

wwPDB X-ray Structure Validation Summary Report (i)

Jan 30, 2024 - 09:32 AM EST

PDB ID 1FPY : Title CRYSTAL STRUCTURE OF GLUTAMINE SYNTHETASE FROM : TYPHIMURIUM SALMONELLA WITH INHIBITOR PHOS-PHINOTHRICIN Authors Gill, H.S.; Eisenberg, D. : Deposited on 2000-08-31

Resolution : 2.89 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.89 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	Similar resolution
	$(\# {\it Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
Clashscore	141614	2172(2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	Qualit	y of chain
-		100	6%	
	A	468	50%	41% 8% •
	-		4%	
1	В	468	52%	40% 8% •
			4%	
1	C	468	50%	41% 8% •
			4%	
1	D	468	51%	40% 8% •
			3%	
1	Ε	468	50%	41% 8% •
			5%	
1	F	468	52%	40% 8% ·
		•		



Mol	Chain	Longth	Quality	of chain
WIOI	Ullain	Length	Quality	
	â		4%	
1	G	468	51%	41% 8% •
-		100	4%	
1	H	468	52%	40% 8% •
			3%	
1	I	468	50%	41% 8% •
			4%	
1	J	468	51%	40% 8% •
			<u>2</u> %	
1	K	468	50%	41% 8% •
	_		4%	
1	L	468	51%	40% 8% •

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
3	ADP	L	4482	-	-	-	Х
4	PPQ	А	5900	-	-	Х	-
4	PPQ	В	5901	-	-	Х	-
4	PPQ	С	5902	-	-	Х	-
4	PPQ	D	5903	-	-	Х	-
4	PPQ	Е	5904	-	-	Х	-
4	PPQ	F	5905	-	-	Х	-
4	PPQ	G	5906	-	-	Х	-
4	PPQ	Н	5907	-	-	Х	-
4	PPQ	Ι	5908	-	-	Х	-
4	PPQ	J	5909	-	-	Х	-
4	PPQ	L	5911	-	-	Х	-



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 47280 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Λ	468	Total	С	Ν	Ο	S	0	26	0
1	A	400	3747	2371	643	713	20	0	20	0
1	В	468	Total	С	Ν	0	S	0	26	0
	D	400	3747	2371	643	713	20	0	20	0
1	С	468	Total	С	Ν	Ο	S	0	26	0
	U	400	3747	2371	643	713	20	0	20	0
1	Л	468	Total	С	Ν	Ο	S	0	26	0
L	D	400	3747	2371	643	713	20	0	20	0
1	F	468	Total	С	Ν	Ο	\mathbf{S}	0	26	0
L	Ľ	400	3747	2371	643	713	20	0	20	0
1	F	468	Total	С	Ν	Ο	\mathbf{S}	0	26	0
L	Ľ	408	3747	2371	643	713	20	0	20	0
1	G	468	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	26	0
1	u	400	3747	2371	643	713	20	0	20	0
1	н	468	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	26	0
	11	400	3747	2371	643	713	20	0	20	0
1	т	468	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	26	0
	1	400	3747	2371	643	713	20	0	20	0
1	Т	468	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	26	0
	0	400	3747	2371	643	713	20	0	20	U
1	K	468	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	26	0
	17	100	3747	2371	643	713	20	0	20	0
1	L	468	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	26	0
L L		100	3747	2371	643	713	20	0	20	U

• Molecule 1 is a protein called GLUTAMINE SYNTHETASE.

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	2	Total Mn 2 2	0	0
2	В	2	Total Mn 2 2	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	С	2	Total Mn 2 2	0	0
2	D	2	Total Mn 2 2	0	0
2	Е	2	Total Mn 2 2	0	0
2	F	2	Total Mn 2 2	0	0
2	G	2	Total Mn 2 2	0	0
2	Н	2	Total Mn 2 2	0	0
2	Ι	2	Total Mn 2 2	0	0
2	J	2	Total Mn 2 2	0	0
2	K	2	Total Mn 2 2	0	0
2	L	2	Total Mn 2 2	0	0

Continued from previous page...

• 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
2	Δ	1	Total	С	Ν	Ο	Р	0	0
0	A	1	27	10	5	10	2	0	0



Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf
2	Р	1	Total	С	Ν	Ο	Р	0	0
J	D	L	27	10	5	10	2	0	0
3	2 C	1	Total	С	Ν	Ο	Р	0	0
0	U	T	27	10	5	10	2	0	0
3	Л	1	Total	\mathbf{C}	Ν	Ο	Р	0	0
0		1	27	10	5	10	2	0	0
3	E	1	Total	С	Ν	Ο	Р	0	0
		1	27	10	5	10	2	0	0
3	F	1	Total	С	Ν	Ο	Р	0	0
	-	T	27	10	5	10	2	0	
3	G	1	Total	С	Ν	Ο	Р	0	0
		1	27	10	5	10	2	0	
3	Н	1	Total	С	Ν	Ο	Р	0	0
		-	27	10	5	10	2	Ŭ	
3	T	1	Total	С	Ν	Ο	Р	0	0
	-	-	27	10	5	10	2	Ŭ	
3	J	1	Total	С	Ν	Ο	Р	0	0
		-	27	10	5	10	2	Ŭ	
3	K	1	Total	С	Ν	Ο	Р	0	0
		-	27	10	5	10	2	Ŭ	
3	L	1	Total	С	Ν	0	Р	0	0
	-		27	10	5	10	2	Ŭ	

• Molecule 4 is PHOSPHINOTHRICIN (three-letter code: PPQ) (formula: $C_5H_{12}NO_4P$).





Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	
4	٨	1	Total	С	Ν	Ο	Р	0	0	
4	A	1	11	5	1	4	1	0	0	
4	D	1	Total	С	Ν	Ο	Р	0	0	
4	D	1	11	5	1	4	1	0	0	
4	C	1	Total	С	Ν	Ο	Р	0	0	
4	C	1	11	5	1	4	1	0	0	
4	Л	1	Total	С	Ν	Ο	Р	0	0	
4	D	1	11	5	1	4	1	0	0	
4	F	1	Total	С	Ν	Ο	Р	0	0	
4	Ľ	1	11	5	1	4	1	0	0	0
4	Б	1	Total	С	Ν	0	Р	0	0	
4	T,	Ľ	1	11	5	1	4	1	0	0
4	С	1	Total	С	Ν	0	Р	0	0	
4	G	1	11	5	1	4	1	0	0	
4	н	1	Total	С	Ν	Ο	Р	0	0	
-1	11	T	11	5	1	4	1	0	0	
4	T	1	Total	С	Ν	Ο	Р	0	0	
-1	1	T	11	5	1	4	1	0	0	
4	T	1	Total	С	Ν	Ο	Р	0	0	
4	J	I	11	5	1	4	1	0	U	
4	K	1	Total	С	Ν	0	Р	0	0	
±	17	L	11	5	1	4	1	U	U	
4	T.	1	Total	C	N	Ō	Р	0	0	
1		L	11	5	1	4	1		U	

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	152	Total O 152 152	0	0
5	В	155	Total O 155 155	0	0
5	С	152	Total O 152 152	0	0
5	D	153	Total O 153 153	0	0
5	Ε	154	Total O 154 154	0	0
5	F	152	Total O 152 152	0	0
5	G	155	Total O 155 155	0	0
5	Н	150	Total O 150 150	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Ι	156	Total O 156 156	0	0
5	J	151	Total O 151 151	0	0
5	К	153	Total O 153 153	0	0
5	L	153	Total O 153 153	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 SYNTHETASE









B

S350
 S355
 S356
 S357
 S356
 S356
 S356
 S356
 <li

• Molecule 1: GLUTAMINE SYNTHETASE

3% Chain E: 50% 41% 8% . 1209 1210 1211 M272 S273 3350 2351 352 406 407 N419 D422 L423 D424 D424 F425 E426 E426 F428 F428 K429 A30 G431 P408 Q409 • Molecule 1: GLUTAMINE SYNTHETASE 5% Chain F: 52% 8% • 40% K27 E28 Q29 H30 A188 Q189 D190 T191 R192 S193 P181 V182 A208 H209 H210 H211 IN DATA BANK











0422 0424 0424 0424 0424 0425 0426 0426 0430 0431 0422 0423 1428 1428 1428 1428 1436 0431 1435 0436 0446 0464 0464 0464



D422 D422 D422 D422 T423 F425 F426 F423 F433 F434 F434 F434 F434 F434 F435 F436 P440 P441 P446 P467 P468 P468 P468 P468 P468 P468 P468



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	230.60Å 132.50Å 195.90Å	Depositor
a, b, c, α , β , γ	90.00° 102.40° 90.00°	Depositor
Bosolution(A)	15.00 - 2.89	Depositor
Resolution (A)	15.00 - 2.89	EDS
% Data completeness	70.0 (15.00-2.89)	Depositor
(in resolution range)	68.7(15.00-2.89)	EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.86 (at 2.91 \text{\AA})$	Xtriage
Refinement program	X-PLOR 3.843	Depositor
B B.	0.248 , 0.263	Depositor
II, II free	0.245 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor $(Å^2)$	51.1	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.24, 69.6	EDS
L-test for $twinning^2$	$ \langle L \rangle = 0.50, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	47280	wwPDB-VP
Average B, all atoms $(Å^2)$	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.37% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: PPQ, ADP, MN

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).

Mal	Chain	Bond lengths		Bond angles		
MIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.63	0/3850	0.90	2/5212~(0.0%)	
1	В	0.63	0/3850	0.90	2/5212~(0.0%)	
1	С	0.63	0/3850	0.90	2/5212~(0.0%)	
1	D	0.63	0/3850	0.90	2/5212~(0.0%)	
1	Е	0.63	0/3850	0.90	2/5212~(0.0%)	
1	F	0.63	0/3850	0.90	2/5212~(0.0%)	
1	G	0.63	0/3850	0.90	2/5212~(0.0%)	
1	Н	0.63	0/3850	0.90	2/5212~(0.0%)	
1	Ι	0.63	0/3850	0.90	2/5212~(0.0%)	
1	J	0.63	0/3850	0.90	2/5212~(0.0%)	
1	Κ	0.63	0/3850	0.90	2/5212~(0.0%)	
1	L	0.63	0/3850	0.90	2/5212~(0.0%)	
All	All	0.63	0/46200	0.90	$24/\overline{62544}~(0.0\%)$	

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	А	0	1
1	В	0	1
1	С	0	1
1	D	0	1
1	Е	0	1
1	F	0	1
1	G	0	1
1	Н	0	1
1	Ι	0	1
1	J	0	1
1	Κ	0	1



Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1
All	All	0	12

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	В	179[A]	TYR	CB-CG-CD2	-5.67	117.60	121.00
1	В	179[B]	TYR	CB-CG-CD2	-5.67	117.60	121.00
1	J	179[A]	TYR	CB-CG-CD2	-5.66	117.60	121.00
1	J	179[B]	TYR	CB-CG-CD2	-5.66	117.60	121.00
1	С	179[A]	TYR	CB-CG-CD2	-5.66	117.60	121.00

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	208	ALA	Mainchain
1	В	208	ALA	Mainchain
1	С	208	ALA	Mainchain
1	D	208	ALA	Mainchain
1	Е	208	ALA	Mainchain

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	А	3747	0	3621	330	0
1	В	3747	0	3621	325	0
1	С	3747	0	3621	330	0
1	D	3747	0	3621	320	0
1	Е	3747	0	3621	322	0
1	F	3747	0	3621	325	0
1	G	3747	0	3621	328	0
1	Н	3747	0	3621	324	0
1	Ι	3747	0	3621	334	0



1	F	Έ	Υ

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	3747		3691	222	
1	J K	3747	0	3621	308	0
1	IX L	3747	0	3621	320	0
$\frac{1}{2}$		0141	0	0	0	0
$\frac{2}{2}$	R R	2	0	0	0	0
$\frac{2}{2}$	D C	2	0	0	0	0
$\frac{2}{2}$		2	0	0	0	0
$\frac{2}{2}$	E E	2	0	0	0	0
$\frac{2}{2}$	E F	2	0	0	0	0
$\frac{2}{2}$	G	2	0	0	0	0
$\frac{2}{2}$	н	2	0	0	0	0
$\frac{2}{2}$	I	2	0	0	0	0
$\frac{2}{2}$	I	2	0	0	0	0
$\frac{2}{2}$	K K	2	0	0	0	0
$\frac{2}{2}$	L	2	0	0	0	0
3		27	0	10	8	0
3	B	27	0	10	8	0
3	C	27	0	10	8	0
3	D	27	0	10	8	0
3	E E	27	0	10	8	0
3	F	27	0	10	8	0
3	G	27	0	10	8	0
3	H	27	0	10	8	0
3	I	27	0	10	8	0
3	J	27	0	10	8	0
3	K	27	0	10	8	0
3	L	27	0	10	8	0
4	А	11	0	10	7	0
4	В	11	0	10	7	0
4	С	11	0	10	6	0
4	D	11	0	10	6	0
4	Е	11	0	10	6	0
4	F	11	0	10	7	0
4	G	11	0	10	6	0
4	Н	11	0	10	7	0
4	Ι	11	0	10	6	0
4	J	11	0	10	6	0
4	K	11	0	10	5	0
4	L	11	0	10	7	0
5	A	152	0	0	89	0
5	В	155	0	0	91	0
5	С	152	0	0	93	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	153	0	0	85	0
5	Ε	154	0	0	91	0
5	F	152	0	0	91	0
5	G	155	0	0	91	0
5	Н	150	0	0	88	0
5	Ι	156	0	0	92	0
5	J	151	0	0	90	0
5	Κ	153	0	0	85	0
5	L	153	0	0	90	0
All	All	47280	0	43692	3738	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 42.

The worst 5 of 3738 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)
3:L:4482:ADP:N9	3:L:4482:ADP:C1'	1.70	1.54
3:C:4473:ADP:N9	3:C:4473:ADP:C1'	1.70	1.53
3:I:4479:ADP:N9	3:I:4479:ADP:C1'	1.70	1.53
3:H:4478:ADP:N9	3:H:4478:ADP:C1'	1.70	1.52
3:B:4472:ADP:N9	3:B:4472:ADP:C1'	1.70	1.52

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	Pe	erc	entil	\mathbf{es}	
1	А	482/468~(103%)	411 (85%)	50 (10%)	21 (4%)		2	10	
1	В	482/468~(103%)	411 (85%)	50 (10%)	21 (4%)		2	10	



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	С	482/468~(103%)	411 (85%)	50 (10%)	21 (4%)	2	10
1	D	482/468~(103%)	411 (85%)	50 (10%)	21 (4%)	2	10
1	Ε	482/468~(103%)	411 (85%)	50 (10%)	21 (4%)	2	10
1	F	482/468~(103%)	411 (85%)	50 (10%)	21 (4%)	2	10
1	G	482/468~(103%)	411 (85%)	50 (10%)	21 (4%)	2	10
1	Н	482/468~(103%)	411 (85%)	50 (10%)	21 (4%)	2	10
1	Ι	482/468~(103%)	411 (85%)	50 (10%)	21 (4%)	2	10
1	J	482/468~(103%)	411 (85%)	50 (10%)	21 (4%)	2	10
1	Κ	482/468~(103%)	411 (85%)	50 (10%)	21 (4%)	2	10
1	L	482/468~(103%)	411 (85%)	50 (10%)	21 (4%)	2	10
All	All	5784/5616~(103%)	4932 (85%)	600 (10%)	252 (4%)	4	10

5 of 252 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	58	LYS
1	А	177[A]	GLY
1	А	177[B]	GLY
1	А	180[A]	PHE
1	А	180[B]	PHE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	395/384~(103%)	350~(89%)	45 (11%)	5	17	
1	В	395/384~(103%)	350~(89%)	45~(11%)	5	17	
1	С	395/384~(103%)	350~(89%)	45 (11%)	5	17	
1	D	395/384~(103%)	350~(89%)	45 (11%)	5	17	
1	Е	395/384~(103%)	350~(89%)	45 (11%)	5	17	
1	F	395/384~(103%)	350~(89%)	45 (11%)	5	17	



Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
1	G	395/384~(103%)	350~(89%)	45 (11%)	5	17	
1	Н	395/384~(103%)	350~(89%)	45 (11%)	5	17	
1	Ι	395/384~(103%)	350~(89%)	45 (11%)	5	17	
1	J	395/384~(103%)	350~(89%)	45 (11%)	5	17	
1	Κ	395/384~(103%)	350~(89%)	45 (11%)	5	17	
1	L	395/384~(103%)	350~(89%)	45 (11%)	5	17	
All	All	4740/4608~(103%)	4200 (89%)	540 (11%)	6	17	

Continued from previous page...

5 of 540 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Κ	115	LEU
1	Κ	337	ARG
1	Κ	101	ASP
1	L	332	LEU
1	Е	125	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	277	ASN
1	Ι	218	GLN
1	L	313	ASN
1	G	384	ASN
1	Н	277	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 monosaccharides in this entry.



5.6 Ligand geometry (i)

Of 48 ligands modelled in this entry, 24 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).

Mal	Tuno	Chain	Dog	Link	Bo	Bond lengths		Bond angles		
IVIOI	Type	Ullalli	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
4	PPQ	L	5911	2	$7,\!10,\!10$	1.23	0	$7,\!14,\!14$	4.61	2 (28%)
3	ADP	С	4473	2	$24,\!29,\!29$	2.62	8 (33%)	$29,\!45,\!45$	3.38	12 (41%)
3	ADP	А	4471	2	$24,\!29,\!29$	2.62	8 (33%)	$29,\!45,\!45$	3.38	12 (41%)
4	PPQ	С	5902	2	7,10,10	1.23	0	7,14,14	4.60	2 (28%)
3	ADP	Е	4475	2	24,29,29	2.61	8 (33%)	$29,\!45,\!45$	<mark>3.38</mark>	12 (41%)
4	PPQ	G	5906	2	7,10,10	1.24	0	7,14,14	4.61	2 (28%)
4	PPQ	К	5910	2	7,10,10	1.22	0	7,14,14	4.60	2 (28%)
4	PPQ	Н	5907	2	7,10,10	1.24	0	7,14,14	4.61	2 (28%)
3	ADP	L	4482	2	24,29,29	2.63	8 (33%)	29,45,45	<mark>3.38</mark>	12 (41%)
3	ADP	D	4474	2	24,29,29	2.61	8 (33%)	29,45,45	3.38	12 (41%)
4	PPQ	В	5901	2	7,10,10	1.23	0	7,14,14	4.61	2 (28%)
4	PPQ	А	5900	2	7,10,10	1.24	0	7,14,14	4.61	2 (28%)
4	PPQ	Е	5904	2	7,10,10	1.24	0	7,14,14	4.61	2 (28%)
3	ADP	Ι	4479	2	24,29,29	2.62	8 (33%)	29,45,45	<mark>3.38</mark>	12 (41%)
4	PPQ	F	5905	2	7,10,10	1.23	0	7,14,14	4.60	2 (28%)
3	ADP	G	4477	2	24,29,29	2.62	8 (33%)	29,45,45	<mark>3.38</mark>	12 (41%)
4	PPQ	D	5903	2	7,10,10	1.24	0	7,14,14	4.61	2 (28%)
3	ADP	F	4476	2	24,29,29	2.61	8 (33%)	29,45,45	<mark>3.38</mark>	12 (41%)
4	PPQ	J	5909	2	7,10,10	1.24	0	7,14,14	4.61	2 (28%)
3	ADP	K	4481	2	24,29,29	2.62	8 (33%)	29,45,45	<mark>3.39</mark>	12 (41%)
3	ADP	Н	4478	2	24,29,29	2.62	8 (33%)	29,45,45	3.38	12 (41%)
3	ADP	В	4472	2	24,29,29	2.61	8 (33%)	29,45,45	3.38	12 (41%)
4	PPQ	Ι	5908	2	7,10,10	1.25	0	7,14,14	4.61	2 (28%)
3	ADP	J	4480	2	24,29,29	2.62	8 (33%)	29,45,45	3.38	12 (41%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PPQ	L	5911	2	-	7/10/10/10	_
3	ADP	С	4473	2	-	5/12/32/32	0/3/3/3
3	ADP	А	4471	2	-	5/12/32/32	0/3/3/3
4	PPQ	С	5902	2	-	7/10/10/10	-
3	ADP	Е	4475	2	-	5/12/32/32	0/3/3/3
4	PPQ	G	5906	2	-	7/10/10/10	-
4	PPQ	K	5910	2	-	7/10/10/10	-
4	PPQ	Н	5907	2	-	7/10/10/10	-
3	ADP	L	4482	2	-	5/12/32/32	0/3/3/3
3	ADP	D	4474	2	-	5/12/32/32	0/3/3/3
4	PPQ	В	5901	2	-	7/10/10/10	-
4	PPQ	А	5900	2	-	7/10/10/10	-
4	PPQ	Е	5904	2	-	7/10/10/10	-
3	ADP	Ι	4479	2	-	5/12/32/32	0/3/3/3
4	PPQ	F	5905	2	-	7/10/10/10	-
3	ADP	G	4477	2	-	5/12/32/32	0/3/3/3
4	PPQ	D	5903	2	-	7/10/10/10	-
3	ADP	F	4476	2	-	5/12/32/32	0/3/3/3
4	PPQ	J	5909	2	-	7/10/10/10	-
3	ADP	K	4481	2	-	5/12/32/32	0/3/3/3
3	ADP	Н	4478	2	-	5/12/32/32	0/3/3/3
3	ADP	В	4472	2	-	5/12/32/32	0/3/3/3
4	PPQ	Ι	5908	2	-	7/10/10/10	-
3	ADP	J	4480	2	-	5/12/32/32	0/3/3/3

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.

The worst 5 of 96 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(\text{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
3	L	4482	ADP	O4'-C1'	7.46	1.51	1.41
3	Κ	4481	ADP	O4'-C1'	7.46	1.51	1.41
3	J	4480	ADP	O4'-C1'	7.45	1.51	1.41
3	Ι	4479	ADP	O4'-C1'	7.44	1.51	1.41
3	G	4477	ADP	O4'-C1'	7.44	1.51	1.41



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	J	4480	ADP	O4'-C1'-C2'	-10.81	91.13	106.93
3	L	4482	ADP	O4'-C1'-C2'	-10.81	91.13	106.93
3	С	4473	ADP	O4'-C1'-C2'	-10.80	91.14	106.93
3	В	4472	ADP	O4'-C1'-C2'	-10.80	91.15	106.93
3	А	4471	ADP	O4'-C1'-C2'	-10.80	91.15	106.93

The worst 5 of 168 bond angle outliers are listed below:

There are no chirality outliers.

5 of 144 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	4471	ADP	C5'-O5'-PA-O1A
3	А	4471	ADP	C5'-O5'-PA-O2A
3	В	4472	ADP	C5'-O5'-PA-O1A
3	В	4472	ADP	C5'-O5'-PA-O2A
3	С	4473	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

24 monomers are involved in 172 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	5911	PPQ	7	0
3	С	4473	ADP	8	0
3	А	4471	ADP	8	0
4	С	5902	PPQ	6	0
3	Е	4475	ADP	8	0
4	G	5906	PPQ	6	0
4	Κ	5910	PPQ	5	0
4	Н	5907	PPQ	7	0
3	L	4482	ADP	8	0
3	D	4474	ADP	8	0
4	В	5901	PPQ	7	0
4	А	5900	PPQ	7	0
4	Е	5904	PPQ	6	0
3	Ι	4479	ADP	8	0
4	F	5905	PPQ	7	0
3	G	4477	ADP	8	0
4	D	5903	PPQ	6	0
3	F	4476	ADP	8	0
4	J	5909	PPQ	6	0
3	Κ	4481	ADP	8	0
3	Н	4478	ADP	8	0



Continued from previous page...

Mol	Chain	\mathbf{Res}	Type	Clashes	Symm-Clashes
3	В	4472	ADP	8	0
4	Ι	5908	PPQ	6	0
3	J	4480	ADP	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





















Torsions

Rings













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, 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		$\mathbf{OWAB}(\mathrm{\AA}^2)$	$\mathbf{Q}{<}0.9$	
1	А	468/468~(100%)	0.10	30~(6%)	19	15	20, 47, 80, 100	94 (20%)
1	В	468/468~(100%)	-0.16	18 (3%)	40	36	20, 47, 80, 100	94 (20%)
1	С	468/468~(100%)	-0.19	20 (4%)	35	31	20, 47, 80, 100	94 (20%)
1	D	468/468~(100%)	-0.29	21 (4%)	33	29	20, 47, 80, 100	94 (20%)
1	Е	468/468 (100%)	-0.22	16 (3%)	45	40	20, 47, 80, 100	94 (20%)
1	F	468/468 (100%)	-0.16	24 (5%)	28	24	20, 47, 80, 100	94 (20%)
1	G	468/468~(100%)	-0.30	18 (3%)	40	36	20, 47, 80, 100	94 (20%)
1	Н	468/468~(100%)	-0.25	20 (4%)	35	31	20, 47, 80, 100	94 (20%)
1	Ι	468/468~(100%)	-0.36	15 (3%)	47	43	20, 47, 80, 100	94 (20%)
1	J	468/468~(100%)	-0.26	18 (3%)	40	36	20, 47, 80, 100	94 (20%)
1	K	468/468~(100%)	-0.35	11 (2%)	59	56	20, 47, 80, 100	94 (20%)
1	L	468/468 (100%)	-0.30	17 (3%)	42	37	20, 47, 80, 100	94 (20%)
All	All	5616/5616~(100%)	-0.23	228 (4%)	37	32	20, 47, 80, 100	1128 (20%)

The worst 5 of 228 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Κ	396	LEU	10.3
1	F	396	LEU	8.7
1	L	396	LEU	7.7
1	D	395	ASN	7.4
1	J	60	ILE	7.3

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 monosaccharides 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, 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	B -factors($Å^2$)	Q<0.9
3	ADP	L	4482	27/27	0.73	0.42	42,80,100,100	27
3	ADP	С	4473	27/27	0.76	0.36	42,80,100,100	27
3	ADP	K	4481	27/27	0.78	0.35	42,80,100,100	27
3	ADP	Ι	4479	27/27	0.78	0.36	42,80,100,100	27
3	ADP	Е	4475	27/27	0.79	0.39	42,80,100,100	27
3	ADP	Н	4478	27/27	0.81	0.32	42,80,100,100	27
3	ADP	В	4472	27/27	0.82	0.31	42,80,100,100	27
3	ADP	F	4476	27/27	0.82	0.41	42,80,100,100	27
3	ADP	J	4480	27/27	0.84	0.30	42,80,100,100	27
3	ADP	А	4471	27/27	0.84	0.35	42,80,100,100	27
3	ADP	G	4477	27/27	0.84	0.28	42,80,100,100	27
3	ADP	D	4474	27/27	0.88	0.34	42,80,100,100	27
2	MN	Н	470	1/1	0.91	0.07	43,43,43,43	0
4	PPQ	В	5901	11/11	0.91	0.20	16,36,70,83	11
2	MN	С	469	1/1	0.92	0.07	41,41,41,41	0
2	MN	G	469	1/1	0.92	0.08	41,41,41,41	0
4	PPQ	F	5905	11/11	0.92	0.20	$16,\!36,\!70,\!83$	11
4	PPQ	D	5903	11/11	0.93	0.19	$16,\!36,\!70,\!83$	11
2	MN	D	469	1/1	0.93	0.07	41,41,41,41	0
4	PPQ	G	5906	11/11	0.93	0.17	16,36,70,83	11
4	PPQ	Н	5907	11/11	0.93	0.20	$16,\!36,\!70,\!83$	11
4	PPQ	Ι	5908	11/11	0.93	0.22	$16,\!36,\!70,\!83$	11
4	PPQ	С	5902	11/11	0.94	0.16	$16,\!36,\!70,\!83$	11
4	PPQ	Е	5904	11/11	0.94	0.15	$16,\!36,\!70,\!83$	11
4	PPQ	K	5910	11/11	0.94	0.17	16,36,70,83	11
4	PPQ	A	5900	11/11	0.95	0.16	16,36,70,83	11
4	PPQ	J	5909	11/11	0.95	0.19	16,36,70,83	11
2	MN	E	469	1/1	0.95	0.04	41,41,41,41	0
4	PPQ	L	5911	11/11	0.95	0.21	16,36,70,83	11
2	MN	Н	469	1/1	0.96	0.10	41,41,41,41	0
2	MN	K	469	1/1	0.97	0.11	41,41,41,41	0
2	MN	F	469	1/1	0.97	0.06	41,41,41,41	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
2	MN	А	470	1/1	0.97	0.03	43,43,43,43	0
2	MN	А	469	1/1	0.97	0.06	41,41,41,41	0
2	MN	Е	470	1/1	0.97	0.06	43,43,43,43	0
2	MN	F	470	1/1	0.98	0.06	43,43,43,43	0
2	MN	D	470	1/1	0.98	0.08	43,43,43,43	0
2	MN	В	469	1/1	0.98	0.04	41,41,41,41	0
2	MN	С	470	1/1	0.98	0.03	43,43,43,43	0
2	MN	В	470	1/1	0.98	0.05	43,43,43,43	0
2	MN	K	470	1/1	0.98	0.04	43,43,43,43	0
2	MN	L	469	1/1	0.98	0.11	41,41,41,41	0
2	MN	L	470	1/1	0.98	0.05	43,43,43,43	0
2	MN	J	469	1/1	0.99	0.07	41,41,41,41	0
2	MN	J	470	1/1	0.99	0.02	43,43,43,43	0
2	MN	G	470	1/1	0.99	0.04	43,43,43,43	0
2	MN	Ι	469	1/1	0.99	0.06	41,41,41,41	0
2	MN	Ι	470	1/1	0.99	0.04	43,43,43,43	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



























6.5 Other polymers (i)

There are no such residues in this entry.

