



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 11:13 PM BST

PDB ID : 4U1W
Title : Full length GluA2-kainate-(R,R)-2b complex crystal form A
Authors : Chen, L.; Gouaux, E.
Deposited on : 2014-07-16
Resolution : 3.25 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 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

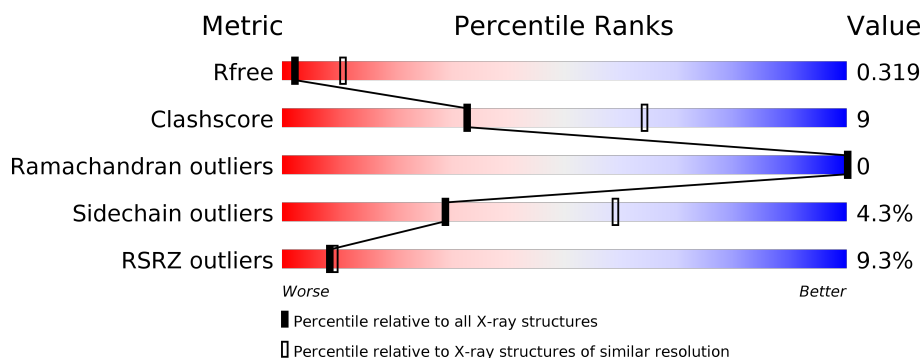
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	<div> <div>9%</div> <div> <div></div> <div>71%</div> <div>16%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	824	<div> <div>7%</div> <div> <div></div> <div>71%</div> <div>19%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	824	<div> <div>8%</div> <div> <div></div> <div>67%</div> <div>22%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	824	<div> <div>10%</div> <div> <div></div> <div>68%</div> <div>21%</div> <div>•</div> <div>9%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23011 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	731	Total	C	N	O	S	0	0	0
			5571	3582	908	1055	26			
1	B	751	Total	C	N	O	S	0	0	0
			5767	3707	952	1083	25			
1	C	736	Total	C	N	O	S	0	0	0
			5713	3668	945	1075	25			
1	D	750	Total	C	N	O	S	0	0	0
			5780	3715	951	1088	26			

There are 72 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	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
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

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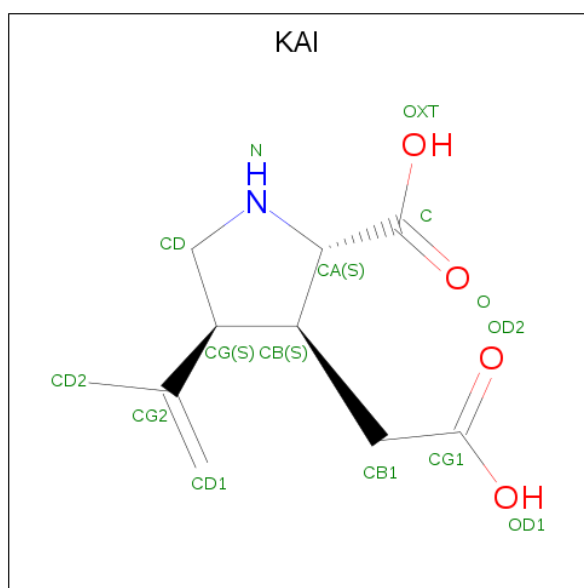
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	SER	deletion	UNP P19491
B	?	-	GLY	deletion	UNP P19491
B	385	ASP	ASN	engineered mutation	UNP P19491
B	392	GLN	ASN	engineered mutation	UNP P19491
B	528	ALA	CYS	engineered mutation	UNP P19491
B	585	PHE	MET	engineered mutation	UNP P19491
B	589	ALA	CYS	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	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
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	585	PHE	MET	engineered mutation	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
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: $C_{10}H_{15}NO_4$).



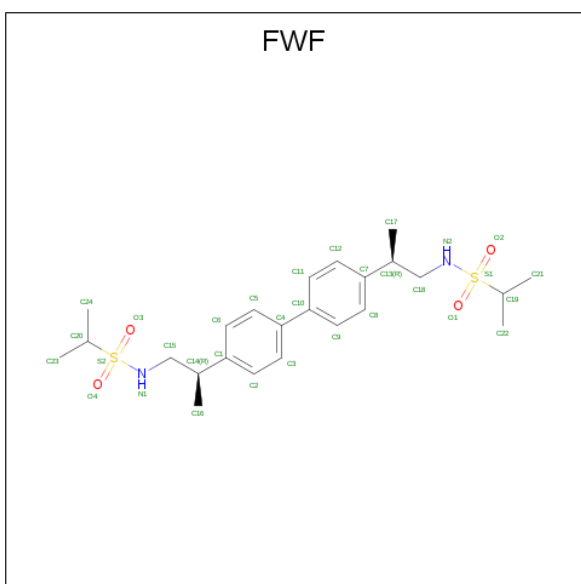
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	10	1	4		
2	B	1	Total	C	N	O	0	0
			15	10	1	4		
2	C	1	Total	C	N	O	0	0
			15	10	1	4		
2	D	1	Total	C	N	O	0	0
			15	10	1	4		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (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]dipropylsulfonamide (three-letter code: FWF) (formula: $C_{24}H_{36}N_2O_4S_2$).

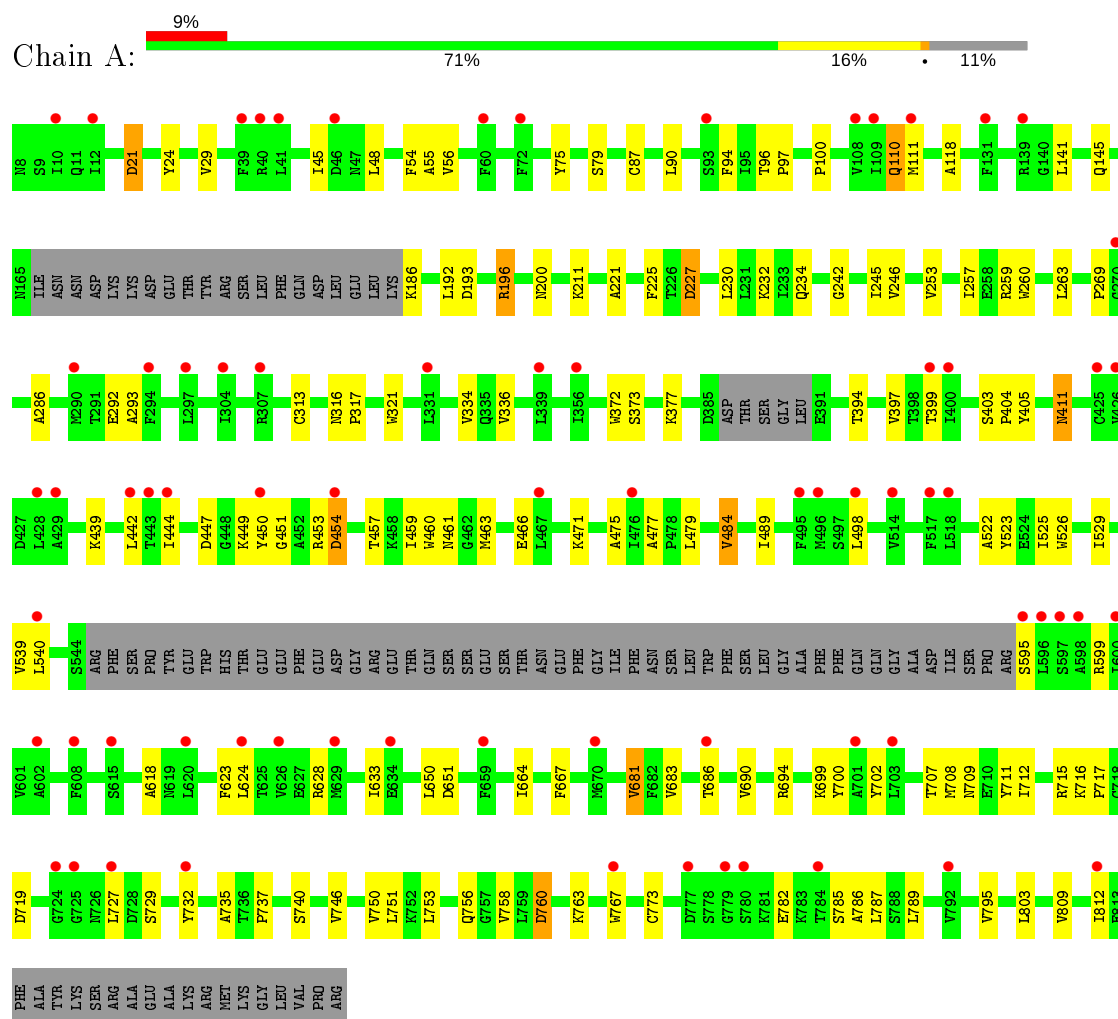


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			32	24	2	4	2		
4	C	1	Total	C	N	O	S	0	0
			32	24	2	4	2		

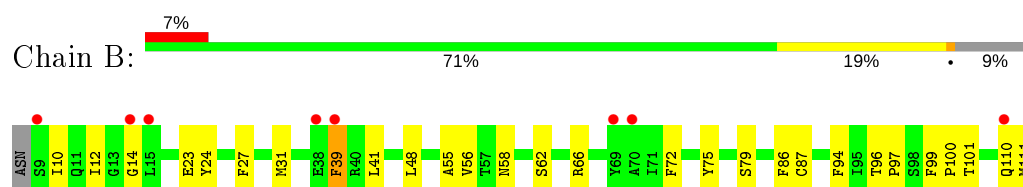
3 Residue-property plots [i](#)

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

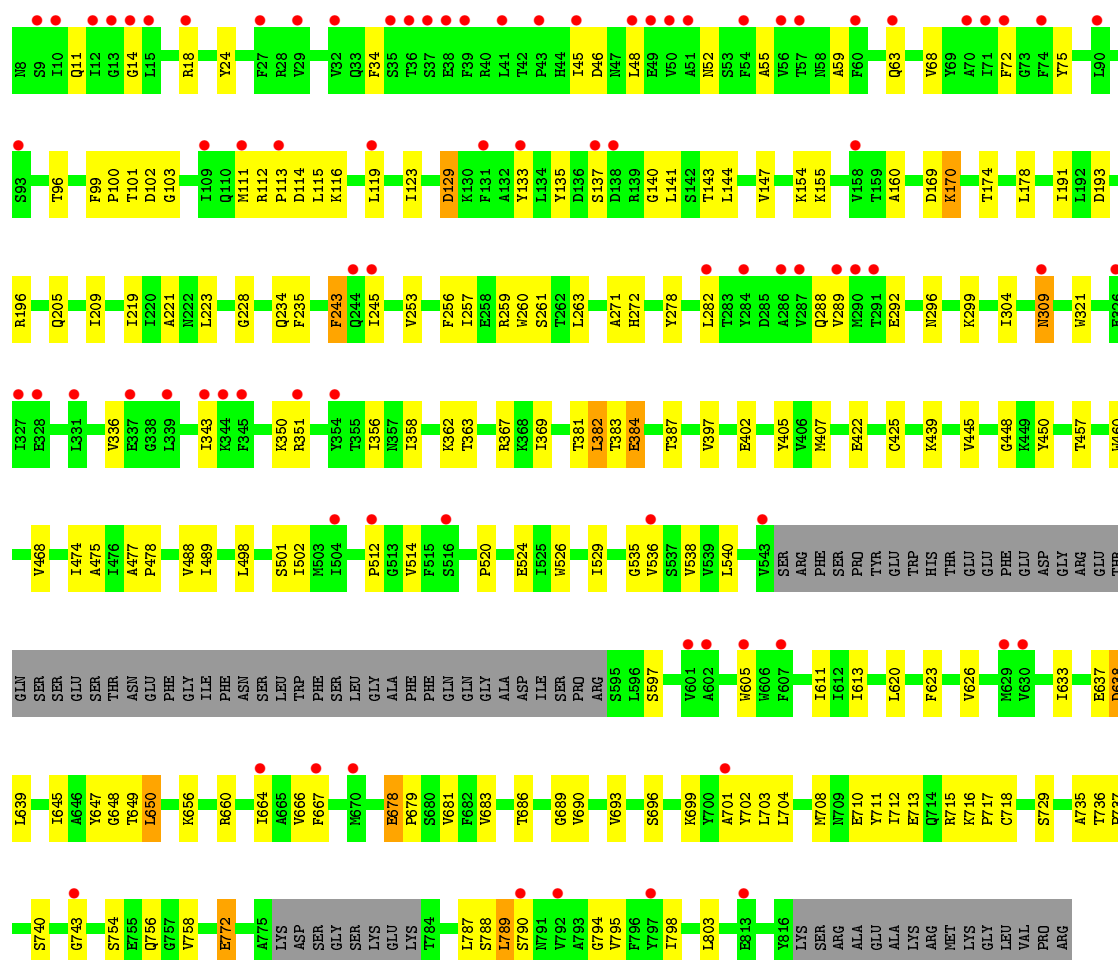


• Molecule 1: Glutamate receptor 2





- Molecule 1: Glutamate receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.50Å 151.11Å 332.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.91 – 3.25 83.21 – 3.25	Depositor EDS
% Data completeness (in resolution range)	79.8 (29.91-3.25) 79.7 (83.21-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 3.26Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.270 , 0.316 0.271 , 0.319	Depositor DCC
R_{free} test set	3359 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	108.0	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	23011	wwPDB-VP
Average B, all atoms (Å ²)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% 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: FWF, KAI, 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	0.25	0/5685	0.44	0/7719
1	B	0.25	0/5884	0.45	0/7974
1	C	0.25	0/5826	0.44	0/7888
1	D	0.25	0/5900	0.46	0/8002
All	All	0.25	0/23295	0.45	0/31583

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	5571	0	5425	90	0
1	B	5767	0	5672	97	0
1	C	5713	0	5643	115	0
1	D	5780	0	5656	113	0
2	A	15	0	13	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	14	0	13	2	0
3	C	14	0	13	0	0
3	D	14	0	13	0	0
4	A	32	0	36	4	0
4	C	32	0	36	5	0
All	All	23011	0	22572	395	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 9.

All (395) 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:112:ARG:HG3	1:D:223:LEU:HD11	1.61	0.81
1:D:75:TYR:HE1	1:D:96:THR:HG21	1.51	0.74
1:B:292:GLU:O	1:B:296:ASN:ND2	2.20	0.73
1:C:649:THR:HG22	1:C:703:LEU:HB2	1.72	0.72
1:B:475:ALA:HB3	1:B:735:ALA:HB3	1.72	0.70
1:A:711:TYR:OH	1:A:715:ARG:NH1	2.24	0.70
1:B:597:SER:H	1:C:810:ALA:HB2	1.56	0.70
1:A:457:THR:HG23	1:A:459:ILE:H	1.56	0.70
1:A:454:ASP:HB2	1:A:457:THR:HG22	1.74	0.69
1:D:656:LYS:HE2	1:D:660:ARG:HH21	1.57	0.69
1:C:493:LYS:HG3	1:C:751:LEU:HD11	1.75	0.68
1:D:99:PHE:HA	1:D:112:ARG:HD2	1.74	0.68
1:C:25:SER:HB3	1:C:268:TYR:HB3	1.75	0.67
1:A:751:LEU:HD23	4:A:903:FWF:H36	1.76	0.67
1:A:447:ASP:HB3	1:A:449:LYS:HG3	1.76	0.67
1:D:116:LYS:HG2	1:D:143:THR:HG22	1.75	0.67
1:B:650:LEU:HD13	2:B:901:KAI:HD23	1.76	0.67
1:B:427:ASP:OD2	1:B:765:LYS:NZ	2.28	0.66
1:D:296:ASN:HA	1:D:299:LYS:HG2	1.77	0.66
1:B:245:ILE:HG23	1:B:246:VAL:HG23	1.77	0.66
1:C:99:PHE:HA	1:C:112:ARG:HD2	1.78	0.66
1:C:193:ASP:HA	1:C:221:ALA:HB3	1.78	0.66
1:A:737:PRO:HG2	1:A:740:SER:HB2	1.77	0.65
1:A:200:ASN:OD1	1:A:232:LYS:NZ	2.30	0.65
1:A:141:LEU:HD21	1:B:145:GLN:HE21	1.62	0.65
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.79	0.64
1:D:696:SER:HB2	1:D:699:LYS:HB3	1.78	0.64
1:C:196:ARG:HD3	1:C:277:LYS:HE3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:THR:HG22	1:A:439:LYS:HB2	1.81	0.63
1:A:681:VAL:HG12	1:A:700:TYR:HE1	1.64	0.62
1:A:411:ASN:N	1:A:411:ASN:OD1	2.31	0.62
1:A:539:VAL:HG21	1:B:803:LEU:HD22	1.82	0.62
1:C:245:ILE:HG23	1:C:246:VAL:HG23	1.80	0.62
1:A:100:PRO:HA	1:A:110:GLN:HG2	1.82	0.61
1:B:411:ASN:OD1	1:B:411:ASN:N	2.31	0.61
1:B:597:SER:HA	1:C:806:ALA:HB1	1.82	0.60
1:D:737:PRO:HG2	1:D:740:SER:HB2	1.84	0.60
1:D:633:ILE:HD11	1:D:645:ILE:HD12	1.84	0.60
1:A:193:ASP:HA	1:A:221:ALA:HB3	1.84	0.60
1:D:129:ASP:N	1:D:129:ASP:OD1	2.34	0.60
1:D:512:PRO:HG3	1:D:790:SER:HB2	1.83	0.60
1:C:292:GLU:HG3	1:C:336:VAL:HG11	1.84	0.60
1:A:145:GLN:OE1	1:B:162:ASN:ND2	2.36	0.59
1:B:208:THR:HG22	1:D:235:PHE:HB2	1.84	0.59
1:B:702:TYR:CE1	1:B:704:LEU:HB3	2.36	0.59
1:D:789:LEU:HD12	1:D:790:SER:N	2.18	0.59
1:C:141:LEU:HD21	1:D:141:LEU:HD13	1.84	0.59
1:C:36:THR:HG23	1:C:39:PHE:H	1.68	0.58
1:C:412:HIS:HA	1:C:415:LEU:HB2	1.85	0.58
1:A:795:VAL:HG21	1:D:611:ILE:HG21	1.85	0.58
1:C:179:PHE:HD2	1:C:211:LYS:HD2	1.68	0.58
1:B:175:TYR:OH	1:B:198:LYS:NZ	2.29	0.58
1:D:647:TYR:HB3	1:D:701:ALA:HB3	1.85	0.58
1:D:11:GLN:HG3	1:D:68:VAL:HG12	1.85	0.57
1:A:460:TRP:HH2	1:A:484:VAL:HB	1.68	0.57
1:B:690:VAL:HG11	1:B:712:ILE:HG21	1.87	0.57
1:D:102:ASP:OD1	1:D:103:GLY:N	2.36	0.57
1:D:514:VAL:HG11	1:D:794:GLY:HA3	1.86	0.57
1:B:48:LEU:HD12	1:B:55:ALA:HB1	1.86	0.56
1:B:729:SER:HB2	4:C:903:FWF:H19	1.87	0.56
1:D:690:VAL:HG11	1:D:712:ILE:HG21	1.87	0.56
1:A:623:PHE:HD1	1:A:624:LEU:HD12	1.70	0.56
1:C:332:LYS:NZ	1:C:347:GLN:O	2.29	0.56
1:C:202:ILE:HA	1:C:205:GLN:HG2	1.87	0.56
1:C:129:ASP:OD1	1:C:129:ASP:N	2.38	0.55
1:C:525:ILE:HD11	1:D:789:LEU:HA	1.88	0.55
1:B:539:VAL:HG11	1:B:601:VAL:HG21	1.87	0.55
1:B:702:TYR:HE1	1:B:704:LEU:HB3	1.71	0.55
1:A:111:MET:HG3	1:A:286:ALA:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:LEU:HD12	1:D:55:ALA:HB1	1.87	0.55
1:A:522:ALA:HB3	1:A:525:ILE:HG13	1.88	0.55
1:C:120:LEU:HD21	1:C:147:VAL:HA	1.89	0.55
1:D:407:MET:N	1:D:422:GLU:O	2.37	0.55
1:D:736:THR:HG21	1:D:743:GLY:HA2	1.89	0.55
1:B:498:LEU:HD23	1:B:705:GLU:HB3	1.89	0.55
1:B:460:TRP:NE1	1:B:488:VAL:HG11	2.21	0.55
1:C:260:TRP:HA	1:C:260:TRP:CE3	2.41	0.55
1:B:175:TYR:HD2	1:B:205:GLN:HG3	1.73	0.54
1:C:28:ARG:NH2	1:C:267:GLU:O	2.40	0.54
1:D:137:SER:HA	1:D:140:GLY:HA3	1.88	0.54
1:B:335:GLN:CD	3:B:902:NAG:H82	2.28	0.54
1:B:56:VAL:HG21	1:B:79:SER:HB2	1.89	0.54
1:C:11:GLN:HG3	1:C:68:VAL:HG12	1.90	0.54
1:A:690:VAL:HG11	1:A:712:ILE:HG21	1.90	0.54
1:C:460:TRP:NE1	1:C:488:VAL:HG11	2.23	0.54
1:C:500:ILE:HD13	1:C:655:THR:HG23	1.90	0.54
1:D:475:ALA:HB3	1:D:735:ALA:HB3	1.89	0.54
1:D:702:TYR:CE1	1:D:704:LEU:HB3	2.43	0.54
1:D:99:PHE:CD1	1:D:100:PRO:HD2	2.42	0.54
1:A:466:GLU:O	1:A:471:LYS:N	2.33	0.54
1:B:696:SER:HB2	1:B:699:LYS:HB2	1.89	0.54
1:B:596:LEU:HD13	1:C:809:VAL:HG12	1.91	0.53
1:C:260:TRP:HA	1:C:260:TRP:HE3	1.72	0.53
1:B:225:PHE:CD1	1:B:242:GLY:HA3	2.44	0.53
1:B:454:ASP:HB3	1:B:457:THR:HG23	1.90	0.53
1:C:460:TRP:HE1	1:C:488:VAL:HG11	1.72	0.53
1:C:751:LEU:HG	4:C:903:FWF:H28	1.91	0.52
1:C:141:LEU:HD11	1:D:141:LEU:HD13	1.91	0.52
1:D:526:TRP:HA	1:D:529:ILE:HG22	1.90	0.52
1:D:191:ILE:HG12	1:D:219:ILE:HB	1.90	0.52
1:A:751:LEU:HD23	4:A:903:FWF:C24	2.38	0.52
4:A:903:FWF:H8	1:D:729:SER:HB2	1.91	0.52
1:B:626:VAL:HG21	1:C:628:ARG:HB3	1.92	0.52
1:C:736:THR:HG21	1:C:743:GLY:HA2	1.92	0.52
1:D:468:VAL:HG21	1:D:488:VAL:HG12	1.91	0.52
1:B:417:GLY:HA2	1:B:420:ARG:HH21	1.75	0.52
1:A:760:ASP:N	1:A:760:ASP:OD1	2.43	0.52
1:A:707:THR:HG21	1:A:732:TYR:HE2	1.74	0.51
1:C:115:LEU:HD21	1:C:243:PHE:CD2	2.45	0.51
1:A:451:GLY:HA2	1:A:461:ASN:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:MET:HB3	1:C:282:LEU:HD22	1.91	0.51
1:D:690:VAL:HG21	1:D:712:ILE:HD12	1.93	0.51
1:D:101:THR:O	1:D:350:LYS:NZ	2.43	0.51
1:D:489:ILE:HD13	1:D:735:ALA:HB1	1.92	0.51
1:C:115:LEU:HD12	1:C:118:ALA:HB3	1.91	0.51
1:C:707:THR:OG1	1:C:708:MET:SD	2.68	0.51
1:A:526:TRP:O	1:A:529:ILE:HG22	2.11	0.51
1:C:489:ILE:HD13	1:C:735:ALA:HB1	1.92	0.51
1:D:633:ILE:HD13	1:D:639:LEU:HD13	1.93	0.51
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.92	0.51
1:C:176:ARG:NH1	1:C:205:GLN:OE1	2.38	0.51
1:A:253:VAL:O	1:A:257:ILE:HG12	2.11	0.50
1:A:230:LEU:O	1:A:234:GLN:HB2	2.11	0.50
1:C:183:GLU:HG2	1:C:211:LYS:NZ	2.26	0.50
1:B:364:ASN:OD1	1:B:365:GLY:N	2.44	0.50
1:D:650:LEU:H	1:D:650:LEU:HD23	1.76	0.50
1:B:520:PRO:HA	1:B:623:PHE:HE2	1.76	0.50
1:C:634:GLU:CB	1:C:635:SER:HB3	2.41	0.50
1:B:500:ILE:HD13	1:B:655:THR:HG23	1.94	0.50
1:B:460:TRP:HE1	1:B:488:VAL:HG11	1.76	0.49
1:C:447:ASP:OD1	1:C:447:ASP:N	2.45	0.49
1:B:504:ILE:HG21	1:B:633:ILE:HD11	1.93	0.49
1:B:94:PHE:HE1	1:B:96:THR:HB	1.78	0.49
1:A:453:ARG:HB2	1:A:460:TRP:CE2	2.48	0.49
1:C:41:LEU:H	1:C:41:LEU:HD12	1.78	0.49
1:C:763:LYS:O	1:C:767:TRP:HB2	2.13	0.49
1:D:14:GLY:HA2	1:D:72:PHE:O	2.12	0.49
1:C:194:CYS:HB2	1:C:199:VAL:HG23	1.95	0.49
1:B:218:TYR:HB2	1:B:240:VAL:HG22	1.95	0.49
1:C:24:TYR:CE2	1:C:28:ARG:HD2	2.48	0.49
1:A:292:GLU:HG3	1:A:336:VAL:HG11	1.95	0.49
1:A:293:ALA:HA	1:A:334:VAL:HG21	1.93	0.49
1:B:689:GLY:HA3	1:B:702:TYR:CE2	2.48	0.49
1:D:309:ASN:N	1:D:309:ASN:OD1	2.28	0.49
1:C:531:PHE:HA	1:C:534:ILE:HG12	1.95	0.48
1:C:737:PRO:HG2	1:C:740:SER:HB2	1.95	0.48
1:D:716:LYS:HB3	1:D:772:GLU:HG2	1.94	0.48
1:C:809:VAL:O	1:C:812:ILE:HG12	2.13	0.48
1:D:135:TYR:HE1	1:D:160:ALA:HB1	1.76	0.48
1:B:451:GLY:HA2	1:B:461:ASN:O	2.14	0.48
1:C:650:LEU:HD13	2:C:901:KAI:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:809:VAL:HA	1:B:812:ILE:HG12	1.94	0.48
1:A:694:ARG:NE	1:A:719:ASP:OD1	2.46	0.48
1:A:650:LEU:HG	1:A:702:TYR:OH	2.12	0.48
1:C:610:LEU:HD21	1:D:613:ILE:HG21	1.96	0.48
1:A:707:THR:OG1	1:A:708:MET:SD	2.71	0.48
1:B:412:HIS:HA	1:B:415:LEU:HD12	1.96	0.48
1:D:34:PHE:CE2	1:D:288:GLN:HB2	2.48	0.48
1:D:536:VAL:HG21	1:D:605:TRP:CE3	2.49	0.48
1:A:24:TYR:HE1	1:A:45:ILE:HD12	1.79	0.48
1:B:711:TYR:O	1:B:715:ARG:HG2	2.14	0.48
1:C:23:GLU:OE1	1:C:23:GLU:N	2.43	0.48
1:A:489:ILE:HD13	1:A:735:ALA:HB1	1.96	0.48
1:B:111:MET:HE1	1:B:289:VAL:HG21	1.96	0.47
1:C:253:VAL:O	1:C:257:ILE:HG12	2.14	0.47
1:D:113:PRO:HA	1:D:351:ARG:HB2	1.95	0.47
1:D:637:GLU:HA	1:D:666:VAL:HG11	1.96	0.47
1:C:494:PRO:HB2	4:C:903:FWF:C8	2.44	0.47
1:A:90:LEU:HD11	1:A:313:CYS:HB2	1.96	0.47
1:C:805:LEU:O	1:C:809:VAL:HG23	2.14	0.47
1:D:144:LEU:HA	1:D:147:VAL:HG22	1.97	0.47
1:A:56:VAL:HG21	1:A:79:SER:HB2	1.96	0.47
1:A:397:VAL:HB	1:A:442:LEU:HD23	1.97	0.47
1:C:711:TYR:O	1:C:715:ARG:HG2	2.15	0.47
1:C:729:SER:HB2	4:C:903:FWF:H8	1.97	0.47
2:D:901:KAI:HD12	2:D:901:KAI:HD2	1.67	0.47
1:B:248:TYR:HA	1:B:253:VAL:HG11	1.96	0.47
1:D:358:ILE:HG22	1:D:369:ILE:HG23	1.96	0.47
1:A:618:ALA:HA	1:B:621:ALA:HB2	1.97	0.47
1:C:171:LYS:O	1:C:174:THR:HG22	2.13	0.47
1:C:445:VAL:HG21	1:C:462:GLY:HA2	1.97	0.47
1:C:642:GLN:NE2	1:C:642:GLN:O	2.47	0.47
1:B:205:GLN:O	1:B:209:ILE:HG13	2.14	0.47
1:C:169:ASP:N	1:C:169:ASP:OD1	2.48	0.47
1:D:362:LYS:HG3	1:D:367:ARG:HD2	1.97	0.47
1:B:175:TYR:CD2	1:B:205:GLN:HG3	2.49	0.46
1:C:163:VAL:HG21	1:C:202:ILE:HD11	1.97	0.46
1:C:370:GLY:HA2	1:C:381:THR:OG1	2.16	0.46
1:D:119:LEU:HD11	1:D:191:ILE:HG21	1.96	0.46
1:C:151:ALA:HB1	1:C:156:TRP:HB2	1.96	0.46
1:C:405:TYR:HB3	1:C:425:CYS:SG	2.56	0.46
1:C:615:SER:HA	1:D:620:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:648:GLY:HA3	1:D:681:VAL:HG12	1.96	0.46
1:D:711:TYR:O	1:D:715:ARG:HG2	2.15	0.46
1:B:793:ALA:HA	1:B:796:PHE:HB2	1.96	0.46
1:D:664:ILE:HB	1:D:667:PHE:HD2	1.79	0.46
1:A:225:PHE:CD1	1:A:242:GLY:HA3	2.51	0.46
1:A:525:ILE:HD13	1:B:792:VAL:HG21	1.98	0.46
1:D:205:GLN:O	1:D:209:ILE:HG13	2.15	0.46
1:D:59:ALA:O	1:D:63:GLN:HG2	2.15	0.46
1:D:756:GLN:HG3	1:D:758:VAL:HG23	1.98	0.46
1:D:111:MET:HE1	1:D:289:VAL:HG21	1.98	0.46
1:A:789:LEU:HD22	1:D:524:GLU:HB3	1.97	0.46
1:A:454:ASP:N	1:A:454:ASP:OD1	2.48	0.46
1:D:115:LEU:HD21	1:D:243:PHE:HE1	1.80	0.46
1:B:405:TYR:HB3	1:B:425:CYS:SG	2.55	0.46
1:B:526:TRP:O	1:B:529:ILE:HG22	2.16	0.46
1:A:716:LYS:HG3	1:A:717:PRO:HA	1.97	0.46
1:B:23:GLU:N	1:B:23:GLU:OE1	2.47	0.46
1:B:253:VAL:O	1:B:257:ILE:HG12	2.16	0.46
1:D:263:LEU:HB2	1:D:271:ALA:HB1	1.97	0.46
1:C:536:VAL:HG22	1:D:803:LEU:HD21	1.97	0.46
1:C:746:VAL:O	1:C:750:VAL:HG23	2.16	0.45
1:D:382:LEU:HD13	1:D:383:THR:HG22	1.97	0.45
1:D:686:THR:HG21	1:D:708:MET:HG2	1.97	0.45
1:B:335:GLN:NE2	3:B:902:NAG:H82	2.31	0.45
1:C:336:VAL:HG23	1:C:343:ILE:HD12	1.98	0.45
1:D:439:LYS:HD2	1:D:439:LYS:HA	1.73	0.45
1:C:358:ILE:HD11	1:C:372:TRP:HB2	1.97	0.45
1:C:539:VAL:HG21	1:D:803:LEU:HD22	1.99	0.45
1:B:14:GLY:HA2	1:B:72:PHE:O	2.16	0.45
1:B:223:LEU:HB3	1:B:245:ILE:HB	1.99	0.45
1:A:729:SER:HB2	4:A:903:FWF:H19	1.99	0.45
1:A:763:LYS:O	1:A:767:TRP:HB2	2.16	0.45
1:B:101:THR:H	1:B:110:GLN:NE2	2.15	0.45
1:C:401:LEU:HA	1:C:406:VAL:HB	1.98	0.45
1:C:94:PHE:O	1:C:109:ILE:N	2.33	0.45
1:C:96:THR:HA	1:C:97:PRO:HD3	1.84	0.45
1:A:118:ALA:HA	1:A:372:TRP:CD1	2.52	0.45
1:A:477:ALA:O	1:A:479:LEU:N	2.47	0.45
1:D:196:ARG:CZ	1:D:228:GLY:HA3	2.46	0.45
1:A:809:VAL:HA	1:A:812:ILE:HG12	1.99	0.45
1:D:119:LEU:HD21	1:D:133:TYR:HE1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:707:THR:OG1	1:B:708:MET:SD	2.75	0.45
1:C:452:ALA:N	1:C:461:ASN:OD1	2.50	0.45
1:C:494:PRO:HB2	4:C:903:FWF:C9	2.47	0.45
1:A:786:ALA:HB1	1:D:520:PRO:O	2.17	0.45
1:B:373:SER:HB3	1:B:376:ASP:HB2	1.99	0.45
1:C:218:TYR:HB2	1:C:240:VAL:HG22	1.98	0.45
1:A:803:LEU:HD11	1:D:536:VAL:HG22	1.99	0.44
1:B:100:PRO:HD3	1:B:112:ARG:HD2	1.98	0.44
1:A:54:PHE:HA	1:B:86:PHE:HE1	1.82	0.44
1:D:638:ASP:OD1	1:D:638:ASP:N	2.49	0.44
1:B:336:VAL:HG23	1:B:343:ILE:HD12	1.99	0.44
1:C:399:THR:O	1:C:444:ILE:HA	2.17	0.44
2:C:901:KAI:HD2	2:C:901:KAI:HD12	1.73	0.44
1:D:100:PRO:HD3	1:D:112:ARG:HB3	1.99	0.44
1:A:628:ARG:CB	1:D:626:VAL:HG11	2.47	0.44
1:C:172:ASP:O	1:C:176:ARG:HG2	2.16	0.44
1:A:686:THR:HG23	1:A:702:TYR:HE2	1.81	0.44
1:A:450:TYR:O	1:A:463:MET:N	2.49	0.44
1:B:511:LYS:HA	1:B:512:PRO:HD3	1.77	0.44
1:D:402:GLU:O	1:D:405:TYR:N	2.51	0.44
1:D:535:GLY:O	1:D:538:VAL:HG12	2.17	0.44
2:A:901:KAI:HD2	2:A:901:KAI:HD12	1.69	0.44
1:B:323:GLN:O	1:B:327:ILE:HG13	2.17	0.44
1:C:620:LEU:HA	1:C:623:PHE:HD2	1.82	0.44
1:C:179:PHE:HE2	1:C:206:VAL:HG22	1.82	0.44
1:A:196:ARG:O	1:A:200:ASN:ND2	2.51	0.43
1:D:193:ASP:HA	1:D:221:ALA:HB3	1.99	0.43
1:D:292:GLU:HG3	1:D:336:VAL:HG11	2.00	0.43
1:C:436:CYS:HB2	1:C:438:PHE:CE2	2.53	0.43
1:D:253:VAL:O	1:D:257:ILE:HG12	2.18	0.43
1:A:523:TYR:HA	1:A:526:TRP:HD1	1.83	0.43
1:D:683:VAL:HG11	1:D:689:GLY:HA2	2.01	0.43
1:D:702:TYR:HE1	1:D:704:LEU:HB3	1.83	0.43
1:D:717:PRO:O	1:D:718:CYS:SG	2.76	0.43
1:B:99:PHE:HA	1:B:100:PRO:HD3	1.92	0.43
1:B:481:ILE:HA	1:B:491:PHE:CE2	2.54	0.43
1:C:24:TYR:O	1:C:27:PHE:HB3	2.19	0.43
1:D:223:LEU:HB2	1:D:278:TYR:CD1	2.53	0.43
1:D:450:TYR:HE2	1:D:478:PRO:HG2	1.84	0.43
1:D:540:LEU:HD23	1:D:540:LEU:HA	1.89	0.43
1:A:21:ASP:HB3	1:A:269:PRO:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ILE:HG23	1:A:246:VAL:HG23	1.99	0.43
1:C:656:LYS:HE2	1:C:660:ARG:NH2	2.33	0.43
1:A:595:SER:O	1:A:599:ARG:HG2	2.19	0.43
1:A:746:VAL:O	1:A:750:VAL:HG23	2.18	0.43
1:C:74:PHE:CZ	1:C:97:PRO:HG2	2.54	0.43
1:B:403:SER:HA	1:B:404:PRO:HA	1.82	0.43
1:B:467:LEU:HG	1:B:737:PRO:HG3	2.01	0.43
1:B:75:TYR:CE2	1:B:96:THR:HG21	2.54	0.43
1:A:87:CYS:SG	1:A:94:PHE:HB2	2.58	0.43
1:D:336:VAL:HG23	1:D:343:ILE:HD12	2.00	0.43
1:A:259:ARG:O	1:A:263:LEU:HG	2.18	0.42
1:B:477:ALA:O	1:B:479:LEU:N	2.47	0.42
1:C:420:ARG:NH1	1:C:421:TYR:OH	2.51	0.42
1:D:257:ILE:HA	1:D:257:ILE:HD13	1.90	0.42
1:A:316:ASN:HA	1:A:317:PRO:HA	1.86	0.42
1:B:499:GLY:HA3	1:B:726:ASN:HB3	2.01	0.42
1:C:29:VAL:HG21	1:C:260:TRP:HZ3	1.83	0.42
1:C:403:SER:HA	1:C:404:PRO:HA	1.83	0.42
1:D:75:TYR:CE1	1:D:96:THR:HG21	2.42	0.42
1:A:141:LEU:O	1:A:145:GLN:HG3	2.18	0.42
1:B:330:ALA:O	1:B:334:VAL:HG23	2.19	0.42
1:B:651:ASP:N	1:B:683:VAL:O	2.52	0.42
1:B:707:THR:OG1	1:B:708:MET:N	2.52	0.42
1:C:690:VAL:HG21	1:C:712:ILE:CD1	2.49	0.42
1:C:404:PRO:HD3	1:C:711:TYR:CG	2.53	0.42
1:D:256:PHE:O	1:D:260:TRP:HB2	2.19	0.42
1:D:710:GLU:O	1:D:713:GLU:HB3	2.19	0.42
1:C:671:TRP:O	1:C:675:ARG:HB2	2.19	0.42
1:B:405:TYR:OH	1:B:732:TYR:HE2	2.03	0.42
1:B:400:ILE:HG21	1:B:450:TYR:CZ	2.54	0.42
1:C:362:LYS:HD3	1:C:362:LYS:HA	1.89	0.42
1:C:683:VAL:HG11	1:C:689:GLY:HA2	2.00	0.42
1:D:99:PHE:HD2	1:D:112:ARG:HH11	1.67	0.42
1:D:282:LEU:HD23	1:D:282:LEU:HA	1.90	0.42
1:D:234:GLN:NE2	1:D:363:THR:O	2.52	0.42
1:D:795:VAL:O	1:D:798:ILE:HG22	2.19	0.42
1:A:475:ALA:HB3	1:A:735:ALA:HB3	2.00	0.42
1:A:664:ILE:HB	1:A:667:PHE:HD2	1.84	0.42
1:A:785:SER:OG	1:A:786:ALA:N	2.53	0.42
1:B:639:LEU:HD23	1:B:639:LEU:HA	1.80	0.42
1:B:12:ILE:HD13	1:B:41:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:CYS:SG	1:C:477:ALA:HA	2.60	0.42
1:D:384:GLU:HG2	1:D:384:GLU:O	2.20	0.42
1:D:52:ASN:OD1	1:D:55:ALA:N	2.39	0.42
1:C:84:THR:HG22	1:C:108:VAL:HG21	2.02	0.42
1:D:245:ILE:HD13	1:D:356:ILE:HG12	2.01	0.42
1:A:405:TYR:CE2	1:A:708:MET:HE3	2.55	0.42
1:A:782:GLU:HG3	1:A:782:GLU:O	2.20	0.42
1:B:726:ASN:OD1	1:B:726:ASN:N	2.52	0.42
1:A:245:ILE:HD12	1:A:245:ILE:HA	1.94	0.42
1:B:10:ILE:HD11	1:B:39:PHE:CD2	2.55	0.42
1:C:667:PHE:HE1	1:C:727:LEU:HD22	1.85	0.42
1:D:445:VAL:HG13	1:D:448:GLY:HA2	2.01	0.42
1:A:372:TRP:HA	1:A:377:LYS:O	2.20	0.41
1:A:651:ASP:N	1:A:683:VAL:O	2.45	0.41
1:A:405:TYR:HE2	1:A:708:MET:HE3	1.85	0.41
1:C:205:GLN:O	1:C:209:ILE:HG13	2.19	0.41
1:C:765:LYS:O	1:C:769:ASP:HB2	2.20	0.41
1:D:397:VAL:HG22	1:D:474:ILE:HG22	2.01	0.41
1:B:87:CYS:SG	1:B:94:PHE:HB2	2.60	0.41
1:C:678:GLU:HA	1:C:679:PRO:C	2.41	0.41
1:A:211:LYS:HA	1:A:211:LYS:HD3	1.68	0.41
1:A:399:THR:O	1:A:444:ILE:HA	2.20	0.41
1:B:96:THR:HA	1:B:97:PRO:HD3	1.84	0.41
1:C:329:ARG:O	1:C:333:GLN:HB2	2.20	0.41
1:D:259:ARG:O	1:D:263:LEU:HG	2.20	0.41
1:C:693:VAL:HG21	1:C:702:TYR:HB2	2.02	0.41
1:C:429:ALA:HA	1:C:476:ILE:HD13	2.01	0.41
1:A:110:GLN:HE21	1:A:110:GLN:H	1.67	0.41
1:A:667:PHE:HE1	1:A:727:LEU:HG	1.85	0.41
2:B:901:KAI:HD12	2:B:901:KAI:HD2	1.68	0.41
1:C:646:ALA:N	1:C:699:LYS:O	2.50	0.41
1:C:808:LEU:O	1:C:811:LEU:HB3	2.21	0.41
1:D:689:GLY:O	1:D:693:VAL:HG23	2.21	0.41
1:A:227:ASP:N	1:A:227:ASP:OD1	2.53	0.41
1:A:403:SER:HA	1:A:404:PRO:HA	1.87	0.41
1:B:27:PHE:O	1:B:31:MET:HG2	2.21	0.41
1:B:624:LEU:HA	1:B:624:LEU:HD23	1.89	0.41
1:B:816:TYR:HD1	1:B:816:TYR:HA	1.77	0.41
1:C:265:GLU:HG2	1:C:272:HIS:HB2	2.03	0.41
1:C:531:PHE:HD1	1:C:534:ILE:HD11	1.86	0.41
1:D:169:ASP:N	1:D:169:ASP:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:LEU:HA	1:A:540:LEU:HD23	1.93	0.41
1:D:501:SER:OG	1:D:502:ILE:N	2.52	0.41
1:A:29:VAL:HG21	1:A:260:TRP:HZ3	1.86	0.41
1:A:753:LEU:HD22	1:A:758:VAL:HG11	2.01	0.41
1:A:75:TYR:CE2	1:A:96:THR:HG21	2.56	0.41
1:B:619:ASN:ND2	1:C:787:LEU:HB2	2.35	0.41
1:B:62:SER:O	1:B:66:ARG:HG3	2.21	0.41
1:B:781:LYS:HD3	1:B:781:LYS:HA	1.85	0.41
1:C:179:PHE:CD2	1:C:211:LYS:HD2	2.52	0.41
1:A:321:TRP:HD1	1:A:321:TRP:H	1.64	0.41
1:A:756:GLN:HG3	1:A:758:VAL:HG23	2.02	0.41
1:C:191:ILE:HG12	1:C:219:ILE:HB	2.03	0.41
1:C:451:GLY:HA2	1:C:461:ASN:O	2.21	0.41
1:B:486:GLU:OE2	1:B:491:PHE:HB2	2.21	0.40
1:B:742:LEU:HD23	1:B:742:LEU:HA	1.83	0.40
1:C:634:GLU:HB3	1:C:635:SER:HB3	2.03	0.40
1:D:460:TRP:CZ2	1:D:488:VAL:HG21	2.56	0.40
1:D:477:ALA:HB1	1:D:478:PRO:HD2	2.03	0.40
1:C:288:GLN:O	1:C:292:GLU:HG2	2.22	0.40
1:D:261:SER:HA	1:D:272:HIS:HA	2.03	0.40
1:D:678:GLU:HA	1:D:679:PRO:C	2.41	0.40
1:B:464:VAL:O	1:B:468:VAL:HG23	2.22	0.40
1:B:678:GLU:HA	1:B:679:PRO:C	2.42	0.40
1:B:795:VAL:O	1:B:798:ILE:HG22	2.21	0.40
1:C:291:THR:HG22	1:C:295:ARG:HH12	1.87	0.40
1:C:323:GLN:O	1:C:327:ILE:HG13	2.22	0.40
1:C:690:VAL:HG21	1:C:712:ILE:HD13	2.03	0.40
1:A:48:LEU:HD12	1:A:55:ALA:HB1	2.04	0.40
1:B:358:ILE:HG12	1:B:378:MET:HE1	2.04	0.40
1:B:450:TYR:CE2	2:B:901:KAI:HD1	2.57	0.40
1:B:683:VAL:HG11	1:B:689:GLY:HA2	2.04	0.40
1:C:210:GLY:HA2	1:C:212:HIS:CE1	2.57	0.40
1:C:762:LEU:HA	1:C:762:LEU:HD12	1.90	0.40
1:D:119:LEU:O	1:D:123:ILE:HG13	2.22	0.40
1:D:169:ASP:HB2	1:D:170:LYS:HD2	2.03	0.40
1:D:787:LEU:HG	1:D:788:SER:N	2.35	0.40
1:A:96:THR:HA	1:A:97:PRO:HD3	1.86	0.40
1:D:154:LYS:HD2	1:D:154:LYS:HA	1.90	0.40
1:D:24:TYR:HE1	1:D:45:ILE:HG13	1.86	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	723/824 (88%)	703 (97%)	20 (3%)	0	100	100
1	B	743/824 (90%)	727 (98%)	16 (2%)	0	100	100
1	C	726/824 (88%)	710 (98%)	16 (2%)	0	100	100
1	D	744/824 (90%)	725 (97%)	19 (3%)	0	100	100
All	All	2936/3296 (89%)	2865 (98%)	71 (2%)	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	580/701 (83%)	562 (97%)	18 (3%)	40	67
1	B	605/701 (86%)	572 (94%)	33 (6%)	21	52
1	C	605/701 (86%)	580 (96%)	25 (4%)	30	60
1	D	604/701 (86%)	577 (96%)	27 (4%)	27	58
All	All	2394/2804 (85%)	2291 (96%)	103 (4%)	29	59

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASP
1	A	110	GLN

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Mol	Chain	Res	Type
1	A	186	LYS
1	A	192	LEU
1	A	196	ARG
1	A	227	ASP
1	A	373	SER
1	A	411	ASN
1	A	454	ASP
1	A	484	VAL
1	A	498	LEU
1	A	633	ILE
1	A	681	VAL
1	A	699	LYS
1	A	709	ASN
1	A	760	ASP
1	A	773	CYS
1	A	787	LEU
1	B	24	TYR
1	B	39	PHE
1	B	58	ASN
1	B	127	GLN
1	B	143	THR
1	B	166	ILE
1	B	178	LEU
1	B	181	ASP
1	B	192	LEU
1	B	252	LEU
1	B	321	TRP
1	B	380	VAL
1	B	383	THR
1	B	411	ASN
1	B	413	GLU
1	B	420	ARG
1	B	435	HIS
1	B	454	ASP
1	B	457	THR
1	B	461	ASN
1	B	490	ASP
1	B	491	PHE
1	B	498	LEU
1	B	509	LYS
1	B	517	PHE
1	B	533	TYR

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Mol	Chain	Res	Type
1	B	626	VAL
1	B	628	ARG
1	B	638	ASP
1	B	708	MET
1	B	721	MET
1	B	726	ASN
1	B	773	CYS
1	C	143	THR
1	C	172	ASP
1	C	260	TRP
1	C	346	ASP
1	C	350	LYS
1	C	373	SER
1	C	376	ASP
1	C	381	THR
1	C	382	LEU
1	C	390	LEU
1	C	394	THR
1	C	413	GLU
1	C	414	MET
1	C	420	ARG
1	C	447	ASP
1	C	454	ASP
1	C	457	THR
1	C	458	LYS
1	C	498	LEU
1	C	639	LEU
1	C	640	SER
1	C	650	LEU
1	C	678	GLU
1	C	736	THR
1	C	744	THR
1	D	18	ARG
1	D	46	ASP
1	D	114	ASP
1	D	129	ASP
1	D	155	LYS
1	D	170	LYS
1	D	174	THR
1	D	178	LEU
1	D	243	PHE
1	D	304	ILE

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Mol	Chain	Res	Type
1	D	309	ASN
1	D	321	TRP
1	D	381	THR
1	D	382	LEU
1	D	384	GLU
1	D	387	THR
1	D	425	CYS
1	D	457	THR
1	D	498	LEU
1	D	597	SER
1	D	623	PHE
1	D	638	ASP
1	D	650	LEU
1	D	678	GLU
1	D	754	SER
1	D	772	GLU
1	D	789	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	300	GLN
1	D	180	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 ⓘ

10 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	D	902	1	14,14,15	0.84	1 (7%)	17,19,21	0.31	0
3	NAG	A	902	1	14,14,15	1.21	1 (7%)	17,19,21	0.74	1 (5%)
3	NAG	C	902	1	14,14,15	0.47	0	17,19,21	0.65	0
2	KAI	C	901	-	6,15,15	0.90	0	8,21,21	1.09	1 (12%)
2	KAI	A	901	-	6,15,15	0.72	0	8,21,21	0.73	0
4	FWF	A	903	-	31,33,33	1.44	2 (6%)	38,48,48	3.56	7 (18%)
2	KAI	B	901	-	6,15,15	0.84	0	8,21,21	1.20	1 (12%)
2	KAI	D	901	-	6,15,15	0.75	0	8,21,21	1.04	0
4	FWF	C	903	-	31,33,33	1.47	2 (6%)	38,48,48	3.22	4 (10%)
3	NAG	B	902	1	14,14,15	0.53	0	17,19,21	0.52	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	D	902	1	-	0/6/23/26	0/1/1/1
3	NAG	A	902	1	-	2/6/23/26	0/1/1/1
3	NAG	C	902	1	-	3/6/23/26	0/1/1/1
2	KAI	C	901	-	-	2/6/25/25	0/1/1/1
2	KAI	A	901	-	-	0/6/25/25	0/1/1/1
4	FWF	A	903	-	-	1/32/36/36	0/2/2/2
2	KAI	B	901	-	-	2/6/25/25	0/1/1/1
2	KAI	D	901	-	-	0/6/25/25	0/1/1/1
4	FWF	C	903	-	-	0/32/36/36	0/2/2/2
3	NAG	B	902	1	-	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	903	FWF	C20-S2	-5.65	1.66	1.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	903	FWF	C19-S1	-5.60	1.66	1.78
4	C	903	FWF	C19-S1	-5.51	1.66	1.78
4	A	903	FWF	C20-S2	-5.33	1.67	1.78
3	A	902	NAG	O5-C1	-4.30	1.36	1.43
3	D	902	NAG	O5-C1	-2.83	1.39	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	903	FWF	O4-S2-O3	-15.72	107.45	119.24
4	C	903	FWF	O2-S1-O1	-13.29	109.27	119.24
4	A	903	FWF	O2-S1-O1	-13.09	109.42	119.24
4	C	903	FWF	O4-S2-O3	-13.05	109.45	119.24
4	A	903	FWF	O4-S2-N1	3.60	112.10	107.76
2	B	901	KAI	CG1-CB1-CB	-2.71	110.36	115.91
4	A	903	FWF	O1-S1-N2	2.30	110.53	107.76
4	A	903	FWF	C3-C4-C10	-2.26	117.44	121.36
2	C	901	KAI	CG1-CB1-CB	-2.22	111.36	115.91
3	A	902	NAG	O3-C3-C2	2.19	114.00	109.47
4	C	903	FWF	O1-S1-N2	2.19	110.40	107.76
4	A	903	FWF	C9-C8-C7	-2.11	119.07	121.20
4	A	903	FWF	C9-C10-C4	-2.03	117.85	121.36
4	C	903	FWF	C3-C4-C10	-2.01	117.86	121.36

There are no chirality outliers.

All (12) torsion outliers are listed below:

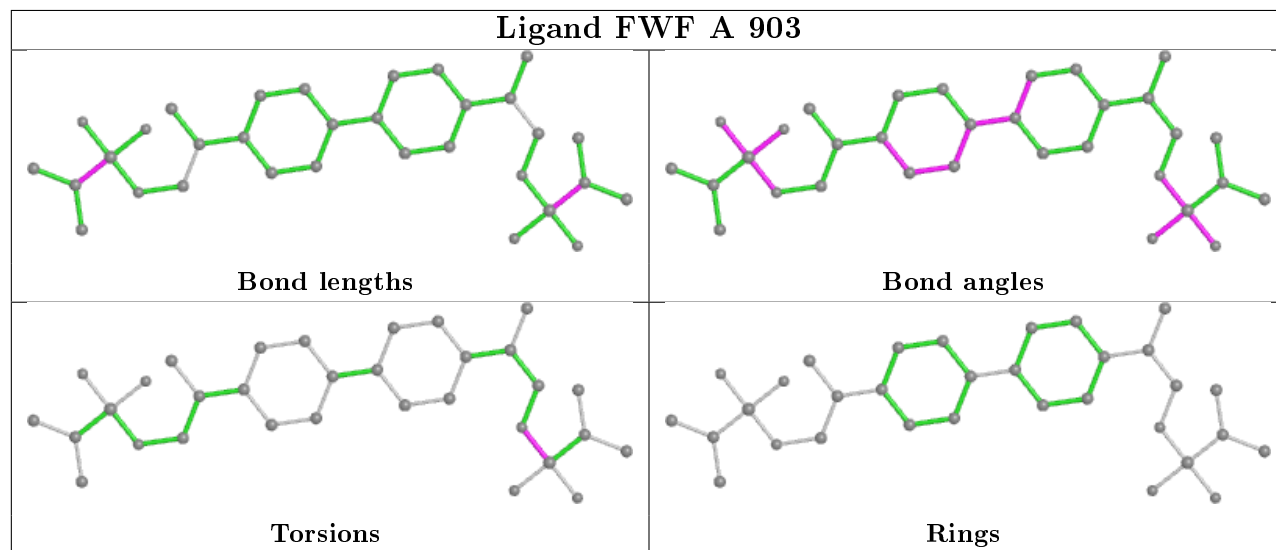
Mol	Chain	Res	Type	Atoms
2	C	901	KAI	CA-CB-CB1-CG1
2	C	901	KAI	CG-CB-CB1-CG1
4	A	903	FWF	C15-N1-S2-O4
2	B	901	KAI	CA-CB-CB1-CG1
2	B	901	KAI	CG-CB-CB1-CG1
3	A	902	NAG	C8-C7-N2-C2
3	A	902	NAG	O7-C7-N2-C2
3	C	902	NAG	C8-C7-N2-C2
3	C	902	NAG	O7-C7-N2-C2
3	B	902	NAG	C8-C7-N2-C2
3	B	902	NAG	O7-C7-N2-C2
3	C	902	NAG	O5-C5-C6-O6

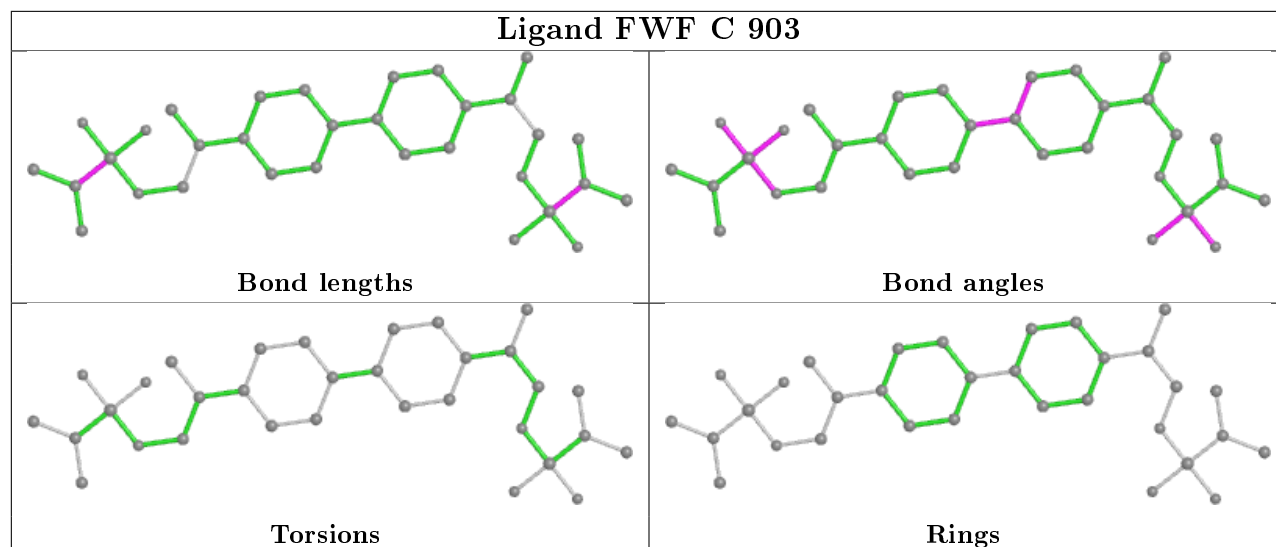
There are no ring outliers.

7 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	901	KAI	2	0
2	A	901	KAI	1	0
4	A	903	FWF	4	0
2	B	901	KAI	3	0
2	D	901	KAI	1	0
4	C	903	FWF	5	0
3	B	902	NAG	2	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	731/824 (88%)	0.55	72 (9%) 7 7	84, 150, 201, 227	0
1	B	751/824 (91%)	0.49	55 (7%) 15 14	59, 127, 207, 262	0
1	C	736/824 (89%)	0.56	66 (8%) 9 10	70, 145, 221, 257	0
1	D	750/824 (91%)	0.63	83 (11%) 5 5	65, 161, 238, 284	0
All	All	2968/3296 (90%)	0.56	276 (9%) 8 9	59, 146, 220, 284	0

All (276) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	14	GLY	14.2
1	C	13	GLY	12.1
1	C	12	ILE	9.0
1	C	15	LEU	8.9
1	B	779	GLY	7.7
1	D	37	SER	6.5
1	C	370	GLY	6.5
1	D	49	GLU	6.5
1	C	42	THR	6.4
1	B	600	ILE	6.4
1	C	73	GLY	6.4
1	C	43	PRO	5.7
1	C	797	TYR	5.5
1	C	69	TYR	5.4
1	A	517	PHE	5.4
1	D	290	MET	5.3
1	A	304	ILE	5.3
1	C	304	ILE	5.3
1	C	60	PHE	5.2
1	A	514	VAL	5.1
1	D	50	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	41	LEU	4.8
1	B	631	SER	4.8
1	B	316	ASN	4.7
1	C	72	PHE	4.5
1	D	629	MET	4.4
1	D	43	PRO	4.4
1	D	516	SER	4.4
1	B	778	SER	4.3
1	C	795	VAL	4.3
1	D	345	PHE	4.3
1	C	70	ALA	4.2
1	A	629	MET	4.2
1	A	615	SER	4.2
1	D	291	THR	4.1
1	B	9	SER	4.1
1	D	331	LEU	4.1
1	C	307	ARG	4.1
1	D	111	MET	4.0
1	B	593	PRO	4.0
1	D	12	ILE	4.0
1	D	32	VAL	3.9
1	D	339	LEU	3.9
1	A	443	THR	3.9
1	A	270	GLY	3.8
1	B	69	TYR	3.8
1	D	351	ARG	3.8
1	A	779	GLY	3.8
1	A	518	LEU	3.8
1	C	41	LEU	3.7
1	B	39	PHE	3.7
1	C	290	MET	3.7
1	D	93	SER	3.7
1	D	131	PHE	3.6
1	D	792	VAL	3.6
1	A	442	LEU	3.6
1	D	287	VAL	3.6
1	D	48	LEU	3.6
1	B	630	VAL	3.6
1	D	51	ALA	3.6
1	A	294	PHE	3.6
1	A	812	ILE	3.5
1	D	10	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	36	THR	3.5
1	D	344	LYS	3.5
1	B	780	SER	3.5
1	C	326	GLU	3.5
1	C	16	PHE	3.4
1	A	339	LEU	3.4
1	B	797	TYR	3.4
1	C	636	ALA	3.4
1	A	425	CYS	3.4
1	C	336	VAL	3.4
1	D	354	TYR	3.4
1	C	245	ILE	3.4
1	D	38	GLU	3.4
1	B	314	LEU	3.4
1	C	11	GLN	3.4
1	D	54	PHE	3.4
1	B	114	ASP	3.4
1	D	327	ILE	3.4
1	D	512	PRO	3.3
1	C	791	ASN	3.3
1	C	798	ILE	3.3
1	D	74	PHE	3.3
1	B	348	ASN	3.3
1	B	14	GLY	3.3
1	B	521	LEU	3.3
1	B	223	LEU	3.2
1	D	630	VAL	3.2
1	C	631	SER	3.2
1	D	113	PRO	3.2
1	A	12	ILE	3.2
1	D	602	ALA	3.2
1	A	39	PHE	3.2
1	D	56	VAL	3.2
1	D	601	VAL	3.1
1	D	18	ARG	3.1
1	D	119	LEU	3.1
1	C	71	ILE	3.1
1	A	400	ILE	3.1
1	A	780	SER	3.1
1	D	63	GLN	3.1
1	A	399	THR	3.1
1	C	371	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	289	VAL	3.1
1	A	727	LEU	3.1
1	B	113	PRO	3.0
1	C	633	ILE	3.0
1	D	13	GLY	3.0
1	C	792	VAL	3.0
1	C	337	GLU	3.0
1	D	326	GLU	3.0
1	A	444	ILE	3.0
1	B	633	ILE	3.0
1	D	9	SER	3.0
1	D	543	VAL	3.0
1	C	732	TYR	3.0
1	A	600	ILE	2.9
1	C	68	VAL	2.9
1	D	14	GLY	2.9
1	C	479	LEU	2.9
1	D	743	GLY	2.9
1	D	245	ILE	2.9
1	B	304	ILE	2.9
1	A	428	LEU	2.9
1	A	290	MET	2.9
1	B	110	GLN	2.9
1	B	634	GLU	2.9
1	C	632	PRO	2.9
1	A	496	MET	2.8
1	A	46	ASP	2.8
1	A	725	GLY	2.8
1	D	607	PHE	2.8
1	C	400	ILE	2.8
1	D	282	LEU	2.8
1	B	15	LEU	2.8
1	C	74	PHE	2.8
1	D	328	GLU	2.8
1	B	425	CYS	2.8
1	D	39	PHE	2.8
1	C	519	ASP	2.8
1	A	767	TRP	2.8
1	A	792	VAL	2.8
1	B	701	ALA	2.8
1	B	527	MET	2.8
1	D	309	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	224	GLY	2.7
1	D	45	ILE	2.7
1	D	664	ILE	2.7
1	D	701	ALA	2.7
1	C	86	PHE	2.7
1	D	72	PHE	2.7
1	C	634	GLU	2.7
1	A	93	SER	2.7
1	C	31	MET	2.7
1	C	478	PRO	2.7
1	B	529	ILE	2.7
1	C	40	ARG	2.7
1	A	476	ILE	2.7
1	B	817	LYS	2.6
1	A	429	ALA	2.6
1	C	529	ILE	2.6
1	D	29	VAL	2.6
1	A	686	THR	2.6
1	C	243	PHE	2.6
1	A	596	LEU	2.6
1	A	732	TYR	2.6
1	A	467	LEU	2.6
1	C	518	LEU	2.6
1	A	724	GLY	2.5
1	D	343	ILE	2.5
1	C	630	VAL	2.5
1	A	701	ALA	2.5
1	A	597	SER	2.5
1	B	768	TYR	2.5
1	A	620	LEU	2.5
1	C	709	ASN	2.5
1	D	70	ALA	2.5
1	D	284	TYR	2.5
1	A	10	ILE	2.5
1	B	525	ILE	2.5
1	D	244	GLN	2.5
1	B	623	PHE	2.5
1	A	626	VAL	2.5
1	B	70	ALA	2.5
1	D	536	VAL	2.5
1	C	796	PHE	2.5
1	A	777	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	602	ALA	2.4
1	D	27	PHE	2.4
1	A	540	LEU	2.4
1	D	790	SER	2.4
1	B	262	THR	2.4
1	C	615	SER	2.4
1	A	108	VAL	2.4
1	A	670	MET	2.4
1	C	9	SER	2.4
1	C	358	ILE	2.4
1	D	670	MET	2.4
1	C	131	PHE	2.4
1	B	720	THR	2.4
1	B	607	PHE	2.4
1	D	15	LEU	2.4
1	B	139	ARG	2.4
1	C	629	MET	2.4
1	A	60	PHE	2.3
1	C	503	MET	2.3
1	A	784	THR	2.3
1	A	307	ARG	2.3
1	B	601	VAL	2.3
1	D	35	SER	2.3
1	B	541	PHE	2.3
1	B	784	THR	2.3
1	D	109	ILE	2.3
1	B	345	PHE	2.3
1	D	133	TYR	2.3
1	D	813	GLU	2.3
1	D	504	ILE	2.3
1	D	286	ALA	2.3
1	D	57	THR	2.3
1	B	327	ILE	2.3
1	B	38	GLU	2.3
1	C	731	GLY	2.3
1	A	356	ILE	2.3
1	D	605	TRP	2.2
1	C	138	ASP	2.2
1	C	356	ILE	2.2
1	D	797	TYR	2.2
1	A	72	PHE	2.2
1	B	504	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	617	THR	2.2
1	B	349	GLY	2.2
1	B	307	ARG	2.2
1	A	297	LEU	2.2
1	A	109	ILE	2.2
1	A	598	ALA	2.2
1	B	506	LYS	2.2
1	B	528	ALA	2.2
1	B	659	PHE	2.2
1	A	426	VAL	2.2
1	B	816	TYR	2.2
1	D	137	SER	2.2
1	C	20	ALA	2.2
1	A	608	PHE	2.2
1	B	282	LEU	2.2
1	A	454	ASP	2.2
1	A	595	SER	2.2
1	A	634	GLU	2.2
1	A	40	ARG	2.1
1	D	337	GLU	2.1
1	D	667	PHE	2.1
1	A	624	LEU	2.1
1	D	138	ASP	2.1
1	A	659	PHE	2.1
1	C	760	ASP	2.1
1	B	596	LEU	2.1
1	C	606	TRP	2.1
1	C	498	LEU	2.1
1	C	515	PHE	2.1
1	A	111	MET	2.1
1	D	90	LEU	2.1
1	D	71	ILE	2.0
1	C	56	VAL	2.0
1	B	703	LEU	2.0
1	D	41	LEU	2.0
1	A	131	PHE	2.0
1	A	495	PHE	2.0
1	A	498	LEU	2.0
1	B	605	TRP	2.0
1	A	139	ARG	2.0
1	A	703	LEU	2.0
1	D	60	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	331	LEU	2.0
1	A	450	TYR	2.0
1	D	158	VAL	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](#)

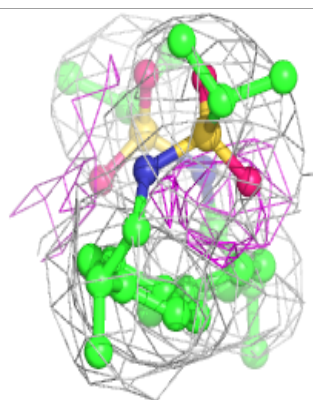
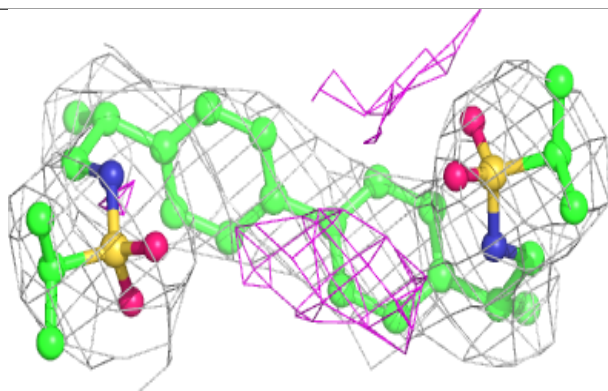
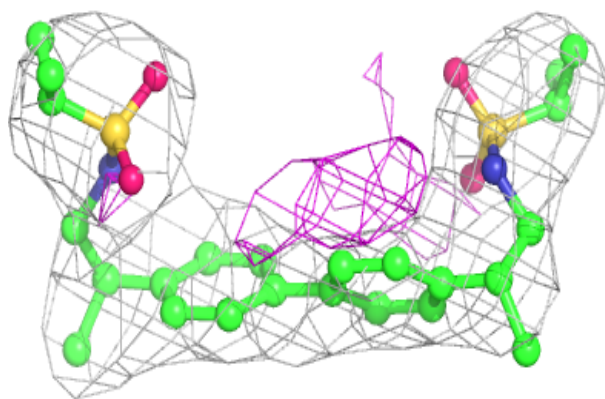
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B	902	14/15	0.65	0.37	140,155,166,170	0
3	NAG	C	902	14/15	0.88	0.24	99,124,138,140	0
3	NAG	A	902	14/15	0.89	0.32	95,132,174,174	0
3	NAG	D	902	14/15	0.90	0.21	136,157,168,172	0
2	KAI	A	901	15/15	0.91	0.33	106,122,133,135	0
2	KAI	D	901	15/15	0.93	0.46	96,118,158,169	0
4	FWF	C	903	32/32	0.94	0.43	43,87,148,165	0
4	FWF	A	903	32/32	0.94	0.53	84,109,162,172	0
2	KAI	B	901	15/15	0.96	0.29	66,81,99,101	0
2	KAI	C	901	15/15	0.96	0.36	91,103,128,132	0

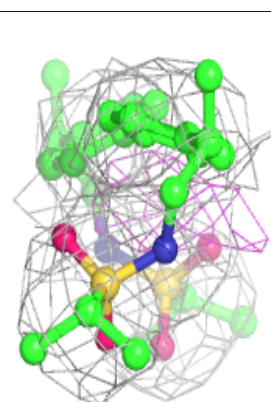
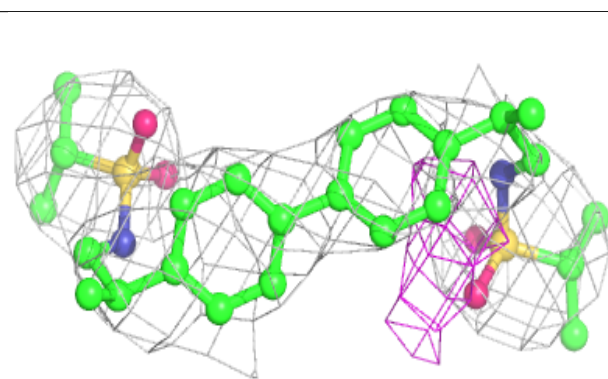
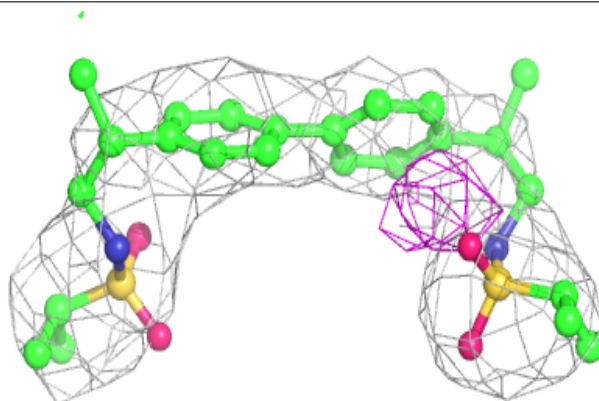
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FWF C 903:

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

**Electron density around FWF A 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.