



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 08:48 pm GMT

PDB ID : 2C5D  
Title : STRUCTURE OF A MINIMAL GAS6-AXL COMPLEX  
Authors : Sasaki, T.; Knyazev, P.G.; Clout, N.J.; Cheburkin, Y.; Goehring, W.; Ullrich, A.; Timpl, R.; Hohenester, E.  
Deposited on : 2005-10-26  
Resolution : 3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

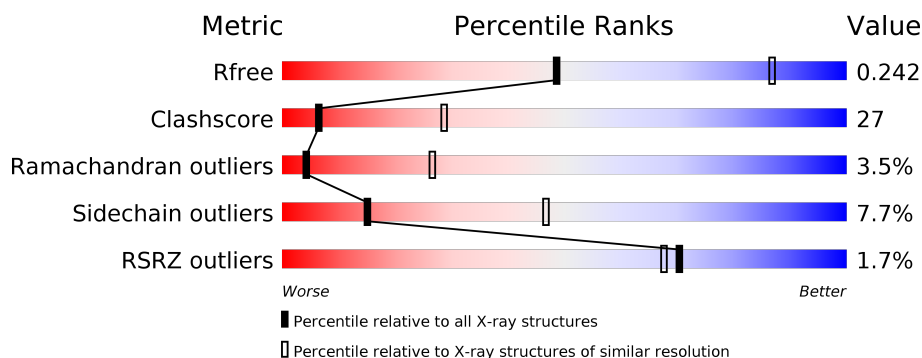
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	100719	1034 (3.36-3.24)
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)

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  $\geq 3$ , 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	422	<div> <div>%</div> <div> <div></div> <div>48%</div> <div>35%</div> <div>7%</div> <div>10%</div> </div> </div>
1	B	422	<div> <div>%</div> <div> <div></div> <div>47%</div> <div>36%</div> <div>7%</div> <div>10%</div> </div> </div>
2	C	195	<div> <div>2%</div> <div> <div></div> <div>53%</div> <div>39%</div> <div>5%</div> <div>••</div> </div> </div>
2	D	195	<div> <div>2%</div> <div> <div></div> <div>54%</div> <div>38%</div> <div>6%</div> <div>••</div> </div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8879 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 GROWTH-ARREST-SPECIFIC PROTEIN 6 PRECURSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	0	1
			2953	1882	518	539	14			
1	B	381	Total	C	N	O	S	0	0	1
			2953	1882	518	539	14			

- Molecule 2 is a protein called TYROSINE-PROTEIN KINASE RECEPTOR UFO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	192	Total	C	N	O	S	0	0	1
			1454	911	251	288	4			
2	D	192	Total	C	N	O	S	0	0	1
			1454	911	251	288	4			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

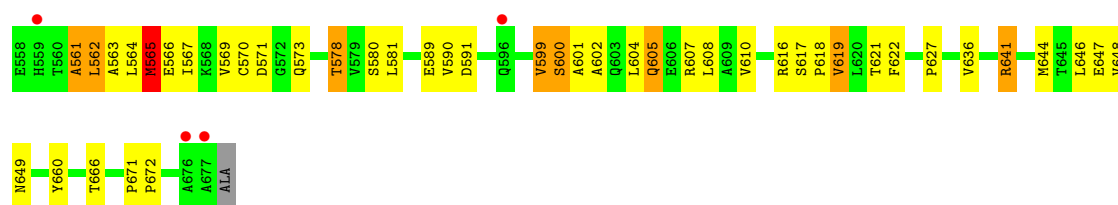
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Ni	0	0
			1	1		
5	C	1	Total	Ni	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

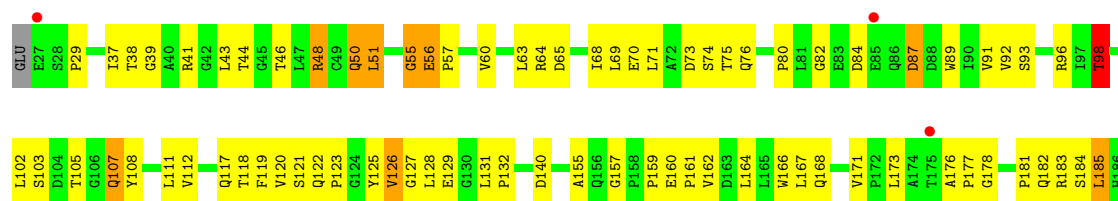


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	S	0	0
			5	4	1		

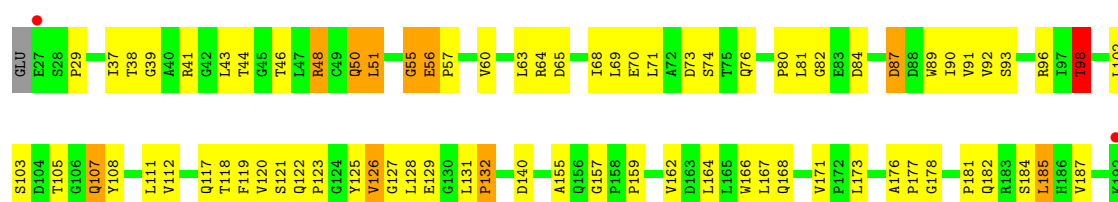




• Molecule 2: TYROSINE-PROTEIN KINASE RECEPTOR UFO



• Molecule 2: TYROSINE-PROTEIN KINASE RECEPTOR UFO



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	292.95Å 292.95Å 63.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.30 19.89 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-3.30) 99.9 (19.89-3.30)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.10 (at 3.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.241 , 0.265 0.218 , 0.242	Depositor DCC
$R_{free}$ test set	2383 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	85.0	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 36.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.034 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8879	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NI, CA, NAG, 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	0.45	0/3017	0.70	0/4107
1	B	0.45	0/3017	0.70	0/4107
2	C	0.52	0/1489	0.69	0/2041
2	D	0.52	0/1489	0.69	0/2041
All	All	0.48	0/9012	0.70	0/12296

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2953	0	2951	151	0
1	B	2953	0	2951	156	0
2	C	1454	0	1401	86	0
2	D	1454	0	1401	85	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	28	0	25	1	0
4	B	28	0	25	2	0
5	C	1	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1	0	0	0	0
6	C	5	0	0	0	0
All	All	8879	0	8754	468	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 27.

The worst 5 of 468 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:622:PHE:CE2	1:A:627:PRO:HD3	2.02	0.94
2:D:51:LEU:HD23	2:D:51:LEU:H	1.32	0.94
2:C:51:LEU:H	2:C:51:LEU:HD23	1.33	0.93
1:B:622:PHE:CE2	1:B:627:PRO:HD3	2.04	0.93
1:B:332:GLY:HA3	1:B:441:LEU:HB2	1.54	0.89

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	375/422 (89%)	296 (79%)	64 (17%)	15 (4%)	3	23
1	B	375/422 (89%)	297 (79%)	63 (17%)	15 (4%)	3	23
2	C	190/195 (97%)	171 (90%)	14 (7%)	5 (3%)	6	33
2	D	190/195 (97%)	171 (90%)	14 (7%)	5 (3%)	6	33
All	All	1130/1234 (92%)	935 (83%)	155 (14%)	40 (4%)	4	26

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	433	LEU
1	A	455	ASP
1	A	456	THR
1	B	433	LEU
1	B	455	ASP

### 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	320/356 (90%)	295 (92%)	25 (8%)	15	46
1	B	320/356 (90%)	296 (92%)	24 (8%)	16	48
2	C	162/166 (98%)	150 (93%)	12 (7%)	16	48
2	D	162/166 (98%)	149 (92%)	13 (8%)	14	45
All	All	964/1044 (92%)	890 (92%)	74 (8%)	15	47

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	375	ASN
1	B	540	VAL
2	D	107	GLN
1	B	391	LEU
1	B	435	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	429	HIS
1	B	465	ASN
2	D	109	GLN
1	B	449	ASN
1	B	573	GLN

### 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 ⓘ

4 carbohydrates 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	$\# Z  > 2$
4	NAG	A	1678	1,4	14,14,15	0.63	0	15,19,21	0.94	0
4	NAG	A	1679	4	14,14,15	0.66	0	15,19,21	0.84	1 (6%)
4	NAG	B	1678	1,4	14,14,15	0.52	0	15,19,21	0.84	1 (6%)
4	NAG	B	1679	4	14,14,15	0.75	0	15,19,21	1.06	2 (13%)

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	NAG	A	1678	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1679	4	-	0/6/23/26	0/1/1/1
4	NAG	B	1678	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1679	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1678	NAG	C2-N2-C7	-2.56	119.22	122.94

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1679	NAG	C2-N2-C7	-2.44	119.38	122.94
4	A	1679	NAG	C2-N2-C7	-2.29	119.61	122.94
4	B	1679	NAG	C4-C3-C2	-2.18	107.82	111.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1678	NAG	1	0
4	B	1678	NAG	2	0

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are 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	$\# Z  > 2$
6	SO4	C	1219	-	4,4,4	0.39	0	6,6,6	0.14	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
6	SO4	C	1219	-	-	0/0/0/0	0/0/0/0

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.

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	381/422 (90%)	-0.27	6 (1%) 72 69	25, 60, 118, 144	2 (0%)
1	B	381/422 (90%)	-0.31	6 (1%) 72 69	25, 60, 118, 144	2 (0%)
2	C	192/195 (98%)	-0.34	4 (2%) 64 61	28, 56, 86, 101	0
2	D	192/195 (98%)	-0.26	4 (2%) 64 61	27, 56, 86, 101	0
All	All	1146/1234 (92%)	-0.29	20 (1%) 70 67	25, 59, 112, 144	4 (0%)

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	677	ALA	4.8
1	A	676	ALA	3.3
2	D	218	PRO	3.2
2	D	192	LYS	3.1
1	B	677	ALA	2.9

### 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](#)

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	1678	14/15	0.85	0.23	0.62	65,73,77,82	0
4	NAG	B	1678	14/15	0.92	0.17	-0.55	62,68,72,80	0
4	NAG	B	1679	14/15	0.86	0.41	-	86,89,91,92	0
4	NAG	A	1679	14/15	0.84	0.57	-	86,91,94,95	0

## 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	CA	A	1677	1/1	0.99	0.18	0.38	40,40,40,40	0
3	CA	B	1677	1/1	0.99	0.17	0.25	45,45,45,45	0
6	SO4	C	1219	5/5	0.95	0.09	-	103,103,104,104	0
5	NI	D	1218	1/1	0.91	0.06	-	134,134,134,134	0
5	NI	C	1218	1/1	0.99	0.03	-	127,127,127,127	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.