



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:36 AM UTC

PDB ID : 4U1X / pdb_00004u1x
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

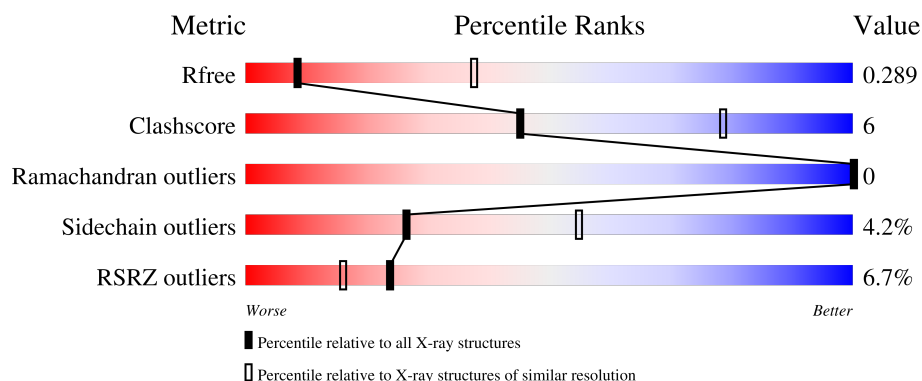
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	6% 75% 14% 10%
1	B	824	4% 75% 13% 10%
1	C	824	8% 73% 18% 8%
1	D	824	7% 74% 15% 10%

2 Entry composition

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
1	A	743	Total	C	N	O	S	0	0	0
			5796	3719	964	1087	26			
1	B	738	Total	C	N	O	S	0	0	0
			5803	3731	961	1085	26			
1	C	755	Total	C	N	O	S	0	0	0
			5882	3778	977	1101	26			
1	D	744	Total	C	N	O	S	0	0	0
			5778	3719	954	1079	26			

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

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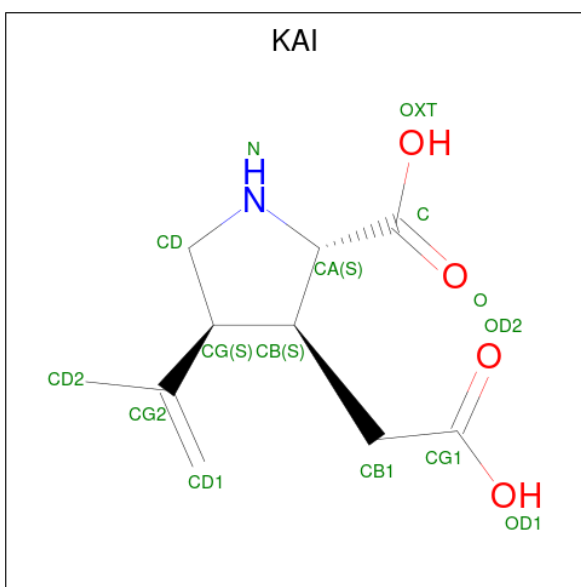
Chain	Residue	Modelled	Actual	Comment	Reference
A	830	PRO	-	expression tag	UNP P19491
A	831	ARG	-	expression tag	UNP P19491
B	239	GLU	ASN	engineered mutation	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	?	-	GLY	deletion	UNP P19491
B	385	ASP	ASN	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
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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
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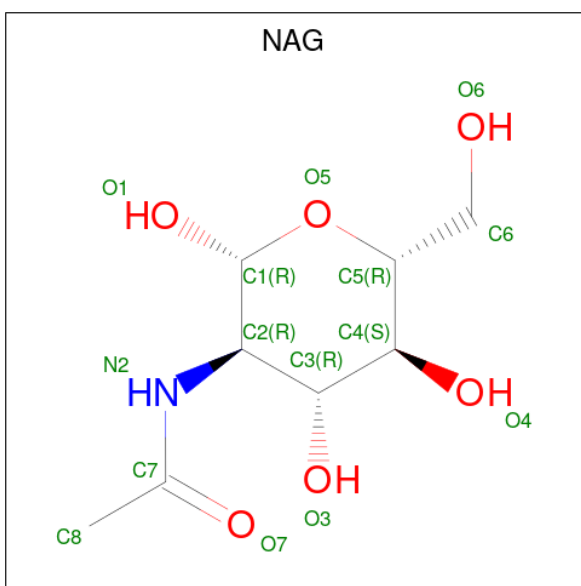
Chain	Residue	Modelled	Actual	Comment	Reference
C	815	ALA	CYS	engineered mutation	UNP P19491
C	827	GLY	-	expression tag	UNP P19491
C	828	LEU	-	expression tag	UNP P19491
C	829	VAL	-	expression tag	UNP P19491
C	830	PRO	-	expression tag	UNP P19491
C	831	ARG	-	expression tag	UNP P19491
D	239	GLU	ASN	engineered 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 (CCD ID: KAI) (formula: C₁₀H₁₅NO₄).



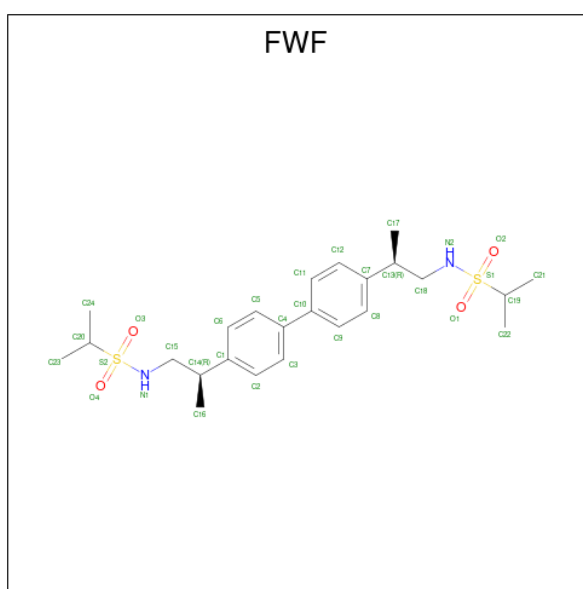
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	10	1	4		
2	B	1	Total	C	N	O	0	0
			15	10	1	4		
2	C	1	Total	C	N	O	0	0
			15	10	1	4		
2	D	1	Total	C	N	O	0	0
			15	10	1	4		

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



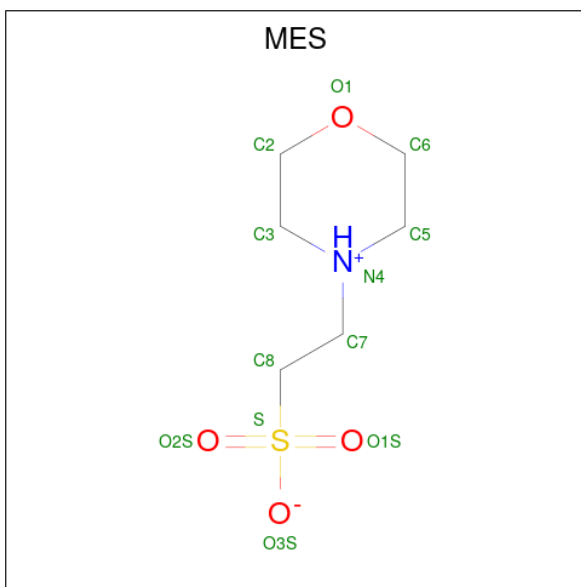
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is N,N'-[biphenyl-4,4'-diyl]di(2R)propane-2,1-diyl]dipropane-2-sulfonamide (CCD ID: FWF) (formula: $C_{24}H_{36}N_2O_4S_2$).



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 (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).

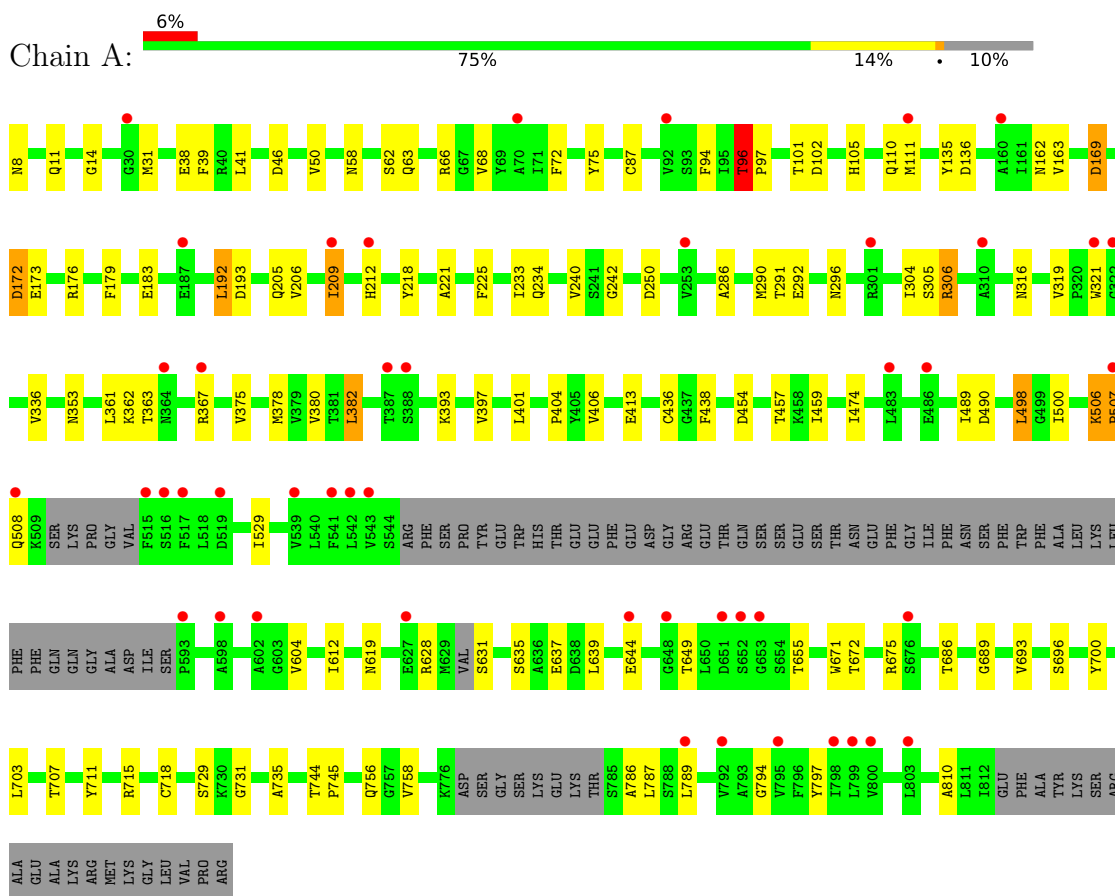


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	D	1	12	6	1	4	1	0	0

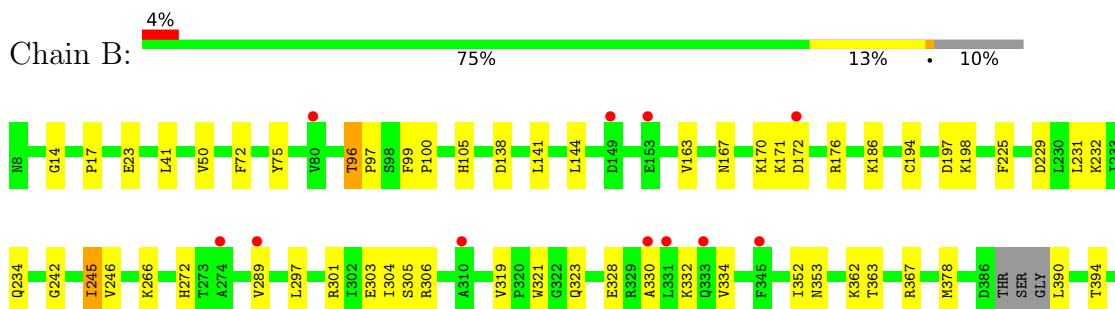
3 Residue-property plots

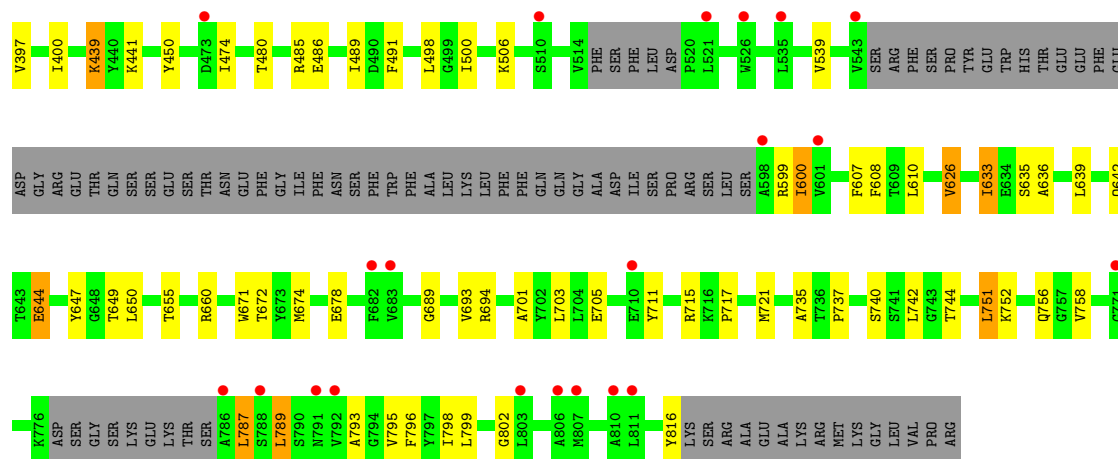
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

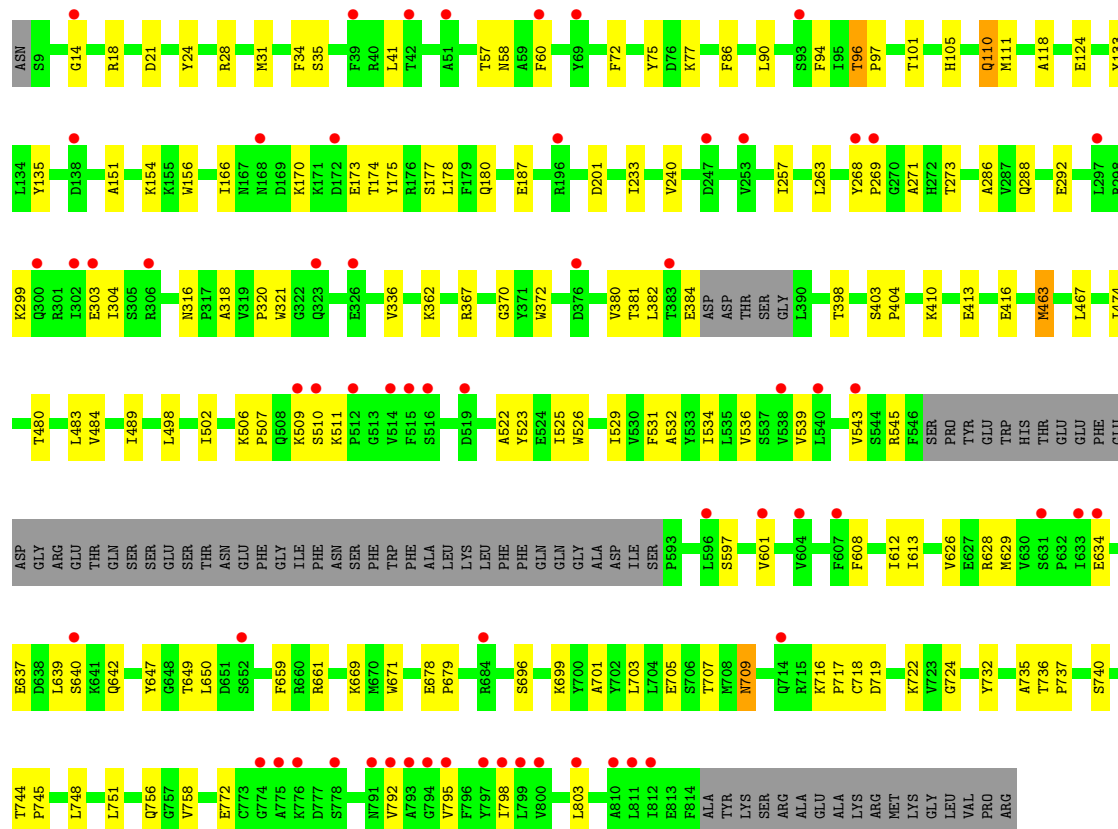
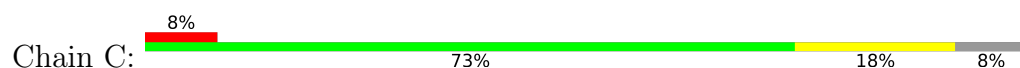


• Molecule 1: Glutamate receptor 2

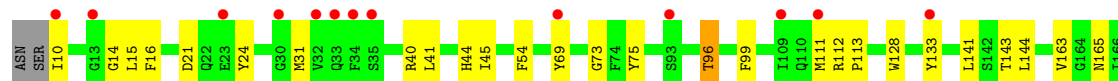
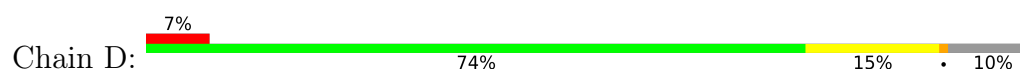


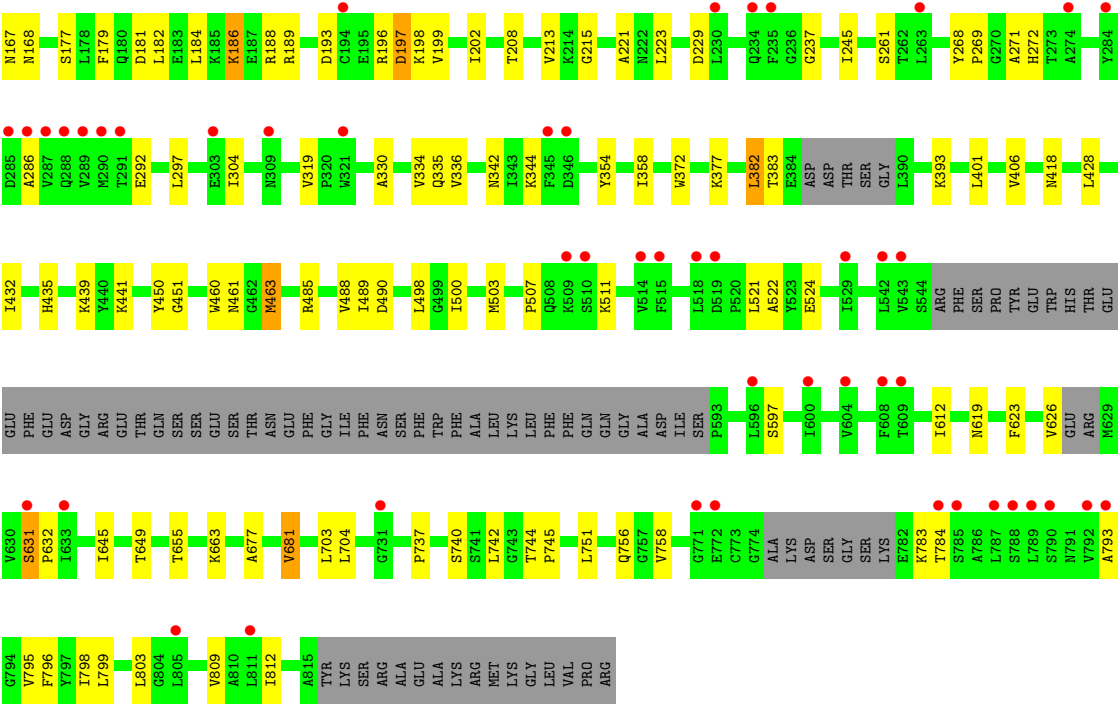


• Molecule 1: Glutamate receptor 2



• 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 29.79 – 3.30	Depositor EDS
% Data completeness (in resolution range)	68.4 (29.79-3.30) 68.3 (29.79-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.33Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.242 , 0.289 0.245 , 0.289	Depositor DCC
R_{free} test set	2773 reflections (3.24%)	wwPDB-VP
Wilson B-factor (Å ²)	75.8	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 20.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	23451	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage'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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FWF, KAI, NAG, MES

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	0.28	0/5911	0.74	7/7997 (0.1%)
1	B	0.28	0/5920	0.74	6/8005 (0.1%)
1	C	0.28	0/6002	0.74	5/8121 (0.1%)
1	D	0.30	0/5895	0.76	8/7978 (0.1%)
All	All	0.29	0/23728	0.74	26/32101 (0.1%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	HIS	CA-C-N	7.30	127.46	120.31
1	A	105	HIS	C-N-CA	7.30	127.46	120.31
1	A	96	THR	CA-C-N	7.07	126.70	119.56
1	A	96	THR	C-N-CA	7.07	126.70	119.56
1	C	96	THR	CA-C-N	6.81	126.44	119.56
1	C	96	THR	C-N-CA	6.81	126.44	119.56
1	C	105	HIS	CA-C-N	6.54	126.72	120.31
1	C	105	HIS	C-N-CA	6.54	126.72	120.31
1	B	96	THR	CA-C-N	6.43	126.06	119.56
1	B	96	THR	C-N-CA	6.43	126.06	119.56
1	D	167	ASN	N-CA-C	6.36	117.91	110.97
1	D	96	THR	CA-C-N	6.20	125.83	119.56
1	D	96	THR	C-N-CA	6.20	125.83	119.56
1	B	105	HIS	CA-C-N	6.17	126.36	120.31
1	B	105	HIS	C-N-CA	6.17	126.36	120.31
1	D	511	LYS	CA-C-N	6.12	125.52	118.85
1	D	511	LYS	C-N-CA	6.12	125.52	118.85
1	A	506	LYS	CA-C-N	5.88	125.85	120.03
1	A	506	LYS	C-N-CA	5.88	125.85	120.03
1	C	545	ARG	CB-CA-C	-5.75	109.96	116.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	377	LYS	CB-CA-C	-5.49	110.22	116.54
1	D	237	GLY	N-CA-C	-5.46	107.24	115.32
1	A	507	PRO	CA-C-O	-5.42	115.14	122.08
1	B	171	LYS	CB-CA-C	-5.29	110.04	117.23
1	B	644	GLU	N-CA-C	5.21	116.65	110.97
1	D	631	SER	N-CA-C	5.14	120.46	113.16

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	5796	0	5761	68	0
1	B	5803	0	5800	73	0
1	C	5882	0	5848	78	0
1	D	5778	0	5748	80	0
2	A	15	0	13	0	0
2	B	15	0	13	3	0
2	C	15	0	13	3	0
2	D	15	0	13	1	0
3	A	14	0	13	0	0
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	277	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 (277) 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:D:31:MET:HE1	1:D:41:LEU:HB2	1.83	0.60
1:A:46:ASP:OD2	1:A:63:GLN:NE2	2.35	0.59
1:B:506:LYS:HG2	1:B:721:MET:HE3	1.83	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:TYR:HH	1:D:143:THR:HG1	1.54	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: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:A:31:MET:HE1	1:A:41:LEU:HB2	1.88	0.54
1:C:380:VAL:HB	1:C:382:LEU:HG	1.89	0.54
1:D:111:MET:HE3	1:D:286:ALA:HA	1.90	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:B:649:THR:HG23	1:B:674:MET:HE1	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
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:B:186:LYS:NZ	1:D:435:HIS:O	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:111:MET:HE3	1:A:286:ALA:HA	1.93	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:321:TRP:H	1:B:321:TRP:CD1	2.29	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:D:128:TRP:CD1	1:D:189:ARG:HE	2.31	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:A:14:GLY:HA2	1:A:72:PHE:O	2.13	0.48
1:A:321:TRP:H	1:A:321:TRP:CD1	2.31	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:678:GLU:HA	1:C:679:PRO:C	2.41	0.45
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:705:GLU:CD	2:C:901:KAI:HB12	2.41	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:742:LEU:C	1:D:745:PRO:HD2	2.43	0.44
1:B:266:LYS:NZ	1:D:21:ASP:OD1	2.47	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: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:503:MET:HE3	1:D:704:LEU:HD21	2.00	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:D:21:ASP:HB3	1:D:269:PRO:HB2	2.00	0.43
1:D:335:GLN:CD	1:D:344:LYS:HE2	2.43	0.43
1:B:306:ARG:HD3	1:B:321:TRP:CD2	2.54	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:719:ASP:OD2	1:C:719:ASP:N	2.52	0.42
1:D:507:PRO:CG	1:D:631:SER:HB2	2.48	0.42
1:A:378:MET:HE3	1:A:378:MET:HB2	1.94	0.42
1:A:693:VAL:O	1:A:696:SER:HB3	2.20	0.42
1:C:321:TRP:H	1:C:321:TRP:CD1	2.37	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:C:31:MET:HE1	1:C:41:LEU:HB2	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:C:696:SER:O	1:C:696:SER:OG	2.38	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

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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:D:450:TYR:HA	1:D:463:MET:HE2	2.03	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:B:378:MET:HE3	1:B:378:MET:HB2	1.96	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 ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 ⓘ

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%)	23	52
1	B	622/703 (88%)	597 (96%)	25 (4%)	28	56
1	C	626/703 (89%)	594 (95%)	32 (5%)	21	50
1	D	614/703 (87%)	595 (97%)	19 (3%)	35	60
All	All	2480/2812 (88%)	2375 (96%)	105 (4%)	26	55

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	163	VAL
1	A	169	ASP
1	A	172	ASP
1	A	192	LEU
1	A	209	ILE
1	A	250	ASP

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Mol	Chain	Res	Type
1	A	291	THR
1	A	306	ARG
1	A	316	ASN
1	A	319	VAL
1	A	353	ASN
1	A	375	VAL
1	A	382	LEU
1	A	393	LYS
1	A	413	GLU
1	A	490	ASP
1	A	498	LEU
1	A	529	ILE
1	A	612	ILE
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	B	23	GLU
1	B	172	ASP
1	B	245	ILE
1	B	272	HIS
1	B	301	ARG
1	B	305	SER
1	B	319	VAL
1	B	390	LEU
1	B	439	LYS
1	B	441	LYS
1	B	599	ARG
1	B	600	ILE
1	B	607	PHE
1	B	626	VAL
1	B	633	ILE
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	787	LEU

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Mol	Chain	Res	Type
1	B	789	LEU
1	B	816	TYR
1	C	18	ARG
1	C	58	ASN
1	C	77	LYS
1	C	110	GLN
1	C	175	TYR
1	C	178	LEU
1	C	187	GLU
1	C	201	ASP
1	C	257	ILE
1	C	273	THR
1	C	299	LYS
1	C	303	GLU
1	C	304	ILE
1	C	384	GLU
1	C	410	LYS
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	612	ILE
1	C	626	VAL
1	C	629	MET
1	C	637	GLU
1	C	642	GLN
1	C	661	ARG
1	C	699	LYS
1	C	709	ASN
1	C	718	CYS
1	C	792	VAL
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	213	VAL

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Mol	Chain	Res	Type
1	D	319	VAL
1	D	382	LEU
1	D	463	MET
1	D	490	ASP
1	D	498	LEU
1	D	612	ILE
1	D	619	ASN
1	D	645	ILE
1	D	663	LYS
1	D	681	VAL
1	D	744	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	157	GLN
1	A	162	ASN
1	A	619	ASN
1	B	145	GLN
1	B	335	GLN
1	C	58	ASN
1	C	244	GLN
1	C	642	GLN
1	C	709	ASN
1	C	791	ASN
1	D	58	ASN
1	D	392	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

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$
4	FWF	D	904	-	31,33,33	0.40	0	40,48,48	1.93	5 (12%)
5	MES	D	903	-	12,12,12	2.18	1 (8%)	15,16,16	5.76	5 (33%)
4	FWF	B	903	-	31,33,33	0.44	0	40,48,48	1.92	5 (12%)
3	NAG	A	902	1	14,14,15	0.37	0	17,19,21	0.42	0
2	KAI	B	901	-	13,15,15	1.13	0	12,21,21	1.12	1 (8%)
2	KAI	A	901	-	13,15,15	1.04	0	12,21,21	1.11	0
3	NAG	C	902	1	14,14,15	0.94	1 (7%)	17,19,21	1.69	4 (23%)
2	KAI	C	901	-	13,15,15	1.09	0	12,21,21	1.16	1 (8%)
2	KAI	D	901	-	13,15,15	1.01	0	12,21,21	1.09	0
3	NAG	B	902	1	14,14,15	0.37	0	17,19,21	0.78	0
3	NAG	D	902	1	14,14,15	0.32	0	17,19,21	0.47	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
4	FWF	D	904	-	-	2/32/36/36	0/2/2/2
5	MES	D	903	-	-	3/6/14/14	0/1/1/1
4	FWF	B	903	-	-	10/32/36/36	0/2/2/2
3	NAG	A	902	1	-	1/6/23/26	0/1/1/1
2	KAI	B	901	-	-	3/12/25/25	0/1/1/1
2	KAI	A	901	-	-	5/12/25/25	0/1/1/1
3	NAG	C	902	1	-	3/6/23/26	0/1/1/1
2	KAI	C	901	-	-	4/12/25/25	0/1/1/1
2	KAI	D	901	-	-	1/12/25/25	0/1/1/1
3	NAG	B	902	1	-	0/6/23/26	0/1/1/1
3	NAG	D	902	1	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	903	MES	C8-S	-7.12	1.67	1.77
3	C	902	NAG	C1-C2	2.83	1.56	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	903	MES	O3S-S-O2S	-11.11	83.62	111.40
5	D	903	MES	O3S-S-C8	-11.05	84.38	106.00
5	D	903	MES	O3S-S-O1S	-10.78	84.42	111.40
5	D	903	MES	O2S-S-C8	8.12	119.00	106.73
5	D	903	MES	O1S-S-C8	7.92	118.69	106.73
4	D	904	FWF	O2-S1-O1	-7.32	108.20	118.88
4	B	903	FWF	O4-S2-O3	-6.73	109.05	118.88
4	B	903	FWF	O2-S1-O1	-6.56	109.30	118.88
4	D	904	FWF	O4-S2-O3	-6.30	109.68	118.88
3	C	902	NAG	O3-C3-C2	-4.43	100.20	109.40
4	D	904	FWF	O1-S1-N2	3.17	111.34	107.65
3	C	902	NAG	O4-C4-C3	3.15	117.80	110.38
4	B	903	FWF	C11-C10-C4	-3.04	116.01	121.25
3	C	902	NAG	O5-C5-C4	-2.59	104.52	110.83
4	B	903	FWF	O2-S1-N2	2.47	110.53	107.65
4	B	903	FWF	O4-S2-N1	2.44	110.50	107.65
4	D	904	FWF	C3-C4-C10	-2.43	117.06	121.25
2	B	901	KAI	CB-CA-C	-2.37	109.22	113.98
4	D	904	FWF	O4-S2-N1	2.21	110.22	107.65
2	C	901	KAI	CB-CA-C	-2.11	109.74	113.98
3	C	902	NAG	C1-C2-N2	2.11	113.76	110.43

There are no chirality outliers.

All (33) 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	C24-C20-S2-O4

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Mol	Chain	Res	Type	Atoms
4	D	904	FWF	C18-N2-S1-O1
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
3	D	902	NAG	O5-C5-C6-O6
3	A	902	NAG	O5-C5-C6-O6
5	D	903	MES	C7-C8-S-O1S
5	D	903	MES	N4-C7-C8-S
2	A	901	KAI	CA-CB-CB1-CG1
3	C	902	NAG	C4-C5-C6-O6
4	B	903	FWF	C17-C13-C18-N2
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	C	901	KAI	CB-CB1-CG1-OD2
3	C	902	NAG	C3-C2-N2-C7
2	A	901	KAI	CB-CB1-CG1-OD1
2	A	901	KAI	CB-CB1-CG1-OD2
2	D	901	KAI	CB-CB1-CG1-OD1

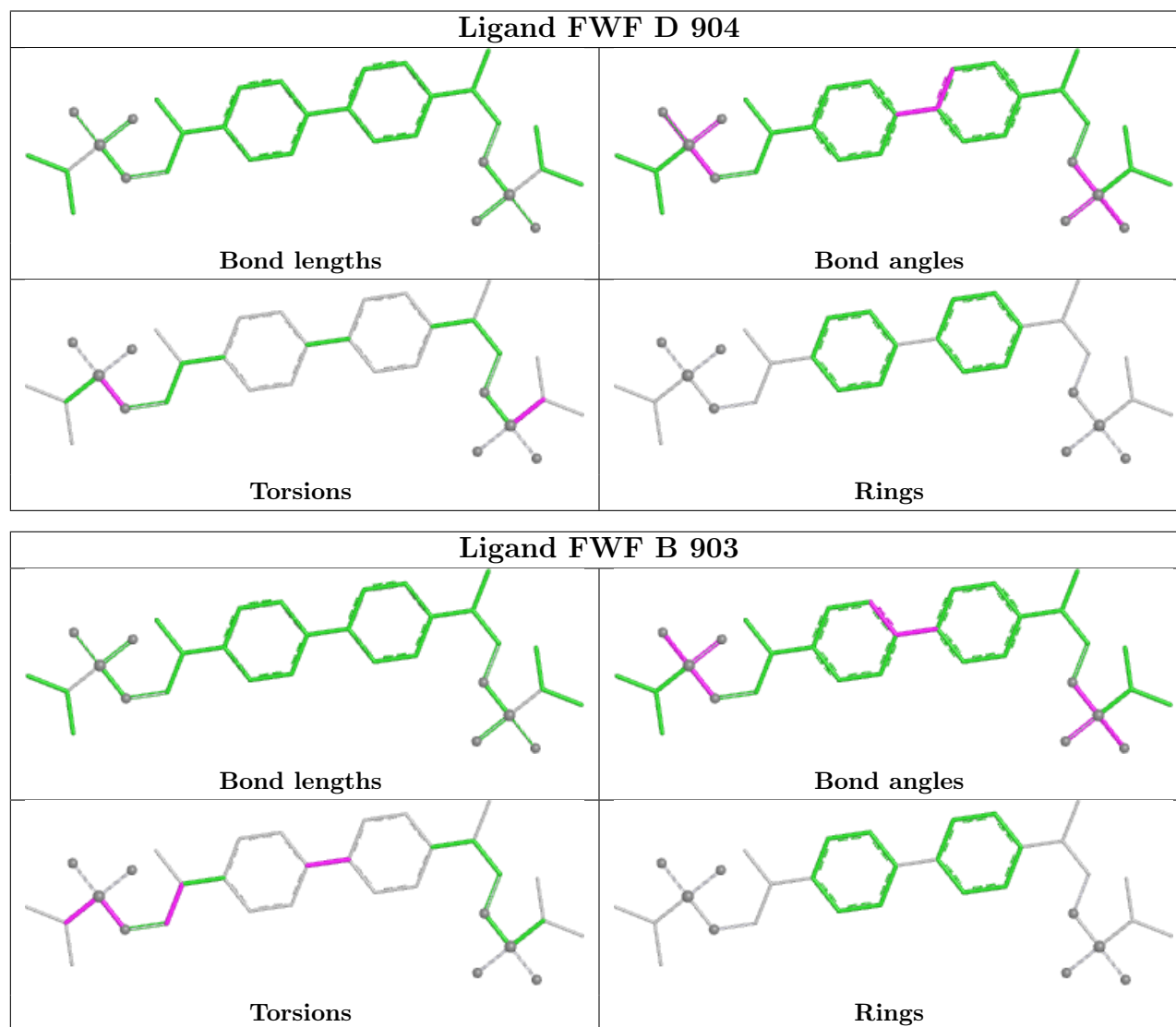
There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	904	FWF	2	0
5	D	903	MES	1	0
4	B	903	FWF	2	0
2	B	901	KAI	3	0
3	C	902	NAG	1	0
2	C	901	KAI	3	0
2	D	901	KAI	1	0
3	D	902	NAG	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.45	46 (6%)	26	18	41, 100, 169, 229	0
1	B	738/824 (89%)	0.36	32 (4%)	40	25	41, 87, 180, 200	0
1	C	755/824 (91%)	0.45	62 (8%)	17	13	38, 86, 191, 233	0
1	D	744/824 (90%)	0.60	61 (8%)	17	13	42, 103, 171, 217	0
All	All	2980/3296 (90%)	0.47	201 (6%)	24	16	38, 95, 180, 233	0

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	542	LEU	8.3
1	C	792	VAL	6.8
1	B	792	VAL	6.8
1	D	510	SER	6.3
1	C	634	GLU	5.6
1	B	788	SER	5.1
1	D	234	GLN	5.0
1	A	516	SER	5.0
1	C	538	VAL	5.0
1	B	786	ALA	4.6
1	C	633	ILE	4.6
1	D	771	GLY	4.6
1	C	519	ASP	4.5
1	A	799	LEU	4.3
1	D	515	PHE	4.3
1	D	346	ASP	4.1
1	D	788	SER	4.1
1	D	289	VAL	4.0
1	D	514	VAL	4.0
1	A	652	SER	4.0
1	D	609	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	302	ILE	4.0
1	B	172	ASP	3.9
1	D	608	PHE	3.9
1	A	627	GLU	3.8
1	A	798	ILE	3.8
1	C	640	SER	3.8
1	C	791	ASN	3.7
1	D	792	VAL	3.7
1	C	794	GLY	3.6
1	A	800	VAL	3.6
1	D	604	VAL	3.4
1	C	14	GLY	3.4
1	D	784	THR	3.4
1	C	383	THR	3.4
1	D	291	THR	3.4
1	A	515	PHE	3.4
1	A	517	PHE	3.4
1	A	644	GLU	3.4
1	C	516	SER	3.3
1	D	33	GLN	3.3
1	B	510	SER	3.3
1	A	651	ASP	3.3
1	C	300	GLN	3.3
1	A	367	ARG	3.2
1	C	510	SER	3.2
1	D	263	LEU	3.2
1	A	70	ALA	3.2
1	A	364	ASN	3.2
1	B	310	ALA	3.2
1	C	684	ARG	3.2
1	B	598	ALA	3.2
1	B	803	LEU	3.1
1	D	321	TRP	3.1
1	C	543	VAL	3.1
1	D	111	MET	3.1
1	C	604	VAL	3.1
1	A	792	VAL	3.1
1	D	284	TYR	3.1
1	A	602	ALA	3.0
1	D	230	LEU	3.0
1	D	34	PHE	3.0
1	A	321	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	326	GLU	3.0
1	B	771	GLY	2.9
1	C	168	ASN	2.9
1	D	789	LEU	2.9
1	A	310	ALA	2.9
1	D	287	VAL	2.9
1	C	303	GLU	2.9
1	D	509	LYS	2.9
1	D	274	ALA	2.9
1	C	778	SER	2.8
1	A	387	THR	2.8
1	C	797	TYR	2.8
1	A	507	PRO	2.8
1	A	539	VAL	2.8
1	C	714	GLN	2.8
1	D	30	GLY	2.8
1	B	543	VAL	2.8
1	D	35	SER	2.8
1	C	596	LEU	2.8
1	D	772	GLU	2.8
1	C	798	ILE	2.8
1	C	812	ILE	2.8
1	D	133	TYR	2.8
1	C	776	LYS	2.8
1	A	253	VAL	2.8
1	D	600	ILE	2.8
1	C	774	GLY	2.7
1	C	297	LEU	2.7
1	D	109	ILE	2.7
1	B	601	VAL	2.7
1	C	60	PHE	2.7
1	C	514	VAL	2.7
1	D	633	ILE	2.7
1	A	30	GLY	2.7
1	A	795	VAL	2.7
1	C	795	VAL	2.6
1	C	172	ASP	2.6
1	B	521	LEU	2.6
1	A	803	LEU	2.6
1	D	793	ALA	2.6
1	C	196	ARG	2.6
1	A	653	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	803	LEU	2.6
1	A	209	ILE	2.5
1	C	269	PRO	2.5
1	C	512	PRO	2.5
1	D	790	SER	2.5
1	B	683	VAL	2.5
1	D	543	VAL	2.5
1	C	509	LYS	2.5
1	D	288	GLN	2.5
1	B	806	ALA	2.4
1	C	51	ALA	2.4
1	C	775	ALA	2.4
1	D	785	SER	2.4
1	D	787	LEU	2.4
1	C	793	ALA	2.4
1	C	306	ARG	2.4
1	D	13	GLY	2.4
1	B	333	GLN	2.4
1	D	23	GLU	2.4
1	B	80	VAL	2.4
1	A	322	GLY	2.4
1	A	598	ALA	2.4
1	B	153	GLU	2.4
1	D	32	VAL	2.4
1	A	519	ASP	2.4
1	C	69	TYR	2.4
1	D	285	ASP	2.4
1	D	345	PHE	2.4
1	D	518	LEU	2.4
1	B	526	TRP	2.4
1	C	631	SER	2.3
1	D	194	CYS	2.3
1	C	799	LEU	2.3
1	C	601	VAL	2.3
1	B	810	ALA	2.3
1	A	212	HIS	2.3
1	A	508	GLN	2.3
1	A	486	GLU	2.2
1	B	535	LEU	2.2
1	B	811	LEU	2.2
1	C	811	LEU	2.2
1	C	515	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	268	TYR	2.2
1	D	631	SER	2.2
1	A	543	VAL	2.2
1	D	10	ILE	2.2
1	B	330	ALA	2.2
1	B	345	PHE	2.2
1	C	42	THR	2.2
1	C	540	LEU	2.2
1	B	149	ASP	2.2
1	C	607	PHE	2.2
1	A	92	VAL	2.2
1	B	473	ASP	2.2
1	D	519	ASP	2.2
1	D	529	ILE	2.1
1	D	542	LEU	2.1
1	A	160	ALA	2.1
1	A	388	SER	2.1
1	C	810	ALA	2.1
1	D	93	SER	2.1
1	D	286	ALA	2.1
1	A	648	GLY	2.1
1	C	800	VAL	2.1
1	A	789	LEU	2.1
1	A	111	MET	2.1
1	A	301	ARG	2.1
1	B	710	GLU	2.1
1	B	791	ASN	2.1
1	D	309	ASN	2.1
1	D	290	MET	2.1
1	A	593	PRO	2.1
1	A	483	LEU	2.1
1	C	247	ASP	2.1
1	D	811	LEU	2.1
1	B	274	ALA	2.1
1	C	39	PHE	2.1
1	D	303	GLU	2.1
1	D	805	LEU	2.1
1	B	289	VAL	2.0
1	C	253	VAL	2.0
1	A	676	SER	2.0
1	C	652	SER	2.0
1	C	376	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	541	PHE	2.0
1	C	323	GLN	2.0
1	B	331	LEU	2.0
1	C	93	SER	2.0
1	B	807	MET	2.0
1	D	69	TYR	2.0
1	C	138	ASP	2.0
1	B	682	PHE	2.0
1	D	235	PHE	2.0
1	D	731	GLY	2.0
1	A	187	GLU	2.0
1	D	596	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

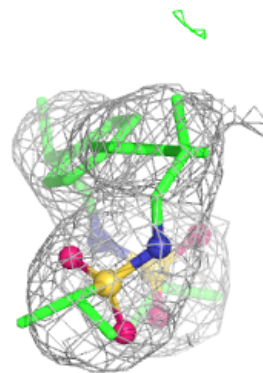
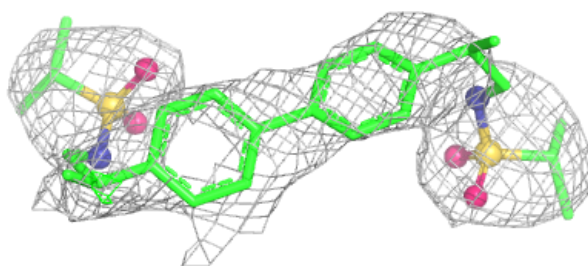
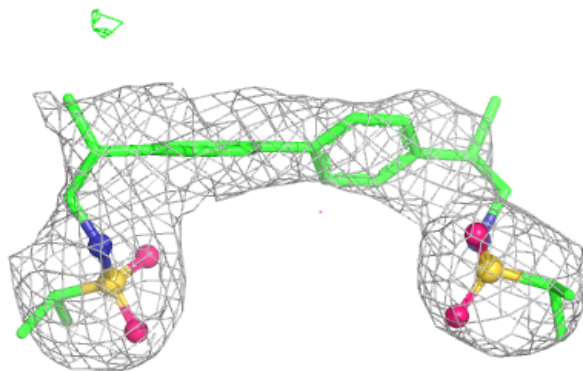
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	D	902	14/15	0.34	0.19	154,174,190,190	0
3	NAG	B	902	14/15	0.62	0.15	128,138,162,170	0
3	NAG	A	902	14/15	0.84	0.16	48,89,106,115	0
2	KAI	D	901	15/15	0.85	0.20	71,90,118,121	0
2	KAI	B	901	15/15	0.85	0.21	55,77,92,101	0
2	KAI	A	901	15/15	0.86	0.21	53,90,108,117	0
5	MES	D	903	12/12	0.86	0.12	70,96,101,103	0
3	NAG	C	902	14/15	0.90	0.10	60,79,105,108	0
2	KAI	C	901	15/15	0.91	0.19	45,58,77,78	0
4	FWF	D	904	32/32	0.94	0.13	56,76,92,101	0
4	FWF	B	903	32/32	0.96	0.10	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.

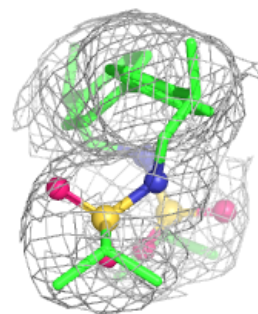
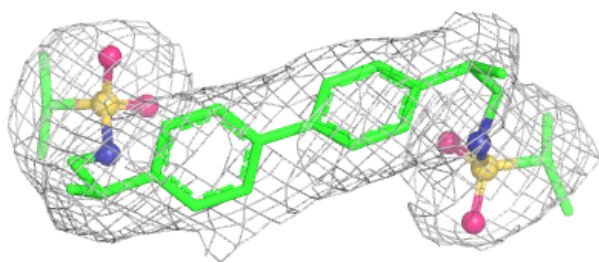
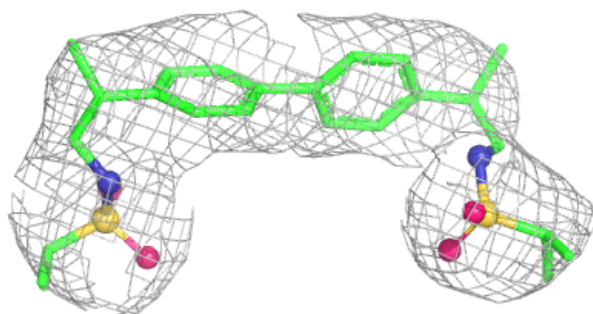
Electron density around FWF D 904:

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



Electron density around FWF B 903:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.