wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 08:37 PM GMT

PDB ID	:	1L5S
Title	:	Human liver glycogen phosphorylase complexed with uric acid, N-Acetyl-beta -D-glucopyranosylamine, and CP-403,700
Authors	:	Ekstrom, J.L.; Pauly, T.A.; Carty, M.D.; Soeller, W.C.; Culp, J.; Danley, D.E.; Hoover, D.J.; Treadway, J.L.; Gibbs, E.M.; Fletterick, R.J.; Day, Y.S.N.; Myszka, D.G.; Rath, V.L.
Deposited on	:	2002-03-07
Resolution	:	2.10 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 (i)) were used in the production of this report:

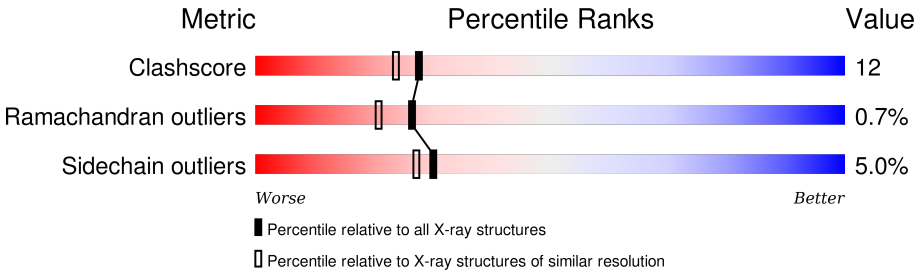
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.10 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))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	847	70% 21% • 6%
1	B	847	69% 22% • 7%

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
6	MRD	B	903	-	-	X	-

2 Entry composition (i)

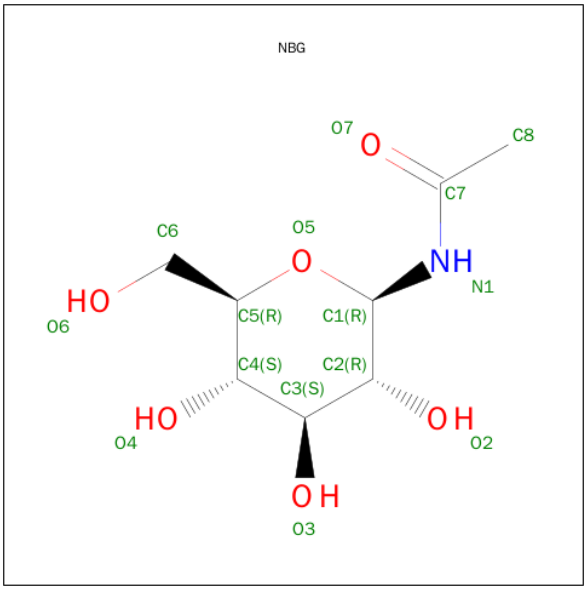
There are 7 unique types of molecules in this entry. The entry contains 13826 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycogen phosphorylase, liver form.

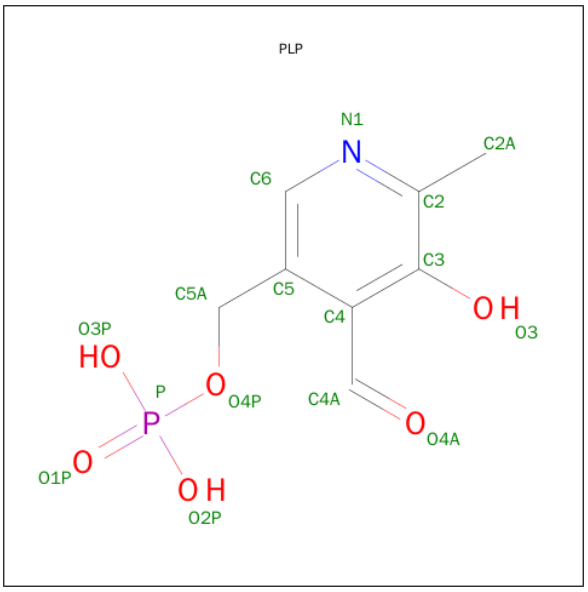
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	793	Total	C	N	O	S	0	0	0
			6437	4134	1092	1182	29			
1	B	791	Total	C	N	O	S	0	0	0
			6420	4125	1090	1176	29			

- Molecule 2 is SUGAR (1-N-ACETYL-BETA-D-GLUCOSAMINE) (three-letter code: NBG) (formula: $C_8H_{15}NO_6$).



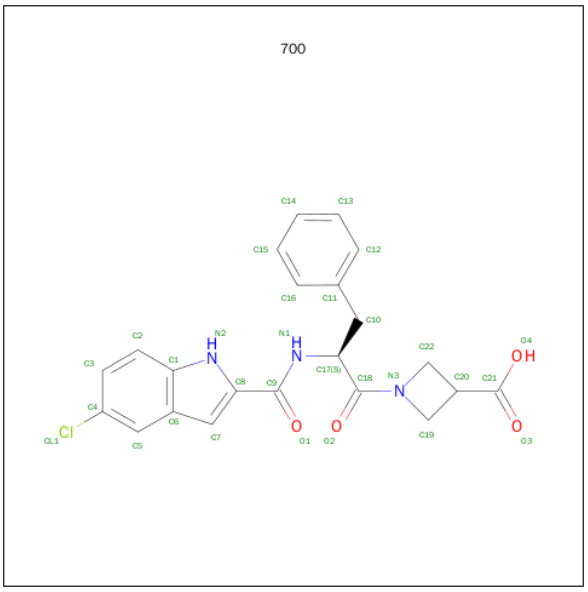
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is [5-CHLORO-1H-INDOL-2-CARBONYL-PHENYLALANINYL]-AZETIDINE -3-CARBOXYLIC ACID (three-letter code: 700) (formula: $C_{22}H_{20}ClN_3O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			30	22	1	3	4		

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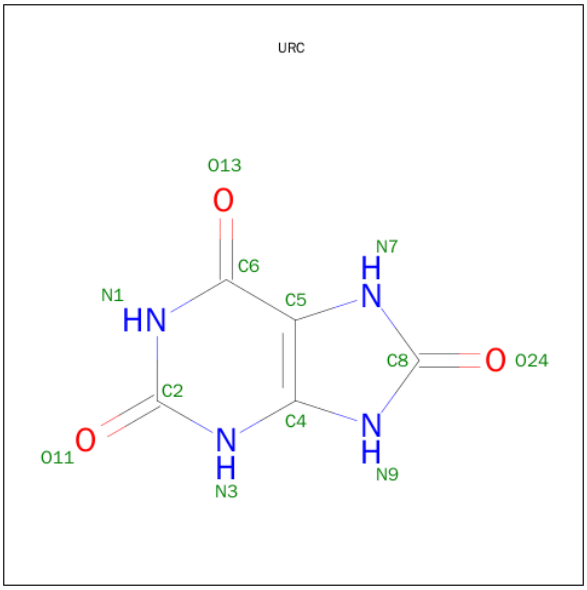
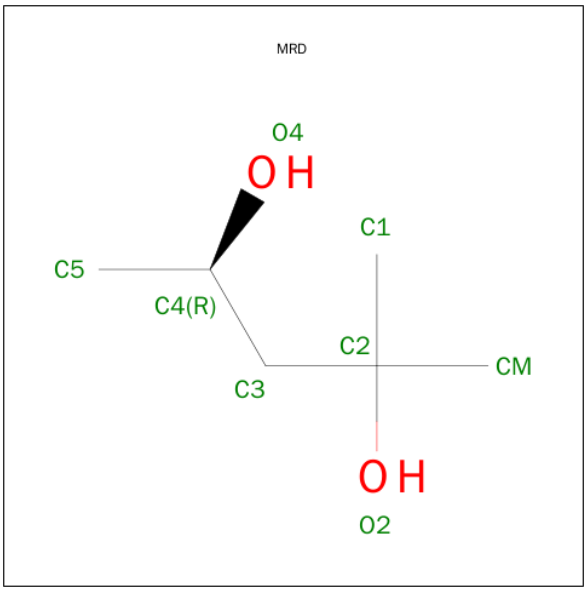
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	Cl	N	O	0	0
			30	22	1	3	4		

- Molecule 5 is URIC ACID (three-letter code: URC) (formula: $C_5H_4N_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			12	5	4	3		
5	B	1	Total	C	N	O	0	0
			12	5	4	3		

- Molecule 6 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 8 6 2	0	0
6	A	1	Total C O 8 6 2	0	0
6	B	1	Total C O 8 6 2	0	0
6	A	1	Total C O 8 6 2	0	0
6	A	1	Total C O 8 6 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	433	Total O 433 433	0	0
7	B	352	Total O 352 352	0	0

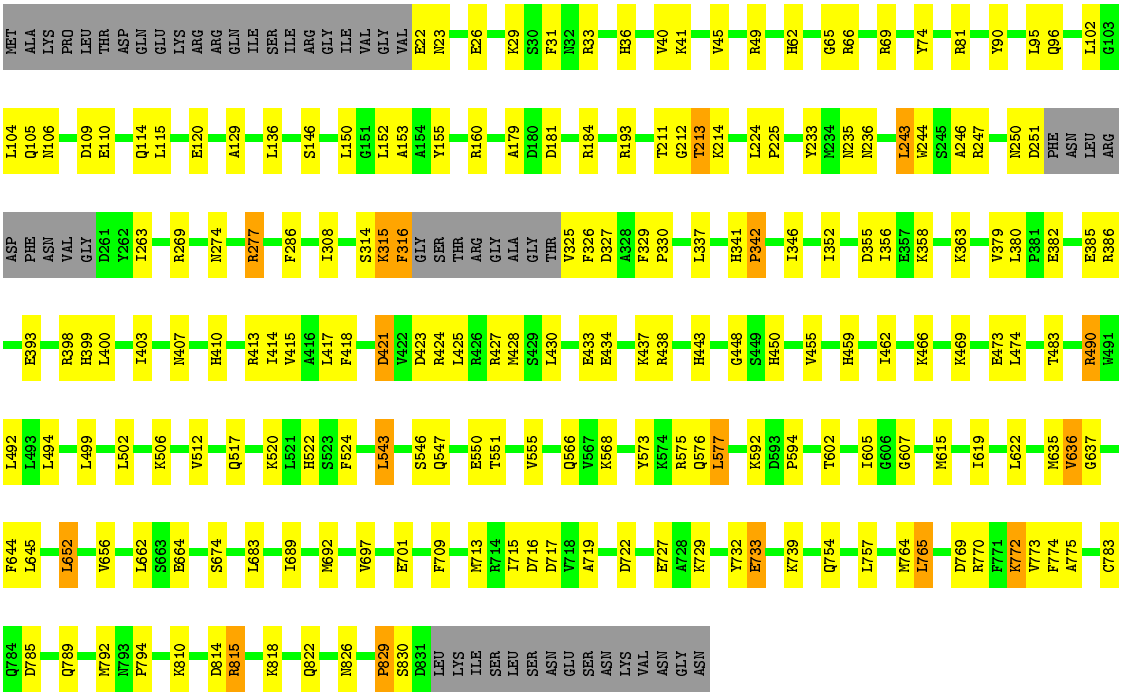
3 Residue-property plots (i)

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.

Note EDS was not executed.

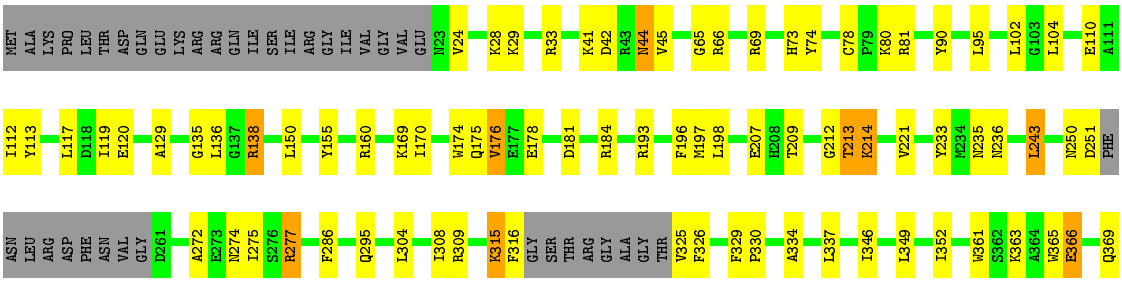
• Molecule 1: Glycogen phosphorylase, liver form

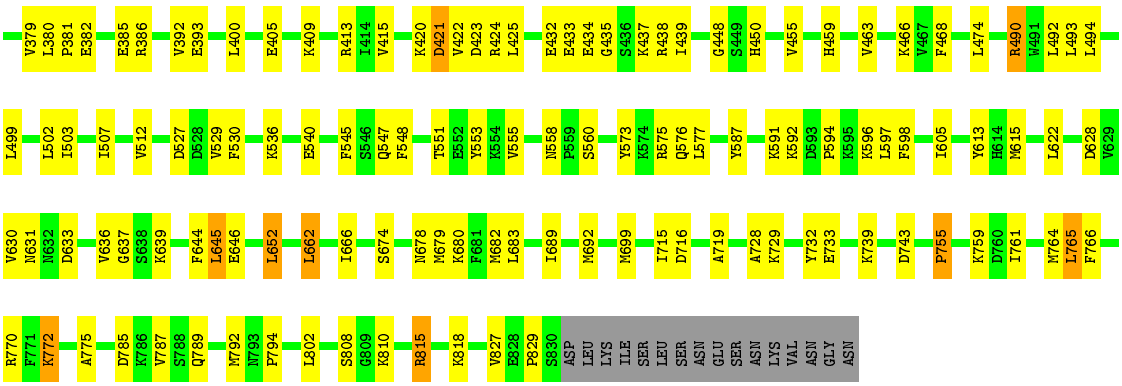
Chain A:



• Molecule 1: Glycogen phosphorylase, liver form

Chain B:




V379 L380 P381 E382
E385 R386
V392 E393
L400
E405
K409
R413 I414 V415
K420 D421 V422 D423 R424 L425
E432 E433 E434 G435 S436 K437 R438 I439
G448 S449 H450
V455
H459
V463
K466 V467 F468
L474
R490 W491 L492 L493 L494
L499 L502 I503
I507
V512
D527 D528 V529 F530
K536
E540
F545 S546 Q547 F548
T551 E552 Y553 K554 V555
N558 P559 S560
Y573 K574 R575 Q576 L577
Y587
K591 K592 D593 P594 K595 K596 L597 F598
I605
Y613 H614 M615
L622
D628 V629
V630 N631 N632 D633
V636 G637 S638 K639
F644 L645 E646
L652
L662
I666
S674
N678 M679 K680 F681 M682 L683
I689
M692
M699
I715 D716
A719
A728 K729
Y732 E733
K739
D743
P755
K759 D760 I761
M764 L765 F766
R770 F771 K772
A775
D785 K786 V787 S788 Q789
M792 N793 P794
L802
S808 G809 K810
R815
K818
V827 E828 P829 S830
ASP LEU LYS ILE SER LEU SER ASN GLU SER ASN LYS VAL ASN GLY ASN

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	124.03Å 124.03Å 123.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.60 – 2.10	Depositor
% Data completeness (in resolution range)	87.8 (40.60-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.194 , 0.236	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13826	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MRD, NBG, URC, 700, PLP

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	0.48	0/6581	0.70	3/8900 (0.0%)
1	B	0.47	0/6564	0.69	2/8877 (0.0%)
All	All	0.47	0/13145	0.69	5/17777 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	490	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	A	490	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	B	129	ALA	N-CA-C	-5.32	96.62	111.00
1	A	129	ALA	N-CA-C	-5.21	96.94	111.00
1	A	602	THR	N-CA-C	-5.08	97.28	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	6437	0	6418	149	0
1	B	6420	0	6408	153	0
2	A	15	0	15	0	0
2	B	15	0	15	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	15	0	7	0	0
3	B	15	0	7	1	0
4	A	30	0	18	0	0
4	B	30	0	18	0	0
5	A	12	0	4	0	0
5	B	12	0	4	0	0
6	A	24	0	42	3	0
6	B	16	0	28	9	0
7	A	433	0	0	16	0
7	B	352	0	0	21	0
All	All	13826	0	12984	307	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 12.

The worst 5 of 307 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:109:ASP:HB3	7:A:2741:HOH:O	1.53	1.05
1:A:49:ARG:HH22	6:A:905:MRD:H1C2	1.26	1.01
1:A:754:GLN:HG2	1:A:757:LEU:HB2	1.43	1.00
1:B:818:LYS:HB3	1:B:818:LYS:NZ	1.81	0.95
1:A:547:GLN:O	1:A:551:THR:HG23	1.72	0.90

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	787/847 (93%)	743 (94%)	38 (5%)	6 (1%)	24 17
1	B	785/847 (93%)	747 (95%)	33 (4%)	5 (1%)	30 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1572/1694 (93%)	1490 (95%)	71 (4%)	11 (1%)	26 21

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	421	ASP
1	A	555	VAL
1	B	421	ASP
1	B	435	GLY
1	A	829	PRO

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	694/740 (94%)	662 (95%)	32 (5%)	33 31
1	B	692/740 (94%)	655 (95%)	37 (5%)	28 25
All	All	1386/1480 (94%)	1317 (95%)	69 (5%)	30 27

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	815	ARG
1	B	138	ARG
1	B	683	LEU
1	B	44	ASN
1	B	95	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	44	ASN
1	B	96	GLN
1	B	459	HIS

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Mol	Chain	Res	Type
1	A	459	HIS
1	B	822	GLN

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

13 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	$\#\|Z\| > 2$
6	MRD	A	1902	-	6,7,7	0.49	0	7,10,10	0.63	0
3	PLP	A	860	1	15,15,16	2.18	9 (60%)	21,22,23	1.20	2 (9%)
2	NBG	A	861	-	15,15,15	1.43	3 (20%)	21,21,21	1.19	2 (9%)
4	700	A	862	-	26,33,33	1.80	8 (30%)	33,47,47	1.65	7 (21%)
5	URC	A	863	-	12,13,13	5.24	6 (50%)	10,19,19	4.56	4 (40%)
6	MRD	A	904	-	6,7,7	0.71	0	7,10,10	1.00	1 (14%)
6	MRD	A	905	-	6,7,7	0.65	0	7,10,10	0.88	0
3	PLP	B	1860	1	15,15,16	2.03	4 (26%)	21,22,23	1.22	2 (9%)
2	NBG	B	1861	-	15,15,15	1.70	4 (26%)	21,21,21	1.34	3 (14%)
4	700	B	1862	-	26,33,33	1.71	8 (30%)	33,47,47	1.63	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	URC	B	1863	-	12,13,13	5.18	7 (58%)	10,19,19	4.69	4 (40%)
6	MRD	B	902	-	6,7,7	0.55	0	7,10,10	0.59	0
6	MRD	B	903	-	6,7,7	1.28	0	7,10,10	0.96	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
6	MRD	A	1902	-	-	0/5/5/5	0/0/0/0
3	PLP	A	860	1	-	0/6/6/8	0/1/1/1
2	NBG	A	861	-	-	0/5/26/26	0/1/1/1
4	700	A	862	-	-	0/15/32/32	0/4/4/4
5	URC	A	863	-	-	0/0/24/24	0/2/2/2
6	MRD	A	904	-	-	0/5/5/5	0/0/0/0
6	MRD	A	905	-	-	0/5/5/5	0/0/0/0
3	PLP	B	1860	1	-	0/6/6/8	0/1/1/1
2	NBG	B	1861	-	-	0/5/26/26	0/1/1/1
4	700	B	1862	-	-	0/15/32/32	0/4/4/4
5	URC	B	1863	-	-	0/0/24/24	0/2/2/2
6	MRD	B	902	-	-	0/5/5/5	0/0/0/0
6	MRD	B	903	-	-	0/5/5/5	0/0/0/0

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	863	URC	C4-N9	-12.02	1.30	1.44
5	B	1863	URC	C4-N9	-11.64	1.30	1.44
5	B	1863	URC	C4-N3	-10.89	1.33	1.46
5	A	863	URC	C4-N3	-10.65	1.33	1.46
5	A	863	URC	C5-N7	-7.01	1.30	1.45

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1863	URC	N7-C8-N9	-5.03	105.41	108.88
5	A	863	URC	N7-C8-N9	-4.69	105.64	108.88
4	B	1862	700	C7-C6-C1	-4.39	102.45	106.27
4	A	862	700	C7-C6-C1	-4.36	102.47	106.27
4	B	1862	700	C4-C5-C6	-3.42	117.04	119.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	904	MRD	1	0
6	A	905	MRD	2	0
3	B	1860	PLP	1	0
2	B	1861	NBG	1	0
6	B	902	MRD	3	0
6	B	903	MRD	8	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.