



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2016 – 01:21 AM EDT

PDB ID : 5BUU
Title : Crystal structure of the GluA2 ligand-binding domain (L483Y-N754S) in complex with glutamate and BPAM-321 at 2.07 Å resolution
Authors : Larsen, A.P.; Tapken, D.; Frydenvang, K.; Kastrup, J.S.
Deposited on : 2015-06-04
Resolution : 2.07 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
<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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0122
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

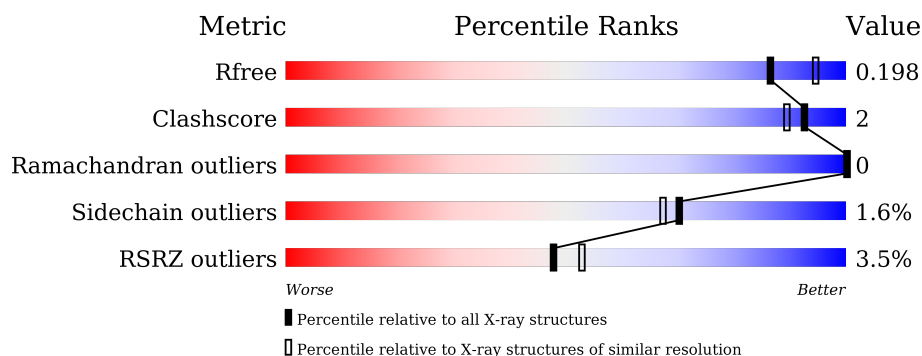
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	1799 (2.08-2.04)
Clashscore	102246	1910 (2.08-2.04)
Ramachandran outliers	100387	1893 (2.08-2.04)
Sidechain outliers	100360	1893 (2.08-2.04)
RSRZ outliers	91569	1802 (2.08-2.04)

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	263	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 93%, yellow 93%, yellow 99%, green 99%, green 100%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> % 93% 6% . </div> </div>
1	B	263	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 6%, orange 6%, orange 89%, yellow 89%, yellow 97%, green 97%, green 100%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> 6% 89% 7% . </div> </div>

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	4V6	A	801[B]	-	-	-	X
5	EDO	B	805	-	-	-	X
5	EDO	B	807	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4440 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.

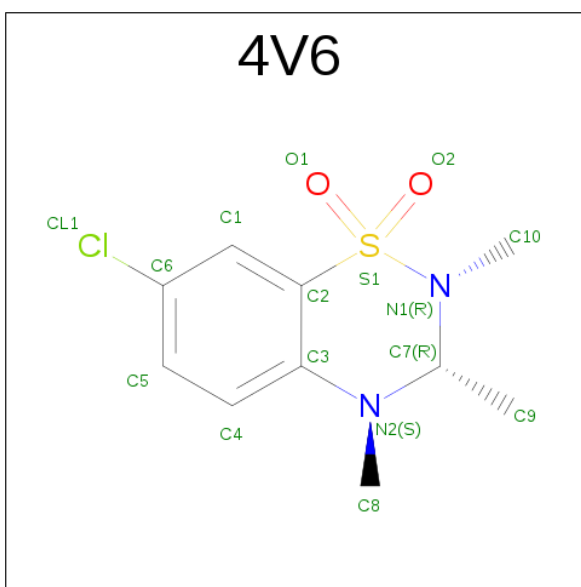
- Molecule 1 is a protein called Glutamate receptor 2, Glutamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	5	0
			2055	1313	340	388	14			
1	B	254	Total	C	N	O	S	0	4	0
			2013	1288	332	380	13			

There are 12 discrepancies between the modelled and reference sequences:

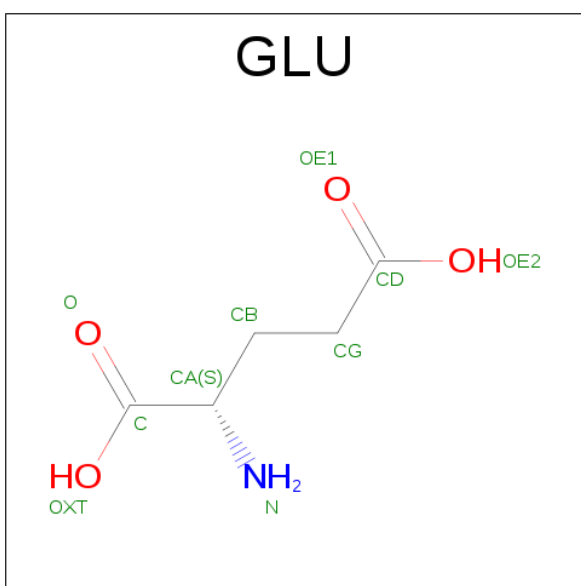
Chain	Residue	Modelled	Actual	Comment	Reference
A	390	GLY	-	expression tag	UNP P19491
A	391	ALA	-	expression tag	UNP P19491
A	483	TYR	LEU	engineered mutation	UNP P19491
A	507	GLY	-	linker	UNP P19491
A	508	THR	-	linker	UNP P19491
A	754	SER	ASN	engineered mutation	UNP P19491
B	390	GLY	-	expression tag	UNP P19491
B	391	ALA	-	expression tag	UNP P19491
B	483	TYR	LEU	engineered mutation	UNP P19491
B	507	GLY	-	linker	UNP P19491
B	508	THR	-	linker	UNP P19491
B	754	SER	ASN	engineered mutation	UNP P19491

- Molecule 2 is (3R)-7-chloro-2,3,4-trimethyl-3,4-dihydro-2H-1,2,4-benzothiadiazine 1,1-dioxide (three-letter code: 4V6) (formula: C₁₀H₁₃ClN₂O₂S).



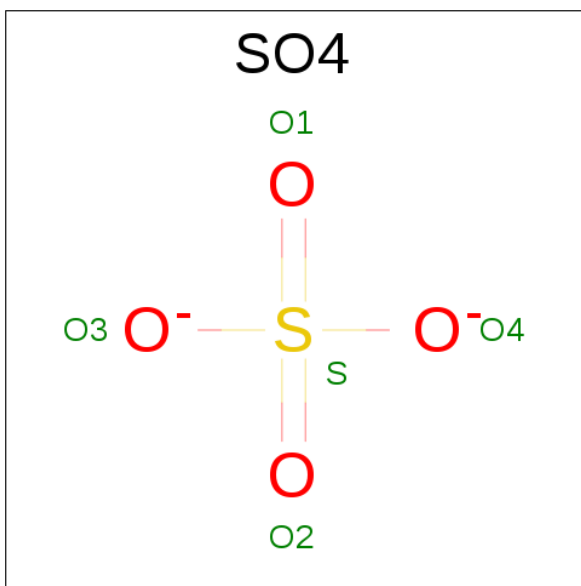
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	1
			16	10	1	2	2	1		
2	B	1	Total	C	Cl	N	O	S	0	1
			16	10	1	2	2	1		

- Molecule 3 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	5	1	4		
3	B	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	165	Total	O	0	1
			165	165		
6	B	110	Total	O	0	0
			110	110		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

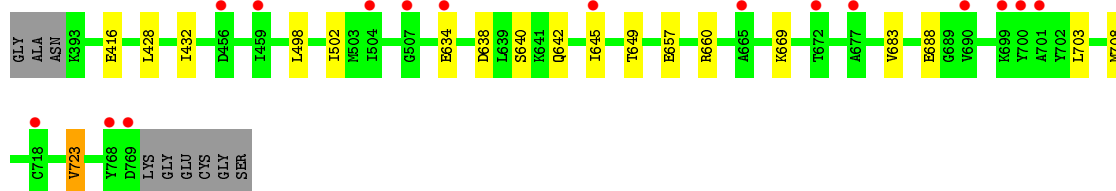
- Molecule 1: Glutamate receptor 2, Glutamate receptor 2

Chain A: 



- Molecule 1: Glutamate receptor 2, Glutamate receptor 2

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	99.21 Å 122.27 Å 47.65 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.65 – 2.07 47.65 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.65-2.07) 99.3 (47.65-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.94 (at 2.07 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.204 , 0.250 0.204 , 0.198	Depositor DCC
R_{free} test set	3335 reflections (4.94%)	DCC
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	4 of 35914 reflections (0.011%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4440	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.77 % 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 5.3292e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4V6, SO4, EDO

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	0.23	0/2108	0.41	0/2835
1	B	0.23	0/2063	0.40	0/2776
All	All	0.23	0/4171	0.41	0/5611

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

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	2055	0	2095	9	0
1	B	2013	0	2051	8	0
2	A	16	0	13	1	0
2	B	16	0	13	0	0
3	A	10	0	5	0	0
3	B	10	0	5	0	0
4	A	15	0	0	0	0
4	B	10	0	0	0	0
5	B	20	0	30	0	0
6	A	165	0	0	2	0
6	B	110	0	0	0	0
All	All	4440	0	4212	17	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 2.

All (17) 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:714:GLN:NE2	6:A:904:HOH:O	2.37	0.57
1:B:640:SER:HB2	1:B:669:LYS:HD2	1.91	0.52
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.92	0.51
1:B:502:ILE:HB	1:B:723:VAL:HG13	1.95	0.48
1:B:428:LEU:O	1:B:432:ILE:HD12	2.14	0.48
1:A:504:ILE:HD12	1:A:508:THR:HB	1.98	0.46
1:B:657:GLU:OE1	1:B:660:ARG:NH1	2.47	0.46
1:B:642:GLN:NE2	1:B:645:ILE:O	2.38	0.46
1:A:637:GLU:HG2	1:A:641:LYS:HE2	1.99	0.45
1:A:695:LYS:NZ	6:A:918:HOH:O	2.45	0.45
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.99	0.43
1:B:634:GLU:HG2	1:B:638:ASP:OD2	2.19	0.43
1:A:453:ARG:NH2	1:A:458:LYS:HD2	2.33	0.43
1:A:497[B]:SER:HB3	2:A:801[B]:4V6:CL1	2.55	0.43
1:A:413:GLU:CD	1:A:413:GLU:H	2.22	0.43
1:A:661:ARG:HA	1:A:661:ARG:HD3	1.83	0.42
1:B:683:VAL:HB	1:B:688:GLU:HB3	2.02	0.41

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	263/263 (100%)	259 (98%)	4 (2%)	0	100	100
1	B	256/263 (97%)	249 (97%)	7 (3%)	0	100	100
All	All	519/526 (99%)	508 (98%)	11 (2%)	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	223/219 (102%)	220 (99%)	3 (1%)	76	74
1	B	218/219 (100%)	214 (98%)	4 (2%)	66	63
All	All	441/438 (101%)	434 (98%)	7 (2%)	70	67

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	498	LEU
1	A	708	MET
1	A	758	LEU
1	B	416	GLU
1	B	498	LEU
1	B	708	MET
1	B	723	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

14 ligands 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	4V6	A	801[B]	-	16,17,17	2.27	6 (37%)	17,27,27	0.72	0
3	GLU	A	802	-	3,9,9	0.15	0	3,11,11	0.98	0
4	SO4	A	803	-	4,4,4	0.20	0	6,6,6	0.05	0
4	SO4	A	804[A]	-	4,4,4	0.27	0	6,6,6	0.09	0
4	SO4	A	805[A]	-	4,4,4	0.28	0	6,6,6	0.06	0
2	4V6	B	801[B]	-	16,17,17	2.25	6 (37%)	17,27,27	0.81	0
3	GLU	B	802	-	3,9,9	0.13	0	3,11,11	1.23	0
4	SO4	B	803	-	4,4,4	0.22	0	6,6,6	0.11	0
4	SO4	B	804	-	4,4,4	0.25	0	6,6,6	0.06	0
5	EDO	B	805	-	3,3,3	0.46	0	2,2,2	0.38	0
5	EDO	B	806	-	3,3,3	0.45	0	2,2,2	0.38	0
5	EDO	B	807	-	3,3,3	0.44	0	2,2,2	0.43	0
5	EDO	B	808	-	3,3,3	0.45	0	2,2,2	0.42	0
5	EDO	B	809	-	3,3,3	0.45	0	2,2,2	0.40	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
2	4V6	A	801[B]	-	-	0/0/24/24	0/1/2/2
3	GLU	A	802	-	-	0/3/9/9	0/0/0/0
4	SO4	A	803	-	-	0/0/0/0	0/0/0/0
4	SO4	A	804[A]	-	-	0/0/0/0	0/0/0/0
4	SO4	A	805[A]	-	-	0/0/0/0	0/0/0/0
2	4V6	B	801[B]	-	-	0/0/24/24	0/1/2/2
3	GLU	B	802	-	-	0/3/9/9	0/0/0/0
4	SO4	B	803	-	-	0/0/0/0	0/0/0/0
4	SO4	B	804	-	-	0/0/0/0	0/0/0/0
5	EDO	B	805	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	806	-	-	0/1/1/1	0/0/0/0
5	EDO	B	807	-	-	0/1/1/1	0/0/0/0
5	EDO	B	808	-	-	0/1/1/1	0/0/0/0
5	EDO	B	809	-	-	0/1/1/1	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801[B]	4V6	C3-C2	2.08	1.42	1.40
2	A	801[B]	4V6	C3-C2	2.17	1.42	1.40
2	A	801[B]	4V6	C2-S1	2.39	1.79	1.76
2	B	801[B]	4V6	C2-S1	2.41	1.79	1.76
2	B	801[B]	4V6	C7-N2	2.46	1.47	1.45
2	A	801[B]	4V6	C7-N2	2.80	1.47	1.45
2	B	801[B]	4V6	O2-S1	3.17	1.47	1.43
2	A	801[B]	4V6	O1-S1	3.18	1.47	1.43
2	A	801[B]	4V6	O2-S1	3.36	1.47	1.43
2	B	801[B]	4V6	O1-S1	3.36	1.47	1.43
2	A	801[B]	4V6	S1-N1	5.60	1.72	1.64
2	B	801[B]	4V6	S1-N1	5.68	1.72	1.64

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 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801[B]	4V6	1	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	260/263 (98%)	0.09	2 (0%) 87 89	21, 35, 64, 87	0
1	B	254/263 (96%)	0.45	16 (6%) 23 25	22, 44, 88, 109	0
All	All	514/526 (97%)	0.27	18 (3%) 48 53	21, 39, 77, 109	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	665	ALA	3.6
1	B	504	ILE	3.2
1	B	677	ALA	3.1
1	B	459	ILE	3.1
1	B	768	TYR	2.9
1	B	700	TYR	2.9
1	B	699	LYS	2.8
1	B	718	CYS	2.8
1	B	645	ILE	2.7
1	B	634	GLU	2.7
1	B	672	THR	2.6
1	B	507	GLY	2.5
1	A	392	ASN	2.4
1	B	701	ALA	2.3
1	A	410	LYS	2.2
1	B	690	VAL	2.2
1	B	456	ASP	2.2
1	B	769	ASP	2.1

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 ⓘ

There are no carbohydrates 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. 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(Å ²)	Q<0.9
5	EDO	B	807	4/4	0.87	0.21	11.50	53,56,59,61	0
5	EDO	B	805	4/4	0.80	0.22	4.69	61,61,62,63	0
2	4V6	A	801[B]	16/16	0.97	0.19	2.28	10,15,23,24	16
2	4V6	B	801[B]	16/16	0.96	0.16	1.67	13,17,27,29	16
4	SO4	B	803	5/5	0.95	0.18	0.46	67,68,70,71	0
4	SO4	A	805[A]	5/5	0.98	0.15	0.41	18,21,23,23	5
3	GLU	A	802	10/10	0.96	0.13	0.22	22,25,28,28	0
4	SO4	A	804[A]	5/5	0.99	0.12	0.17	20,23,25,26	5
3	GLU	B	802	10/10	0.94	0.11	-0.59	21,26,31,31	0
4	SO4	A	803	5/5	0.96	0.11	-1.55	49,49,51,52	0
4	SO4	B	804	5/5	0.82	0.24	-	115,116,116,117	0
5	EDO	B	808	4/4	0.86	0.11	-	64,65,65,65	0
5	EDO	B	809	4/4	0.86	0.10	-	61,61,62,63	0
5	EDO	B	806	4/4	0.83	0.29	-	71,72,72,73	0

6.5 Other polymers ⓘ

There are no such residues in this entry.