



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:43 AM GMT

PDB ID : 2NVA
Title : The X-ray crystal structure of the Paramecium bursaria Chlorella virus arginine decarboxylase bound to agmatine
Authors : Shah, R.H.; Akella, R.; Goldsmith, E.; Phillips, M.A.
Deposited on : 2006-11-11
Resolution : 1.80 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
<http://wwpdb.org/validation/2016/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 (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

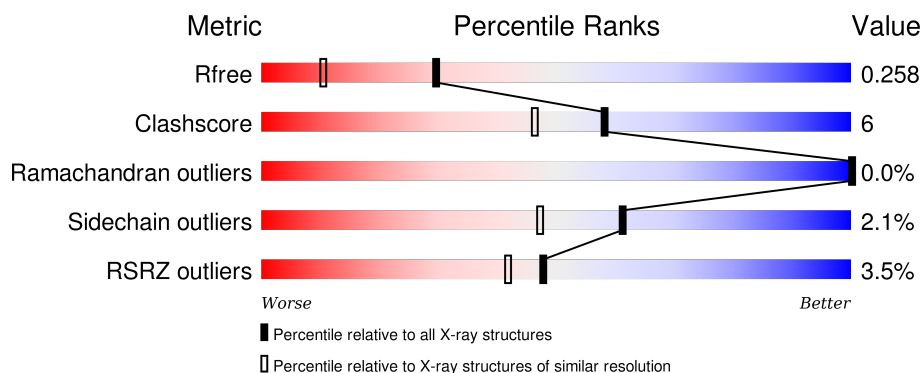
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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.




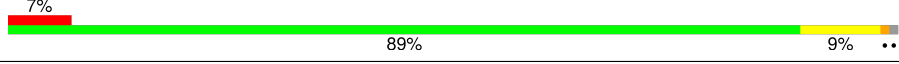
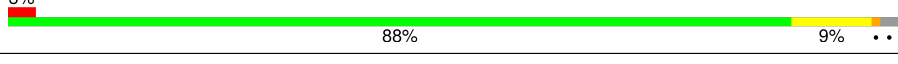
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	372	<div> <div>3%</div> <div>92%</div> <div>6% ..</div> </div>
1	B	372	<div> <div>2%</div> <div>91%</div> <div>8% .</div> </div>
1	C	372	<div> <div>5%</div> <div>87%</div> <div>12% ..</div> </div>
1	D	372	<div> <div>5%</div> <div>88%</div> <div>10% ..</div> </div>
1	E	372	<div> <div>%</div> <div>88%</div> <div>11% ..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	372	
1	G	372	
1	H	372	

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	PL2	H	2008	-	-	-	X

2 Entry composition

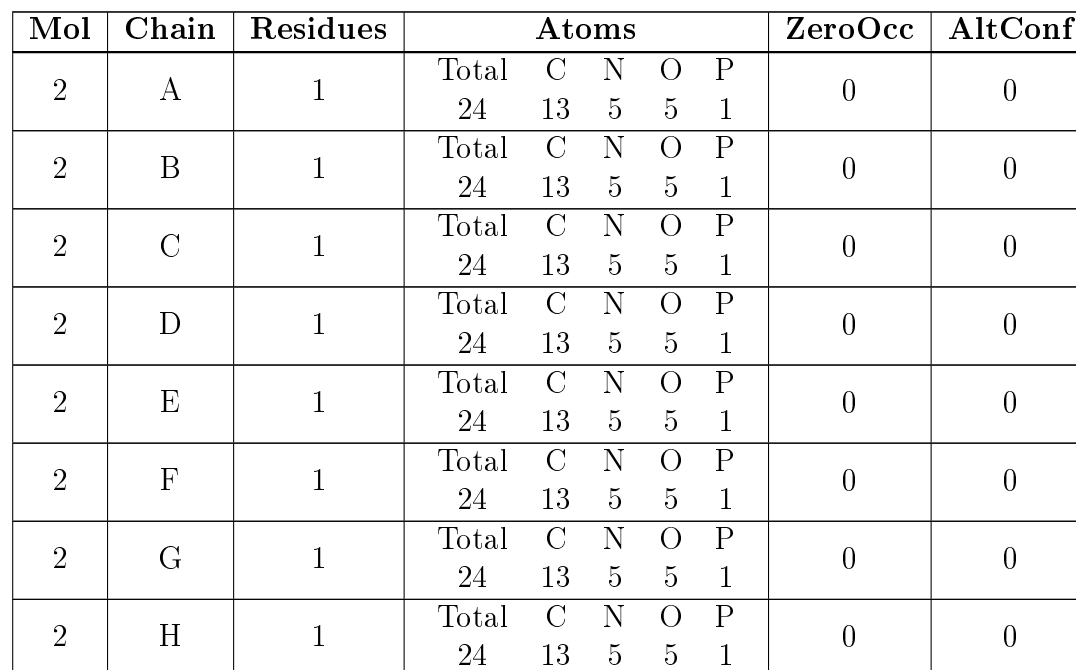
There are 3 unique types of molecules in this entry. The entry contains 25034 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 arginine decarboxylase, A207R protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	1	0
			2939	1884	480	562	13			
1	B	369	Total	C	N	O	S	0	1	0
			2933	1880	478	562	13			
1	C	367	Total	C	N	O	S	0	1	0
			2916	1867	475	561	13			
1	D	371	Total	C	N	O	S	0	1	0
			2941	1884	480	564	13			
1	E	370	Total	C	N	O	S	0	1	0
			2945	1886	479	567	13			
1	F	368	Total	C	N	O	S	0	1	0
			2917	1869	476	559	13			
1	G	368	Total	C	N	O	S	0	1	0
			2902	1858	475	556	13			
1	H	364	Total	C	N	O	S	0	1	0
			2882	1845	469	555	13			

- Molecule 2 is (4-{{(4-{{[AMINO(IMINO)METHYL]AMINO}BUTYL)AMINO]METHYL}-5-HYDROXY-6-METHYLPYRIDIN-3-YL)METHYL DIHYDROGEN PHOSPHATE (three-letter code: PL2) (formula: C₁₃H₂₄N₅O₅P).



- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	219	Total O 219 219	0	0
3	B	193	Total O 193 193	0	0
3	C	163	Total O 163 163	0	0
3	D	173	Total O 173 173	0	0

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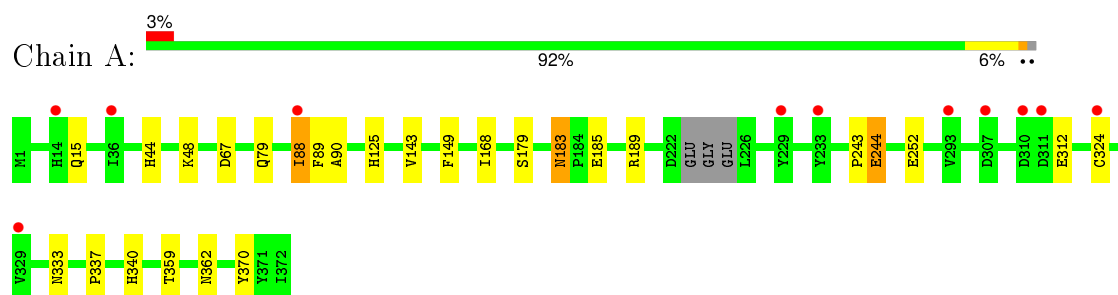
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	211	Total 211	O 211	0	0
3	F	174	Total 174	O 174	0	0
3	G	149	Total 149	O 149	0	0
3	H	185	Total 185	O 185	0	0

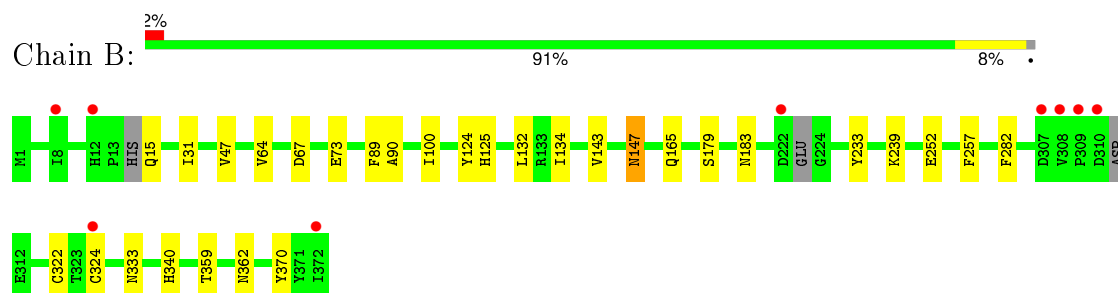
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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.

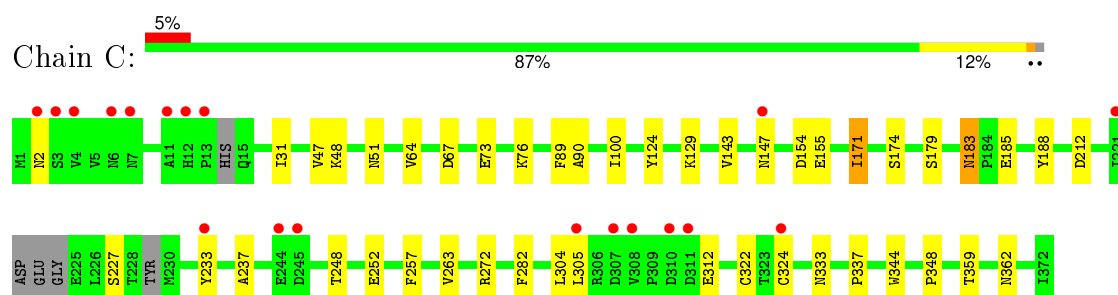
- Molecule 1: arginine decarboxylase, A207R protein



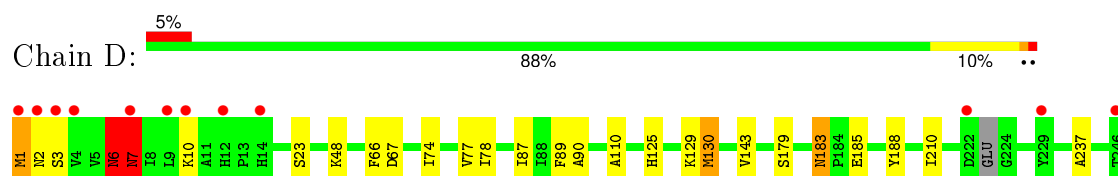
- Molecule 1: arginine decarboxylase, A207R protein

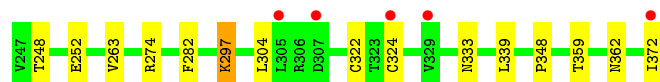


- Molecule 1: arginine decarboxylase, A207R protein

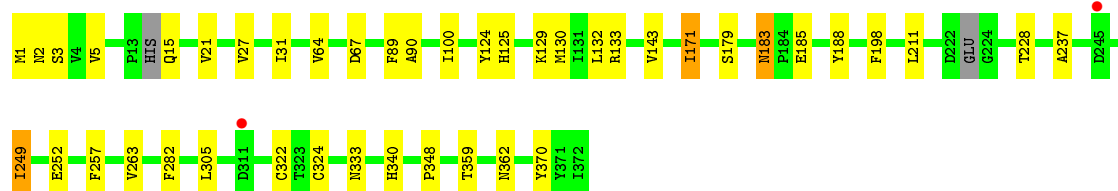
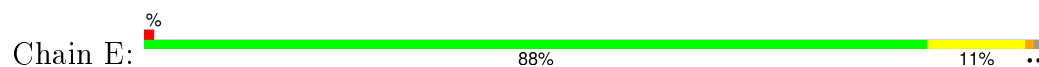


- Molecule 1: arginine decarboxylase, A207R protein

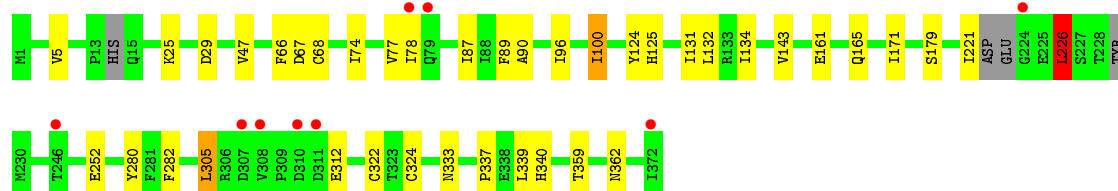
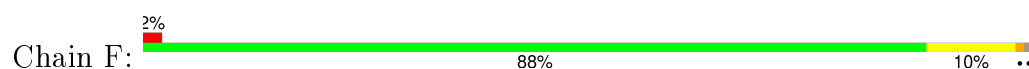




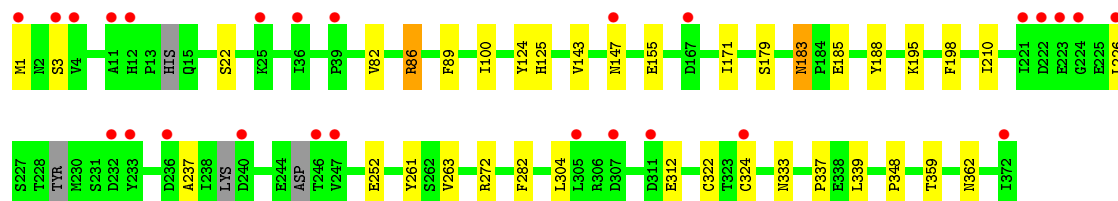
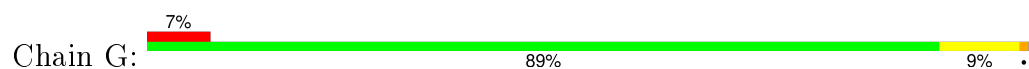
- Molecule 1: arginine decarboxylase, A207R protein



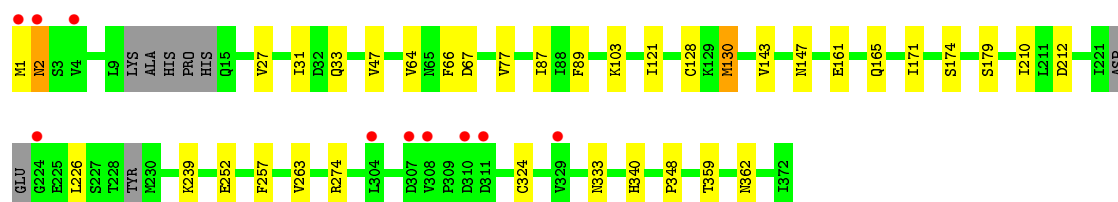
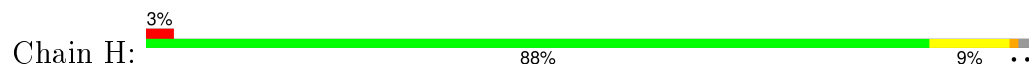
- Molecule 1: arginine decarboxylase, A207R protein



- Molecule 1: arginine decarboxylase, A207R protein



- Molecule 1: arginine decarboxylase, A207R protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.21Å 117.28Å 268.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.74 – 1.80 44.77 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.74-1.80) 99.7 (44.77-1.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.219 , 0.238 0.233 , 0.258	Depositor DCC
R_{free} test set	2052 reflections (0.61%)	DCC
Wilson B-factor (Å ²)	15.6	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 43.3	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	2 of 336913 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25034	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.93 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.2439e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: PL2

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	0.53	0/3014	0.58	0/4095
1	B	0.51	0/3005	0.55	0/4079
1	C	0.51	0/2987	0.59	2/4056 (0.0%)
1	D	0.53	0/3015	0.59	2/4095 (0.0%)
1	E	0.50	0/3018	0.55	0/4099
1	F	0.51	0/2988	0.58	2/4055 (0.0%)
1	G	0.52	0/2972	0.59	2/4033 (0.0%)
1	H	0.52	0/2951	0.57	0/4004
All	All	0.52	0/23950	0.57	8/32516 (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	D	0	1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	86	ARG	CB-CA-C	-6.88	96.63	110.40
1	D	7	ASN	N-CA-C	5.95	127.06	111.00
1	F	226	LEU	CA-CB-CG	5.49	127.92	115.30
1	C	272	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	G	272	ARG	NE-CZ-NH2	-5.39	117.61	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	6	ASN	Peptide

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	2939	0	2834	27	0
1	B	2933	0	2828	33	0
1	C	2916	0	2807	39	0
1	D	2941	0	2832	39	0
1	E	2945	0	2836	37	0
1	F	2917	0	2814	47	0
1	G	2902	0	2786	25	0
1	H	2882	0	2772	38	0
2	A	24	0	21	2	0
2	B	24	0	21	3	0
2	C	24	0	21	3	0
2	D	24	0	21	4	0
2	E	24	0	21	3	0
2	F	24	0	21	4	0
2	G	24	0	21	3	0
2	H	24	0	21	5	0
3	A	219	0	0	3	0
3	B	193	0	0	1	0
3	C	163	0	0	0	0
3	D	173	0	0	0	0
3	E	211	0	0	1	0
3	F	174	0	0	2	0
3	G	149	0	0	0	0
3	H	185	0	0	3	0
All	All	25034	0	22677	271	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 6.

The worst 5 of 271 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:G:324[B]:CYS:SG	2:H:2008:PL2:HA2	1.65	1.33
2:G:2007:PL2:HA2	1:H:324[B]:CYS:SG	1.83	1.18
1:H:121:ILE:HG13	1:H:130:MET:HE3	1.22	1.16
1:G:324[B]:CYS:SG	2:H:2008:PL2:CA	2.36	1.13
1:D:130:MET:HA	1:D:130:MET:HE2	1.28	1.13

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	366/372 (98%)	357 (98%)	9 (2%)	0	100	100
1	B	362/372 (97%)	354 (98%)	8 (2%)	0	100	100
1	C	360/372 (97%)	350 (97%)	10 (3%)	0	100	100
1	D	368/372 (99%)	358 (97%)	9 (2%)	1 (0%)	46	29
1	E	365/372 (98%)	355 (97%)	10 (3%)	0	100	100
1	F	361/372 (97%)	352 (98%)	9 (2%)	0	100	100
1	G	359/372 (96%)	350 (98%)	9 (2%)	0	100	100
1	H	357/372 (96%)	348 (98%)	9 (2%)	0	100	100
All	All	2898/2976 (97%)	2824 (97%)	73 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	7	ASN

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	326/329 (99%)	320 (98%)	6 (2%)	66	54
1	B	325/329 (99%)	319 (98%)	6 (2%)	66	54
1	C	324/329 (98%)	315 (97%)	9 (3%)	51	35
1	D	325/329 (99%)	316 (97%)	9 (3%)	51	35
1	E	327/329 (99%)	319 (98%)	8 (2%)	57	41
1	F	323/329 (98%)	319 (99%)	4 (1%)	78	71
1	G	320/329 (97%)	314 (98%)	6 (2%)	65	52
1	H	319/329 (97%)	313 (98%)	6 (2%)	65	52
All	All	2589/2632 (98%)	2535 (98%)	54 (2%)	61	47

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	10	LYS
1	E	2	ASN
1	H	2	ASN
1	D	89	PHE
1	D	130	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	7	ASN
1	D	362	ASN
1	G	362	ASN
1	D	79	GLN
1	D	218	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	PL2	A	2001	-	21,24,24	1.43	4 (19%)	26,32,32	1.77	4 (15%)
2	PL2	B	2002	-	21,24,24	1.28	3 (14%)	26,32,32	1.51	4 (15%)
2	PL2	C	2003	-	21,24,24	1.30	3 (14%)	26,32,32	1.56	5 (19%)
2	PL2	D	2004	-	21,24,24	1.24	2 (9%)	26,32,32	1.51	3 (11%)
2	PL2	E	2005	-	21,24,24	1.43	3 (14%)	26,32,32	1.69	4 (15%)
2	PL2	F	2006	-	21,24,24	1.30	4 (19%)	26,32,32	1.61	5 (19%)
2	PL2	G	2007	-	21,24,24	1.27	3 (14%)	26,32,32	1.76	4 (15%)
2	PL2	H	2008	-	21,24,24	1.31	4 (19%)	26,32,32	1.59	5 (19%)

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	PL2	A	2001	-	-	0/14/16/16	0/1/1/1
2	PL2	B	2002	-	-	0/14/16/16	0/1/1/1
2	PL2	C	2003	-	-	0/14/16/16	0/1/1/1
2	PL2	D	2004	-	-	0/14/16/16	0/1/1/1
2	PL2	E	2005	-	-	0/14/16/16	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PL2	F	2006	-	-	0/14/16/16	0/1/1/1
2	PL2	G	2007	-	-	0/14/16/16	0/1/1/1
2	PL2	H	2008	-	-	0/14/16/16	0/1/1/1

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2006	PL2	P-OP3	2.02	1.62	1.54
2	B	2002	PL2	C2A-C2	2.03	1.54	1.50
2	H	2008	PL2	P-OP3	2.06	1.62	1.54
2	H	2008	PL2	P-OP2	2.10	1.58	1.51
2	A	2001	PL2	C2A-C2	2.14	1.54	1.50

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2007	PL2	C3-C4-C5	-3.19	115.46	118.82
2	F	2006	PL2	C3-C4-C5	-2.84	115.82	118.82
2	E	2005	PL2	C3-C4-C5	-2.65	116.03	118.82
2	D	2004	PL2	C3-C4-C5	-2.59	116.09	118.82
2	H	2008	PL2	C3-C4-C5	-2.52	116.16	118.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	PL2	2	0
2	B	2002	PL2	3	0
2	C	2003	PL2	3	0
2	D	2004	PL2	4	0
2	E	2005	PL2	3	0
2	F	2006	PL2	4	0
2	G	2007	PL2	3	0
2	H	2008	PL2	5	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	369/372 (99%)	0.33	11 (2%) 54 48	12, 13, 16, 17	0
1	B	369/372 (99%)	0.27	9 (2%) 62 57	11, 13, 16, 18	0
1	C	367/372 (98%)	0.32	19 (5%) 31 25	12, 14, 17, 19	0
1	D	371/372 (99%)	0.24	17 (4%) 36 30	13, 14, 17, 19	0
1	E	370/372 (99%)	0.20	2 (0%) 91 90	12, 13, 16, 18	0
1	F	368/372 (98%)	0.30	9 (2%) 62 57	12, 14, 16, 19	0
1	G	368/372 (98%)	0.37	26 (7%) 19 15	12, 14, 17, 20	0
1	H	364/372 (97%)	0.17	10 (2%) 58 53	13, 14, 16, 19	0
All	All	2946/2976 (98%)	0.28	103 (3%) 48 42	11, 14, 16, 20	0

The worst 5 of 103 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	229	TYR	4.7
1	F	224	GLY	4.4
1	H	310	ASP	3.8
1	G	372	ILE	3.8
1	G	247	VAL	3.6

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	PL2	H	2008	24/24	0.90	0.18	2.23	14,16,17,17	0
2	PL2	G	2007	24/24	0.91	0.16	1.89	14,17,18,18	0
2	PL2	F	2006	24/24	0.91	0.15	1.09	13,16,17,18	0
2	PL2	B	2002	24/24	0.91	0.16	0.71	13,16,17,17	0
2	PL2	C	2003	24/24	0.91	0.15	0.70	14,16,18,18	0
2	PL2	D	2004	24/24	0.92	0.14	0.69	15,16,17,18	0
2	PL2	E	2005	24/24	0.92	0.13	0.06	12,16,17,17	0
2	PL2	A	2001	24/24	0.92	0.13	-0.10	13,16,17,17	0

6.5 Other polymers

There are no such residues in this entry.