wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 06:31 PM GMT

PDB ID	:	4LNI
Title	:	B. subtilis glutamine synthetase structures reveal large active site conformational changes and basis for isoenzyme specific regulation: structure of the transition state complex
Authors	:	Schumacher, M.A.; Chinnam, N.; Tonthat, N.; Fisher, S.; Wray, L.
Deposited on	:	2013-07-11
Resolution	:	2.58 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

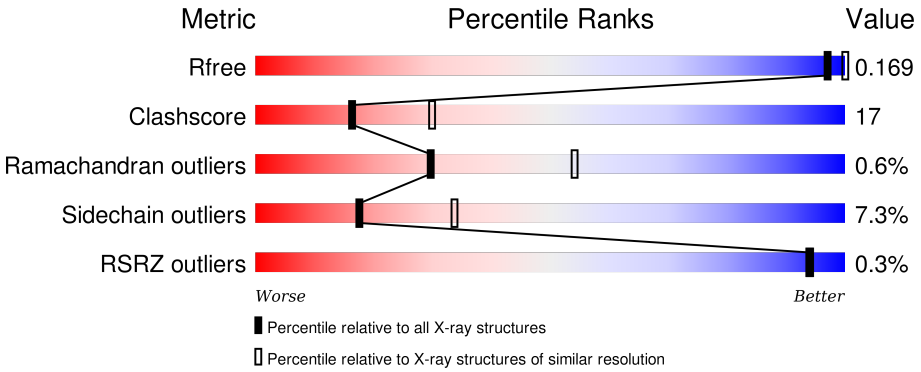
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.58 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	2636 (2.60-2.56)
Clashscore	102246	3003 (2.60-2.56)
Ramachandran outliers	100387	2956 (2.60-2.56)
Sidechain outliers	100360	2956 (2.60-2.56)
RSRZ outliers	91569	2642 (2.60-2.56)

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	443	67% 28% 5%
1	B	443	67% 27% 6%
1	C	443	68% 27%
1	D	443	65% 29% 5%
1	E	443	68% 27% 5%

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Mol	Chain	Length	Quality of chain
1	F	443	63% 33%
1	G	443	% 65% 31%
1	H	443	67% 27%
1	I	443	67% 28% 5%
1	J	443	67% 28%
1	K	443	70% 26%
1	L	443	67% 27% 6%

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	P3S	A	501	-	-	-	X
2	P3S	D	501	-	-	X	X
2	P3S	F	601	-	-	X	X
2	P3S	G	601	-	-	X	-
2	P3S	K	501	-	-	-	X
4	MG	A	503	-	-	-	X
4	MG	B	503	-	-	-	X
4	MG	B	504	-	-	-	X
4	MG	C	503	-	-	-	X
4	MG	C	505	-	-	-	X
4	MG	D	503	-	-	-	X
4	MG	D	505	-	-	-	X
4	MG	E	503	-	-	-	X
4	MG	H	603	-	-	-	X
4	MG	I	503	-	-	-	X
4	MG	K	503	-	-	-	X
4	MG	L	503	-	-	-	X

2 Entry composition (i)

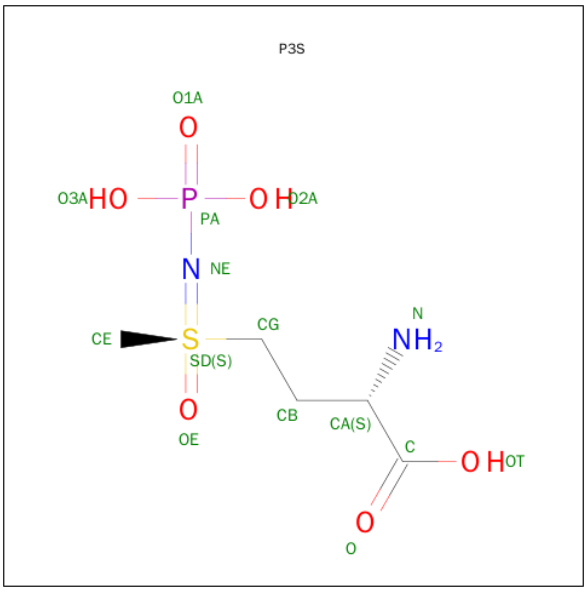
There are 5 unique types of molecules in this entry. The entry contains 86960 atoms, of which 41847 are hydrogens and 0 are deuteriums.

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 Glutamine synthetase.

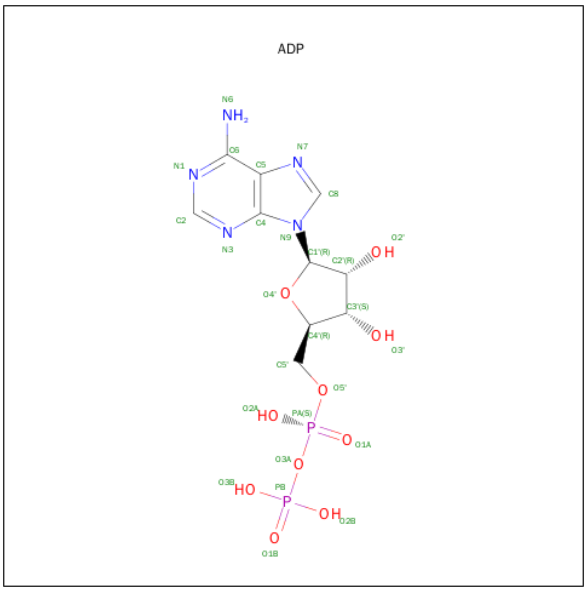
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	443	Total	C	H	N	O	S	0	0	0
			7012	2259	3477	590	670	16			
1	B	443	Total	C	H	N	O	S	0	0	0
			7012	2259	3477	590	670	16			
1	C	443	Total	C	H	N	O	S	0	0	0
			7012	2259	3477	590	670	16			
1	D	443	Total	C	H	N	O	S	0	0	0
			7012	2259	3477	590	670	16			
1	E	443	Total	C	H	N	O	S	0	0	0
			7012	2259	3477	590	670	16			
1	F	443	Total	C	H	N	O	S	0	0	0
			7012	2259	3477	590	670	16			
1	G	443	Total	C	H	N	O	S	0	0	0
			7009	2259	3474	590	670	16			
1	H	443	Total	C	H	N	O	S	0	0	0
			7012	2259	3477	590	670	16			
1	I	443	Total	C	H	N	O	S	0	0	0
			7012	2259	3477	590	670	16			
1	J	441	Total	C	H	N	O	S	0	0	0
			6980	2250	3459	587	668	16			
1	K	443	Total	C	H	N	O	S	0	0	0
			7012	2259	3477	590	670	16			
1	L	443	Total	C	H	N	O	S	0	0	0
			7012	2259	3477	590	670	16			

- Molecule 2 is L-METHIONINE-S-SULFOXIMINE PHOSPHATE (three-letter code: P3S) (formula: $C_5H_{13}N_2O_6PS$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	B	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	C	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	D	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	E	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	F	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	G	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	H	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	I	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	J	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	K	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	L	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	3	Total Mg 3 3	0	0
4	J	3	Total Mg 3 3	0	0
4	D	3	Total Mg 3 3	0	0
4	K	3	Total Mg 3 3	0	0
4	E	3	Total Mg 3 3	0	0
4	H	3	Total Mg 3 3	0	0
4	B	3	Total Mg 3 3	0	0
4	I	3	Total Mg 3 3	0	0
4	C	3	Total Mg 3 3	0	0
4	A	3	Total Mg 3 3	0	0
4	L	3	Total Mg 3 3	0	0
4	F	3	Total Mg 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	177	Total O 177 177	0	0
5	B	178	Total O 178 178	0	0
5	C	183	Total O 183 183	0	0
5	D	200	Total O 200 200	0	0
5	E	168	Total O 168 168	0	0
5	F	166	Total O 166 166	0	0
5	G	184	Total O 184 184	0	0
5	H	174	Total O 174 174	0	0

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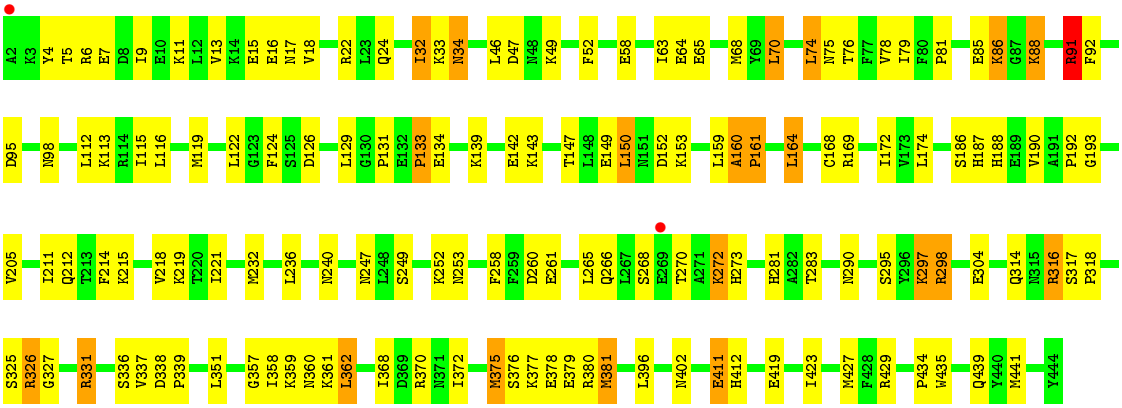
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	189	Total O 189 189	0	0
5	J	194	Total O 194 194	0	0
5	K	191	Total O 191 191	0	0
5	L	163	Total O 163 163	0	0

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.

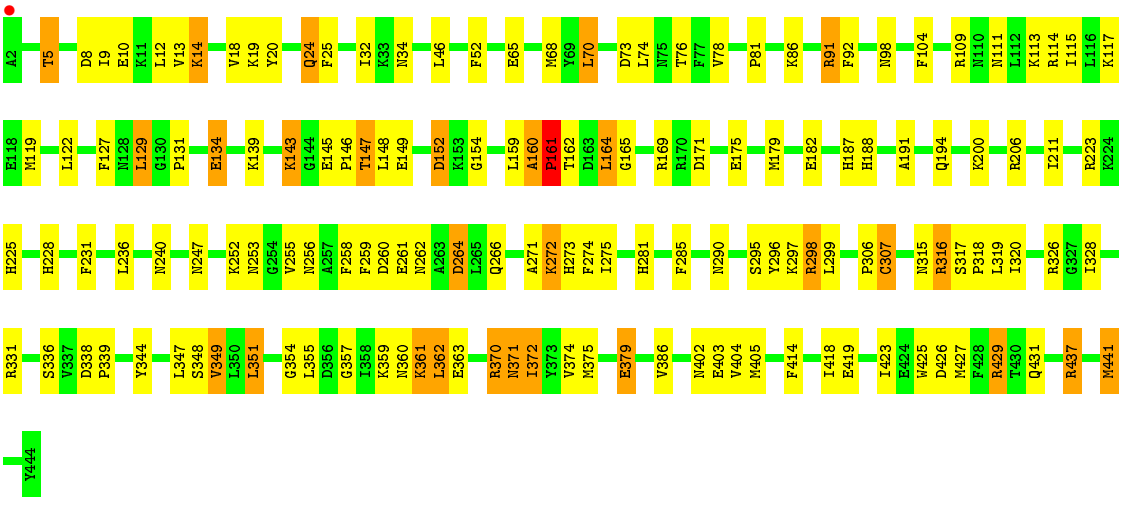
- Molecule 1: Glutamine synthetase

Chain A:



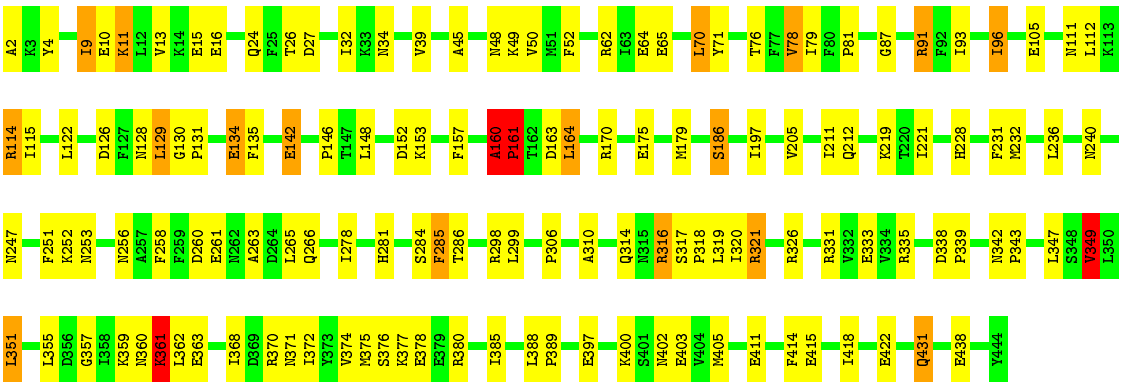
- Molecule 1: Glutamine synthetase

Chain B:



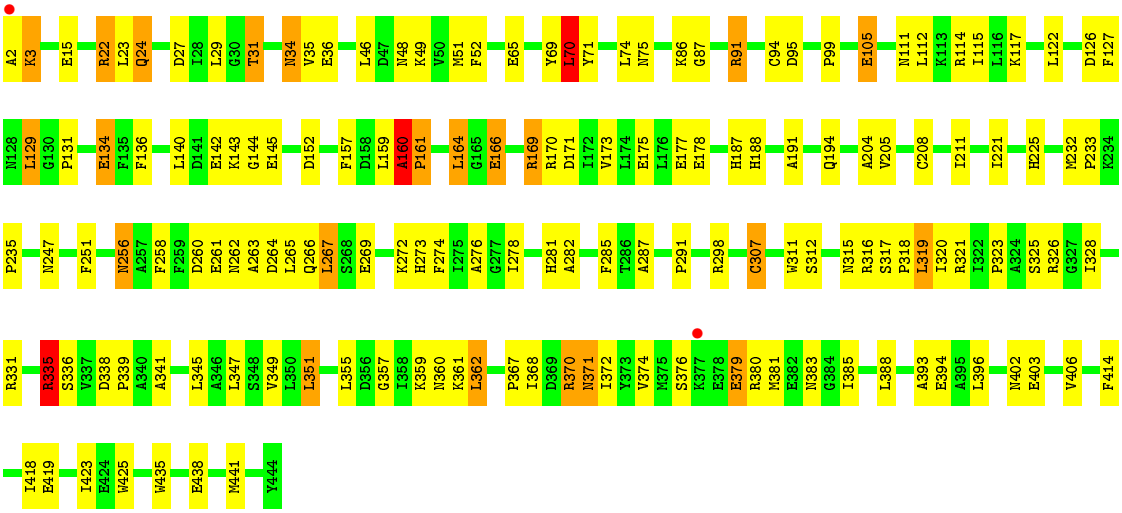
- Molecule 1: Glutamine synthetase

Chain C:



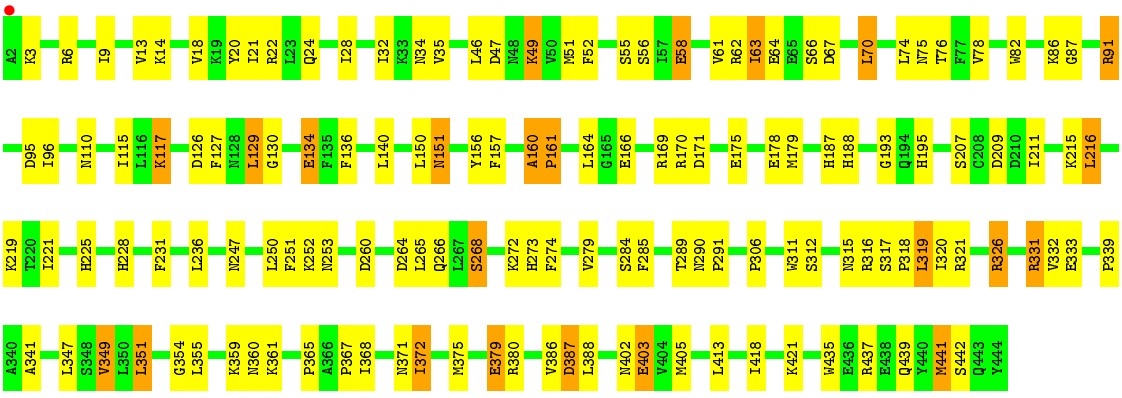
• Molecule 1: Glutamine synthetase

Chain D:



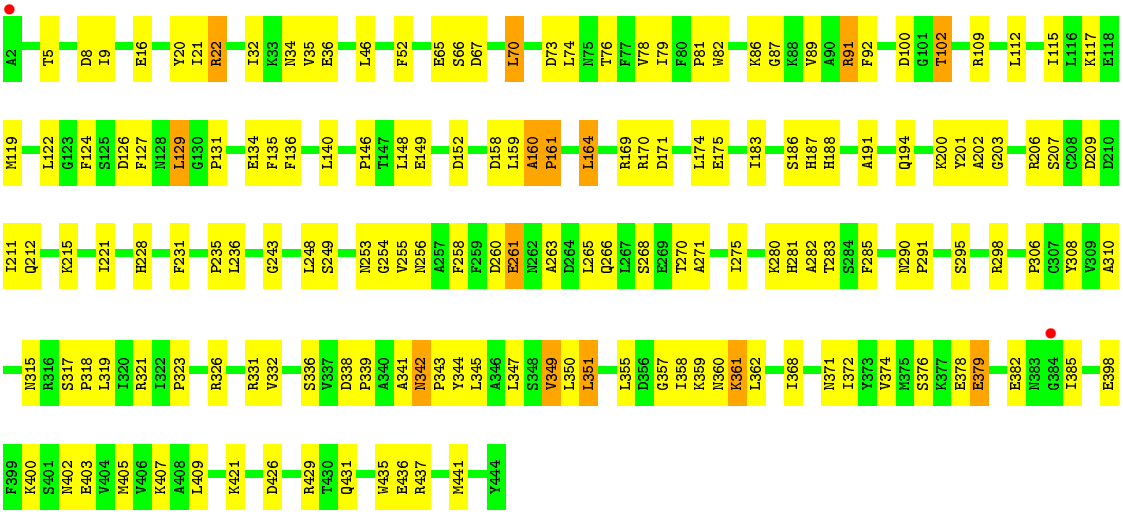
• Molecule 1: Glutamine synthetase

Chain E:



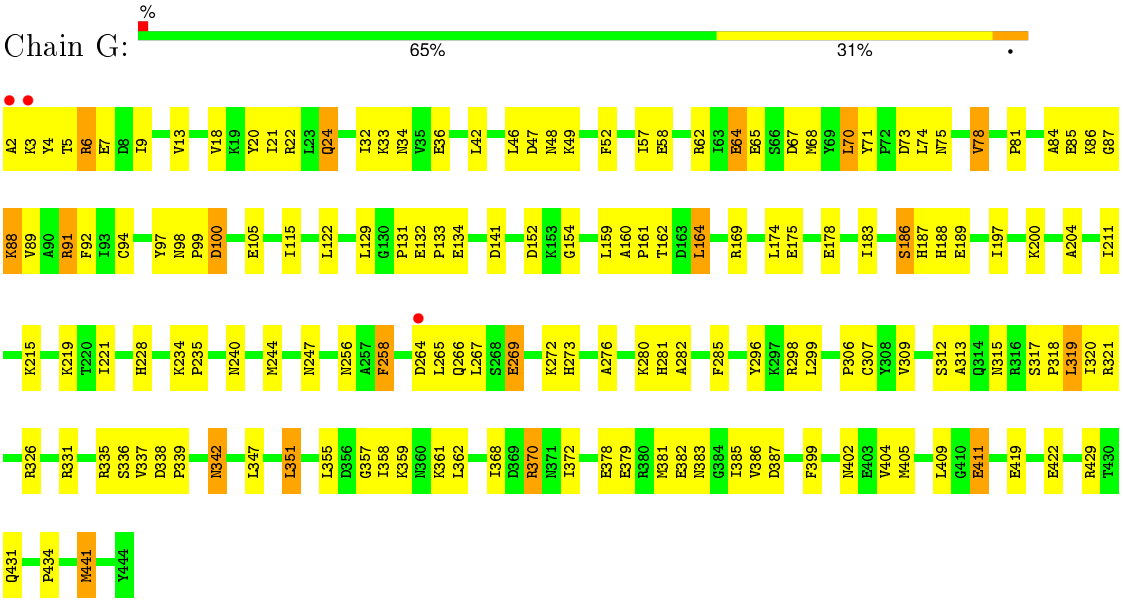
• Molecule 1: Glutamine synthetase

Chain F:



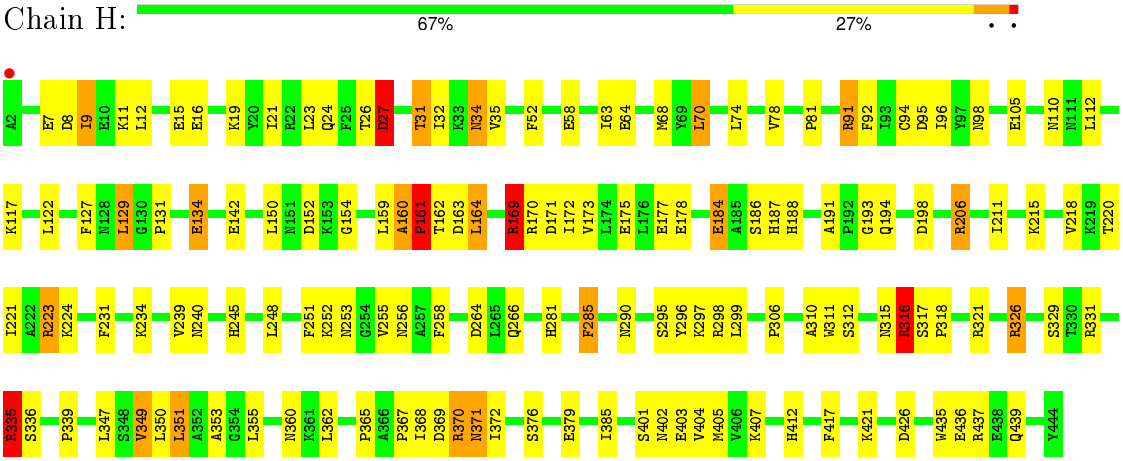
• Molecule 1: Glutamine synthetase

Chain G:



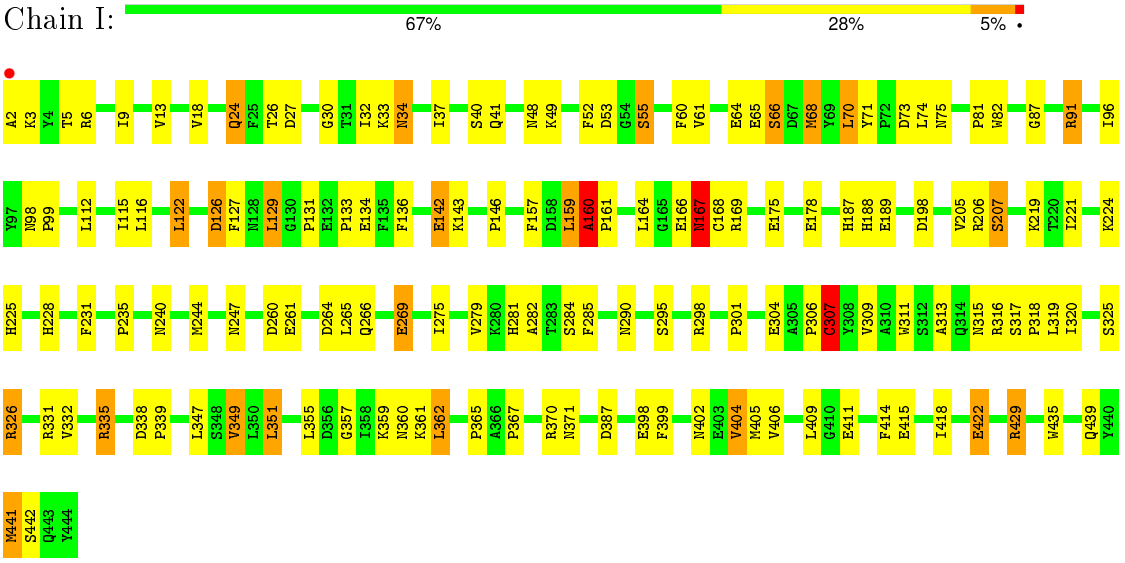
• Molecule 1: Glutamine synthetase

Chain H:



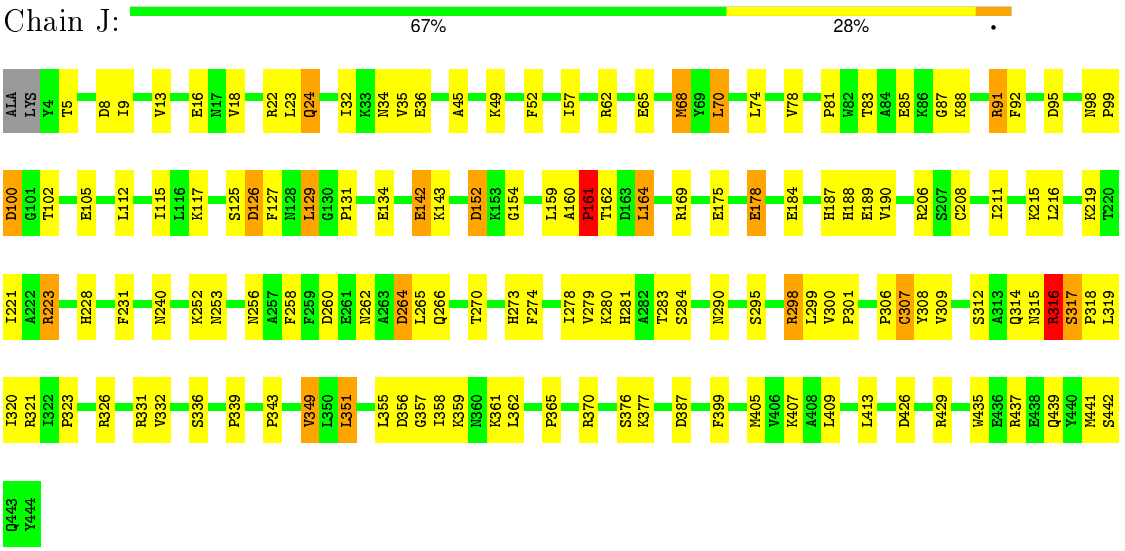
• Molecule 1: Glutamine synthetase

Chain I:



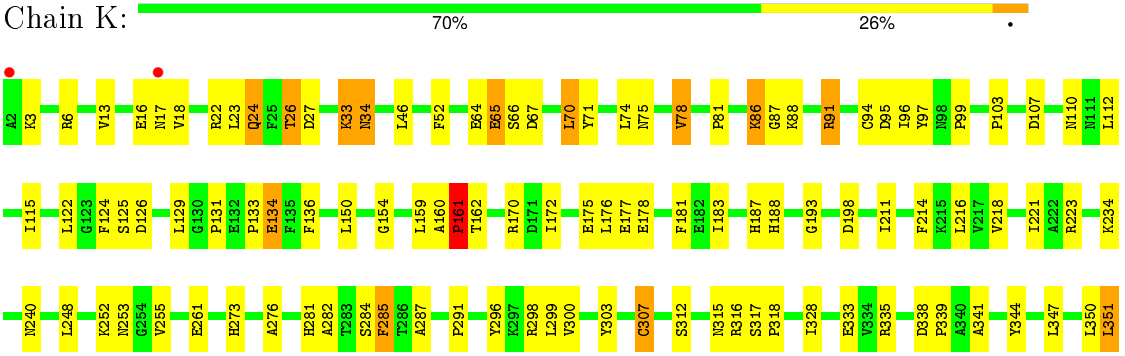
• Molecule 1: Glutamine synthetase

Chain J:



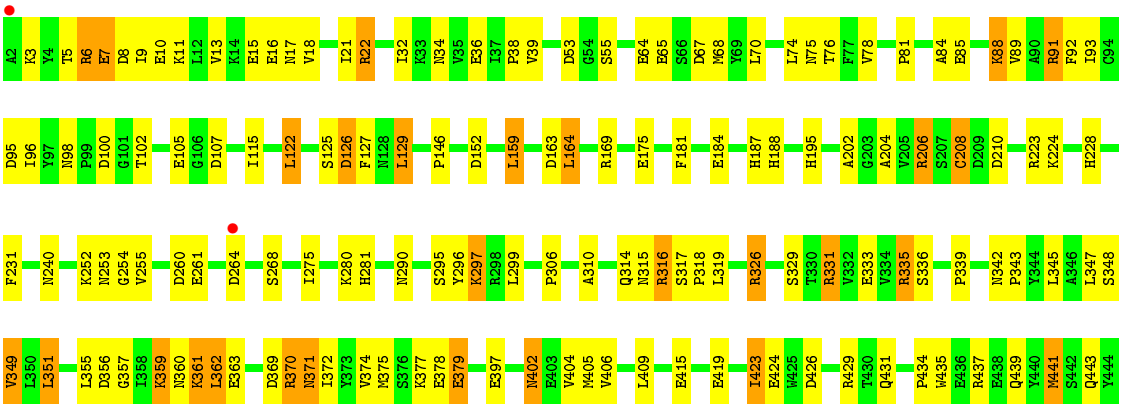
• Molecule 1: Glutamine synthetase

Chain K:



- Molecule 1: Glutamine synthetase

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	110.20Å 141.60Å 142.10Å 60.29° 67.38° 76.20°	Depositor
Resolution (Å)	117.10 – 2.58 117.10 – 2.58	Depositor EDS
% Data completeness (in resolution range)	90.8 (117.10-2.58) 77.8 (117.10-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.14 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.165 , 0.223 0.166 , 0.169	Depositor DCC
R_{free} test set	21985 reflections (12.59%)	DCC
Wilson B-factor (Å^2)	19.1	Xtriage
Anisotropy	1.014	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 45.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 196659 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	86960	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.84% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: P3S, 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	0.96	0/3618	0.95	6/4895 (0.1%)
1	B	0.98	3/3618 (0.1%)	0.97	10/4895 (0.2%)
1	C	0.98	4/3618 (0.1%)	1.02	10/4895 (0.2%)
1	D	0.97	4/3618 (0.1%)	0.96	9/4895 (0.2%)
1	E	0.97	3/3618 (0.1%)	1.03	14/4895 (0.3%)
1	F	0.95	1/3618 (0.0%)	0.96	5/4895 (0.1%)
1	G	0.95	3/3618 (0.1%)	0.92	6/4895 (0.1%)
1	H	0.97	2/3618 (0.1%)	0.99	9/4895 (0.2%)
1	I	0.96	2/3618 (0.1%)	0.99	11/4895 (0.2%)
1	J	0.98	6/3604 (0.2%)	1.01	10/4877 (0.2%)
1	K	1.01	2/3618 (0.1%)	1.00	8/4895 (0.2%)
1	L	0.96	2/3618 (0.1%)	0.89	2/4895 (0.0%)
All	All	0.97	32/43402 (0.1%)	0.98	100/58722 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	2
1	D	0	1
1	E	0	1
1	F	0	1
1	H	0	1
1	I	0	1
All	All	0	9

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	161	PRO	N-CD	7.91	1.58	1.47
1	D	166	GLU	CG-CD	7.69	1.63	1.51
1	C	134	GLU	CG-CD	7.57	1.63	1.51
1	I	307	CYS	CB-SG	-6.89	1.70	1.82
1	J	105	GLU	CG-CD	6.76	1.62	1.51

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	160	ALA	C-N-CD	-26.90	61.42	120.60
1	K	160	ALA	C-N-CD	-23.72	68.41	120.60
1	C	160	ALA	C-N-CD	-22.46	71.20	120.60
1	H	160	ALA	C-N-CD	-22.29	71.56	120.60
1	J	160	ALA	C-N-CD	-22.20	71.76	120.60

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	ALA	Peptide
1	B	160	ALA	Peptide
1	C	160	ALA	Mainchain,Peptide
1	D	160	ALA	Peptide
1	E	160	ALA	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	3535	3477	3466	118	0
1	B	3535	3477	3466	113	0
1	C	3535	3477	3466	114	0
1	D	3535	3477	3466	128	0
1	E	3535	3477	3466	117	0
1	F	3535	3477	3466	140	0
1	G	3535	3474	3466	141	0
1	H	3535	3477	3466	126	0
1	I	3535	3477	3466	129	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	3521	3459	3448	115	0
1	K	3535	3477	3466	111	0
1	L	3535	3477	3466	129	0
2	A	15	12	10	4	0
2	B	15	12	10	1	0
2	C	15	12	10	4	0
2	D	15	12	10	6	0
2	E	15	12	10	1	0
2	F	15	12	10	6	0
2	G	15	12	10	8	0
2	H	15	12	10	5	0
2	I	15	12	10	2	0
2	J	15	12	10	3	0
2	K	15	12	10	2	0
2	L	15	12	10	1	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	0	0
3	E	27	0	12	1	0
3	F	27	0	12	1	0
3	G	27	0	12	0	0
3	H	27	0	12	0	0
3	I	27	0	12	0	0
3	J	27	0	12	0	0
3	K	27	0	12	0	0
3	L	27	0	12	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
4	E	3	0	0	0	0
4	F	3	0	0	0	0
4	G	3	0	0	0	0
4	H	3	0	0	0	0
4	I	3	0	0	0	0
4	J	3	0	0	0	0
4	K	3	0	0	0	0
4	L	3	0	0	0	0
5	A	177	0	0	11	0
5	B	178	0	0	14	0
5	C	183	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	200	0	0	13	0
5	E	168	0	0	11	0
5	F	166	0	0	15	0
5	G	184	0	0	19	0
5	H	174	0	0	17	0
5	I	189	0	0	16	0
5	J	194	0	0	20	0
5	K	191	0	0	19	0
5	L	163	0	0	11	0
All	All	45113	41847	41838	1414	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 17.

The worst 5 of 1414 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)
2:H:601:P3S:SD	2:H:601:P3S:CE	2.01	1.48
2:G:601:P3S:CE	2:G:601:P3S:SD	2.01	1.46
2:F:601:P3S:CE	2:F:601:P3S:SD	2.02	1.45
2:D:501:P3S:CE	2:D:501:P3S:SD	2.03	1.43
1:I:357:GLY:HA2	1:I:362:LEU:CD1	1.64	1.27

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	441/443 (100%)	407 (92%)	32 (7%)	2 (0%)	34	58
1	B	441/443 (100%)	417 (95%)	22 (5%)	2 (0%)	34	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	441/443 (100%)	414 (94%)	22 (5%)	5 (1%)	17	35
1	D	441/443 (100%)	407 (92%)	31 (7%)	3 (1%)	26	49
1	E	441/443 (100%)	417 (95%)	21 (5%)	3 (1%)	26	49
1	F	441/443 (100%)	410 (93%)	28 (6%)	3 (1%)	26	49
1	G	441/443 (100%)	403 (91%)	34 (8%)	4 (1%)	21	41
1	H	441/443 (100%)	420 (95%)	20 (4%)	1 (0%)	52	75
1	I	441/443 (100%)	414 (94%)	24 (5%)	3 (1%)	26	49
1	J	439/443 (99%)	413 (94%)	23 (5%)	3 (1%)	26	49
1	K	441/443 (100%)	416 (94%)	23 (5%)	2 (0%)	34	58
1	L	441/443 (100%)	416 (94%)	24 (5%)	1 (0%)	52	75
All	All	5290/5316 (100%)	4954 (94%)	304 (6%)	32 (1%)	30	54

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	PRO
1	B	161	PRO
1	C	161	PRO
1	C	361	LYS
1	D	161	PRO

5.3.2 Protein sidechains

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	382/382 (100%)	353 (92%)	29 (8%)	16	31
1	B	382/382 (100%)	354 (93%)	28 (7%)	17	34
1	C	382/382 (100%)	358 (94%)	24 (6%)	22	43
1	D	382/382 (100%)	358 (94%)	24 (6%)	22	43
1	E	382/382 (100%)	357 (94%)	25 (6%)	21	40
1	F	382/382 (100%)	363 (95%)	19 (5%)	30	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	382/382 (100%)	354 (93%)	28 (7%)	17 34
1	H	382/382 (100%)	350 (92%)	32 (8%)	14 25
1	I	382/382 (100%)	349 (91%)	33 (9%)	13 24
1	J	381/382 (100%)	349 (92%)	32 (8%)	14 25
1	K	382/382 (100%)	359 (94%)	23 (6%)	24 45
1	L	382/382 (100%)	346 (91%)	36 (9%)	11 20
All	All	4583/4584 (100%)	4250 (93%)	333 (7%)	17 34

5 of 333 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	24	GLN
1	H	91	ARG
1	L	126	ASP
1	G	78	VAL
1	G	307	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 148 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	240	ASN
1	G	342	ASN
1	L	167	ASN
1	F	253	ASN
1	G	167	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 60 ligands modelled in this entry, 36 are monoatomic - leaving 24 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	P3S	A	501	4	10,14,14	5.07	4 (40%)	6,21,21	8.69	3 (50%)
3	ADP	A	502	4	22,29,29	0.98	1 (4%)	27,45,45	2.50	6 (22%)
2	P3S	B	501	4	10,14,14	5.36	3 (30%)	6,21,21	7.44	3 (50%)
3	ADP	B	502	4	22,29,29	0.95	1 (4%)	27,45,45	2.74	10 (37%)
2	P3S	C	501	4	10,14,14	5.57	4 (40%)	6,21,21	12.17	3 (50%)
3	ADP	C	502	4	22,29,29	0.94	1 (4%)	27,45,45	3.08	7 (25%)
2	P3S	D	501	4	10,14,14	5.12	5 (50%)	6,21,21	11.24	3 (50%)
3	ADP	D	502	4	22,29,29	1.01	1 (4%)	27,45,45	2.68	8 (29%)
2	P3S	E	501	4	10,14,14	5.58	4 (40%)	6,21,21	7.84	4 (66%)
3	ADP	E	502	4	22,29,29	0.98	2 (9%)	27,45,45	3.48	7 (25%)
2	P3S	F	601	4	10,14,14	4.72	5 (50%)	6,21,21	11.05	4 (66%)
3	ADP	F	602	4	22,29,29	1.07	2 (9%)	27,45,45	3.07	9 (33%)
2	P3S	G	601	4	10,14,14	5.49	4 (40%)	6,21,21	9.00	3 (50%)
3	ADP	G	602	4	22,29,29	1.02	1 (4%)	27,45,45	2.32	10 (37%)
2	P3S	H	601	4	10,14,14	5.30	6 (60%)	6,21,21	7.92	3 (50%)
3	ADP	H	602	4	22,29,29	1.06	1 (4%)	27,45,45	2.60	5 (18%)
2	P3S	I	501	4	10,14,14	4.76	4 (40%)	6,21,21	6.32	3 (50%)
3	ADP	I	502	4	22,29,29	1.17	3 (13%)	27,45,45	2.51	8 (29%)
2	P3S	J	501	4	10,14,14	4.75	3 (30%)	6,21,21	8.56	3 (50%)
3	ADP	J	502	4	22,29,29	0.88	1 (4%)	27,45,45	2.36	5 (18%)
2	P3S	K	501	4	10,14,14	5.02	3 (30%)	6,21,21	7.23	3 (50%)
3	ADP	K	502	4	22,29,29	0.96	1 (4%)	27,45,45	3.17	8 (29%)
2	P3S	L	501	4	10,14,14	5.26	4 (40%)	6,21,21	9.26	3 (50%)
3	ADP	L	502	4	22,29,29	1.20	2 (9%)	27,45,45	2.35	8 (29%)

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	P3S	A	501	4	-	0/5/16/16	0/0/0/0
3	ADP	A	502	4	-	0/12/32/32	0/3/3/3
2	P3S	B	501	4	-	0/5/16/16	0/0/0/0
3	ADP	B	502	4	-	0/12/32/32	0/3/3/3
2	P3S	C	501	4	-	0/5/16/16	0/0/0/0
3	ADP	C	502	4	-	0/12/32/32	0/3/3/3
2	P3S	D	501	4	-	0/5/16/16	0/0/0/0
3	ADP	D	502	4	-	0/12/32/32	0/3/3/3
2	P3S	E	501	4	-	0/5/16/16	0/0/0/0
3	ADP	E	502	4	-	0/12/32/32	0/3/3/3
2	P3S	F	601	4	-	0/5/16/16	0/0/0/0
3	ADP	F	602	4	-	0/12/32/32	0/3/3/3
2	P3S	G	601	4	-	0/5/16/16	0/0/0/0
3	ADP	G	602	4	-	0/12/32/32	0/3/3/3
2	P3S	H	601	4	-	0/5/16/16	0/0/0/0
3	ADP	H	602	4	-	0/12/32/32	0/3/3/3
2	P3S	I	501	4	-	0/5/16/16	0/0/0/0
3	ADP	I	502	4	-	0/12/32/32	0/3/3/3
2	P3S	J	501	4	-	0/5/16/16	0/0/0/0
3	ADP	J	502	4	-	0/12/32/32	0/3/3/3
2	P3S	K	501	4	-	0/5/16/16	0/0/0/0
3	ADP	K	502	4	-	0/12/32/32	0/3/3/3
2	P3S	L	501	4	-	0/5/16/16	0/0/0/0
3	ADP	L	502	4	-	0/12/32/32	0/3/3/3

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	P3S	CB-CG	-4.00	1.48	1.52
3	F	602	ADP	PB-O2B	-3.06	1.43	1.54
3	D	502	ADP	PB-O2B	-2.54	1.45	1.54
2	I	501	P3S	PA-O2A	-2.38	1.49	1.54
3	L	502	ADP	PB-O2B	-2.35	1.46	1.54

The worst 5 of 129 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	502	ADP	N3-C2-N1	-15.04	117.38	128.89
3	C	502	ADP	N3-C2-N1	-12.69	119.18	128.89
3	K	502	ADP	N3-C2-N1	-12.62	119.23	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	602	ADP	N3-C2-N1	-11.48	120.10	128.89
3	H	602	ADP	N3-C2-N1	-10.76	120.65	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	P3S	4	0
2	B	501	P3S	1	0
2	C	501	P3S	4	0
2	D	501	P3S	6	0
2	E	501	P3S	1	0
3	E	502	ADP	1	0
2	F	601	P3S	6	0
3	F	602	ADP	1	0
2	G	601	P3S	8	0
2	H	601	P3S	5	0
2	I	501	P3S	2	0
2	J	501	P3S	3	0
2	K	501	P3S	2	0
2	L	501	P3S	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	443/443 (100%)	-0.16	2 (0%) 91 90	8, 19, 44, 77	0
1	B	443/443 (100%)	-0.15	1 (0%) 95 95	9, 19, 45, 79	0
1	C	443/443 (100%)	-0.20	0 100 100	8, 19, 45, 61	0
1	D	443/443 (100%)	-0.16	2 (0%) 91 90	9, 19, 42, 67	0
1	E	443/443 (100%)	-0.17	1 (0%) 95 95	7, 19, 42, 72	0
1	F	443/443 (100%)	-0.16	2 (0%) 91 90	9, 20, 45, 74	0
1	G	443/443 (100%)	-0.16	3 (0%) 89 87	8, 19, 45, 73	0
1	H	443/443 (100%)	-0.13	1 (0%) 95 95	7, 19, 44, 74	0
1	I	443/443 (100%)	-0.20	1 (0%) 95 95	7, 19, 43, 70	0
1	J	441/443 (99%)	-0.16	0 100 100	7, 19, 42, 65	0
1	K	443/443 (100%)	-0.17	2 (0%) 91 90	7, 19, 44, 67	0
1	L	443/443 (100%)	-0.17	2 (0%) 91 90	9, 21, 45, 72	0
All	All	5314/5316 (99%)	-0.17	17 (0%) 94 94	7, 19, 44, 79	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	8.6
1	E	2	ALA	7.2
1	B	2	ALA	6.3
1	K	2	ALA	5.1
1	F	2	ALA	4.4

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

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
4	MG	B	503	1/1	0.99	0.23	9.39	0,0,0,0	0
4	MG	D	503	1/1	0.97	0.19	8.98	5,5,5,5	0
4	MG	E	503	1/1	0.99	0.22	4.59	1,1,1,1	0
4	MG	C	503	1/1	0.99	0.20	3.91	0,0,0,0	0
4	MG	I	503	1/1	0.99	0.19	2.86	0,0,0,0	0
2	P3S	D	501	15/15	0.99	0.17	2.81	8,18,34,41	0
4	MG	K	503	1/1	1.00	0.16	2.64	0,0,0,0	0
4	MG	L	503	1/1	0.99	0.16	2.53	2,2,2,2	0
4	MG	A	503	1/1	0.99	0.17	2.35	4,4,4,4	0
2	P3S	K	501	15/15	0.98	0.17	2.33	10,15,21,23	0
2	P3S	F	601	15/15	0.98	0.18	2.32	12,21,32,45	0
4	MG	B	504	1/1	0.97	0.17	2.23	4,4,4,4	0
4	MG	C	505	1/1	0.98	0.16	2.20	5,5,5,5	0
2	P3S	A	501	15/15	0.98	0.18	2.20	8,16,28,34	0
4	MG	D	505	1/1	0.97	0.17	2.06	1,1,1,1	0
4	MG	H	603	1/1	0.99	0.17	2.04	1,1,1,1	0
4	MG	J	503	1/1	0.99	0.18	1.67	5,5,5,5	0
2	P3S	C	501	15/15	0.98	0.16	1.48	4,13,27,40	0
2	P3S	I	501	15/15	0.98	0.17	1.38	9,13,27,28	0
2	P3S	G	601	15/15	0.98	0.16	1.31	13,24,38,39	0
2	P3S	J	501	15/15	0.99	0.16	1.13	8,16,22,24	0
2	P3S	E	501	15/15	0.98	0.16	0.93	7,15,26,33	0
2	P3S	L	501	15/15	0.98	0.15	0.86	13,18,26,32	0
2	P3S	B	501	15/15	0.99	0.15	0.84	7,15,22,31	0
4	MG	F	603	1/1	0.99	0.15	0.78	5,5,5,5	0
4	MG	G	603	1/1	0.98	0.15	0.54	4,4,4,4	0
2	P3S	H	601	15/15	0.98	0.15	0.36	9,13,21,26	0
4	MG	A	504	1/1	1.00	0.15	0.28	4,4,4,4	0
3	ADP	J	502	27/27	0.99	0.14	0.25	13,18,24,33	0
3	ADP	C	502	27/27	0.99	0.14	0.21	11,18,21,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	ADP	A	502	27/27	0.98	0.14	0.02	14,18,24,25	0
4	MG	F	604	1/1	0.98	0.14	-0.15	6,6,6,6	0
4	MG	F	605	1/1	0.99	0.14	-0.21	5,5,5,5	0
3	ADP	L	502	27/27	0.99	0.14	-0.25	16,24,35,37	0
3	ADP	D	502	27/27	0.98	0.14	-0.25	11,19,28,32	0
3	ADP	K	502	27/27	0.98	0.13	-0.25	8,15,22,25	0
3	ADP	F	602	27/27	0.99	0.14	-0.36	10,20,27,30	0
3	ADP	I	502	27/27	0.98	0.14	-0.39	13,18,25,26	0
3	ADP	H	602	27/27	0.99	0.13	-0.48	11,18,23,25	0
4	MG	I	504	1/1	0.98	0.14	-0.55	5,5,5,5	0
4	MG	H	604	1/1	0.99	0.14	-0.56	5,5,5,5	0
4	MG	E	504	1/1	0.96	0.14	-0.62	3,3,3,3	0
3	ADP	B	502	27/27	0.98	0.13	-0.67	11,19,23,28	0
3	ADP	G	602	27/27	0.98	0.12	-0.75	16,22,31,32	0
3	ADP	E	502	27/27	0.99	0.11	-1.23	8,15,23,31	0
4	MG	G	604	1/1	0.99	0.13	-1.37	10,10,10,10	0
4	MG	J	504	1/1	0.99	0.12	-1.48	4,4,4,4	0
4	MG	C	504	1/1	0.99	0.11	-1.62	6,6,6,6	0
4	MG	K	504	1/1	0.98	0.11	-1.94	5,5,5,5	0
4	MG	D	504	1/1	0.98	0.09	-3.18	2,2,2,2	0
4	MG	L	504	1/1	0.99	0.12	-3.92	7,7,7,7	0
4	MG	I	505	1/1	0.97	0.17	-	6,6,6,6	0
4	MG	L	505	1/1	0.99	0.15	-	0,0,0,0	0
4	MG	A	505	1/1	0.99	0.17	-	6,6,6,6	0
4	MG	J	505	1/1	0.98	0.17	-	0,0,0,0	0
4	MG	B	505	1/1	0.96	0.17	-	7,7,7,7	0
4	MG	E	505	1/1	0.99	0.16	-	4,4,4,4	0
4	MG	H	605	1/1	0.99	0.17	-	1,1,1,1	0
4	MG	G	605	1/1	0.93	0.12	-	7,7,7,7	0
4	MG	K	505	1/1	0.98	0.20	-	1,1,1,1	0

6.5 Other polymers

There are no such residues in this entry.