



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1SIU / pdb_00001siu
Title : KUMAMOLISIN-AS E78H MUTANT
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Deposited on : 2004-03-01
Resolution : 2.31 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

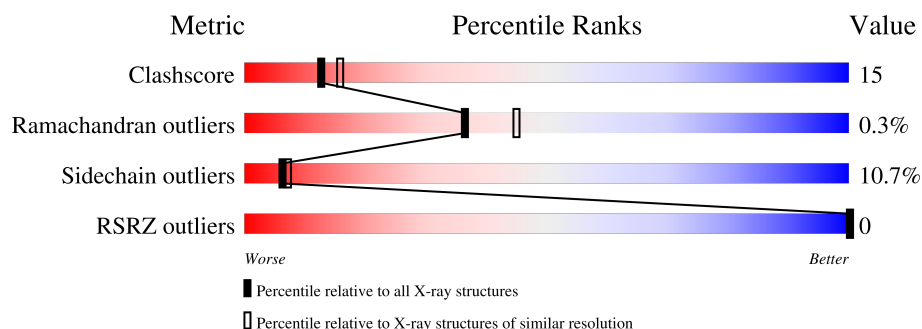
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	364	

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	400	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2711 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.

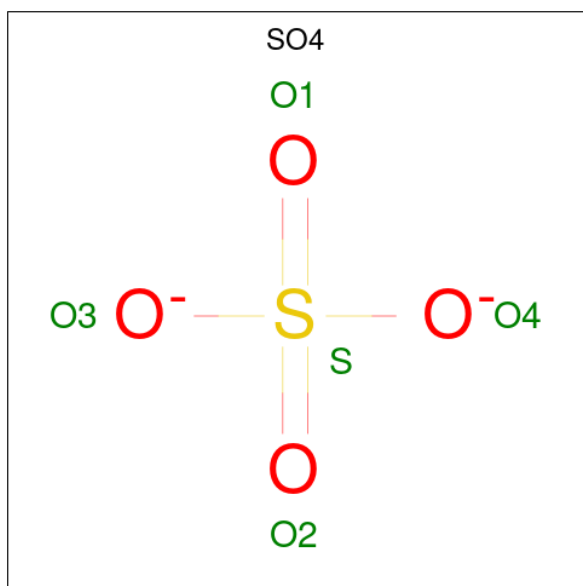
- Molecule 1 is a protein called kumamolisin-As.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	355	2528	1593	425	506	4	0	0	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	HIS	GLU	engineered mutation	UNP Q8GB88

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is water.

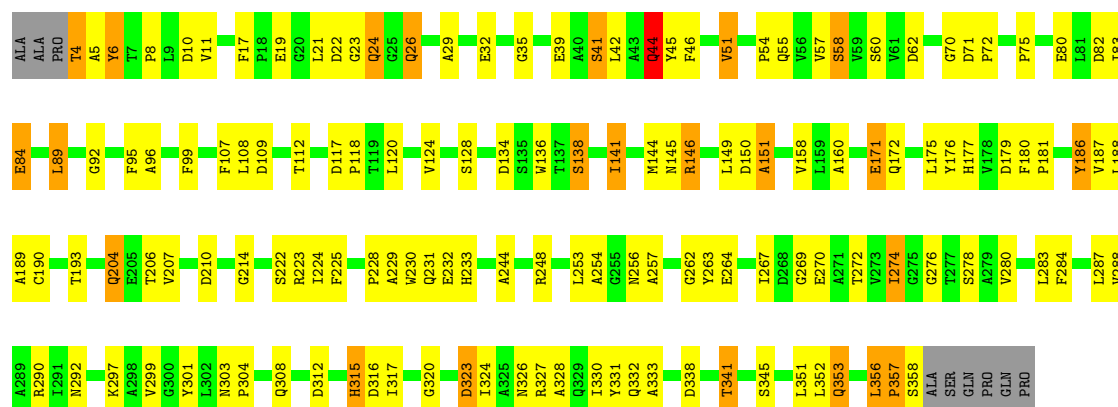
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	177	Total 177	O 177	0	0

3 Residue-property plots

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: kumamolisin-As

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	42.16Å 45.04Å 49.43Å 114.82° 106.36° 102.03°	Depositor
Resolution (Å)	10.00 – 2.31 10.00 – 2.31	Depositor EDS
% Data completeness (in resolution range)	89.2 (10.00-2.31) 91.4 (10.00-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.59 (at 2.31Å)	Xtriage
Refinement program	SHELXL, SHELXL-97	Depositor
R, R_{free}	0.162 , 0.287 0.159 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 78.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2711	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.44% 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: SO4, CA

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	0.58	1/2592 (0.0%)	1.79	53/3562 (1.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	357	PRO	C-N	-5.85	1.25	1.33

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	ASP	CA-CB-CG	9.32	121.92	112.60
1	A	179	ASP	CA-CB-CG	9.25	121.85	112.60
1	A	171	GLU	CA-C-N	8.34	137.48	121.54
1	A	171	GLU	C-N-CA	8.34	137.48	121.54
1	A	26	GLN	CA-C-N	-7.80	111.62	122.93
1	A	26	GLN	C-N-CA	-7.80	111.62	122.93
1	A	60	SER	CA-C-N	-7.80	113.04	123.10
1	A	60	SER	C-N-CA	-7.80	113.04	123.10
1	A	323	ASP	CA-CB-CG	7.78	120.38	112.60
1	A	233	HIS	CA-CB-CG	-7.31	106.49	113.80
1	A	189	ALA	CA-C-N	6.83	132.81	123.11
1	A	189	ALA	C-N-CA	6.83	132.81	123.11
1	A	17	PHE	CA-CB-CG	6.57	120.37	113.80
1	A	224	ILE	CB-CA-C	-6.54	105.02	111.30
1	A	316	ASP	CA-C-N	-6.29	114.84	122.90
1	A	316	ASP	C-N-CA	-6.29	114.84	122.90
1	A	84	GLU	CB-CG-CD	6.07	122.93	112.60
1	A	70	GLY	CA-C-O	5.85	125.47	119.10
1	A	312	ASP	CA-CB-CG	5.80	118.40	112.60
1	A	138	SER	CA-C-O	5.78	126.54	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	256	ASN	CA-C-O	5.75	126.29	120.88
1	A	146	ARG	CA-C-O	5.74	126.63	120.55
1	A	29	ALA	CA-C-N	-5.74	115.02	122.99
1	A	29	ALA	C-N-CA	-5.74	115.02	122.99
1	A	134	ASP	CA-CB-CG	5.71	118.31	112.60
1	A	315	HIS	CA-CB-CG	-5.70	108.10	113.80
1	A	315	HIS	CA-C-O	5.61	126.76	120.92
1	A	324	ILE	N-CA-C	-5.56	107.56	112.90
1	A	176	TYR	O-C-N	-5.54	116.74	123.16
1	A	151	ALA	CA-C-N	5.52	129.10	120.82
1	A	151	ALA	C-N-CA	5.52	129.10	120.82
1	A	6	TYR	CA-C-N	-5.46	113.63	122.48
1	A	6	TYR	C-N-CA	-5.46	113.63	122.48
1	A	95	PHE	CA-C-N	5.33	130.43	122.86
1	A	95	PHE	C-N-CA	5.33	130.43	122.86
1	A	44	GLN	CA-C-O	5.28	126.10	120.24
1	A	186	TYR	CA-C-O	5.27	125.81	119.43
1	A	262	GLY	N-CA-C	5.25	121.16	112.66
1	A	244	ALA	O-C-N	-5.24	116.02	122.57
1	A	141	ILE	CA-C-N	-5.23	113.32	120.44
1	A	141	ILE	C-N-CA	-5.23	113.32	120.44
1	A	58	SER	CA-C-N	-5.21	115.76	122.99
1	A	58	SER	C-N-CA	-5.21	115.76	122.99
1	A	287	LEU	CA-C-N	5.16	127.06	120.56
1	A	287	LEU	C-N-CA	5.16	127.06	120.56
1	A	8	PRO	N-CA-C	-5.15	106.70	113.65
1	A	353	GLN	CA-C-O	5.12	126.38	120.90
1	A	324	ILE	CA-C-O	5.12	124.72	119.35
1	A	320	GLY	CA-C-O	-5.11	117.20	122.26
1	A	356	LEU	O-C-N	5.11	125.85	121.30
1	A	323	ASP	CA-C-N	-5.11	115.08	122.69
1	A	323	ASP	C-N-CA	-5.11	115.08	122.69
1	A	341	THR	CA-C-O	5.07	124.75	119.03

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	2528	0	2416	75	0
2	A	5	0	0	2	0
3	A	1	0	0	0	0
4	A	177	0	0	12	0
All	All	2711	0	2416	75	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 15.

All (75) 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:292:ASN:OD1	1:A:299:VAL:HG22	1.83	0.77
1:A:128:SER:HB2	1:A:278:SER:HB2	1.67	0.76
1:A:107:PHE:HB3	4:A:657:HOH:O	1.84	0.76
1:A:24:GLN:HA	1:A:92:GLY:O	1.87	0.74
1:A:352:LEU:HD23	4:A:551:HOH:O	1.90	0.70
1:A:327:ARG:HG3	4:A:619:HOH:O	1.92	0.69
1:A:80:GLU:O	1:A:84:GLU:HG3	1.93	0.68
1:A:46:PHE:HB3	1:A:51:VAL:HG22	1.75	0.68
1:A:284:PHE:O	1:A:288:VAL:HG23	1.94	0.67
1:A:188:LEU:HD21	1:A:253:LEU:HD12	1.76	0.66
1:A:6:TYR:O	1:A:264:GLU:HG3	1.96	0.66
1:A:315:HIS:HB3	1:A:345:SER:OG	1.97	0.64
1:A:248:ARG:HB3	4:A:668:HOH:O	1.97	0.64
1:A:223:ARG:HG3	2:A:400:SO4:O2	1.98	0.64
1:A:225:PHE:HB2	4:A:668:HOH:O	1.98	0.63
1:A:358:SER:N	4:A:623:HOH:O	2.31	0.62
1:A:136:TRP:CH2	1:A:144:MET:HE2	2.33	0.62
1:A:4:THR:HG22	1:A:5:ALA:H	1.65	0.62
1:A:6:TYR:HB3	1:A:10:ASP:HB2	1.81	0.61
1:A:108:LEU:O	1:A:112:THR:HG23	2.05	0.56
1:A:229:ALA:O	1:A:232:GLU:HG3	2.04	0.56
1:A:35:GLY:HA3	1:A:75:PRO:HB2	1.87	0.56
1:A:22:ASP:OD1	1:A:24:GLN:HB3	2.06	0.56
1:A:193:THR:HB	1:A:206:THR:O	2.05	0.56
1:A:45:TYR:CE2	1:A:84:GLU:HB3	2.43	0.53
1:A:32:GLU:O	1:A:99:PHE:HA	2.10	0.52
1:A:42:LEU:HD13	1:A:83:ILE:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:GLY:O	1:A:26:GLN:HB2	2.11	0.51
1:A:62:ASP:OD2	1:A:109:ASP:OD2	2.29	0.50
1:A:128:SER:HB2	1:A:278:SER:CB	2.41	0.49
1:A:323:ASP:OD2	1:A:326:ASN:OD1	2.30	0.49
1:A:58:SER:HB2	4:A:569:HOH:O	2.13	0.48
1:A:96:ALA:CB	1:A:120:LEU:HD13	2.44	0.48
1:A:204:GLN:HE21	1:A:204:GLN:HB2	1.57	0.47
1:A:32:GLU:OE2	1:A:82:ASP:OD2	2.33	0.46
1:A:228:PRO:HG2	1:A:231:GLN:HB2	1.97	0.46
1:A:146:ARG:NH1	1:A:150:ASP:OD1	2.49	0.46
1:A:21:LEU:HD13	1:A:290:ARG:O	2.15	0.46
1:A:80:GLU:HB2	1:A:267:ILE:HD12	1.97	0.46
1:A:190:CYS:HB3	1:A:280:VAL:HG12	1.97	0.45
1:A:267:ILE:O	1:A:270:GLU:HG2	2.17	0.45
1:A:180:PHE:CG	1:A:181:PRO:HA	2.52	0.45
1:A:55:GLN:NE2	4:A:550:HOH:O	2.50	0.45
1:A:41:SER:O	1:A:44:GLN:NE2	2.50	0.45
1:A:204:GLN:NE2	4:A:666:HOH:O	2.50	0.45
1:A:326:ASN:OD1	1:A:328:ALA:HB3	2.17	0.44
1:A:89:LEU:HD23	1:A:283:LEU:HD12	1.99	0.44
1:A:11:VAL:HG21	1:A:263:TYR:CE2	2.53	0.44
1:A:96:ALA:HB2	1:A:120:LEU:HD13	2.00	0.44
1:A:223:ARG:NE	2:A:400:SO4:O2	2.50	0.44
1:A:257:ALA:O	1:A:276:GLY:N	2.49	0.43
1:A:323:ASP:HB2	1:A:330:ILE:O	2.18	0.43
1:A:210:ASP:HB2	1:A:214:GLY:HA3	1.99	0.43
1:A:254:ALA:HB2	1:A:341:THR:HA	2.00	0.43
1:A:272:THR:HG23	1:A:274:ILE:HD12	2.00	0.43
1:A:117:ASP:HA	1:A:118:PRO:HD2	1.74	0.43
1:A:328:ALA:CB	1:A:330:ILE:HD12	2.49	0.43
1:A:207:VAL:CG2	1:A:333:ALA:HB2	2.49	0.42
1:A:330:ILE:HA	1:A:331:TYR:HA	1.83	0.42
1:A:44:GLN:HE21	1:A:44:GLN:HB3	1.65	0.42
1:A:57:VAL:HA	4:A:620:HOH:O	2.18	0.42
1:A:151:ALA:HB3	4:A:534:HOH:O	2.19	0.42
1:A:328:ALA:HB1	1:A:330:ILE:HD12	2.01	0.42
1:A:71:ASP:HA	1:A:72:PRO:HD3	1.91	0.42
1:A:264:GLU:HG3	1:A:264:GLU:H	1.63	0.42
1:A:303:ASN:HB2	1:A:304:PRO:HD3	2.02	0.42
1:A:46:PHE:CD2	1:A:54:PRO:HD2	2.55	0.41
1:A:4:THR:O	1:A:5:ALA:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ALA:HB3	1:A:187:VAL:HG11	2.02	0.41
1:A:186:TYR:HA	1:A:301:TYR:CE1	2.56	0.41
1:A:257:ALA:HB1	1:A:276:GLY:C	2.46	0.41
1:A:269:GLY:HA2	4:A:635:HOH:O	2.20	0.41
1:A:42:LEU:CD1	1:A:83:ILE:HG21	2.50	0.40
1:A:171:GLU:HB3	1:A:177:HIS:CD2	2.56	0.40
1:A:190:CYS:HB3	1:A:280:VAL:CG1	2.52	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	353/364 (97%)	337 (96%)	15 (4%)	1 (0%)	36 45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	357	PRO

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	253/260 (97%)	226 (89%)	27 (11%)	6 7

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	19	GLU
1	A	24	GLN
1	A	39	GLU
1	A	41	SER
1	A	44	GLN
1	A	51	VAL
1	A	89	LEU
1	A	124	VAL
1	A	138	SER
1	A	141	ILE
1	A	145	ASN
1	A	149	LEU
1	A	158	VAL
1	A	172	GLN
1	A	175	LEU
1	A	204	GLN
1	A	222	SER
1	A	230	TRP
1	A	274	ILE
1	A	297	LYS
1	A	308	GLN
1	A	317	ILE
1	A	332	GLN
1	A	351	LEU
1	A	353	GLN
1	A	356	LEU

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

Mol	Chain	Res	Type
1	A	16	GLN
1	A	44	GLN
1	A	55	GLN
1	A	102	ASN
1	A	145	ASN
1	A	204	GLN
1	A	256	ASN
1	A	329	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z > 2$
2	SO4	A	400	-	4,4,4	0.47	0	6,6,6	0.18	0

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	SO4	2	0

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	355/364 (97%)	-0.63	0 100 100	11, 22, 43, 78	0

There are no RSRZ outliers to report.

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 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(Å ²)	Q<0.9
2	SO4	A	400	5/5	0.98	0.06	32,33,46,52	0
3	CA	A	401	1/1	0.99	0.03	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.