



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:39 PM GMT

PDB ID : 4A2M
Title : Structure of the periplasmic domain of the heparin and heparan sulphate sensing hybrid two component system BT4663 in apo and ligand bound forms
Authors : Lowe, E.C.; Basle, A.; Czjzek, M.; Firbank, S.J.; Bolam, D.N.
Deposited on : 2011-09-27
Resolution : 3.40 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
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

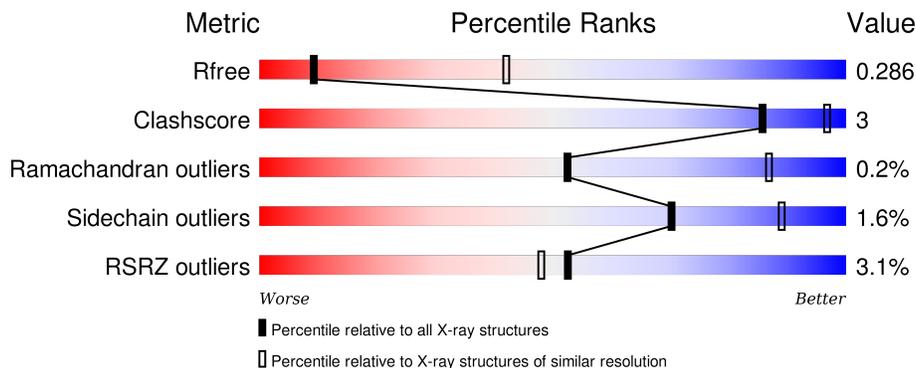
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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 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	795	
1	B	795	
1	C	795	
1	D	795	

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	NGS	B	1785	X	-	-	-
2	NGS	C	1785	X	-	-	-

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 23370 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 TWO-COMPONENT SYSTEM SENSOR HISTIDINE KINASE/RESPONSE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	741	5791	3684	956	1139	12	0	0	0
1	B	750	5893	3741	983	1157	12	0	0	0
1	C	743	5794	3683	960	1139	12	0	0	0
1	D	745	5772	3671	951	1138	12	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	788	LEU	-	EXPRESSION TAG	UNP Q89YR8
A	789	GLU	-	EXPRESSION TAG	UNP Q89YR8
A	790	HIS	-	EXPRESSION TAG	UNP Q89YR8
A	791	HIS	-	EXPRESSION TAG	UNP Q89YR8
A	792	HIS	-	EXPRESSION TAG	UNP Q89YR8
A	793	HIS	-	EXPRESSION TAG	UNP Q89YR8
A	794	HIS	-	EXPRESSION TAG	UNP Q89YR8
A	795	HIS	-	EXPRESSION TAG	UNP Q89YR8
B	788	LEU	-	EXPRESSION TAG	UNP Q89YR8
B	789	GLU	-	EXPRESSION TAG	UNP Q89YR8
B	790	HIS	-	EXPRESSION TAG	UNP Q89YR8
B	791	HIS	-	EXPRESSION TAG	UNP Q89YR8
B	792	HIS	-	EXPRESSION TAG	UNP Q89YR8
B	793	HIS	-	EXPRESSION TAG	UNP Q89YR8
B	794	HIS	-	EXPRESSION TAG	UNP Q89YR8
B	795	HIS	-	EXPRESSION TAG	UNP Q89YR8
C	788	LEU	-	EXPRESSION TAG	UNP Q89YR8
C	789	GLU	-	EXPRESSION TAG	UNP Q89YR8
C	790	HIS	-	EXPRESSION TAG	UNP Q89YR8
C	791	HIS	-	EXPRESSION TAG	UNP Q89YR8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	792	HIS	-	EXPRESSION TAG	UNP Q89YR8
C	793	HIS	-	EXPRESSION TAG	UNP Q89YR8
C	794	HIS	-	EXPRESSION TAG	UNP Q89YR8
C	795	HIS	-	EXPRESSION TAG	UNP Q89YR8
D	788	LEU	-	EXPRESSION TAG	UNP Q89YR8
D	789	GLU	-	EXPRESSION TAG	UNP Q89YR8
D	790	HIS	-	EXPRESSION TAG	UNP Q89YR8
D	791	HIS	-	EXPRESSION TAG	UNP Q89YR8
D	792	HIS	-	EXPRESSION TAG	UNP Q89YR8
D	793	HIS	-	EXPRESSION TAG	UNP Q89YR8
D	794	HIS	-	EXPRESSION TAG	UNP Q89YR8
D	795	HIS	-	EXPRESSION TAG	UNP Q89YR8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	2	30	14	1	14	1	0	0
2	B	2	30	14	1	14	1	0	0
2	C	2	30	14	1	14	1	0	0
2	D	2	30	14	1	14	1	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.12Å 80.83Å 228.94Å 90.00° 93.96° 90.00°	Depositor
Resolution (Å)	55.73 – 3.40 55.73 – 3.40	Depositor EDS
% Data completeness (in resolution range)	97.5 (55.73-3.40) 97.6 (55.73-3.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 3.40Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.268 , 0.286 0.267 , 0.286	Depositor DCC
R_{free} test set	2544 reflections (4.85%)	DCC
Wilson B-factor (Å ²)	58.9	Xtrriage
Anisotropy	0.457	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 52.2	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtrriage
Outliers	0 of 55028 reflections	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	23370	wwPDB-VP
Average B, all atoms (Å ²)	131.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GCD, NGS

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	0.43	0/5926	0.46	0/8076
1	B	0.43	2/6028 (0.0%)	0.47	0/8205
1	C	0.43	6/5929 (0.1%)	0.46	0/8081
1	D	0.43	5/5907 (0.1%)	0.46	0/8060
All	All	0.43	13/23790 (0.1%)	0.46	0/32422

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
2	B	1	0
2	C	1	0
All	All	2	0

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	371	TRP	CD2-CE2	5.11	1.47	1.41
1	D	557	TRP	CD2-CE2	5.08	1.47	1.41
1	D	102	TRP	CD2-CE2	5.05	1.47	1.41
1	C	102	TRP	CD2-CE2	5.05	1.47	1.41
1	C	512	TRP	CD2-CE2	5.04	1.47	1.41

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1785	NGS	C4

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Mol	Chain	Res	Type	Atom
2	C	1785	NGS	C4

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	5791	0	5420	30	0
1	B	5893	0	5554	31	0
1	C	5794	0	5419	29	0
1	D	5772	0	5349	33	0
2	A	30	0	19	0	0
2	B	30	0	19	1	0
2	C	30	0	19	4	0
2	D	30	0	19	0	0
All	All	23370	0	21818	126	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 3.

The worst 5 of 126 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:C:707:THR:HG22	1:C:750:ASN:HA	1.72	0.72
1:C:470:LEU:HD22	1:C:499:GLN:HE21	1.62	0.62
1:A:265:ILE:HG12	1:A:280:THR:HG22	1.84	0.59
1:C:609:CYS:HB3	1:C:618:ARG:HB3	1.84	0.59
1:D:609:CYS:HB3	1:D:618:ARG:HB3	1.85	0.59

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	735/795 (92%)	703 (96%)	30 (4%)	2 (0%)	46	82
1	B	744/795 (94%)	707 (95%)	35 (5%)	2 (0%)	46	82
1	C	737/795 (93%)	701 (95%)	34 (5%)	2 (0%)	46	82
1	D	739/795 (93%)	707 (96%)	31 (4%)	1 (0%)	56	89
All	All	2955/3180 (93%)	2818 (95%)	130 (4%)	7 (0%)	52	87

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	427	GLY
1	B	427	GLY
1	D	427	GLY
1	C	750	ASN
1	C	751	LEU

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	620/712 (87%)	610 (98%)	10 (2%)	70	89
1	B	635/712 (89%)	621 (98%)	14 (2%)	60	86
1	C	620/712 (87%)	609 (98%)	11 (2%)	66	88
1	D	611/712 (86%)	606 (99%)	5 (1%)	86	94
All	All	2486/2848 (87%)	2446 (98%)	40 (2%)	70	89

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	386	THR
1	B	633	THR
1	D	313	ARG
1	B	537	VAL
1	B	672	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	241	ASN
1	B	448	GLN
1	C	678	ASN
1	B	132	GLN
1	C	499	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](#)

8 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
2	GCD	A	1784	2	9,12,12	1.73	1 (11%)	9,17,17	0.81	0
2	NGS	A	1785	2	17,18,19	0.64	0	18,26,28	1.16	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GCD	B	1784	2	9,12,12	1.79	1 (11%)	9,17,17	1.04	1 (11%)
2	NGS	B	1785	2	17,18,19	0.78	0	18,26,28	0.83	0
2	GCD	C	1784	2	9,12,12	1.68	1 (11%)	9,17,17	1.17	2 (22%)
2	NGS	C	1785	2	17,18,19	0.93	0	18,26,28	1.56	3 (16%)
2	GCD	D	1784	2	9,12,12	1.68	1 (11%)	9,17,17	0.81	0
2	NGS	D	1785	2	17,18,19	0.67	0	18,26,28	1.06	2 (11%)

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
2	GCD	A	1784	2	-	0/0/20/20	0/1/1/1
2	NGS	A	1785	2	-	0/10/26/30	0/1/1/1
2	GCD	B	1784	2	-	0/0/20/20	0/1/1/1
2	NGS	B	1785	2	1/1/6/8	0/10/26/30	0/1/1/1
2	GCD	C	1784	2	-	0/0/20/20	0/1/1/1
2	NGS	C	1785	2	1/1/6/8	0/10/26/30	1/1/1/1
2	GCD	D	1784	2	-	0/0/20/20	0/1/1/1
2	NGS	D	1785	2	-	0/10/26/30	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1784	GCD	O5-C5	4.29	1.46	1.37
2	B	1784	GCD	O5-C5	4.36	1.46	1.37
2	A	1784	GCD	O5-C5	4.47	1.46	1.37
2	D	1784	GCD	O5-C5	4.48	1.46	1.37

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1784	GCD	O5-C5-C4	-2.39	120.65	124.12
2	D	1785	NGS	C3-C2-N	-2.34	105.33	110.41
2	A	1785	NGS	C3-C2-N	-2.19	105.64	110.41
2	C	1784	GCD	O5-C5-C4	-2.19	120.95	124.12
2	A	1785	NGS	C4-C3-C2	2.29	114.02	111.47

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1785	NGS	C4
2	C	1785	NGS	C4

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1785	NGS	C1-C2-C3-C4-C5-O5

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1784	GCD	1	0
2	B	1785	NGS	1	0
2	C	1784	GCD	2	0
2	C	1785	NGS	4	0

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	741/795 (93%)	0.24	14 (1%) 70 64	76, 109, 211, 243	0
1	B	750/795 (94%)	0.22	20 (2%) 58 53	72, 105, 208, 257	0
1	C	743/795 (93%)	0.53	31 (4%) 40 35	129, 144, 167, 184	0
1	D	745/795 (93%)	0.47	27 (3%) 46 41	124, 139, 163, 179	0
All	All	2979/3180 (93%)	0.36	92 (3%) 52 48	72, 135, 191, 257	0

The worst 5 of 92 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	102	TRP	5.2
1	D	204	THR	4.6
1	A	520	SER	3.9
1	B	263	ASN	3.9
1	A	412	TYR	3.4

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, 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	GCD	D	1784	12/12	0.91	0.25	-0.24	57,57,57,57	0
2	GCD	C	1784	12/12	0.87	0.27	-0.38	57,57,57,57	0
2	GCD	B	1784	12/12	0.88	0.28	-0.44	57,57,57,57	0
2	NGS	B	1785	18/19	0.87	0.24	-0.91	57,57,57,57	0
2	NGS	D	1785	18/19	0.90	0.23	-0.92	57,57,57,57	0
2	NGS	A	1785	18/19	0.93	0.18	-1.63	57,57,57,57	0
2	NGS	C	1785	18/19	0.91	0.20	-1.72	57,57,57,57	0
2	GCD	A	1784	12/12	0.94	0.19	-1.98	57,57,57,57	0

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.