



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:33 PM UTC

PDB ID : 3B6W / pdb_00003b6w
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

<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
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

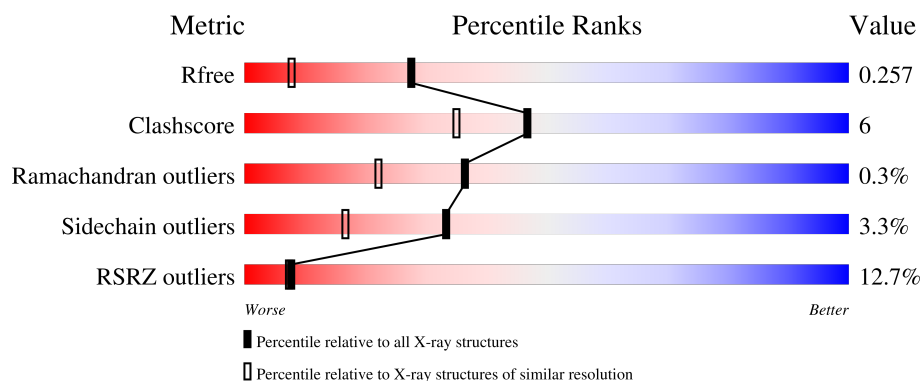
1 Overall quality at a glance

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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 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 $\leq 5\%$. 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	5% 87% 9% ..
1	B	263	7% 91% 7% .
1	C	263	3% 90% 8% .
1	D	263	35% 77% 19% ..

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.

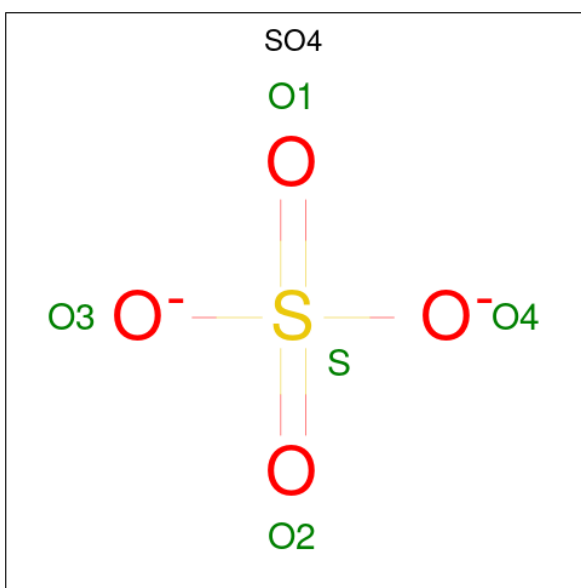
- Molecule 1 is a protein called Glutamate receptor 2.

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:

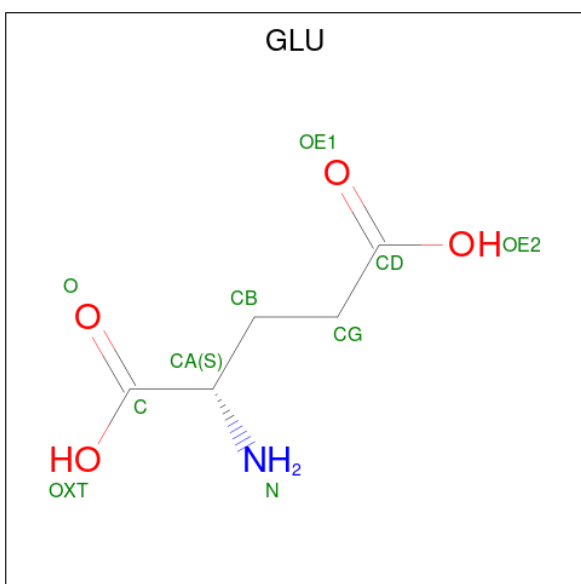
Chain	Residue	Modelled	Actual	Comment	Reference
A	390	GLY	-	expression tag	UNP P19491
A	391	ALA	-	expression tag	UNP P19491
A	630	GLY	-	linker	UNP P19491
A	631	THR	-	linker	UNP P19491
A	686	SER	THR	engineered mutation	UNP P19491
B	390	GLY	-	expression tag	UNP P19491
B	391	ALA	-	expression tag	UNP P19491
B	630	GLY	-	linker	UNP P19491
B	631	THR	-	linker	UNP P19491
B	686	SER	THR	engineered mutation	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 mutation	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 mutation	UNP P19491

- Molecule 2 is SULFATE ION (CCD ID: 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 (CCD ID: 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		

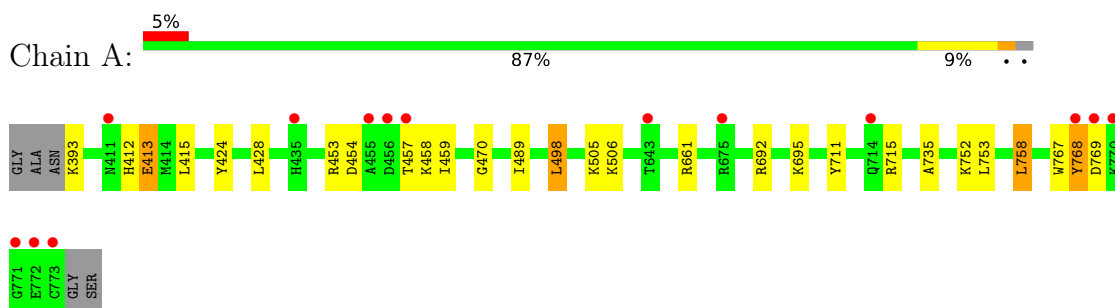
- Molecule 4 is water.

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

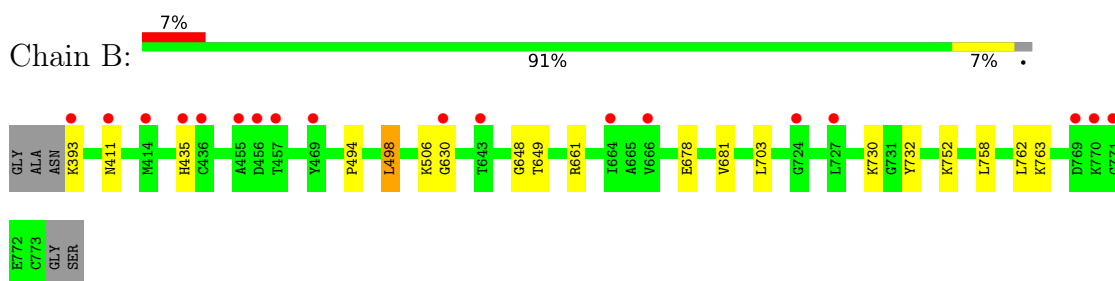
3 Residue-property plots [i](#)

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.

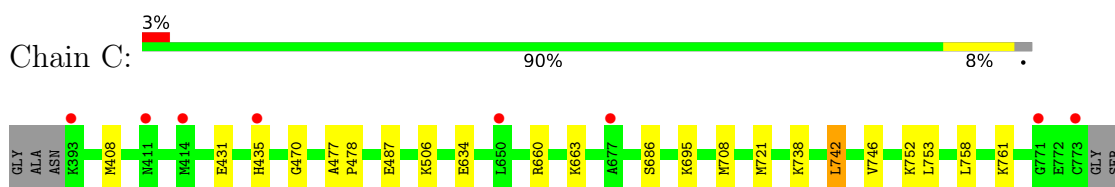
- Molecule 1: Glutamate receptor 2



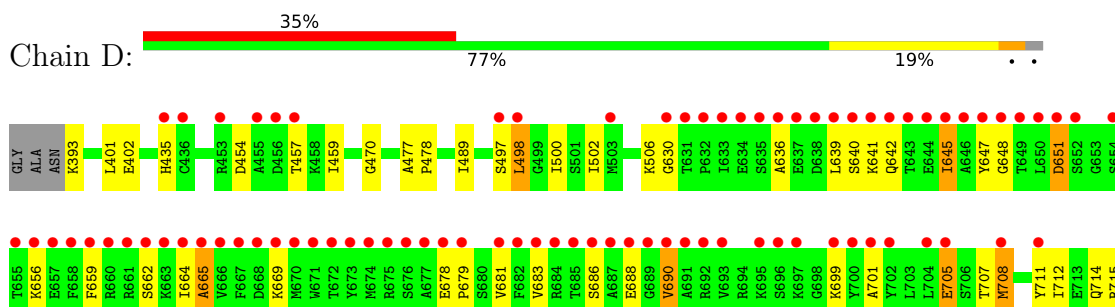
- Molecule 1: Glutamate receptor 2



- 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 – 1.70 122.67 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (123.00-1.70) 98.3 (122.67-1.70)	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 (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 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: 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	0.88	1/2027 (0.0%)	0.91	0/2728
1	B	0.74	0/1998	0.89	0/2693
1	C	0.86	1/2008 (0.0%)	0.90	0/2710
1	D	0.73	0/1903	0.98	3/2577 (0.1%)
All	All	0.81	2/7936 (0.0%)	0.92	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	10.20	1.49	1.33
1	A	506	LYS	C-N	9.72	1.47	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	651	ASP	N-CA-C	8.54	120.37	111.14
1	D	645	ILE	N-CA-C	5.73	115.59	106.88
1	D	435	HIS	N-CA-C	5.20	116.95	111.28

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	22	0
1	B	1959	0	1944	10	0
1	C	1967	0	1949	13	0
1	D	1872	0	1747	44	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	0	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	88	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 6.

All (88) 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:506:LYS:C	1:D:630:GLY:N	2.17	1.01
1:D:659:PHE:HB2	4:D:868:HOH:O	1.61	1.00
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:B:506:LYS:C	1:B:630:GLY:N	2.31	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: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:A:413:GLU:H	1:A:413:GLU:CD	2.13	0.57
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:A:498:LEU:C	1:A:498:LEU:HD22	2.31	0.55
1:B:506:LYS:C	1:B:630:GLY:CA	2.80	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:D:506:LYS:NZ	4:D:776:HOH:O	2.42	0.52
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:D:506:LYS:C	1:D:630:GLY:CA	2.85	0.50
1:C:695:LYS:HE2	4:C:1059:HOH:O	2.11	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:C:435:HIS:NE2	1:C:752:LYS:HD2	2.29	0.47
1:D:678:GLU:HA	1:D:679:PRO:C	2.38	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: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:D:705:GLU:H	1:D:705:GLU:CD	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:HIS:CD2	1:C:752:LYS:HD2	2.52	0.44
1:C:487:GLU:O	1:C:738:LYS:HE3	2.18	0.44
1:C:431:GLU:CD	1:C:758:LEU:HD21	2.43	0.43
1:C:660:ARG:HH11	1:C:660:ARG:HG2	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:424:TYR:C	1:A:424:TYR:CD1	2.97	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:B:498:LEU:C	1:B:498:LEU:HD22	2.44	0.42
1:C:761:LYS:HB3	1:C:761:LYS:HE3	1.87	0.42
1:D:502:ILE:CD1	1:D:636:ALA:HA	2.38	0.42
1:D:640:SER:C	1:D:642:GLN:H	2.26	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:506:LYS:C	1:B:630:GLY:HA3	2.45	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:A:767:TRP:O	1:A:768:TYR:C	2.64	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 [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	257/263 (98%)	254 (99%)	2 (1%)	1 (0%)	30	16
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%)	16	5
All	All	1023/1052 (97%)	1007 (98%)	13 (1%)	3 (0%)	36	22

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%)	206 (98%)	5 (2%)	43	26
1	B	203/219 (93%)	196 (97%)	7 (3%)	32	16
1	C	206/219 (94%)	201 (98%)	5 (2%)	43	26
1	D	177/219 (81%)	168 (95%)	9 (5%)	21	7
All	All	797/876 (91%)	771 (97%)	26 (3%)	33	17

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	393	LYS
1	A	413	GLU
1	A	428	LEU
1	A	498	LEU
1	A	758	LEU
1	B	393	LYS
1	B	498	LEU
1	B	661	ARG

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Mol	Chain	Res	Type
1	B	730	LYS
1	B	758	LEU
1	B	762	LEU
1	B	763	LYS
1	C	408	MET
1	C	634	GLU
1	C	663	LYS
1	C	721	MET
1	C	742	LEU
1	D	393	LYS
1	D	401	LEU
1	D	497	SER
1	D	498	LEU
1	D	500	ILE
1	D	690	VAL
1	D	705	GLU
1	D	708	MET
1	D	730	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	411	ASN
1	A	764	ASN
1	B	726	ASN
1	C	435	HIS
1	C	756	GLN
1	D	411	ASN
1	D	714	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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
2	SO4	A	903	-	4,4,4	0.21	0	6,6,6	0.54	0
3	GLU	B	801	-	8,9,9	1.37	2 (25%)	8,11,11	1.04	0
2	SO4	C	902	-	4,4,4	0.27	0	6,6,6	0.45	0
2	SO4	B	904	-	4,4,4	0.26	0	6,6,6	0.32	0
2	SO4	A	901	-	4,4,4	0.22	0	6,6,6	0.17	0
3	GLU	A	801	-	8,9,9	1.07	0	8,11,11	0.90	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	B	801	-	-	1/9/9/9	-
3	GLU	A	801	-	-	1/9/9/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	GLU	OXT-C	-2.63	1.22	1.30
3	B	801	GLU	CG-CD	2.14	1.55	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	801	GLU	O-C-CA-N
3	A	801	GLU	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	506:LYS	C	630:GLY	N	2.31
1	D	506:LYS	C	630:GLY	N	2.17

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%)	0.11	14 (5%) 31 34	9, 16, 29, 40	1 (0%)
1	B	258/263 (98%)	0.65	18 (6%) 22 24	12, 21, 34, 39	1 (0%)
1	C	258/263 (98%)	0.18	8 (3%) 51 55	10, 17, 28, 35	1 (0%)
1	D	258/263 (98%)	1.92	91 (35%) 1 1	15, 26, 49, 52	0
All	All	1032/1052 (98%)	0.72	131 (12%) 8 7	9, 20, 39, 52	3 (0%)

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	666	VAL	9.0
1	D	690	VAL	7.8
1	D	673	TYR	7.7
1	D	647	TYR	7.6
1	D	664	ILE	7.4
1	D	671	TRP	7.3
1	D	665	ALA	7.1
1	D	667	PHE	6.8
1	D	650	LEU	6.4
1	D	689	GLY	6.3
1	D	639	LEU	5.9
1	D	646	ALA	5.9
1	D	645	ILE	5.9
1	D	677	ALA	5.8
1	D	681	VAL	5.8
1	D	701	ALA	5.8
1	D	700	TYR	5.7
1	D	636	ALA	5.7
1	D	655	THR	5.3
1	A	769	ASP	5.3
1	D	679	PRO	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	640	SER	5.2
1	D	659	PHE	5.2
1	D	691	ALA	5.2
1	D	683	VAL	5.1
1	A	770	LYS	5.1
1	D	642	GLN	5.1
1	D	641	LYS	5.1
1	D	670	MET	5.0
1	D	648	GLY	4.9
1	D	682	PHE	4.9
1	A	771	GLY	4.9
1	D	651	ASP	4.9
1	B	630	GLY	4.9
1	A	457	THR	4.8
1	D	686	SER	4.7
1	D	687	ALA	4.6
1	B	411	ASN	4.6
1	A	773	CYS	4.6
1	D	643	THR	4.6
1	D	685	THR	4.6
1	D	693	VAL	4.6
1	D	635	SER	4.5
1	D	672	THR	4.5
1	D	675	ARG	4.3
1	D	771	GLY	4.3
1	D	456	ASP	4.3
1	D	633	ILE	4.3
1	D	649	THR	4.2
1	D	660	ARG	4.2
1	D	455	ALA	4.2
1	B	456	ASP	4.1
1	D	708	MET	4.1
1	D	652	SER	4.1
1	B	664	ILE	4.1
1	B	770	LYS	4.0
1	A	768	TYR	4.0
1	D	773	CYS	4.0
1	D	684	ARG	3.9
1	B	435	HIS	3.8
1	D	644	GLU	3.7
1	D	657	GLU	3.7
1	D	678	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	662	SER	3.7
1	D	668	ASP	3.6
1	A	455	ALA	3.5
1	D	654	SER	3.5
1	D	630	GLY	3.5
1	D	768	TYR	3.5
1	A	456	ASP	3.4
1	D	702	TYR	3.3
1	D	658	PHE	3.3
1	D	435	HIS	3.3
1	D	699	LYS	3.3
1	D	638	ASP	3.2
1	D	770	LYS	3.2
1	D	674	MET	3.1
1	D	631	THR	3.1
1	D	669	LYS	3.1
1	D	632	PRO	3.1
1	D	503	MET	3.1
1	D	729	SER	3.1
1	D	453	ARG	2.9
1	D	661	ARG	2.9
1	D	656	LYS	2.9
1	B	455	ALA	2.9
1	C	393	LYS	2.8
1	D	705	GLU	2.7
1	D	457	THR	2.7
1	C	414	MET	2.6
1	B	666	VAL	2.6
1	D	711	TYR	2.6
1	D	772	GLU	2.6
1	D	704	LEU	2.6
1	B	469	TYR	2.6
1	B	724	GLY	2.5
1	D	697	LYS	2.5
1	D	696	SER	2.5
1	D	676	SER	2.5
1	A	675	ARG	2.5
1	B	436	CYS	2.5
1	D	498	LEU	2.5
1	B	643	THR	2.5
1	B	769	ASP	2.4
1	D	663	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	762	LEU	2.4
1	C	677	ALA	2.4
1	A	714	GLN	2.4
1	D	497	SER	2.3
1	D	688	GLU	2.3
1	B	771	GLY	2.3
1	A	411	ASN	2.2
1	D	695	LYS	2.2
1	C	771	GLY	2.2
1	B	393	LYS	2.2
1	B	414	MET	2.2
1	A	643	THR	2.2
1	C	773	CYS	2.2
1	D	767	TRP	2.2
1	D	634	GLU	2.1
1	D	436	CYS	2.1
1	D	761	LYS	2.1
1	A	772	GLU	2.1
1	D	692	ARG	2.1
1	D	637	GLU	2.1
1	B	727	LEU	2.1
1	C	650	LEU	2.1
1	A	435	HIS	2.1
1	C	435	HIS	2.1
1	B	457	THR	2.0
1	C	411	ASN	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 [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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	901	5/5	0.91	0.09	40,41,41,41	0
2	SO4	C	902	5/5	0.92	0.10	36,37,39,40	0
2	SO4	A	903	5/5	0.93	0.15	28,32,33,35	0
2	SO4	B	904	5/5	0.94	0.11	25,28,31,31	0
3	GLU	B	801	10/10	0.94	0.08	12,13,15,16	0
3	GLU	A	801	10/10	0.96	0.05	8,10,12,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.