



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:42 PM UTC

PDB ID : 4U1W / pdb_00004u1w
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 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

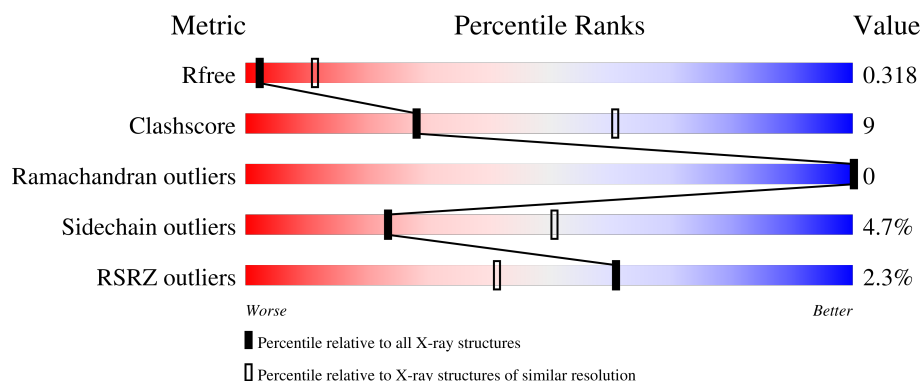
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (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 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	2% 70% 17% 11%
1	B	824	2% 71% 19% 9%
1	C	824	2% 66% 22% 11%
1	D	824	2% 67% 22% 9%

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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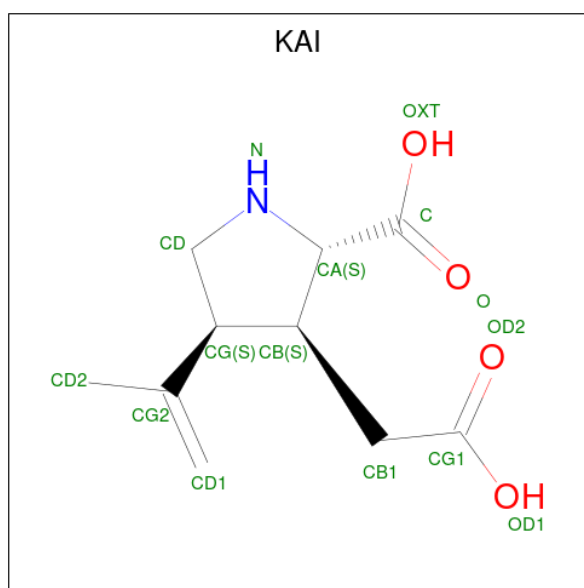
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	SER	deletion	UNP P19491
B	?	-	GLY	deletion	UNP P19491
B	385	ASP	ASN	engineered mutation	UNP P19491
B	392	GLN	ASN	engineered mutation	UNP P19491
B	528	ALA	CYS	engineered mutation	UNP P19491
B	585	PHE	MET	engineered mutation	UNP P19491
B	589	ALA	CYS	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 (CCD ID: KAI) (formula: $C_{10}H_{15}NO_4$).



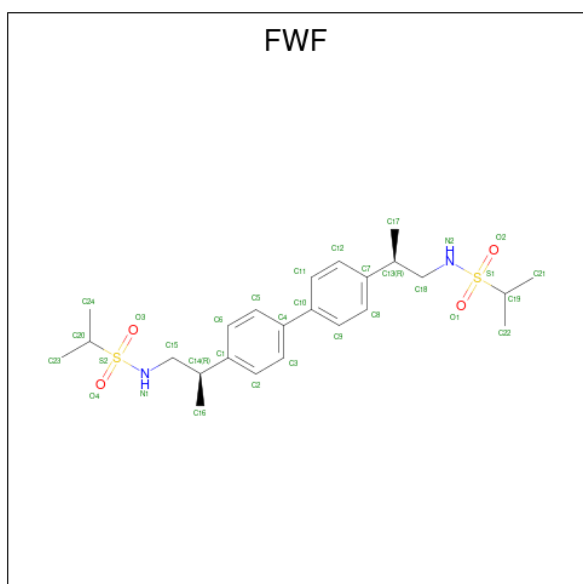
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	10	1	4		
2	B	1	Total	C	N	O	0	0
			15	10	1	4		
2	C	1	Total	C	N	O	0	0
			15	10	1	4		
2	D	1	Total	C	N	O	0	0
			15	10	1	4		

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

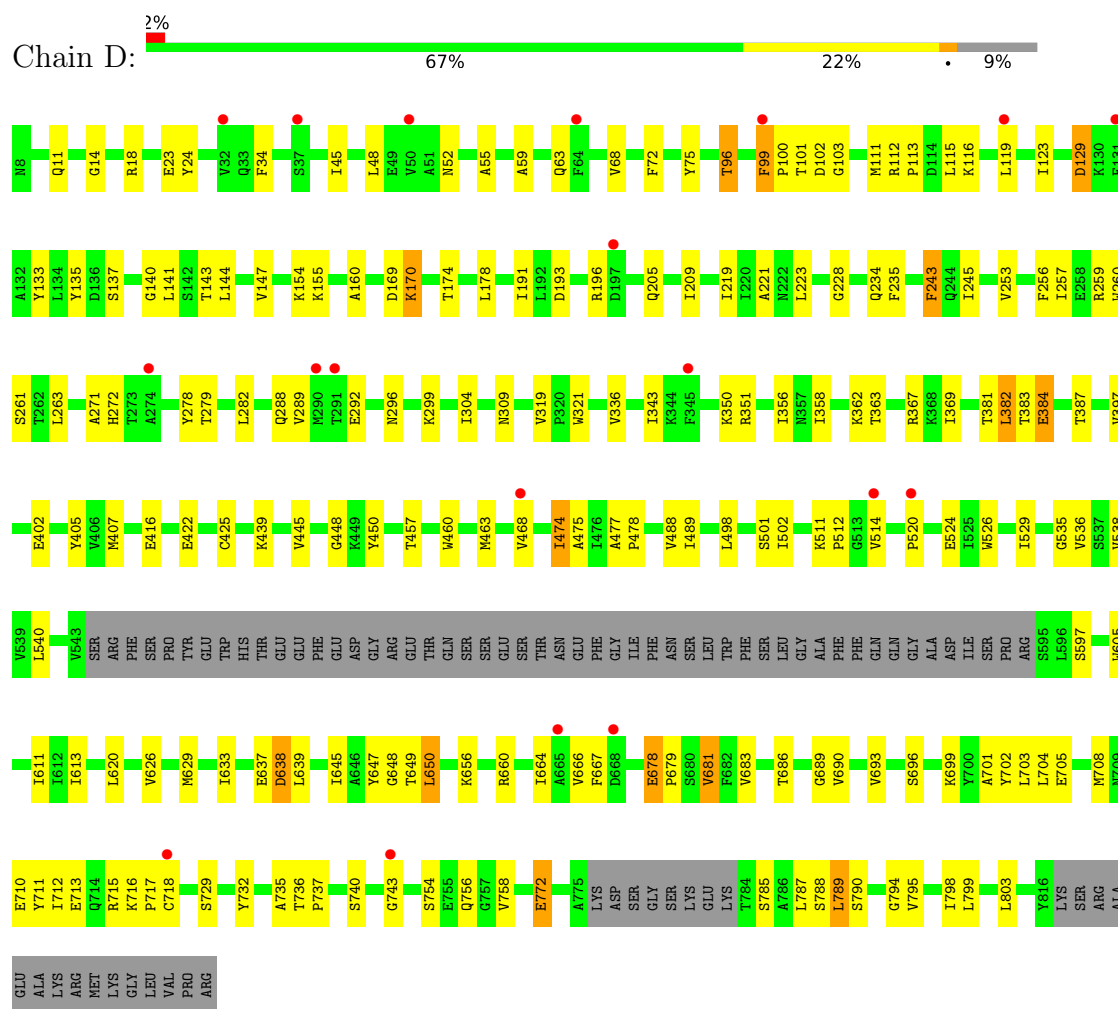


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- 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	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		



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 29.91 – 3.25	Depositor EDS
% Data completeness (in resolution range)	79.8 (29.91-3.25) 79.6 (29.91-3.25)	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 0.272 , 0.318	Depositor DCC
R_{free} test set	3359 reflections (3.97%)	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)	0.24 , 57.0	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	0.90	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 ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.30	0/5685	0.77	5/7719 (0.1%)
1	B	0.31	0/5884	0.79	6/7974 (0.1%)
1	C	0.30	0/5826	0.77	5/7888 (0.1%)
1	D	0.31	0/5900	0.79	6/8002 (0.1%)
All	All	0.31	0/23295	0.78	22/31583 (0.1%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	99	PHE	CA-C-N	7.17	127.20	119.89
1	D	99	PHE	C-N-CA	7.17	127.20	119.89
1	B	105	HIS	CA-C-N	6.84	127.01	120.31
1	B	105	HIS	C-N-CA	6.84	127.01	120.31
1	A	96	THR	CA-C-N	6.78	126.40	119.56
1	A	96	THR	C-N-CA	6.78	126.40	119.56
1	C	105	HIS	CA-C-N	6.73	126.90	120.31
1	C	105	HIS	C-N-CA	6.73	126.90	120.31
1	B	511	LYS	CA-C-N	6.46	125.69	118.97
1	B	511	LYS	C-N-CA	6.46	125.69	118.97
1	B	96	THR	CA-C-N	6.43	126.05	119.56
1	B	96	THR	C-N-CA	6.43	126.05	119.56
1	C	96	THR	CA-C-N	6.24	125.86	119.56
1	C	96	THR	C-N-CA	6.24	125.86	119.56
1	D	511	LYS	CA-C-N	6.23	125.64	118.85
1	D	511	LYS	C-N-CA	6.23	125.64	118.85
1	A	105	HIS	CA-C-N	6.17	126.36	120.31
1	A	105	HIS	C-N-CA	6.17	126.36	120.31
1	D	96	THR	CA-C-N	5.83	125.45	119.56
1	D	96	THR	C-N-CA	5.83	125.45	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	171	LYS	CB-CA-C	-5.64	110.06	116.54
1	A	786	ALA	CB-CA-C	-5.15	110.66	116.63

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	5571	0	5425	91	0
1	B	5767	0	5672	101	0
1	C	5713	0	5643	118	0
1	D	5780	0	5656	117	0
2	A	15	0	13	2	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
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	407	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 (407) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ILE:HG12	1:B:378:MET:HE1	1.72	0.71
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:C:625:THR:HG22	1:C:629:MET:HE3	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
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:OD1	1:A:411:ASN:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:335:GLN:CD	3:B:902:NAG:H82	2.28	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:A:321:TRP:H	1:A:321:TRP:CD1	2.21	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
1:D:48:LEU:HD12	1:D:55:ALA:HB1	1.87	0.55
1:B:31:MET:HE1	1:B:41:LEU:HB2	1.88	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:56:VAL:HG21	1:B:79:SER:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:99:PHE:CD1	1:D:100:PRO:HD2	2.42	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: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:141:LEU:HD11	1:D:141:LEU:HD13	1.91	0.52
1:C:751:LEU:HG	4:C:903:FWF:H28	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:D:101:THR:O	1:D:350:LYS:NZ	2.43	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:OD1	1:A:760:ASP:N	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:321:TRP:H	1:C:321:TRP:CD1	2.30	0.49
1:C:447:ASP:OD1	1:C:447:ASP:N	2.45	0.49
1:B:111:MET:HE1	1:B:289:VAL:HG21	1.94	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: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
1:B:809:VAL:HA	1:B:812:ILE:HG12	1.94	0.48
1:A:650:LEU:HG	1:A:702:TYR:OH	2.12	0.48
1:A:694:ARG:NE	1:A:719:ASP:OD1	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:C:642:GLN:NE2	2.47	0.47
1:B:205:GLN:O	1:B:209:ILE:HG13	2.14	0.47
1:C:169:ASP:OD1	1:C:169:ASP:N	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
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:C:678:GLU:HA	1:C:679:PRO:C	2.41	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:59:ALA:O	1:D:63:GLN:HG2	2.15	0.46
1:D:205:GLN:O	1:D:209:ILE:HG13	2.15	0.46
1:D:756:GLN:HG3	1:D:758:VAL:HG23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:TRP:CD1	1:D:321:TRP:H	2.33	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:OE1	1:B:23:GLU:N	2.47	0.46
1:B:253:VAL:O	1:B:257:ILE:HG12	2.16	0.46
1:C:536:VAL:HG22	1:D:803:LEU:HD21	1.97	0.46
1:D:263:LEU:HB2	1:D:271:ALA:HB1	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:450:TYR:HA	1:D:463:MET:HE2	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:B:450:TYR:HA	1:B:463:MET:HE2	1.97	0.45
1:C:336:VAL:HG23	1:C:343:ILE:HD12	1.98	0.45
1:D:111:MET:HE1	1:D:289:VAL:HG21	1.97	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: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:C:401:LEU:HA	1:C:406:VAL:HB	1.98	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:B:678:GLU:HA	1:B:679:PRO:C	2.42	0.45
1:D:119:LEU:HD21	1:D:133:TYR:HE1	1.81	0.45
1:A:786:ALA:HB1	1:D:520:PRO:O	2.17	0.45
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:D:678:GLU:HA	1:D:679:PRO:C	2.41	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:54:PHE:HA	1:B:86:PHE:HE1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HD12	2:A:901:KAI:HD2	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:D:638:ASP:OD1	1:D:638:ASP:N	2.49	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:C:20:ALA:HB1	1:C:23:GLU:CD	2.43	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
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:708:MET:HE2	2:A:901:KAI:HD12	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:TYR:CE2	1:B:96:THR:HG21	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: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:HD13	1:D:257:ILE:HA	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:404:PRO:HD3	1:C:711:TYR:CG	2.53	0.42
1:C:690:VAL:HG21	1:C:712:ILE:CD1	2.49	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:400:ILE:HG21	1:B:450:TYR:CZ	2.54	0.42
1:B:405:TYR:OH	1:B:732:TYR:HE2	2.03	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:234:GLN:NE2	1:D:363:THR:O	2.52	0.42
1:D:282:LEU:HD23	1:D:282:LEU:HA	1.90	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:HA	1:B:639:LEU:HD23	1.80	0.42
1:B:671:TRP:HA	1:B:674:MET:HE3	2.01	0.42
1:B:12:ILE:HD13	1:B:41:LEU:HD23	2.01	0.42
1:C:425:CYS:SG	1:C:477:ALA:HA	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:782:GLU:O	1:A:782:GLU:HG3	2.20	0.42
1:B:463:MET:HE3	1:B:463:MET:HB2	1.81	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:463:MET:HE1	1:A:477:ALA:HB3	2.02	0.41
1:A:651:ASP:N	1:A:683:VAL:O	2.45	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:A:211:LYS:HD3	1:A:211:LYS:HA	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:D:384:GLU:O	1:D:384:GLU:HG2	2.20	0.41
1:A:110:GLN:H	1:A:110:GLN:HE21	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:OD1	1:A:227:ASP:N	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:HD23	1:B:624:LEU:HA	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
1:A:29:VAL:HG21	1:A:260:TRP:HZ3	1.86	0.41
1:A:75:TYR:CE2	1:A:96:THR:HG21	2.56	0.41
1:A:540:LEU:HD23	1:A:540:LEU:HA	1.93	0.41
1:A:753:LEU:HD22	1:A:758:VAL:HG11	2.01	0.41
1:B:62:SER:O	1:B:66:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:619:ASN:ND2	1:C:787:LEU:HB2	2.35	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:D:501:SER:OG	1:D:502:ILE:N	2.52	0.41
1:D:705:GLU:OE2	1:D:732:TYR:OH	2.33	0.41
1:A:321:TRP:H	1:A:321:TRP:HD1	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:B:464:VAL:O	1:B:468:VAL:HG23	2.22	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: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:HD12	1:C:762:LEU:HA	1.90	0.40
1:D:23:GLU:OE2	1:D:279:THR:OG1	2.32	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:629:MET:HE3	1:D:629:MET:HB3	1.89	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:24:TYR:HE1	1:D:45:ILE:HG13	1.86	0.40
1:D:154:LYS:HD2	1:D:154:LYS:HA	1.90	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%)	553 (95%)	27 (5%)	23	51
1	B	605/701 (86%)	576 (95%)	29 (5%)	23	50
1	C	605/701 (86%)	577 (95%)	28 (5%)	24	51
1	D	604/701 (86%)	575 (95%)	29 (5%)	23	50
All	All	2394/2804 (85%)	2281 (95%)	113 (5%)	23	51

All (113) 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	163	VAL
1	A	186	LYS
1	A	187	GLU
1	A	192	LEU
1	A	196	ARG
1	A	227	ASP
1	A	319	VAL
1	A	373	SER
1	A	382	LEU
1	A	392	GLN
1	A	411	ASN
1	A	454	ASP
1	A	464	VAL
1	A	484	VAL
1	A	498	LEU
1	A	538	VAL
1	A	626	VAL
1	A	633	ILE
1	A	650	LEU
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	39	PHE
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	319	VAL
1	B	359	MET
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

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Mol	Chain	Res	Type
1	B	457	THR
1	B	461	ASN
1	B	490	ASP
1	B	498	LEU
1	B	509	LYS
1	B	612	ILE
1	B	626	VAL
1	B	628	ARG
1	B	721	MET
1	B	723	VAL
1	B	726	ASN
1	B	773	CYS
1	C	129	ASP
1	C	143	THR
1	C	169	ASP
1	C	170	LYS
1	C	260	TRP
1	C	319	VAL
1	C	346	ASP
1	C	350	LYS
1	C	369	ILE
1	C	373	SER
1	C	375	VAL
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	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	129	ASP

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Mol	Chain	Res	Type
1	D	155	LYS
1	D	170	LYS
1	D	174	THR
1	D	178	LEU
1	D	243	PHE
1	D	304	ILE
1	D	309	ASN
1	D	319	VAL
1	D	381	THR
1	D	382	LEU
1	D	384	GLU
1	D	387	THR
1	D	416	GLU
1	D	425	CYS
1	D	457	THR
1	D	474	ILE
1	D	498	LEU
1	D	597	SER
1	D	638	ASP
1	D	650	LEU
1	D	678	GLU
1	D	681	VAL
1	D	754	SER
1	D	772	GLU
1	D	785	SER
1	D	789	LEU
1	D	799	LEU

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

Mol	Chain	Res	Type
1	A	217	HIS
1	B	145	GLN
1	B	200	ASN
1	C	333	GLN
1	C	714	GLN
1	C	764	ASN
1	D	180	GLN
1	D	300	GLN
1	D	333	GLN
1	D	619	ASN

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 ⓘ

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	$\# Z > 2$
2	KAI	A	901	-	13,15,15	1.02	0	12,21,21	1.17	0
3	NAG	B	902	1	14,14,15	0.53	0	17,19,21	0.53	0
3	NAG	C	902	1	14,14,15	0.46	0	17,19,21	0.65	0
2	KAI	D	901	-	13,15,15	1.04	0	12,21,21	1.21	1 (8%)
2	KAI	B	901	-	13,15,15	1.09	0	12,21,21	1.21	1 (8%)
3	NAG	D	902	1	14,14,15	0.81	1 (7%)	17,19,21	0.33	0
2	KAI	C	901	-	13,15,15	1.14	1 (7%)	12,21,21	1.16	1 (8%)
4	FWF	C	903	-	31,33,33	0.42	0	40,48,48	1.86	4 (10%)
4	FWF	A	903	-	31,33,33	0.42	0	40,48,48	2.09	6 (15%)
3	NAG	A	902	1	14,14,15	1.15	1 (7%)	17,19,21	0.75	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KAI	A	901	-	-	4/12/25/25	0/1/1/1
3	NAG	B	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	D	901	-	-	4/12/25/25	0/1/1/1
2	KAI	B	901	-	-	4/12/25/25	0/1/1/1
3	NAG	D	902	1	-	0/6/23/26	0/1/1/1
2	KAI	C	901	-	-	4/12/25/25	0/1/1/1
4	FWF	C	903	-	-	0/32/36/36	0/2/2/2
4	FWF	A	903	-	-	1/32/36/36	0/2/2/2
3	NAG	A	902	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	NAG	O5-C1	-4.07	1.36	1.43
3	D	902	NAG	O5-C1	-2.68	1.39	1.43
2	C	901	KAI	CB-CA	-2.05	1.51	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	903	FWF	O4-S2-O3	-7.83	107.45	118.88
4	C	903	FWF	O2-S1-O1	-6.58	109.27	118.88
4	A	903	FWF	O2-S1-O1	-6.48	109.42	118.88
4	C	903	FWF	O4-S2-O3	-6.46	109.45	118.88
4	A	903	FWF	O4-S2-N1	3.82	112.10	107.65
4	A	903	FWF	O1-S1-N2	2.47	110.53	107.65
2	D	901	KAI	CB-CA-C	-2.45	109.05	113.98
4	C	903	FWF	O1-S1-N2	2.36	110.40	107.65
2	B	901	KAI	CB-CA-C	-2.28	109.41	113.98
3	A	902	NAG	O3-C3-C2	2.22	114.00	109.40
4	A	903	FWF	C3-C4-C10	-2.21	117.44	121.25
4	C	903	FWF	O4-S2-N1	2.15	110.15	107.65
2	C	901	KAI	CB-CA-C	-2.12	109.73	113.98
4	A	903	FWF	C9-C8-C7	-2.11	119.07	121.18

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	KAI	O-C-CA-N

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Mol	Chain	Res	Type	Atoms
2	A	901	KAI	OXT-C-CA-N
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	A	903	FWF	C15-N1-S2-O4
3	A	902	NAG	C8-C7-N2-C2
3	A	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	C8-C7-N2-C2
3	C	902	NAG	O7-C7-N2-C2
2	D	901	KAI	OXT-C-CA-N
3	C	902	NAG	O5-C5-C6-O6
2	D	901	KAI	O-C-CA-N
2	B	901	KAI	CG-CB-CB1-CG1
2	D	901	KAI	CB-CB1-CG1-OD1
2	D	901	KAI	CB-CB1-CG1-OD2
2	B	901	KAI	CB-CB1-CG1-OD1
2	B	901	KAI	CB-CB1-CG1-OD2
2	A	901	KAI	CB-CB1-CG1-OD1
2	C	901	KAI	CB-CB1-CG1-OD2
2	A	901	KAI	CB-CB1-CG1-OD2
2	C	901	KAI	CB-CB1-CG1-OD1

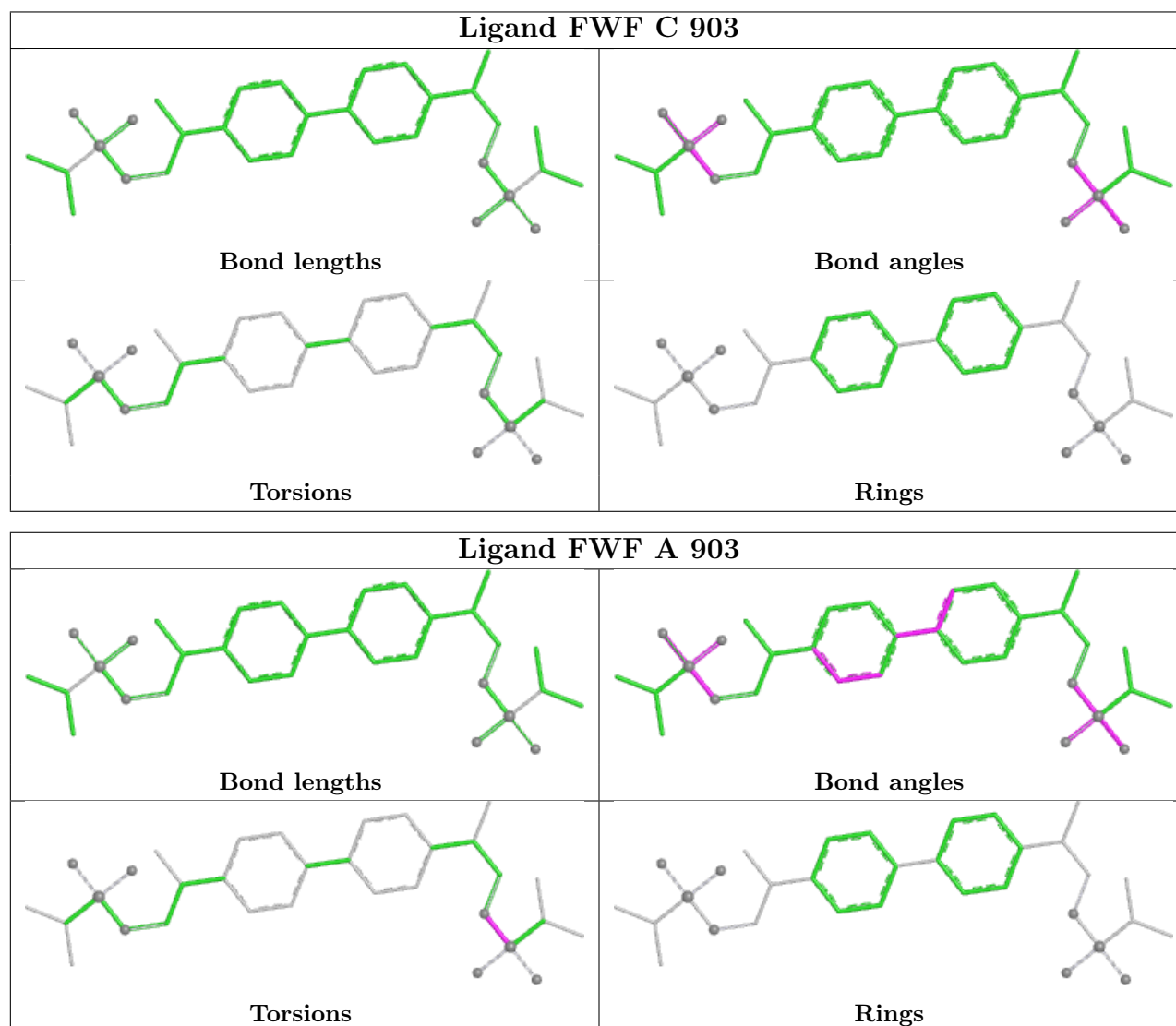
There are no ring outliers.

7 monomers are involved in 19 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.07	11 (1%) 72 53	84, 150, 201, 227	0
1	B	751/824 (91%)	0.02	19 (2%) 58 39	59, 126, 207, 262	0
1	C	736/824 (89%)	0.08	19 (2%) 57 38	70, 145, 221, 257	0
1	D	750/824 (91%)	0.13	19 (2%) 58 39	65, 161, 238, 284	0
All	All	2968/3296 (90%)	0.08	68 (2%) 61 41	59, 146, 220, 284	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	779	GLY	4.5
1	A	376	ASP	4.4
1	C	12	ILE	4.3
1	D	37	SER	4.3
1	C	370	GLY	4.2
1	B	187	GLU	4.0
1	D	345	PHE	3.7
1	B	316	ASN	3.7
1	A	339	LEU	3.5
1	C	20	ALA	3.4
1	B	348	ASN	3.4
1	A	615	SER	3.4
1	A	517	PHE	3.3
1	B	314	LEU	3.3
1	B	768	TYR	3.3
1	C	13	GLY	3.3
1	D	668	ASP	3.2
1	D	64	PHE	3.2
1	C	676	SER	3.1
1	C	42	THR	3.0
1	B	235	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	809	VAL	2.9
1	C	791	ASN	2.9
1	D	291	THR	2.8
1	D	32	VAL	2.8
1	C	304	ILE	2.8
1	B	113	PRO	2.8
1	B	9	SER	2.8
1	B	184	LEU	2.8
1	A	204	ASP	2.8
1	D	290	MET	2.7
1	C	479	LEU	2.7
1	C	14	GLY	2.6
1	D	119	LEU	2.6
1	C	358	ILE	2.5
1	C	808	LEU	2.5
1	B	793	ALA	2.4
1	B	593	PRO	2.4
1	A	138	ASP	2.4
1	B	797	TYR	2.4
1	C	15	LEU	2.4
1	D	718	CYS	2.4
1	D	197	ASP	2.3
1	D	99	PHE	2.3
1	B	258	GLU	2.3
1	D	520	PRO	2.3
1	D	274	ALA	2.3
1	A	792	VAL	2.3
1	C	527	MET	2.2
1	D	514	VAL	2.2
1	A	205	GLN	2.2
1	A	385	ASP	2.2
1	D	468	VAL	2.2
1	D	665	ALA	2.2
1	B	194	CYS	2.2
1	C	760	ASP	2.2
1	D	131	PHE	2.2
1	B	223	LEU	2.1
1	C	138	ASP	2.1
1	D	50	VAL	2.1
1	B	355	THR	2.1
1	B	231	LEU	2.1
1	C	815	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	743	GLY	2.1
1	C	195	GLU	2.1
1	A	454	ASP	2.0
1	A	655	THR	2.0
1	C	519	ASP	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](#)

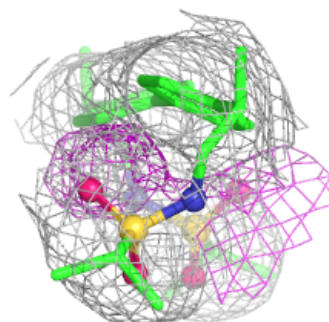
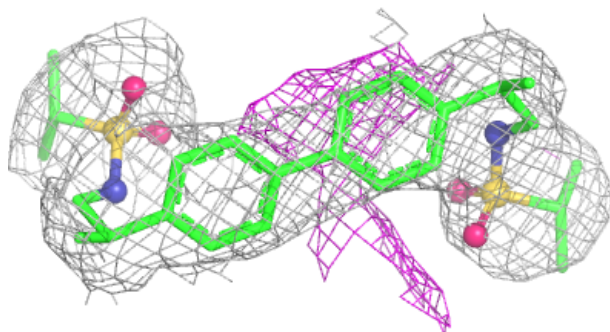
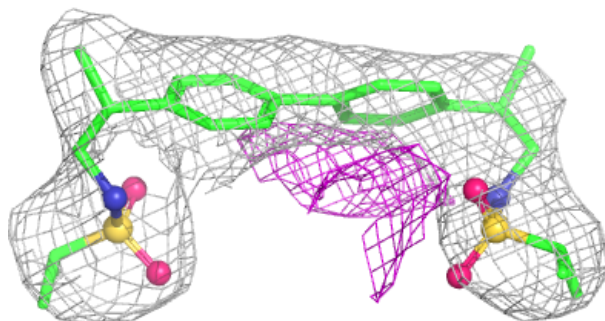
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B	902	14/15	0.19	0.13	140,155,166,170	0
3	NAG	D	902	14/15	0.57	0.09	136,157,168,172	0
3	NAG	C	902	14/15	0.81	0.10	99,124,138,140	0
3	NAG	A	902	14/15	0.86	0.19	95,132,174,174	0
2	KAI	A	901	15/15	0.89	0.11	106,122,133,135	0
2	KAI	C	901	15/15	0.91	0.14	91,103,128,132	0
4	FWF	C	903	32/32	0.92	0.12	43,87,148,165	0
4	FWF	A	903	32/32	0.93	0.14	84,109,162,172	0
2	KAI	B	901	15/15	0.94	0.10	66,81,99,101	0
2	KAI	D	901	15/15	0.94	0.13	96,118,158,169	0

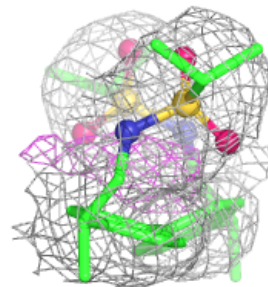
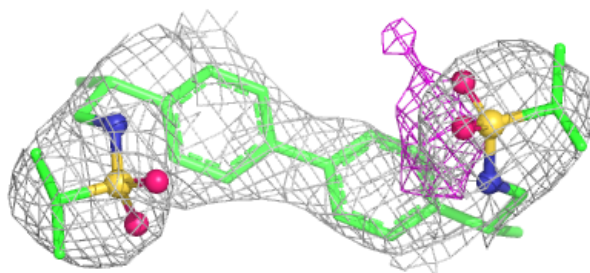
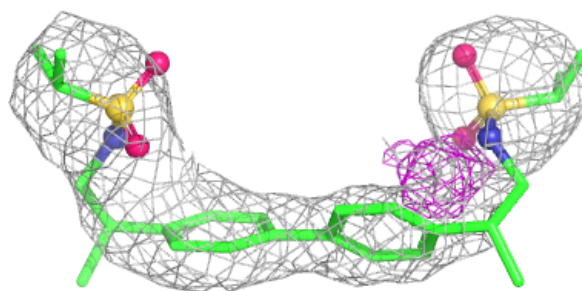
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

There are no such residues in this entry.