



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:13 PM GMT

PDB ID : 1SQA
Title : Substituted 2-Naphthamidine Inhibitors of Urokinase
Authors : Wendt, M.D.; Geyer, A.; McClellan, W.J.; Rockway, T.W.; Weitzberg, M.;
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Deposited on : 2004-03-18
Resolution : 2.00 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
<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

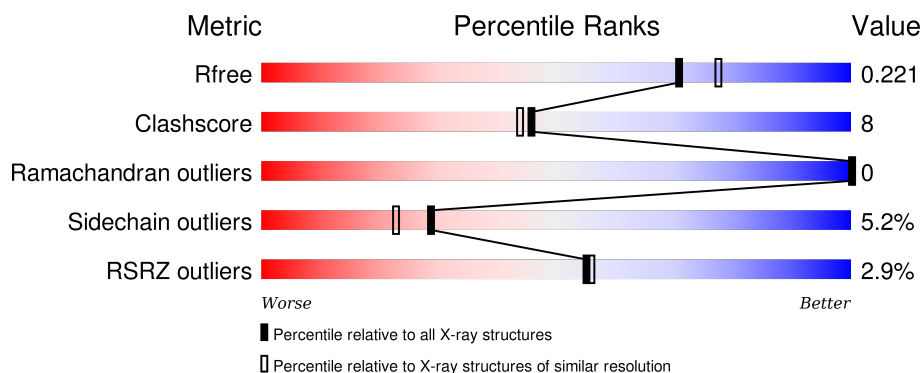
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

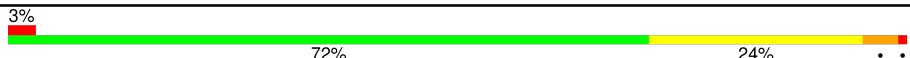
The reported resolution of this entry is 2.00 Å.

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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	245	

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	SO4	A	302	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	UI1	A	1001	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2041 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 Urokinase-type plasminogen activator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	245	1934	1219	338	361	16	0	0	0

There is a discrepancy between the modelled and reference sequences:

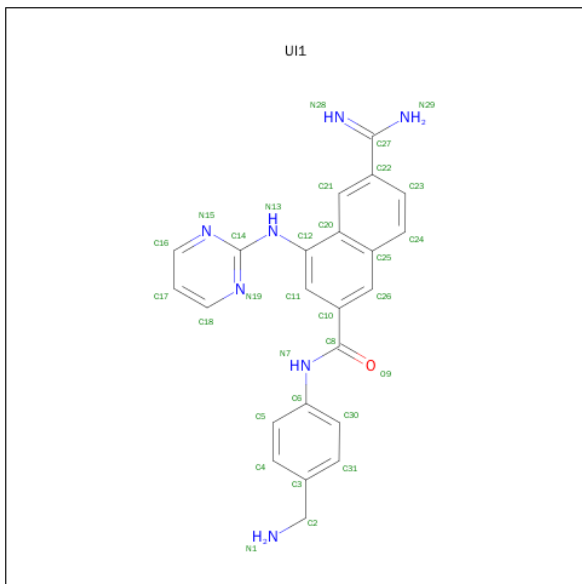
Chain	Residue	Modelled	Actual	Comment	Reference
A	156	GLN	ASN	CONFLICT	UNP P00749

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0

- Molecule 3 is 6-[(Z)-AMINO(IMINO)METHYL]-N-[4-(AMINOMETHYL)PHENYL]-4-(PYRIMIDIN-2-YLAMINO)-2-NAPHTHAMIDE (three-letter code: UI1) (formula: C₂₃H₂₁N₇O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			31	23	7	1		

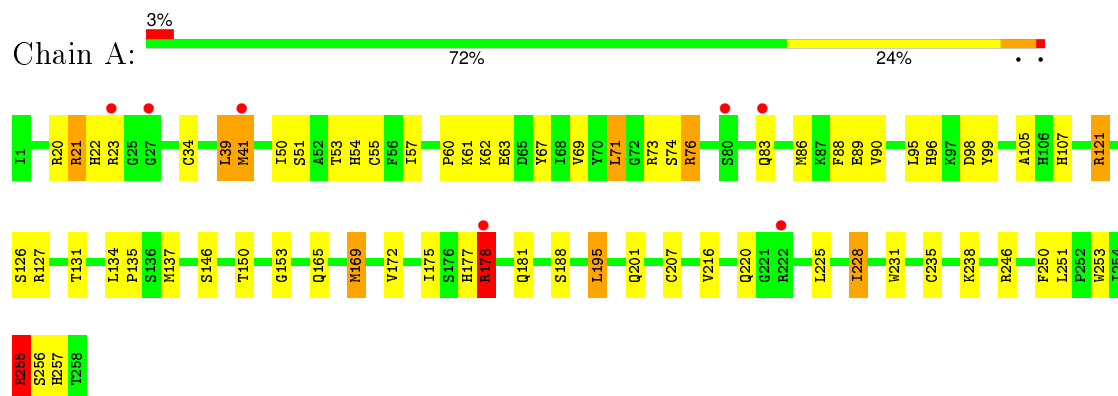
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	61	Total	O	0	0
			61	61		

3 Residue-property plots

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.

- Molecule 1: Urokinase-type plasminogen activator



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.16Å 53.00Å 82.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00 22.94 – 1.92	Depositor EDS
% Data completeness (in resolution range)	67.4 (10.00-2.00) 88.9 (22.94-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 1.92Å)	Xtriage
Refinement program	X-PLOR 98.0	Depositor
R, R_{free}	0.210 , 0.266 0.218 , 0.221	Depositor DCC
R_{free} test set	1160 reflections (6.83%)	DCC
Wilson B-factor (Å ²)	11.6	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 47.9	EDS
Estimated twinning fraction	0.069 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 16972 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	2041	wwPDB-VP
Average B, all atoms (Å ²)	7.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.88% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: UI1, SO4

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	1.36	11/1983 (0.6%)	1.63	36/2685 (1.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	SER	CA-CB	10.22	1.68	1.52
1	A	126	SER	CB-OG	-6.45	1.33	1.42
1	A	146	SER	CA-CB	-5.83	1.44	1.52
1	A	74	SER	CA-CB	5.79	1.61	1.52
1	A	169	MET	CA-CB	5.62	1.66	1.53
1	A	63	GLU	CD-OE1	5.59	1.31	1.25
1	A	146	SER	CB-OG	-5.59	1.34	1.42
1	A	50	ILE	CA-CB	5.35	1.67	1.54
1	A	228	ILE	CA-CB	5.27	1.67	1.54
1	A	172	VAL	CA-CB	5.18	1.65	1.54
1	A	41	MET	CB-CG	-5.03	1.35	1.51

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	ARG	NE-CZ-NH1	-13.93	113.33	120.30
1	A	20	ARG	NE-CZ-NH2	13.25	126.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	MET	CA-CB-CG	12.79	135.05	113.30
1	A	21	ARG	NE-CZ-NH2	-12.36	114.12	120.30
1	A	255	ARG	NE-CZ-NH2	-12.02	114.29	120.30
1	A	21	ARG	NE-CZ-NH1	10.40	125.50	120.30
1	A	73	ARG	NE-CZ-NH2	-10.37	115.11	120.30
1	A	41	MET	CA-CB-CG	-10.35	95.70	113.30
1	A	69	VAL	CG1-CB-CG2	-9.50	95.69	110.90
1	A	71	LEU	CB-CG-CD2	-8.15	97.14	111.00
1	A	255	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	A	127	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	A	73	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	A	175	ILE	O-C-N	-7.51	110.68	122.70
1	A	216	VAL	CG1-CB-CG2	-7.25	99.29	110.90
1	A	178	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	A	71	LEU	CB-CG-CD1	6.76	122.49	111.00
1	A	74	SER	O-C-N	-6.26	112.68	122.70
1	A	53	THR	O-C-N	-6.22	112.75	122.70
1	A	220	GLN	CA-CB-CG	-5.99	100.22	113.40
1	A	67	TYR	O-C-N	5.77	131.94	122.70
1	A	57	ILE	CG1-CB-CG2	-5.72	98.81	111.40
1	A	195	LEU	CB-CG-CD2	5.49	120.33	111.00
1	A	95	LEU	O-C-N	-5.47	113.94	122.70
1	A	175	ILE	CA-C-N	5.45	129.19	117.20
1	A	23	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	39	LEU	C-N-CA	5.23	134.78	121.70
1	A	238	LYS	C-N-CA	5.20	134.71	121.70
1	A	86	MET	CA-CB-CG	5.17	122.09	113.30
1	A	188	SER	O-C-N	-5.16	114.45	122.70
1	A	127	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	89	GLU	O-C-N	-5.10	114.54	122.70
1	A	201	GLN	O-C-N	-5.10	114.54	122.70
1	A	181	GLN	O-C-N	-5.09	114.55	122.70
1	A	175	ILE	CG1-CB-CG2	5.06	122.54	111.40
1	A	121	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	153	GLY	Mainchain
1	A	250	PHE	Mainchain
1	A	255	ARG	Sidechain

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	1934	0	1880	27	0
2	A	15	0	0	0	0
3	A	31	0	20	0	0
4	A	61	0	0	3	0
All	All	2041	0	1900	27	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 8.

All (27) 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:96:HIS:HD2	1:A:98:ASP:H	1.26	0.82
1:A:76:ARG:HG2	1:A:76:ARG:HH11	1.57	0.68
1:A:137:MET:HG2	1:A:251:LEU:HD12	1.80	0.64
1:A:255:ARG:HH11	1:A:255:ARG:HG2	1.61	0.64
1:A:76:ARG:NH1	1:A:76:ARG:HG2	2.18	0.59
1:A:41:MET:HE2	1:A:225:LEU:HD22	1.83	0.59
1:A:62:LYS:HD2	1:A:90:VAL:O	2.04	0.58
1:A:195:LEU:HB3	4:A:1029:HOH:O	2.05	0.55
1:A:253:TRP:O	1:A:257:HIS:HD2	1.92	0.53
1:A:195:LEU:HG	1:A:246:ARG:HB2	1.90	0.52
1:A:71:LEU:HD12	1:A:88:PHE:CE1	2.49	0.48
1:A:39:LEU:HG	1:A:131:THR:HG22	1.96	0.48
1:A:34:CYS:CB	1:A:55:CYS:SG	3.01	0.47
1:A:41:MET:HE3	1:A:134:LEU:HD21	1.97	0.47
1:A:105:ALA:HA	1:A:231:TRP:CE2	2.51	0.46
1:A:99:TYR:HA	1:A:107:HIS:O	2.16	0.45
1:A:96:HIS:CD2	1:A:98:ASP:H	2.18	0.45
1:A:41:MET:HE2	1:A:225:LEU:CD2	2.47	0.44
1:A:177:HIS:HD2	4:A:1010:HOH:O	2.01	0.43
1:A:76:ARG:HH11	1:A:165:GLN:HE21	1.68	0.42
1:A:135:PRO:O	1:A:251:LEU:HD11	2.20	0.41
1:A:178:ARG:HD3	1:A:178:ARG:HA	1.87	0.41
1:A:225:LEU:HD21	1:A:228:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ARG:HH11	1:A:121:ARG:HD2	1.77	0.41
1:A:207:CYS:HA	1:A:235:CYS:SG	2.61	0.40
1:A:76:ARG:HH11	1:A:165:GLN:NE2	2.19	0.40
1:A:22:HIS:HD2	4:A:1043:HOH:O	2.04	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	243/245 (99%)	234 (96%)	9 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	213/214 (100%)	202 (95%)	11 (5%)	29	23

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	54	HIS

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Mol	Chain	Res	Type
1	A	60	PRO
1	A	61	LYS
1	A	76	ARG
1	A	83	GLN
1	A	150	THR
1	A	169	MET
1	A	178	ARG
1	A	255	ARG
1	A	256	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	22	HIS
1	A	96	HIS
1	A	107	HIS
1	A	156	GLN
1	A	165	GLN
1	A	177	HIS
1	A	257	HIS

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](#)

4 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$
3	UI1	A	1001	-	34,34,34	1.52	7 (20%)	41,47,47	2.07	10 (24%)
2	SO4	A	301	-	4,4,4	2.09	1 (25%)	6,6,6	1.23	1 (16%)
2	SO4	A	302	-	4,4,4	1.29	0	6,6,6	1.91	1 (16%)
2	SO4	A	303	-	4,4,4	1.35	0	6,6,6	0.44	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
3	UI1	A	1001	-	-	0/18/18/18	0/4/4/4
2	SO4	A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	A	302	-	-	0/0/0/0	0/0/0/0
2	SO4	A	303	-	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	SO4	O4-S	-3.52	1.34	1.47
3	A	1001	UI1	C12-N13	2.02	1.44	1.39
3	A	1001	UI1	C21-C22	2.53	1.41	1.37
3	A	1001	UI1	C5-C6	2.55	1.43	1.39
3	A	1001	UI1	C24-C23	2.62	1.42	1.36
3	A	1001	UI1	C31-C30	2.69	1.43	1.38
3	A	1001	UI1	C14-N13	3.50	1.42	1.36
3	A	1001	UI1	C26-C10	3.77	1.43	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	UI1	N19-C14-N15	-6.08	120.83	126.50
2	A	302	SO4	O4-S-O3	-4.13	92.19	108.98
3	A	1001	UI1	C6-N7-C8	-2.34	121.25	126.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	UI1	C17-C16-N15	-2.25	119.69	123.44
3	A	1001	UI1	C17-C18-N19	-2.19	119.78	123.44
3	A	1001	UI1	C12-N13-C14	-2.14	123.58	129.22
3	A	1001	UI1	C21-C22-C27	-2.09	117.31	120.24
3	A	1001	UI1	C5-C6-N7	-2.05	113.57	120.41
3	A	1001	UI1	C12-C20-C25	2.10	120.84	118.43
2	A	301	SO4	O2-S-O1	2.26	116.67	109.50
3	A	1001	UI1	C16-N15-C14	6.11	120.80	115.49
3	A	1001	UI1	C18-N19-C14	6.19	120.87	115.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	245/245 (100%)	0.24	7 (2%) 55 56	2, 5, 18, 33	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	23	ARG	3.6
1	A	27	GLY	3.2
1	A	83	GLN	2.8
1	A	41	MET	2.6
1	A	222	ARG	2.3
1	A	178	ARG	2.3
1	A	80	SER	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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(\AA^2)	Q<0.9
2	SO4	A	302	5/5	0.83	0.26	6.95	21,21,26,29	0
3	UI1	A	1001	31/31	0.80	0.19	3.03	2,9,15,19	0
2	SO4	A	301	5/5	0.97	0.09	-2.69	8,11,13,13	0
2	SO4	A	303	5/5	0.95	0.12	-	35,36,37,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.