Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:53 PM UTC

PDB ID	:	5WLU / pdb_00005wlu
Title	:	Carbonic Anhydrase IX-mimic in complex with aryloxy-2-hydroxypropylamm ine sulfonamide
Authors	:	Lomelino, C.L.; Andring, J.T.; McKenna, R.
Deposited on	:	2017-07-27
Resolution	:	1.39 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:

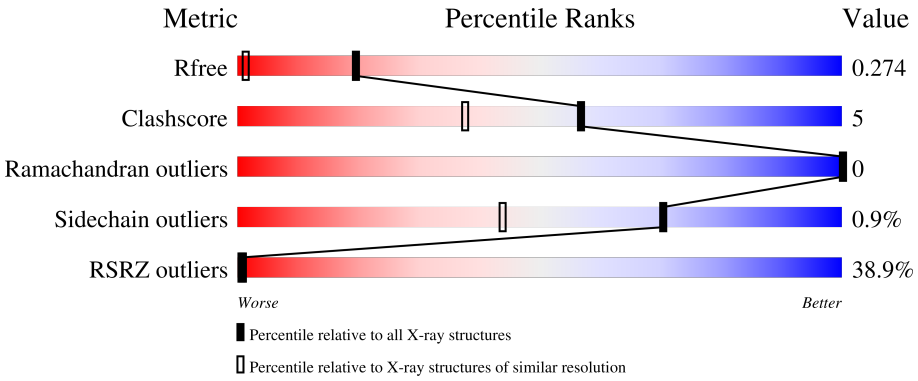
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.39 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}	180053	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	Quality of chain
1	A	257	39% 90% 9%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2191 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 Carbonic Anhydrase IX-mimic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	7	5	0
			2077	1331	356	388	2			

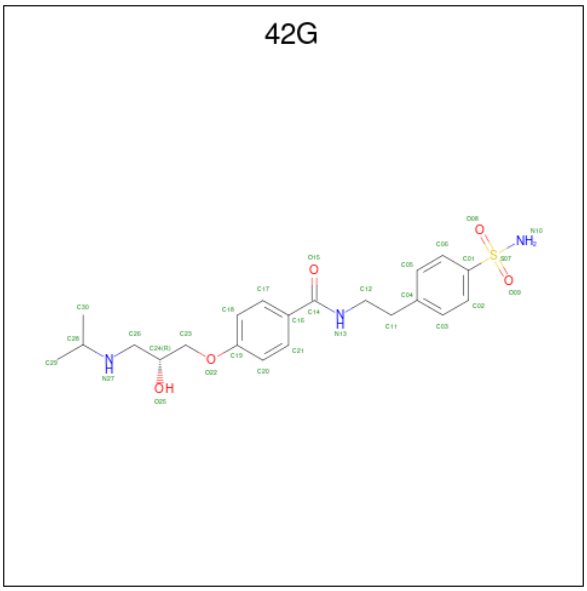
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	SER	ALA	conflict	UNP P00918
A	67	GLN	ASN	conflict	UNP P00918
A	69	THR	GLU	conflict	UNP P00918
A	91	LEU	ILE	conflict	UNP P00918
A	131	VAL	PHE	conflict	UNP P00918
A	170	GLU	LYS	conflict	UNP P00918
A	204	ALA	LEU	conflict	UNP P00918

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 4-{(2R)-2-hydroxy-3-[(propan-2-yl)amino]propoxy}-N-[2-(4-sulfamoylphenyl)ethyl]benzamide (CCD ID: 42G) (formula: $C_{21}H_{29}N_3O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			30	21	3	5	1		

- Molecule 4 is water.

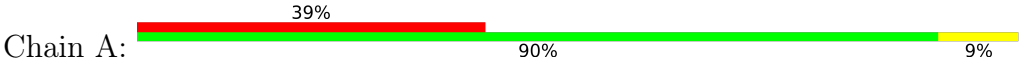
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	83	Total	O	0	0
			83	83		

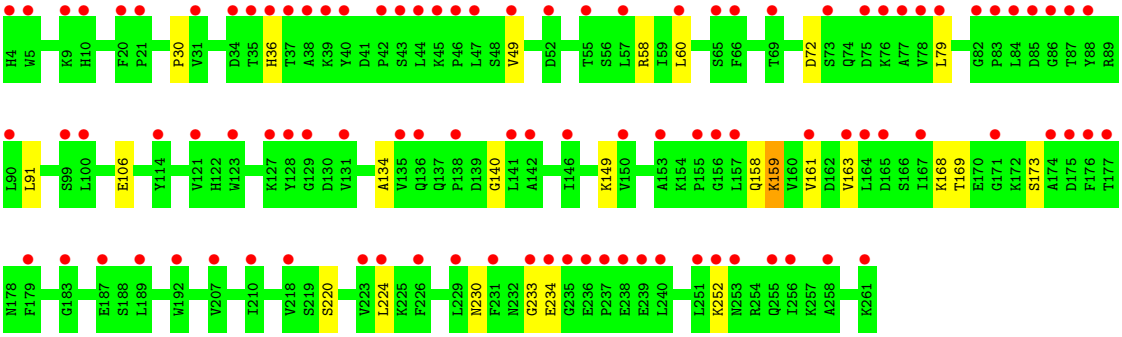
3 Residue-property plots (i)

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: Carbonic Anhydrase IX-mimic

Chain A:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	42.14Å 41.50Å 72.26Å 90.00° 104.02° 90.00°	Depositor
Resolution (Å)	35.10 – 1.39 35.10 – 1.39	Depositor EDS
% Data completeness (in resolution range)	91.7 (35.10-1.39) 92.2 (35.10-1.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 1.39Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.247 , 0.271 0.252 , 0.274	Depositor DCC
R_{free} test set	2019 reflections (4.10%)	wwPDB-VP
Wilson B-factor (Å^2)	14.4	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 39.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	2191	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 42G, ZN

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	0.37	1/2138 (0.0%)	0.54	0/2903

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	159	LYS	C-O	-5.45	1.17	1.24

There are no bond angle outliers.

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	2077	0	2028	19	0
2	A	1	0	0	0	0
3	A	30	0	0	0	0
4	A	83	0	0	10	0
All	All	2191	0	2028	19	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 5.

All (19) 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:252:LYS:HB2	4:A:402:HOH:O	1.74	0.88
1:A:163:VAL:CG2	4:A:454:HOH:O	2.24	0.86
1:A:220:SER:O	1:A:224:LEU:HD13	1.82	0.80
1:A:163:VAL:HB	4:A:454:HOH:O	1.92	0.70
1:A:163:VAL:HG23	4:A:454:HOH:O	1.87	0.66
1:A:58:ARG:NH1	1:A:173:SER:OG	2.30	0.65
1:A:168:LYS:NZ	1:A:230:ASN:OD1	2.26	0.61
1:A:163:VAL:CB	4:A:454:HOH:O	2.47	0.57
1:A:234:GLU:HG2	4:A:405:HOH:O	2.08	0.53
1:A:79:LEU:HD13	4:A:474:HOH:O	2.11	0.49
1:A:149:LYS:HE3	4:A:404:HOH:O	2.16	0.45
1:A:158:GLN:HA	1:A:161[A]:VAL:HG22	1.99	0.45
1:A:49:VAL:HG13	4:A:474:HOH:O	2.19	0.42
1:A:72:ASP:OD2	1:A:91:LEU:HD13	2.19	0.42
1:A:134:ALA:O	1:A:140:GLY:HA3	2.20	0.42
1:A:169:THR:HB	1:A:233:GLY:HA2	2.01	0.42
1:A:30:PRO:HG3	1:A:106:GLU:HB3	2.02	0.41
1:A:234:GLU:HG2	1:A:234:GLU:H	1.69	0.41
1:A:36:HIS:ND1	4:A:401:HOH:O	2.25	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	260/257 (101%)	253 (97%)	7 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	227/222 (102%)	225 (99%)	2 (1%)	70 44

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	LEU
1	A	159	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	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 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	$\#\|Z\| > 2$
3	42G	A	302	2	31,31,31	1.53	3 (9%)	42,42,42	1.39	4 (9%)

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	42G	A	302	2	-	7/26/26/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	42G	C14-N13	5.25	1.45	1.33
3	A	302	42G	S07-N10	4.36	1.68	1.60
3	A	302	42G	C01-S07	3.02	1.81	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	302	42G	O09-S07-O08	-5.47	110.38	118.80
3	A	302	42G	O09-S07-N10	4.03	113.16	107.35
3	A	302	42G	C21-C16-C17	2.23	121.40	118.57
3	A	302	42G	C12-C11-C04	-2.09	108.12	112.83

There are no chirality outliers.

All (7) torsion outliers are listed below:

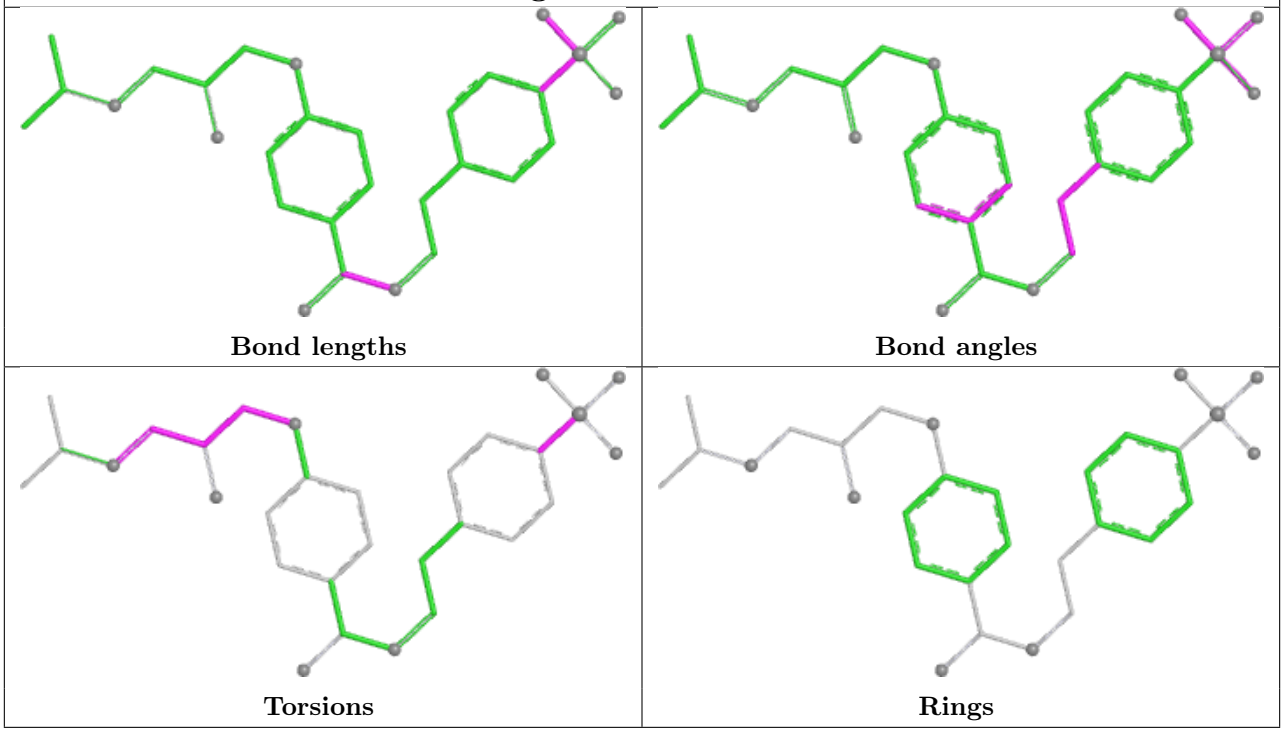
Mol	Chain	Res	Type	Atoms
3	A	302	42G	O22-C23-C24-O25
3	A	302	42G	O22-C23-C24-C26
3	A	302	42G	C23-C24-C26-N27
3	A	302	42G	C24-C23-O22-C19
3	A	302	42G	C24-C26-N27-C28
3	A	302	42G	C06-C01-S07-O08
3	A	302	42G	C02-C01-S07-O08

There are no ring outliers.

No monomer is involved in short contacts.

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 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.

Ligand 42G A 302



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

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, 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	OWAB(Å^2)	Q<0.9
1	A	257/257 (100%)	1.87	100 (38%) 1 1	7, 17, 31, 51	5 (1%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	PRO	7.7
1	A	224	LEU	6.0
1	A	4	HIS	5.8
1	A	235	GLY	5.6
1	A	40	TYR	5.6
1	A	155	PRO	4.7
1	A	100	LEU	4.7
1	A	240	LEU	4.6
1	A	85	ASP	4.4
1	A	82	GLY	4.4
1	A	49	VAL	4.3
1	A	78	VAL	4.3
1	A	47	LEU	4.2
1	A	77	ALA	4.1
1	A	129	GLY	4.1
1	A	167	ILE	4.0
1	A	9	LYS	3.9
1	A	46	PRO	3.9
1	A	44	LEU	3.9
1	A	153	ALA	3.9
1	A	38	ALA	3.8
1	A	163	VAL	3.7
1	A	161[A]	VAL	3.7
1	A	179	PHE	3.6
1	A	238	GLU	3.5
1	A	233	GLY	3.5
1	A	21	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	135[A]	VAL	3.3
1	A	87	THR	3.3
1	A	146	ILE	3.3
1	A	176	PHE	3.2
1	A	86	GLY	3.2
1	A	234	GLU	3.2
1	A	75	ASP	3.2
1	A	37	THR	3.1
1	A	175	ASP	3.1
1	A	253	ASN	3.0
1	A	231	PHE	3.0
1	A	183	GLY	3.0
1	A	43	SER	3.0
1	A	42	PRO	3.0
1	A	229	LEU	3.0
1	A	60	LEU	2.9
1	A	52	ASP	2.9
1	A	165	ASP	2.9
1	A	251	LEU	2.9
1	A	5	TRP	2.8
1	A	131	VAL	2.8
1	A	255	GLN	2.8
1	A	261	LYS	2.8
1	A	256	ILE	2.8
1	A	157	LEU	2.8
1	A	164	LEU	2.8
1	A	236	GLU	2.8
1	A	55	THR	2.7
1	A	73	SER	2.7
1	A	207	VAL	2.7
1	A	141	LEU	2.7
1	A	121	VAL	2.6
1	A	20	PHE	2.6
1	A	192	TRP	2.5
1	A	39	LYS	2.5
1	A	10	HIS	2.5
1	A	88	TYR	2.5
1	A	252	LYS	2.5
1	A	156	GLY	2.5
1	A	65	SER	2.4
1	A	45	LYS	2.4
1	A	36	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	57	LEU	2.4
1	A	123	TRP	2.4
1	A	258	ALA	2.4
1	A	127	LYS	2.3
1	A	223	VAL	2.3
1	A	35	THR	2.3
1	A	177	THR	2.3
1	A	76	LYS	2.3
1	A	138	PRO	2.3
1	A	83	PRO	2.3
1	A	31	VAL	2.3
1	A	34	ASP	2.3
1	A	84	LEU	2.2
1	A	142	ALA	2.2
1	A	66	PHE	2.2
1	A	150	VAL	2.2
1	A	79	LEU	2.1
1	A	136	GLN	2.1
1	A	239	GLU	2.1
1	A	189	LEU	2.1
1	A	69	THR	2.1
1	A	210	ILE	2.1
1	A	171	GLY	2.1
1	A	90	LEU	2.1
1	A	187	GLU	2.1
1	A	174	ALA	2.1
1	A	128	TYR	2.1
1	A	99	SER	2.0
1	A	226	PHE	2.0
1	A	114	TYR	2.0
1	A	218	VAL	2.0

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

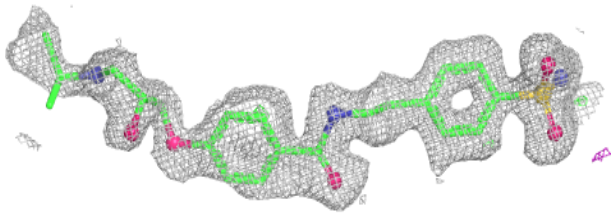
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

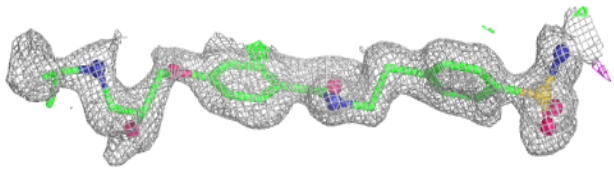
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	42G	A	302	30/30	0.94	0.14	8,25,40,49	0
2	ZN	A	301	1/1	1.00	0.02	9,9,9,9	0

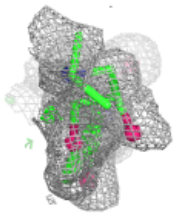
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 42G A 302:

$2mF_o$-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

There are no such residues in this entry.