



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:32 AM GMT

PDB ID : 3B6W
Title : Crystal Structure of the GLUR2 Ligand Binding Core (S1S2J) T686S Mutant
in Complex with Glutamate at 1.7 Resolution
Authors : Cho, Y.; Lolis, E.; Howe, J.R.
Deposited on : 2007-10-29
Resolution : 1.70 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 (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

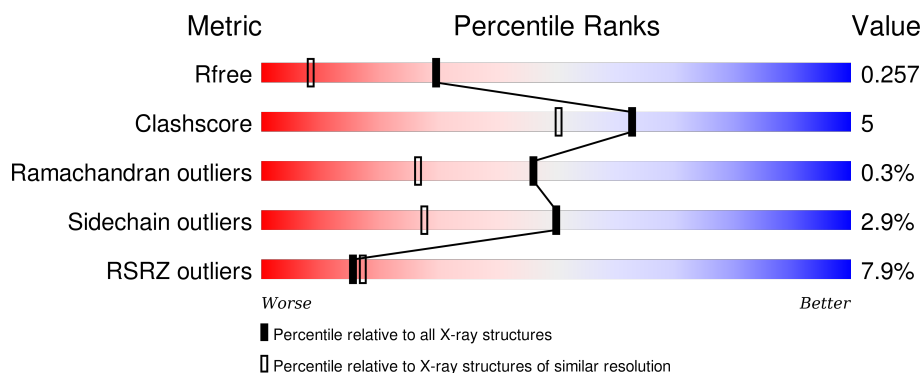
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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>3%</div> <div>88%</div> <div>9%</div> <div>••</div> </div>
1	B	263	<div> <div>3%</div> <div>90%</div> <div>8%</div> <div>•</div> </div>
1	C	263	<div> <div>90%</div> <div>8%</div> <div>•</div> </div>
1	D	263	<div> <div>25%</div> <div>78%</div> <div>18%</div> <div>••</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	SO4	A	903	-	-	-	X
3	GLU	B	801	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8407 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	1	0
			1988	1266	332	375	15			
1	B	258	Total	C	N	O	S	0	1	0
			1959	1249	326	369	15			
1	C	258	Total	C	N	O	S	0	1	0
			1967	1256	321	375	15			
1	D	258	Total	C	N	O	S	0	0	0
			1872	1188	310	361	13			

There are 20 discrepancies between the modelled and reference sequences:

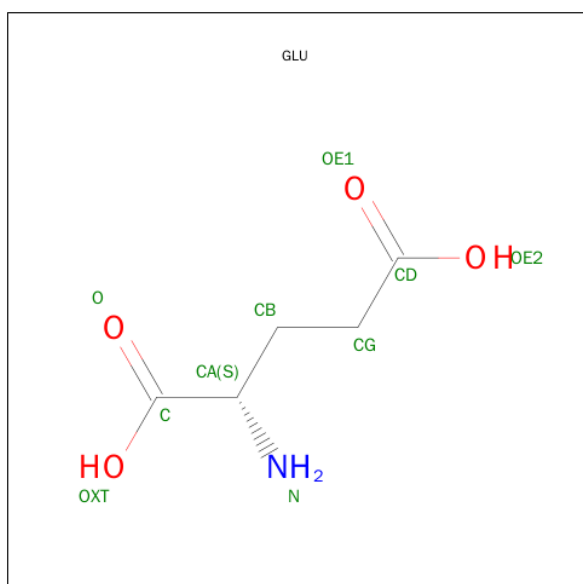
Chain	Residue	Modelled	Actual	Comment	Reference
A	390	GLY	-	EXPRESSION TAG	UNP P19491
A	391	ALA	-	EXPRESSION TAG	UNP P19491
A	630	GLY	-	LINKER	UNP P19491
A	631	THR	-	LINKER	UNP P19491
A	686	SER	THR	ENGINEERED	UNP P19491
B	390	GLY	-	EXPRESSION TAG	UNP P19491
B	391	ALA	-	EXPRESSION TAG	UNP P19491
B	630	GLY	-	LINKER	UNP P19491
B	631	THR	-	LINKER	UNP P19491
B	686	SER	THR	ENGINEERED	UNP P19491
C	390	GLY	-	EXPRESSION TAG	UNP P19491
C	391	ALA	-	EXPRESSION TAG	UNP P19491
C	630	GLY	-	LINKER	UNP P19491
C	631	THR	-	LINKER	UNP P19491
C	686	SER	THR	ENGINEERED	UNP P19491
D	390	GLY	-	EXPRESSION TAG	UNP P19491
D	391	ALA	-	EXPRESSION TAG	UNP P19491
D	630	GLY	-	LINKER	UNP P19491
D	631	THR	-	LINKER	UNP P19491
D	686	SER	THR	ENGINEERED	UNP P19491

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is GLUTAMIC ACID (three-letter code: GLU) (formula: C₅H₉NO₄).



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		

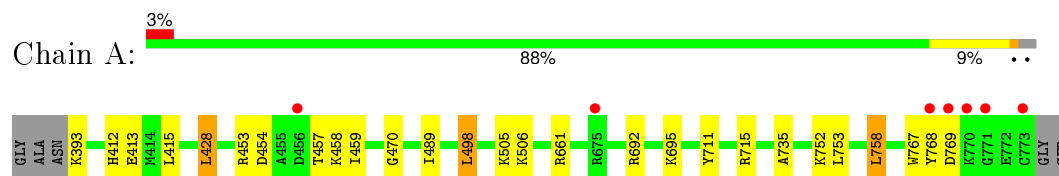
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	189	Total	O	0	0
			189	189		
4	C	171	Total	O	0	0
			171	171		
4	D	104	Total	O	0	0
			104	104		
4	B	117	Total	O	0	0
			117	117		

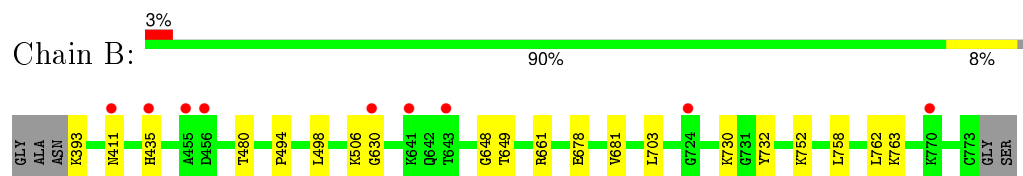
3 Residue-property plots [i](#)

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.

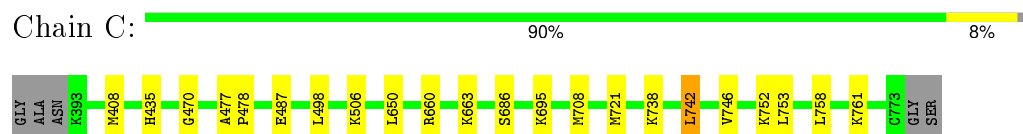
• Molecule 1: Glutamate receptor 2



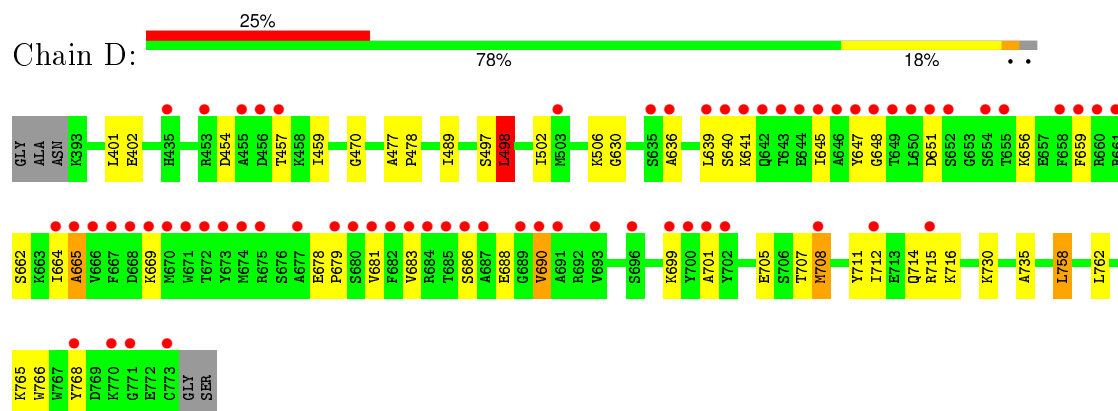
• Molecule 1: Glutamate receptor 2



• Molecule 1: Glutamate receptor 2



• Molecule 1: Glutamate receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.82Å 95.84Å 122.89Å 90.00° 93.43° 90.00°	Depositor
Resolution (Å)	123.00 – 1.70 51.66 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (123.00-1.70) 98.3 (51.66-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.225 , 0.260 0.223 , 0.257	Depositor DCC
R_{free} test set	6005 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 119286 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8407	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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 21.52 % 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 6.8883e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.79	1/2027 (0.0%)	0.75	1/2728 (0.0%)
1	B	0.61	0/1998	0.68	0/2693
1	C	0.77	1/2008 (0.0%)	0.72	1/2710 (0.0%)
1	D	0.59	0/1903	0.69	1/2577 (0.0%)
All	All	0.70	2/7936 (0.0%)	0.71	3/10708 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	506	LYS	C-N	9.26	1.49	1.33
1	A	506	LYS	C-N	8.19	1.47	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	498	LEU	CA-CB-CG	5.44	127.82	115.30
1	C	650	LEU	CA-CB-CG	5.24	127.35	115.30
1	A	428	LEU	CB-CG-CD2	5.10	119.67	111.00

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	1988	0	2007	20	0
1	B	1959	0	1944	9	0
1	C	1967	0	1949	12	0
1	D	1872	0	1747	42	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	10	0	5	0	0
3	B	10	0	5	1	0
4	A	189	0	0	5	0
4	B	117	0	0	1	0
4	C	171	0	0	4	0
4	D	104	0	0	12	0
All	All	8407	0	7657	82	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 (82) 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:D:647:TYR:HB3	1:D:701:ALA:O	1.43	1.15
1:D:645:ILE:HA	1:D:699:LYS:O	1.51	1.11
1:D:659:PHE:HB2	4:D:868:HOH:O	1.61	1.00
1:D:506:LYS:C	1:D:630:GLY:N	2.17	0.97
1:D:683:VAL:HB	4:D:863:HOH:O	1.70	0.89
1:D:502:ILE:HD11	1:D:636:ALA:HA	1.55	0.89
1:C:753:LEU:HD22	1:C:758:LEU:HD23	1.55	0.88
1:A:752:LYS:HD2	4:A:1076:HOH:O	1.71	0.87
1:D:640:SER:HB3	4:D:864:HOH:O	1.73	0.87
1:D:639:LEU:HD21	1:D:701:ALA:HB3	1.55	0.85
1:B:506:LYS:C	1:B:630:GLY:N	2.31	0.83
1:A:457:THR:HG21	4:A:1057:HOH:O	1.79	0.82
1:A:453:ARG:HH21	1:A:458:LYS:HD3	1.47	0.80
1:A:505:LYS:HE2	4:A:1070:HOH:O	1.80	0.79
1:D:639:LEU:CD2	1:D:701:ALA:HB3	2.14	0.77
1:A:454:ASP:HB3	1:A:457:THR:HG22	1.66	0.76
1:D:454:ASP:HB3	1:D:457:THR:HG22	1.67	0.76
1:D:639:LEU:HD21	1:D:701:ALA:CB	2.16	0.75
1:D:659:PHE:HA	4:D:849:HOH:O	1.87	0.73
1:A:767:TRP:O	1:A:769:ASP:N	2.22	0.71
1:D:647:TYR:CB	1:D:701:ALA:O	2.33	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:THR:HG23	1:A:459:ILE:H	1.59	0.66
1:D:647:TYR:HB2	4:D:852:HOH:O	1.96	0.66
1:D:640:SER:HB2	1:D:669:LYS:HD2	1.79	0.64
1:A:470:GLY:HA2	4:A:1055:HOH:O	1.97	0.63
1:D:502:ILE:HD11	1:D:636:ALA:CA	2.29	0.62
1:C:470:GLY:HA2	4:C:1051:HOH:O	2.01	0.61
1:A:695:LYS:HG3	4:A:1062:HOH:O	1.99	0.60
1:D:688:GLU:CB	4:D:863:HOH:O	2.48	0.60
1:D:454:ASP:CB	1:D:457:THR:HG22	2.32	0.60
1:A:453:ARG:NH2	1:A:458:LYS:HD3	2.17	0.58
1:D:714:GLN:HE21	1:D:768:TYR:HD1	1.53	0.57
1:D:716:LYS:CB	4:D:854:HOH:O	2.53	0.56
1:D:656:LYS:HA	4:D:868:HOH:O	2.06	0.56
1:D:470:GLY:HA2	4:D:843:HOH:O	2.06	0.55
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.88	0.55
1:D:690:VAL:HG13	1:D:712:ILE:HG21	1.91	0.53
1:A:412:HIS:HA	1:A:415:LEU:HD12	1.90	0.53
1:D:664:ILE:O	1:D:665:ALA:HB2	2.08	0.53
1:C:686:SER:HB3	1:C:708[B]:MET:SD	2.49	0.52
1:A:413:GLU:H	1:A:413:GLU:CD	2.13	0.52
1:A:498:LEU:C	1:A:498:LEU:HD22	2.31	0.51
1:A:453:ARG:HH21	1:A:458:LYS:CD	2.19	0.51
1:D:489:ILE:HD12	1:D:735:ALA:HB1	1.92	0.51
1:C:695:LYS:HE2	4:C:1059:HOH:O	2.11	0.50
1:B:506:LYS:C	1:B:630:GLY:CA	2.80	0.50
1:D:711:TYR:O	1:D:715:ARG:HG2	2.11	0.49
1:D:651:ASP:O	1:D:656:LYS:HD3	2.12	0.49
1:D:402:GLU:OE1	1:D:686:SER:HB2	2.13	0.49
1:A:692:ARG:HD2	1:B:678:GLU:OE1	2.13	0.48
1:B:480:THR:HG1	3:B:801:GLU:N	2.11	0.48
1:D:506:LYS:NZ	4:D:776:HOH:O	2.42	0.47
1:C:435:HIS:NE2	1:C:752:LYS:HD2	2.29	0.47
1:C:695:LYS:CE	4:C:1059:HOH:O	2.62	0.47
1:A:454:ASP:CB	1:A:457:THR:HG22	2.39	0.47
1:D:765:LYS:HE2	1:D:766:TRP:CE2	2.51	0.46
1:D:662:SER:CB	4:D:849:HOH:O	2.62	0.46
1:D:506:LYS:C	1:D:630:GLY:CA	2.85	0.46
1:A:753:LEU:HD22	1:A:758:LEU:HD23	1.97	0.46
1:D:690:VAL:CG1	1:D:712:ILE:HG21	2.46	0.45
1:A:711:TYR:O	1:A:715:ARG:HG2	2.17	0.45
1:C:435:HIS:CD2	1:C:752:LYS:HD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:487:GLU:O	1:C:738:LYS:HE3	2.18	0.44
1:D:678:GLU:HA	1:D:679:PRO:C	2.38	0.43
1:C:660:ARG:HG2	1:C:660:ARG:HH11	1.82	0.43
1:D:498:LEU:HB3	1:D:707:THR:HG23	2.00	0.43
1:D:477:ALA:HB1	1:D:478:PRO:HD2	2.00	0.43
1:A:661:ARG:HD3	4:C:1021:HOH:O	2.19	0.43
1:C:477:ALA:HB1	1:C:478:PRO:HD2	2.01	0.43
1:B:648:GLY:HA3	1:B:681:VAL:O	2.19	0.43
1:D:758:LEU:O	1:D:762:LEU:HD13	2.18	0.43
1:D:502:ILE:CD1	1:D:636:ALA:HA	2.38	0.42
1:C:761:LYS:HB3	1:C:761:LYS:HE3	1.87	0.42
1:C:742:LEU:HD22	1:C:746:VAL:HG13	2.00	0.42
1:A:489:ILE:HD12	1:A:735:ALA:HB1	2.02	0.42
1:D:648:GLY:HA3	1:D:681:VAL:HB	2.02	0.41
1:D:648:GLY:N	4:D:852:HOH:O	2.52	0.41
1:B:494:PRO:HA	1:B:732:TYR:O	2.20	0.41
1:D:705:GLU:OE2	1:D:708:MET:HG2	2.21	0.41
1:B:435:HIS:CD2	1:B:752:LYS:HD3	2.56	0.40
1:D:457:THR:HG23	1:D:459:ILE:H	1.85	0.40
1:B:411:ASN:CB	4:B:999:HOH:O	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	257/263 (98%)	254 (99%)	2 (1%)	1 (0%)	39	20
1	B	255/263 (97%)	249 (98%)	6 (2%)	0	100	100
1	C	257/263 (98%)	255 (99%)	2 (1%)	0	100	100
1	D	254/263 (97%)	249 (98%)	3 (1%)	2 (1%)	24	7
All	All	1023/1052 (97%)	1007 (98%)	13 (1%)	3 (0%)	46	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	768	TYR
1	D	665	ALA
1	D	641	LYS

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	211/219 (96%)	207 (98%)	4 (2%)	65	46
1	B	203/219 (93%)	196 (97%)	7 (3%)	44	21
1	C	206/219 (94%)	201 (98%)	5 (2%)	57	36
1	D	177/219 (81%)	170 (96%)	7 (4%)	38	16
All	All	797/876 (91%)	774 (97%)	23 (3%)	50	27

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	393	LYS
1	A	428	LEU
1	A	498	LEU
1	A	758	LEU
1	B	393	LYS
1	B	498	LEU
1	B	661	ARG
1	B	730	LYS
1	B	758	LEU
1	B	762	LEU
1	B	763	LYS
1	C	408	MET
1	C	498	LEU
1	C	663	LYS
1	C	721	MET
1	C	742	LEU
1	D	401	LEU

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Mol	Chain	Res	Type
1	D	497	SER
1	D	498	LEU
1	D	690	VAL
1	D	708	MET
1	D	730	LYS
1	D	758	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	764	ASN
1	B	726	ASN
1	C	756	GLN
1	D	411	ASN
1	D	714	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 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
3	GLU	A	801	-	3,9,9	0.28	0	2,11,11	0.21	0
2	SO4	A	901	-	4,4,4	0.16	0	6,6,6	0.16	0
2	SO4	A	903	-	4,4,4	0.23	0	6,6,6	0.39	0
3	GLU	B	801	-	3,9,9	0.30	0	2,11,11	0.36	0
2	SO4	B	904	-	4,4,4	0.17	0	6,6,6	0.36	0
2	SO4	C	902	-	4,4,4	0.20	0	6,6,6	0.34	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
3	GLU	A	801	-	-	0/3/9/9	0/0/0/0
2	SO4	A	901	-	-	0/0/0/0	0/0/0/0
2	SO4	A	903	-	-	0/0/0/0	0/0/0/0
3	GLU	B	801	-	-	0/3/9/9	0/0/0/0
2	SO4	B	904	-	-	0/0/0/0	0/0/0/0
2	SO4	C	902	-	-	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	801	GLU	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 ⓘ

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, 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	258/263 (98%)	0.29	7 (2%) 58 62	9, 16, 29, 40	0
1	B	258/263 (98%)	0.40	9 (3%) 48 52	12, 21, 34, 39	0
1	C	258/263 (98%)	0.21	0 100 100	10, 17, 28, 35	0
1	D	258/263 (98%)	1.36	66 (25%) 1 1	15, 26, 49, 52	0
All	All	1032/1052 (98%)	0.57	82 (7%) 15 17	9, 20, 39, 52	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	646	ALA	8.2
1	D	671	TRP	7.5
1	D	700	TYR	7.2
1	D	670	MET	7.2
1	D	679	PRO	6.9
1	D	665	ALA	6.7
1	D	650	LEU	6.6
1	D	667	PHE	6.5
1	D	664	ILE	6.4
1	A	770	LYS	6.3
1	D	647	TYR	5.6
1	D	684	ARG	5.6
1	D	686	SER	5.5
1	D	690	VAL	5.5
1	B	455	ALA	5.4
1	D	639	LEU	5.2
1	D	640	SER	5.0
1	D	651	ASP	5.0
1	D	701	ALA	4.9
1	D	683	VAL	4.8
1	D	655	THR	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	630	GLY	4.5
1	D	673	TYR	4.5
1	D	666	VAL	4.4
1	D	687	ALA	4.4
1	D	682	PHE	4.3
1	D	648	GLY	4.2
1	D	668	ASP	4.2
1	D	693	VAL	4.2
1	D	455	ALA	4.0
1	D	636	ALA	4.0
1	D	645	ILE	4.0
1	D	643	THR	4.0
1	D	677	ALA	3.8
1	D	699	LYS	3.8
1	D	642	GLN	3.7
1	A	773	CYS	3.7
1	B	456	ASP	3.7
1	D	771	GLY	3.7
1	D	689	GLY	3.6
1	D	658	PHE	3.6
1	D	641	LYS	3.5
1	D	674	MET	3.5
1	D	456	ASP	3.5
1	B	411	ASN	3.4
1	D	649	THR	3.4
1	A	769	ASP	3.3
1	D	659	PHE	3.2
1	D	708	MET	3.2
1	D	685	THR	3.2
1	D	770	LYS	3.1
1	D	644	GLU	3.1
1	D	672	THR	3.1
1	D	457	THR	3.0
1	D	675	ARG	2.9
1	D	680	SER	2.9
1	D	691	ALA	2.9
1	D	635	SER	2.8
1	A	768	TYR	2.8
1	B	435	HIS	2.8
1	A	771	GLY	2.7
1	D	660	ARG	2.7
1	B	770	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	456	ASP	2.7
1	D	652	SER	2.7
1	D	712	ILE	2.4
1	D	669	LYS	2.3
1	D	696	SER	2.3
1	D	435	HIS	2.3
1	D	715	ARG	2.2
1	D	681	VAL	2.2
1	A	675	ARG	2.2
1	B	643	THR	2.1
1	B	641	LYS	2.1
1	D	661	ARG	2.1
1	D	702	TYR	2.1
1	B	724	GLY	2.1
1	D	453	ARG	2.1
1	D	768	TYR	2.1
1	D	773	CYS	2.0
1	D	654	SER	2.0
1	D	503	MET	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 carbohydrates 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. 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
2	SO4	A	903	5/5	0.96	0.13	2.53	28,32,33,35	0
3	GLU	B	801	10/10	0.91	0.12	2.30	12,13,15,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	GLU	A	801	10/10	0.94	0.11	0.68	8,10,12,13	0
2	SO4	C	902	5/5	0.96	0.12	0.08	36,37,39,40	0
2	SO4	B	904	5/5	0.96	0.09	-0.72	25,28,31,31	0
2	SO4	A	901	5/5	0.94	0.13	-	40,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.