



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:17 PM UTC

PDB ID : 1OIH / pdb_00001oih
Title : Crystal structure of the alkylsulfatase AtsK, a non-heme Fe(II) alphaketoglutarate dependent Dioxygenase
Authors : Mueller, I.; Kahnert, A.; Pape, T.; Dierks, T.; Meyer-Klauke, W.; Kertesz, M.; Uson, I.
Deposited on : 2003-06-18
Resolution : 1.89 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

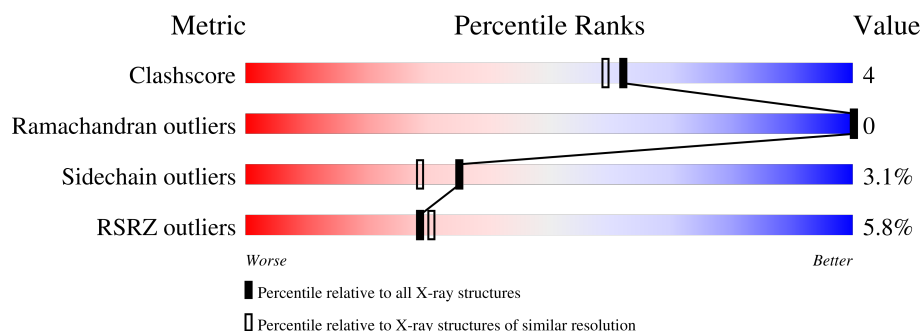
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 $\leq 5\%$. 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	301	2% 76% 8% • 16%
1	B	301	3% 78% 6% • 15%
1	C	301	4% 75% 5% • 20%
1	D	301	10% 74% 7% • 19%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8416 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 PUTATIVE ALKYL SULFATASE ATSK.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	0	1	0
			1971	1246	365	360			
1	B	255	Total	C	N	O	0	1	0
			1970	1245	362	363			
1	C	242	Total	C	N	O	0	0	0
			1846	1171	336	339			
1	D	244	Total	C	N	O	0	1	0
			1865	1183	340	342			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	1
			1	1		
2	B	1	Total	Na	0	1
			1	1		
2	C	1	Total	Na	0	1
			1	1		
2	D	1	Total	Na	0	1
			1	1		

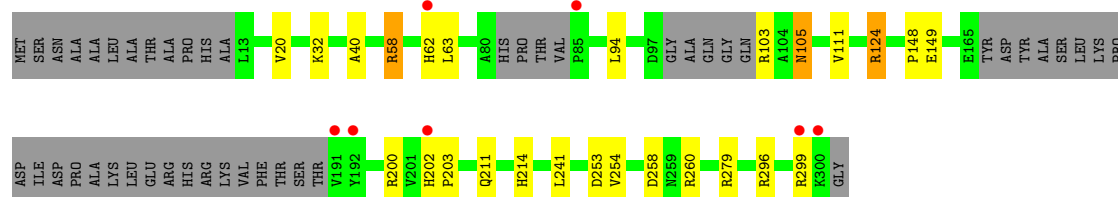
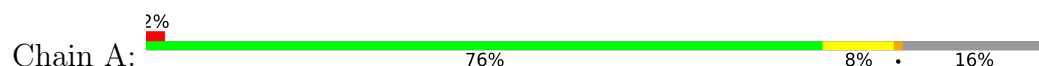
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	214	Total	O	0	0
			214	214		
3	B	225	Total	O	0	0
			225	225		
3	C	168	Total	O	0	0
			168	168		
3	D	153	Total	O	0	0
			153	153		

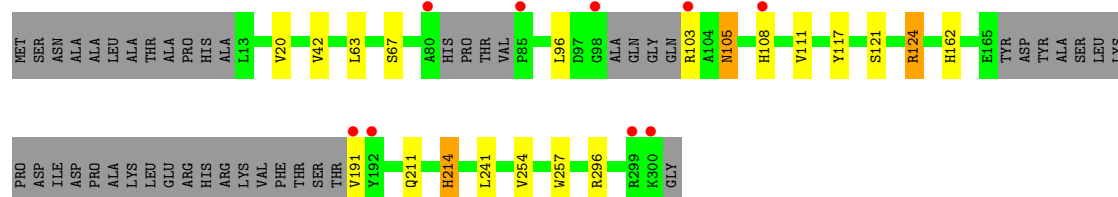
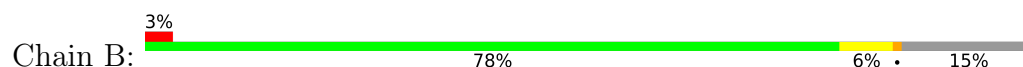
3 Residue-property plots [i](#)

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.

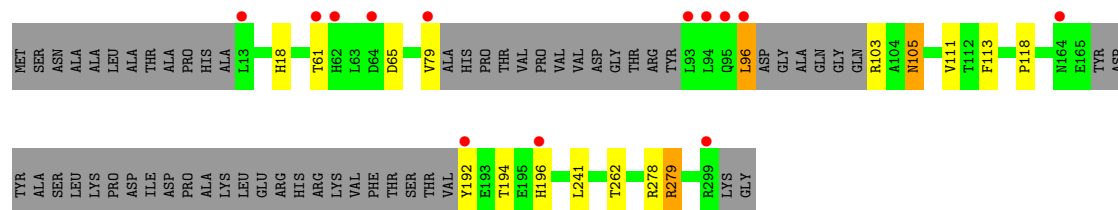
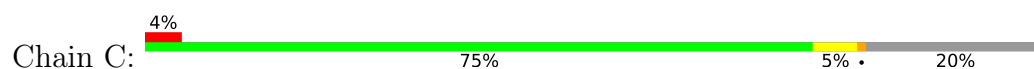
• Molecule 1: PUTATIVE ALKYL SULFATASE ATSK



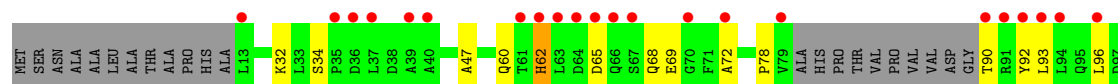
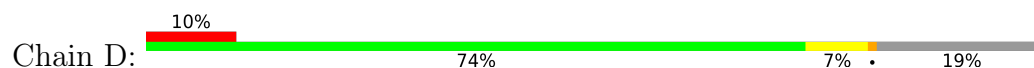
• Molecule 1: PUTATIVE ALKYL SULFATASE ATSK

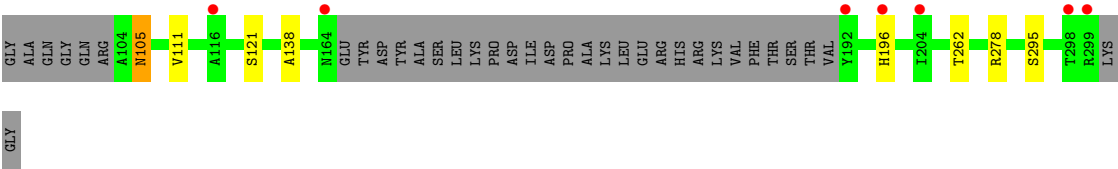


• Molecule 1: PUTATIVE ALKYL SULFATASE ATSK



• Molecule 1: PUTATIVE ALKYL SULFATASE ATSK





GLY

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.24Å 145.34Å 159.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.89 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-1.89) 99.1 (20.00-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.79 (at 1.90Å)	Xtrriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.170 , 0.191 0.184 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtrriage
Anisotropy	0.428	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8416	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.68 % 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 3.6624e-03. 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, 0.333 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: NA

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	1.21	4/2018 (0.2%)	1.06	1/2749 (0.0%)
1	B	1.20	3/2017 (0.1%)	1.02	0/2751
1	C	1.16	2/1888 (0.1%)	1.00	0/2579
1	D	1.27	3/1911 (0.2%)	1.05	4/2610 (0.2%)
All	All	1.21	12/7834 (0.2%)	1.03	5/10689 (0.0%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	20	VAL	CA-CB	-7.24	1.47	1.55
1	D	121	SER	CA-C	-6.37	1.45	1.52
1	A	149	GLU	CA-CB	6.11	1.61	1.53
1	C	262	THR	CA-C	-6.06	1.45	1.52
1	A	20	VAL	CA-CB	-5.84	1.48	1.55
1	B	42	VAL	CA-CB	-5.51	1.47	1.54
1	A	148	PRO	CA-C	-5.47	1.46	1.52
1	D	47	ALA	CA-CB	-5.36	1.44	1.53
1	A	40	ALA	CA-CB	-5.24	1.45	1.53
1	D	72	ALA	CA-CB	-5.18	1.45	1.53
1	C	18	HIS	CA-C	5.11	1.58	1.52
1	B	67	SER	CA-C	5.09	1.59	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	ARG	NE-CZ-NH2	5.67	124.30	119.20
1	D	34	SER	N-CA-C	5.45	113.03	108.13
1	D	68	GLN	N-CA-C	-5.41	104.94	112.45
1	D	60	GLN	CA-C-N	5.20	127.25	120.28
1	D	60	GLN	C-N-CA	5.20	127.25	120.28

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	1971	0	1932	25	0
1	B	1970	0	1915	10	0
1	C	1846	0	1771	15	0
1	D	1865	0	1780	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	214	0	0	2	0
3	B	225	0	0	3	0
3	C	168	0	0	1	0
3	D	153	0	0	0	0
All	All	8416	0	7398	61	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 4.

All (61) 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:202:HIS:HD2	1:A:203:PRO:HD2	1.30	0.96
1:C:194:THR:HG21	1:C:196:HIS:HE1	1.34	0.93
1:A:62:HIS:HD2	1:A:63:LEU:N	1.74	0.86
1:A:32:LYS:HG3	1:A:62:HIS:CE1	2.12	0.84
1:A:62:HIS:CD2	1:A:63:LEU:N	2.50	0.79
1:C:194:THR:HG21	1:C:196:HIS:CE1	2.19	0.77
1:C:105:ASN:HD22	1:C:105:ASN:H	1.33	0.76
1:A:202:HIS:CD2	1:A:203:PRO:HD2	2.19	0.75
1:C:194:THR:CG2	1:C:196:HIS:CE1	2.70	0.74
1:B:105:ASN:H	1:B:105:ASN:HD22	1.35	0.73
1:A:105:ASN:H	1:A:105:ASN:HD22	1.38	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LYS:CG	1:A:62:HIS:CE1	2.73	0.71
1:D:69:GLU:OE2	1:D:92:TYR:N	2.24	0.70
1:D:105:ASN:HD22	1:D:105:ASN:H	1.41	0.69
1:A:103:ARG:HB3	3:A:2188:HOH:O	1.98	0.64
1:D:62:HIS:C	1:D:62:HIS:CD2	2.78	0.62
1:A:202:HIS:HD2	1:A:203:PRO:CD	2.11	0.60
1:A:32:LYS:CG	1:A:62:HIS:HE1	2.13	0.59
1:A:32:LYS:HG3	1:A:62:HIS:ND1	2.16	0.59
1:A:241:LEU:HD23	3:A:2169:HOH:O	2.03	0.58
1:D:196:HIS:ND1	1:D:295:SER:HB3	2.19	0.57
1:A:202:HIS:CD2	1:A:260:ARG:HD2	2.40	0.56
1:A:62:HIS:HD2	1:A:63:LEU:H	1.51	0.54
1:A:200:ARG:HB2	1:A:211[B]:GLN:HG3	1.89	0.54
1:A:62:HIS:CD2	1:A:62:HIS:C	2.86	0.53
1:C:111:VAL:O	1:C:111:VAL:HG22	2.10	0.52
1:A:32:LYS:HE3	1:A:62:HIS:ND1	2.26	0.50
1:C:194:THR:HG22	1:C:196:HIS:CE1	2.46	0.50
1:B:162:HIS:HE1	3:B:2157:HOH:O	1.94	0.50
1:A:202:HIS:HE1	1:A:258:ASP:OD2	1.95	0.49
1:C:111:VAL:HG23	1:C:113:PHE:CZ	2.47	0.49
1:A:32:LYS:HG2	1:A:62:HIS:CE1	2.48	0.49
1:D:65:ASP:HA	1:D:93:LEU:HD22	1.95	0.48
1:C:111:VAL:HG13	1:C:118:PRO:CD	2.43	0.48
1:C:96:LEU:HD21	1:C:279:ARG:HH11	1.79	0.48
1:B:241:LEU:HD23	3:B:2179:HOH:O	2.13	0.47
1:D:196:HIS:ND1	1:D:295:SER:CB	2.79	0.46
1:B:103:ARG:HB3	3:B:2197:HOH:O	2.16	0.46
1:C:105:ASN:HD22	1:C:105:ASN:N	2.03	0.45
1:A:202:HIS:CE1	1:A:258:ASP:OD2	2.69	0.45
1:B:105:ASN:HD22	1:B:105:ASN:N	2.06	0.44
1:D:93:LEU:HD21	1:D:278:ARG:HD3	2.00	0.44
1:C:96:LEU:HD21	1:C:279:ARG:NH1	2.33	0.43
1:B:117:TYR:OH	1:B:211[A]:GLN:NE2	2.51	0.43
1:A:124:ARG:HB2	1:A:254:VAL:HG22	1.99	0.43
1:B:108:HIS:HD1	1:B:214:HIS:CE1	2.35	0.43
1:B:96:LEU:HD22	1:B:96:LEU:N	2.33	0.43
1:D:78:PRO:HB2	1:D:92:TYR:CG	2.54	0.43
1:A:32:LYS:HG2	1:A:62:HIS:HE1	1.82	0.42
1:A:58:ARG:NH1	1:A:253:ASP:OD1	2.53	0.42
1:C:111:VAL:CG1	1:C:118:PRO:CD	2.98	0.42
1:C:65:ASP:OD2	1:C:278:ARG:HD2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:VAL:HG13	1:C:118:PRO:HD2	2.01	0.41
1:A:214:HIS:CD2	1:A:214:HIS:C	2.98	0.41
1:C:241:LEU:HD23	3:C:2127:HOH:O	2.21	0.41
1:D:65:ASP:CA	1:D:93:LEU:HD22	2.51	0.41
1:D:138:ALA:O	1:D:262:THR:HA	2.20	0.41
1:B:124:ARG:HB2	1:B:254:VAL:HG22	2.02	0.40
1:D:32:LYS:CB	1:D:62:HIS:HE1	2.34	0.40
1:A:94:LEU:HD23	1:A:279:ARG:NH1	2.37	0.40
1:B:121:SER:HB2	1:B:257:TRP:CZ2	2.56	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	247/301 (82%)	238 (96%)	9 (4%)	0	100	100
1	B	248/301 (82%)	238 (96%)	10 (4%)	0	100	100
1	C	234/301 (78%)	225 (96%)	9 (4%)	0	100	100
1	D	237/301 (79%)	228 (96%)	9 (4%)	0	100	100
All	All	966/1204 (80%)	929 (96%)	37 (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	201/244 (82%)	196 (98%)	5 (2%)	42	37
1	B	200/244 (82%)	193 (96%)	7 (4%)	32	24
1	C	183/244 (75%)	176 (96%)	7 (4%)	29	21
1	D	184/244 (75%)	179 (97%)	5 (3%)	39	34
All	All	768/976 (79%)	744 (97%)	24 (3%)	35	29

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ARG
1	A	105	ASN
1	A	111	VAL
1	A	296	ARG
1	A	299	ARG
1	B	63	LEU
1	B	105	ASN
1	B	111	VAL
1	B	124	ARG
1	B	191	VAL
1	B	214	HIS
1	B	296	ARG
1	C	61	THR
1	C	79	VAL
1	C	96	LEU
1	C	103	ARG
1	C	105	ASN
1	C	192	TYR
1	C	279	ARG
1	D	62	HIS
1	D	90	THR
1	D	96	LEU
1	D	105	ASN
1	D	111	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	105	ASN
1	B	105	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	162	HIS
1	B	293	GLN
1	C	105	ASN
1	C	145	GLN
1	C	264	HIS
1	D	105	ASN
1	D	264	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 ⓘ

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	254/301 (84%)	-0.12	7 (2%) 55 59	15, 24, 44, 70	1 (0%)
1	B	255/301 (84%)	-0.13	9 (3%) 47 50	15, 24, 43, 70	1 (0%)
1	C	242/301 (80%)	0.08	13 (5%) 31 33	17, 28, 50, 63	0
1	D	244/301 (81%)	0.58	29 (11%) 9 9	17, 31, 58, 79	1 (0%)
All	All	995/1204 (82%)	0.10	58 (5%) 29 30	15, 26, 51, 79	3 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	92	TYR	6.8
1	D	67	SER	5.8
1	D	192	TYR	5.5
1	C	93	LEU	5.4
1	D	91	ARG	5.3
1	D	13	LEU	5.1
1	D	79	VAL	4.8
1	C	192	TYR	4.6
1	B	191	VAL	4.5
1	D	61	THR	4.5
1	D	90	THR	4.5
1	D	66	GLN	4.4
1	C	13	LEU	4.2
1	C	94	LEU	4.1
1	D	93	LEU	4.1
1	A	191	VAL	4.0
1	A	300	LYS	3.9
1	C	299	ARG	3.9
1	C	96	LEU	3.8
1	D	63	LEU	3.7
1	D	64	ASP	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	85	PRO	3.6
1	D	299	ARG	3.4
1	D	65	ASP	3.3
1	D	62	HIS	3.3
1	D	94	LEU	3.2
1	D	40	ALA	3.2
1	D	164	ASN	3.1
1	C	196	HIS	3.1
1	D	196	HIS	3.1
1	B	192	TYR	2.8
1	D	39	ALA	2.8
1	D	96	LEU	2.7
1	B	85	PRO	2.7
1	D	37	LEU	2.7
1	D	70	GLY	2.6
1	A	62	HIS	2.6
1	B	80	ALA	2.6
1	C	95	GLN	2.5
1	C	79	VAL	2.5
1	D	298	THR	2.5
1	B	300	LYS	2.5
1	C	62	HIS	2.5
1	A	202	HIS	2.4
1	B	108	HIS	2.3
1	B	98	GLY	2.3
1	A	192	TYR	2.3
1	D	36	ASP	2.3
1	C	61	THR	2.2
1	B	299	ARG	2.2
1	D	35	PRO	2.2
1	D	204	ILE	2.2
1	D	72	ALA	2.2
1	C	164	ASN	2.1
1	D	116	ALA	2.1
1	C	64	ASP	2.1
1	A	299	ARG	2.1
1	B	103	ARG	2.1

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 [i](#)

There are no oligosaccharides 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, 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($\text{\AA}^2$)	Q<0.9
2	NA	C	1300[A]	1/1	0.81	0.41	38,38,38,38	1
2	NA	D	1300[A]	1/1	0.82	0.15	38,38,38,38	1
2	NA	A	1301[A]	1/1	0.83	0.10	31,31,31,31	1
2	NA	B	1301[A]	1/1	0.87	0.17	30,30,30,30	1

6.5 Other polymers [i](#)

There are no such residues in this entry.