



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 02:01 PM GMT

PDB ID : 2D3A
Title : Crystal Structure of the Maize Glutamine Synthetase complexed with ADP and Methionine sulfoximine Phosphate
Authors : Unno, H.; Uchida, T.; Sugawara, H.; Kurisu, G.; Sugiyama, T.; Yamaya, T.; Sakakibara, H.; Hase, T.; Kusunoki, M.
Deposited on : 2005-09-26
Resolution : 2.63 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

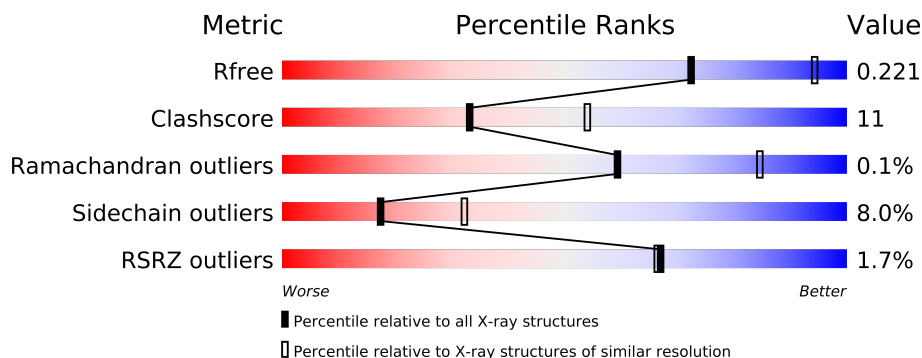
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.63 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}	66092	2393 (2.68-2.60)
Clashscore	79885	2915 (2.68-2.60)
Ramachandran outliers	78287	2865 (2.68-2.60)
Sidechain outliers	78261	2865 (2.68-2.60)
RSRZ outliers	66119	2393 (2.68-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	356	
1	B	356	
1	C	356	
1	D	356	
1	E	356	
1	F	356	
1	G	356	
1	H	356	
1	I	356	
1	J	356	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28621 atoms, of which 0 are hydrogen and 0 are deuterium.

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	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	B	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	C	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	D	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	E	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	F	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	G	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	H	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	I	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	J	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

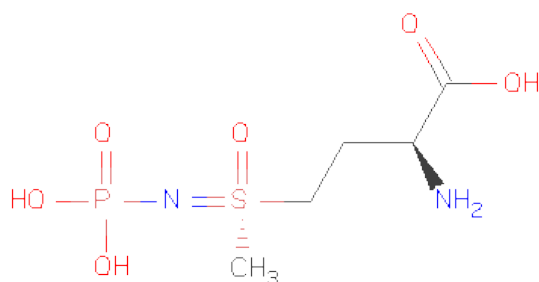
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	3	Total	Mn	0	0
			3	3		
2	J	3	Total	Mn	0	0
			3	3		
2	D	3	Total	Mn	0	0
			3	3		
2	E	3	Total	Mn	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	3	Total	Mn	0	0
			3	3		
2	B	3	Total	Mn	0	0
			3	3		
2	I	3	Total	Mn	0	0
			3	3		
2	C	3	Total	Mn	0	0
			3	3		
2	A	3	Total	Mn	0	0
			3	3		
2	F	3	Total	Mn	0	0
			3	3		

- Molecule 3 is L-METHIONINE-S-SULFOXIMINEPHOSPHATE (three-letter code: P3S) (formula: C₅H₁₃N₂O₆PS).



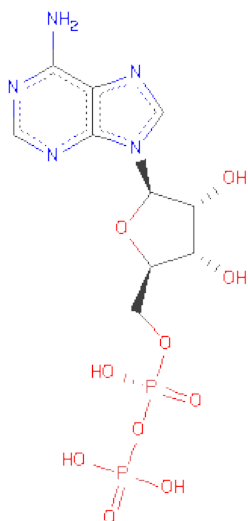
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
3	B	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
3	C	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
3	D	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
3	E	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total	C	N	O	P	S	
			15	5	2	6	1	1	
3	F	1	Total	C	N	O	P	S	
			15	5	2	6	1	1	
3	I	1	Total	C	N	O	P	S	
			15	5	2	6	1	1	
3	J	1	Total	C	N	O	P	S	
			15	5	2	6	1	1	
3	H	1	Total	C	N	O	P	S	
			15	5	2	6	1	1	

- 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		
			27	10	5	10	2	0	0
4	B	1	Total	C	N	O	P		
			27	10	5	10	2	0	0
4	C	1	Total	C	N	O	P		
			27	10	5	10	2	0	0
4	E	1	Total	C	N	O	P		
			27	10	5	10	2	0	0
4	D	1	Total	C	N	O	P		
			27	10	5	10	2	0	0
4	G	1	Total	C	N	O	P		
			27	10	5	10	2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	F	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		
4	J	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		

- Molecule 5 is water.

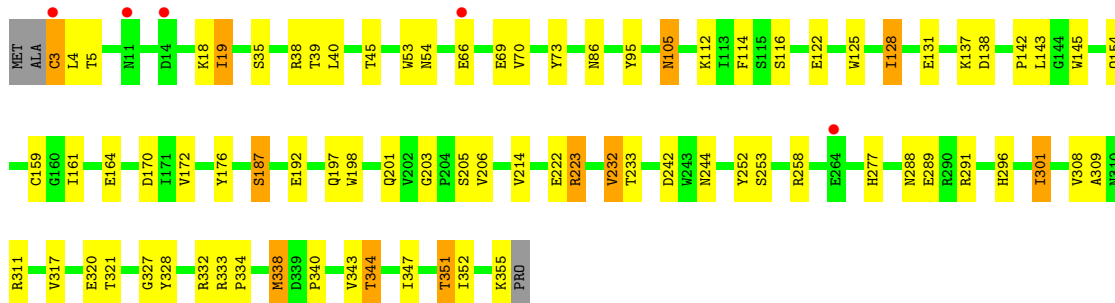
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	70	Total	O	0	0
			70	70		
5	B	100	Total	O	0	0
			100	100		
5	C	63	Total	O	0	0
			63	63		
5	D	63	Total	O	0	0
			63	63		
5	E	57	Total	O	0	0
			57	57		
5	F	58	Total	O	0	0
			58	58		
5	G	54	Total	O	0	0
			54	54		
5	H	88	Total	O	0	0
			88	88		
5	I	76	Total	O	0	0
			76	76		
5	J	92	Total	O	0	0
			92	92		

3 Residue-property plots

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

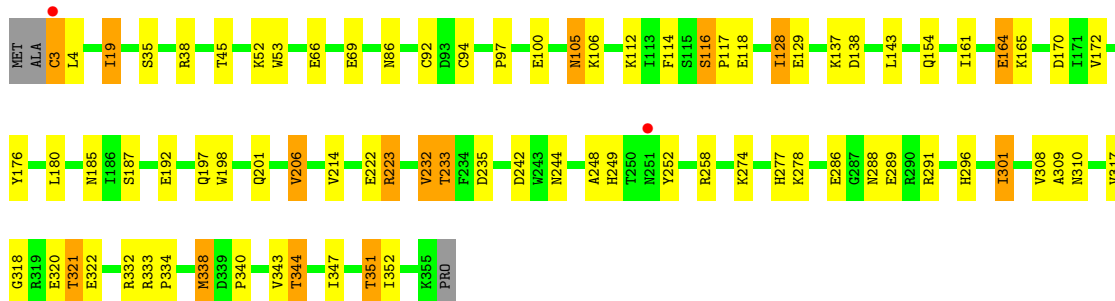
- Molecule 1: glutamine synthetase

Chain A: 



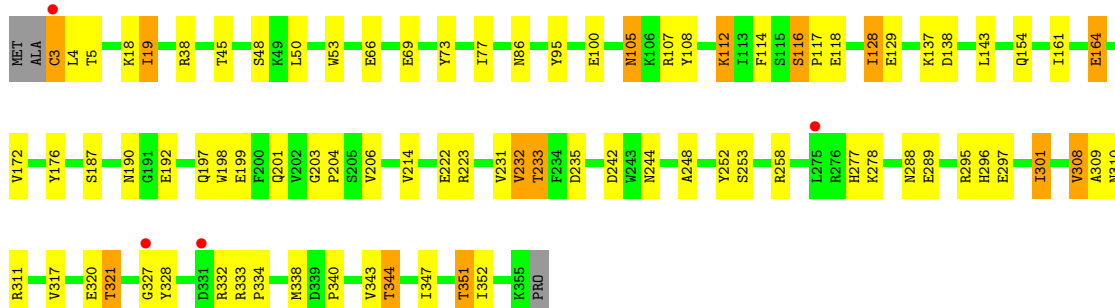
- Molecule 1: glutamine synthetase

Chain B: 



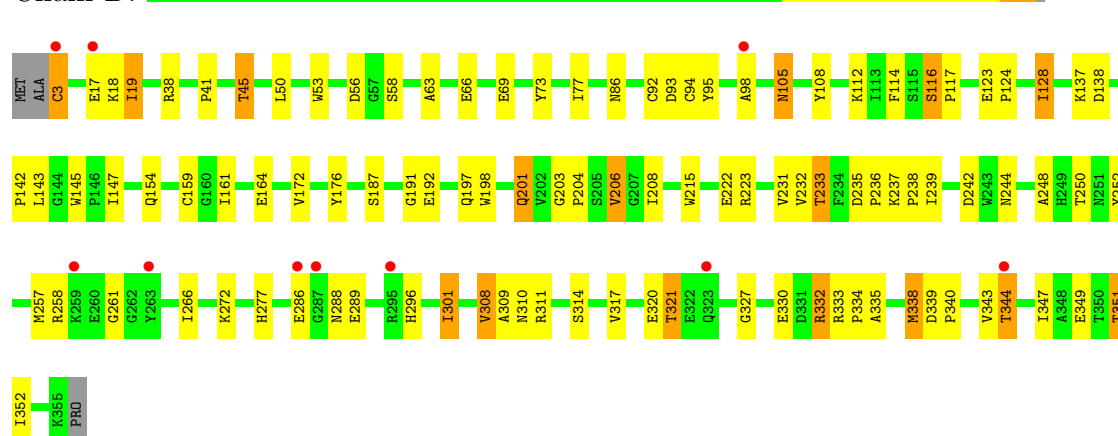
- Molecule 1: glutamine synthetase

Chain C: 



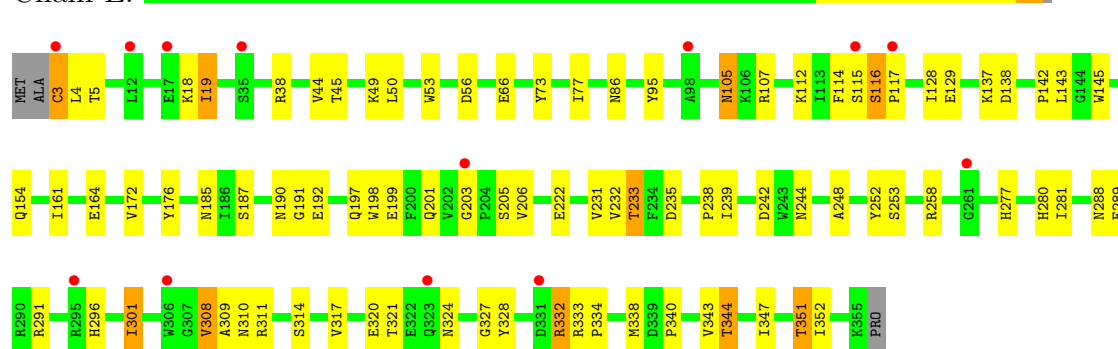
- Molecule 1: glutamine synthetase

Chain D:



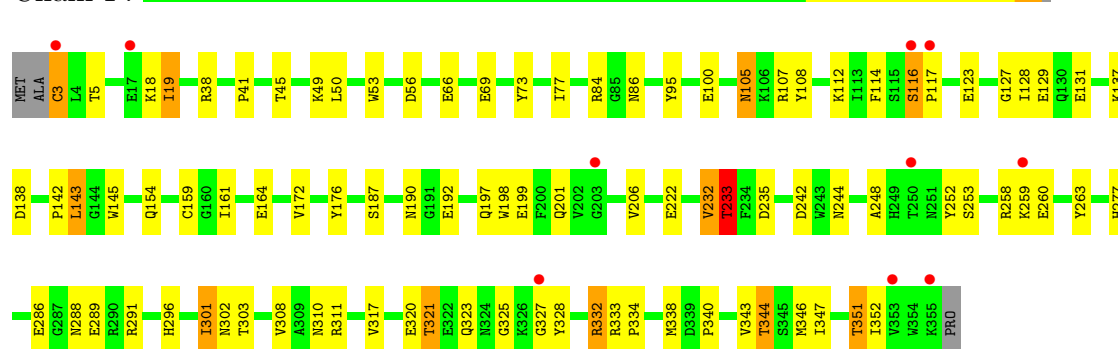
- Molecule 1: glutamine synthetase

Chain E:



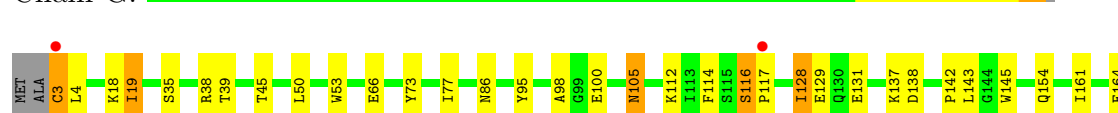
- Molecule 1: glutamine synthetase

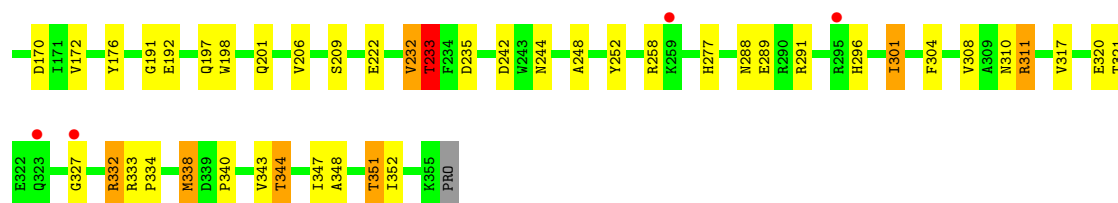
Chain F:



- Molecule 1: glutamine synthetase

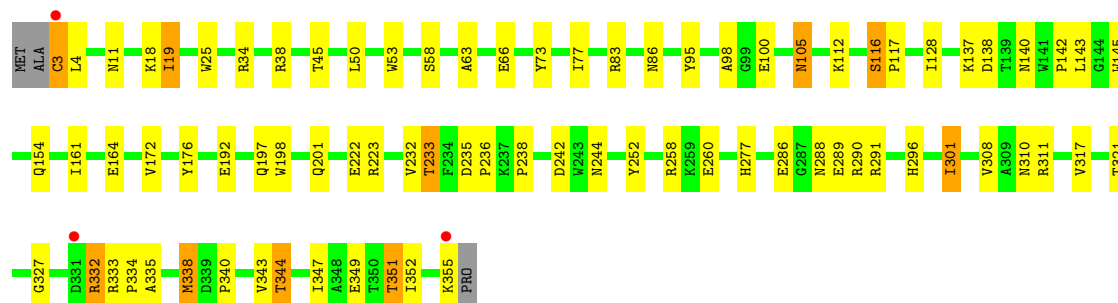
Chain G:





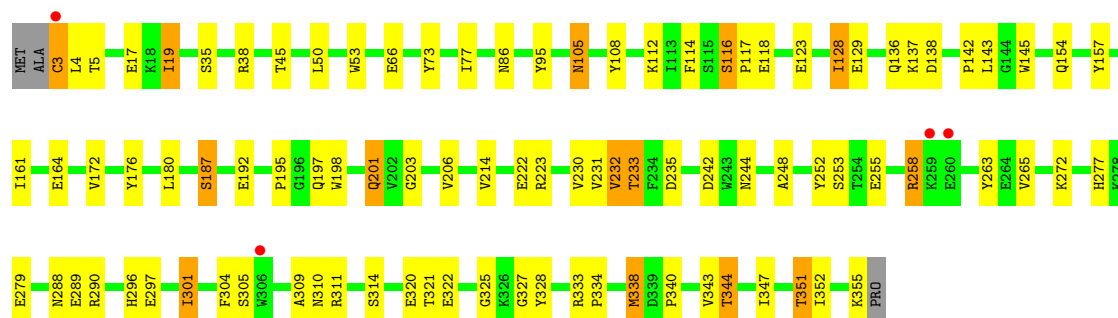
• Molecule 1: glutamine synthetase

Chain H:



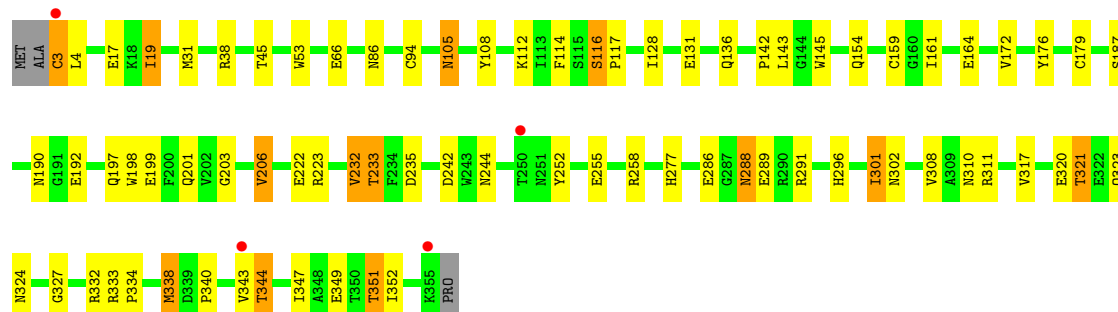
• Molecule 1: glutamine synthetase

Chain I:



• Molecule 1: glutamine synthetase

Chain J:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.80Å 191.04Å 118.10Å 90.00° 101.47° 90.00°	Depositor
Resolution (Å)	26.13 – 2.63 26.13 – 2.63	Depositor EDS
% Data completeness (in resolution range)	86.8 (26.13-2.63) 86.8 (26.13-2.63)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.64Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.184 , 0.220 0.185 , 0.221	Depositor DCC
R_{free} test set	5400 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	63.1	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 35.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 106990 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	28621	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: P3S, MN, 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	0.79	0/2819	0.79	5/3834 (0.1%)
1	B	0.79	2/2819 (0.1%)	0.78	3/3834 (0.1%)
1	C	0.76	0/2819	0.76	1/3834 (0.0%)
1	D	0.88	1/2819 (0.0%)	0.80	2/3834 (0.1%)
1	E	0.86	0/2819	0.79	3/3834 (0.1%)
1	F	0.80	0/2819	0.78	6/3834 (0.2%)
1	G	0.82	0/2819	0.79	6/3834 (0.2%)
1	H	0.78	0/2819	0.79	2/3834 (0.1%)
1	I	0.77	0/2819	0.76	2/3834 (0.1%)
1	J	0.80	2/2819 (0.1%)	0.79	3/3834 (0.1%)
All	All	0.80	5/28190 (0.0%)	0.78	33/38340 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	179	CYS	CB-SG	-7.34	1.69	1.82
1	D	92	CYS	CB-SG	-6.80	1.70	1.82
1	B	94	CYS	CB-SG	-6.15	1.71	1.82
1	B	92	CYS	CB-SG	-5.60	1.72	1.81
1	J	94	CYS	CB-SG	-5.47	1.72	1.81

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	291	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	B	332	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	J	291	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	H	332	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	A	291	ARG	NE-CZ-NH1	6.69	123.64	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2745	0	2653	56	0
1	B	2745	0	2653	57	0
1	C	2745	0	2653	60	0
1	D	2745	0	2653	86	0
1	E	2745	0	2653	62	0
1	F	2745	0	2653	66	0
1	G	2745	0	2653	64	0
1	H	2745	0	2653	60	0
1	I	2745	0	2653	70	0
1	J	2745	0	2653	57	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
2	I	3	0	0	0	0
2	J	3	0	0	0	0
3	A	15	0	10	2	0
3	B	15	0	10	2	0
3	C	15	0	10	1	0
3	D	15	0	10	2	0
3	E	15	0	10	1	0
3	F	15	0	10	2	0
3	G	15	0	10	4	0
3	H	15	0	10	2	0
3	I	15	0	10	1	0
3	J	15	0	10	3	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	27	0	12	0	0
4	D	27	0	12	3	0
4	E	27	0	12	1	0
4	F	27	0	12	1	0
4	G	27	0	12	0	0
4	H	27	0	12	0	0
4	I	27	0	12	0	0
4	J	27	0	12	1	0
5	A	70	0	0	11	0
5	B	100	0	0	18	0
5	C	63	0	0	16	0
5	D	63	0	0	31	0
5	E	57	0	0	16	0
5	F	58	0	0	22	0
5	G	54	0	0	17	0
5	H	88	0	0	20	0
5	I	76	0	0	20	0
5	J	92	0	0	17	0
All	All	28621	0	26750	605	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

The worst 5 of 605 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:206:VAL:HB	5:J:6073:HOH:O	1.37	1.23
1:C:203:GLY:HA3	5:C:6039:HOH:O	1.39	1.20
1:H:321:THR:HG23	5:H:6097:HOH:O	1.47	1.13
1:H:344:THR:HG21	5:H:6011:HOH:O	1.51	1.09
1:G:321:THR:HG23	5:G:6024:HOH:O	1.53	1.09

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	351/356 (99%)	333 (95%)	18 (5%)	0	100	100
1	B	351/356 (99%)	334 (95%)	17 (5%)	0	100	100
1	C	351/356 (99%)	333 (95%)	17 (5%)	1 (0%)	50	77
1	D	351/356 (99%)	332 (95%)	18 (5%)	1 (0%)	50	77
1	E	351/356 (99%)	330 (94%)	19 (5%)	2 (1%)	33	61
1	F	351/356 (99%)	331 (94%)	20 (6%)	0	100	100
1	G	351/356 (99%)	331 (94%)	20 (6%)	0	100	100
1	H	351/356 (99%)	334 (95%)	17 (5%)	0	100	100
1	I	351/356 (99%)	332 (95%)	19 (5%)	0	100	100
1	J	351/356 (99%)	333 (95%)	18 (5%)	0	100	100
All	All	3510/3560 (99%)	3323 (95%)	183 (5%)	4 (0%)	59	84

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	308	VAL
1	C	308	VAL
1	D	308	VAL
1	E	281	ILE

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	288/290 (99%)	265 (92%)	23 (8%)	17	32
1	B	288/290 (99%)	264 (92%)	24 (8%)	16	29
1	C	288/290 (99%)	265 (92%)	23 (8%)	17	32
1	D	288/290 (99%)	263 (91%)	25 (9%)	15	27
1	E	288/290 (99%)	266 (92%)	22 (8%)	19	35
1	F	288/290 (99%)	265 (92%)	23 (8%)	17	32
1	G	288/290 (99%)	266 (92%)	22 (8%)	19	35
1	H	288/290 (99%)	267 (93%)	21 (7%)	20	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	288/290 (99%)	264 (92%)	24 (8%)	16	29
1	J	288/290 (99%)	264 (92%)	24 (8%)	16	29
All	All	2880/2900 (99%)	2649 (92%)	231 (8%)	17	32

5 of 231 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	176	TYR
1	F	206	VAL
1	J	128	ILE
1	E	206	VAL
1	F	3	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	277	HIS
1	F	201	GLN
1	J	190	ASN
1	E	288	ASN
1	F	105	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 50 ligands modelled in this entry, 30 are monoatomic - leaving 20 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
3	P3S	A	5001	2	14,14,14	4.04	4 (28%)	19,21,21	2.78	5 (26%)
4	ADP	A	6001	2	29,29,29	0.85	1 (3%)	45,45,45	2.40	10 (22%)
3	P3S	B	5002	2	14,14,14	3.71	4 (28%)	19,21,21	3.53	8 (42%)
4	ADP	B	6002	2	29,29,29	0.97	3 (10%)	45,45,45	3.20	13 (28%)
3	P3S	C	5003	2	14,14,14	3.69	3 (21%)	19,21,21	2.39	4 (21%)
4	ADP	C	6003	2	29,29,29	0.91	1 (3%)	45,45,45	2.16	6 (13%)
3	P3S	D	5004	2	14,14,14	4.35	4 (28%)	19,21,21	3.12	6 (31%)
4	ADP	D	6005	2	29,29,29	0.99	2 (6%)	45,45,45	1.98	9 (20%)
3	P3S	E	5005	2	14,14,14	4.04	4 (28%)	19,21,21	2.56	4 (21%)
4	ADP	E	6004	2	29,29,29	0.94	2 (6%)	45,45,45	2.54	12 (26%)
3	P3S	F	5007	2	14,14,14	4.05	4 (28%)	19,21,21	3.01	7 (36%)
4	ADP	F	6007	2	29,29,29	1.15	4 (13%)	45,45,45	2.42	8 (17%)
3	P3S	G	5006	2	14,14,14	3.90	3 (21%)	19,21,21	1.92	5 (26%)
4	ADP	G	6006	2	29,29,29	0.90	2 (6%)	45,45,45	2.04	10 (22%)
3	P3S	H	5010	2	14,14,14	3.89	5 (35%)	19,21,21	2.79	7 (36%)
4	ADP	H	6010	2	29,29,29	1.13	1 (3%)	45,45,45	2.13	14 (31%)
3	P3S	I	5008	2	14,14,14	3.90	3 (21%)	19,21,21	3.08	5 (26%)
4	ADP	I	6008	2	29,29,29	1.01	2 (6%)	45,45,45	2.55	11 (24%)
3	P3S	J	5009	2	14,14,14	3.64	3 (21%)	19,21,21	3.03	9 (47%)
4	ADP	J	6009	2	29,29,29	1.25	3 (10%)	45,45,45	2.54	13 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	P3S	A	5001	2	-	1/13/16/16	0/0/0/0
4	ADP	A	6001	2	-	0/16/32/32	0/1/3/3
3	P3S	B	5002	2	-	1/13/16/16	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	B	6002	2	-	0/16/32/32	0/1/3/3
3	P3S	C	5003	2	-	1/13/16/16	0/0/0/0
4	ADP	C	6003	2	-	0/16/32/32	0/1/3/3
3	P3S	D	5004	2	-	1/13/16/16	0/0/0/0
4	ADP	D	6005	2	-	0/16/32/32	0/1/3/3
3	P3S	E	5005	2	-	1/13/16/16	0/0/0/0
4	ADP	E	6004	2	-	0/16/32/32	0/1/3/3
3	P3S	F	5007	2	-	1/13/16/16	0/0/0/0
4	ADP	F	6007	2	-	0/16/32/32	0/1/3/3
3	P3S	G	5006	2	-	1/13/16/16	0/0/0/0
4	ADP	G	6006	2	-	0/16/32/32	0/1/3/3
3	P3S	H	5010	2	-	1/13/16/16	0/0/0/0
4	ADP	H	6010	2	-	0/16/32/32	0/1/3/3
3	P3S	I	5008	2	-	1/13/16/16	0/0/0/0
4	ADP	I	6008	2	-	0/16/32/32	0/1/3/3
3	P3S	J	5009	2	-	1/13/16/16	0/0/0/0
4	ADP	J	6009	2	-	1/16/32/32	0/1/3/3

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	5007	P3S	CG-SD	-12.64	1.64	1.79
3	D	5004	P3S	CG-SD	-11.71	1.65	1.79
3	A	5001	P3S	CG-SD	-11.03	1.66	1.79
3	C	5003	P3S	CG-SD	-10.70	1.66	1.79
3	G	5006	P3S	CG-SD	-10.69	1.66	1.79

The worst 5 of 166 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	6002	ADP	N3-C2-N1	-13.30	117.59	128.71
4	J	6009	ADP	N3-C2-N1	-12.24	118.48	128.71
4	B	6002	ADP	O4'-C1'-N9	12.08	119.67	108.44
4	A	6001	ADP	N3-C2-N1	-11.64	118.97	128.71
4	E	6004	ADP	N3-C2-N1	-11.08	119.44	128.71

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	5009	P3S	CB-CG-SD-NE

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Mol	Chain	Res	Type	Atoms
3	A	5001	P3S	CB-CG-SD-NE
3	D	5004	P3S	CB-CG-SD-NE
3	I	5008	P3S	CB-CG-SD-NE
3	G	5006	P3S	CB-CG-SD-NE

There are no ring outliers.

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, 95th 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	353/356 (99%)	-0.25	5 (1%) 72 72	46, 64, 86, 99	0
1	B	353/356 (99%)	-0.19	2 (0%) 86 88	46, 64, 86, 99	0
1	C	353/356 (99%)	-0.24	4 (1%) 77 79	46, 64, 86, 99	0
1	D	353/356 (99%)	-0.11	10 (2%) 50 48	46, 64, 86, 99	0
1	E	353/356 (99%)	-0.13	13 (3%) 39 36	46, 64, 86, 99	0
1	F	353/356 (99%)	-0.16	10 (2%) 50 48	46, 64, 86, 99	0
1	G	353/356 (99%)	-0.17	6 (1%) 67 66	46, 64, 86, 99	0
1	H	353/356 (99%)	-0.08	3 (0%) 83 85	46, 64, 86, 99	0
1	I	353/356 (99%)	-0.29	4 (1%) 77 79	46, 64, 86, 99	0
1	J	353/356 (99%)	-0.17	4 (1%) 77 79	46, 64, 86, 99	0
All	All	3530/3560 (99%)	-0.18	61 (1%) 67 66	46, 64, 87, 99	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	3	CYS	6.6
1	B	3	CYS	6.5
1	A	3	CYS	6.3
1	E	3	CYS	6.3
1	C	327	GLY	6.2

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

There are no carbohydrates in this entry.

6.4 Ligands

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MN	C	1021	1/1	0.23	1.52	73,73,73,73	0
2	MN	D	1033	1/1	0.20	0.41	68,68,68,68	0
2	MN	E	1041	1/1	0.14	0.23	66,66,66,66	0
3	P3S	A	5001	15/15	0.16	-0.07	41,51,59,62	0
3	P3S	I	5008	15/15	0.15	-0.18	43,48,53,54	0
3	P3S	D	5004	15/15	0.15	-0.21	55,63,71,72	0
3	P3S	E	5005	15/15	0.15	-0.42	65,68,70,70	0
3	P3S	F	5007	15/15	0.14	-0.51	59,64,69,71	0
4	ADP	E	6004	27/27	0.15	-0.53	67,86,94,95	0
2	MN	G	1061	1/1	0.12	-0.57	57,57,57,57	0
4	ADP	C	6003	27/27	0.15	-0.58	62,75,80,81	0
2	MN	A	1003	1/1	0.18	-0.59	53,53,53,53	0
3	P3S	C	5003	15/15	0.13	-0.68	53,57,61,61	0
3	P3S	G	5006	15/15	0.12	-0.73	52,59,63,63	0
4	ADP	G	6006	27/27	0.12	-0.76	47,68,76,77	0
3	P3S	J	5009	15/15	0.14	-0.86	40,47,49,49	0
3	P3S	B	5002	15/15	0.13	-0.95	32,41,45,51	0
4	ADP	F	6007	27/27	0.12	-0.95	61,78,84,84	0
4	ADP	I	6008	27/27	0.14	-1.01	54,68,70,70	0
4	ADP	D	6005	27/27	0.12	-1.12	55,78,85,86	0
2	MN	G	1063	1/1	0.10	-1.13	53,53,53,53	0
4	ADP	B	6002	27/27	0.14	-1.18	39,50,52,53	0
3	P3S	H	5010	15/15	0.10	-1.42	33,40,52,53	0
2	MN	C	1022	1/1	0.12	-1.47	59,59,59,59	0
2	MN	F	1051	1/1	0.12	-1.52	66,66,66,66	0
2	MN	H	1073	1/1	0.17	-1.57	47,47,47,47	0
2	MN	J	1091	1/1	0.17	-1.60	47,47,47,47	0
4	ADP	A	6001	27/27	0.13	-1.62	48,62,73,74	0
2	MN	F	1053	1/1	0.07	-1.67	67,67,67,67	0
2	MN	H	1071	1/1	0.14	-1.79	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MN	E	1043	1/1	0.09	-1.86	58,58,58,58	0
2	MN	G	1062	1/1	0.10	-1.92	60,60,60,60	0
2	MN	C	1023	1/1	0.09	-1.92	62,62,62,62	0
4	ADP	J	6009	27/27	0.12	-1.94	42,54,60,61	0
2	MN	I	1083	1/1	0.11	-1.99	54,54,54,54	0
4	ADP	H	6010	27/27	0.11	-1.99	38,44,47,48	0
2	MN	F	1052	1/1	0.13	-2.05	66,66,66,66	0
2	MN	I	1081	1/1	0.13	-2.07	56,56,56,56	0
2	MN	E	1042	1/1	0.12	-2.26	70,70,70,70	0
2	MN	D	1031	1/1	0.07	-2.34	58,58,58,58	0
2	MN	J	1093	1/1	0.14	-2.38	45,45,45,45	0
2	MN	B	1012	1/1	0.14	-2.73	51,51,51,51	0
2	MN	B	1011	1/1	0.14	-2.74	49,49,49,49	0
2	MN	B	1013	1/1	0.11	-2.87	46,46,46,46	0
2	MN	A	1002	1/1	0.13	-2.89	56,56,56,56	0
2	MN	D	1032	1/1	0.10	-2.96	63,63,63,63	0
2	MN	A	1001	1/1	0.12	-2.98	47,47,47,47	0
2	MN	I	1082	1/1	0.12	-3.64	56,56,56,56	0
2	MN	H	1072	1/1	0.13	-4.19	44,44,44,44	0
2	MN	J	1092	1/1	0.12	-4.28	53,53,53,53	0

6.5 Other polymers ⓘ

There are no such residues in this entry.