



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 03:02 PM EST

PDB ID : 4U1X
Title : Full length GluA2-kainate-(R,R)-2b complex crystal form B
Authors : Chen, L.; Gouaux, E.
Deposited on : 2014-07-16
Resolution : 3.30 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

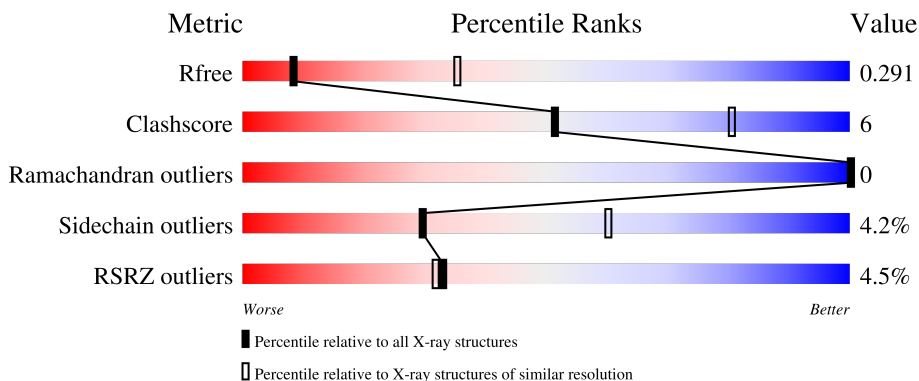
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	824	 4% 76% 13% • 10%
1	B	824	 3% 75% 13% • 10%
1	C	824	 5% 75% 17% 8%
1	D	824	 4% 75% 14% • 10%

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
3	NAG	D	902	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 23451 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
			Total	C	N	O	S			
1	A	743	5796	3719	964	1087	26	0	0	0
1	B	738	5803	3731	961	1085	26	0	0	0
1	C	755	5882	3778	977	1101	26	0	0	0
1	D	744	5778	3719	954	1079	26	0	0	0

There are 92 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	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
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

Continued on next page...

Continued from previous page...

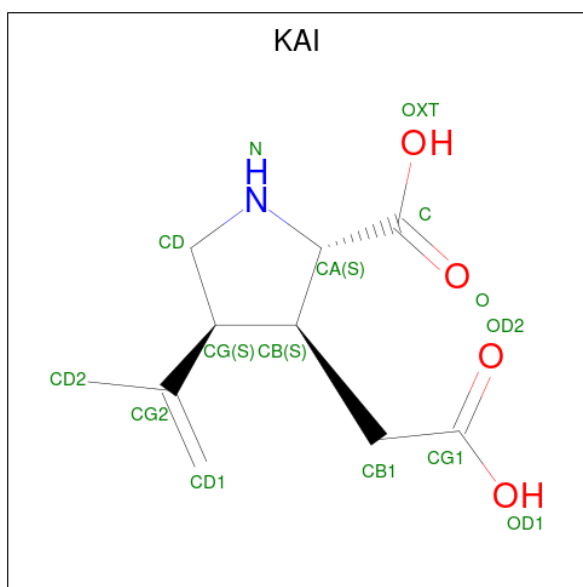
Chain	Residue	Modelled	Actual	Comment	Reference
A	830	PRO	-	expression tag	UNP P19491
A	831	ARG	-	expression tag	UNP P19491
B	239	GLU	ASN	engineered mutation	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	?	-	GLY	deletion	UNP P19491
B	385	ASP	ASN	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	577	PHE	LEU	engineered mutation	UNP P19491
B	580	ALA	SER	engineered mutation	UNP P19491
B	582	LYS	GLY	engineered mutation	UNP P19491
B	583	LEU	ALA	engineered mutation	UNP P19491
B	585	PHE	MET	engineered mutation	UNP P19491
B	589	ALA	CYS	engineered mutation	UNP P19491
B	598	ALA	GLY	engineered mutation	UNP P19491
B	602	ALA	GLY	engineered mutation	UNP P19491
B	815	ALA	CYS	engineered mutation	UNP P19491
B	827	GLY	-	expression tag	UNP P19491
B	828	LEU	-	expression tag	UNP P19491
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
C	385	ASP	ASN	engineered mutation	UNP P19491
C	392	GLN	ASN	engineered mutation	UNP P19491
C	528	ALA	CYS	engineered mutation	UNP P19491
C	535	LEU	GLY	engineered mutation	UNP P19491
C	577	PHE	LEU	engineered mutation	UNP P19491
C	580	ALA	SER	engineered mutation	UNP P19491
C	582	LYS	GLY	engineered mutation	UNP P19491
C	583	LEU	ALA	engineered mutation	UNP P19491
C	585	PHE	MET	engineered mutation	UNP P19491
C	589	ALA	CYS	engineered mutation	UNP P19491
C	598	ALA	GLY	engineered mutation	UNP P19491
C	602	ALA	GLY	engineered mutation	UNP P19491

Continued on next page...

Continued from previous page...

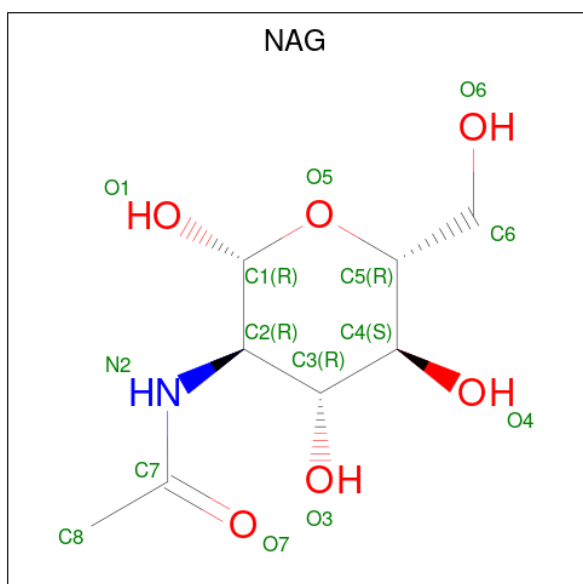
Chain	Residue	Modelled	Actual	Comment	Reference
C	815	ALA	CYS	engineered mutation	UNP P19491
C	827	GLY	-	expression tag	UNP P19491
C	828	LEU	-	expression tag	UNP P19491
C	829	VAL	-	expression tag	UNP P19491
C	830	PRO	-	expression tag	UNP P19491
C	831	ARG	-	expression tag	UNP P19491
D	239	GLU	ASN	engineered 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	577	PHE	LEU	engineered mutation	UNP P19491
D	580	ALA	SER	engineered mutation	UNP P19491
D	582	LYS	GLY	engineered mutation	UNP P19491
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 3-(CARBOXYMETHYL)-4-ISOPROPENYLPROLINE (three-letter code: KAI) (formula: C₁₀H₁₅NO₄).



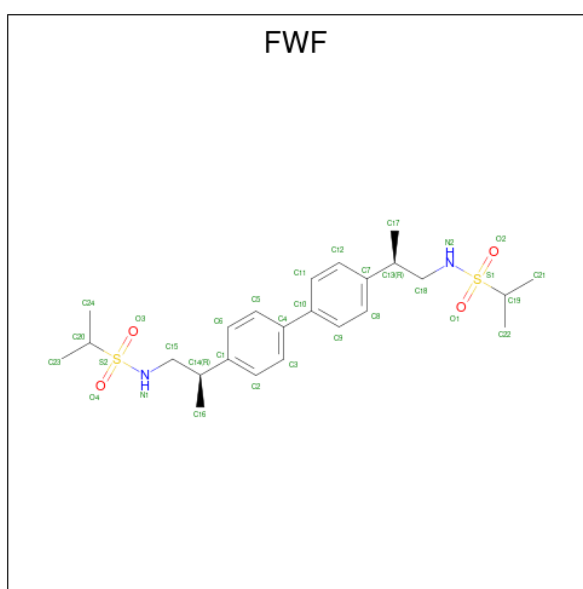
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total	C	N	O	0	0
			15	10	1	4		
2	B	1	Total	C	N	O	0	0
			15	10	1	4		
2	C	1	Total	C	N	O	0	0
			15	10	1	4		
2	D	1	Total	C	N	O	0	0
			15	10	1	4		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



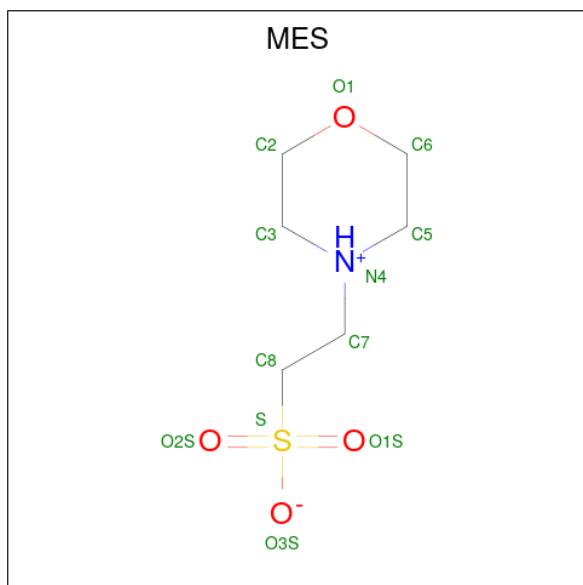
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is N,N'-[biphenyl-4,4'-diyl-di(2R)propane-2,1-diyl]dipropane-2-sulfonamide (three-letter code: FWF) (formula: C₂₄H₃₆N₂O₄S₂).



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

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).

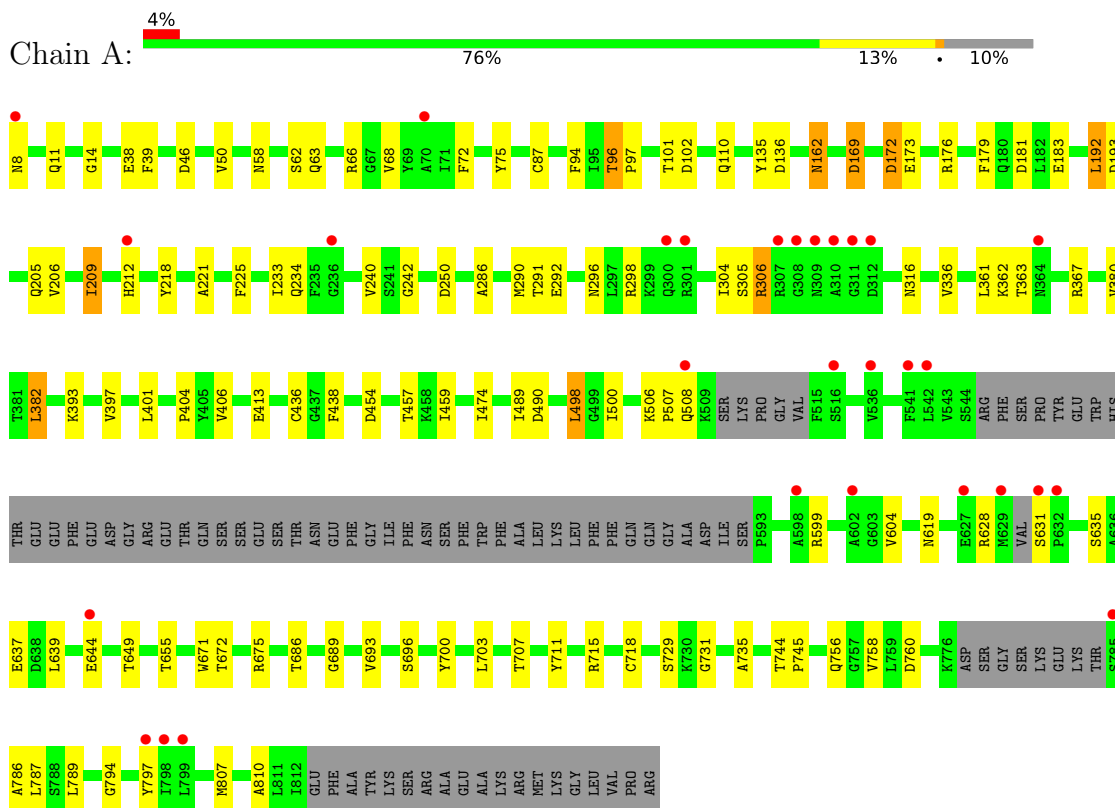


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	D	1	12	6	1	4	1	0	0

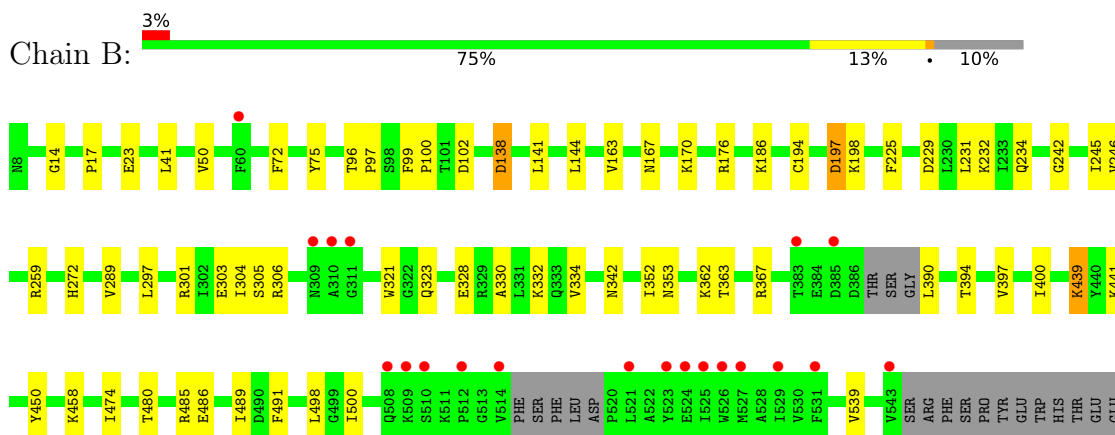
3 Residue-property plots [i](#)

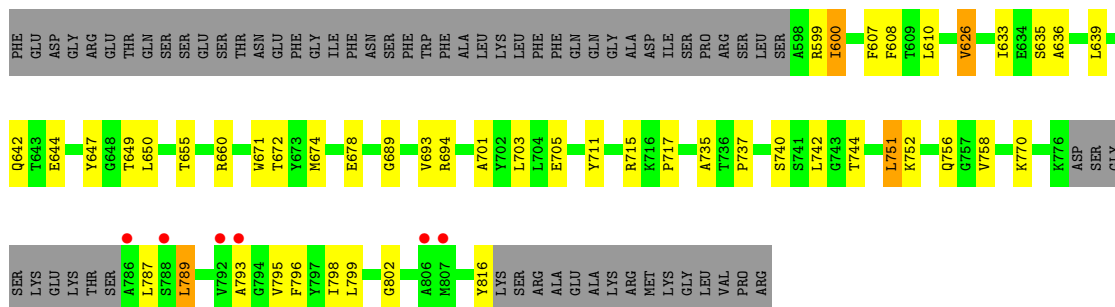
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

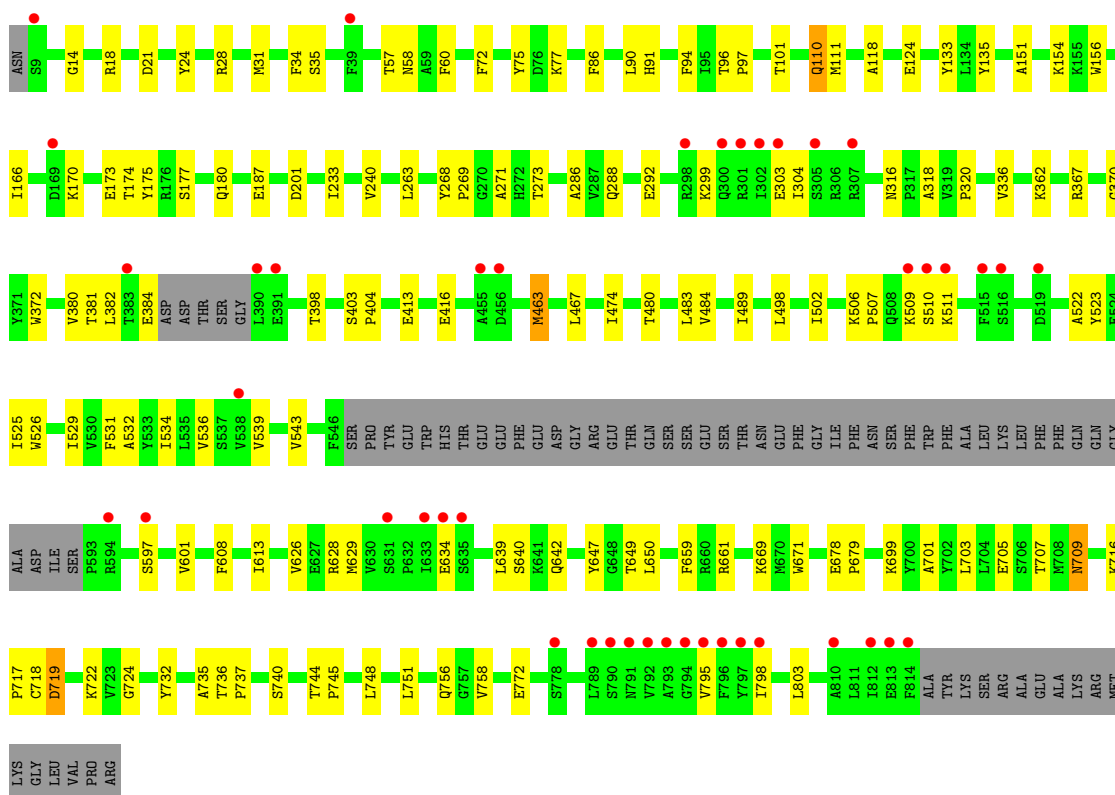
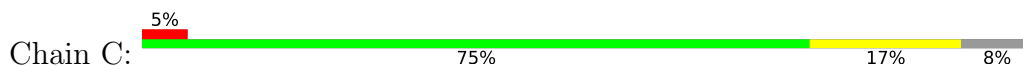


- Molecule 1: Glutamate receptor 2

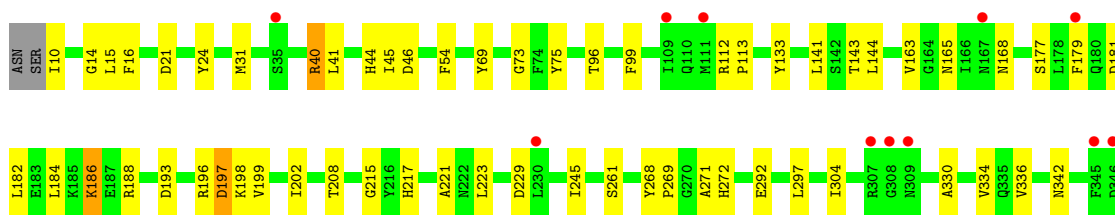
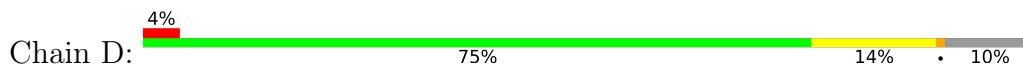


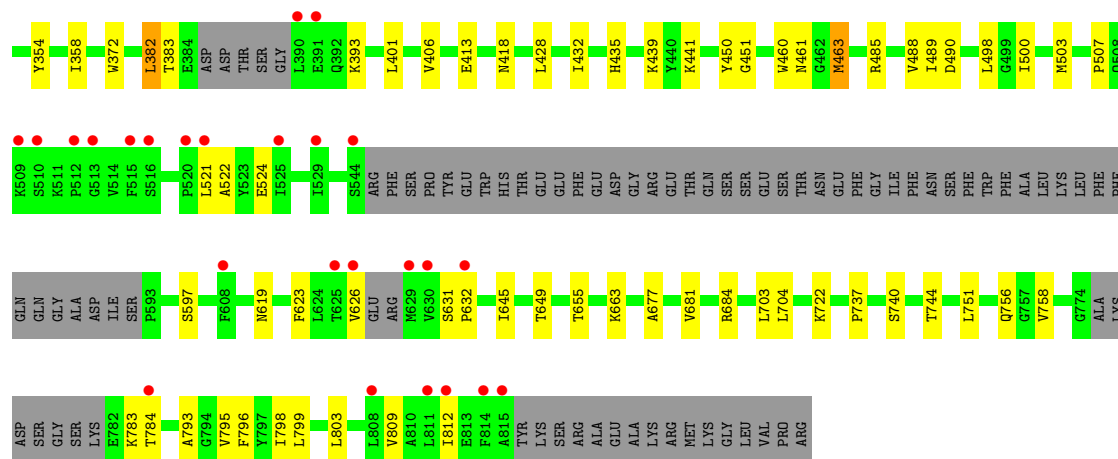


- Molecule 1: Glutamate receptor 2



- Molecule 1: Glutamate receptor 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.52Å 160.73Å 338.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.79 – 3.30 73.38 – 3.30	Depositor EDS
% Data completeness (in resolution range)	68.4 (29.79-3.30) 68.5 (73.38-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.33Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.242 , 0.289 0.246 , 0.291	Depositor DCC
R_{free} test set	2773 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	75.8	Xtrriage
Anisotropy	0.072	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 26.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	23451	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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: MES, KAI, 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	0.23	0/5911	0.42	0/7997
1	B	0.23	0/5920	0.41	0/8005
1	C	0.23	0/6002	0.41	0/8121
1	D	0.23	0/5895	0.42	0/7978
All	All	0.23	0/23728	0.42	0/32101

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	5796	0	5761	64	0
1	B	5803	0	5800	69	0
1	C	5882	0	5848	74	0
1	D	5778	0	5748	74	0
2	A	15	0	13	0	0
2	B	15	0	13	3	0
2	C	15	0	13	2	0
2	D	15	0	13	1	0
3	A	14	0	13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	14	0	13	0	0
3	C	14	0	13	1	0
3	D	14	0	13	1	0
4	B	32	0	36	2	0
4	D	32	0	36	2	0
5	D	12	0	13	1	0
All	All	23451	0	23346	260	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 (260) 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:677:ALA:HB1	1:D:681:VAL:HG23	1.65	0.79
1:A:507:PRO:HA	1:A:508:GLN:HB2	1.69	0.75
1:D:99:PHE:HA	1:D:112:ARG:HD2	1.68	0.74
1:C:21:ASP:HB3	1:C:269:PRO:HB2	1.72	0.71
1:D:75:TYR:HE2	1:D:96:THR:HG21	1.55	0.70
1:D:793:ALA:HA	1:D:796:PHE:HD1	1.57	0.69
1:A:75:TYR:HE2	1:A:96:THR:HG21	1.58	0.69
1:D:268:TYR:HB2	1:D:271:ALA:HB2	1.75	0.68
1:D:342:ASN:HB2	3:D:902:NAG:H82	1.75	0.67
1:A:234:GLN:HA	1:A:361:LEU:HD21	1.76	0.66
1:A:789:LEU:HD22	1:D:524:GLU:HB3	1.77	0.66
1:C:233:ILE:HD12	1:C:240:VAL:HG21	1.78	0.66
1:D:24:TYR:HE1	1:D:45:ILE:HG21	1.61	0.65
1:D:163:VAL:HG21	1:D:202:ILE:HG12	1.79	0.65
1:B:711:TYR:OH	1:B:715:ARG:NH1	2.30	0.65
1:B:610:LEU:HD21	1:C:613:ILE:HG21	1.79	0.64
1:D:197:ASP:OD2	1:D:197:ASP:N	2.28	0.64
1:A:179:PHE:O	1:A:183:GLU:HG2	1.98	0.62
1:B:167:ASN:HB2	1:B:170:LYS:HG2	1.82	0.61
1:B:650:LEU:HD13	2:B:901:KAI:HD23	1.83	0.60
1:A:292:GLU:O	1:A:296:ASN:ND2	2.32	0.60
1:A:46:ASP:OD2	1:A:63:GLN:NE2	2.35	0.59
1:D:261:SER:HA	1:D:272:HIS:HB2	1.84	0.59
1:A:169:ASP:OD2	1:A:169:ASP:N	2.35	0.59
1:B:303:GLU:O	1:B:323:GLN:NE2	2.35	0.59
1:B:500:ILE:HD13	1:B:655:THR:HG23	1.84	0.59
1:A:135:TYR:O	1:A:162:ASN:ND2	2.33	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:705:GLU:OE2	1:C:732:TYR:OH	2.18	0.58
1:C:362:LYS:HE3	1:C:367:ARG:HH21	1.67	0.58
1:C:659:PHE:HB3	1:C:671:TRP:HB2	1.85	0.58
1:C:649:THR:HG22	1:C:703:LEU:HB2	1.84	0.58
1:C:166:ILE:HG13	1:C:174:THR:HG21	1.86	0.57
1:D:418:ASN:HD21	1:D:441:LYS:HA	1.69	0.57
1:A:173:GLU:OE2	1:A:176:ARG:NH2	2.38	0.57
1:C:756:GLN:HG3	1:C:758:VAL:HG23	1.86	0.57
1:D:751:LEU:HD23	4:D:904:FWF:H30	1.86	0.57
1:B:397:VAL:HG13	1:B:474:ILE:HG23	1.85	0.57
1:B:400:ILE:HD13	1:B:450:TYR:HE1	1.68	0.57
1:D:500:ILE:HD13	1:D:655:THR:HG23	1.85	0.57
1:B:626:VAL:HG21	1:C:628:ARG:HE	1.68	0.56
1:A:193:ASP:HB2	1:A:221:ALA:HB3	1.88	0.55
1:C:268:TYR:HB2	1:C:271:ALA:HB2	1.86	0.55
1:D:292:GLU:HG3	1:D:336:VAL:HG11	1.87	0.55
1:C:292:GLU:HG3	1:C:336:VAL:HG11	1.87	0.55
1:B:400:ILE:HG21	1:B:450:TYR:CE1	2.41	0.55
1:C:650:LEU:HD13	2:C:901:KAI:HD23	1.88	0.55
1:D:133:TYR:HH	1:D:143:THR:HG1	1.55	0.55
1:D:223:LEU:HB3	1:D:245:ILE:HB	1.88	0.55
1:A:234:GLN:NE2	1:A:363:THR:O	2.39	0.55
1:A:11:GLN:HG2	1:A:68:VAL:HG12	1.88	0.55
1:A:401:LEU:HD23	1:A:406:VAL:HG12	1.88	0.55
1:C:380:VAL:HB	1:C:382:LEU:HG	1.89	0.54
1:D:756:GLN:HG3	1:D:758:VAL:HG23	1.89	0.54
1:C:716:LYS:HB2	1:C:772:GLU:HG3	1.90	0.54
1:B:633:ILE:HD13	1:B:639:LEU:HD21	1.90	0.54
1:C:57:THR:HG23	1:C:86:PHE:HE2	1.72	0.54
1:B:14:GLY:HA2	1:B:72:PHE:O	2.08	0.54
1:B:756:GLN:HG3	1:B:758:VAL:HG23	1.89	0.54
1:D:40:ARG:H	1:D:40:ARG:HD3	1.72	0.54
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.89	0.53
1:A:233:ILE:HD12	1:A:240:VAL:HG21	1.89	0.53
1:A:498:LEU:HB3	1:A:707:THR:HG23	1.91	0.53
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.91	0.53
1:A:500:ILE:HD13	1:A:655:THR:HG23	1.91	0.53
1:D:168:ASN:OD1	1:D:168:ASN:N	2.42	0.52
1:C:709:ASN:ND2	1:C:722:LYS:HB2	2.24	0.52
1:A:8:ASN:ND2	1:A:38:GLU:O	2.37	0.52
1:A:628:ARG:HB3	1:D:626:VAL:HG21	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:TYR:HE2	1:C:96:THR:HG21	1.74	0.52
1:C:316:ASN:O	1:C:318:ALA:N	2.42	0.52
1:C:370:GLY:HA2	1:C:381:THR:OG1	2.08	0.52
1:C:640:SER:HB2	1:C:669:LYS:HD2	1.92	0.52
1:A:292:GLU:HG3	1:A:336:VAL:HG11	1.90	0.52
3:C:902:NAG:O7	3:C:902:NAG:O3	2.24	0.51
1:A:756:GLN:HG3	1:A:758:VAL:HG23	1.93	0.51
1:B:231:LEU:HD11	1:D:208:THR:HG22	1.91	0.51
1:A:454:ASP:HB3	1:A:457:THR:HG22	1.92	0.51
1:C:634:GLU:HA	1:C:724:GLY:HA2	1.92	0.51
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.93	0.51
1:D:297:LEU:HD13	1:D:304:ILE:HG21	1.92	0.51
1:D:393:LYS:O	1:D:439:LYS:NZ	2.43	0.51
1:B:225:PHE:CD1	1:B:242:GLY:HA3	2.46	0.51
1:B:498:LEU:HD22	1:B:705:GLU:HB3	1.92	0.51
1:D:193:ASP:HB2	1:D:221:ALA:HB3	1.92	0.50
1:B:141:LEU:HD23	1:B:144:LEU:HD23	1.94	0.50
1:B:793:ALA:HA	1:B:796:PHE:HD1	1.77	0.50
1:A:489:ILE:HD12	1:A:735:ALA:HB1	1.93	0.50
1:B:489:ILE:HD12	1:B:735:ALA:HB1	1.94	0.50
1:D:488:VAL:HG23	1:D:489:ILE:HG23	1.94	0.50
1:B:795:VAL:O	1:B:798:ILE:HG22	2.11	0.49
1:A:304:ILE:HG13	1:A:305:SER:H	1.77	0.49
1:A:729:SER:HB2	4:D:904:FWF:H19	1.93	0.49
1:B:694:ARG:CZ	1:B:717:PRO:HD2	2.41	0.49
1:A:457:THR:HG23	1:A:459:ILE:H	1.77	0.49
1:C:24:TYR:CE2	1:C:28:ARG:HD2	2.48	0.49
1:D:737:PRO:HG2	1:D:740:SER:HB2	1.94	0.49
1:B:75:TYR:CE2	1:B:96:THR:HG21	2.48	0.49
1:C:523:TYR:HA	1:C:526:TRP:HD1	1.78	0.49
1:D:358:ILE:HD11	1:D:372:TRP:HB2	1.95	0.49
1:A:498:LEU:HD13	1:A:731:GLY:HA2	1.95	0.49
1:B:649:THR:HG23	1:B:674:MET:HE1	1.95	0.48
1:A:14:GLY:HA2	1:A:72:PHE:O	2.13	0.48
1:A:696:SER:HB2	1:A:700:TYR:HB3	1.94	0.48
1:A:205:GLN:O	1:A:209:ILE:HG12	2.13	0.48
1:D:198:LYS:O	1:D:202:ILE:HG13	2.14	0.48
1:B:647:TYR:HB3	1:B:701:ALA:HB3	1.95	0.48
1:C:101:THR:N	1:C:110:GLN:OE1	2.39	0.48
1:A:286:ALA:O	1:A:290:MET:HG3	2.14	0.48
1:C:151:ALA:HA	1:C:156:TRP:HB2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:GLY:HA2	1:C:72:PHE:O	2.14	0.48
1:A:787:LEU:HG	1:D:521:LEU:N	2.29	0.47
1:C:522:ALA:H	1:C:525:ILE:HD12	1.79	0.47
1:A:397:VAL:HG13	1:A:474:ILE:HG23	1.96	0.47
1:B:450:TYR:CE2	2:B:901:KAI:HG	2.48	0.47
1:B:17:PRO:HG3	1:B:50:VAL:HB	1.97	0.47
1:C:94:PHE:HE2	1:C:96:THR:HB	1.79	0.47
1:D:382:LEU:HB3	1:D:383:THR:H	1.53	0.47
1:B:328:GLU:OE1	1:B:332:LYS:NZ	2.46	0.47
1:A:380:VAL:HB	1:A:382:LEU:HD23	1.95	0.47
1:B:229:ASP:HB3	1:B:232:LYS:HE2	1.97	0.47
1:C:737:PRO:HG2	1:C:740:SER:HB2	1.97	0.47
1:D:451:GLY:HA2	1:D:461:ASN:O	2.14	0.47
1:B:752:LYS:HD3	1:C:483:LEU:HD22	1.97	0.46
1:C:531:PHE:O	1:C:534:ILE:HG12	2.14	0.46
1:B:41:LEU:HD12	1:B:41:LEU:H	1.79	0.46
1:B:186:LYS:NZ	1:D:435:HIS:O	2.40	0.46
1:B:789:LEU:HD12	1:B:789:LEU:H	1.80	0.46
1:A:787:LEU:HB2	1:D:522:ALA:HB2	1.96	0.46
1:B:400:ILE:HD13	1:B:450:TYR:CE1	2.50	0.46
1:B:751:LEU:HG	4:B:903:FWF:H31	1.97	0.46
1:C:124:GLU:OE2	1:C:154:LYS:NZ	2.48	0.46
2:D:901:KAI:HD12	2:D:901:KAI:HD2	1.62	0.46
1:B:163:VAL:HG13	1:B:198:LYS:HE3	1.98	0.46
1:D:485:ARG:O	1:D:489:ILE:HG12	2.16	0.46
1:B:176:ARG:NH2	1:D:439:LYS:HE3	2.30	0.46
1:A:62:SER:OG	1:A:66:ARG:NH2	2.49	0.46
1:C:31:MET:O	1:C:35:SER:HB2	2.16	0.45
1:B:796:PHE:O	1:B:799:LEU:HB3	2.17	0.45
1:C:263:LEU:HD21	1:C:268:TYR:CD2	2.52	0.45
1:C:529:ILE:HA	1:D:796:PHE:HE2	1.82	0.45
1:C:707:THR:HG21	1:C:732:TYR:HE2	1.82	0.45
1:B:480:THR:O	1:B:485:ARG:NH1	2.50	0.44
1:B:486:GLU:OE2	1:B:491:PHE:HB2	2.17	0.44
1:D:31:MET:HE1	1:D:41:LEU:HB2	1.98	0.44
1:B:660:ARG:HA	1:B:671:TRP:CE2	2.53	0.44
1:C:403:SER:HA	1:C:404:PRO:HA	1.76	0.44
1:C:597:SER:O	1:C:601:VAL:HG23	2.17	0.44
1:A:635:SER:OG	1:A:637:GLU:HG2	2.18	0.44
1:C:60:PHE:CE2	1:C:86:PHE:HB3	2.52	0.44
1:A:172:ASP:OD2	1:A:172:ASP:N	2.41	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:LYS:NZ	1:A:718:CYS:SG	2.91	0.44
1:C:398:THR:HG23	1:C:463:MET:HG3	1.98	0.44
1:C:502:ILE:HD13	1:C:639:LEU:HD12	1.99	0.44
1:C:716:LYS:HG3	1:C:717:PRO:HA	1.99	0.44
1:D:15:LEU:O	1:D:73:GLY:HA2	2.18	0.44
1:A:628:ARG:HD3	1:D:626:VAL:HB	2.00	0.44
1:C:647:TYR:HB3	1:C:701:ALA:HB3	2.00	0.44
1:B:737:PRO:HG2	1:B:740:SER:HB2	1.99	0.44
1:A:436:CYS:SG	1:A:745:PRO:HB2	2.58	0.44
1:D:186:LYS:HE3	1:D:186:LYS:HB3	1.82	0.44
1:B:96:THR:HA	1:B:97:PRO:HD3	1.87	0.44
1:C:34:PHE:CE2	1:C:288:GLN:HB2	2.52	0.44
1:B:297:LEU:HD13	1:B:304:ILE:HG21	2.00	0.43
1:B:635:SER:OG	1:B:636:ALA:N	2.50	0.43
1:C:795:VAL:HA	1:C:798:ILE:HG22	2.00	0.43
1:B:689:GLY:O	1:B:693:VAL:HG23	2.18	0.43
1:C:413:GLU:OE2	1:C:413:GLU:N	2.46	0.43
1:D:141:LEU:HD23	1:D:144:LEU:HD23	2.00	0.43
1:D:503:MET:HE3	1:D:704:LEU:HD21	2.00	0.43
1:D:112:ARG:HA	1:D:113:PRO:HD3	1.84	0.43
1:D:133:TYR:OH	1:D:143:THR:OG1	2.29	0.43
1:D:795:VAL:O	1:D:798:ILE:HG22	2.17	0.43
1:A:192:LEU:HD21	1:A:218:TYR:HD1	1.83	0.43
1:D:401:LEU:HD23	1:D:406:VAL:HG12	2.00	0.43
1:C:118:ALA:HA	1:C:372:TRP:CD1	2.53	0.43
1:C:474:ILE:HG13	1:C:736:THR:HG22	2.01	0.43
2:C:901:KAI:HD2	2:C:901:KAI:HD12	1.70	0.43
1:D:809:VAL:HA	1:D:812:ILE:HG12	2.00	0.43
1:A:136:ASP:HA	1:A:162:ASN:HD21	1.83	0.43
1:C:748:LEU:HA	1:C:751:LEU:HD12	2.01	0.43
1:A:794:GLY:HA2	1:A:797:TYR:HD1	1.83	0.43
1:B:600:ILE:H	1:B:600:ILE:HG12	1.60	0.43
1:B:751:LEU:HA	4:B:903:FWF:H34	2.01	0.43
1:D:631:SER:N	1:D:632:PRO:HD2	2.33	0.43
1:A:306:ARG:H	1:A:306:ARG:HE	1.67	0.43
1:C:522:ALA:HB3	1:C:525:ILE:HG13	1.99	0.43
1:D:188:ARG:N	1:D:215:GLY:O	2.42	0.43
1:C:539:VAL:O	1:C:543:VAL:HG23	2.19	0.43
1:C:719:ASP:OD2	1:C:719:ASP:N	2.52	0.43
1:D:21:ASP:HB3	1:D:269:PRO:HB2	2.00	0.43
1:B:306:ARG:HD3	1:B:321:TRP:CD2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:PRO:HB3	1:D:354:TYR:CG	2.54	0.43
1:A:711:TYR:O	1:A:715:ARG:HG2	2.19	0.42
1:A:810:ALA:HB2	1:D:597:SER:HB3	1.99	0.42
2:B:901:KAI:HD2	2:B:901:KAI:HD12	1.77	0.42
1:C:177:SER:HA	1:C:180:GLN:HG2	2.01	0.42
1:A:436:CYS:HB2	1:A:438:PHE:CE2	2.54	0.42
1:A:671:TRP:NE1	1:A:675:ARG:HD2	2.33	0.42
1:B:99:PHE:HA	1:B:100:PRO:HD3	1.88	0.42
1:B:194:CYS:HB3	1:B:198:LYS:HB3	2.01	0.42
1:B:245:ILE:HG23	1:B:246:VAL:HG23	2.01	0.42
1:C:489:ILE:HD12	1:C:735:ALA:HB1	2.01	0.42
1:D:507:PRO:CG	1:D:631:SER:HB2	2.48	0.42
1:A:693:VAL:O	1:A:696:SER:HB3	2.20	0.42
1:D:113:PRO:HG2	1:D:245:ILE:HD11	2.01	0.42
5:D:903:MES:H31	5:D:903:MES:H81	1.80	0.42
1:C:509:LYS:O	1:C:510:SER:HB3	2.20	0.42
1:D:196:ARG:NH1	1:D:229:ASP:O	2.52	0.42
1:B:394:THR:HG22	1:B:439:LYS:HG3	2.02	0.42
1:A:225:PHE:CD1	1:A:242:GLY:HA3	2.55	0.42
1:A:689:GLY:O	1:A:693:VAL:HG23	2.19	0.42
1:B:75:TYR:HE2	1:B:96:THR:HG21	1.85	0.42
1:B:197:ASP:N	1:B:197:ASP:OD2	2.52	0.42
1:B:289:VAL:HG13	1:B:334:VAL:HG11	2.01	0.42
1:B:610:LEU:HD11	1:C:613:ILE:HD12	2.02	0.42
1:C:362:LYS:HG3	1:C:367:ARG:HE	1.84	0.42
1:A:96:THR:HA	1:A:97:PRO:HD3	1.84	0.42
1:A:206:VAL:HG12	1:A:212:HIS:HB3	2.01	0.42
1:D:14:GLY:O	1:D:16:PHE:HD2	2.03	0.42
1:D:113:PRO:HB3	1:D:354:TYR:CD1	2.55	0.42
1:D:450:TYR:O	1:D:463:MET:N	2.52	0.42
1:C:744:THR:OG1	1:C:745:PRO:HD3	2.20	0.42
1:C:111:MET:HG3	1:C:286:ALA:HB2	2.02	0.42
1:D:177:SER:O	1:D:181:ASP:HB2	2.19	0.42
1:A:786:ALA:HB1	1:D:623:PHE:HZ	1.85	0.41
1:A:362:LYS:HG3	1:A:367:ARG:HE	1.85	0.41
1:A:619:ASN:ND2	1:B:787:LEU:HB2	2.35	0.41
1:D:460:TRP:NE1	1:D:488:VAL:HG11	2.34	0.41
1:A:604:VAL:HG21	1:B:802:GLY:HA3	2.02	0.41
1:B:138:ASP:OD2	1:B:138:ASP:N	2.52	0.41
1:B:234:GLN:NE2	1:B:363:THR:O	2.51	0.41
1:C:678:GLU:HA	1:C:679:PRO:C	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:GLY:HA3	1:D:44:HIS:O	2.21	0.41
1:D:428:LEU:O	1:D:432:ILE:HG12	2.20	0.41
1:B:539:VAL:HG11	1:C:803:LEU:HD22	2.02	0.41
1:B:539:VAL:HG21	1:C:803:LEU:HB3	2.02	0.41
1:C:133:TYR:CE1	1:C:135:TYR:HB3	2.56	0.41
1:D:330:ALA:O	1:D:334:VAL:HG23	2.19	0.41
1:C:608:PHE:HZ	1:D:796:PHE:CE2	2.38	0.41
1:B:400:ILE:HG21	1:B:450:TYR:HE1	1.84	0.41
1:B:608:PHE:HD1	1:C:795:VAL:HG12	1.86	0.41
1:A:101:THR:N	1:A:110:GLN:OE1	2.45	0.41
1:A:404:PRO:HD3	1:A:711:TYR:CG	2.56	0.41
1:A:628:ARG:HH11	1:D:626:VAL:HB	1.86	0.41
1:B:330:ALA:O	1:B:334:VAL:HG23	2.21	0.41
1:D:783:LYS:O	1:D:784:THR:OG1	2.35	0.41
1:B:352:ILE:O	1:B:353:ASN:HB3	2.21	0.41
1:A:87:CYS:SG	1:A:94:PHE:HB2	2.61	0.40
1:C:506:LYS:HA	1:C:507:PRO:HD3	1.86	0.40
1:C:86:PHE:HE1	1:D:54:PHE:HA	1.86	0.40
1:C:90:LEU:HA	1:C:320:PRO:HB3	2.03	0.40
1:C:536:VAL:HG22	1:D:803:LEU:HD21	2.03	0.40
1:C:532:ALA:HB1	1:D:799:LEU:HD23	2.04	0.40
1:A:102:ASP:OD2	1:A:102:ASP:N	2.42	0.40
1:B:626:VAL:HG23	1:C:628:ARG:HH11	1.86	0.40
1:C:96:THR:HA	1:C:97:PRO:HD3	1.87	0.40
1:B:362:LYS:HG3	1:B:367:ARG:NE	2.36	0.40
1:C:170:LYS:HE2	1:C:173:GLU:HG3	2.02	0.40
1:D:10:ILE:HA	1:D:69:TYR:CE2	2.57	0.40
1:D:186:LYS:O	1:D:186:LYS:HG2	2.21	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	733/824 (89%)	722 (98%)	11 (2%)	0	100	100
1	B	728/824 (88%)	708 (97%)	20 (3%)	0	100	100
1	C	749/824 (91%)	728 (97%)	21 (3%)	0	100	100
1	D	734/824 (89%)	708 (96%)	26 (4%)	0	100	100
All	All	2944/3296 (89%)	2866 (97%)	78 (3%)	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	618/703 (88%)	589 (95%)	29 (5%)	26	57
1	B	622/703 (88%)	595 (96%)	27 (4%)	29	59
1	C	626/703 (89%)	598 (96%)	28 (4%)	27	58
1	D	614/703 (87%)	593 (97%)	21 (3%)	37	65
All	All	2480/2812 (88%)	2375 (96%)	105 (4%)	30	60

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	PHE
1	A	50	VAL
1	A	58	ASN
1	A	96	THR
1	A	162	ASN
1	A	169	ASP
1	A	172	ASP
1	A	181	ASP
1	A	192	LEU
1	A	209	ILE
1	A	250	ASP
1	A	291	THR
1	A	298	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	306	ARG
1	A	316	ASN
1	A	382	LEU
1	A	393	LYS
1	A	413	GLU
1	A	490	ASP
1	A	498	LEU
1	A	599	ARG
1	A	631	SER
1	A	639	LEU
1	A	644	GLU
1	A	672	THR
1	A	686	THR
1	A	744	THR
1	A	760	ASP
1	A	807	MET
1	B	23	GLU
1	B	102	ASP
1	B	138	ASP
1	B	197	ASP
1	B	259	ARG
1	B	272	HIS
1	B	301	ARG
1	B	305	SER
1	B	342	ASN
1	B	390	LEU
1	B	439	LYS
1	B	441	LYS
1	B	458	LYS
1	B	599	ARG
1	B	600	ILE
1	B	607	PHE
1	B	626	VAL
1	B	642	GLN
1	B	644	GLU
1	B	672	THR
1	B	678	GLU
1	B	742	LEU
1	B	744	THR
1	B	751	LEU
1	B	770	LYS
1	B	789	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	816	TYR
1	C	18	ARG
1	C	58	ASN
1	C	77	LYS
1	C	91	HIS
1	C	110	GLN
1	C	175	TYR
1	C	187	GLU
1	C	201	ASP
1	C	273	THR
1	C	299	LYS
1	C	303	GLU
1	C	304	ILE
1	C	384	GLU
1	C	416	GLU
1	C	463	MET
1	C	467	LEU
1	C	480	THR
1	C	484	VAL
1	C	498	LEU
1	C	511	LYS
1	C	626	VAL
1	C	629	MET
1	C	642	GLN
1	C	661	ARG
1	C	699	LYS
1	C	709	ASN
1	C	718	CYS
1	C	719	ASP
1	D	40	ARG
1	D	46	ASP
1	D	165	ASN
1	D	179	PHE
1	D	182	LEU
1	D	184	LEU
1	D	186	LYS
1	D	197	ASP
1	D	199	VAL
1	D	217	HIS
1	D	382	LEU
1	D	413	GLU
1	D	463	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	490	ASP
1	D	498	LEU
1	D	619	ASN
1	D	645	ILE
1	D	663	LYS
1	D	684	ARG
1	D	722	LYS
1	D	744	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	ASN
1	C	642	GLN
1	C	709	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 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	NAG	A	902	1	14,14,15	0.37	0	17,19,21	0.41	0
4	FWF	B	903	-	31,33,33	1.43	2 (6%)	38,48,48	3.30	5 (13%)
2	KAI	C	901	-	13,15,15	1.06	0	14,21,21	0.91	0
4	FWF	D	904	-	31,33,33	1.45	2 (6%)	38,48,48	3.36	5 (13%)
3	NAG	B	902	1	14,14,15	0.38	0	17,19,21	0.76	0
5	MES	D	903	-	12,12,12	2.13	1 (8%)	14,16,16	6.69	5 (35%)
2	KAI	A	901	-	13,15,15	1.01	0	14,21,21	0.96	0
3	NAG	D	902	1	14,14,15	0.30	0	17,19,21	0.45	0
2	KAI	B	901	-	13,15,15	1.09	0	14,21,21	0.86	0
3	NAG	C	902	1	14,14,15	0.90	1 (7%)	17,19,21	1.69	3 (17%)
2	KAI	D	901	-	13,15,15	0.98	0	14,21,21	0.95	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	NAG	A	902	1	-	1/6/23/26	0/1/1/1
4	FWF	B	903	-	-	10/32/36/36	0/2/2/2
2	KAI	C	901	-	-	4/12/25/25	0/1/1/1
4	FWF	D	904	-	-	3/32/36/36	0/2/2/2
3	NAG	B	902	1	-	0/6/23/26	0/1/1/1
5	MES	D	903	-	-	3/6/14/14	0/1/1/1
2	KAI	A	901	-	-	5/12/25/25	0/1/1/1
3	NAG	D	902	1	-	1/6/23/26	0/1/1/1
2	KAI	B	901	-	-	3/12/25/25	0/1/1/1
3	NAG	C	902	1	-	4/6/23/26	0/1/1/1
2	KAI	D	901	-	-	0/12/25/25	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	903	MES	C8-S	-6.97	1.67	1.77
4	D	904	FWF	C19-S1	-5.53	1.66	1.78
4	D	904	FWF	C20-S2	-5.52	1.66	1.78
4	B	903	FWF	C20-S2	-5.41	1.66	1.78
4	B	903	FWF	C19-S1	-5.35	1.67	1.78
3	C	902	NAG	C1-C2	2.58	1.56	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	904	FWF	O2-S1-O1	-14.72	108.20	119.24
4	B	903	FWF	O4-S2-O3	-13.58	109.05	119.24
4	B	903	FWF	O2-S1-O1	-13.25	109.30	119.24
5	D	903	MES	O3S-S-C8	-13.22	84.38	105.77
4	D	904	FWF	O4-S2-O3	-12.75	109.68	119.24
5	D	903	MES	O3S-S-O2S	-11.32	83.62	111.27
5	D	903	MES	O3S-S-O1S	-10.99	84.42	111.27
5	D	903	MES	O2S-S-C8	10.03	119.00	106.92
5	D	903	MES	O1S-S-C8	9.78	118.69	106.92
3	C	902	NAG	O3-C3-C2	-4.48	100.20	109.47
3	C	902	NAG	O4-C4-C3	3.22	117.80	110.35
4	B	903	FWF	C11-C10-C4	-3.09	116.01	121.36
4	D	904	FWF	O1-S1-N2	2.97	111.34	107.76
3	C	902	NAG	O5-C5-C4	-2.59	104.52	110.83
4	D	904	FWF	C3-C4-C10	-2.48	117.06	121.36
4	B	903	FWF	O2-S1-N2	2.30	110.53	107.76
4	B	903	FWF	O4-S2-N1	2.27	110.50	107.76
4	D	904	FWF	O4-S2-N1	2.04	110.22	107.76

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	901	KAI	CA-CB-CB1-CG1
2	C	901	KAI	CA-CB-CB1-CG1
2	C	901	KAI	CG-CB-CB1-CG1
4	B	903	FWF	C18-N2-S1-O2
4	B	903	FWF	C21-C19-S1-O1
4	B	903	FWF	C22-C19-S1-O1
4	B	903	FWF	C21-C19-S1-O2
4	B	903	FWF	C22-C19-S1-O2
4	D	904	FWF	C18-N2-S1-O1
5	D	903	MES	N4-C7-C8-S
3	C	902	NAG	O5-C5-C6-O6
4	B	903	FWF	C11-C10-C4-C3
4	B	903	FWF	C9-C10-C4-C3
4	B	903	FWF	C11-C10-C4-C5
4	B	903	FWF	C9-C10-C4-C5
2	A	901	KAI	O-C-CA-N
2	A	901	KAI	OXT-C-CA-N
5	D	903	MES	C7-C8-S-O3S

Continued on next page...

Continued from previous page...

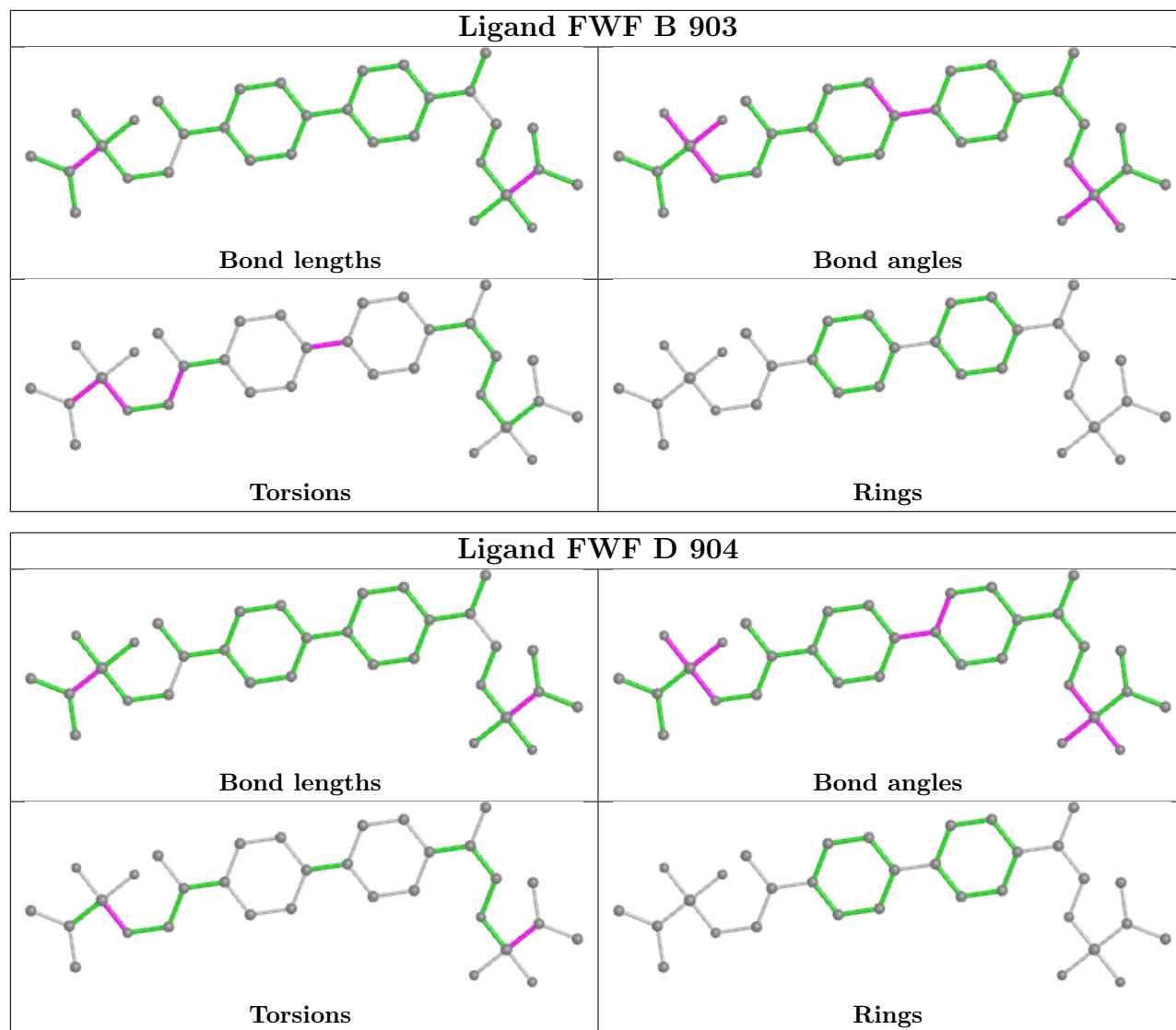
Mol	Chain	Res	Type	Atoms
3	D	902	NAG	O5-C5-C6-O6
3	A	902	NAG	O5-C5-C6-O6
3	C	902	NAG	C1-C2-N2-C7
4	B	903	FWF	C17-C13-C18-N2
4	D	904	FWF	C24-C20-S2-O4
2	A	901	KAI	CA-CB-CB1-CG1
5	D	903	MES	C7-C8-S-O1S
3	C	902	NAG	C4-C5-C6-O6
2	B	901	KAI	CB-CB1-CG1-OD1
2	B	901	KAI	CB-CB1-CG1-OD2
2	C	901	KAI	CB-CB1-CG1-OD1
2	A	901	KAI	CB-CB1-CG1-OD1
2	C	901	KAI	CB-CB1-CG1-OD2
3	C	902	NAG	C3-C2-N2-C7
4	D	904	FWF	C23-C20-S2-O3
2	A	901	KAI	CB-CB1-CG1-OD2

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	903	FWF	2	0
2	C	901	KAI	2	0
4	D	904	FWF	2	0
5	D	903	MES	1	0
3	D	902	NAG	1	0
2	B	901	KAI	3	0
3	C	902	NAG	1	0
2	D	901	KAI	1	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, 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	743/824 (90%)	-0.01	29 (3%) 39 37	41, 100, 169, 229	0
1	B	738/824 (89%)	-0.09	26 (3%) 44 42	41, 87, 180, 200	0
1	C	755/824 (91%)	-0.05	43 (5%) 23 23	38, 86, 191, 233	0
1	D	744/824 (90%)	-0.03	36 (4%) 30 28	42, 103, 171, 217	0
All	All	2980/3296 (90%)	-0.04	134 (4%) 33 32	38, 95, 180, 233	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	792	VAL	8.1
1	D	307	ARG	8.0
1	C	793	ALA	7.3
1	C	794	GLY	7.2
1	C	797	TYR	7.1
1	A	310	ALA	6.9
1	B	510	SER	5.9
1	B	786	ALA	5.8
1	C	383	THR	5.8
1	A	309	ASN	5.7
1	A	631	SER	5.3
1	C	9	SER	5.3
1	C	634	GLU	5.2
1	D	35	SER	4.9
1	A	516	SER	4.8
1	D	510	SER	4.8
1	A	311	GLY	4.6
1	C	510	SER	4.6
1	B	792	VAL	4.5
1	C	633	ILE	4.3
1	D	309	ASN	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	391	GLU	4.2
1	C	812	ILE	4.2
1	C	631	SER	4.1
1	B	806	ALA	4.1
1	C	303	GLU	4.1
1	D	515	PHE	4.1
1	B	529	ILE	4.0
1	A	212	HIS	3.9
1	B	526	TRP	3.9
1	C	301	ARG	3.9
1	C	795	VAL	3.9
1	A	629	MET	3.9
1	A	542	LEU	3.8
1	D	544	SER	3.8
1	A	308	GLY	3.7
1	C	519	ASP	3.7
1	D	308	GLY	3.6
1	B	788	SER	3.6
1	C	302	ILE	3.5
1	D	811	LEU	3.5
1	B	514	VAL	3.5
1	B	310	ALA	3.5
1	C	390	LEU	3.5
1	C	778	SER	3.5
1	A	307	ARG	3.5
1	A	797	TYR	3.4
1	D	784	THR	3.4
1	A	508	GLN	3.3
1	D	608	PHE	3.3
1	C	789	LEU	3.3
1	C	814	PHE	3.3
1	C	39	PHE	3.3
1	D	629	MET	3.2
1	A	627	GLU	3.1
1	D	512	PRO	3.1
1	A	632	PRO	3.1
1	A	798	ILE	3.1
1	C	516	SER	3.1
1	D	814	PHE	3.1
1	D	626	VAL	3.0
1	C	169	ASP	3.0
1	D	346	ASP	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	796	PHE	2.9
1	B	523	TYR	2.9
1	B	385	ASP	2.9
1	B	383	THR	2.9
1	A	301	ARG	2.8
1	C	456	ASP	2.8
1	D	815	ALA	2.8
1	C	597	SER	2.8
1	A	644	GLU	2.8
1	A	799	LEU	2.8
1	A	8	ASN	2.7
1	C	791	ASN	2.7
1	D	111	MET	2.7
1	C	635	SER	2.7
1	D	390	LEU	2.7
1	C	813	GLU	2.7
1	C	391	GLU	2.6
1	D	516	SER	2.6
1	D	529	ILE	2.6
1	A	536	VAL	2.5
1	B	309	ASN	2.5
1	B	521	LEU	2.5
1	C	810	ALA	2.5
1	D	509	LYS	2.5
1	B	525	ILE	2.5
1	B	524	GLU	2.4
1	D	513	GLY	2.4
1	D	625	THR	2.4
1	B	543	VAL	2.4
1	C	305	SER	2.4
1	A	541	PHE	2.4
1	C	798	ILE	2.4
1	C	455	ALA	2.4
1	D	632	PRO	2.4
1	C	307	ARG	2.3
1	D	808	LEU	2.3
1	D	109	ILE	2.3
1	C	538	VAL	2.3
1	B	793	ALA	2.3
1	A	312	ASP	2.3
1	C	790	SER	2.3
1	C	594	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	345	PHE	2.3
1	C	511	LYS	2.3
1	A	236	GLY	2.3
1	B	509	LYS	2.2
1	A	300	GLN	2.2
1	B	527	MET	2.2
1	A	364	ASN	2.2
1	C	509	LYS	2.2
1	B	531	PHE	2.2
1	B	60	PHE	2.2
1	C	515	PHE	2.2
1	A	70	ALA	2.2
1	B	508	GLN	2.2
1	B	311	GLY	2.2
1	B	512	PRO	2.1
1	D	167	ASN	2.1
1	A	602	ALA	2.1
1	D	812	ILE	2.1
1	D	520	PRO	2.1
1	B	807	MET	2.1
1	D	525	ILE	2.1
1	A	598	ALA	2.1
1	D	630	VAL	2.1
1	D	230	LEU	2.1
1	C	298	ARG	2.1
1	A	785	SER	2.0
1	D	179	PHE	2.0
1	C	300	GLN	2.0
1	D	521	LEU	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](#)

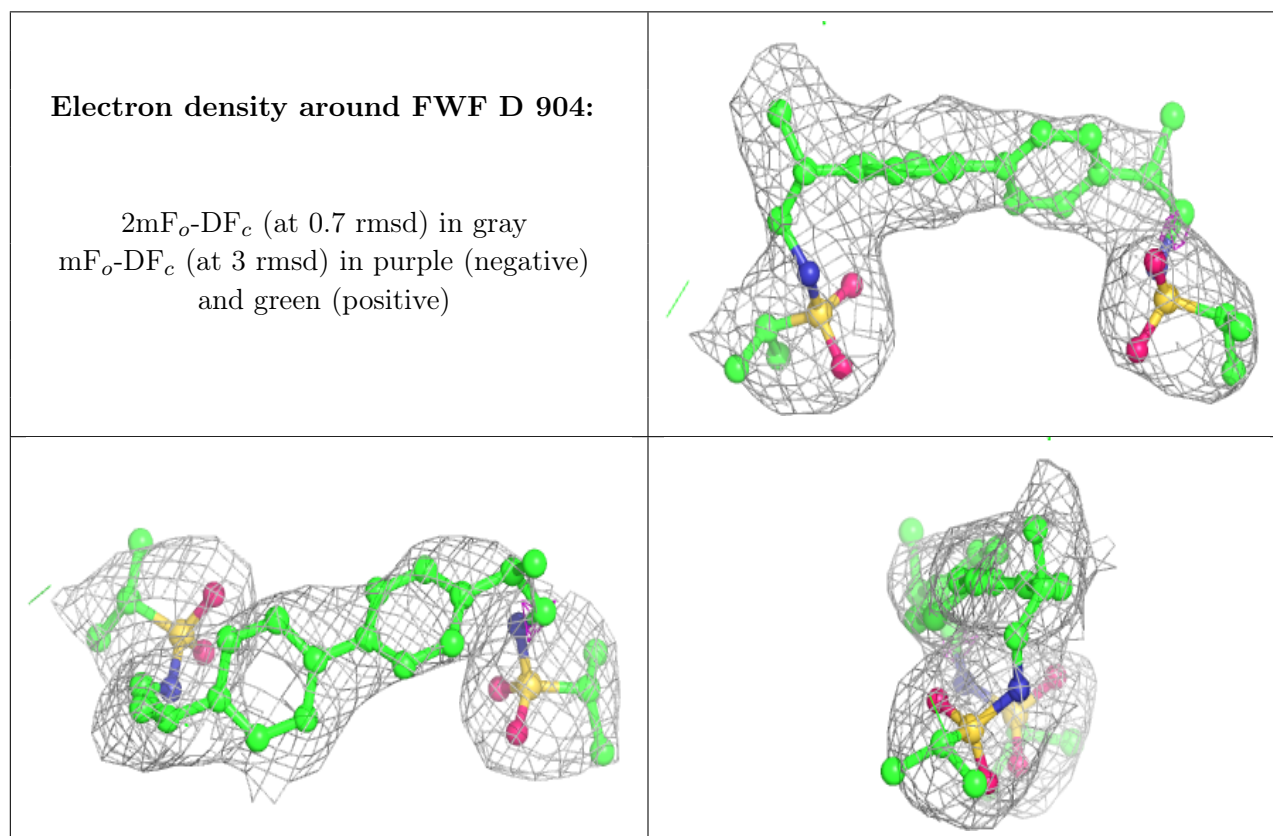
There are no monosaccharides in this entry.

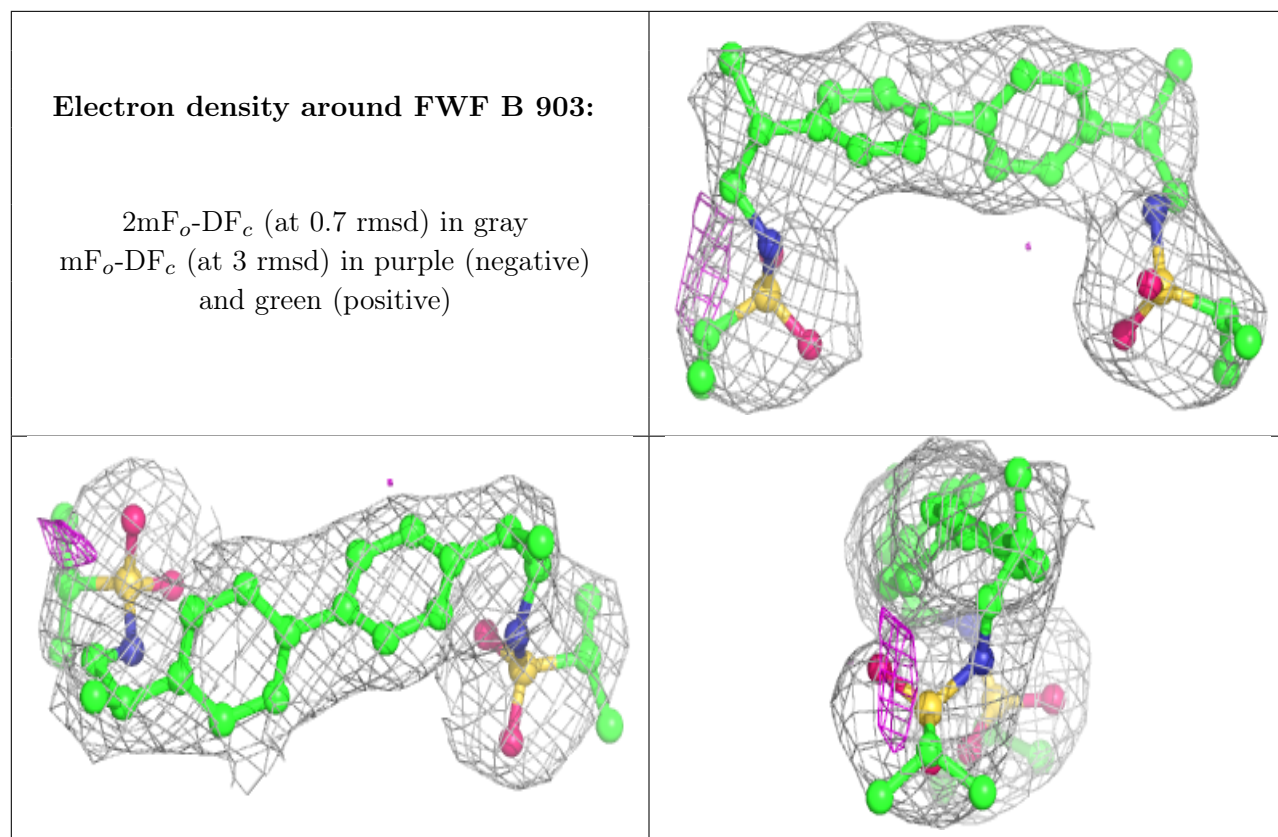
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
3	NAG	D	902	14/15	0.73	0.52	154,174,190,190	0
3	NAG	B	902	14/15	0.80	0.38	128,138,162,170	0
2	KAI	B	901	15/15	0.87	0.34	55,77,92,101	0
2	KAI	D	901	15/15	0.87	0.40	71,90,118,121	0
2	KAI	A	901	15/15	0.90	0.41	53,90,108,117	0
3	NAG	A	902	14/15	0.90	0.26	48,89,106,115	0
3	NAG	C	902	14/15	0.93	0.26	60,79,105,108	0
5	MES	D	903	12/12	0.94	0.20	70,96,101,103	0
4	FWF	D	904	32/32	0.95	0.28	56,76,92,101	0
2	KAI	C	901	15/15	0.95	0.31	45,58,77,78	0
4	FWF	B	903	32/32	0.97	0.24	43,58,75,78	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.