



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2018 – 10:43 am GMT

PDB ID : 1AO0
Title : GLUTAMINE PHOSPHORIBOSYLPYROPHOSPHATE (PRPP) AMI-
DOTRANSFERASE FROM B. SUBTILIS COMPLEXED WITH ADP AND
GMP
Authors : Tomchick, D.R.; Smith, J.L.
Deposited on : 1997-07-15
Resolution : 2.80 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

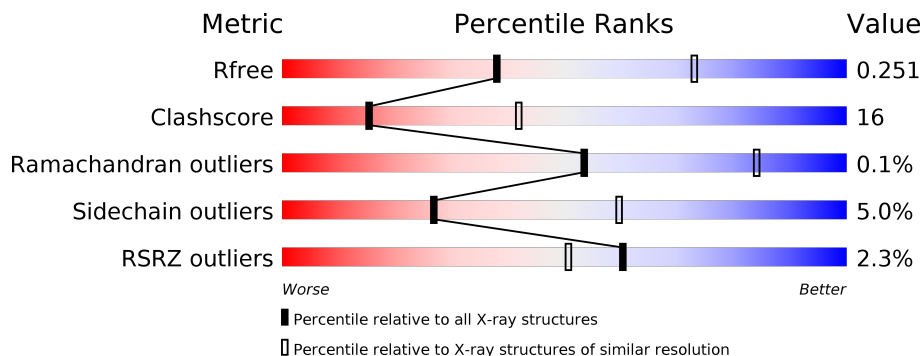
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	111664	2792 (2.80-2.80)
Clashscore	122126	3209 (2.80-2.80)
Ramachandran outliers	120053	3158 (2.80-2.80)
Sidechain outliers	120020	3160 (2.80-2.80)
RSRZ outliers	108989	2726 (2.80-2.80)

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 $\leq 5\%$. 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	459	
1	B	459	
1	C	459	
1	D	459	

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 14152 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 GLUTAMINE PHOSPHORIBOSYLPYROPHOSPHATE AMIDOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	455	3477	2175	609	673	20	21	0	0
1	B	455	3477	2175	609	673	20	44	0	0
1	C	455	3477	2175	609	673	20	22	0	0
1	D	455	3477	2175	609	673	20	17	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	402	GLU	GLY	SEQUENCE CORRECTION	UNP P00497
B	402	GLU	GLY	SEQUENCE CORRECTION	UNP P00497
C	402	GLU	GLY	SEQUENCE CORRECTION	UNP P00497
D	402	GLU	GLY	SEQUENCE CORRECTION	UNP P00497

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

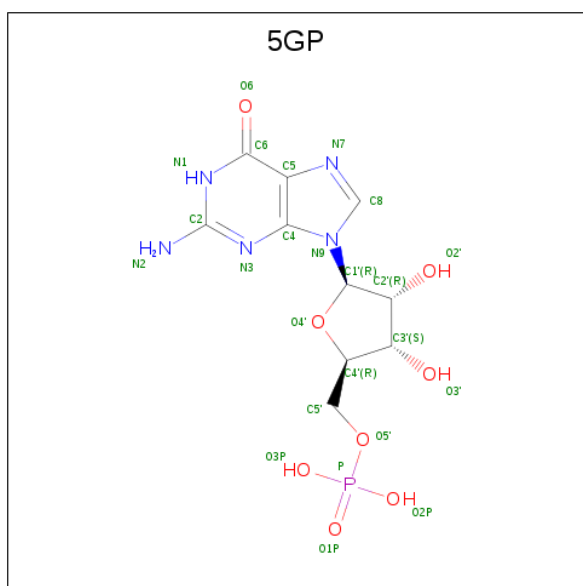
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Mg 1	0	0
2	A	1	Total 1	Mg 1	0	0
2	D	1	Total 1	Mg 1	0	0
2	C	1	Total 1	Mg 1	0	0

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



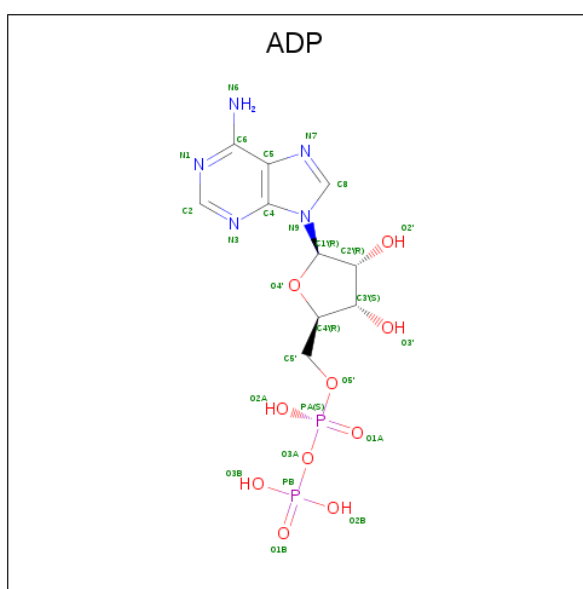
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe S	0	0
			8	4 4		
3	B	1	Total	Fe S	0	0
			8	4 4		
3	C	1	Total	Fe S	0	0
			8	4 4		
3	D	1	Total	Fe S	0	0
			8	4 4		

- Molecule 4 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula: $C_{10}H_{14}N_5O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
4	B	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
4	C	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
4	D	1	Total	C	N	O	P	0	0
			24	10	5	8	1		

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



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		

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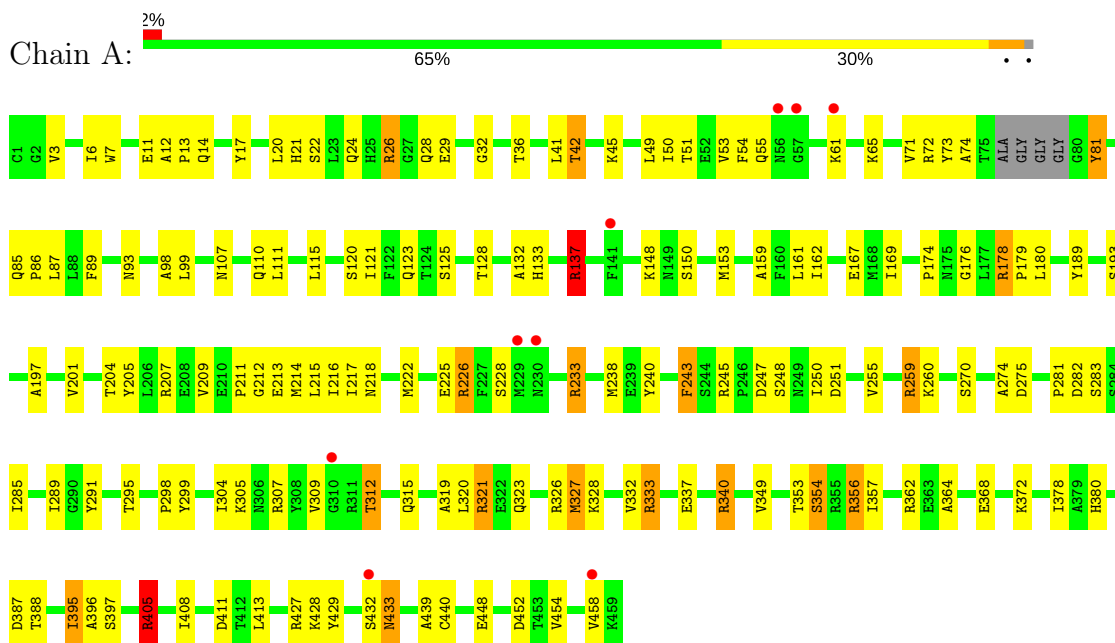
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total O 1 1	0	0
6	C	1	Total O 1 1	0	0
6	D	1	Total O 1 1	0	0

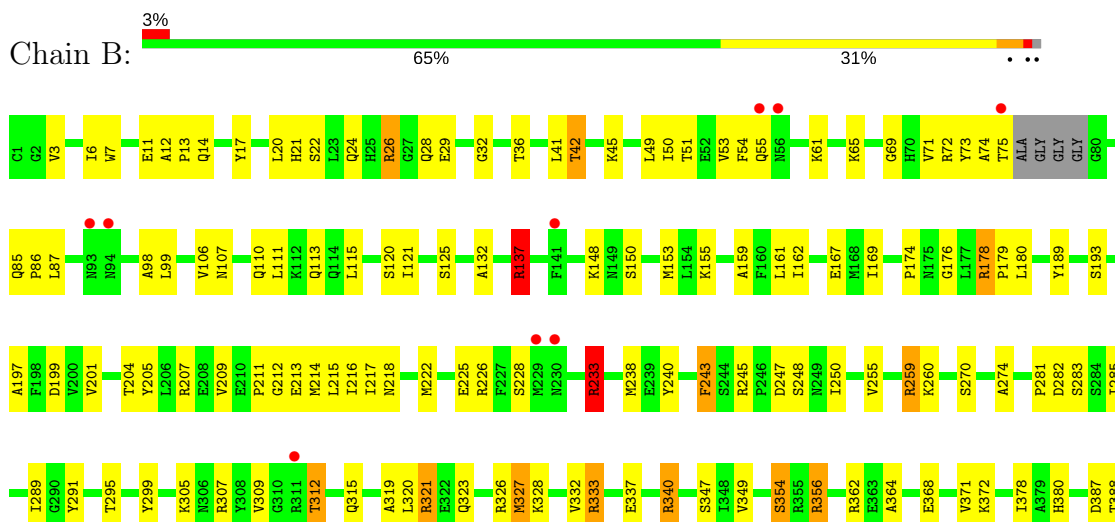
3 Residue-property plots [\(i\)](#)

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

- Molecule 1: GLUTAMINE PHOSPHORIBOSYLPYROPHOSPHATE AMIDOTRANSFERASE

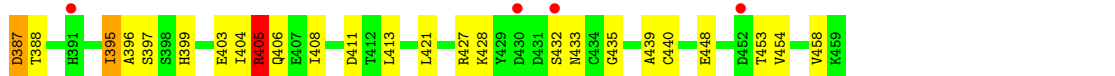
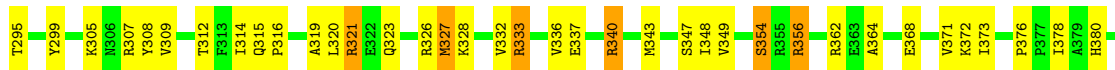
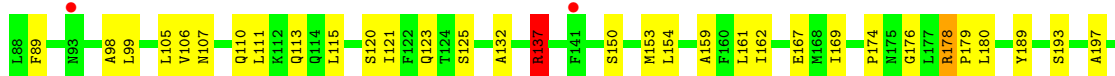
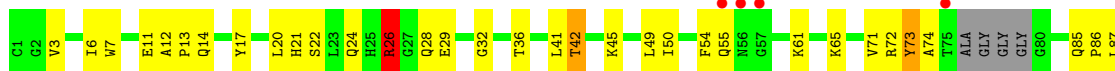


- Molecule 1: GLUTAMINE PHOSPHORIBOSYLPYROPHOSPHATE AMIDOTRANSFERASE

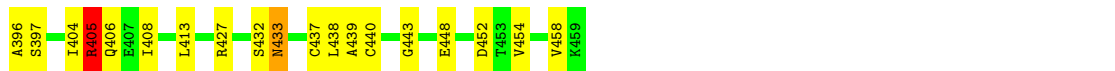
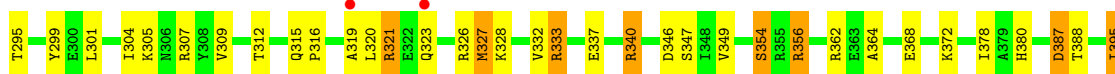
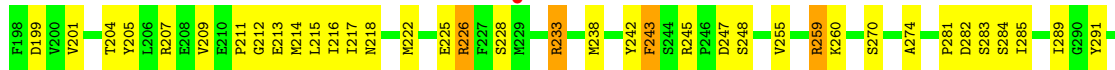
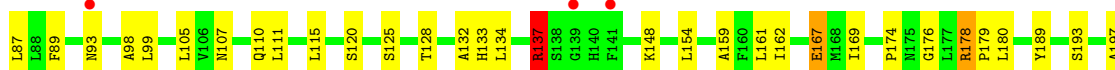
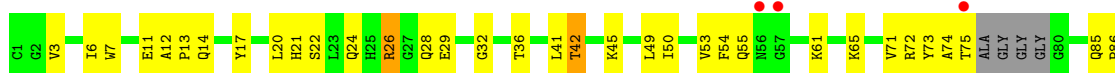




• Molecule 1: GLUTAMINE PHOSPHORIBOSYLPYROPHOSPHATE AMIDOTRANSFERASE



• Molecule 1: GLUTAMINE PHOSPHORIBOSYLPYROPHOSPHATE AMIDOTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	160.30Å 70.40Å 182.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 19.97 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.0 (15.00-2.80) 91.0 (19.97-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.03 (at 2.79Å)	Xtrriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.214 , 0.264 0.205 , 0.251	Depositor DCC
R_{free} test set	2348 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtrriage
Anisotropy	0.821	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14152	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, 5GP, 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	0.70	0/3534	0.74	0/4772
1	B	0.69	0/3534	0.75	0/4772
1	C	0.70	0/3534	0.75	2/4772 (0.0%)
1	D	0.70	0/3534	0.74	0/4772
All	All	0.70	0/14136	0.74	2/19088 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	22
1	B	0	22
1	C	0	21
1	D	0	23
All	All	0	88

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	247	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	C	26	ARG	NE-CZ-NH1	-5.30	117.65	120.30

There are no chirality outliers.

5 of 88 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	ARG	Sidechain
1	A	178	ARG	Sidechain
1	A	26	ARG	Sidechain
1	A	72	ARG	Sidechain
1	A	73	TYR	Sidechain

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	3477	0	3459	120	0
1	B	3477	0	3459	110	0
1	C	3477	0	3459	124	0
1	D	3477	0	3459	118	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	8	0	0	1	0
3	B	8	0	0	1	0
3	C	8	0	0	1	0
3	D	8	0	0	1	0
4	A	24	0	11	2	0
4	B	24	0	11	3	0
4	C	24	0	11	3	0
4	D	24	0	11	6	0
5	A	27	0	12	1	0
5	B	27	0	12	2	0
5	C	27	0	12	1	0
5	D	27	0	12	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
All	All	14152	0	13928	443	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 16.

The worst 5 of 443 close contacts within the same asymmetric unit are listed below, sorted by

their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ARG:NH2	1:C:137:ARG:HH22	1.49	1.10
1:A:137:ARG:HH22	1:C:137:ARG:NH2	1.50	1.08
1:A:20:LEU:HD22	1:A:71:VAL:HG23	1.52	0.92
1:A:340:ARG:HB2	1:A:368:GLU:HB2	1.52	0.91
1:B:20:LEU:HD22	1:B:71:VAL:HG23	1.54	0.89

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	451/459 (98%)	429 (95%)	22 (5%)	0	100	100
1	B	451/459 (98%)	429 (95%)	21 (5%)	1 (0%)	49	81
1	C	451/459 (98%)	427 (95%)	24 (5%)	0	100	100
1	D	451/459 (98%)	428 (95%)	23 (5%)	0	100	100
All	All	1804/1836 (98%)	1713 (95%)	90 (5%)	1 (0%)	53	84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	430	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	377/377 (100%)	358 (95%)	19 (5%)	27	60
1	B	377/377 (100%)	358 (95%)	19 (5%)	27	60
1	C	377/377 (100%)	359 (95%)	18 (5%)	28	61
1	D	377/377 (100%)	357 (95%)	20 (5%)	25	57
All	All	1508/1508 (100%)	1432 (95%)	76 (5%)	27	60

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	405	ARG
1	C	233	ARG
1	D	395	ILE
1	B	427	ARG
1	C	42	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	380	HIS
1	C	21	HIS
1	D	380	HIS
1	B	433	ASN
1	C	14	GLN

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 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	SF4	A	466	1	0,12,12	0.00	-	0,24,24	0.00	-
4	5GP	A	467	2,5	22,26,26	1.18	1 (4%)	25,40,40	2.73	6 (24%)
5	ADP	A	468	4	25,29,29	0.85	0	25,45,45	1.28	4 (16%)
3	SF4	B	466	1	0,12,12	0.00	-	0,24,24	0.00	-
4	5GP	B	467	2,5	22,26,26	1.25	2 (9%)	25,40,40	2.63	8 (32%)
5	ADP	B	468	4	25,29,29	0.85	0	25,45,45	1.19	4 (16%)
3	SF4	C	466	1	0,12,12	0.00	-	0,24,24	0.00	-
4	5GP	C	467	2,5	22,26,26	1.43	4 (18%)	25,40,40	2.68	6 (24%)
5	ADP	C	468	4	25,29,29	0.87	0	25,45,45	1.22	3 (12%)
3	SF4	D	466	1	0,12,12	0.00	-	0,24,24	0.00	-
4	5GP	D	467	2,5	22,26,26	1.22	1 (4%)	25,40,40	2.62	6 (24%)
5	ADP	D	468	4	25,29,29	0.90	1 (4%)	25,45,45	1.22	3 (12%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	A	466	1	-	0/0/48/48	0/6/5/5
4	5GP	A	467	2,5	-	0/6/26/26	0/3/3/3
5	ADP	A	468	4	-	0/12/32/32	0/3/3/3
3	SF4	B	466	1	-	0/0/48/48	0/6/5/5
4	5GP	B	467	2,5	-	0/6/26/26	0/3/3/3
5	ADP	B	468	4	-	0/12/32/32	0/3/3/3
3	SF4	C	466	1	-	0/0/48/48	0/6/5/5
4	5GP	C	467	2,5	-	0/6/26/26	0/3/3/3
5	ADP	C	468	4	-	0/12/32/32	0/3/3/3
3	SF4	D	466	1	-	0/0/48/48	0/6/5/5
4	5GP	D	467	2,5	-	0/6/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	D	468	4	-	0/12/32/32	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	467	5GP	C8-N7	-2.27	1.30	1.34
4	B	467	5GP	C8-N7	-2.18	1.30	1.34
5	D	468	ADP	C8-N7	-2.04	1.30	1.34
4	C	467	5GP	C2-N1	2.18	1.39	1.35
4	C	467	5GP	C8-N9	2.25	1.39	1.36

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	467	5GP	C5-C6-N1	-9.08	110.56	123.47
4	D	467	5GP	C5-C6-N1	-8.96	110.73	123.47
4	B	467	5GP	C5-C6-N1	-8.86	110.88	123.47
4	A	467	5GP	C5-C6-N1	-8.64	111.18	123.47
4	C	467	5GP	C2-N3-C4	-4.82	109.53	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	466	SF4	1	0
4	A	467	5GP	2	0
5	A	468	ADP	1	0
3	B	466	SF4	1	0
4	B	467	5GP	3	0
5	B	468	ADP	2	0
3	C	466	SF4	1	0
4	C	467	5GP	3	0
5	C	468	ADP	1	0
3	D	466	SF4	1	0
4	D	467	5GP	6	0
5	D	468	ADP	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	455/459 (99%)	-0.45	9 (1%) 65 56	10, 24, 65, 96	7 (1%)
1	B	454/459 (98%)	-0.16	13 (2%) 51 41	11, 31, 69, 99	8 (1%)
1	C	455/459 (99%)	-0.30	11 (2%) 59 49	11, 29, 69, 98	9 (1%)
1	D	455/459 (99%)	-0.37	9 (1%) 65 56	11, 28, 65, 96	6 (1%)
All	All	1819/1836 (99%)	-0.32	42 (2%) 60 51	10, 28, 67, 99	30 (1%)

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	56	ASN	10.3
1	B	429	TYR	6.6
1	A	229	MET	4.7
1	D	56	ASN	4.7
1	B	93	ASN	4.4

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. 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	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	B	469	1/1	0.94	0.07	22,22,22,22	0
2	MG	A	469	1/1	0.95	0.06	10,10,10,10	0
5	ADP	A	468	27/27	0.96	0.13	12,24,58,67	0
4	5GP	C	467	24/24	0.97	0.12	10,26,47,53	0
4	5GP	A	467	24/24	0.97	0.12	10,20,52,59	0
5	ADP	B	468	27/27	0.97	0.15	10,22,53,67	0
4	5GP	D	467	24/24	0.97	0.14	10,19,46,53	0
4	5GP	B	467	24/24	0.97	0.13	12,28,50,58	0
5	ADP	D	468	27/27	0.97	0.17	10,20,59,69	0
5	ADP	C	468	27/27	0.97	0.13	10,19,65,73	0
2	MG	C	469	1/1	0.98	0.05	12,12,12,12	0
2	MG	D	469	1/1	0.99	0.03	10,10,10,10	0
3	SF4	A	466	8/8	0.99	0.07	12,15,15,15	0
3	SF4	B	466	8/8	0.99	0.08	12,21,25,29	0
3	SF4	C	466	8/8	0.99	0.07	20,22,24,28	0
3	SF4	D	466	8/8	0.99	0.07	15,18,24,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.