



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 07:13 pm BST

PDB ID : 6KG1
Title : NifS from Helicobacter pylori, soaked with L-cysteine for 180 sec
Authors : Nakamura, R.; Takahashi, Y.; Fujishiro, T.
Deposited on : 2019-07-09
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

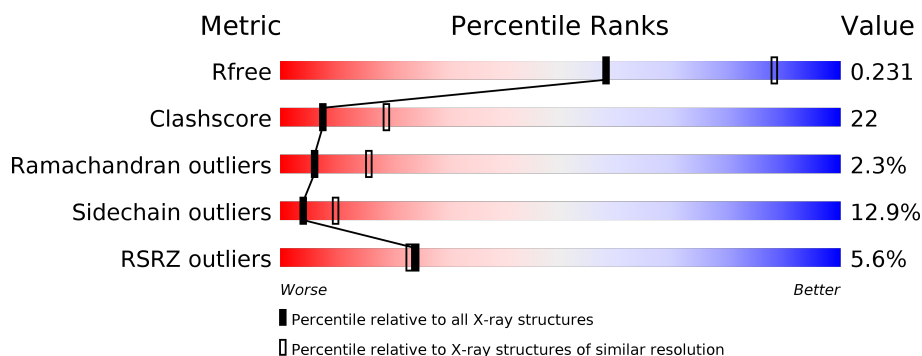
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 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 $\leq 5\%$. 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	401	<div> <div>5%</div> <div>56%</div> <div>24%</div> <div>9%</div> <div>10%</div> </div>

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
4	PDA	A	503	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2814 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 Cysteine desulfurase IscS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2780	1757	487	525	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	LEU	engineered mutation	UNP O25008
A	138	ARG	LYS	engineered mutation	UNP O25008
A	388	VAL	-	expression tag	UNP O25008
A	389	ASP	-	expression tag	UNP O25008
A	390	LEU	-	expression tag	UNP O25008
A	391	VAL	-	expression tag	UNP O25008
A	392	PRO	-	expression tag	UNP O25008
A	393	ARG	-	expression tag	UNP O25008
A	394	GLY	-	expression tag	UNP O25008
A	395	SER	-	expression tag	UNP O25008
A	396	HIS	-	expression tag	UNP O25008
A	397	HIS	-	expression tag	UNP O25008
A	398	HIS	-	expression tag	UNP O25008
A	399	HIS	-	expression tag	UNP O25008
A	400	HIS	-	expression tag	UNP O25008
A	401	HIS	-	expression tag	UNP O25008

- Molecule 2 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).

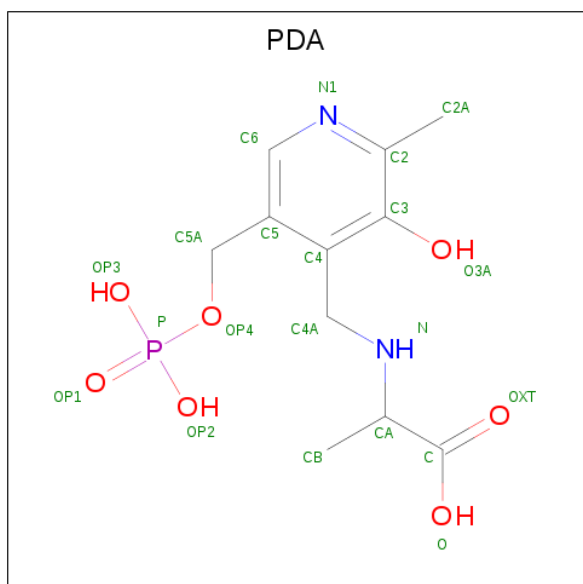


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	3	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is 2-[(3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YLMETHYL)-AMINO]-PROPIONIC ACID (three-letter code: PDA) (formula: C₁₁H₁₇N₂O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			21	11	2	7	1		

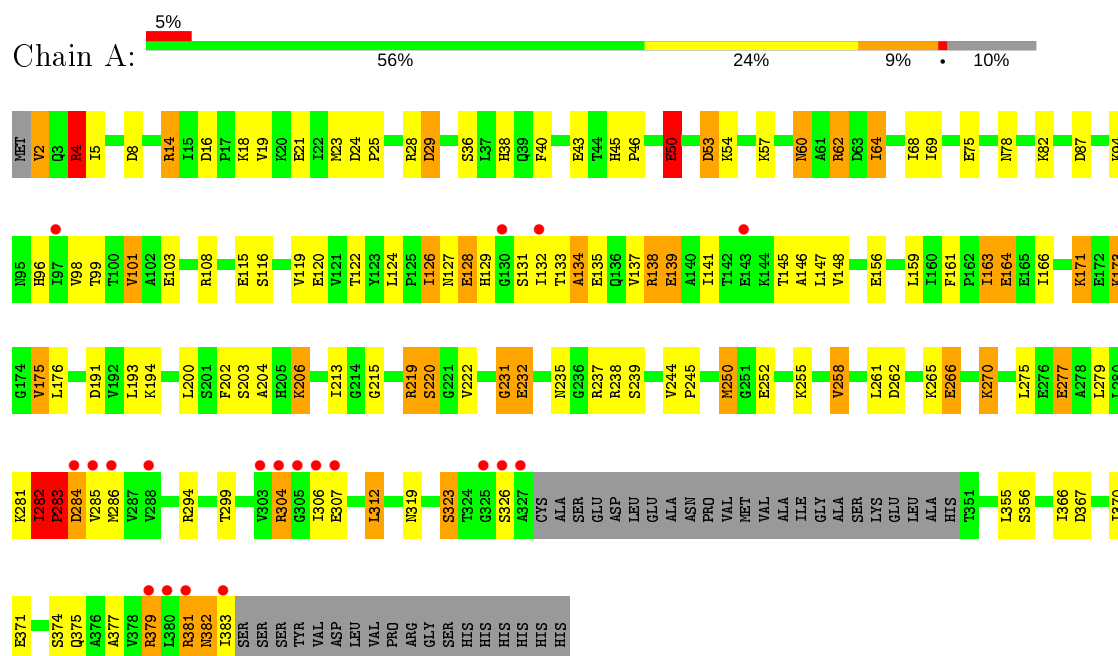
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	8	Total	O	0	0
			8	8		

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: Cysteine desulfurase IscS



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	102.90 Å 102.90 Å 133.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.18 – 2.70 49.13 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.18-2.70) 100.0 (49.13-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.69 Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.180 , 0.231 0.180 , 0.231	Depositor DCC
R_{free} test set	1014 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	75.0	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.6	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	0.96	EDS
Total number of atoms	2814	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IPA, PDA, CL

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	0.84	8/2830 (0.3%)	1.46	35/3833 (0.9%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	103	GLU	CD-OE1	9.86	1.36	1.25
1	A	43	GLU	CD-OE2	9.06	1.35	1.25
1	A	43	GLU	CD-OE1	7.67	1.34	1.25
1	A	139	GLU	CD-OE2	6.24	1.32	1.25
1	A	232	GLU	CD-OE2	5.73	1.31	1.25
1	A	252	GLU	CD-OE2	5.73	1.31	1.25
1	A	75	GLU	CD-OE2	-5.26	1.19	1.25
1	A	21	GLU	CD-OE1	5.17	1.31	1.25

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	ARG	NE-CZ-NH1	-11.31	114.64	120.30
1	A	173	LYS	CB-CA-C	9.02	128.45	110.40
1	A	4	ARG	CB-CA-C	8.93	128.26	110.40
1	A	28	ARG	CB-CA-C	7.92	126.23	110.40
1	A	14	ARG	CG-CD-NE	7.66	127.88	111.80
1	A	250	MET	CG-SD-CE	-7.63	87.99	100.20
1	A	28	ARG	NE-CZ-NH1	-7.50	116.55	120.30
1	A	138	ARG	CB-CG-CD	7.32	130.63	111.60
1	A	270	LYS	CB-CA-C	7.27	124.94	110.40
1	A	108	ARG	NE-CZ-NH2	-7.15	116.73	120.30
1	A	283	PRO	N-CD-CG	-6.57	93.34	103.20
1	A	371	GLU	CB-CA-C	6.34	123.08	110.40
1	A	173	LYS	CB-CG-CD	6.11	127.48	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	PRO	N-CA-CB	-6.10	95.89	102.60
1	A	60	ASN	CB-CA-C	6.05	122.51	110.40
1	A	219	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	A	237	ARG	CG-CD-NE	-5.93	99.35	111.80
1	A	235	ASN	CB-CA-C	-5.89	98.62	110.40
1	A	128	GLU	CB-CA-C	5.86	122.13	110.40
1	A	4	ARG	CG-CD-NE	5.79	123.96	111.80
1	A	50	GLU	CB-CG-CD	-5.76	98.64	114.20
1	A	4	ARG	N-CA-CB	-5.73	100.28	110.60
1	A	258	VAL	N-CA-CB	5.73	124.10	111.50
1	A	28	ARG	C-N-CA	-5.72	107.40	121.70
1	A	2	VAL	CA-CB-CG2	5.51	119.17	110.90
1	A	29	ASP	CB-CA-C	-5.48	99.44	110.40
1	A	171	LYS	CB-CA-C	5.48	121.36	110.40
1	A	62	ARG	CG-CD-NE	5.47	123.29	111.80
1	A	231	GLY	C-N-CA	-5.46	108.05	121.70
1	A	4	ARG	CA-CB-CG	5.43	125.34	113.40
1	A	2	VAL	C-N-CA	5.42	135.26	121.70
1	A	266	GLU	CB-CA-C	-5.33	99.74	110.40
1	A	282	ILE	CB-CA-C	5.33	122.26	111.60
1	A	25	PRO	N-CD-CG	-5.14	95.49	103.20
1	A	138	ARG	CB-CA-C	-5.04	100.31	110.40

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	2780	0	2798	124	0
2	A	4	0	8	0	0
3	A	1	0	0	0	0
4	A	21	0	13	8	0
5	A	8	0	0	0	0
All	All	2814	0	2819	124	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 22.

All (124) 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:206:LYS:NZ	4:A:503:PDA:H4A1	1.49	1.27
1:A:204:ALA:HB2	1:A:250:MET:CE	1.67	1.24
1:A:213:ILE:HG23	1:A:250:MET:HE3	1.26	1.12
1:A:204:ALA:HB2	1:A:250:MET:HE2	1.19	1.09
1:A:206:LYS:CE	4:A:503:PDA:H4A1	1.85	1.05
1:A:213:ILE:HG23	1:A:250:MET:CE	1.86	1.04
1:A:282:ILE:HG13	1:A:283:PRO:HD3	1.37	1.03
1:A:206:LYS:HZ1	4:A:503:PDA:H4A1	1.20	0.93
1:A:206:LYS:NZ	4:A:503:PDA:C4A	2.31	0.92
1:A:283:PRO:HD2	1:A:285:VAL:HG13	1.52	0.91
1:A:282:ILE:HG13	1:A:283:PRO:CD	2.00	0.90
1:A:379:ARG:HG2	1:A:379:ARG:HH11	1.36	0.90
1:A:282:ILE:CG1	1:A:283:PRO:HD3	2.02	0.89
1:A:204:ALA:HB2	1:A:250:MET:HE1	1.55	0.87
1:A:98:VAL:HG12	1:A:148:VAL:HG22	1.58	0.86
1:A:312:LEU:HD11	1:A:323:SER:HA	1.58	0.84
1:A:382:ASN:N	1:A:382:ASN:HD22	1.75	0.84
1:A:126:ILE:HD12	1:A:127:ASN:H	1.44	0.82
1:A:262:ASP:O	1:A:266:GLU:HG2	1.80	0.82
1:A:382:ASN:H	1:A:382:ASN:ND2	1.77	0.81
1:A:213:ILE:CG2	1:A:250:MET:HE3	2.09	0.79
1:A:163:ILE:O	1:A:164:GLU:HB3	1.83	0.79
1:A:382:ASN:ND2	1:A:382:ASN:N	2.31	0.78
1:A:126:ILE:HD11	1:A:131:SER:C	2.04	0.78
1:A:126:ILE:CD1	1:A:131:SER:O	2.33	0.76
1:A:139:GLU:O	1:A:139:GLU:HG2	1.85	0.76
1:A:231:GLY:H	1:A:239:SER:HB2	1.51	0.75
1:A:283:PRO:CD	1:A:285:VAL:HG13	2.15	0.75
1:A:206:LYS:CE	4:A:503:PDA:C4A	2.65	0.74
1:A:231:GLY:N	1:A:239:SER:HB2	2.04	0.72
1:A:163:ILE:O	1:A:164:GLU:CB	2.39	0.71
1:A:204:ALA:CB	1:A:250:MET:HE2	2.11	0.70
1:A:96:HIS:NE2	1:A:122:THR:HG23	2.10	0.67
1:A:206:LYS:HZ3	4:A:503:PDA:C4A	2.11	0.64
1:A:60:ASN:HD21	1:A:193:LEU:HD12	1.62	0.64
1:A:133:THR:O	1:A:134:ALA:HB3	1.98	0.63
1:A:133:THR:O	1:A:134:ALA:CB	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ILE:HD12	1:A:127:ASN:N	2.13	0.62
1:A:206:LYS:HZ1	4:A:503:PDA:C4A	2.04	0.62
1:A:60:ASN:ND2	1:A:193:LEU:HD12	2.14	0.62
1:A:284:ASP:CG	1:A:304:ARG:HD2	2.19	0.62
1:A:284:ASP:OD1	1:A:304:ARG:HD2	1.99	0.62
1:A:282:ILE:HG23	1:A:285:VAL:HG11	1.81	0.61
1:A:219:ARG:O	1:A:222:VAL:HG23	2.00	0.60
1:A:304:ARG:HG3	1:A:381:ARG:NH2	2.17	0.60
1:A:54:LYS:HD3	1:A:255:LYS:HD2	1.83	0.60
1:A:375:GLN:O	1:A:379:ARG:HB3	2.02	0.59
1:A:16:ASP:HB3	1:A:19:VAL:HG23	1.85	0.59
1:A:137:VAL:HG21	1:A:166:ILE:HG23	1.84	0.59
1:A:98:VAL:CG1	1:A:148:VAL:HG22	2.30	0.58
1:A:19:VAL:O	1:A:23:MET:HG3	2.03	0.58
1:A:134:ALA:O	1:A:137:VAL:HG22	2.02	0.58
1:A:98:VAL:HG13	1:A:148:VAL:HG13	1.85	0.58
1:A:204:ALA:CB	1:A:250:MET:CE	2.62	0.58
1:A:126:ILE:CD1	1:A:131:SER:C	2.72	0.58
1:A:306:ILE:HG22	1:A:307:GLU:O	2.04	0.57
1:A:38:HIS:CE1	1:A:40:PHE:HB2	2.39	0.57
1:A:279:LEU:O	1:A:285:VAL:HG21	2.05	0.56
1:A:135:GLU:OE2	1:A:138:ARG:HD2	2.05	0.56
1:A:275:LEU:HD21	1:A:355:LEU:HD13	1.88	0.56
1:A:64:ILE:HG13	1:A:220:SER:HB2	1.88	0.55
1:A:244:VAL:N	1:A:245:PRO:HD2	2.21	0.55
1:A:379:ARG:HG2	1:A:379:ARG:NH1	2.11	0.55
1:A:275:LEU:O	1:A:279:LEU:HG	2.07	0.55
1:A:206:LYS:HE3	4:A:503:PDA:H4A1	1.83	0.54
1:A:244:VAL:HB	1:A:245:PRO:HD3	1.88	0.54
1:A:213:ILE:HG23	1:A:250:MET:HE2	1.85	0.54
1:A:244:VAL:N	1:A:245:PRO:CD	2.71	0.54
1:A:148:VAL:HG23	1:A:175:VAL:HG11	1.91	0.53
1:A:204:ALA:CB	1:A:250:MET:HE1	2.35	0.52
1:A:200:LEU:C	1:A:200:LEU:HD23	2.29	0.52
1:A:213:ILE:CG2	1:A:250:MET:CE	2.74	0.51
1:A:53:ASP:O	1:A:57:LYS:HG2	2.10	0.51
1:A:50:GLU:O	1:A:54:LYS:HG3	2.10	0.51
1:A:126:ILE:CD1	1:A:127:ASN:H	2.19	0.51
1:A:78:ASN:O	1:A:82:LYS:HG3	2.11	0.51
1:A:45:HIS:HB2	1:A:46:PRO:HD3	1.92	0.51
1:A:304:ARG:HG3	1:A:381:ARG:HH22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ARG:HB2	1:A:138:ARG:NH1	2.26	0.50
1:A:312:LEU:HD11	1:A:323:SER:CA	2.37	0.50
1:A:191:ASP:CG	1:A:194:LYS:HG3	2.32	0.50
1:A:94:LYS:O	1:A:146:ALA:HB2	2.12	0.50
1:A:159:LEU:HD23	1:A:294:ARG:HG3	1.93	0.49
1:A:283:PRO:HG2	1:A:381:ARG:NH2	2.27	0.49
1:A:126:ILE:HD11	1:A:131:SER:CA	2.43	0.48
1:A:279:LEU:O	1:A:282:ILE:CG2	2.62	0.48
1:A:282:ILE:HG13	1:A:283:PRO:CG	2.42	0.48
1:A:374:SER:O	1:A:377:ALA:HB3	2.14	0.47
1:A:98:VAL:CG1	1:A:148:VAL:HG13	2.45	0.47
1:A:101:VAL:HG22	1:A:124:LEU:O	2.13	0.47
1:A:96:HIS:HA	1:A:120:GLU:O	2.15	0.47
1:A:147:LEU:HD12	1:A:176:LEU:O	2.15	0.47
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.77	0.47
1:A:4:ARG:HB2	1:A:319:ASN:HB3	1.97	0.46
1:A:78:ASN:OD1	1:A:82:LYS:HE3	2.14	0.46
1:A:312:LEU:CD1	1:A:323:SER:HA	2.38	0.46
1:A:156:GLU:OE2	1:A:326:SER:N	2.48	0.46
1:A:126:ILE:HD13	1:A:126:ILE:HA	1.47	0.46
1:A:36:SER:HB3	1:A:38:HIS:NE2	2.32	0.45
1:A:277:GLU:O	1:A:281:LYS:HG3	2.16	0.45
1:A:8:ASP:OD1	1:A:323:SER:OG	2.35	0.45
1:A:135:GLU:O	1:A:138:ARG:HB3	2.17	0.43
1:A:366:ILE:O	1:A:367:ASP:C	2.56	0.43
1:A:68:ILE:HG22	1:A:69:ILE:N	2.33	0.43
1:A:62:ARG:HD3	1:A:193:LEU:HD21	2.00	0.43
1:A:202:PHE:CZ	1:A:215:GLY:HA3	2.53	0.43
1:A:53:ASP:OD1	1:A:57:LYS:HE3	2.18	0.43
1:A:219:ARG:O	1:A:222:VAL:CG2	2.65	0.43
1:A:231:GLY:H	1:A:239:SER:CB	2.26	0.43
1:A:115:GLU:HA	1:A:119:VAL:O	2.19	0.42
1:A:124:LEU:CD1	1:A:137:VAL:HG12	2.50	0.42
1:A:213:ILE:HG12	1:A:250:MET:HE3	2.00	0.42
1:A:367:ASP:HA	1:A:370:ILE:HD12	2.02	0.42
1:A:367:ASP:O	1:A:370:ILE:HB	2.20	0.42
1:A:145:THR:HG22	1:A:175:VAL:HG21	2.02	0.42
1:A:279:LEU:O	1:A:282:ILE:HG22	2.19	0.42
1:A:283:PRO:HG2	1:A:381:ARG:HH21	1.85	0.41
1:A:68:ILE:O	1:A:215:GLY:HA2	2.19	0.41
1:A:159:LEU:HD23	1:A:294:ARG:CG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ASP:N	1:A:284:ASP:OD1	2.54	0.41
1:A:161:PHE:CD1	1:A:161:PHE:N	2.89	0.41
1:A:36:SER:HB3	1:A:38:HIS:CE1	2.55	0.41
1:A:282:ILE:HG13	1:A:283:PRO:HG3	2.03	0.40
1:A:5:ILE:HG21	1:A:5:ILE:HD13	1.72	0.40

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	355/401 (88%)	328 (92%)	19 (5%)	8 (2%)	6 16

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	ALA
1	A	164	GLU
1	A	282	ILE
1	A	283	PRO
1	A	381	ARG
1	A	220	SER
1	A	141	ILE
1	A	163	ILE

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	302/337 (90%)	263 (87%)	39 (13%)	4 10

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	4	ARG
1	A	14	ARG
1	A	18	LYS
1	A	24	ASP
1	A	29	ASP
1	A	50	GLU
1	A	53	ASP
1	A	64	ILE
1	A	87	ASP
1	A	99	THR
1	A	101	VAL
1	A	116	SER
1	A	126	ILE
1	A	128	GLU
1	A	129	HIS
1	A	132	ILE
1	A	171	LYS
1	A	173	LYS
1	A	175	VAL
1	A	203	SER
1	A	206	LYS
1	A	232	GLU
1	A	238	ARG
1	A	258	VAL
1	A	265	LYS
1	A	270	LYS
1	A	277	GLU
1	A	282	ILE
1	A	284	ASP
1	A	286	MET
1	A	299	THR
1	A	304	ARG
1	A	312	LEU
1	A	323	SER
1	A	356	SER

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Mol	Chain	Res	Type
1	A	379	ARG
1	A	382	ASN
1	A	383	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	382	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z > 2$
4	PDA	A	503	-	18,21,21	3.53	5 (27%)	23,30,30	2.77	7 (30%)
2	IPA	A	501	-	3,3,3	0.55	0	3,3,3	0.95	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
4	PDA	A	503	-	-	2/11/15/15	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	PDA	C3-C2	10.83	1.51	1.40
4	A	503	PDA	C5-C4	7.29	1.50	1.40
4	A	503	PDA	C3-C4	5.13	1.47	1.40
4	A	503	PDA	C4A-C4	3.23	1.56	1.51
4	A	503	PDA	C6-C5	2.08	1.42	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	PDA	C3-C4-C5	-6.72	112.27	118.72
4	A	503	PDA	C4A-C4-C5	6.28	126.69	119.71
4	A	503	PDA	C6-C5-C4	5.56	122.05	118.12
4	A	503	PDA	CB-CA-C	4.17	117.32	110.93
4	A	503	PDA	OP4-P-OP1	-3.95	95.40	106.47
4	A	503	PDA	OP3-P-OP1	2.64	121.00	110.68
4	A	503	PDA	C2A-C2-C3	-2.24	118.13	120.89

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	PDA	CB-CA-N-C4A
4	A	503	PDA	C-CA-N-C4A

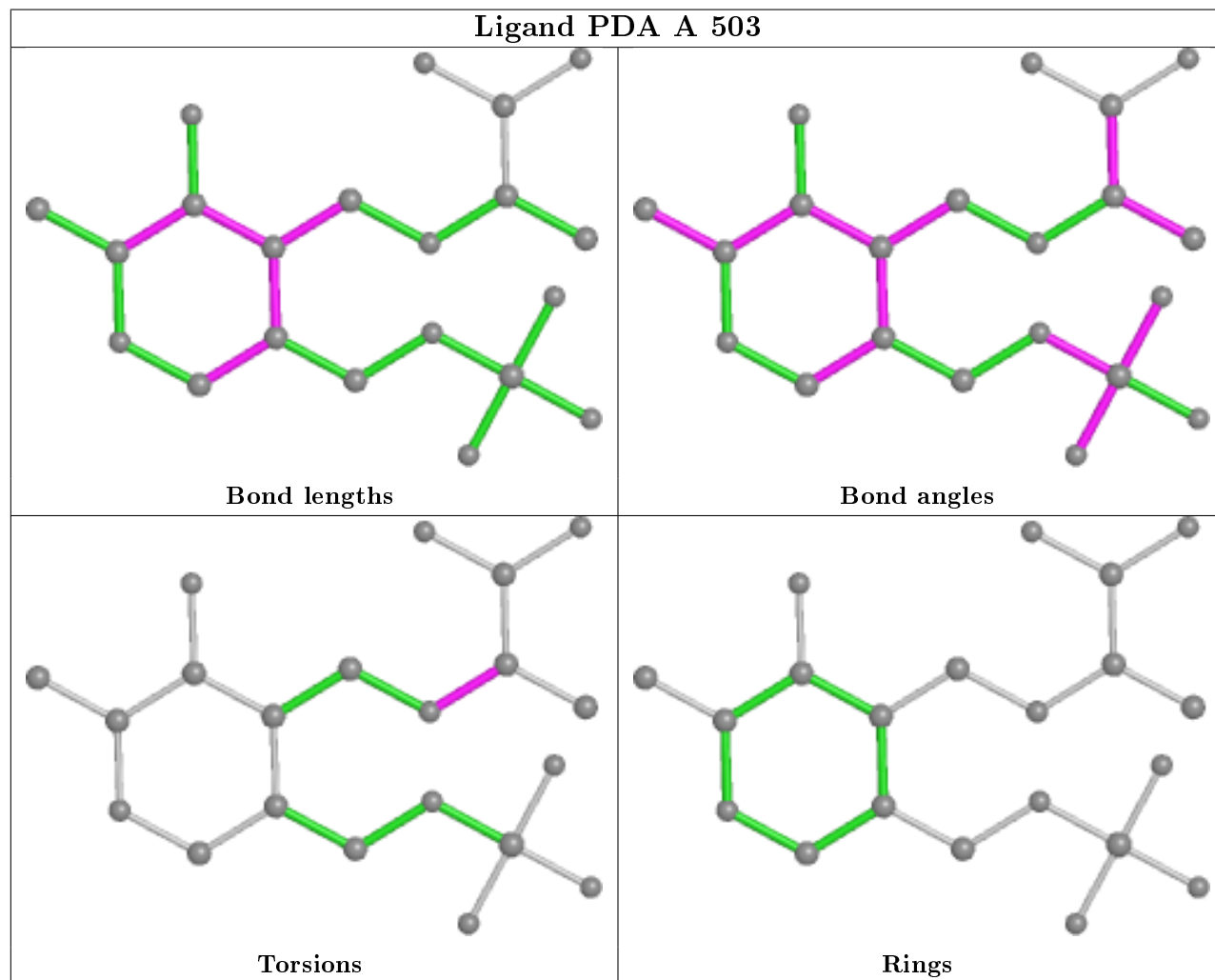
There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	PDA	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 than 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 any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	359/401 (89%)	0.19	20 (5%) 24 23	47, 88, 151, 190	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	306	ILE	5.9
1	A	383	ILE	5.4
1	A	305	GLY	4.3
1	A	325	GLY	3.8
1	A	326	SER	3.6
1	A	381	ARG	3.6
1	A	380	LEU	3.5
1	A	286	MET	3.4
1	A	327	ALA	2.9
1	A	307	GLU	2.7
1	A	379	ARG	2.7
1	A	285	VAL	2.7
1	A	143	GLU	2.5
1	A	284	ASP	2.5
1	A	304	ARG	2.5
1	A	132	ILE	2.4
1	A	97	ILE	2.3
1	A	303	VAL	2.2
1	A	288	VAL	2.1
1	A	130	GLY	2.1

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

There are no carbohydrates in this entry.

6.4 Ligands

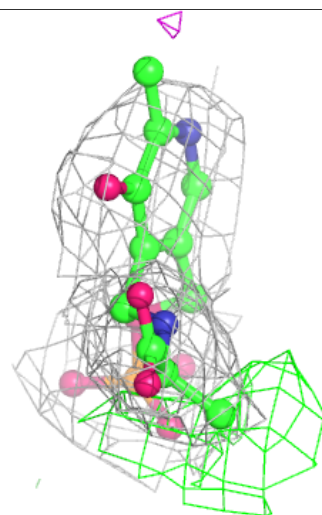
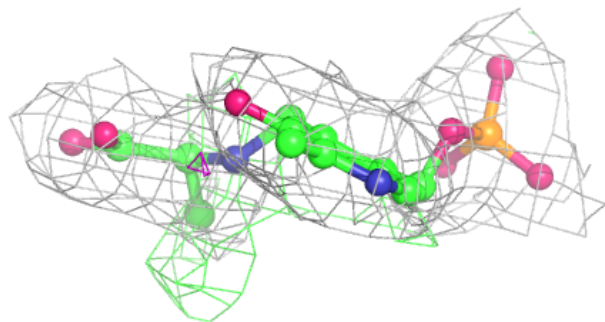
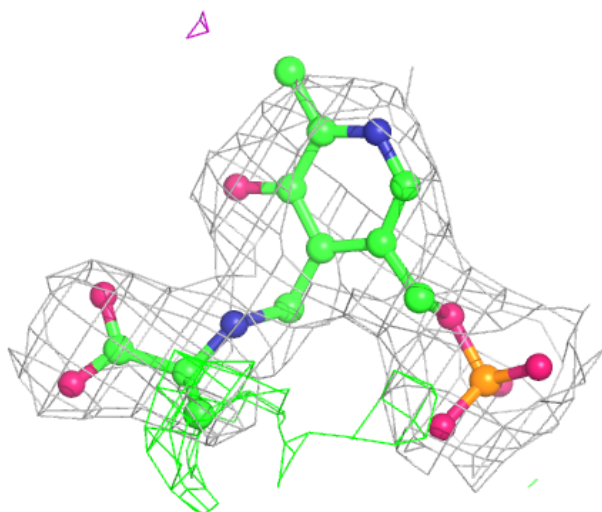
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	IPA	A	501	4/4	0.94	0.34	66,67,81,84	0
3	CL	A	502	1/1	0.97	0.24	83,83,83,83	0
4	PDA	A	503	21/21	0.97	0.25	51,74,94,104	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.

Electron density around PDA A 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.