.45	0.48
1:D:418:THR:HG22	1:D:420:GLU:H	1.79	0.48
1:C:41:ALA:HB2	1:C:75:TYR:O	2.14	0.47
1:C:107:ARG:HB2	1:C:115:ARG:HD2	1.95	0.47
1:K:386:ARG:NH2	2:K:503:SO4:O4	2.48	0.47
1:E:40:ARG:NH2	1:E:385:ASP:OD1	2.47	0.47
1:G:44:ALA:O	1:G:52:ARG:NH1	2.40	0.47
1:E:126:ASP:OD1	1:E:126:ASP:N	2.48	0.47
1:H:237:SER:OG	1:H:243:ASP:OD2	2.23	0.47
1:D:406:ARG:HB3	1:D:425:LEU:HD21	1.95	0.47
1:I:307:ARG:NH1	1:L:94:GLU:OE2	2.47	0.47
1:N:23:LEU:HD21	1:N:128:ILE:HD13	1.97	0.47
1:E:237:SER:OG	1:E:243:ASP:OD2	2.23	0.47
1:H:44:ALA:O	1:H:52:ARG:NH1	2.45	0.47
1:B:16:LEU:HD11	1:B:157:VAL:HG21	1.96	0.46
1:L:41:ALA:HB2	1:L:75:TYR:O	2.16	0.46
1:L:16:LEU:HD21	1:L:157:VAL:HG21	1.98	0.46
1:G:201:SER:HB3	1:G:206:PRO:HA	1.97	0.46
1:A:46:HIS:HB3	1:A:351:PHE:CE2	2.51	0.45
1:E:387:ALA:O	1:E:419:ARG:NH1	2.43	0.45
1:B:93:GLU:HG2	1:D:86:ARG:NE	2.30	0.45
1:K:46:HIS:HB3	1:K:351:PHE:CE2	2.52	0.45
1:D:429:GLN:O	1:D:431:ARG:HB2	2.16	0.45
1:F:46:HIS:HB3	1:F:351:PHE:CE2	2.52	0.45
1:A:427:HIS:CD2	1:A:427:HIS:H	2.34	0.45
1:D:46:HIS:HB3	1:D:351:PHE:CE2	2.51	0.45
1:E:86:ARG:HB3	1:E:309:TYR:CD1	2.52	0.45
1:K:183:VAL:HG12	1:K:189:ILE:HA	1.98	0.45
1:F:44:ALA:O	1:F:52:ARG:NH1	2.44	0.45
1:L:46:HIS:HB3	1:L:351:PHE:CE2	2.52	0.45
1:A:233:ASP:HA	1:A:234:GLU:HA	1.64	0.45
1:B:10:LEU:HD22	1:B:10:LEU:H	1.82	0.45
1:F:387:ALA:O	1:F:419:ARG:HD3	2.16	0.44
1:L:201:SER:HB2	1:L:206:PRO:HA	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:ALA:O	1:C:52:ARG:NH1	2.48	0.44
1:D:396:ILE:HD13	1:D:417:VAL:HG21	1.99	0.44
1:G:389:VAL:H	1:G:429:GLN:HE21	1.65	0.44
1:H:46:HIS:HB3	1:H:351:PHE:CE2	2.52	0.44
1:K:370:GLU:O	1:K:431:ARG:NH1	2.45	0.44
1:L:40:ARG:NH2	1:L:385:ASP:OD1	2.51	0.44
1:D:386:ARG:NH1	2:D:503:SO4:O3	2.51	0.43
1:J:307:ARG:HB3	1:K:95:MET:HE3	2.00	0.43
1:B:14:ARG:NH2	1:C:63:ASN:O	2.51	0.43
1:G:46:HIS:HB3	1:G:351:PHE:CE2	2.53	0.43
1:I:430:GLU:O	1:I:431:ARG:HB3	2.17	0.43
1:F:40:ARG:NH2	1:F:385:ASP:OD1	2.51	0.43
1:B:95:MET:CE	1:C:307:ARG:HB3	2.49	0.43
1:C:186:ASN:O	1:C:187:ASP:HB2	2.18	0.43
1:F:20:SER:HA	1:F:135:TYR:O	2.19	0.43
1:N:46:HIS:HB3	1:N:351:PHE:CE2	2.53	0.43
1:C:42:LYS:HA	1:C:45:VAL:HG23	2.01	0.43
1:A:328:MET:SD	1:B:326:HIS:NE2	2.92	0.43
1:E:29:ARG:HG3	1:E:31:THR:HG23	2.01	0.43
1:L:418:THR:HG22	1:L:420:GLU:H	1.84	0.43
1:K:40:ARG:NE	2:K:503:SO4:O1	2.40	0.43
1:L:357:ASN:ND2	2:L:502:SO4:O4	2.52	0.43
1:A:40:ARG:NE	2:A:502:SO4:O3	2.51	0.42
1:P:321:ASP:OD2	1:P:325:SER:OG	2.37	0.42
1:I:40:ARG:NH2	1:I:385:ASP:OD1	2.52	0.42
1:C:201:SER:HB2	1:C:206:PRO:HA	2.01	0.42
1:B:46:HIS:HB3	1:B:351:PHE:CE2	2.55	0.42
1:C:16:LEU:HD21	1:C:157:VAL:HG21	2.01	0.42
1:F:14:ARG:HA	1:G:14:ARG:HG3	2.01	0.42
1:H:10:LEU:O	1:H:13:ALA:HB3	2.19	0.42
1:N:44:ALA:O	1:N:52:ARG:NH1	2.48	0.42
1:J:46:HIS:HB3	1:J:351:PHE:CE2	2.54	0.42
1:J:41:ALA:HB2	1:J:75:TYR:O	2.19	0.42
1:G:10:LEU:O	1:G:13:ALA:HB3	2.19	0.42
1:L:237:SER:OG	1:L:243:ASP:OD2	2.26	0.42
1:L:18:LEU:HA	1:L:18:LEU:HD13	1.90	0.42
1:L:14:ARG:NH1	1:L:18:LEU:HD21	2.35	0.42
1:C:326:HIS:CD2	1:D:330:LEU:HB2	2.55	0.42
1:H:339:VAL:HB	1:H:355:ARG:HD2	2.02	0.42
1:G:419:ARG:HH12	1:G:431:ARG:HD3	1.85	0.42
1:C:226:LEU:HD22	1:C:244:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:HIS:HB3	1:E:351:PHE:CE2	2.55	0.41
1:K:10:LEU:O	1:K:13:ALA:HB3	2.19	0.41
1:F:20:SER:HB3	1:F:135:TYR:HB2	2.02	0.41
1:E:330:LEU:HB3	1:E:346:VAL:HG22	2.02	0.41
1:A:428:LYS:HG3	1:A:430:GLU:H	1.85	0.41
1:B:347:GLN:O	1:B:364:SER:HA	2.21	0.41
1:C:86:ARG:HB3	1:C:309:TYR:CD1	2.54	0.41
1:J:201:SER:OG	1:J:206:PRO:HA	2.21	0.41
1:C:14:ARG:O	1:C:18:LEU:HD23	2.21	0.41
1:J:226:LEU:HD11	1:J:248:ILE:HG12	2.03	0.41
1:M:335:SER:HA	1:N:315:PRO:HB3	2.03	0.41
1:A:10:LEU:O	1:A:13:ALA:HB3	2.21	0.41
1:H:52:ARG:HD2	1:H:83:HIS:CG	2.56	0.41
1:J:307:ARG:NH1	1:K:94:GLU:OE1	2.54	0.41
1:F:357:ASN:ND2	1:F:373:VAL:O	2.47	0.40
1:L:72:ILE:HG21	1:L:120:ALA:HB1	2.03	0.40
1:C:52:ARG:HD2	1:C:83:HIS:CG	2.57	0.40
1:E:244:LEU:O	1:E:248:ILE:HG13	2.21	0.40
1:H:363:ASP:O	1:H:380:ARG:HA	2.21	0.40
1:P:347:GLN:O	1:P:364:SER:HA	2.20	0.40
1:C:339:VAL:HB	1:C:355:ARG:HD2	2.03	0.40
1:C:46:HIS:HB3	1:C:351:PHE:CE2	2.57	0.40
1:D:363:ASP:OD1	1:L:322:ARG:NH2	2.34	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:392:GLU:OE1	1:I:325:SER:OG[2_445]	2.19	0.01

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	405/431 (94%)	387 (96%)	17 (4%)	1 (0%)	52 87
1	B	413/431 (96%)	397 (96%)	15 (4%)	1 (0%)	52 87
1	C	416/431 (96%)	403 (97%)	13 (3%)	0	100 100
1	D	394/431 (91%)	381 (97%)	13 (3%)	0	100 100
1	E	402/431 (93%)	388 (96%)	14 (4%)	0	100 100
1	F	394/431 (91%)	383 (97%)	11 (3%)	0	100 100
1	G	401/431 (93%)	391 (98%)	10 (2%)	0	100 100
1	H	402/431 (93%)	387 (96%)	14 (4%)	1 (0%)	52 87
1	I	403/431 (94%)	390 (97%)	13 (3%)	0	100 100
1	J	403/431 (94%)	392 (97%)	11 (3%)	0	100 100
1	K	401/431 (93%)	388 (97%)	13 (3%)	0	100 100
1	L	411/431 (95%)	396 (96%)	15 (4%)	0	100 100
1	M	221/431 (51%)	216 (98%)	5 (2%)	0	100 100
1	N	359/431 (83%)	348 (97%)	10 (3%)	1 (0%)	46 82
1	O	348/431 (81%)	338 (97%)	10 (3%)	0	100 100
1	P	327/431 (76%)	318 (97%)	9 (3%)	0	100 100
All	All	6100/6896 (88%)	5903 (97%)	193 (3%)	4 (0%)	56 89

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	187	ASP
1	A	187	ASP
1	H	76	GLN
1	N	187	ASP

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	296/373 (79%)	291 (98%)	5 (2%)	68 90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	335/373 (90%)	327 (98%)	8 (2%)	57 86
1	C	352/373 (94%)	348 (99%)	4 (1%)	80 94
1	D	286/373 (77%)	281 (98%)	5 (2%)	68 90
1	E	322/373 (86%)	317 (98%)	5 (2%)	70 91
1	F	319/373 (86%)	315 (99%)	4 (1%)	76 93
1	G	331/373 (89%)	326 (98%)	5 (2%)	72 91
1	H	313/373 (84%)	307 (98%)	6 (2%)	65 89
1	I	330/373 (88%)	323 (98%)	7 (2%)	61 88
1	J	317/373 (85%)	311 (98%)	6 (2%)	65 89
1	K	324/373 (87%)	317 (98%)	7 (2%)	60 87
1	L	337/373 (90%)	330 (98%)	7 (2%)	61 88
1	M	19/373 (5%)	19 (100%)	0	100 100
1	N	150/373 (40%)	148 (99%)	2 (1%)	76 93
1	O	102/373 (27%)	102 (100%)	0	100 100
1	P	57/373 (15%)	57 (100%)	0	100 100
All	All	4190/5968 (70%)	4119 (98%)	71 (2%)	68 90

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
1	A	77	SER
1	A	226	LEU
1	A	230	ASP
1	A	427	HIS
1	B	10	LEU
1	B	16	LEU
1	B	35	ASP
1	B	77	SER
1	B	94	GLU
1	B	186	ASN
1	B	226	LEU
1	B	341	SER
1	C	35	ASP
1	C	40	ARG
1	C	187	ASP
1	C	226	LEU

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Mol	Chain	Res	Type
1	D	35	ASP
1	D	37	THR
1	D	77	SER
1	D	423	ARG
1	D	431	ARG
1	E	18	LEU
1	E	35	ASP
1	E	94	GLU
1	E	189	ILE
1	E	307	ARG
1	F	31	THR
1	F	94	GLU
1	F	208	LYS
1	F	418	THR
1	G	35	ASP
1	G	94	GLU
1	G	187	ASP
1	G	226	LEU
1	G	386	ARG
1	H	35	ASP
1	H	77	SER
1	H	94	GLU
1	H	190	ILE
1	H	372	TRP
1	H	386	ARG
1	I	29	ARG
1	I	35	ASP
1	I	94	GLU
1	I	187	ASP
1	I	307	ARG
1	I	386	ARG
1	I	431	ARG
1	J	35	ASP
1	J	94	GLU
1	J	181	MET
1	J	183	VAL
1	J	352	SER
1	J	430	GLU
1	K	10	LEU
1	K	35	ASP
1	K	181	MET
1	K	226	LEU

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Mol	Chain	Res	Type
1	K	329	THR
1	K	386	ARG
1	K	430	GLU
1	L	14	ARG
1	L	18	LEU
1	L	77	SER
1	L	173	GLU
1	L	307	ARG
1	L	311	GLU
1	L	386	ARG
1	N	68	ARG
1	N	418	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	78	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

43 ligands are modelled in this entry.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	501	-	4,4,4	0.25	0	6,6,6	0.09	0
2	SO4	A	502	-	4,4,4	0.28	0	6,6,6	0.08	0
2	SO4	A	503	-	4,4,4	0.25	0	6,6,6	0.09	0
2	SO4	B	501	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	B	502	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	B	503	-	4,4,4	0.26	0	6,6,6	0.09	0
2	SO4	C	501	-	4,4,4	0.26	0	6,6,6	0.05	0
2	SO4	C	502	-	4,4,4	0.27	0	6,6,6	0.09	0
2	SO4	C	503	-	4,4,4	0.26	0	6,6,6	0.07	0
3	FBP	C	504	-	18,20,20	0.60	0	22,32,32	0.65	0
2	SO4	D	501	-	4,4,4	0.27	0	6,6,6	0.14	0
2	SO4	D	502	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	D	503	-	4,4,4	0.26	0	6,6,6	0.06	0
2	SO4	D	504	-	4,4,4	0.26	0	6,6,6	0.08	0
2	SO4	E	501	-	4,4,4	0.26	0	6,6,6	0.10	0
2	SO4	E	502	-	4,4,4	0.26	0	6,6,6	0.10	0
2	SO4	E	503	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	F	501	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	F	502	-	4,4,4	0.26	0	6,6,6	0.09	0
2	SO4	G	501	-	4,4,4	0.26	0	6,6,6	0.08	0
2	SO4	G	502	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	G	503	-	4,4,4	0.27	0	6,6,6	0.09	0
3	FBP	G	504	-	18,20,20	0.46	0	22,32,32	0.60	0
2	SO4	H	501	-	4,4,4	0.25	0	6,6,6	0.06	0
2	SO4	H	502	-	4,4,4	0.28	0	6,6,6	0.07	0
2	SO4	H	503	-	4,4,4	0.25	0	6,6,6	0.06	0
2	SO4	H	504	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	I	501	-	4,4,4	0.27	0	6,6,6	0.08	0
2	SO4	I	502	-	4,4,4	0.27	0	6,6,6	0.05	0
2	SO4	I	503	-	4,4,4	0.25	0	6,6,6	0.10	0
3	FBP	I	504	-	18,20,20	0.47	0	22,32,32	0.61	0
2	SO4	J	501	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	J	502	-	4,4,4	0.26	0	6,6,6	0.06	0
2	SO4	J	503	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	K	501	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	K	502	-	4,4,4	0.27	0	6,6,6	0.08	0
2	SO4	K	503	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	L	501	-	4,4,4	0.25	0	6,6,6	0.06	0
2	SO4	L	502	-	4,4,4	0.27	0	6,6,6	0.09	0
2	SO4	L	503	-	4,4,4	0.25	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	FBP	L	504	-	18,20,20	0.61	0	22,32,32	0.71	0
2	SO4	P	501	-	4,4,4	0.25	0	6,6,6	0.06	0
2	SO4	P	502	-	4,4,4	0.25	0	6,6,6	0.09	0

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	SO4	A	501	-	-	0/0/0/0	0/0/0/0
2	SO4	A	502	-	-	0/0/0/0	0/0/0/0
2	SO4	A	503	-	-	0/0/0/0	0/0/0/0
2	SO4	B	501	-	-	0/0/0/0	0/0/0/0
2	SO4	B	502	-	-	0/0/0/0	0/0/0/0
2	SO4	B	503	-	-	0/0/0/0	0/0/0/0
2	SO4	C	501	-	-	0/0/0/0	0/0/0/0
2	SO4	C	502	-	-	0/0/0/0	0/0/0/0
2	SO4	C	503	-	-	0/0/0/0	0/0/0/0
3	FBP	C	504	-	-	0/13/32/32	0/1/1/1
2	SO4	D	501	-	-	0/0/0/0	0/0/0/0
2	SO4	D	502	-	-	0/0/0/0	0/0/0/0
2	SO4	D	503	-	-	0/0/0/0	0/0/0/0
2	SO4	D	504	-	-	0/0/0/0	0/0/0/0
2	SO4	E	501	-	-	0/0/0/0	0/0/0/0
2	SO4	E	502	-	-	0/0/0/0	0/0/0/0
2	SO4	E	503	-	-	0/0/0/0	0/0/0/0
2	SO4	F	501	-	-	0/0/0/0	0/0/0/0
2	SO4	F	502	-	-	0/0/0/0	0/0/0/0
2	SO4	G	501	-	-	0/0/0/0	0/0/0/0
2	SO4	G	502	-	-	0/0/0/0	0/0/0/0
2	SO4	G	503	-	-	0/0/0/0	0/0/0/0
3	FBP	G	504	-	-	0/13/32/32	0/1/1/1
2	SO4	H	501	-	-	0/0/0/0	0/0/0/0
2	SO4	H	502	-	-	0/0/0/0	0/0/0/0
2	SO4	H	503	-	-	0/0/0/0	0/0/0/0
2	SO4	H	504	-	-	0/0/0/0	0/0/0/0
2	SO4	I	501	-	-	0/0/0/0	0/0/0/0
2	SO4	I	502	-	-	0/0/0/0	0/0/0/0
2	SO4	I	503	-	-	0/0/0/0	0/0/0/0
3	FBP	I	504	-	-	0/13/32/32	0/1/1/1
2	SO4	J	501	-	-	0/0/0/0	0/0/0/0
2	SO4	J	502	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	J	503	-	-	0/0/0/0	0/0/0/0
2	SO4	K	501	-	-	0/0/0/0	0/0/0/0
2	SO4	K	502	-	-	0/0/0/0	0/0/0/0
2	SO4	K	503	-	-	0/0/0/0	0/0/0/0
2	SO4	L	501	-	-	0/0/0/0	0/0/0/0
2	SO4	L	502	-	-	0/0/0/0	0/0/0/0
2	SO4	L	503	-	-	0/0/0/0	0/0/0/0
3	FBP	L	504	-	-	0/13/32/32	0/1/1/1
2	SO4	P	501	-	-	0/0/0/0	0/0/0/0
2	SO4	P	502	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	SO4	1	0
2	B	503	SO4	1	0
2	C	502	SO4	1	0
2	D	503	SO4	1	0
2	E	501	SO4	3	0
2	F	501	SO4	3	0
2	G	501	SO4	1	0
3	G	504	FBP	1	0
2	I	501	SO4	2	0
2	J	501	SO4	2	0
2	K	503	SO4	2	0
2	L	501	SO4	1	0
2	L	502	SO4	1	0
3	L	504	FBP	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	409/431 (94%)	0.09	15 (3%) 45 19	59, 96, 145, 179	0
1	B	417/431 (96%)	-0.24	2 (0%) 91 77	44, 78, 119, 152	0
1	C	418/431 (96%)	-0.34	0 100 100	25, 53, 97, 129	0
1	D	402/431 (93%)	0.01	14 (3%) 48 21	24, 75, 160, 187	0
1	E	408/431 (94%)	0.07	11 (2%) 58 28	39, 90, 166, 193	0
1	F	402/431 (93%)	0.08	12 (2%) 54 25	44, 84, 155, 187	0
1	G	409/431 (94%)	-0.23	0 100 100	35, 69, 113, 136	0
1	H	408/431 (94%)	0.05	13 (3%) 51 23	31, 84, 148, 180	0
1	I	409/431 (94%)	-0.20	0 100 100	36, 68, 113, 154	0
1	J	407/431 (94%)	0.14	17 (4%) 40 17	41, 88, 156, 179	0
1	K	409/431 (94%)	-0.07	8 (1%) 68 39	32, 78, 130, 170	0
1	L	415/431 (96%)	-0.17	6 (1%) 78 51	30, 67, 124, 168	0
1	M	229/431 (53%)	1.58	77 (33%) 0 0	120, 197, 256, 270	0
1	N	369/431 (85%)	0.82	65 (17%) 2 1	85, 153, 207, 239	0
1	O	364/431 (84%)	0.50	42 (11%) 6 2	70, 147, 196, 211	0
1	P	339/431 (78%)	0.47	33 (9%) 10 4	67, 141, 202, 244	0
All	All	6214/6896 (90%)	0.11	315 (5%) 32 13	24, 89, 186, 270	0

All (315) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	383	VAL	8.6
1	P	237	SER	7.4
1	M	366	VAL	7.3
1	M	416	LEU	7.0
1	M	391	PRO	6.5

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Mol	Chain	Res	Type	RSRZ
1	M	145	TYR	6.4
1	O	253	LEU	6.3
1	N	254	ALA	6.2
1	M	382	CYS	6.1
1	M	143	HIS	6.0
1	N	255	TYR	6.0
1	P	141	GLY	5.9
1	M	398	GLU	5.9
1	N	390	ILE	5.8
1	N	316	ALA	5.7
1	J	255	TYR	5.7
1	M	414	ILE	5.7
1	M	415	VAL	5.7
1	O	391	PRO	5.6
1	M	374	GLY	5.6
1	N	297	LEU	5.5
1	M	399	ASN	5.4
1	N	382	CYS	5.3
1	O	390	ILE	5.2
1	M	329	THR	5.1
1	E	209	SER	5.1
1	O	35	ASP	5.0
1	N	153	LEU	5.0
1	O	211	ALA	4.9
1	O	167	CYS	4.8
1	N	272	PRO	4.8
1	M	332	SER	4.8
1	M	384	ILE	4.7
1	J	253	LEU	4.7
1	J	254	ALA	4.6
1	N	144	ILE	4.6
1	M	340	ILE	4.6
1	N	256	ALA	4.6
1	O	196	PRO	4.5
1	O	182	ALA	4.5
1	P	163	CYS	4.4
1	M	365	ALA	4.4
1	J	267	ASP	4.4
1	M	420	GLU	4.4
1	N	147	GLN	4.4
1	M	151	ARG	4.3
1	N	374	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	M	153	LEU	4.3
1	J	256	ALA	4.2
1	N	393	GLY	4.2
1	M	305	PRO	4.2
1	M	134	GLU	4.2
1	M	297	LEU	4.2
1	P	140	ALA	4.1
1	M	293	VAL	4.0
1	O	163	CYS	4.0
1	M	390	ILE	4.0
1	N	183	VAL	4.0
1	M	385	ASP	3.9
1	N	381	ARG	3.9
1	M	316	ALA	3.8
1	O	206	PRO	3.8
1	M	96	ASN	3.8
1	M	320	GLN	3.8
1	D	219	ASP	3.7
1	A	181	MET	3.7
1	O	256	ALA	3.7
1	A	211	ALA	3.7
1	N	414	ILE	3.7
1	H	163	CYS	3.7
1	N	394	MET	3.7
1	N	373	VAL	3.7
1	P	272	PRO	3.7
1	P	65	GLY	3.7
1	M	133	ALA	3.6
1	O	254	ALA	3.6
1	M	333	LEU	3.6
1	N	348	SER	3.6
1	M	397	GLY	3.6
1	J	249	THR	3.6
1	N	152	MET	3.5
1	N	267	ASP	3.5
1	N	318	PHE	3.5
1	O	383	VAL	3.5
1	D	256	ALA	3.5
1	O	197	ALA	3.5
1	M	146	LYS	3.5
1	M	323	SER	3.5
1	N	136	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	M	386	ARG	3.5
1	N	397	GLY	3.5
1	M	147	GLN	3.4
1	O	209	SER	3.4
1	P	160	GLY	3.4
1	M	140	ALA	3.4
1	N	248	ILE	3.4
1	N	396	ILE	3.4
1	E	180	VAL	3.4
1	O	212	SER	3.4
1	M	348	SER	3.4
1	P	241	GLY	3.3
1	N	150	SER	3.3
1	N	135	TYR	3.3
1	A	210	LEU	3.3
1	N	226	LEU	3.3
1	A	326	HIS	3.3
1	N	340	ILE	3.3
1	M	334	VAL	3.3
1	M	150	SER	3.3
1	M	326	HIS	3.3
1	O	282	ALA	3.3
1	M	136	VAL	3.3
1	O	174	GLU	3.3
1	N	250	GLU	3.3
1	M	350	LEU	3.3
1	O	218	PHE	3.3
1	J	209	SER	3.2
1	M	367	LEU	3.2
1	O	349	VAL	3.2
1	O	183	VAL	3.2
1	P	169	PRO	3.2
1	M	287	ASN	3.2
1	K	74	GLN	3.2
1	M	408	TYR	3.2
1	O	176	SER	3.2
1	N	218	PHE	3.2
1	N	271	GLU	3.1
1	M	306	ILE	3.1
1	E	173	GLU	3.1
1	N	298	ASP	3.1
1	N	253	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	K	222	TYR	3.0
1	M	339	VAL	3.0
1	M	67	ARG	3.0
1	M	325	SER	3.0
1	D	254	ALA	3.0
1	P	120	ALA	3.0
1	P	217	VAL	3.0
1	E	255	TYR	2.9
1	M	349	VAL	2.9
1	O	258	PRO	2.9
1	M	322	ARG	2.9
1	N	329	THR	2.9
1	P	135	TYR	2.9
1	K	9	HIS	2.9
1	P	96	ASN	2.9
1	M	372	TRP	2.9
1	O	166	ALA	2.8
1	P	243	ASP	2.8
1	H	249	THR	2.8
1	E	253	LEU	2.8
1	F	253	LEU	2.8
1	P	177	ALA	2.8
1	M	403	ASP	2.8
1	N	211	ALA	2.8
1	N	417	VAL	2.8
1	M	63	ASN	2.8
1	N	317	LYS	2.8
1	P	242	LYS	2.8
1	M	64	SER	2.8
1	O	382	CYS	2.8
1	P	227	LEU	2.7
1	P	235	ASN	2.7
1	H	161	ALA	2.7
1	L	190	ILE	2.7
1	P	236	SER	2.7
1	F	163	CYS	2.7
1	D	241	GLY	2.7
1	N	262	SER	2.7
1	P	294	VAL	2.7
1	M	317	LYS	2.7
1	D	196	PRO	2.7
1	D	163	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	28	GLY	2.6
1	D	200	PRO	2.6
1	N	32	ARG	2.6
1	O	210	LEU	2.6
1	M	373	VAL	2.6
1	N	235	ASN	2.6
1	M	426	GLY	2.6
1	M	396	ILE	2.6
1	F	240	PHE	2.6
1	H	192	PHE	2.6
1	H	222	TYR	2.6
1	J	183	VAL	2.6
1	P	83	HIS	2.6
1	N	33	LEU	2.6
1	N	379	LEU	2.6
1	N	407	PHE	2.6
1	F	105	GLN	2.6
1	L	116	GLY	2.6
1	P	95	MET	2.6
1	J	235	ASN	2.6
1	O	405	ARG	2.5
1	O	396	ILE	2.5
1	A	165	VAL	2.5
1	P	164	THR	2.5
1	J	192	PHE	2.5
1	M	274	TRP	2.5
1	M	401	GLU	2.5
1	N	358	SER	2.5
1	F	192	PHE	2.5
1	A	203	PRO	2.5
1	D	255	TYR	2.5
1	J	210	LEU	2.5
1	D	245	ILE	2.5
1	O	397	GLY	2.5
1	D	218	PHE	2.4
1	N	265	GLN	2.4
1	N	149	TYR	2.4
1	M	413	GLY	2.4
1	N	415	VAL	2.4
1	O	326	HIS	2.4
1	M	347	GLN	2.4
1	K	183	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	O	73	THR	2.4
1	H	211	ALA	2.4
1	O	162	ARG	2.4
1	L	221	ASP	2.4
1	K	253	LEU	2.4
1	N	332	SER	2.4
1	O	377	CYS	2.4
1	O	249	THR	2.4
1	J	189	ILE	2.4
1	A	180	VAL	2.4
1	F	203	PRO	2.4
1	O	255	TYR	2.4
1	N	36	LEU	2.4
1	O	241	GLY	2.3
1	H	182	ALA	2.3
1	K	249	THR	2.3
1	J	187	ASP	2.3
1	A	12	LEU	2.3
1	A	182	ALA	2.3
1	M	70	GLY	2.3
1	P	246	PRO	2.3
1	N	268	PRO	2.3
1	P	223	LEU	2.3
1	F	206	PRO	2.3
1	M	141	GLY	2.3
1	B	330	LEU	2.3
1	M	139	LEU	2.3
1	P	231	ASP	2.3
1	A	255	TYR	2.3
1	O	385	ASP	2.3
1	E	125	LEU	2.3
1	F	222	TYR	2.3
1	M	71	VAL	2.3
1	N	146	LYS	2.3
1	N	290	LEU	2.3
1	O	389	VAL	2.3
1	A	327	GLY	2.2
1	E	249	THR	2.2
1	H	253	LEU	2.2
1	J	222	TYR	2.2
1	N	264	VAL	2.2
1	P	300	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	276	ASP	2.2
1	N	212	SER	2.2
1	O	36	LEU	2.2
1	B	329	THR	2.2
1	M	356	VAL	2.2
1	F	255	TYR	2.2
1	E	222	TYR	2.2
1	H	255	TYR	2.2
1	P	393	GLY	2.2
1	N	58	LEU	2.2
1	E	210	LEU	2.2
1	N	323	SER	2.2
1	O	412	GLU	2.2
1	P	225	GLU	2.2
1	M	364	SER	2.2
1	N	365	ALA	2.2
1	H	250	GLU	2.2
1	N	376	SER	2.2
1	N	426	GLY	2.2
1	D	182	ALA	2.2
1	M	135	TYR	2.2
1	M	387	ALA	2.2
1	L	253	LEU	2.2
1	O	175	ALA	2.2
1	J	180	VAL	2.2
1	A	218	PHE	2.1
1	D	168	MET	2.1
1	J	414	ILE	2.1
1	M	417	VAL	2.1
1	F	193	VAL	2.1
1	L	181	MET	2.1
1	O	76	GLN	2.1
1	J	75	TYR	2.1
1	H	218	PHE	2.1
1	P	211	ALA	2.1
1	A	187	ASP	2.1
1	D	75	TYR	2.1
1	E	207	SER	2.1
1	N	54	ILE	2.1
1	F	170	VAL	2.1
1	K	269	ASP	2.1
1	M	62	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	N	164	THR	2.1
1	A	200	PRO	2.1
1	K	180	VAL	2.1
1	P	162	ARG	2.1
1	H	236	SER	2.1
1	L	113	TRP	2.1
1	N	326	HIS	2.1
1	P	122	THR	2.1
1	D	195	LYS	2.0
1	P	233	ASP	2.0
1	M	381	ARG	2.0
1	M	321	ASP	2.0
1	M	406	ARG	2.0
1	E	174	GLU	2.0
1	H	219	ASP	2.0
1	N	273	TYR	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	FBP	G	504	20/20	0.83	0.33	1.75	72,152,203,206	0
3	FBP	L	504	20/20	0.82	0.32	1.57	81,139,188,189	0
3	FBP	C	504	20/20	0.89	0.23	0.51	67,122,166,185	0
2	SO4	C	502	5/5	0.98	0.23	0.49	61,62,68,76	0
2	SO4	A	502	5/5	0.97	0.20	0.40	77,81,104,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	A	503	5/5	0.89	0.27	0.38	95,124,132,170	0
3	FBP	I	504	20/20	0.78	0.25	0.34	79,138,171,209	0
2	SO4	K	503	5/5	0.91	0.19	0.02	73,89,109,110	0
2	SO4	I	502	5/5	0.94	0.18	-0.30	69,80,89,98	0
2	SO4	B	503	5/5	0.96	0.19	-0.50	69,81,88,100	0
2	SO4	H	502	5/5	0.99	0.15	-0.68	42,46,49,52	0
2	SO4	L	503	5/5	0.95	0.15	-0.82	77,79,96,100	0
2	SO4	E	503	5/5	0.94	0.14	-0.83	96,97,118,122	0
2	SO4	L	501	5/5	0.99	0.18	-0.98	55,63,82,97	0
2	SO4	G	502	5/5	0.96	0.10	-1.02	79,79,104,106	0
2	SO4	E	502	5/5	0.98	0.12	-1.11	43,62,69,82	0
2	SO4	D	501	5/5	0.99	0.14	-1.17	33,41,44,47	0
2	SO4	I	501	5/5	0.97	0.22	-1.20	58,62,89,97	0
2	SO4	I	503	5/5	0.93	0.15	-1.22	66,66,117,120	0
2	SO4	B	502	5/5	0.94	0.12	-1.42	75,97,117,126	0
2	SO4	D	503	5/5	0.97	0.15	-1.43	60,80,95,96	0
2	SO4	C	501	5/5	0.97	0.14	-1.62	53,73,81,108	0
2	SO4	P	502	5/5	0.86	0.20	-1.66	79,82,137,151	0
2	SO4	C	503	5/5	0.98	0.15	-1.66	47,52,61,80	0
2	SO4	J	502	5/5	0.97	0.08	-1.76	67,71,96,129	0
2	SO4	G	503	5/5	0.97	0.12	-1.78	48,60,70,89	0
2	SO4	D	502	5/5	0.95	0.11	-1.84	83,105,110,111	0
2	SO4	B	501	5/5	0.95	0.08	-1.87	102,128,135,146	0
2	SO4	L	502	5/5	0.99	0.15	-2.04	37,40,48,54	0
2	SO4	K	501	5/5	0.93	0.09	-2.07	112,117,131,144	0
2	SO4	K	502	5/5	0.97	0.11	-2.27	62,73,85,93	0
2	SO4	H	501	5/5	0.94	0.12	-2.36	74,95,102,105	0
2	SO4	F	502	5/5	0.95	0.11	-2.45	67,68,94,100	0
2	SO4	J	501	5/5	0.98	0.12	-2.45	70,73,88,90	0
2	SO4	H	504	5/5	0.98	0.14	-2.84	60,61,81,113	0
2	SO4	P	501	5/5	0.95	0.09	-2.85	66,92,123,145	0
2	SO4	F	501	5/5	0.94	0.16	-2.86	77,78,105,111	0
2	SO4	E	501	5/5	0.97	0.14	-3.28	71,72,88,120	0
2	SO4	A	501	5/5	0.93	0.13	-3.41	92,101,111,132	0
2	SO4	G	501	5/5	0.99	0.10	-11.32	57,72,80,85	0
2	SO4	H	503	5/5	0.97	0.17	-	70,72,87,98	0
2	SO4	J	503	5/5	0.79	0.18	-	117,132,142,157	0
2	SO4	D	504	5/5	0.91	0.25	-	77,84,97,116	0

6.5 Other polymers (i)

There are no such residues in this entry.