



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:17 AM UTC

PDB ID : 5L1F / pdb_0000511f
Title : AMPA subtype ionotropic glutamate receptor GluA2 in complex with non-competitive inhibitor Perampanel
Authors : Yelshanskaya, M.V.; Singh, A.K.; Sampson, J.M.; Sobolevsky, A.I.
Deposited on : 2016-07-29
Resolution : 4.00 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

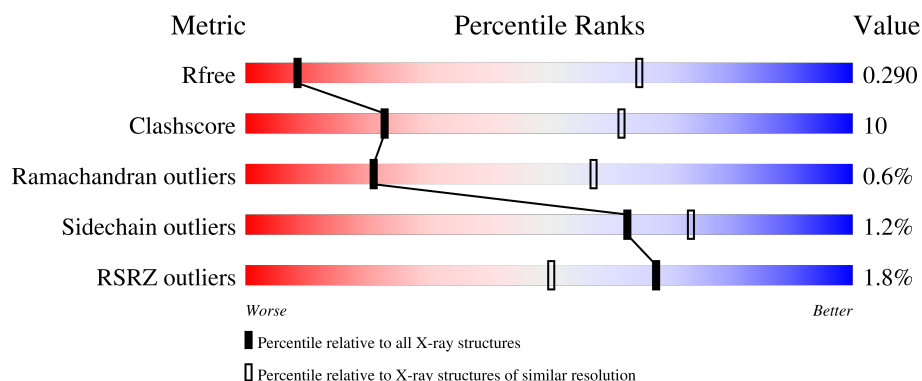
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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	803	80% 15% ..
1	B	803	2% 78% 17% ..
1	C	803	80% 16% ..
1	D	803	2% 81% 14% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24073 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	777	Total	C	N	O	S	0	0	0
			5988	3848	992	1119	29			
1	B	773	Total	C	N	O	S	0	0	0
			5990	3843	989	1129	29			
1	C	773	Total	C	N	O	S	0	0	0
			5952	3825	985	1114	28			
1	D	777	Total	C	N	O	S	0	0	0
			5979	3840	990	1121	28			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	engineered mutation	UNP P19491
A	?	-	VAL	deletion	UNP P19491
A	?	-	THR	deletion	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	564	ASP	-	linker	UNP P19491
A	565	THR	-	linker	UNP P19491
A	566	ASP	-	linker	UNP P19491
A	589	ALA	CYS	engineered mutation	UNP P19491
A	827	GLY	-	cloning artifact	UNP P19491
A	828	LEU	-	cloning artifact	UNP P19491
A	829	VAL	-	cloning artifact	UNP P19491
A	830	PRO	-	cloning artifact	UNP P19491
A	831	ARG	-	cloning artifact	UNP P19491
B	241	GLU	ASN	engineered mutation	UNP P19491
B	?	-	VAL	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491

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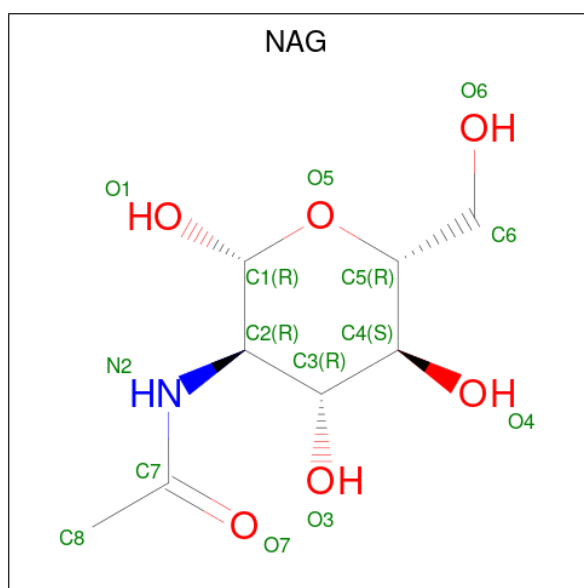
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	?	-	GLY	deletion	UNP P19491
B	385	ASP	ASN	engineered mutation	UNP P19491
B	392	GLN	ASN	engineered mutation	UNP P19491
B	564	ASP	-	linker	UNP P19491
B	565	THR	-	linker	UNP P19491
B	566	ASP	-	linker	UNP P19491
B	589	ALA	CYS	engineered mutation	UNP P19491
B	827	GLY	-	cloning artifact	UNP P19491
B	828	LEU	-	cloning artifact	UNP P19491
B	829	VAL	-	cloning artifact	UNP P19491
B	830	PRO	-	cloning artifact	UNP P19491
B	831	ARG	-	cloning artifact	UNP P19491
C	241	GLU	ASN	engineered mutation	UNP P19491
C	?	-	VAL	deletion	UNP P19491
C	?	-	THR	deletion	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	564	ASP	-	linker	UNP P19491
C	565	THR	-	linker	UNP P19491
C	566	ASP	-	linker	UNP P19491
C	589	ALA	CYS	engineered mutation	UNP P19491
C	827	GLY	-	cloning artifact	UNP P19491
C	828	LEU	-	cloning artifact	UNP P19491
C	829	VAL	-	cloning artifact	UNP P19491
C	830	PRO	-	cloning artifact	UNP P19491
C	831	ARG	-	cloning artifact	UNP P19491
D	241	GLU	ASN	engineered mutation	UNP P19491
D	?	-	VAL	deletion	UNP P19491
D	?	-	THR	deletion	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

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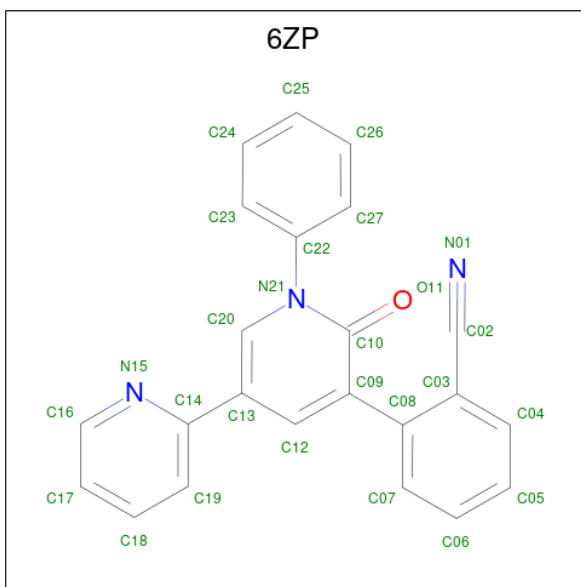
Chain	Residue	Modelled	Actual	Comment	Reference
D	564	ASP	-	linker	UNP P19491
D	565	THR	-	linker	UNP P19491
D	566	ASP	-	linker	UNP P19491
D	589	ALA	CYS	engineered mutation	UNP P19491
D	827	GLY	-	cloning artifact	UNP P19491
D	828	LEU	-	cloning artifact	UNP P19491
D	829	VAL	-	cloning artifact	UNP P19491
D	830	PRO	-	cloning artifact	UNP P19491
D	831	ARG	-	cloning artifact	UNP P19491

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



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

- Molecule 3 is 2-(6'-oxo-1'-phenyl[1',6'-dihydro[2,3'-bipyridine]]-5'-yl)benzonitrile (CCD ID: 6ZP) (formula: $C_{23}H_{15}N_3O$).

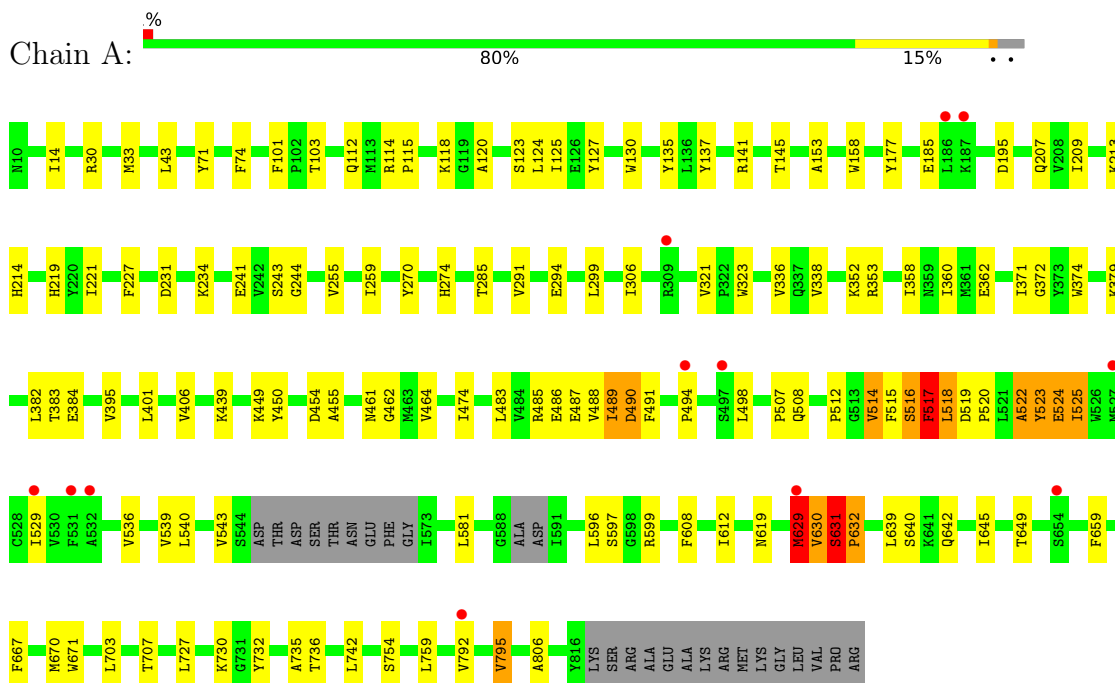


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			27	23	3	1		
3	B	1	Total	C	N	O	0	0
			27	23	3	1		
3	C	1	Total	C	N	O	0	0
			27	23	3	1		
3	D	1	Total	C	N	O	0	0
			27	23	3	1		

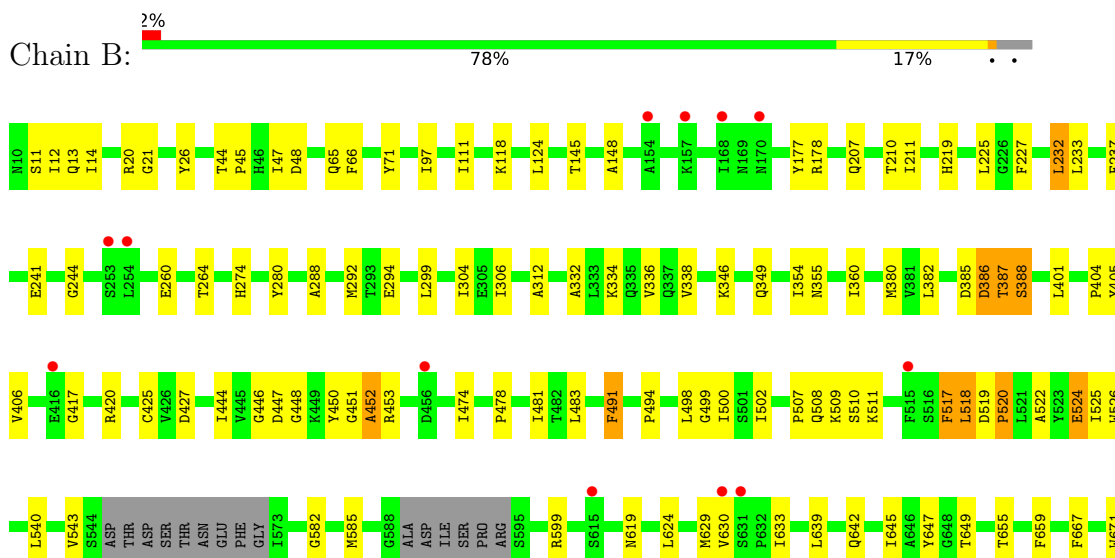
3 Residue-property plots [i](#)

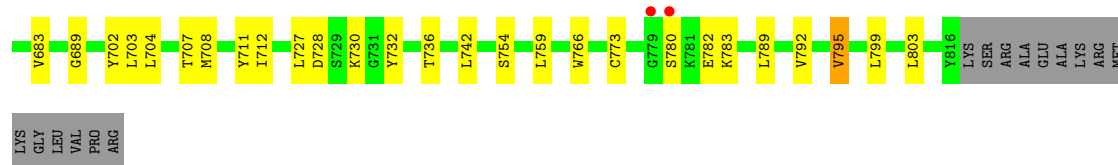
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Glutamate receptor 2

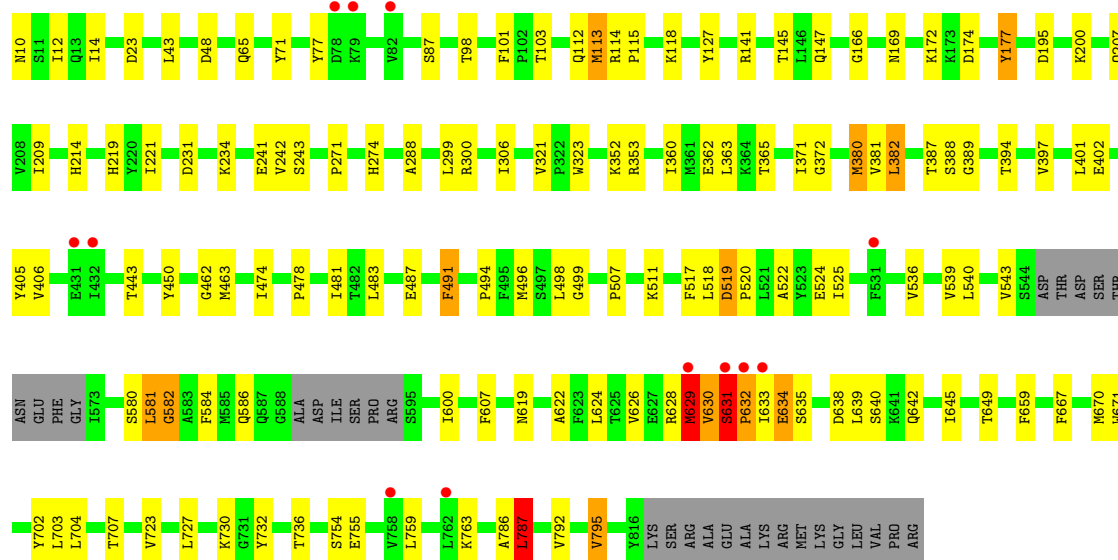
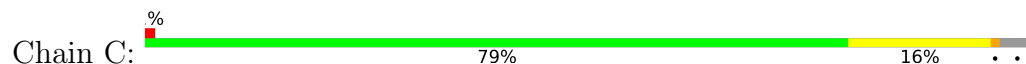


• Molecule 1: Glutamate receptor 2

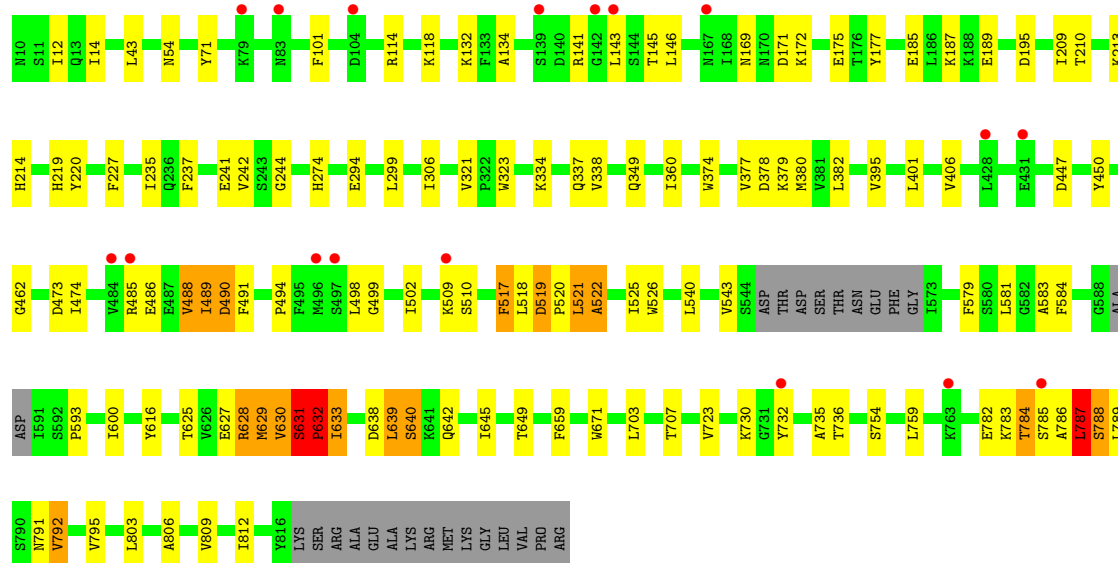
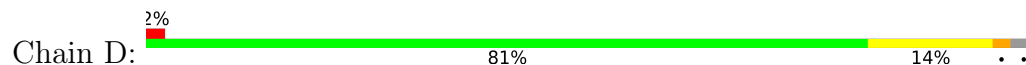




• Molecule 1: Glutamate receptor 2



• Molecule 1: Glutamate receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.74Å 109.34Å 594.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.57 – 4.00 49.57 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.57-4.00) 99.4 (49.57-4.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.10.1 _2155	Depositor
R, R_{free}	0.237 , 0.272 0.264 , 0.290	Depositor DCC
R_{free} test set	2581 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	196.2	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 194.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	24073	wwPDB-VP
Average B, all atoms (Å ²)	239.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% 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: NAG, 6ZP

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	0.16	1/6111 (0.0%)	0.58	20/8272 (0.2%)
1	B	0.20	2/6112 (0.0%)	0.62	22/8270 (0.3%)
1	C	0.19	1/6074 (0.0%)	0.50	17/8225 (0.2%)
1	D	0.30	5/6102 (0.1%)	0.63	32/8263 (0.4%)
All	All	0.22	9/24399 (0.0%)	0.59	91/33030 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	787	LEU	CA-C	13.68	1.73	1.53
1	B	232	LEU	CA-C	9.20	1.64	1.52
1	C	581	LEU	CA-C	7.61	1.63	1.52
1	D	639	LEU	CA-C	7.27	1.62	1.52
1	D	784	THR	N-CA	5.65	1.52	1.46
1	D	518	LEU	CA-C	5.52	1.61	1.52
1	B	388	SER	N-CA	5.45	1.56	1.46
1	D	632	PRO	N-CD	5.21	1.55	1.47
1	A	632	PRO	N-CD	5.15	1.55	1.47

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	524	GLU	N-CA-C	18.07	135.14	112.92
1	B	388	SER	N-CA-CB	-17.48	80.78	110.50
1	B	452	ALA	CB-CA-C	-16.74	85.40	110.50
1	D	518	LEU	N-CA-C	15.51	130.41	112.72
1	D	783	LYS	N-CA-C	14.92	127.26	111.14
1	A	524	GLU	N-CA-CB	-14.11	89.97	110.56
1	A	522	ALA	N-CA-C	13.94	130.93	109.60
1	D	521	LEU	N-CA-C	-13.67	88.67	109.86
1	A	518	LEU	N-CA-C	11.86	125.98	112.57
1	C	629	MET	CB-CA-C	-11.76	91.99	110.81
1	B	452	ALA	N-CA-C	11.63	143.58	111.00
1	A	629	MET	CB-CA-C	-11.19	91.98	110.79
1	D	638	ASP	N-CA-C	11.15	124.75	111.82
1	B	387	THR	N-CA-C	10.99	130.69	112.99
1	C	787	LEU	N-CA-C	10.70	126.04	110.10
1	B	453	ARG	N-CA-CB	-10.60	94.34	110.45
1	B	233	LEU	N-CA-C	-10.54	99.68	112.54
1	B	232	LEU	CA-C-O	9.78	129.15	119.08
1	D	786	ALA	N-CA-C	-9.63	95.08	109.81
1	B	783	LYS	N-CA-CB	-9.59	95.60	110.56
1	C	580	SER	N-CA-C	9.20	122.46	111.33
1	B	453	ARG	N-CA-C	9.10	122.84	110.55
1	D	640	SER	N-CA-CB	8.95	124.41	110.44
1	B	232	LEU	CB-CA-C	-8.78	94.72	110.35
1	C	382	LEU	N-CA-C	8.76	123.87	109.24
1	B	388	SER	N-CA-C	8.74	135.47	111.00
1	A	522	ALA	CB-CA-C	-8.67	94.78	112.99
1	D	489	ILE	N-CA-C	8.58	121.48	109.29
1	C	582	GLY	N-CA-C	-8.53	101.94	113.37
1	A	518	LEU	N-CA-CB	-8.37	97.68	110.91
1	D	522	ALA	N-CA-CB	-8.35	94.31	109.10
1	D	787	LEU	N-CA-CB	-8.29	98.95	111.64
1	D	631	SER	C-N-CD	8.24	138.74	120.60
1	C	786	ALA	N-CA-C	-8.19	93.36	110.80
1	A	489	ILE	N-CA-C	8.15	121.84	109.20
1	D	522	ALA	N-CA-C	8.14	123.65	109.80
1	D	518	LEU	N-CA-CB	-8.12	98.61	110.70
1	B	524	GLU	N-CA-C	8.04	123.43	112.90
1	D	640	SER	N-CA-C	-7.75	103.61	113.23
1	A	630	VAL	CB-CA-C	-7.66	86.60	110.97
1	C	630	VAL	CB-CA-C	-7.65	86.64	110.97
1	A	516	SER	N-CA-C	-7.49	103.94	113.23
1	D	787	LEU	CB-CA-C	-7.49	99.84	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	388	SER	CB-CA-C	-7.47	95.91	110.10
1	D	639	LEU	CA-C-O	7.24	128.04	119.28
1	B	232	LEU	N-CA-C	7.02	124.28	113.19
1	C	581	LEU	CA-C-O	6.87	127.35	119.18
1	D	489	ILE	N-CA-CB	-6.78	104.61	112.34
1	D	639	LEU	CB-CA-C	-6.72	97.91	110.01
1	B	783	LYS	N-CA-C	6.67	120.76	110.42
1	D	786	ALA	CB-CA-C	-6.58	97.86	110.24
1	D	783	LYS	CB-CA-C	-6.50	100.63	110.90
1	B	522	ALA	N-CA-C	6.47	118.22	110.19
1	D	518	LEU	CA-C-O	6.46	127.47	119.78
1	A	597	SER	N-CA-C	6.40	119.07	111.71
1	D	519	ASP	N-CA-C	6.13	123.36	109.81
1	A	517	PHE	CB-CA-C	6.11	122.59	110.42
1	D	792	VAL	N-CA-C	-6.08	104.05	112.50
1	C	113	MET	N-CA-CB	-6.04	100.26	110.41
1	A	525	ILE	N-CA-C	-6.02	104.44	111.00
1	C	586	GLN	N-CA-CB	5.99	118.00	110.45
1	B	386	ASP	N-CA-C	5.97	119.44	109.95
1	C	380	MET	N-CA-C	5.94	123.45	110.80
1	D	488	VAL	N-CA-C	-5.82	107.24	112.12
1	A	629	MET	N-CA-C	-5.78	104.34	111.40
1	C	581	LEU	CB-CA-C	-5.78	98.62	109.72
1	D	632	PRO	CA-N-CD	-5.75	103.45	111.50
1	C	365	THR	N-CA-C	5.72	117.59	111.36
1	D	639	LEU	N-CA-C	5.70	120.23	113.16
1	C	629	MET	N-CA-C	-5.64	104.35	111.11
1	A	631	SER	C-N-CD	5.61	132.95	120.60
1	A	514	VAL	N-CA-C	5.60	120.28	112.50
1	B	524	GLU	N-CA-CB	-5.57	101.98	110.33
1	D	517	PHE	CA-C-N	5.53	131.63	122.73
1	D	517	PHE	C-N-CA	5.53	131.63	122.73
1	B	518	LEU	N-CA-CB	-5.52	103.19	111.64
1	B	386	ASP	N-CA-CB	-5.52	102.02	110.85
1	A	523	TYR	CB-CA-C	-5.46	101.68	110.74
1	D	788	SER	N-CA-C	-5.45	99.20	110.80
1	B	233	LEU	N-CA-CB	5.37	119.30	110.39
1	A	516	SER	N-CA-CB	5.27	118.66	110.44
1	A	490	ASP	N-CA-CB	5.24	119.01	110.37
1	B	782	GLU	N-CA-C	-5.22	99.69	110.80
1	A	519	ASP	N-CA-C	5.19	121.28	109.81
1	C	631	SER	CA-C-N	-5.18	113.37	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	631	SER	C-N-CA	-5.18	113.37	119.84
1	D	628	ARG	N-CA-C	5.17	116.60	111.07
1	D	786	ALA	CA-C-N	5.14	131.22	123.04
1	D	786	ALA	C-N-CA	5.14	131.22	123.04
1	C	381	VAL	N-CA-CB	-5.08	104.11	111.52
1	D	490	ASP	N-CA-CB	5.00	118.77	110.47

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	629	MET	Peptide
1	C	629	MET	Peptide

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	5988	0	5887	127	0
1	B	5990	0	5903	109	0
1	C	5952	0	5835	156	0
1	D	5979	0	5866	154	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	1	0
2	D	14	0	13	1	0
3	A	27	0	0	3	0
3	B	27	0	0	2	0
3	C	27	0	0	2	0
3	D	27	0	0	3	0
All	All	24073	0	23543	497	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 10.

All (497) 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:628:ARG:CB	1:D:630:VAL:HG22	1.33	1.58
1:D:628:ARG:CB	1:D:630:VAL:CG2	1.93	1.43
1:C:629:MET:HB2	1:C:630:VAL:CA	1.47	1.36
1:A:629:MET:HB2	1:A:630:VAL:CA	1.47	1.30
1:D:787:LEU:O	1:D:787:LEU:HD22	1.30	1.29
1:C:629:MET:CB	1:C:630:VAL:HA	1.66	1.26
1:A:629:MET:CB	1:A:630:VAL:HA	1.65	1.24
1:C:633:ILE:CG2	1:C:723:VAL:CG1	2.16	1.23
1:C:633:ILE:HG21	1:C:723:VAL:CG1	1.68	1.23
1:B:518:LEU:HD12	1:B:518:LEU:O	1.48	1.11
1:A:631:SER:HB2	1:A:632:PRO:HA	1.32	1.11
1:C:633:ILE:HG21	1:C:723:VAL:HG12	1.20	1.08
1:C:634:GLU:HG3	1:C:635:SER:H	1.17	1.08
1:C:633:ILE:HG23	1:C:723:VAL:HG11	1.34	1.06
1:A:485:ARG:HB3	1:A:491:PHE:HZ	1.20	1.05
1:C:382:LEU:O	1:C:382:LEU:HD12	1.54	1.03
1:C:633:ILE:CG2	1:C:723:VAL:HB	1.89	1.03
1:B:599:ARG:CB	1:C:581:LEU:HD11	1.89	1.02
1:B:582:GLY:HA2	1:B:585:MET:HE3	1.38	1.01
1:D:632:PRO:O	1:D:633:ILE:O	1.80	0.99
1:C:633:ILE:CG2	1:C:723:VAL:CB	2.41	0.98
1:C:633:ILE:HG23	1:C:723:VAL:CG1	1.91	0.97
1:D:489:ILE:HG21	1:D:735:ALA:HB1	1.42	0.97
1:C:581:LEU:HA	1:C:584:PHE:HB3	1.45	0.97
1:A:631:SER:CB	1:A:632:PRO:HA	1.95	0.95
1:D:787:LEU:O	1:D:787:LEU:CD2	2.14	0.94
1:C:619:ASN:ND2	1:D:787:LEU:HB3	1.81	0.94
1:D:485:ARG:HB3	1:D:491:PHE:HZ	1.30	0.93
1:D:789:LEU:HA	1:D:792:VAL:HG13	1.52	0.91
1:A:489:ILE:HG21	1:A:735:ALA:HB1	1.49	0.91
1:C:619:ASN:HD21	1:D:787:LEU:HB3	1.36	0.90
1:C:522:ALA:HB2	1:D:787:LEU:HD21	1.52	0.90
1:D:629:MET:HA	1:D:630:VAL:CG2	2.01	0.89
1:D:629:MET:HA	1:D:630:VAL:HG23	1.53	0.89
1:A:485:ARG:HB3	1:A:491:PHE:CZ	2.09	0.88
1:D:628:ARG:CB	1:D:630:VAL:HG21	2.03	0.88
1:C:522:ALA:CA	1:D:787:LEU:HD21	2.04	0.88
1:C:518:LEU:HD12	1:C:518:LEU:O	1.75	0.87
1:B:232:LEU:C	1:B:232:LEU:HD12	2.00	0.85
1:C:633:ILE:CG2	1:C:723:VAL:HG11	1.93	0.85
1:A:629:MET:CB	1:A:630:VAL:CA	2.40	0.85
1:D:791:ASN:O	1:D:791:ASN:OD1	1.95	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:ARG:C	1:A:491:PHE:HE2	1.85	0.84
1:D:488:VAL:HG23	1:D:489:ILE:HG12	1.58	0.83
1:A:599:ARG:HA	1:B:585:MET:HE1	1.60	0.83
1:C:629:MET:CB	1:C:630:VAL:CA	2.40	0.83
1:C:522:ALA:CB	1:D:787:LEU:HD21	2.08	0.82
1:C:633:ILE:HG22	1:C:723:VAL:HB	1.60	0.82
1:A:488:VAL:HG23	1:A:489:ILE:HG12	1.62	0.81
1:C:581:LEU:C	1:C:581:LEU:HD12	2.05	0.81
1:D:485:ARG:HB3	1:D:491:PHE:CZ	2.15	0.80
1:D:631:SER:CB	1:D:632:PRO:HA	2.14	0.78
1:B:518:LEU:O	1:B:518:LEU:CD1	2.32	0.78
1:D:485:ARG:C	1:D:491:PHE:HE2	1.92	0.78
1:C:371:ILE:O	1:C:382:LEU:CD2	2.31	0.77
1:D:519:ASP:O	1:D:521:LEU:O	2.02	0.77
1:C:371:ILE:O	1:C:382:LEU:HD22	1.83	0.77
1:D:628:ARG:N	1:D:629:MET:HB3	2.00	0.76
1:A:524:GLU:OE1	1:B:789:LEU:HD22	1.85	0.76
1:C:522:ALA:HB2	1:D:787:LEU:CD2	2.15	0.75
1:A:486:GLU:OE1	1:A:491:PHE:HD2	1.69	0.75
1:B:451:GLY:HA2	1:B:452:ALA:HB3	1.68	0.75
1:C:522:ALA:N	1:D:787:LEU:HD21	2.01	0.74
1:D:628:ARG:CB	1:D:629:MET:HA	2.17	0.74
1:D:639:LEU:C	1:D:639:LEU:HD12	2.12	0.74
1:A:631:SER:HB2	1:A:632:PRO:CA	2.16	0.74
1:C:581:LEU:HA	1:C:584:PHE:CB	2.18	0.74
1:B:502:ILE:HD13	1:B:639:LEU:HD13	1.70	0.74
1:D:628:ARG:CA	1:D:630:VAL:HG22	2.18	0.74
1:D:632:PRO:O	1:D:633:ILE:C	2.31	0.73
1:C:630:VAL:O	1:C:631:SER:HB2	1.89	0.73
1:D:377:VAL:HG13	1:D:378:ASP:H	1.53	0.73
1:D:787:LEU:H	1:D:787:LEU:HD13	1.53	0.73
1:C:360:ILE:HB	1:C:372:GLY:HA3	1.71	0.73
1:A:629:MET:HB2	1:A:630:VAL:HA	0.74	0.72
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.70	0.72
1:C:634:GLU:HG3	1:C:635:SER:N	1.98	0.72
1:C:581:LEU:CA	1:C:584:PHE:HB3	2.18	0.72
1:C:630:VAL:O	1:C:631:SER:CB	2.37	0.72
1:C:147:GLN:HE21	1:D:143:LEU:HD21	1.53	0.72
1:D:486:GLU:OE1	1:D:491:PHE:HD2	1.72	0.72
1:D:627:GLU:CB	1:D:629:MET:HG2	2.20	0.72
1:C:629:MET:HB2	1:C:630:VAL:HA	0.74	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:630:VAL:O	1:C:630:VAL:HG22	1.90	0.71
1:A:631:SER:CB	1:A:632:PRO:CA	2.69	0.71
1:D:787:LEU:H	1:D:787:LEU:CD1	2.02	0.71
1:B:346:LYS:HG3	1:B:354:ILE:HG13	1.70	0.71
1:A:485:ARG:CB	1:A:491:PHE:HZ	2.01	0.70
1:B:494:PRO:HG3	1:C:494:PRO:HG3	1.72	0.70
1:C:525:ILE:HD11	1:D:789:LEU:HB3	1.72	0.70
1:A:630:VAL:HG22	1:A:630:VAL:O	1.90	0.70
1:A:485:ARG:C	1:A:491:PHE:CE2	2.68	0.70
1:A:485:ARG:CB	1:A:491:PHE:CZ	2.76	0.69
1:B:387:THR:O	1:B:387:THR:OG1	2.09	0.69
1:B:387:THR:N	1:B:388:SER:HA	2.08	0.69
1:C:649:THR:HG22	1:C:703:LEU:HB2	1.74	0.68
1:C:522:ALA:N	1:D:787:LEU:CD2	2.56	0.68
1:B:274:HIS:O	1:B:274:HIS:ND1	2.27	0.67
1:A:486:GLU:N	1:A:491:PHE:HE2	1.91	0.67
1:C:382:LEU:HD12	1:C:382:LEU:C	2.20	0.67
1:C:498:LEU:HD21	1:C:732:TYR:CZ	2.30	0.67
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.76	0.66
1:D:628:ARG:H	1:D:629:MET:HB3	1.61	0.66
1:D:489:ILE:HG22	1:D:490:ASP:N	2.11	0.66
1:B:232:LEU:C	1:B:232:LEU:CD1	2.69	0.66
1:B:518:LEU:HB2	1:B:526:TRP:CD1	2.32	0.66
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.77	0.66
1:C:98:THR:O	1:C:112:GLN:HA	1.95	0.65
1:C:394:THR:HG23	1:C:394:THR:O	1.94	0.65
1:D:377:VAL:HG13	1:D:378:ASP:N	2.10	0.65
1:B:474:ILE:HG13	1:B:736:THR:HG22	1.79	0.64
1:A:599:ARG:CA	1:B:585:MET:HE1	2.26	0.64
1:C:581:LEU:HD12	1:C:582:GLY:N	2.11	0.64
1:D:450:TYR:HA	1:D:462:GLY:HA3	1.78	0.64
1:C:147:GLN:HE21	1:D:143:LEU:CD2	2.10	0.63
1:B:633:ILE:HD13	1:B:639:LEU:HD12	1.80	0.63
1:D:519:ASP:C	1:D:521:LEU:O	2.41	0.63
1:D:632:PRO:C	1:D:633:ILE:O	2.40	0.63
1:A:619:ASN:HA	1:B:624:LEU:HD13	1.81	0.63
1:C:402:GLU:OE1	1:C:450:TYR:OH	2.15	0.63
1:D:509:LYS:N	1:D:510:SER:HB2	2.13	0.62
1:A:608:PHE:CD2	1:B:799:LEU:HD22	2.35	0.62
1:C:633:ILE:HG23	1:C:723:VAL:CB	2.24	0.62
1:D:789:LEU:HB2	1:D:792:VAL:HG22	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:THR:H	1:B:388:SER:HA	1.63	0.62
1:D:502:ILE:HD13	1:D:639:LEU:CD2	2.29	0.62
1:C:519:ASP:HB2	3:C:902:6ZP:C20	2.29	0.62
1:D:581:LEU:HA	1:D:584:PHE:HB3	1.81	0.62
1:B:498:LEU:HD21	1:B:732:TYR:CZ	2.35	0.61
1:C:177:TYR:HB3	1:C:207:GLN:HG2	1.82	0.61
1:C:642:GLN:HE22	1:C:645:ILE:HB	1.65	0.61
1:A:486:GLU:HA	1:A:491:PHE:CE2	2.36	0.61
1:B:502:ILE:HD13	1:B:639:LEU:CD1	2.30	0.61
1:C:524:GLU:HB2	1:D:789:LEU:CD2	2.30	0.61
1:C:633:ILE:HG21	1:C:723:VAL:CB	2.18	0.61
1:C:382:LEU:O	1:C:382:LEU:CD1	2.41	0.61
1:B:334:LYS:NZ	1:B:349:GLN:O	2.34	0.61
1:B:510:SER:H	1:B:511:LYS:HA	1.66	0.61
1:A:523:TYR:CD2	1:A:524:GLU:HG3	2.36	0.60
1:B:26:TYR:HE1	1:B:47:ILE:HG12	1.66	0.60
1:D:169:ASN:ND2	1:D:171:ASP:OD1	2.35	0.60
1:D:485:ARG:CB	1:D:491:PHE:CZ	2.84	0.60
1:D:629:MET:HA	1:D:630:VAL:HG22	1.80	0.60
1:A:299:LEU:HD13	1:A:306:ILE:HG21	1.82	0.60
1:A:489:ILE:HG22	1:A:490:ASP:N	2.15	0.60
1:C:12:ILE:HG23	1:C:71:TYR:HD2	1.67	0.60
1:B:177:TYR:HB3	1:B:207:GLN:HG2	1.84	0.60
1:C:101:PHE:HA	1:C:114:ARG:HD2	1.84	0.60
1:C:581:LEU:C	1:C:581:LEU:CD1	2.74	0.59
1:D:628:ARG:N	1:D:629:MET:CB	2.65	0.59
1:C:498:LEU:CD1	1:C:730:LYS:HD2	2.33	0.59
1:D:143:LEU:HD23	1:D:146:LEU:HD23	1.84	0.59
1:B:260:GLU:O	1:B:264:THR:OG1	2.19	0.59
1:C:522:ALA:H	1:C:525:ILE:HD12	1.67	0.59
1:C:112:GLN:NE2	1:C:352:LYS:HD3	2.17	0.59
1:C:634:GLU:CG	1:C:635:SER:H	2.01	0.59
1:C:299:LEU:HD13	1:C:306:ILE:HG21	1.85	0.58
1:D:628:ARG:C	1:D:630:VAL:HG22	2.28	0.58
1:C:474:ILE:HG13	1:C:736:THR:HG22	1.84	0.58
1:B:447:ASP:N	1:B:448:GLY:HA2	2.18	0.58
1:C:141:ARG:NH2	1:C:195:ASP:OD1	2.36	0.58
1:A:362:GLU:HG3	1:A:371:ILE:HG21	1.85	0.58
1:D:374:TRP:CD1	1:D:379:LYS:O	2.57	0.58
1:C:640:SER:HB3	1:C:670:MET:HG2	1.86	0.57
1:D:485:ARG:C	1:D:491:PHE:CE2	2.78	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:632:PRO:HG2	1:C:633:ILE:HD12	1.86	0.57
1:B:385:ASP:OD1	1:B:386:ASP:N	2.37	0.57
1:A:103:THR:O	1:A:352:LYS:NZ	2.37	0.57
1:A:474:ILE:HG13	1:A:736:THR:HG22	1.88	0.56
1:C:498:LEU:HD11	1:C:730:LYS:CD	2.35	0.56
1:C:619:ASN:ND2	1:D:787:LEU:CB	2.64	0.56
1:D:377:VAL:HG13	1:D:378:ASP:OD1	2.04	0.56
1:C:371:ILE:O	1:C:382:LEU:HD23	2.05	0.56
1:B:11:SER:OG	1:B:44:THR:OG1	2.23	0.56
1:B:599:ARG:CA	1:C:581:LEU:HD11	2.36	0.56
1:D:629:MET:N	1:D:630:VAL:HA	2.21	0.56
1:A:14:ILE:HD13	1:A:43:LEU:HD23	1.88	0.56
1:D:631:SER:HB2	1:D:632:PRO:HA	1.88	0.56
1:B:639:LEU:HD21	1:B:647:TYR:CG	2.40	0.56
1:C:219:HIS:HD2	1:C:241:GLU:O	1.89	0.56
1:D:631:SER:HB2	1:D:632:PRO:CA	2.36	0.56
1:A:71:TYR:HA	1:A:323:TRP:HH2	1.71	0.56
1:B:124:LEU:HA	1:B:380:MET:HE1	1.88	0.55
1:C:522:ALA:HB3	1:C:525:ILE:HG13	1.86	0.55
1:D:382:LEU:HD12	1:D:382:LEU:C	2.32	0.55
1:D:502:ILE:HD13	1:D:639:LEU:HD23	1.86	0.55
1:D:639:LEU:C	1:D:639:LEU:CD1	2.80	0.55
1:B:508:GLN:N	1:B:509:LYS:HA	2.21	0.55
1:A:118:LYS:HG2	1:A:145:THR:HG22	1.89	0.55
1:A:358:ILE:HD12	1:A:374:TRP:HE1	1.71	0.55
1:A:449:LYS:HD3	1:A:461:ASN:HB2	1.89	0.55
1:D:631:SER:CB	1:D:632:PRO:CA	2.85	0.55
1:D:789:LEU:HD12	1:D:789:LEU:C	2.32	0.55
1:B:517:PHE:C	3:B:902:6ZP:C18	2.80	0.55
1:D:489:ILE:CG2	1:D:735:ALA:HB1	2.29	0.54
1:D:498:LEU:HD21	1:D:732:TYR:CZ	2.42	0.54
1:A:642:GLN:HE22	1:A:645:ILE:HB	1.72	0.54
1:A:372:GLY:HA2	1:A:382:LEU:HB3	1.90	0.54
1:B:483:LEU:N	1:C:755:GLU:OE2	2.37	0.54
1:C:630:VAL:HG13	1:C:631:SER:N	2.11	0.54
1:C:634:GLU:HG2	1:C:638:ASP:HB2	1.88	0.54
1:D:784:THR:HA	1:D:785:SER:HB3	1.90	0.54
1:C:540:LEU:HA	1:C:543:VAL:HG22	1.89	0.54
1:D:628:ARG:CB	1:D:630:VAL:HG23	2.21	0.54
2:C:901:NAG:H83	2:C:901:NAG:H3	1.89	0.54
1:A:659:PHE:HB3	1:A:671:TRP:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:450:TYR:HA	1:C:463:MET:HE2	1.90	0.54
1:C:754:SER:HB2	1:C:759:LEU:HD12	1.90	0.54
1:A:486:GLU:CA	1:A:491:PHE:HE2	2.21	0.54
1:C:169:ASN:HD21	1:C:172:LYS:HD3	1.72	0.54
1:A:177:TYR:CD2	1:A:207:GLN:HG3	2.43	0.53
1:C:600:ILE:HD11	1:D:806:ALA:HA	1.90	0.53
1:D:474:ILE:HG13	1:D:736:THR:HG22	1.90	0.53
1:A:515:PHE:O	1:A:515:PHE:CD2	2.62	0.53
1:C:14:ILE:HD13	1:C:43:LEU:HD23	1.90	0.53
1:D:141:ARG:NH2	1:D:195:ASP:OD1	2.40	0.53
1:D:789:LEU:HA	1:D:792:VAL:CG1	2.31	0.53
1:B:517:PHE:O	3:B:902:6ZP:C18	2.56	0.53
1:D:498:LEU:HB3	1:D:707:THR:HG23	1.91	0.53
1:A:494:PRO:HG3	1:D:494:PRO:HG3	1.90	0.53
1:B:498:LEU:HB3	1:B:707:THR:HG23	1.89	0.53
1:D:517:PHE:HA	3:D:902:6ZP:C18	2.39	0.52
1:D:540:LEU:HA	1:D:543:VAL:HG22	1.91	0.52
1:A:536:VAL:HG22	1:B:803:LEU:HD21	1.91	0.52
1:C:498:LEU:HB3	1:C:707:THR:HG23	1.89	0.52
1:C:518:LEU:O	1:C:518:LEU:CD1	2.53	0.52
1:D:377:VAL:CG1	1:D:378:ASP:H	2.20	0.52
1:A:209:ILE:HA	1:A:214:HIS:CD2	2.44	0.52
1:A:498:LEU:HD12	1:A:730:LYS:HG3	1.91	0.52
1:C:362:GLU:HG3	1:C:371:ILE:HG21	1.91	0.52
1:C:607:PHE:HE1	1:D:584:PHE:HZ	1.56	0.52
1:B:659:PHE:HB3	1:B:671:TRP:HB2	1.91	0.52
1:D:209:ILE:HA	1:D:214:HIS:CD2	2.45	0.52
1:A:221:ILE:HG12	1:A:243:SER:HB2	1.92	0.52
1:A:274:HIS:O	1:A:274:HIS:CG	2.63	0.52
1:C:112:GLN:HE21	1:C:352:LYS:HD3	1.73	0.51
1:D:334:LYS:NZ	1:D:349:GLN:O	2.32	0.51
1:A:515:PHE:O	1:A:515:PHE:CG	2.63	0.51
1:D:337:GLN:NE2	2:D:901:NAG:O7	2.41	0.51
1:A:517:PHE:O	3:A:902:6ZP:C18	2.58	0.51
1:C:87:SER:OG	1:D:54:ASN:OD1	2.29	0.51
1:A:135:TYR:CE1	1:A:137:TYR:HB3	2.46	0.51
1:B:97:ILE:HD12	1:B:292:MET:HE3	1.92	0.51
1:B:427:ASP:OD2	1:B:766:TRP:NE1	2.37	0.51
1:C:498:LEU:CD1	1:C:730:LYS:CD	2.88	0.51
1:A:124:LEU:HD13	1:A:360:ILE:HD13	1.92	0.51
1:C:450:TYR:O	1:C:462:GLY:HA3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:ILE:HG23	1:D:71:TYR:HD2	1.75	0.51
1:A:630:VAL:HG13	1:A:631:SER:N	2.15	0.51
1:D:486:GLU:N	1:D:491:PHE:HE2	2.09	0.51
1:D:489:ILE:CG2	1:D:490:ASP:N	2.74	0.51
1:A:742:LEU:O	1:A:742:LEU:HD12	2.11	0.51
1:C:498:LEU:CD2	1:C:732:TYR:CZ	2.94	0.51
1:D:498:LEU:CD1	1:D:730:LYS:HD2	2.41	0.50
1:B:540:LEU:HA	1:B:543:VAL:HG22	1.94	0.50
1:D:299:LEU:HD13	1:D:306:ILE:HG21	1.92	0.50
1:A:630:VAL:O	1:A:631:SER:CB	2.60	0.50
1:B:12:ILE:HG23	1:B:71:TYR:HD2	1.77	0.50
1:A:754:SER:HB2	1:A:759:LEU:HD12	1.92	0.50
1:D:101:PHE:HA	1:D:114:ARG:HD2	1.94	0.50
1:B:360:ILE:HD13	1:B:380:MET:HE2	1.94	0.49
1:B:508:GLN:H	1:B:509:LYS:HA	1.77	0.49
1:C:498:LEU:HD12	1:C:730:LYS:HG3	1.94	0.49
1:C:626:VAL:HG11	1:D:782:GLU:O	2.12	0.49
1:D:629:MET:CA	1:D:630:VAL:CG2	2.82	0.49
1:A:525:ILE:HG12	1:B:792:VAL:HG21	1.94	0.49
1:B:498:LEU:HD12	1:B:730:LYS:HG3	1.94	0.49
1:C:166:GLY:HA2	1:C:200:LYS:HE2	1.94	0.49
1:B:642:GLN:HE22	1:B:645:ILE:HB	1.78	0.49
1:B:227:PHE:CD1	1:B:244:GLY:HA3	2.48	0.49
1:A:539:VAL:HG21	1:B:803:LEU:HD22	1.93	0.49
1:B:754:SER:HB2	1:B:759:LEU:HD12	1.95	0.49
1:C:388:SER:H	1:C:389:GLY:HA2	1.76	0.49
1:A:522:ALA:O	1:A:523:TYR:C	2.56	0.49
1:D:71:TYR:HA	1:D:323:TRP:HH2	1.78	0.49
1:A:498:LEU:HB3	1:A:707:THR:HG23	1.95	0.49
1:A:294:GLU:HG3	1:A:338:VAL:HG11	1.95	0.48
1:C:23:ASP:HB3	1:C:271:PRO:HG2	1.95	0.48
1:C:387:THR:HA	1:C:388:SER:HA	1.55	0.48
1:A:540:LEU:HA	1:A:543:VAL:HG22	1.95	0.48
1:A:599:ARG:O	1:B:585:MET:CE	2.62	0.48
1:A:454:ASP:OD1	1:A:455:ALA:N	2.46	0.48
1:B:232:LEU:HD12	1:B:232:LEU:O	2.13	0.48
1:B:237:PHE:HB2	1:D:210:THR:HG22	1.95	0.48
1:C:48:ASP:OD1	1:C:65:GLN:NE2	2.46	0.48
1:C:103:THR:O	1:C:352:LYS:NZ	2.46	0.48
1:A:599:ARG:O	1:B:585:MET:HE1	2.13	0.48
1:A:177:TYR:HD2	1:A:207:GLN:HG3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:ALA:O	1:B:292:MET:HG3	2.14	0.48
1:B:498:LEU:HD12	1:B:499:GLY:N	2.28	0.48
1:D:498:LEU:HD11	1:D:730:LYS:HD2	1.95	0.48
1:D:787:LEU:CD1	1:D:787:LEU:N	2.73	0.48
1:A:608:PHE:CG	1:B:799:LEU:HD22	2.49	0.48
1:A:486:GLU:OE1	1:A:491:PHE:CD2	2.59	0.48
1:B:20:ARG:HG3	1:B:21:GLY:N	2.29	0.48
1:C:622:ALA:O	1:C:626:VAL:HG23	2.14	0.48
1:D:521:LEU:HB2	1:D:526:TRP:NE1	2.29	0.48
1:C:630:VAL:CG1	1:C:631:SER:N	2.64	0.47
1:A:489:ILE:CG2	1:A:490:ASP:N	2.78	0.47
1:C:498:LEU:HD11	1:C:730:LYS:HD2	1.96	0.47
1:D:639:LEU:HD12	1:D:640:SER:N	2.29	0.47
1:A:516:SER:O	1:A:518:LEU:N	2.47	0.47
1:A:498:LEU:CD1	1:A:730:LYS:HG3	2.44	0.47
1:C:77:TYR:HE2	1:C:98:THR:HG21	1.80	0.47
1:D:274:HIS:CG	1:D:274:HIS:O	2.67	0.47
1:B:444:ILE:HG22	1:B:446:GLY:H	1.80	0.47
1:D:294:GLU:HG3	1:D:338:VAL:HG11	1.95	0.47
1:C:628:ARG:O	1:C:629:MET:C	2.58	0.47
1:C:10:ASN:HB3	1:C:300:ARG:HH22	1.79	0.47
1:D:377:VAL:CG1	1:D:378:ASP:N	2.77	0.47
1:B:386:ASP:OD1	1:B:386:ASP:O	2.32	0.47
1:B:498:LEU:CD2	1:B:732:TYR:CE2	2.98	0.47
1:A:115:PRO:HA	1:A:353:ARG:HB2	1.98	0.46
1:C:632:PRO:CG	1:C:633:ILE:H	2.27	0.46
1:D:14:ILE:HD13	1:D:43:LEU:HD23	1.97	0.46
1:D:498:LEU:HD11	1:D:730:LYS:CD	2.45	0.46
1:A:120:ALA:HB2	1:A:374:TRP:NE1	2.30	0.46
1:B:274:HIS:O	1:B:274:HIS:CG	2.68	0.46
1:B:401:LEU:HD23	1:B:406:VAL:HG12	1.98	0.46
1:B:417:GLY:O	1:B:420:ARG:NE	2.46	0.46
1:C:481:ILE:HA	1:C:491:PHE:CE2	2.50	0.46
1:A:486:GLU:CA	1:A:491:PHE:CE2	2.98	0.46
1:B:14:ILE:O	1:B:45:PRO:HA	2.16	0.46
1:C:127:TYR:HB2	1:C:380:MET:HE3	1.97	0.46
1:A:219:HIS:HA	1:A:241:GLU:O	2.15	0.46
1:B:294:GLU:HG3	1:B:338:VAL:HG11	1.98	0.46
1:C:174:ASP:OD1	1:C:207:GLN:NE2	2.49	0.46
1:C:524:GLU:HB2	1:D:789:LEU:HD21	1.96	0.46
1:A:449:LYS:HB2	1:A:462:GLY:HA2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:ALA:HB2	1:D:189:GLU:HG2	1.98	0.46
1:A:33:MET:HE1	1:A:43:LEU:HB2	1.98	0.46
1:C:517:PHE:CE1	1:C:795:VAL:HG22	2.51	0.46
1:D:789:LEU:HB2	1:D:792:VAL:CG2	2.44	0.46
1:C:242:VAL:HB	1:C:363:LEU:HB3	1.98	0.46
1:B:66:PHE:CZ	1:B:312:ALA:HB1	2.51	0.46
1:D:486:GLU:HA	1:D:491:PHE:CE2	2.51	0.46
1:C:522:ALA:H	1:D:787:LEU:CD2	2.27	0.46
1:C:634:GLU:CG	1:C:638:ASP:HB2	2.46	0.46
1:C:118:LYS:HG2	1:C:145:THR:HG22	1.97	0.45
1:C:274:HIS:CG	1:C:274:HIS:O	2.68	0.45
1:A:123:SER:O	1:A:127:TYR:N	2.49	0.45
1:A:498:LEU:HD12	1:A:498:LEU:C	2.41	0.45
1:A:524:GLU:OE1	1:B:789:LEU:CD2	2.60	0.45
1:B:219:HIS:HA	1:B:241:GLU:O	2.17	0.45
1:C:659:PHE:HB3	1:C:671:TRP:HB2	1.98	0.45
1:A:485:ARG:O	1:A:491:PHE:CE2	2.69	0.45
1:A:498:LEU:HD11	1:A:730:LYS:CD	2.46	0.45
1:A:792:VAL:HG21	1:D:525:ILE:HG12	1.97	0.45
1:D:520:PRO:C	1:D:521:LEU:O	2.49	0.45
1:A:383:THR:HA	1:A:384:GLU:HA	1.64	0.45
1:C:494:PRO:HA	1:C:732:TYR:O	2.17	0.45
1:C:517:PHE:HE1	1:C:795:VAL:HG22	1.81	0.45
1:B:225:LEU:HB2	1:B:280:TYR:CD2	2.52	0.45
1:D:522:ALA:HB3	1:D:525:ILE:HD12	1.99	0.45
1:D:227:PHE:CD2	1:D:244:GLY:HA3	2.52	0.45
1:A:523:TYR:HD2	1:A:524:GLU:HG3	1.79	0.45
1:A:630:VAL:CG1	1:A:631:SER:N	2.68	0.45
1:C:394:THR:O	1:C:394:THR:CG2	2.63	0.45
1:A:219:HIS:HD2	1:A:241:GLU:O	2.00	0.45
1:A:291:VAL:HA	1:A:336:VAL:HG11	1.98	0.45
1:A:498:LEU:HD21	1:A:732:TYR:CZ	2.52	0.45
1:D:521:LEU:HD13	1:D:616:TYR:HD2	1.80	0.45
1:B:507:PRO:N	1:B:508:GLN:HA	2.32	0.44
1:C:112:GLN:OE1	1:C:112:GLN:N	2.44	0.44
1:C:536:VAL:HG22	1:D:803:LEU:HD21	1.98	0.44
1:C:634:GLU:HG2	1:C:638:ASP:CB	2.47	0.44
1:D:788:SER:HB2	3:D:902:6ZP:C06	2.47	0.44
1:A:489:ILE:HG21	1:A:735:ALA:CB	2.35	0.44
1:B:498:LEU:HD12	1:B:498:LEU:C	2.43	0.44
1:C:219:HIS:HA	1:C:241:GLU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:502:ILE:HB	1:D:723:VAL:HG23	2.00	0.44
1:C:498:LEU:HD12	1:C:730:LYS:CG	2.48	0.44
1:C:522:ALA:N	1:D:787:LEU:HD23	2.32	0.44
1:D:395:VAL:HG13	1:D:473:ASP:HB2	1.99	0.44
1:A:101:PHE:HA	1:A:114:ARG:HD2	1.99	0.44
1:C:98:THR:HG23	1:C:112:GLN:HA	1.99	0.44
1:C:498:LEU:HD12	1:C:498:LEU:C	2.42	0.44
1:C:632:PRO:CD	1:C:633:ILE:H	2.30	0.44
1:C:401:LEU:HD23	1:C:406:VAL:HG12	1.99	0.44
1:D:659:PHE:HB3	1:D:671:TRP:HB2	1.99	0.44
1:D:754:SER:HB2	1:D:759:LEU:HD12	1.98	0.44
1:A:474:ILE:HD12	1:A:742:LEU:HD13	1.99	0.43
1:B:20:ARG:HG3	1:B:21:GLY:H	1.83	0.43
1:B:118:LYS:HB3	1:B:145:THR:HG22	2.00	0.43
1:D:360:ILE:HD13	1:D:380:MET:HE1	1.98	0.43
1:A:529:ILE:HD13	1:A:612:ILE:HD12	2.00	0.43
1:B:667:PHE:HE1	1:B:727:LEU:HD13	1.81	0.43
1:C:522:ALA:H	1:D:787:LEU:HD23	1.82	0.43
1:D:494:PRO:HA	1:D:732:TYR:O	2.18	0.43
1:B:498:LEU:CD1	1:B:730:LYS:HG3	2.49	0.43
1:D:213:LYS:O	1:D:220:TYR:OH	2.31	0.43
1:A:486:GLU:HA	1:A:491:PHE:HE2	1.75	0.43
1:C:112:GLN:NE2	1:C:352:LYS:HA	2.34	0.43
1:A:517:PHE:C	3:A:902:6ZP:C18	2.92	0.43
1:A:742:LEU:HD12	1:A:742:LEU:C	2.43	0.43
1:A:185:GLU:OE1	1:A:213:LYS:NZ	2.41	0.43
1:A:629:MET:SD	1:A:630:VAL:HA	2.59	0.43
1:B:299:LEU:HD13	1:B:306:ILE:HG21	2.01	0.43
1:C:113:MET:HE3	1:C:288:ALA:HA	1.99	0.43
1:A:141:ARG:HH22	1:A:195:ASP:C	2.26	0.43
1:B:517:PHE:CE1	1:B:795:VAL:HG22	2.54	0.43
1:C:221:ILE:HG12	1:C:243:SER:HB2	2.01	0.43
1:A:464:VAL:HG13	1:A:489:ILE:HG13	2.01	0.43
1:B:118:LYS:HE2	1:B:148:ALA:HB2	2.01	0.43
1:D:118:LYS:HG2	1:D:145:THR:HG22	2.01	0.43
1:D:498:LEU:HD12	1:D:498:LEU:C	2.44	0.43
1:B:178:ARG:HD3	1:B:211:ILE:HG22	2.01	0.42
1:C:520:PRO:HD3	3:C:902:6ZP:C20	2.49	0.42
1:C:667:PHE:HE1	1:C:727:LEU:HD13	1.84	0.42
1:D:579:PHE:O	1:D:583:ALA:N	2.46	0.42
1:A:667:PHE:HE1	1:A:727:LEU:HD13	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:ILE:HG12	1:C:792:VAL:HG21	2.01	0.42
1:C:71:TYR:HA	1:C:323:TRP:HH2	1.83	0.42
1:C:231:ASP:HB3	1:C:234:LYS:HE2	2.02	0.42
1:C:496:MET:HE2	1:C:763:LYS:HD3	2.01	0.42
1:A:379:LYS:O	1:A:379:LYS:HG3	2.19	0.42
1:B:97:ILE:HG12	1:B:111:ILE:HB	2.01	0.42
1:B:405:TYR:CD1	1:B:478:PRO:HG3	2.55	0.42
1:D:132:LYS:NZ	1:D:187:LYS:HB3	2.34	0.42
1:A:507:PRO:HA	1:A:508:GLN:CB	2.50	0.42
1:B:520:PRO:O	1:C:787:LEU:HB2	2.19	0.42
1:B:728:ASP:OD1	1:B:728:ASP:N	2.52	0.42
1:C:581:LEU:HA	1:C:584:PHE:H	1.84	0.42
1:A:231:ASP:HB3	1:A:234:LYS:HE2	2.01	0.42
1:C:112:GLN:H	1:C:112:GLN:CD	2.27	0.42
1:D:185:GLU:OE1	1:D:213:LYS:NZ	2.40	0.42
1:D:219:HIS:HA	1:D:241:GLU:O	2.19	0.42
1:A:486:GLU:N	1:A:491:PHE:CE2	2.80	0.42
1:A:608:PHE:HD1	1:B:795:VAL:HG12	1.84	0.42
1:B:210:THR:HG22	1:D:237:PHE:HB2	2.01	0.42
1:D:522:ALA:O	1:D:526:TRP:HD1	2.01	0.42
1:A:514:VAL:O	1:A:514:VAL:HG22	2.20	0.42
1:B:498:LEU:HD23	1:B:707:THR:HG21	2.02	0.42
1:C:498:LEU:HD12	1:C:499:GLY:N	2.34	0.42
1:D:520:PRO:HD3	3:D:902:6ZP:C19	2.50	0.42
1:A:125:ILE:HG23	1:A:130:TRP:HB2	2.02	0.42
1:C:388:SER:N	1:C:389:GLY:HA2	2.34	0.42
1:C:629:MET:SD	1:C:630:VAL:HA	2.59	0.42
1:D:172:LYS:NZ	1:D:175:GLU:OE1	2.52	0.42
1:A:401:LEU:HD23	1:A:406:VAL:HG12	2.02	0.42
1:D:642:GLN:HE22	1:D:645:ILE:HB	1.85	0.42
1:D:791:ASN:OD1	1:D:791:ASN:C	2.62	0.42
1:D:809:VAL:HA	1:D:812:ILE:HG12	2.02	0.42
1:A:255:VAL:O	1:A:259:ILE:HG12	2.20	0.41
1:B:346:LYS:HE3	1:B:355:ASN:HD22	1.85	0.41
1:B:619:ASN:HA	1:C:624:LEU:HD13	2.02	0.41
1:D:498:LEU:HD12	1:D:730:LYS:HG3	2.01	0.41
1:A:517:PHE:HE1	1:A:795:VAL:HG22	1.85	0.41
1:B:405:TYR:HB3	1:B:425:CYS:SG	2.60	0.41
1:C:702:TYR:CE2	1:C:704:LEU:HB3	2.55	0.41
1:D:447:ASP:OD1	1:D:447:ASP:N	2.53	0.41
1:B:404:PRO:HB3	1:B:711:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481:ILE:HA	1:B:491:PHE:CE2	2.55	0.41
1:A:486:GLU:HA	1:A:491:PHE:CD2	2.54	0.41
1:A:596:LEU:HD12	1:A:596:LEU:HA	1.80	0.41
1:B:332:ALA:O	1:B:336:VAL:HG23	2.20	0.41
1:C:405:TYR:CD2	1:C:478:PRO:HG3	2.56	0.41
1:D:171:ASP:OD1	1:D:172:LYS:N	2.49	0.41
1:D:632:PRO:O	1:D:632:PRO:HD2	2.20	0.41
1:A:619:ASN:HA	1:B:624:LEU:CD1	2.49	0.41
1:A:640:SER:HB3	1:A:670:MET:HG2	2.02	0.41
1:C:115:PRO:HA	1:C:353:ARG:HB2	2.02	0.41
1:D:485:ARG:O	1:D:491:PHE:HE2	2.01	0.41
1:D:509:LYS:HA	1:D:510:SER:C	2.46	0.41
1:A:30:ARG:HD2	1:A:270:TYR:CE2	2.55	0.41
1:A:517:PHE:HA	3:A:902:6ZP:C18	2.51	0.41
1:B:48:ASP:OD1	1:B:65:GLN:NE2	2.54	0.41
1:C:98:THR:O	1:C:113:MET:N	2.45	0.41
1:D:502:ILE:HD13	1:D:639:LEU:HD21	2.00	0.41
1:A:227:PHE:CD1	1:A:244:GLY:HA3	2.55	0.41
1:B:500:ILE:HD12	1:B:655:THR:HG23	2.03	0.41
1:B:524:GLU:CD	1:B:524:GLU:N	2.78	0.41
1:C:397:VAL:O	1:C:443:THR:OG1	2.35	0.41
1:A:153:ALA:HA	1:A:158:TRP:HB2	2.02	0.41
1:D:498:LEU:HD12	1:D:499:GLY:N	2.35	0.41
1:A:483:LEU:O	1:A:487:GLU:HG3	2.21	0.41
1:A:494:PRO:HA	1:A:732:TYR:O	2.21	0.41
1:C:209:ILE:HA	1:C:214:HIS:CD2	2.56	0.41
1:C:633:ILE:O	1:C:634:GLU:O	2.39	0.41
1:A:395:VAL:N	1:A:439:LYS:O	2.51	0.41
1:C:483:LEU:O	1:C:487:GLU:HG3	2.21	0.41
1:D:235:ILE:HD12	1:D:242:VAL:HG21	2.03	0.41
1:D:521:LEU:HB3	1:D:525:ILE:HB	2.03	0.41
1:B:13:GLN:H	1:B:13:GLN:HG2	1.66	0.40
1:B:219:HIS:HD2	1:B:241:GLU:O	2.04	0.40
1:B:702:TYR:CE2	1:B:704:LEU:HB3	2.56	0.40
1:C:622:ALA:HA	1:D:625:THR:HG22	2.04	0.40
1:A:74:PHE:CZ	1:A:285:THR:HG23	2.57	0.40
1:A:498:LEU:HD12	1:A:730:LYS:CG	2.51	0.40
1:A:806:ALA:HA	1:D:600:ILE:HD11	2.03	0.40
1:B:507:PRO:CD	1:B:508:GLN:HA	2.52	0.40
1:B:683:VAL:HG11	1:B:689:GLY:HA2	2.03	0.40
1:B:708:MET:O	1:B:712:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:498:LEU:HD23	1:D:707:THR:HG21	2.04	0.40
1:A:498:LEU:CD1	1:A:730:LYS:HD2	2.52	0.40
1:C:539:VAL:HG21	1:D:803:LEU:HD22	2.03	0.40
1:D:401:LEU:HD23	1:D:406:VAL:HG12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	771/803 (96%)	715 (93%)	52 (7%)	4 (0%)	24	60
1	B	767/803 (96%)	708 (92%)	55 (7%)	4 (0%)	24	60
1	C	767/803 (96%)	718 (94%)	43 (6%)	6 (1%)	16	52
1	D	771/803 (96%)	718 (93%)	49 (6%)	4 (0%)	24	60
All	All	3076/3212 (96%)	2859 (93%)	199 (6%)	18 (1%)	21	57

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	631	SER
1	C	632	PRO
1	C	634	GLU
1	D	633	ILE
1	D	630	VAL
1	A	512	PRO
1	A	517	PHE
1	A	631	SER
1	B	520	PRO
1	B	780	SER
1	A	520	PRO

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Mol	Chain	Res	Type
1	B	517	PHE
1	C	519	ASP
1	B	519	ASP
1	C	507	PRO
1	D	593	PRO
1	C	511	LYS
1	D	632	PRO

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	628/683 (92%)	621 (99%)	7 (1%)	65	74
1	B	635/683 (93%)	626 (99%)	9 (1%)	59	71
1	C	622/683 (91%)	614 (99%)	8 (1%)	61	72
1	D	626/683 (92%)	620 (99%)	6 (1%)	68	76
All	All	2511/2732 (92%)	2481 (99%)	30 (1%)	63	73

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	321	VAL
1	A	450	TYR
1	A	581	LEU
1	A	629	MET
1	A	639	LEU
1	A	795	VAL
1	B	304	ILE
1	B	382	LEU
1	B	450	TYR
1	B	491	PHE
1	B	629	MET
1	B	630	VAL
1	B	742	LEU

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Mol	Chain	Res	Type
1	B	773	CYS
1	B	795	VAL
1	C	177	TYR
1	C	321	VAL
1	C	491	PHE
1	C	629	MET
1	C	631	SER
1	C	639	LEU
1	C	787	LEU
1	C	795	VAL
1	D	177	TYR
1	D	321	VAL
1	D	629	MET
1	D	631	SER
1	D	787	LEU
1	D	795	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	290	GLN
1	B	112	GLN
1	B	791	ASN
1	C	49	ASN
1	C	147	GLN
1	C	219	HIS
1	C	274	HIS
1	C	290	GLN
1	C	298	ASN
1	C	302	GLN
1	D	93	HIS
1	D	274	HIS
1	D	764	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	C	901	1	14,14,15	0.41	0	17,19,21	1.38	2 (11%)
3	6ZP	B	902	-	30,30,30	2.55	7 (23%)	37,41,41	1.66	6 (16%)
3	6ZP	A	902	-	30,30,30	2.54	7 (23%)	37,41,41	1.67	7 (18%)
2	NAG	D	901	1	14,14,15	0.24	0	17,19,21	0.41	0
3	6ZP	D	902	-	30,30,30	2.54	7 (23%)	37,41,41	1.64	7 (18%)
2	NAG	B	901	1	14,14,15	0.24	0	17,19,21	0.44	0
3	6ZP	C	902	-	30,30,30	2.54	7 (23%)	37,41,41	1.65	6 (16%)
2	NAG	A	901	1	14,14,15	0.30	0	17,19,21	0.38	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
2	NAG	C	901	1	-	5/6/23/26	0/1/1/1
3	6ZP	B	902	-	-	0/13/14/14	0/4/4/4
3	6ZP	A	902	-	-	0/13/14/14	0/4/4/4
2	NAG	D	901	1	-	2/6/23/26	0/1/1/1
3	6ZP	D	902	-	-	0/13/14/14	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	901	1	-	0/6/23/26	0/1/1/1
3	6ZP	C	902	-	-	1/13/14/14	0/4/4/4
2	NAG	A	901	1	-	2/6/23/26	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	902	6ZP	C08-C09	-8.26	1.39	1.49
3	C	902	6ZP	C08-C09	-8.23	1.39	1.49
3	A	902	6ZP	C08-C09	-8.18	1.39	1.49
3	D	902	6ZP	C08-C09	-8.18	1.39	1.49
3	B	902	6ZP	C22-N21	-6.27	1.33	1.44
3	A	902	6ZP	C22-N21	-6.26	1.33	1.44
3	D	902	6ZP	C22-N21	-6.25	1.33	1.44
3	C	902	6ZP	C22-N21	-6.20	1.33	1.44
3	A	902	6ZP	C03-C02	6.20	1.53	1.44
3	B	902	6ZP	C03-C02	6.20	1.53	1.44
3	D	902	6ZP	C03-C02	6.15	1.53	1.44
3	C	902	6ZP	C03-C02	6.14	1.53	1.44
3	D	902	6ZP	C09-C10	-3.60	1.40	1.46
3	B	902	6ZP	C09-C10	-3.58	1.40	1.46
3	A	902	6ZP	C09-C10	-3.57	1.40	1.46
3	C	902	6ZP	C09-C10	-3.54	1.40	1.46
3	C	902	6ZP	C10-N21	-2.95	1.35	1.41
3	A	902	6ZP	C10-N21	-2.94	1.35	1.41
3	B	902	6ZP	C10-N21	-2.92	1.35	1.41
3	D	902	6ZP	C10-N21	-2.88	1.35	1.41
3	D	902	6ZP	C20-N21	-2.88	1.32	1.37
3	B	902	6ZP	C20-N21	-2.86	1.32	1.37
3	C	902	6ZP	C20-N21	-2.86	1.32	1.37
3	A	902	6ZP	C20-N21	-2.83	1.32	1.37
3	D	902	6ZP	C14-C13	-2.56	1.39	1.48
3	B	902	6ZP	C14-C13	-2.55	1.39	1.48
3	A	902	6ZP	C14-C13	-2.54	1.39	1.48
3	C	902	6ZP	C14-C13	-2.54	1.39	1.48

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	6ZP	O11-C10-C09	-5.38	118.33	125.37
3	B	902	6ZP	O11-C10-C09	-5.37	118.35	125.37
3	C	902	6ZP	O11-C10-C09	-5.37	118.35	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	902	6ZP	O11-C10-C09	-5.34	118.38	125.37
3	A	902	6ZP	C22-N21-C10	4.85	122.17	118.74
3	B	902	6ZP	C22-N21-C10	4.84	122.16	118.74
3	C	902	6ZP	C22-N21-C10	4.75	122.10	118.74
3	D	902	6ZP	C22-N21-C10	4.75	122.10	118.74
2	C	901	NAG	C2-N2-C7	4.66	129.14	122.90
3	A	902	6ZP	C16-N15-C14	3.72	121.72	116.93
3	B	902	6ZP	C16-N15-C14	3.69	121.69	116.93
3	C	902	6ZP	C16-N15-C14	3.69	121.68	116.93
3	D	902	6ZP	C16-N15-C14	3.65	121.64	116.93
3	A	902	6ZP	C08-C09-C10	2.43	121.61	119.41
3	B	902	6ZP	C08-C09-C10	2.41	121.59	119.41
3	C	902	6ZP	C08-C09-C10	2.39	121.58	119.41
3	D	902	6ZP	C08-C09-C10	2.38	121.57	119.41
3	A	902	6ZP	C20-C13-C12	2.33	120.11	117.65
2	C	901	NAG	C1-C2-N2	2.29	114.05	110.43
3	C	902	6ZP	C20-C13-C12	2.29	120.06	117.65
3	B	902	6ZP	C20-C13-C12	2.28	120.05	117.65
3	D	902	6ZP	C20-C13-C12	2.25	120.03	117.65
3	C	902	6ZP	C17-C16-N15	-2.07	120.14	123.42
3	A	902	6ZP	C17-C16-N15	-2.05	120.17	123.42
3	D	902	6ZP	C17-C16-N15	-2.03	120.20	123.42
3	B	902	6ZP	C17-C16-N15	-2.03	120.21	123.42
3	A	902	6ZP	C08-C09-C12	-2.02	119.56	122.30
3	D	902	6ZP	C08-C09-C12	-2.01	119.56	122.30

There are no chirality outliers.

All (10) torsion outliers are listed below:

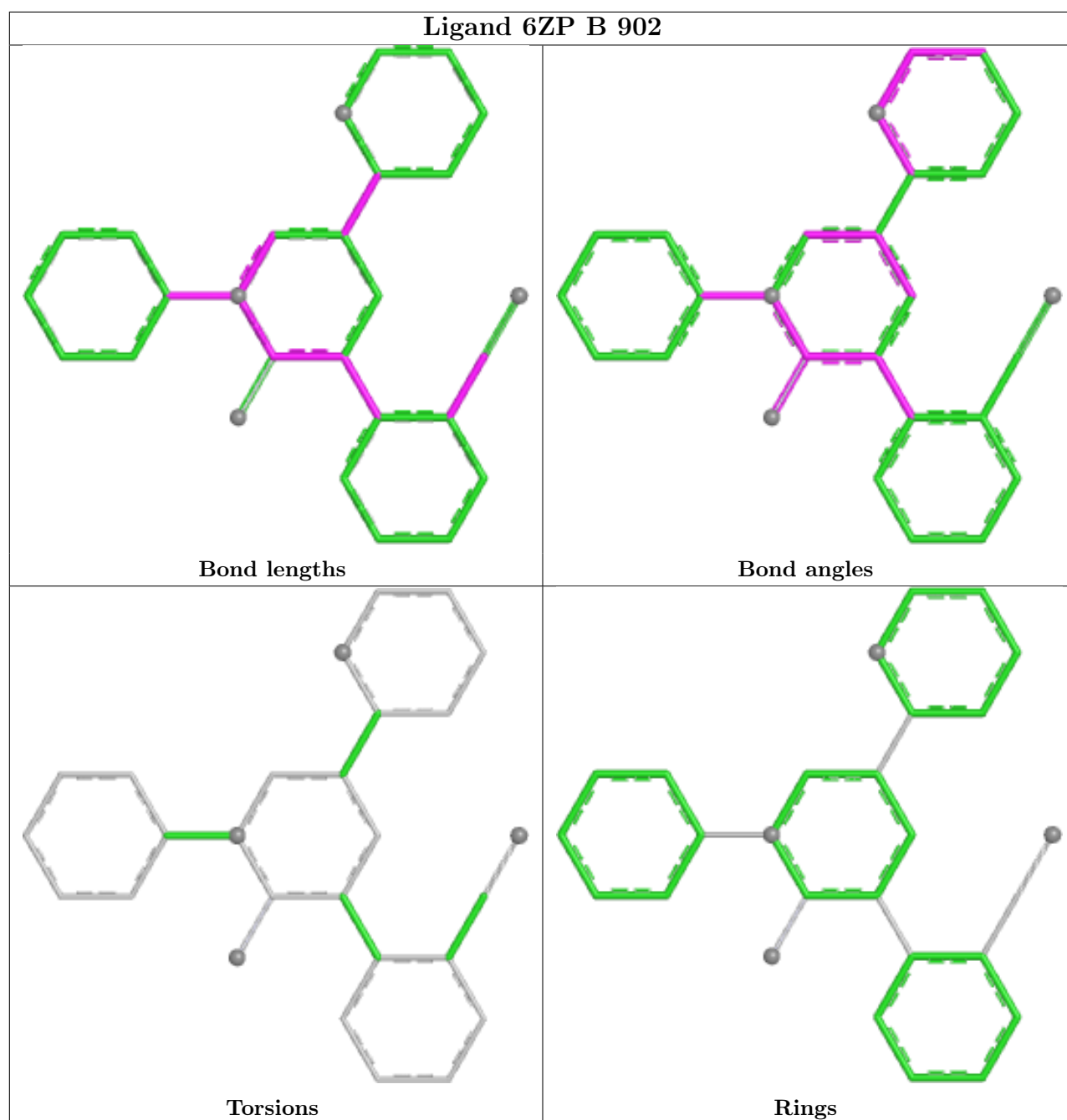
Mol	Chain	Res	Type	Atoms
2	A	901	NAG	O5-C5-C6-O6
2	A	901	NAG	C4-C5-C6-O6
2	C	901	NAG	C8-C7-N2-C2
2	C	901	NAG	O7-C7-N2-C2
2	D	901	NAG	C4-C5-C6-O6
2	D	901	NAG	O5-C5-C6-O6
2	C	901	NAG	C1-C2-N2-C7
2	C	901	NAG	C3-C2-N2-C7
2	C	901	NAG	C4-C5-C6-O6
3	C	902	6ZP	N01-C02-C03-C08

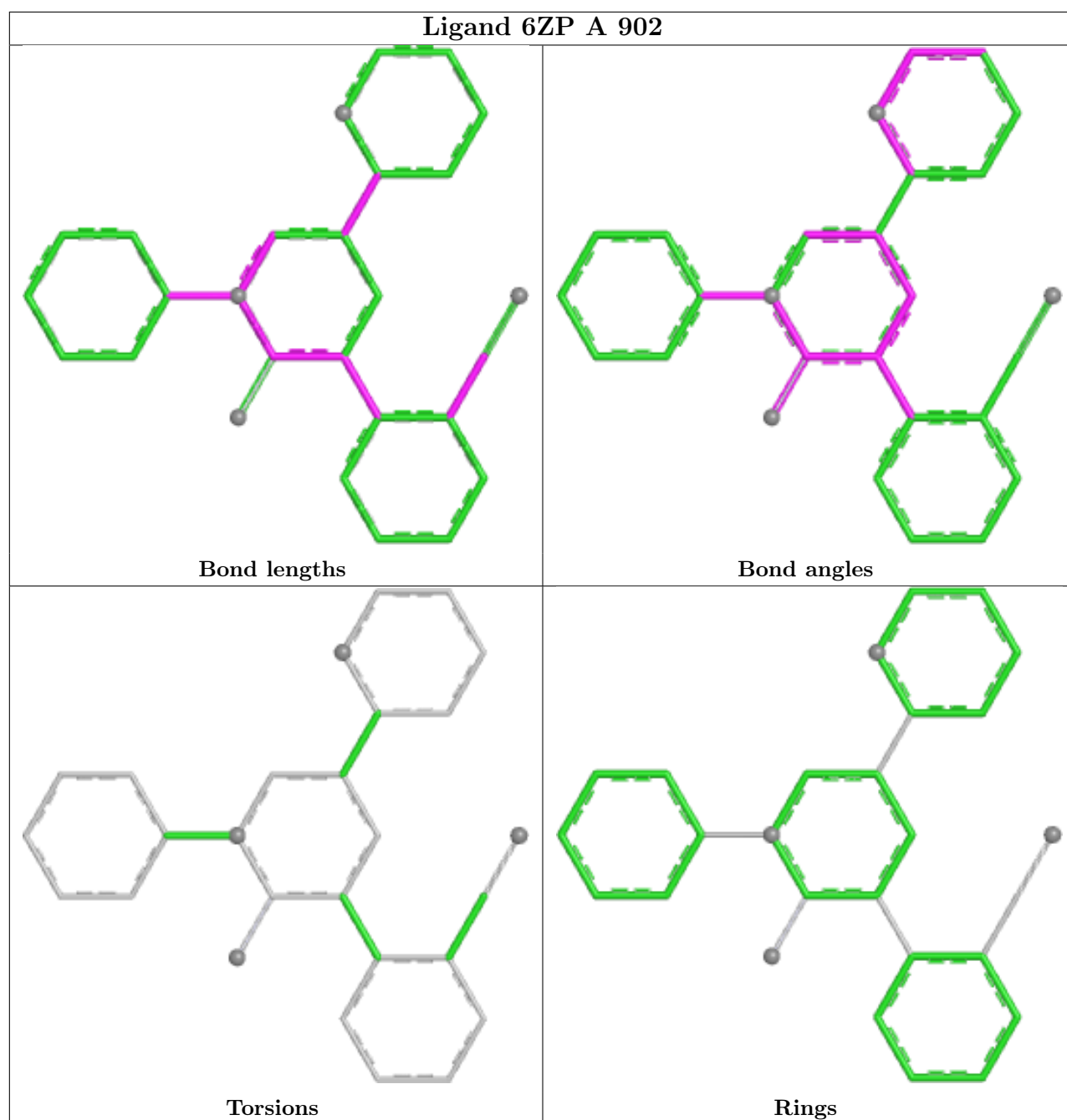
There are no ring outliers.

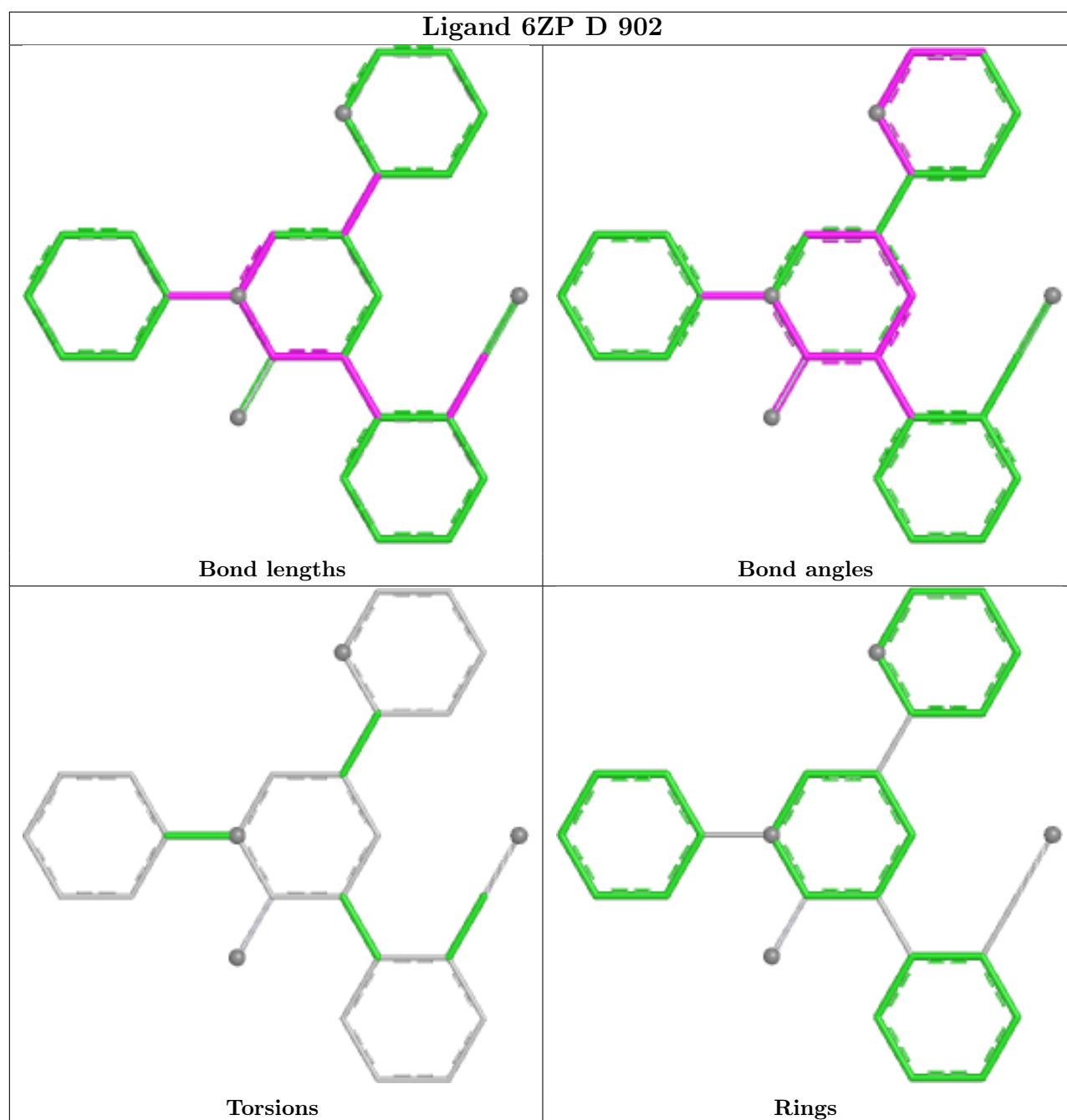
6 monomers are involved in 12 short contacts:

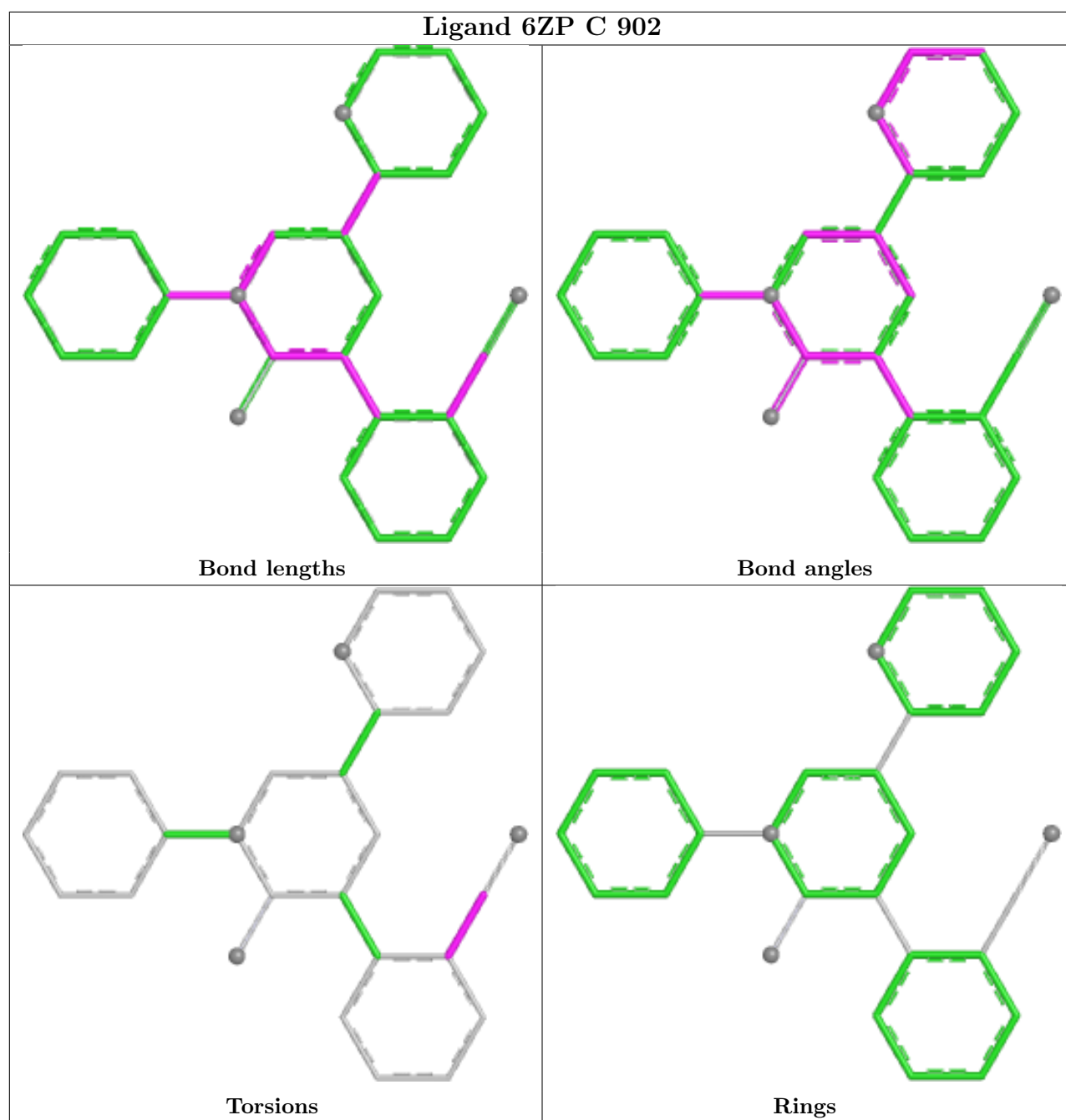
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	901	NAG	1	0
3	B	902	6ZP	2	0
3	A	902	6ZP	3	0
2	D	901	NAG	1	0
3	D	902	6ZP	3	0
3	C	902	6ZP	2	0

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	777/803 (96%)	-0.35	12 (1%)	72 54	121, 219, 345, 425	0
1	B	773/803 (96%)	-0.28	14 (1%)	67 50	126, 208, 343, 403	0
1	C	773/803 (96%)	-0.34	12 (1%)	70 52	26, 245, 351, 418	0
1	D	777/803 (96%)	-0.21	17 (2%)	62 46	137, 260, 387, 440	0
All	All	3100/3212 (96%)	-0.29	55 (1%)	67 50	26, 232, 355, 440	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	632	PRO	6.4
1	A	186	LEU	6.1
1	D	79	LYS	5.2
1	C	762	LEU	4.7
1	B	157	LYS	4.7
1	C	79	LYS	4.6
1	B	780	SER	4.3
1	B	253	SER	4.1
1	A	187	LYS	4.0
1	D	484	VAL	3.9
1	A	531	PHE	3.9
1	C	631	SER	3.9
1	D	104	ASP	3.8
1	C	629	MET	3.7
1	B	630	VAL	3.3
1	B	631	SER	3.3
1	A	309	ARG	3.2
1	B	254	LEU	3.2
1	D	497	SER	3.1
1	A	529	ILE	3.0
1	B	779	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	496	MET	2.8
1	D	485	ARG	2.8
1	B	170	ASN	2.8
1	C	78	ASP	2.7
1	D	143	LEU	2.7
1	A	532	ALA	2.6
1	D	167	ASN	2.6
1	C	82	VAL	2.5
1	C	633	ILE	2.5
1	D	431	GLU	2.5
1	D	139	SER	2.5
1	D	428	LEU	2.5
1	B	154	ALA	2.5
1	C	531	PHE	2.4
1	C	432	ILE	2.4
1	A	654	SER	2.4
1	B	615	SER	2.3
1	D	785	SER	2.3
1	C	431	GLU	2.3
1	A	527	MET	2.3
1	A	497	SER	2.3
1	D	509	LYS	2.3
1	A	792	VAL	2.2
1	D	763	LYS	2.2
1	B	515	PHE	2.2
1	D	732	TYR	2.2
1	B	416	GLU	2.2
1	C	758	VAL	2.2
1	B	456	ASP	2.2
1	A	494	PRO	2.2
1	B	168	ILE	2.2
1	A	629	MET	2.1
1	D	142	GLY	2.1
1	D	83	ASN	2.0

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

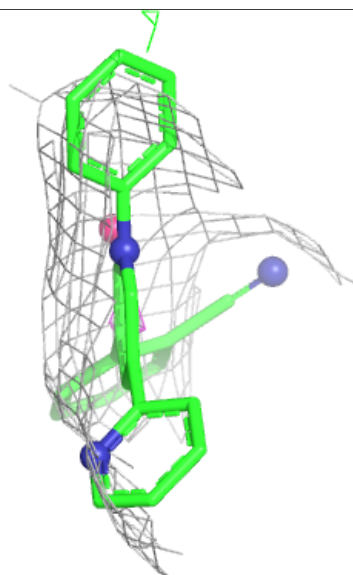
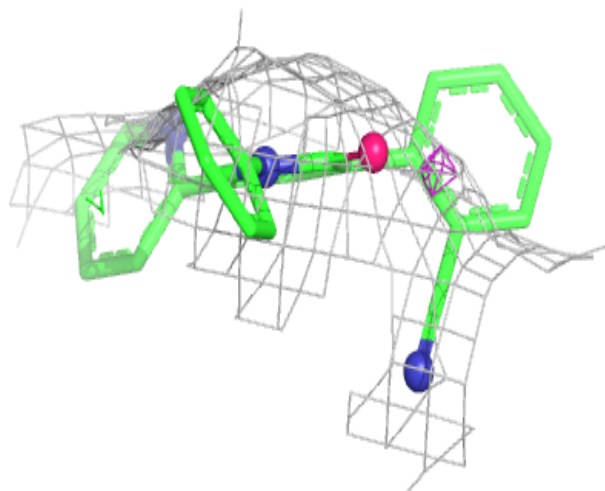
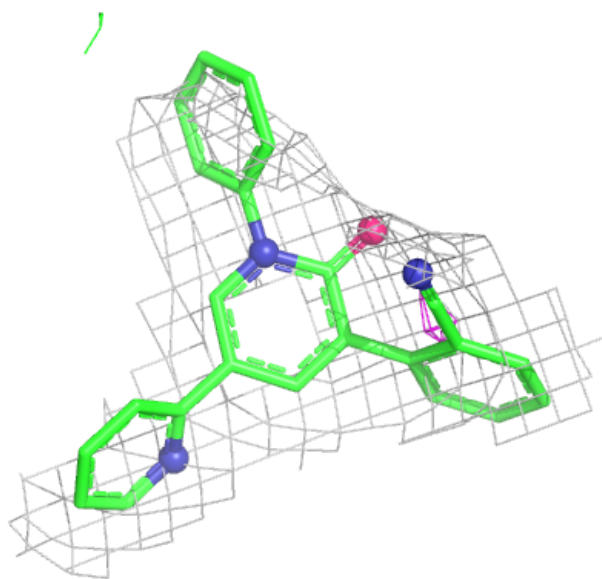
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	D	901	14/15	0.10	0.09	213,248,273,287	0
2	NAG	A	901	14/15	0.59	0.10	129,179,249,257	0
2	NAG	B	901	14/15	0.74	0.08	174,197,262,323	0
3	6ZP	B	902	27/27	0.77	0.10	135,215,215,215	0
3	6ZP	C	902	27/27	0.78	0.11	144,215,215,215	0
3	6ZP	D	902	27/27	0.79	0.08	152,203,215,215	0
3	6ZP	A	902	27/27	0.83	0.09	144,210,215,215	0
2	NAG	C	901	14/15	0.83	0.06	158,248,297,304	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.

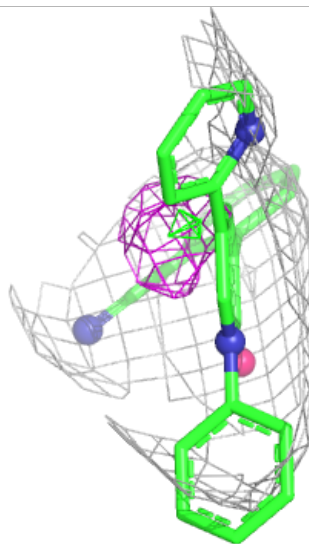
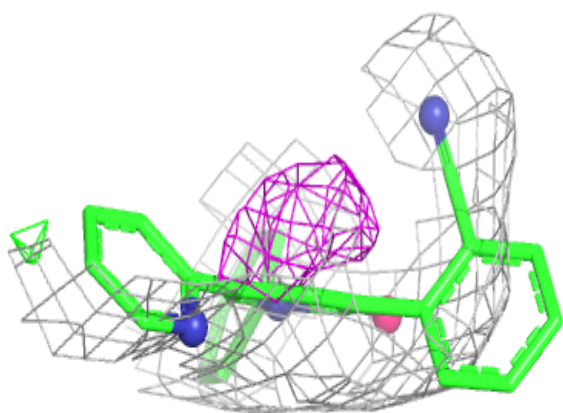
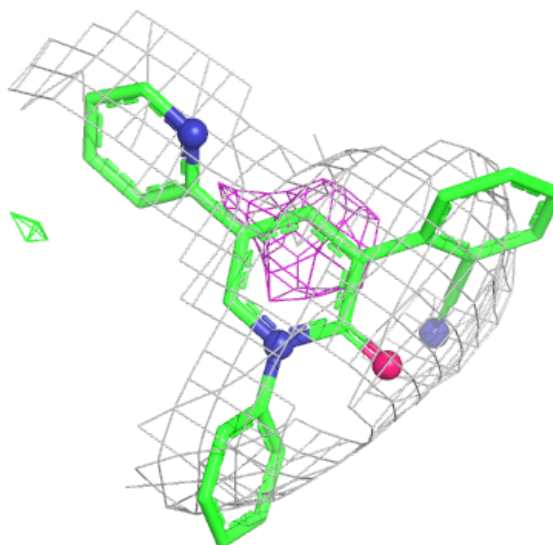
Electron density around 6ZP B 902:

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



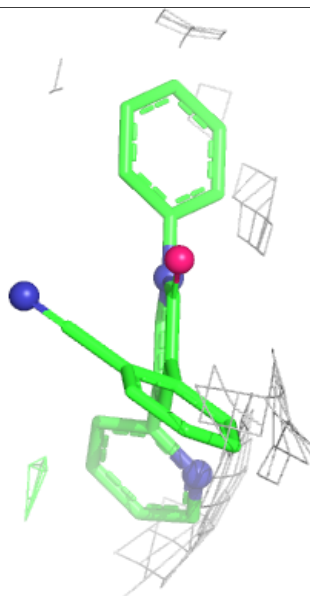
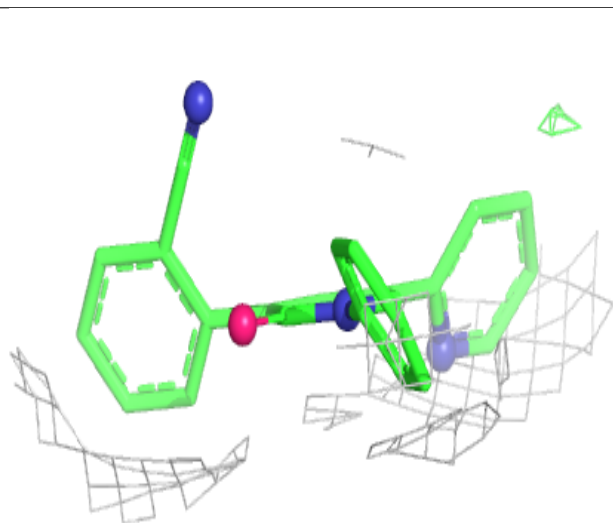
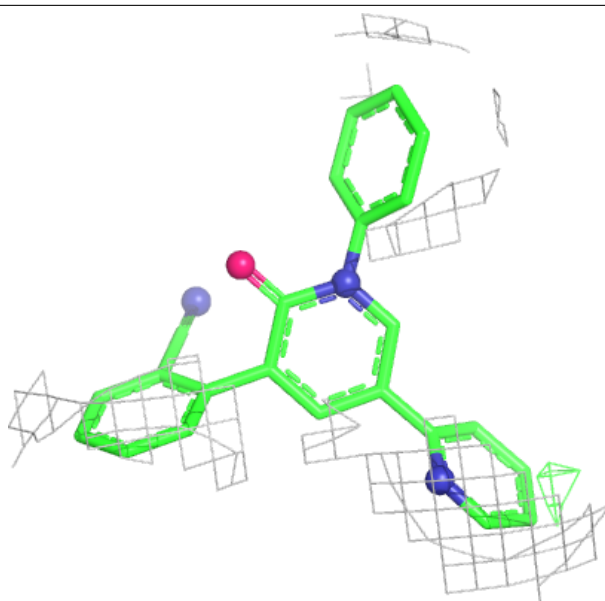
Electron density around 6ZP C 902:

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



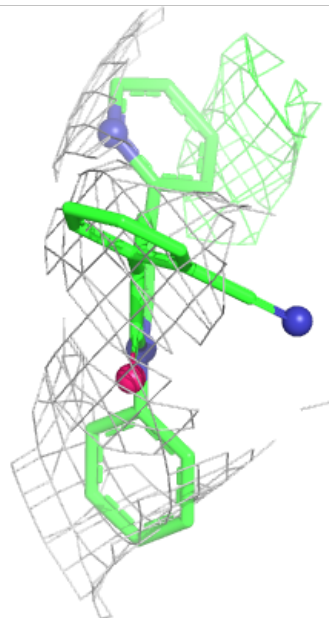
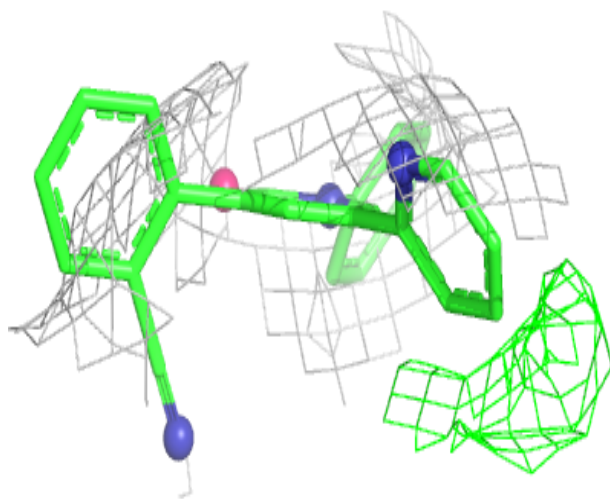
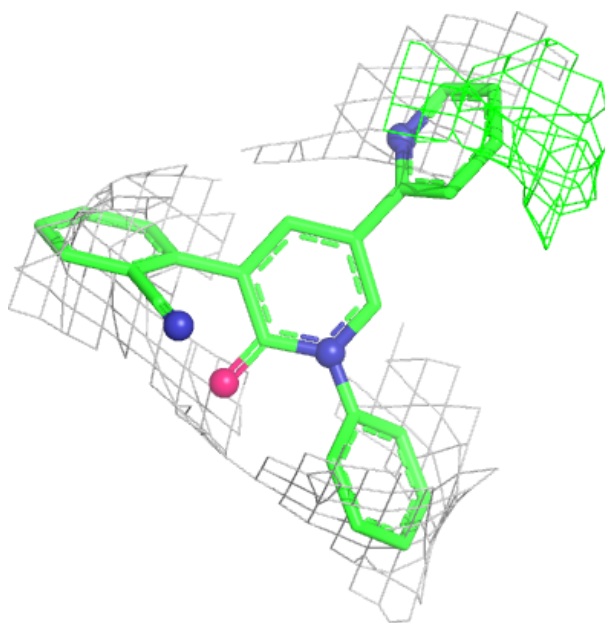
Electron density around 6ZP D 902:

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



Electron density around 6ZP A 902:

$2mF_o-DF_c$ (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.