



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2020 – 09:48 AM BST

PDB ID : 4U1Y  
Title : Full length GluA2-FW-(R,R)-2b complex  
Authors : Chen, L.; Gouaux, E.  
Deposited on : 2014-07-16  
Resolution : 3.90 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

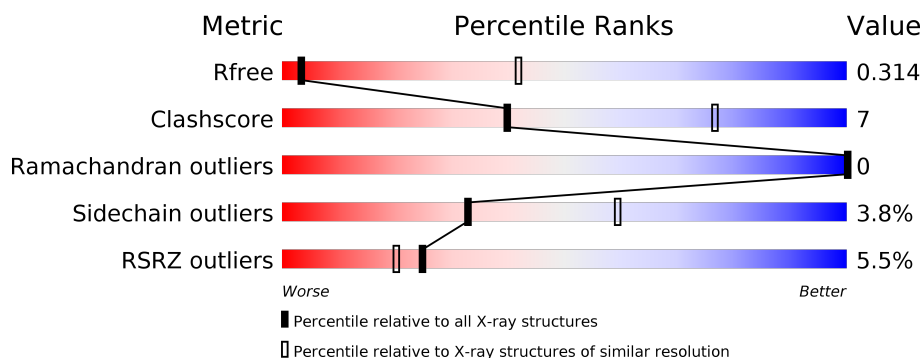
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.90 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))
$R_{free}$	130704	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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 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	819	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>17%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	819	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>14%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	819	<div> <div>6%</div> <div> <div></div> <div>72%</div> <div>16%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	819	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>15%</div> <div>•</div> <div>11%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22259 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	720	Total	C	N	O	S	0	0	0
			5467	3527	898	1017	25			
1	B	731	Total	C	N	O	S	0	0	0
			5574	3591	915	1045	23			
1	C	730	Total	C	N	O	S	0	0	0
			5547	3576	909	1037	25			
1	D	727	Total	C	N	O	S	0	0	0
			5505	3546	904	1031	24			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	239	GLU	ASN	engineered mutation	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	?	-	GLY	deletion	UNP P19491
A	385	ASP	ASN	engineered mutation	UNP P19491
A	392	GLN	ASN	engineered mutation	UNP P19491
A	528	ALA	CYS	engineered mutation	UNP P19491
A	535	LEU	GLY	engineered mutation	UNP P19491
A	?	-	ARG	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLN	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	565	GLU	SER	engineered mutation	UNP P19491
A	577	PHE	LEU	engineered mutation	UNP P19491
A	580	ALA	SER	engineered mutation	UNP P19491
A	582	LYS	GLY	engineered mutation	UNP P19491
A	583	LEU	ALA	engineered mutation	UNP P19491
A	585	PHE	MET	engineered mutation	UNP P19491
A	589	ALA	CYS	engineered mutation	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
A	598	ALA	GLY	engineered mutation	UNP P19491
A	602	ALA	GLY	engineered mutation	UNP P19491
A	815	ALA	CYS	engineered mutation	UNP P19491
A	827	GLY	-	expression tag	UNP P19491
A	828	LEU	-	expression tag	UNP P19491
A	829	VAL	-	expression tag	UNP P19491
A	830	PRO	-	expression tag	UNP P19491
A	831	ARG	-	expression tag	UNP P19491
B	239	GLU	ASN	engineered mutation	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	?	-	GLY	deletion	UNP P19491
B	385	ASP	ASN	engineered mutation	UNP P19491
B	392	GLN	ASN	engineered mutation	UNP P19491
B	528	ALA	CYS	engineered mutation	UNP P19491
B	535	LEU	GLY	engineered mutation	UNP P19491
B	?	-	ARG	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLN	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	565	GLU	SER	engineered mutation	UNP P19491
B	577	PHE	LEU	engineered mutation	UNP P19491
B	580	ALA	SER	engineered mutation	UNP P19491
B	582	LYS	GLY	engineered mutation	UNP P19491
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B	829	VAL	-	expression tag	UNP P19491
B	830	PRO	-	expression tag	UNP P19491
B	831	ARG	-	expression tag	UNP P19491
C	239	GLU	ASN	engineered mutation	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	?	-	GLY	deletion	UNP P19491

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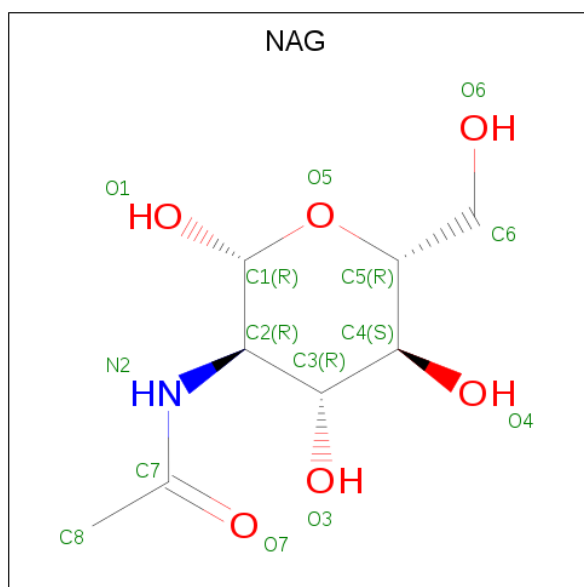
Chain	Residue	Modelled	Actual	Comment	Reference
C	385	ASP	ASN	engineered mutation	UNP P19491
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C	828	LEU	-	expression tag	UNP P19491
C	829	VAL	-	expression tag	UNP P19491
C	830	PRO	-	expression tag	UNP P19491
C	831	ARG	-	expression tag	UNP P19491
D	239	GLU	ASN	engineered mutation	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	?	-	GLY	deletion	UNP P19491
D	385	ASP	ASN	engineered mutation	UNP P19491
D	392	GLN	ASN	engineered mutation	UNP P19491
D	528	ALA	CYS	engineered mutation	UNP P19491
D	535	LEU	GLY	engineered mutation	UNP P19491
D	?	-	ARG	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLN	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	565	GLU	SER	engineered mutation	UNP P19491
D	577	PHE	LEU	engineered mutation	UNP P19491
D	580	ALA	SER	engineered mutation	UNP P19491
D	582	LYS	GLY	engineered mutation	UNP P19491

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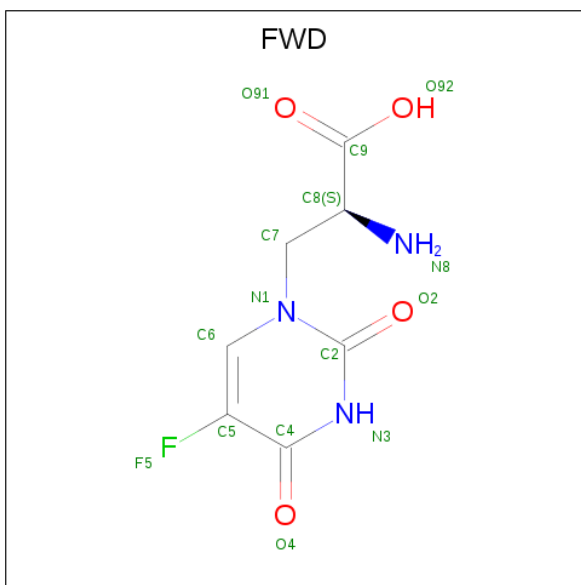
Chain	Residue	Modelled	Actual	Comment	Reference
D	583	LEU	ALA	engineered mutation	UNP P19491
D	585	PHE	MET	engineered mutation	UNP P19491
D	589	ALA	CYS	engineered mutation	UNP P19491
D	598	ALA	GLY	engineered mutation	UNP P19491
D	602	ALA	GLY	engineered mutation	UNP P19491
D	815	ALA	CYS	engineered mutation	UNP P19491
D	827	GLY	-	expression tag	UNP P19491
D	828	LEU	-	expression tag	UNP P19491
D	829	VAL	-	expression tag	UNP P19491
D	830	PRO	-	expression tag	UNP P19491
D	831	ARG	-	expression tag	UNP P19491

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



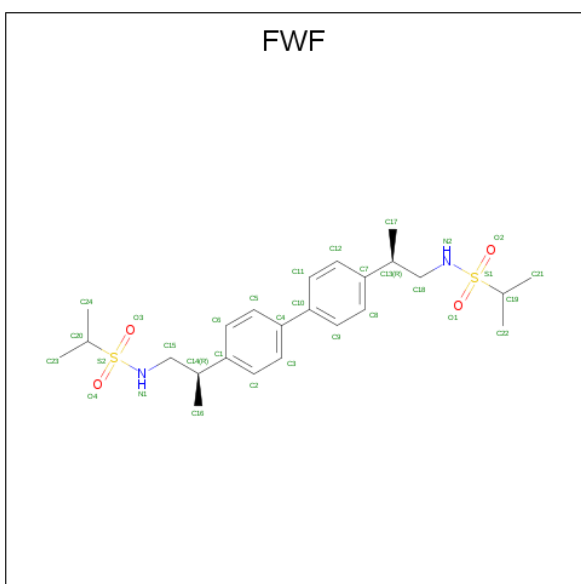
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is 2-AMINO-3-(5-FLUORO-2,4-DIOXO-3,4-DIHYDRO-2H-PYRIMIDIN-1-YL)-PROPIONIC ACID (three-letter code: FWD) (formula:  $C_7H_8FN_3O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 15	C 7	F 1	N 3	O 4	0	0
3	B	1	Total 15	C 7	F 1	N 3	O 4	0	0
3	C	1	Total 15	C 7	F 1	N 3	O 4	0	0
3	D	1	Total 15	C 7	F 1	N 3	O 4	0	0

- Molecule 4 is N,N'-[biphenyl-4,4'-diyl-di(2R)propane-2,1-diyl]dipropane-2-sulfonamide (three-letter code: FWF) (formula: C<sub>24</sub>H<sub>36</sub>N<sub>2</sub>O<sub>4</sub>S<sub>2</sub>).



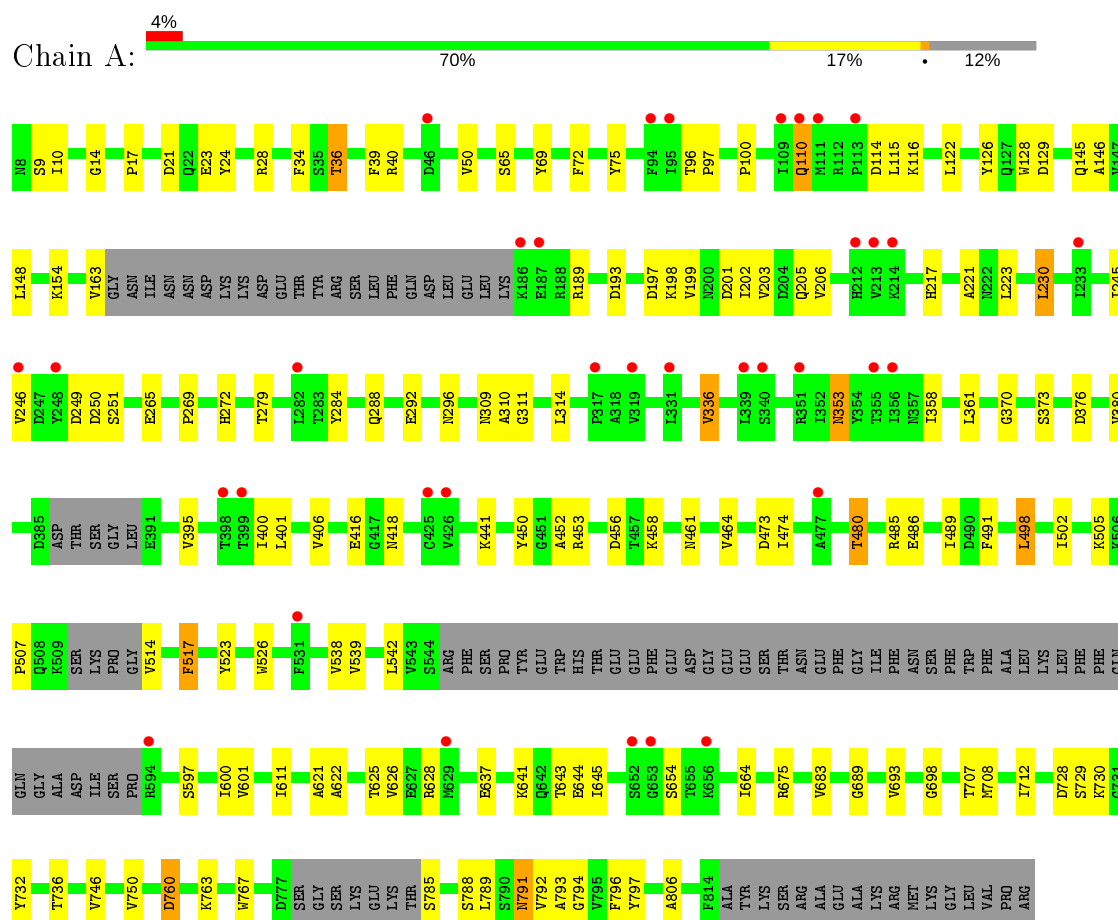
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			32	24	2	4	2		
4	B	1	Total	C	N	O	S	0	0
			32	24	2	4	2		



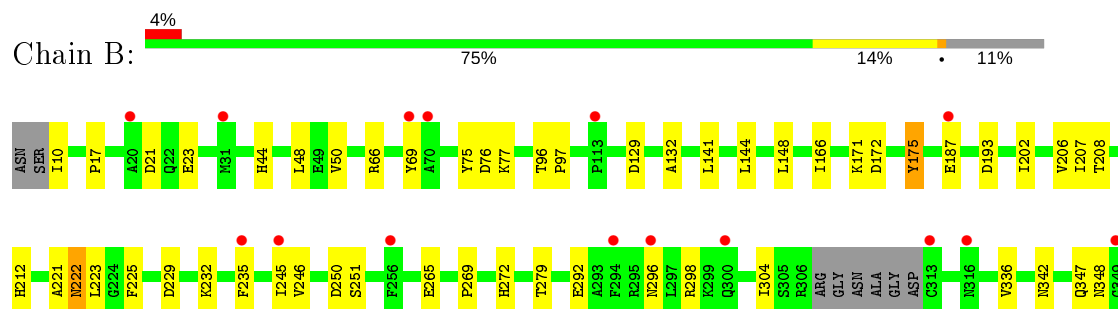
### 3 Residue-property plots

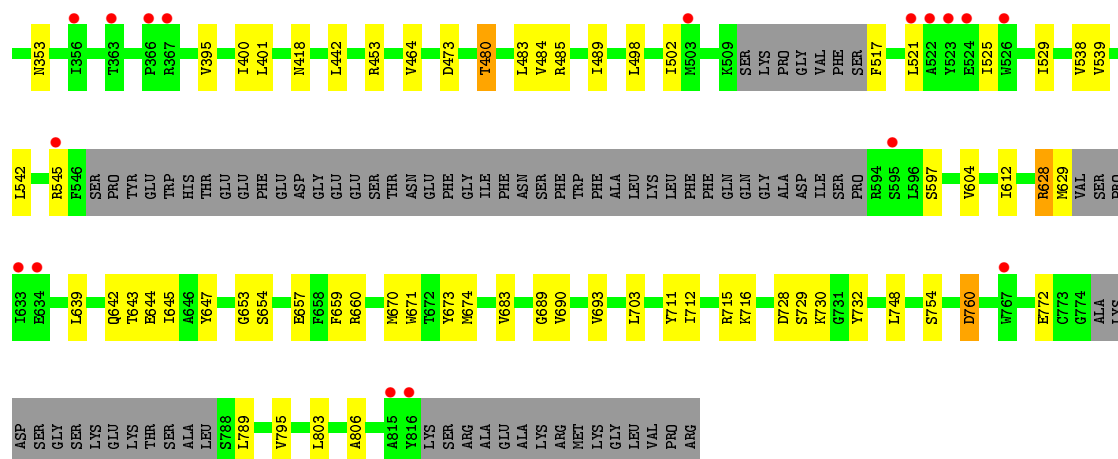
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

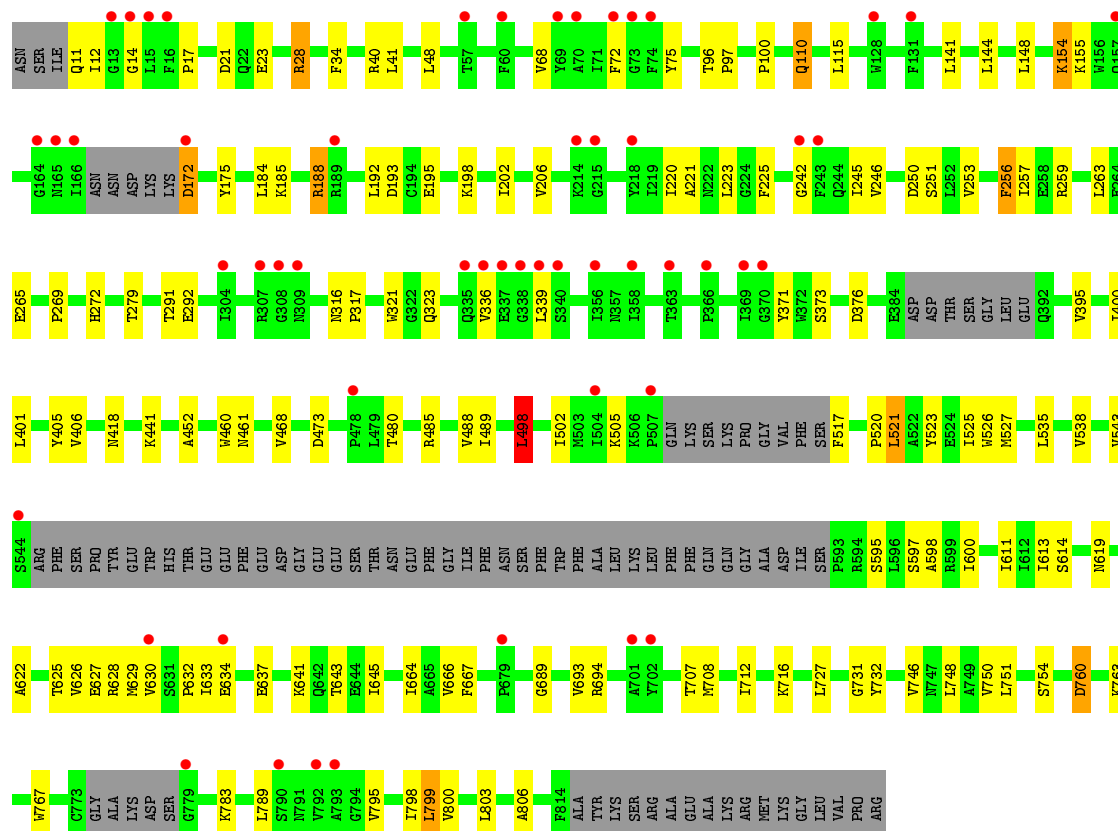


#### • Molecule 1: Glutamate receptor 2

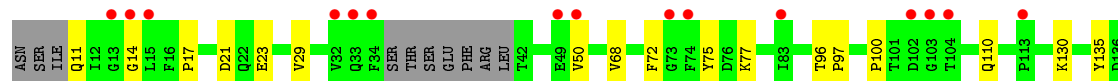
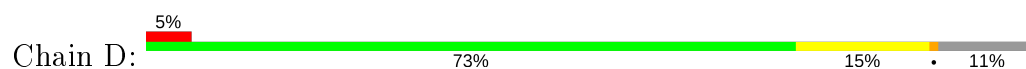




• Molecule 1: Glutamate receptor 2



• Molecule 1: Glutamate receptor 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.25Å 151.44Å 330.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 3.90 49.90 – 3.90	Depositor EDS
% Data completeness (in resolution range)	93.7 (19.97-3.90) 93.7 (49.90-3.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 3.88Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.268 , 0.303 0.278 , 0.314	Depositor DCC
$R_{free}$ test set	2297 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	140.4	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.20 , 56.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	22259	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	175.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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: FWD, FWF, NAG

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	0.30	0/5579	0.52	0/7580
1	B	0.29	0/5689	0.52	0/7725
1	C	0.28	0/5658	0.52	1/7676 (0.0%)
1	D	0.32	0/5616	0.54	1/7628 (0.0%)
All	All	0.30	0/22542	0.52	2/30609 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	498	LEU	CA-CB-CG	5.33	127.57	115.30
1	C	498	LEU	CA-CB-CG	5.22	127.31	115.30

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	5467	0	5281	95	0
1	B	5574	0	5372	78	0
1	C	5547	0	5396	90	0
1	D	5505	0	5320	83	0
2	A	14	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	14	0	13	4	0
2	D	14	0	13	0	0
3	A	15	0	7	1	0
3	B	15	0	7	1	0
3	C	15	0	7	0	0
3	D	15	0	7	0	0
4	A	32	0	36	2	0
4	B	32	0	36	2	0
All	All	22259	0	21507	320	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 7.

All (320) 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:622:ALA:O	1:C:626:VAL:HG23	1.52	1.10
1:A:122:LEU:HD13	1:A:358:ILE:HD11	1.50	0.93
1:D:627:GLU:HG2	1:D:628:ARG:H	1.41	0.83
1:C:172:ASP:N	1:C:172:ASP:OD2	2.15	0.78
1:D:646:ALA:HB1	1:D:681:VAL:HG11	1.67	0.77
1:A:637:GLU:O	1:A:641:LYS:HG3	1.86	0.76
1:C:543:VAL:HG11	1:C:598:ALA:HB2	1.65	0.76
1:D:507:PRO:HG2	1:D:630:VAL:HG12	1.69	0.74
1:C:628:ARG:CB	1:C:783:LYS:HA	2.18	0.73
1:D:514:VAL:HG11	1:D:794:GLY:HA3	1.71	0.73
1:D:637:GLU:HA	1:D:666:VAL:HG11	1.71	0.72
1:A:418:ASN:HD21	1:A:441:LYS:HA	1.54	0.70
1:D:508:GLN:O	1:D:630:VAL:HG13	1.92	0.70
1:A:114:ASP:OD2	1:A:116:LYS:NZ	2.25	0.69
1:D:77:LYS:HG2	1:D:138:ASP:HA	1.75	0.69
1:C:525:ILE:HD11	1:D:789:LEU:HA	1.75	0.67
1:B:172:ASP:HA	1:B:175:TYR:HD2	1.60	0.67
1:A:230:LEU:HD23	1:A:230:LEU:H	1.59	0.66
1:B:342:ASN:HD22	2:B:2001:NAG:H5	1.61	0.66
1:D:418:ASN:HD21	1:D:441:LYS:HA	1.60	0.66
1:D:166:ILE:HG21	1:D:174:THR:HG21	1.76	0.66
1:C:418:ASN:HD21	1:C:441:LYS:HA	1.61	0.65
1:A:517:PHE:HB2	1:A:791:ASN:ND2	2.12	0.64
1:D:627:GLU:HG2	1:D:628:ARG:N	2.10	0.64
1:B:44:HIS:HB2	1:B:66:ARG:NH1	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:514:VAL:CG1	1:D:794:GLY:HA3	2.29	0.62
1:B:17:PRO:HB3	1:B:50:VAL:HB	1.79	0.62
1:A:625:THR:HG22	1:D:622:ALA:HA	1.80	0.62
1:D:21:ASP:HB3	1:D:269:PRO:HB2	1.81	0.62
1:A:201:ASP:O	1:A:205:GLN:HG2	1.98	0.62
1:A:122:LEU:HD13	1:A:358:ILE:CD1	2.26	0.61
1:A:292:GLU:HG3	1:A:336:VAL:HG11	1.82	0.61
1:A:75:TYR:HE2	1:A:96:THR:HG21	1.66	0.61
1:B:464:VAL:HG13	1:B:489:ILE:HD13	1.83	0.61
1:A:163:VAL:HG13	1:A:198:LYS:HE3	1.82	0.60
1:C:75:TYR:HE2	1:C:96:THR:HG21	1.67	0.60
1:D:130:LYS:HA	1:D:157:GLN:O	2.01	0.60
1:D:650:LEU:O	1:D:656:LYS:HD2	2.02	0.60
1:B:21:ASP:HB3	1:B:269:PRO:HB2	1.85	0.59
1:D:654:SER:O	1:D:658:PHE:N	2.32	0.59
1:D:211:LYS:NZ	1:D:216:TYR:OH	2.35	0.59
1:D:670:MET:O	1:D:674:MET:HG3	2.02	0.59
1:A:128:TRP:CE2	1:A:189:ARG:HG2	2.39	0.58
1:A:395:VAL:HG13	1:A:473:ASP:HB2	1.86	0.58
1:D:75:TYR:HE2	1:D:96:THR:HG21	1.68	0.58
1:B:525:ILE:HG12	1:C:789:LEU:HB2	1.85	0.58
1:C:626:VAL:O	1:C:630:VAL:N	2.27	0.57
1:A:600:ILE:HD11	1:B:806:ALA:HA	1.86	0.57
1:B:657:GLU:OE2	1:B:660:ARG:HD2	2.04	0.57
1:D:626:VAL:HG12	1:D:627:GLU:H	1.68	0.57
1:B:292:GLU:HG3	1:B:336:VAL:HG11	1.86	0.57
1:C:100:PRO:HA	1:C:110:GLN:HG2	1.87	0.57
1:B:172:ASP:HA	1:B:175:TYR:CD2	2.38	0.57
1:A:100:PRO:HA	1:A:110:GLN:HG2	1.86	0.56
1:A:453:ARG:CB	1:A:458:LYS:HB3	2.34	0.56
1:A:230:LEU:HD12	1:A:361:LEU:HD13	1.86	0.56
1:B:542:LEU:HD22	1:B:545:ARG:HH21	1.70	0.56
1:B:166:ILE:HG21	1:B:171:LYS:HA	1.87	0.56
1:A:23:GLU:N	1:A:23:GLU:OE1	2.39	0.55
1:A:641:LYS:HB3	1:B:772:GLU:O	2.05	0.55
1:C:707:THR:OG1	1:C:708:MET:SD	2.64	0.55
1:C:23:GLU:N	1:C:23:GLU:OE2	2.40	0.55
1:D:100:PRO:HA	1:D:110:GLN:HG2	1.89	0.55
1:D:17:PRO:HB3	1:D:50:VAL:HB	1.88	0.55
1:B:647:TYR:CE2	1:B:674:MET:HE3	2.42	0.55
1:B:674:MET:HE1	1:B:703:LEU:HD12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ILE:HG23	1:A:69:TYR:HD2	1.72	0.55
1:D:23:GLU:N	1:D:23:GLU:OE1	2.40	0.55
1:D:627:GLU:CG	1:D:628:ARG:H	2.16	0.54
1:A:122:LEU:CD1	1:A:358:ILE:HD11	2.31	0.54
1:D:138:ASP:HB2	1:D:198:LYS:NZ	2.22	0.54
1:A:14:GLY:HA2	1:A:72:PHE:O	2.08	0.54
1:B:23:GLU:N	1:B:23:GLU:OE2	2.41	0.54
1:C:597:SER:O	1:C:600:ILE:HG12	2.07	0.54
1:D:645:ILE:O	1:D:646:ALA:HB2	2.07	0.53
1:D:795:VAL:O	1:D:798:ILE:HG22	2.08	0.53
1:C:12:ILE:HD13	1:C:41:LEU:HD23	1.91	0.53
1:C:760:ASP:N	1:C:760:ASP:OD2	2.43	0.52
1:C:292:GLU:HG3	1:C:336:VAL:HG11	1.91	0.52
1:C:632:PRO:O	1:C:633:ILE:HG22	2.09	0.52
1:D:151:ALA:HA	1:D:156:TRP:CE3	2.45	0.52
1:C:192:LEU:HD23	1:C:220:ILE:HD13	1.91	0.52
1:A:10:ILE:HG23	1:A:69:TYR:CD2	2.44	0.52
1:C:597:SER:HB2	1:D:809:VAL:HG12	1.91	0.52
1:C:498:LEU:HD13	1:C:731:GLY:HA2	1.92	0.52
1:B:647:TYR:CZ	1:B:673:TYR:CD2	2.97	0.52
1:D:452:ALA:N	1:D:461:ASN:OD1	2.37	0.52
1:D:760:ASP:N	1:D:760:ASP:OD2	2.43	0.51
1:B:10:ILE:HG23	1:B:69:TYR:HD2	1.75	0.51
1:A:689:GLY:O	1:A:693:VAL:HG23	2.10	0.51
1:A:707:THR:OG1	1:A:708:MET:SD	2.65	0.51
1:A:793:ALA:HB1	1:A:797:TYR:HE1	1.76	0.51
1:C:14:GLY:HA2	1:C:72:PHE:O	2.11	0.51
1:C:622:ALA:O	1:C:626:VAL:CG2	2.42	0.51
1:C:611:ILE:HG21	1:D:795:VAL:HG21	1.91	0.51
1:A:452:ALA:N	1:A:461:ASN:OD1	2.39	0.51
1:B:539:VAL:HG11	1:C:803:LEU:HD22	1.91	0.51
1:B:193:ASP:HA	1:B:221:ALA:HB3	1.92	0.51
1:B:730:LYS:HA	4:B:2003:FWF:O4	2.10	0.51
1:D:135:TYR:O	1:D:162:ASN:HA	2.10	0.51
1:C:641:LYS:O	1:D:772:GLU:O	2.29	0.51
1:A:122:LEU:HD11	1:A:126:TYR:CE1	2.46	0.51
1:C:632:PRO:C	1:C:633:ILE:CG2	2.79	0.51
1:D:193:ASP:HA	1:D:221:ALA:HB3	1.92	0.51
1:A:643:THR:C	1:A:645:ILE:H	2.14	0.51
1:B:342:ASN:HD21	2:B:2001:NAG:H3	1.75	0.51
1:C:632:PRO:C	1:C:633:ILE:HG23	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ALA:HB2	1:B:187:GLU:HG2	1.93	0.51
1:C:628:ARG:CB	1:C:783:LYS:CA	2.88	0.51
1:D:163:VAL:HG21	1:D:175:TYR:CZ	2.46	0.50
1:D:521:LEU:HD13	1:D:616:TYR:HD1	1.75	0.50
1:A:197:ASP:OD1	1:A:198:LYS:N	2.39	0.50
1:C:627:GLU:HA	1:C:627:GLU:OE2	2.11	0.50
1:C:643:THR:C	1:C:645:ILE:H	2.14	0.50
1:A:760:ASP:N	1:A:760:ASP:OD2	2.43	0.50
1:C:505:LYS:HD3	1:C:694:ARG:HA	1.94	0.50
1:A:198:LYS:O	1:A:202:ILE:HG13	2.10	0.50
1:C:395:VAL:HG13	1:C:473:ASP:HB2	1.93	0.50
1:D:507:PRO:HG2	1:D:630:VAL:CG1	2.39	0.50
1:A:358:ILE:HG22	1:A:370:GLY:C	2.32	0.50
1:B:529:ILE:HD11	1:B:612:ILE:HD12	1.94	0.50
1:C:488:VAL:HG23	1:C:489:ILE:HG23	1.93	0.50
1:B:212:HIS:HE1	1:D:212:HIS:HE1	1.59	0.49
1:D:14:GLY:HA2	1:D:72:PHE:O	2.11	0.49
1:B:604:VAL:HG11	1:C:799:LEU:HA	1.94	0.49
1:B:485:ARG:O	1:B:489:ILE:HG12	2.13	0.49
1:D:488:VAL:HG23	1:D:489:ILE:HG23	1.95	0.49
1:D:650:LEU:HD23	1:D:652:SER:H	1.78	0.49
1:C:11:GLN:HG3	1:C:68:VAL:HG12	1.95	0.48
1:D:654:SER:OG	1:D:730:LYS:NZ	2.46	0.48
1:B:674:MET:HE1	1:B:703:LEU:CD1	2.43	0.48
1:C:521:LEU:HB3	1:C:526:TRP:CE2	2.48	0.48
1:A:728:ASP:OD2	1:A:730:LYS:HE3	2.14	0.48
1:C:632:PRO:O	1:C:633:ILE:CG2	2.62	0.48
1:C:245:ILE:HG23	1:C:246:VAL:HG23	1.96	0.48
1:B:202:ILE:O	1:B:206:VAL:HG23	2.14	0.48
1:C:225:PHE:CD1	1:C:242:GLY:HA3	2.49	0.48
1:B:265:GLU:HB3	1:B:272:HIS:HB2	1.97	0.47
1:C:795:VAL:O	1:C:798:ILE:HG22	2.14	0.47
1:A:34:PHE:HE2	1:A:284:TYR:CE2	2.33	0.47
1:A:36:THR:HG23	1:A:39:PHE:O	2.15	0.47
1:A:9:SER:HA	1:A:40:ARG:O	2.14	0.47
1:A:485:ARG:O	1:A:489:ILE:HG12	2.15	0.47
1:A:597:SER:O	1:A:601:VAL:HG23	2.14	0.47
1:B:643:THR:C	1:B:645:ILE:H	2.18	0.47
1:B:418:ASN:ND2	1:B:442:LEU:H	2.12	0.47
1:D:395:VAL:HG13	1:D:473:ASP:HB2	1.97	0.47
1:B:229:ASP:HB3	1:B:232:LYS:HE2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:ASN:N	1:D:168:ASN:OD1	2.46	0.47
1:C:485:ARG:O	1:C:489:ILE:HG12	2.15	0.47
1:D:474:ILE:HG13	1:D:736:THR:HG22	1.95	0.47
1:D:689:GLY:O	1:D:693:VAL:HG23	2.14	0.47
1:B:395:VAL:HG13	1:B:473:ASP:HB2	1.96	0.47
1:D:597:SER:O	1:D:600:ILE:HG12	2.14	0.47
1:C:265:GLU:HB3	1:C:272:HIS:HB2	1.97	0.46
1:A:21:ASP:HB3	1:A:269:PRO:HB2	1.96	0.46
1:B:689:GLY:O	1:B:693:VAL:HG23	2.16	0.46
1:B:654:SER:OG	1:B:730:LYS:NZ	2.49	0.46
1:C:373:SER:HB3	1:C:376:ASP:HB2	1.97	0.46
1:A:474:ILE:HG13	1:A:736:THR:HG22	1.96	0.46
1:A:788:SER:O	1:A:792:VAL:HG23	2.16	0.46
1:B:342:ASN:ND2	2:B:2001:NAG:H5	2.28	0.46
1:A:763:LYS:O	1:A:767:TRP:HB2	2.15	0.46
1:B:342:ASN:ND2	2:B:2001:NAG:H3	2.30	0.46
1:D:485:ARG:O	1:D:489:ILE:HG12	2.15	0.46
1:A:538:VAL:O	1:A:542:LEU:HG	2.16	0.45
1:B:245:ILE:HG23	1:B:246:VAL:HG23	1.98	0.45
1:C:175:TYR:OH	1:C:198:LYS:NZ	2.49	0.45
1:D:245:ILE:HG23	1:D:246:VAL:HG23	1.98	0.45
1:A:708:MET:O	1:A:712:ILE:HG12	2.16	0.45
1:C:193:ASP:HA	1:C:221:ALA:HB3	1.99	0.45
1:A:115:LEU:HD22	1:A:223:LEU:HD12	1.99	0.45
1:A:116:LYS:HD2	1:A:146:ALA:HB2	1.98	0.45
1:A:193:ASP:HA	1:A:221:ALA:HB3	1.99	0.45
1:C:110:GLN:HB2	1:C:110:GLN:HE21	1.50	0.45
1:C:202:ILE:O	1:C:206:VAL:HG23	2.15	0.45
1:B:597:SER:OG	1:C:806:ALA:HB1	2.15	0.45
1:D:683:VAL:HG11	1:D:689:GLY:HA2	1.98	0.45
1:B:538:VAL:O	1:B:542:LEU:HG	2.16	0.45
1:A:126:TYR:HE2	1:A:217:HIS:NE2	2.14	0.45
1:A:643:THR:HG21	1:B:716:LYS:HD2	1.99	0.45
1:D:11:GLN:HG3	1:D:68:VAL:HG12	1.98	0.45
1:C:626:VAL:O	1:C:630:VAL:CB	2.64	0.45
1:B:141:LEU:HD23	1:B:144:LEU:HD23	1.99	0.45
1:B:728:ASP:OD2	1:B:730:LYS:HE2	2.17	0.45
1:C:746:VAL:O	1:C:750:VAL:HG23	2.16	0.45
1:A:793:ALA:HB1	1:A:797:TYR:CE1	2.52	0.45
1:B:207:ILE:HA	1:B:212:HIS:ND1	2.31	0.45
1:C:689:GLY:O	1:C:693:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:GLU:HB3	1:A:272:HIS:HB2	1.99	0.45
1:A:400:ILE:O	1:A:406:VAL:HB	2.17	0.45
1:B:44:HIS:HB2	1:B:66:ARG:CZ	2.46	0.45
1:B:674:MET:CE	1:B:703:LEU:HD12	2.46	0.45
1:A:17:PRO:HB3	1:A:50:VAL:HB	1.99	0.45
1:C:184:LEU:HD12	1:C:185:LYS:N	2.32	0.45
1:B:483:LEU:HA	1:C:751:LEU:HD13	1.98	0.44
1:A:145:GLN:HE21	1:B:141:LEU:HD21	1.81	0.44
1:A:250:ASP:OD2	1:A:251:SER:N	2.50	0.44
1:A:498:LEU:HB3	1:A:707:THR:HG23	1.99	0.44
1:C:253:VAL:O	1:C:257:ILE:HG12	2.16	0.44
1:B:208:THR:HG22	1:D:235:PHE:HB2	1.98	0.44
1:B:480:THR:HG23	1:B:732:TYR:CE1	2.52	0.44
1:D:505:LYS:HD3	1:D:694:ARG:HA	1.97	0.44
1:C:460:TRP:NE1	1:C:488:VAL:HG11	2.33	0.44
1:B:401:LEU:HD23	1:B:401:LEU:HA	1.82	0.44
1:C:520:PRO:O	1:C:619:ASN:ND2	2.51	0.44
1:C:664:ILE:HB	1:C:667:PHE:HD2	1.82	0.44
1:C:708:MET:O	1:C:712:ILE:HG12	2.17	0.44
1:D:626:VAL:HG12	1:D:627:GLU:N	2.31	0.44
1:A:480:THR:HG23	1:A:732:TYR:CE1	2.53	0.44
1:B:683:VAL:HG11	1:B:689:GLY:HA2	1.98	0.44
1:D:649:THR:HG21	1:D:659:PHE:CE2	2.53	0.44
1:D:658:PHE:O	1:D:662:SER:OG	2.23	0.44
1:A:65:SER:HA	1:A:311:GLY:O	2.18	0.44
1:C:28:ARG:C	1:C:28:ARG:HD3	2.38	0.44
1:C:400:ILE:O	1:C:406:VAL:HB	2.18	0.44
1:C:763:LYS:O	1:C:767:TRP:HB2	2.18	0.44
1:D:763:LYS:O	1:D:767:TRP:HB2	2.17	0.44
1:A:729:SER:OG	4:A:2003:FWF:C16	2.66	0.43
1:C:452:ALA:N	1:C:461:ASN:OD1	2.47	0.43
1:D:138:ASP:HB2	1:D:198:LYS:HZ2	1.83	0.43
1:D:538:VAL:O	1:D:542:LEU:HG	2.18	0.43
1:A:645:ILE:HG23	1:A:698:GLY:O	2.18	0.43
1:C:498:LEU:HB3	1:C:707:THR:HG23	1.99	0.43
1:C:535:LEU:O	1:C:538:VAL:HG12	2.18	0.43
1:B:222:ASN:ND2	1:B:223:LEU:O	2.45	0.43
1:D:218:TYR:HB2	1:D:240:VAL:HG22	1.99	0.43
1:A:456:ASP:O	1:A:458:LYS:NZ	2.51	0.43
1:A:539:VAL:HG21	1:B:803:LEU:HD21	2.00	0.43
1:B:76:ASP:OD2	1:B:77:LYS:N	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:ASP:HB3	1:C:269:PRO:HB2	2.00	0.43
1:D:800:VAL:HA	1:D:803:LEU:HD12	2.00	0.43
1:B:10:ILE:HG23	1:B:69:TYR:CD2	2.54	0.43
1:B:17:PRO:HA	1:B:48:LEU:O	2.18	0.43
1:C:400:ILE:HG12	1:C:401:LEU:N	2.33	0.43
1:A:628:ARG:HB3	1:D:626:VAL:HG11	2.01	0.43
1:A:746:VAL:O	1:A:750:VAL:HG23	2.19	0.43
1:B:659:PHE:HB3	1:B:671:TRP:HB2	1.99	0.43
1:A:245:ILE:HG23	1:A:246:VAL:HG23	1.99	0.43
1:A:622:ALA:O	1:A:626:VAL:HG23	2.17	0.43
1:B:653:GLY:HA3	3:B:2002:FWD:H72	2.01	0.43
1:D:626:VAL:CG1	1:D:627:GLU:H	2.32	0.43
1:D:707:THR:OG1	1:D:708:MET:SD	2.75	0.43
1:C:401:LEU:HA	1:C:401:LEU:HD23	1.85	0.43
1:C:800:VAL:HA	1:C:803:LEU:HD12	2.01	0.43
1:B:628:ARG:HB3	1:B:629:MET:H	1.49	0.43
1:B:760:ASP:OD2	1:B:760:ASP:N	2.51	0.43
1:A:450:TYR:CD1	3:A:2002:FWD:H71	2.54	0.42
1:C:17:PRO:HA	1:C:48:LEU:O	2.18	0.42
1:C:595:SER:HB2	1:D:813:GLU:OE2	2.19	0.42
1:C:141:LEU:HD22	1:D:141:LEU:HD22	2.01	0.42
1:D:169:ASP:OD2	1:D:169:ASP:N	2.51	0.42
1:B:235:PHE:HB2	1:D:208:THR:HG22	2.01	0.42
1:D:250:ASP:OD1	1:D:251:SER:N	2.52	0.42
1:C:625:THR:O	1:C:629:MET:HG2	2.19	0.42
1:A:309:ASN:O	1:A:310:ALA:HB3	2.19	0.42
1:B:659:PHE:CZ	1:B:703:LEU:HD13	2.53	0.42
1:C:154:LYS:O	1:C:155:LYS:HB3	2.20	0.42
1:A:729:SER:O	4:A:2003:FWF:H8	2.19	0.42
1:A:464:VAL:HG13	1:A:489:ILE:HD13	2.01	0.42
1:B:647:TYR:CD2	1:B:674:MET:HE3	2.53	0.42
1:B:711:TYR:O	1:B:715:ARG:HG2	2.20	0.42
1:C:321:TRP:CE3	1:C:323:GLN:HB2	2.55	0.42
1:A:505:LYS:O	1:A:507:PRO:HD3	2.19	0.42
1:D:597:SER:O	1:D:601:VAL:HG23	2.19	0.42
1:A:401:LEU:HA	1:A:401:LEU:HD23	1.83	0.42
1:B:250:ASP:OD2	1:B:251:SER:N	2.53	0.42
1:B:96:THR:HA	1:B:97:PRO:HD3	1.77	0.42
1:C:195:GLU:H	1:C:195:GLU:CD	2.23	0.42
1:C:96:THR:HA	1:C:97:PRO:HD3	1.76	0.42
1:A:621:ALA:O	1:A:625:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:VAL:HG13	1:A:794:GLY:HA2	2.02	0.42
1:B:729:SER:OG	4:B:2003:FWF:C16	2.68	0.42
1:B:690:VAL:HG11	1:B:712:ILE:HG21	2.02	0.42
1:A:202:ILE:O	1:A:206:VAL:HG23	2.19	0.42
1:C:316:ASN:HA	1:C:317:PRO:HA	1.93	0.42
1:C:460:TRP:HE1	1:C:488:VAL:HG11	1.84	0.42
1:C:667:PHE:HE1	1:C:727:LEU:HG	1.84	0.42
1:A:129:ASP:O	1:A:129:ASP:OD1	2.38	0.42
1:A:199:VAL:O	1:A:203:VAL:HG23	2.19	0.42
1:B:639:LEU:HG	1:B:639:LEU:O	2.20	0.42
1:C:141:LEU:HD23	1:C:144:LEU:HD23	2.00	0.42
1:C:75:TYR:CE2	1:C:96:THR:HG21	2.53	0.42
1:A:796:PHE:CE2	1:D:528:ALA:HB1	2.54	0.42
1:D:711:TYR:O	1:D:715:ARG:HG2	2.19	0.42
1:B:298:ARG:NH2	1:B:304:ILE:HG12	2.35	0.41
1:A:373:SER:HB3	1:A:376:ASP:HB2	2.01	0.41
1:A:96:THR:HA	1:A:97:PRO:HD3	1.76	0.41
1:D:506:LYS:HA	1:D:507:PRO:HD2	1.86	0.41
1:A:288:GLN:NE2	1:A:336:VAL:HB	2.35	0.41
1:B:172:ASP:O	1:B:175:TYR:CD2	2.72	0.41
1:C:405:TYR:OH	1:C:732:TYR:HE2	2.04	0.41
1:A:400:ILE:HG12	1:A:401:LEU:N	2.35	0.41
1:B:670:MET:O	1:B:674:MET:HG3	2.20	0.41
1:C:256:PHE:CE2	1:C:339:LEU:HD11	2.55	0.41
1:D:171:LYS:O	1:D:175:TYR:HD1	2.03	0.41
1:A:110:GLN:HB2	1:A:110:GLN:HE21	1.52	0.41
1:A:128:TRP:CD2	1:A:189:ARG:HG2	2.55	0.41
1:A:24:TYR:CE2	1:A:28:ARG:HD2	2.55	0.41
1:A:353:ASN:N	1:A:353:ASN:ND2	2.68	0.41
1:A:683:VAL:HG11	1:A:689:GLY:HA2	2.02	0.41
1:D:96:THR:HA	1:D:97:PRO:HD3	1.77	0.41
1:A:416:GLU:OE1	1:A:416:GLU:N	2.54	0.41
1:B:347:GLN:HG3	1:B:348:ASN:OD1	2.21	0.41
1:C:614:SER:HG	1:D:616:TYR:HD2	1.67	0.41
1:D:373:SER:HB3	1:D:376:ASP:HB2	2.02	0.41
1:A:806:ALA:HA	1:D:600:ILE:HD11	2.02	0.41
1:A:486:GLU:OE2	1:A:491:PHE:HB2	2.20	0.40
1:A:523:TYR:HA	1:A:526:TRP:HD1	1.85	0.40
1:C:250:ASP:OD2	1:C:251:SER:N	2.54	0.40
1:C:637:GLU:HA	1:C:666:VAL:HG11	2.02	0.40
1:A:611:ILE:HG21	1:B:795:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:788:SER:OG	1:A:789:LEU:N	2.55	0.40
1:C:188:ARG:NH2	1:C:468:VAL:O	2.50	0.40
1:D:29:VAL:HG21	1:D:260:TRP:HZ3	1.86	0.40
1:B:525:ILE:HG12	1:C:789:LEU:HD13	2.02	0.40
1:C:115:LEU:HD22	1:C:223:LEU:HD12	2.03	0.40
1:C:34:PHE:HB3	1:C:291:THR:HG21	2.03	0.40
1:D:202:ILE:O	1:D:206:VAL:HG23	2.22	0.40
1:D:405:TYR:CE1	1:D:478:PRO:HB3	2.57	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	708/819 (86%)	693 (98%)	15 (2%)	0	100	100
1	B	719/819 (88%)	702 (98%)	17 (2%)	0	100	100
1	C	718/819 (88%)	701 (98%)	17 (2%)	0	100	100
1	D	715/819 (87%)	694 (97%)	21 (3%)	0	100	100
All	All	2860/3276 (87%)	2790 (98%)	70 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	556/698 (80%)	533 (96%)	23 (4%)	30	58
1	B	569/698 (82%)	545 (96%)	24 (4%)	30	57
1	C	569/698 (82%)	543 (95%)	26 (5%)	27	55
1	D	559/698 (80%)	546 (98%)	13 (2%)	50	71
All	All	2253/2792 (81%)	2167 (96%)	86 (4%)	33	59

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	THR
1	A	110	GLN
1	A	148	LEU
1	A	154	LYS
1	A	230	LEU
1	A	249	ASP
1	A	279	THR
1	A	296	ASN
1	A	314	LEU
1	A	336	VAL
1	A	353	ASN
1	A	380	VAL
1	A	480	THR
1	A	498	LEU
1	A	502	ILE
1	A	517	PHE
1	A	644	GLU
1	A	654	SER
1	A	664	ILE
1	A	675	ARG
1	A	760	ASP
1	A	785	SER
1	A	791	ASN
1	B	75	TYR
1	B	129	ASP
1	B	148	LEU
1	B	175	TYR
1	B	222	ASN
1	B	225	PHE
1	B	279	THR
1	B	296	ASN
1	B	353	ASN
1	B	400	ILE

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Mol	Chain	Res	Type
1	B	453	ARG
1	B	480	THR
1	B	484	VAL
1	B	498	LEU
1	B	502	ILE
1	B	517	PHE
1	B	521	LEU
1	B	628	ARG
1	B	642	GLN
1	B	644	GLU
1	B	748	LEU
1	B	754	SER
1	B	760	ASP
1	B	789	LEU
1	C	28	ARG
1	C	40	ARG
1	C	110	GLN
1	C	148	LEU
1	C	154	LYS
1	C	172	ASP
1	C	188	ARG
1	C	256	PHE
1	C	259	ARG
1	C	263	LEU
1	C	279	THR
1	C	371	TYR
1	C	480	THR
1	C	498	LEU
1	C	502	ILE
1	C	517	PHE
1	C	521	LEU
1	C	523	TYR
1	C	527	MET
1	C	613	ILE
1	C	634	GLU
1	C	716	LYS
1	C	748	LEU
1	C	754	SER
1	C	760	ASP
1	C	799	LEU
1	D	168	ASN
1	D	187	GLU

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Mol	Chain	Res	Type
1	D	194	CYS
1	D	279	THR
1	D	400	ILE
1	D	480	THR
1	D	498	LEU
1	D	502	ILE
1	D	538	VAL
1	D	650	LEU
1	D	748	LEU
1	D	754	SER
1	D	760	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	145	GLN
1	A	234	GLN
1	A	288	GLN
1	A	791	ASN
1	B	342	ASN
1	C	110	GLN
1	D	110	GLN
1	D	145	GLN
1	D	335	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 monosaccharides in this entry.

## 5.6 Ligand geometry

9 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	NAG	A	2001	1	14,14,15	1.21	1 (7%)	17,19,21	3.74	9 (52%)
4	FWF	B	2003	-	31,33,33	1.62	2 (6%)	38,48,48	3.09	6 (15%)
3	FWD	C	1001	-	9,15,15	2.93	1 (11%)	7,21,21	2.92	2 (28%)
4	FWF	A	2003	-	31,33,33	1.53	2 (6%)	38,48,48	3.19	6 (15%)
3	FWD	D	2002	-	9,15,15	3.89	2 (22%)	7,21,21	3.83	2 (28%)
3	FWD	B	2002	-	9,15,15	2.84	1 (11%)	7,21,21	2.91	2 (28%)
3	FWD	A	2002	-	9,15,15	2.89	1 (11%)	7,21,21	2.88	2 (28%)
2	NAG	B	2001	1	14,14,15	0.83	0	17,19,21	1.05	1 (5%)
2	NAG	D	2001	1	14,14,15	0.56	0	17,19,21	1.59	1 (5%)

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	NAG	A	2001	1	-	5/6/23/26	0/1/1/1
4	FWF	B	2003	-	-	0/32/36/36	0/2/2/2
3	FWD	C	1001	-	-	0/4/8/8	0/1/1/1
4	FWF	A	2003	-	-	2/32/36/36	0/2/2/2
3	FWD	D	2002	-	-	0/4/8/8	0/1/1/1
3	FWD	B	2002	-	-	0/4/8/8	0/1/1/1
3	FWD	A	2002	-	-	0/4/8/8	0/1/1/1
2	NAG	B	2001	1	-	2/6/23/26	0/1/1/1
2	NAG	D	2001	1	-	0/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2002	FWD	C4-C5	11.18	1.52	1.38
3	C	1001	FWD	C4-C5	8.43	1.48	1.38
3	A	2002	FWD	C4-C5	8.33	1.48	1.38
3	B	2002	FWD	C4-C5	8.16	1.48	1.38
4	B	2003	FWF	C20-S2	-6.21	1.65	1.78
4	B	2003	FWF	C19-S1	-6.06	1.65	1.78
4	A	2003	FWF	C19-S1	-6.02	1.65	1.78
4	A	2003	FWF	C20-S2	-5.54	1.66	1.78
2	A	2001	NAG	O7-C7	-2.87	1.16	1.23
3	D	2002	FWD	C4-N3	2.80	1.37	1.33

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2003	FWF	O2-S1-O1	-12.78	109.65	119.24
4	A	2003	FWF	O4-S2-O3	-12.67	109.74	119.24
4	A	2003	FWF	O2-S1-O1	-12.55	109.82	119.24
4	B	2003	FWF	O4-S2-O3	-11.57	110.56	119.24
2	A	2001	NAG	C2-N2-C7	11.10	138.71	122.90
3	D	2002	FWD	C4-N3-C2	9.00	122.74	115.14
3	C	1001	FWD	C4-N3-C2	6.63	120.74	115.14
3	B	2002	FWD	C4-N3-C2	6.61	120.72	115.14
3	A	2002	FWD	C4-N3-C2	6.48	120.61	115.14
2	D	2001	NAG	C1-O5-C5	5.64	119.83	112.19
2	A	2001	NAG	C1-O5-C5	5.52	119.68	112.19
2	A	2001	NAG	O3-C3-C2	4.35	118.47	109.47
2	A	2001	NAG	C1-C2-N2	-4.24	103.25	110.49
3	D	2002	FWD	C5-C4-N3	-4.10	118.06	122.39
3	C	1001	FWD	C5-C4-N3	-3.47	118.73	122.39
3	B	2002	FWD	C5-C4-N3	-3.46	118.74	122.39
3	A	2002	FWD	C5-C4-N3	-3.31	118.90	122.39
4	A	2003	FWF	O1-S1-N2	3.31	111.74	107.76
2	A	2001	NAG	O7-C7-C8	-2.96	116.56	122.06
4	B	2003	FWF	O4-S2-N1	2.73	111.05	107.76
4	B	2003	FWF	O1-S1-N2	2.66	110.97	107.76
2	A	2001	NAG	O4-C4-C3	2.61	116.38	110.35
2	A	2001	NAG	C6-C5-C4	2.55	118.98	113.00
2	A	2001	NAG	O5-C1-C2	-2.50	107.33	111.29
2	A	2001	NAG	C3-C4-C5	-2.33	106.09	110.24
4	A	2003	FWF	C22-C19-S1	-2.29	103.89	109.62
4	A	2003	FWF	O4-S2-N1	2.18	110.39	107.76
4	A	2003	FWF	C2-C1-C6	2.18	121.01	118.29
4	B	2003	FWF	C22-C19-S1	-2.15	104.25	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2003	FWF	O2-S1-N2	2.11	110.30	107.76
2	B	2001	NAG	O5-C1-C2	-2.00	108.13	111.29

There are no chirality outliers.

All (9) torsion outliers are listed below:

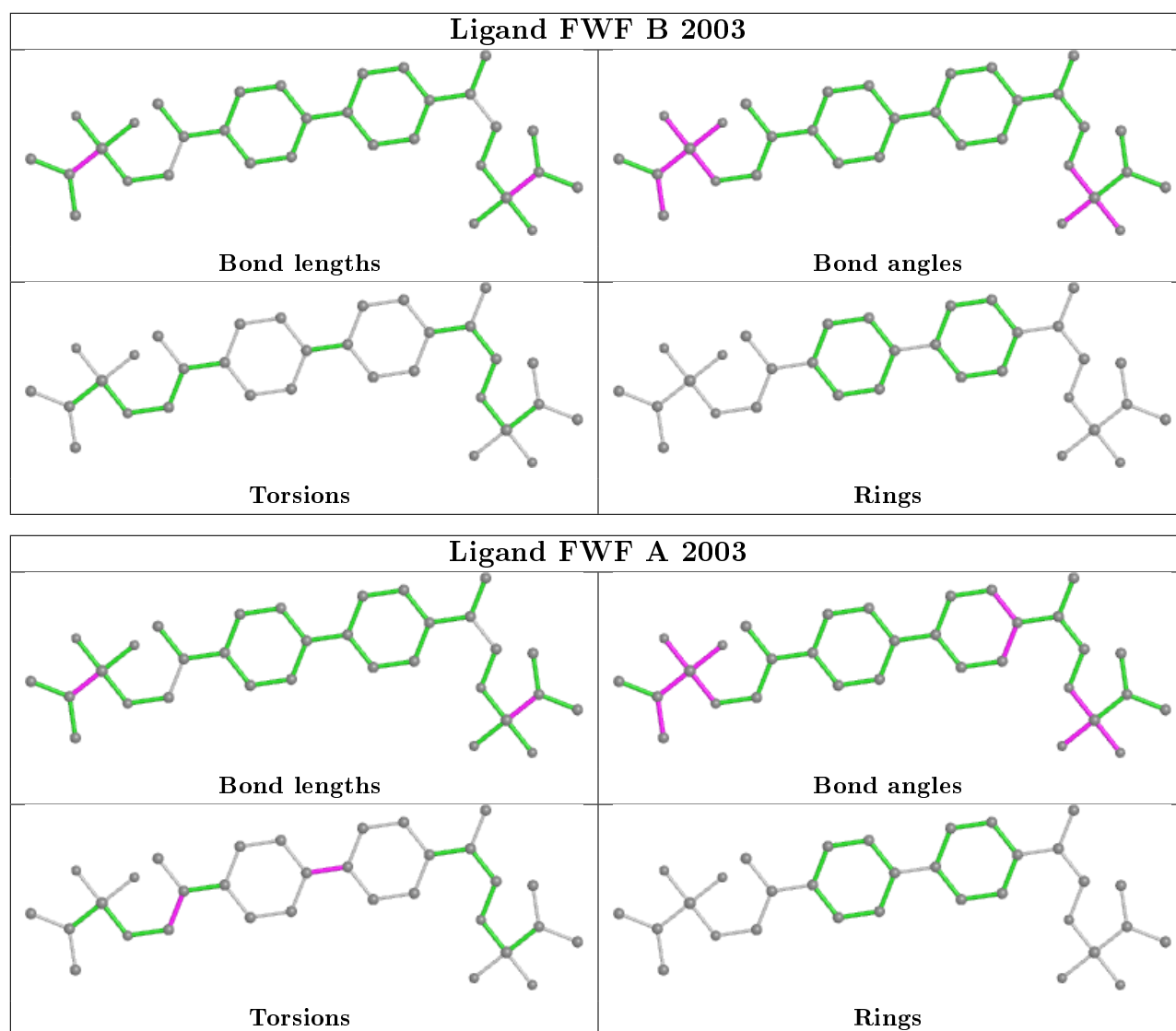
Mol	Chain	Res	Type	Atoms
2	A	2001	NAG	C8-C7-N2-C2
2	A	2001	NAG	O7-C7-N2-C2
2	B	2001	NAG	C8-C7-N2-C2
2	B	2001	NAG	O7-C7-N2-C2
2	A	2001	NAG	C4-C5-C6-O6
4	A	2003	FWF	C17-C13-C18-N2
2	A	2001	NAG	O5-C5-C6-O6
2	A	2001	NAG	C1-C2-N2-C7
4	A	2003	FWF	C9-C10-C4-C5

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2003	FWF	2	0
4	A	2003	FWF	2	0
3	B	2002	FWD	1	0
3	A	2002	FWD	1	0
2	B	2001	NAG	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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, 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	720/819 (87%)	-0.07	35 (4%)	29	24	98, 166, 237, 304	0
1	B	731/819 (89%)	-0.06	32 (4%)	34	28	68, 140, 237, 301	0
1	C	730/819 (89%)	0.10	53 (7%)	15	11	72, 192, 269, 397	0
1	D	727/819 (88%)	0.05	41 (5%)	24	19	77, 203, 265, 315	0
All	All	2908/3276 (88%)	0.01	161 (5%)	25	20	68, 176, 260, 397	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	370	GLY	9.2
1	D	13	GLY	8.2
1	C	14	GLY	7.5
1	B	523	TYR	7.0
1	B	634	GLU	6.7
1	C	358	ILE	6.7
1	C	13	GLY	6.4
1	D	14	GLY	6.2
1	D	291	THR	5.9
1	C	336	VAL	5.9
1	C	218	TYR	5.6
1	A	653	GLY	5.6
1	D	32	VAL	5.6
1	C	337	GLU	5.5
1	D	102	ASP	4.8
1	D	163	VAL	4.7
1	C	15	LEU	4.7
1	D	652	SER	4.5
1	D	74	PHE	4.4
1	A	652	SER	4.3
1	D	34	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	57	THR	4.2
1	A	113	PRO	4.1
1	A	339	LEU	4.0
1	C	165	ASN	4.0
1	B	69	TYR	3.9
1	D	15	LEU	3.9
1	B	816	TYR	3.9
1	C	166	ILE	3.8
1	A	425	CYS	3.8
1	C	356	ILE	3.7
1	B	526	TRP	3.7
1	C	73	GLY	3.7
1	A	214	LYS	3.6
1	C	69	TYR	3.6
1	D	50	VAL	3.6
1	D	631	SER	3.5
1	A	111	MET	3.5
1	D	138	ASP	3.4
1	B	296	ASN	3.4
1	C	338	GLY	3.4
1	A	212	HIS	3.4
1	C	308	GLY	3.4
1	B	70	ALA	3.3
1	B	367	ARG	3.3
1	C	304	ILE	3.2
1	C	189	ARG	3.2
1	B	366	PRO	3.2
1	C	131	PHE	3.2
1	C	339	LEU	3.1
1	B	633	ILE	3.1
1	D	290	MET	3.1
1	C	70	ALA	3.1
1	A	399	THR	3.0
1	C	792	VAL	3.0
1	B	349	GLY	3.0
1	A	246	VAL	3.0
1	C	793	ALA	3.0
1	C	215	GLY	3.0
1	D	33	GLN	2.9
1	C	307	ARG	2.9
1	A	356	ILE	2.9
1	B	522	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	194	CYS	2.9
1	D	345	PHE	2.9
1	D	218	TYR	2.9
1	C	779	GLY	2.8
1	B	815	ALA	2.8
1	C	478	PRO	2.7
1	C	16	PHE	2.7
1	A	340	SER	2.7
1	C	340	SER	2.7
1	B	521	LEU	2.7
1	C	504	ILE	2.7
1	B	31	MET	2.7
1	C	157	GLN	2.7
1	A	186	LYS	2.7
1	D	686	THR	2.7
1	D	49	GLU	2.6
1	B	313	CYS	2.6
1	C	172	ASP	2.6
1	A	477	ALA	2.6
1	B	545	ARG	2.6
1	A	331	LEU	2.6
1	C	679	PRO	2.6
1	A	656	LYS	2.6
1	B	294	PHE	2.6
1	C	74	PHE	2.6
1	C	366	PRO	2.6
1	C	507	PRO	2.6
1	A	319	VAL	2.6
1	A	94	PHE	2.6
1	D	381	THR	2.6
1	D	380	VAL	2.6
1	A	355	THR	2.5
1	D	113	PRO	2.5
1	C	243	PHE	2.5
1	C	701	ALA	2.5
1	D	476	ILE	2.5
1	B	113	PRO	2.5
1	C	363	THR	2.5
1	B	20	ALA	2.5
1	A	594	ARG	2.5
1	D	137	SER	2.5
1	A	629	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	187	GLU	2.5
1	C	630	VAL	2.5
1	A	351	ARG	2.5
1	D	650	LEU	2.4
1	B	300	GLN	2.4
1	C	242	GLY	2.4
1	A	426	VAL	2.4
1	C	634	GLU	2.4
1	B	235	PHE	2.4
1	D	642	GLN	2.4
1	A	213	VAL	2.4
1	C	702	TYR	2.4
1	D	268	TYR	2.4
1	C	335	GLN	2.4
1	D	402	GLU	2.4
1	C	164	GLY	2.3
1	C	544	SER	2.3
1	B	316	ASN	2.3
1	D	455	ALA	2.3
1	B	245	ILE	2.3
1	D	732	TYR	2.3
1	D	456	ASP	2.3
1	C	369	ILE	2.3
1	D	73	GLY	2.3
1	A	110	GLN	2.3
1	A	233	ILE	2.2
1	B	524	GLU	2.2
1	A	531	PHE	2.2
1	C	128	TRP	2.2
1	D	450	TYR	2.2
1	D	684	ARG	2.2
1	D	83	ILE	2.2
1	B	503	MET	2.2
1	B	767	TRP	2.2
1	A	317	PRO	2.1
1	A	187	GLU	2.1
1	D	676	SER	2.1
1	D	375	VAL	2.1
1	B	356	ILE	2.1
1	B	363	THR	2.1
1	D	179	PHE	2.1
1	C	72	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	60	PHE	2.1
1	A	95	ILE	2.1
1	A	46	ASP	2.1
1	A	398	THR	2.1
1	B	256	PHE	2.1
1	D	103	GLY	2.1
1	D	104	THR	2.0
1	A	248	TYR	2.0
1	B	595	SER	2.0
1	C	790	SER	2.0
1	A	282	LEU	2.0
1	C	309	ASN	2.0
1	A	109	ILE	2.0
1	C	214	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

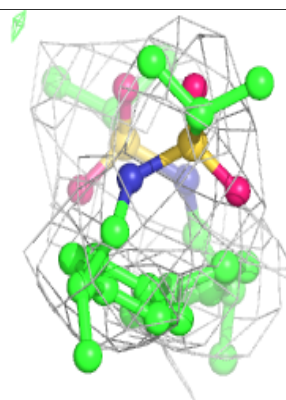
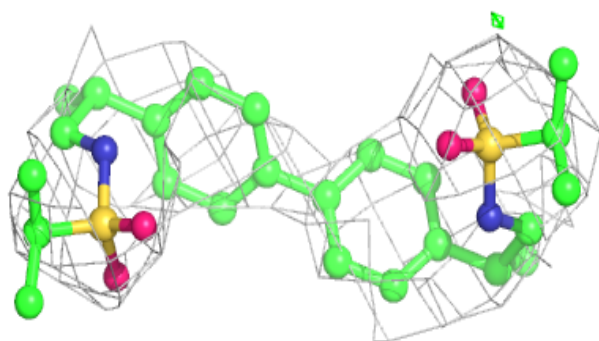
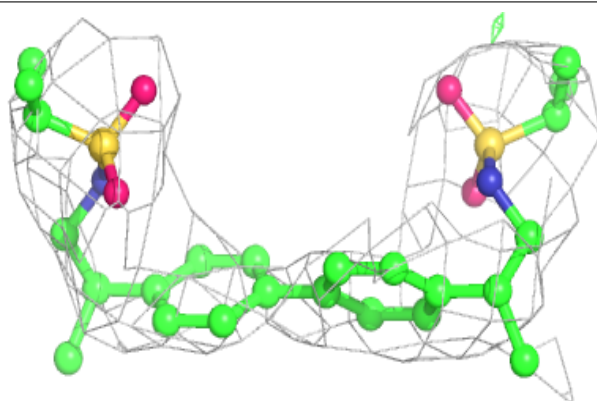
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FWD	A	2002	15/15	0.73	0.24	209,229,269,276	0
2	NAG	D	2001	14/15	0.78	0.35	194,264,298,311	0
2	NAG	A	2001	14/15	0.82	0.33	95,112,279,312	0
3	FWD	D	2002	15/15	0.85	0.55	120,172,252,266	0
3	FWD	B	2002	15/15	0.85	0.29	86,104,211,216	0
2	NAG	B	2001	14/15	0.86	0.20	171,220,263,306	0
3	FWD	C	1001	15/15	0.90	0.20	100,124,170,184	0
4	FWF	A	2003	32/32	0.92	0.28	73,126,184,207	0
4	FWF	B	2003	32/32	0.93	0.25	69,102,150,215	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

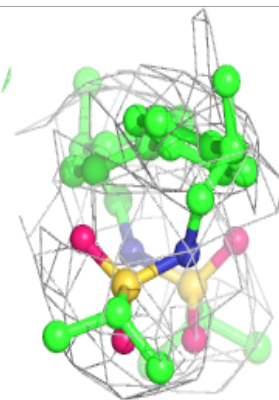
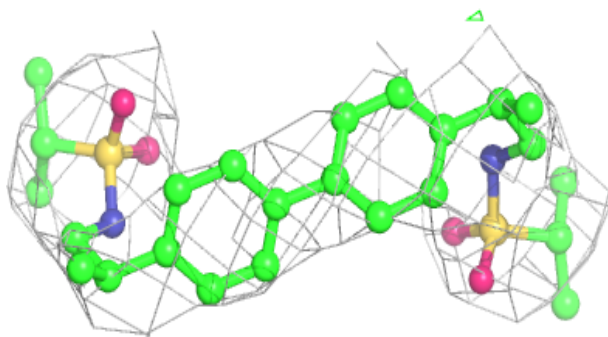
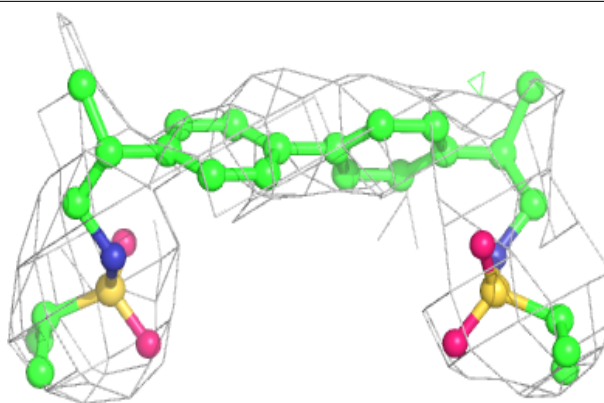
**Electron density around FWF A 2003:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FWF B 2003:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.