



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:35 PM UTC

PDB ID : 1UK1 / pdb_00001uk1
Title : Crystal structure of human poly(ADP-ribose) polymerase complexed with a potent inhibitor
Authors : Kinoshita, T.
Deposited on : 2003-08-14
Resolution : 3.00 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

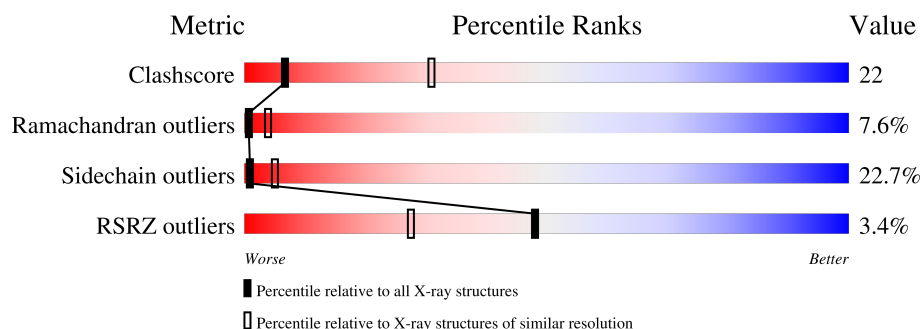
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	350	
1	B	350	

2 Entry composition [i](#)

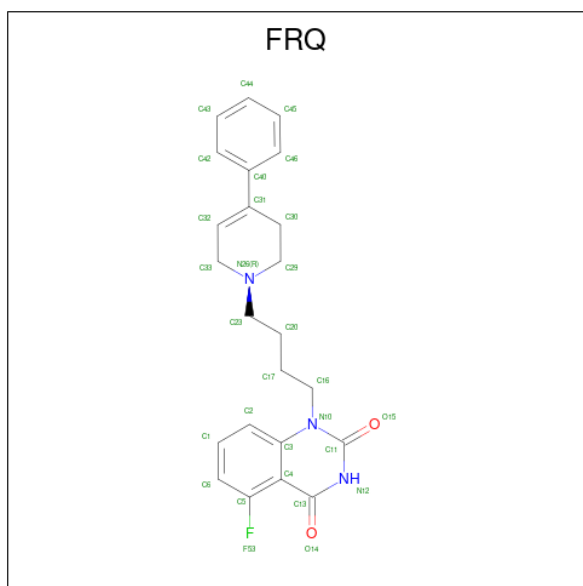
There are 3 unique types of molecules in this entry. The entry contains 5757 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Poly [ADP-ribose] polymerase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2754	1752	465	526	11			
1	B	350	Total	C	N	O	S	0	0	0
			2754	1752	465	526	11			

- Molecule 2 is 5-FLUORO-1-[4-(4-PHENYL-3,6-DIHYDROPYRIDIN-1(2H)-YL)BUTYL]QUINAZOLINE-2,4(1H,3H)-DIONE (CCD ID: FRQ) (formula: C₂₃H₂₄FN₃O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			29	23	1	3	2		
2	B	1	Total	C	F	N	O	0	0
			29	23	1	3	2		

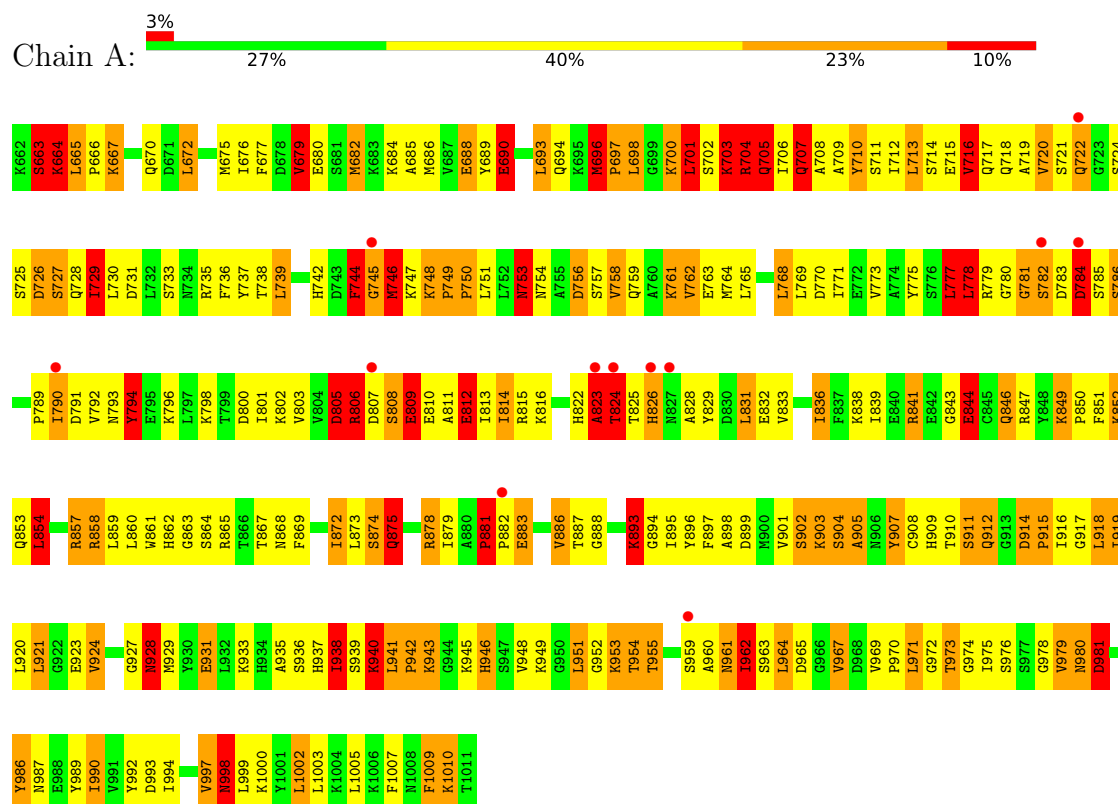
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	101	Total 101	O 101	0	0
3	B	90	Total 90	O 90	0	0

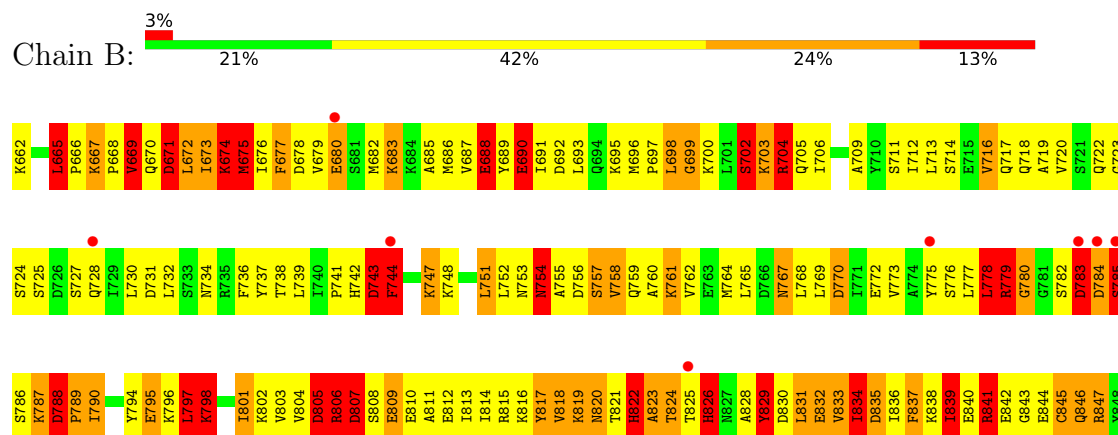
3 Residue-property plots

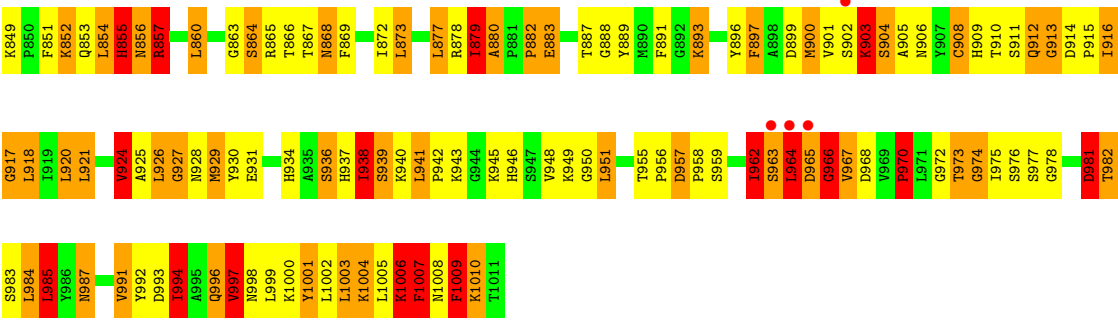
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Poly [ADP-ribose] polymerase-1



• Molecule 1: Poly [ADP-ribose] polymerase-1





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	179.96Å 53.27Å 91.47Å 90.00° 113.80° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 30.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.00) 99.5 (30.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.96Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.242 , 0.274 0.281 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	53.0	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	5757	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.49% 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: FRQ

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	1.26	2/2806 (0.1%)	2.56	251/3786 (6.6%)
1	B	1.35	8/2806 (0.3%)	2.65	267/3786 (7.1%)
All	All	1.31	10/5612 (0.2%)	2.61	518/7572 (6.8%)

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	14
1	B	0	28
All	All	0	42

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	806	ARG	NE-CZ	6.29	1.40	1.33
1	B	909	HIS	ND1-CE1	6.15	1.38	1.32
1	B	742	HIS	CA-C	6.10	1.61	1.53
1	B	742	HIS	CG-CD2	6.04	1.42	1.35
1	B	742	HIS	ND1-CE1	5.90	1.38	1.32
1	B	964	LEU	CA-C	5.57	1.60	1.52
1	A	936	SER	CA-C	-5.53	1.47	1.53
1	B	924	VAL	CA-CB	5.27	1.60	1.54
1	B	807	ASP	CA-C	5.26	1.59	1.52
1	B	909	HIS	CE1-NE2	5.20	1.37	1.32

All (518) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	782	SER	N-CA-C	12.52	128.84	111.56
1	A	828	ALA	CA-C-N	11.03	141.55	121.70
1	A	828	ALA	C-N-CA	11.03	141.55	121.70
1	B	822	HIS	CA-CB-CG	-10.81	102.99	113.80
1	B	926	LEU	N-CA-C	10.35	122.56	111.28
1	A	744	PHE	N-CA-C	10.22	123.68	111.82
1	A	744	PHE	CA-CB-CG	-10.17	103.63	113.80
1	B	879	ILE	N-CA-C	10.01	123.12	109.80
1	B	906	ASN	CA-CB-CG	-10.01	102.59	112.60
1	B	709	ALA	N-CA-C	9.77	122.01	111.36
1	A	839	ILE	N-CA-C	9.64	122.00	108.12
1	B	744	PHE	N-CA-C	9.61	124.55	113.02
1	B	757	SER	N-CA-C	9.59	122.94	111.82
1	B	1006	LYS	CA-C-N	-9.53	110.45	122.84
1	B	1006	LYS	C-N-CA	-9.53	110.45	122.84
1	B	753	ASN	CA-C-O	9.52	131.47	119.95
1	B	691	ILE	CA-C-N	-9.51	108.43	122.41
1	B	691	ILE	C-N-CA	-9.51	108.43	122.41
1	B	1009	PHE	N-CA-C	9.46	124.81	110.14
1	A	914	ASP	CA-CB-CG	9.41	122.01	112.60
1	B	853	GLN	CA-C-N	-9.40	107.02	122.81
1	B	853	GLN	C-N-CA	-9.40	107.02	122.81
1	A	1009	PHE	CA-CB-CG	-9.38	104.42	113.80
1	B	1009	PHE	CA-CB-CG	9.34	123.14	113.80
1	A	902	SER	N-CA-C	9.06	121.24	111.36
1	B	669	VAL	N-CA-C	9.01	119.56	110.82
1	A	833	VAL	N-CA-C	8.88	120.62	108.89
1	A	812	GLU	N-CA-C	8.86	120.93	111.28
1	A	808	SER	N-CA-C	8.84	123.24	110.24
1	B	767	ASN	CA-CB-CG	-8.83	103.77	112.60
1	B	832	GLU	CA-C-N	-8.79	111.69	123.12
1	B	832	GLU	C-N-CA	-8.79	111.69	123.12
1	A	963	SER	CA-C-N	-8.78	106.76	122.74
1	A	963	SER	C-N-CA	-8.78	106.76	122.74
1	B	976	SER	N-CA-C	8.75	124.03	110.20
1	A	672	LEU	N-CA-C	8.69	120.75	111.28
1	B	916	ILE	CA-CB-CG1	8.64	125.09	110.40
1	A	971	LEU	CA-C-N	-8.63	116.03	122.33
1	A	971	LEU	C-N-CA	-8.63	116.03	122.33
1	B	856	ASN	CA-C-N	8.60	137.18	121.70
1	B	856	ASN	C-N-CA	8.60	137.18	121.70
1	B	959	SER	N-CA-C	8.59	123.01	112.54
1	A	852	LYS	CA-C-N	-8.58	110.08	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	852	LYS	C-N-CA	-8.58	110.08	123.12
1	A	733	SER	N-CA-C	8.57	121.40	111.11
1	A	775	TYR	N-CA-C	8.52	121.33	111.11
1	A	878	ARG	CA-C-N	-8.51	108.01	121.62
1	A	878	ARG	C-N-CA	-8.51	108.01	121.62
1	B	982	THR	N-CA-C	8.47	121.95	109.07
1	B	998	ASN	CA-C-N	-8.47	109.38	121.50
1	B	998	ASN	C-N-CA	-8.47	109.38	121.50
1	B	787	LYS	N-CA-C	8.46	125.23	109.24
1	A	791	ASP	N-CA-C	8.28	125.03	111.37
1	B	902	SER	N-CA-C	8.27	119.99	110.97
1	B	833	VAL	CA-C-N	-8.24	114.67	122.66
1	B	833	VAL	C-N-CA	-8.24	114.67	122.66
1	B	788	ASP	N-CA-C	8.22	127.97	109.81
1	B	832	GLU	N-CA-C	8.17	121.79	108.55
1	A	823	ALA	N-CA-C	8.17	122.21	109.96
1	A	781	GLY	CA-C-N	-8.12	109.34	122.34
1	A	781	GLY	C-N-CA	-8.12	109.34	122.34
1	A	696	MET	CA-C-O	8.12	126.29	119.71
1	A	960	ALA	CA-C-N	-8.12	110.78	122.06
1	A	960	ALA	C-N-CA	-8.12	110.78	122.06
1	B	670	GLN	N-CA-C	8.10	120.83	111.11
1	A	832	GLU	N-CA-C	8.09	121.59	108.32
1	A	941	LEU	CB-CA-C	8.07	119.24	109.31
1	B	938	ILE	N-CA-CB	-8.06	100.34	112.35
1	A	874	SER	N-CA-C	8.01	122.31	112.54
1	B	839	ILE	CA-C-N	-7.95	110.76	123.23
1	B	839	ILE	C-N-CA	-7.95	110.76	123.23
1	B	883	GLU	N-CA-C	7.94	127.71	110.80
1	B	856	ASN	N-CA-C	7.93	121.78	109.96
1	A	997	VAL	CA-C-N	-7.89	109.94	122.73
1	A	997	VAL	C-N-CA	-7.89	109.94	122.73
1	A	938	ILE	CA-C-O	7.88	129.17	120.59
1	B	826	HIS	CA-C-N	-7.86	111.92	122.85
1	B	826	HIS	C-N-CA	-7.86	111.92	122.85
1	B	784	ASP	N-CA-C	7.84	127.51	110.80
1	A	980	ASN	N-CA-C	7.78	121.26	111.69
1	A	789	PRO	N-CA-C	7.78	123.82	113.40
1	B	725	SER	N-CA-C	7.74	121.92	110.30
1	A	696	MET	N-CA-C	7.70	123.67	108.59
1	B	834	ILE	CA-C-O	7.67	127.51	120.30
1	A	1005	LEU	CA-C-N	-7.63	112.00	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1005	LEU	C-N-CA	-7.63	112.00	122.30
1	A	919	ILE	N-CA-C	7.62	119.26	108.36
1	B	802	LYS	CA-C-N	-7.62	113.33	122.93
1	B	802	LYS	C-N-CA	-7.62	113.33	122.93
1	A	945	LYS	CA-CB-CG	-7.56	98.98	114.10
1	B	739	LEU	CA-C-N	-7.54	114.95	123.25
1	B	739	LEU	C-N-CA	-7.54	114.95	123.25
1	A	781	GLY	N-CA-C	7.53	125.16	113.86
1	A	717	GLN	CA-C-N	-7.53	110.39	120.63
1	A	717	GLN	C-N-CA	-7.53	110.39	120.63
1	B	805	ASP	CA-CB-CG	7.52	120.12	112.60
1	A	707	GLN	N-CA-C	7.52	121.70	112.23
1	B	975	ILE	CA-C-N	-7.45	110.77	121.42
1	B	975	ILE	C-N-CA	-7.45	110.77	121.42
1	A	761	LYS	N-CA-C	7.43	121.59	112.23
1	A	712	ILE	N-CA-C	7.43	118.20	110.62
1	A	701	LEU	CA-C-N	-7.40	111.63	122.65
1	A	701	LEU	C-N-CA	-7.40	111.63	122.65
1	B	806	ARG	N-CA-C	7.38	126.53	110.80
1	B	946	HIS	CA-CB-CG	-7.37	106.43	113.80
1	B	751	LEU	CA-C-N	-7.34	111.18	122.05
1	B	751	LEU	C-N-CA	-7.34	111.18	122.05
1	A	750	PRO	CB-CA-C	7.28	117.98	111.87
1	A	951	LEU	N-CA-C	7.26	120.36	109.25
1	B	758	VAL	N-CA-C	7.26	118.05	110.72
1	B	803	VAL	N-CA-C	7.26	118.74	108.36
1	B	760	ALA	CA-C-N	-7.26	111.24	122.49
1	B	760	ALA	C-N-CA	-7.26	111.24	122.49
1	B	993	ASP	CA-C-N	-7.23	110.11	121.02
1	B	993	ASP	C-N-CA	-7.23	110.11	121.02
1	B	834	ILE	CA-C-N	-7.21	111.38	122.62
1	B	834	ILE	C-N-CA	-7.21	111.38	122.62
1	B	665	LEU	CA-C-N	-7.20	112.90	120.03
1	B	665	LEU	C-N-CA	-7.20	112.90	120.03
1	A	792	VAL	N-CA-C	7.20	117.30	110.53
1	B	795	GLU	N-CA-C	7.20	121.16	112.38
1	A	782	SER	CA-C-N	-7.19	107.81	121.54
1	A	782	SER	C-N-CA	-7.19	107.81	121.54
1	A	962	ILE	CA-C-N	-7.17	112.19	123.23
1	A	962	ILE	C-N-CA	-7.17	112.19	123.23
1	A	868	ASN	N-CA-C	7.16	121.25	112.23
1	A	786	SER	N-CA-C	7.14	121.83	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	721	SER	N-CA-C	7.13	121.80	113.18
1	B	716	VAL	N-CA-C	7.12	117.89	110.62
1	A	746	MET	N-CA-C	7.11	120.68	108.02
1	B	754	ASN	N-CA-CB	-7.08	98.97	111.08
1	A	770	ASP	N-CA-C	7.07	119.84	111.71
1	B	671	ASP	CA-CB-CG	7.07	119.67	112.60
1	A	979	VAL	N-CA-C	7.05	116.77	106.55
1	B	966	GLY	CA-C-N	6.97	134.25	121.70
1	B	966	GLY	C-N-CA	6.97	134.25	121.70
1	A	748	LYS	N-CA-C	6.96	119.61	109.04
1	B	790	ILE	N-CA-C	6.95	120.77	111.17
1	B	994	ILE	CA-CB-CG1	6.93	122.19	110.40
1	A	693	LEU	N-CA-C	6.92	121.47	112.89
1	B	783	ASP	N-CA-C	6.92	122.00	112.04
1	B	845	CYS	N-CA-C	6.91	118.89	111.36
1	A	710	TYR	CA-C-O	6.90	127.73	120.42
1	A	981	ASP	N-CA-C	6.89	125.48	110.80
1	B	809	GLU	N-CA-C	6.87	119.35	111.11
1	B	869	PHE	CA-CB-CG	-6.80	107.00	113.80
1	A	993	ASP	CA-CB-CG	6.79	119.39	112.60
1	B	929	MET	N-CA-C	6.79	119.80	108.73
1	A	964	LEU	CB-CA-C	6.79	121.00	109.80
1	B	977	SER	N-CA-C	6.79	118.76	110.41
1	A	759	GLN	CB-CG-CD	-6.78	101.07	112.60
1	B	807	ASP	N-CA-C	6.77	121.51	112.30
1	B	824	THR	N-CA-C	6.76	119.23	111.11
1	B	673	ILE	CA-C-N	-6.76	109.42	120.71
1	B	673	ILE	C-N-CA	-6.76	109.42	120.71
1	B	991	VAL	N-CA-C	6.74	118.31	108.53
1	A	936	SER	CB-CA-C	-6.74	102.87	111.70
1	B	1010	LYS	N-CA-CB	-6.74	101.42	111.25
1	B	738	THR	CA-C-N	6.70	129.81	120.29
1	B	738	THR	C-N-CA	6.70	129.81	120.29
1	A	851	PHE	CA-CB-CG	-6.68	107.12	113.80
1	B	872	ILE	N-CA-C	6.68	118.24	110.62
1	A	794	TYR	CA-C-N	-6.66	109.19	120.58
1	A	794	TYR	C-N-CA	-6.66	109.19	120.58
1	A	705	GLN	N-CA-C	6.66	118.54	111.28
1	B	844	GLU	N-CA-C	6.66	119.36	111.71
1	A	697	PRO	CA-C-N	-6.64	109.02	122.31
1	A	697	PRO	C-N-CA	-6.64	109.02	122.31
1	A	759	GLN	N-CA-C	6.64	119.53	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	929	MET	CA-C-N	-6.64	111.30	121.66
1	A	929	MET	C-N-CA	-6.64	111.30	121.66
1	B	949	LYS	CA-C-N	-6.60	113.33	120.92
1	B	949	LYS	C-N-CA	-6.60	113.33	120.92
1	B	831	LEU	N-CA-C	6.58	120.10	110.17
1	B	915	PRO	CA-C-N	-6.58	114.66	122.22
1	B	915	PRO	C-N-CA	-6.58	114.66	122.22
1	B	754	ASN	CA-CB-CG	-6.56	106.04	112.60
1	B	770	ASP	N-CA-C	6.55	119.75	111.69
1	B	909	HIS	CA-C-O	6.52	129.04	121.28
1	A	826	HIS	N-CA-C	6.51	122.06	113.20
1	A	965	ASP	N-CA-C	6.51	120.15	111.30
1	B	717	GLN	CA-C-O	6.48	127.43	119.97
1	A	756	ASP	CA-C-N	-6.48	108.35	121.18
1	A	756	ASP	C-N-CA	-6.48	108.35	121.18
1	A	688	GLU	CA-C-O	6.46	127.32	119.38
1	B	968	ASP	N-CA-C	6.45	120.42	110.42
1	A	729	ILE	CA-C-N	-6.45	109.71	120.68
1	A	729	ILE	C-N-CA	-6.45	109.71	120.68
1	A	978	GLY	CA-C-N	-6.44	114.81	122.22
1	A	978	GLY	C-N-CA	-6.44	114.81	122.22
1	A	764	MET	N-CA-C	6.43	118.83	111.11
1	A	719	ALA	CA-C-N	-6.43	109.23	120.29
1	A	719	ALA	C-N-CA	-6.43	109.23	120.29
1	A	731	ASP	N-CA-C	6.42	118.28	111.28
1	A	914	ASP	N-CA-CB	6.41	121.78	110.37
1	B	675	MET	N-CA-C	6.41	121.95	111.37
1	A	893	LYS	N-CA-C	6.40	120.31	111.55
1	B	822	HIS	CA-C-N	-6.39	112.56	122.59
1	B	822	HIS	C-N-CA	-6.39	112.56	122.59
1	B	665	LEU	CB-CA-C	-6.38	100.02	108.76
1	B	727	SER	CA-C-N	-6.38	111.10	120.28
1	B	727	SER	C-N-CA	-6.38	111.10	120.28
1	A	921	LEU	CA-C-N	-6.37	116.62	122.80
1	A	921	LEU	C-N-CA	-6.37	116.62	122.80
1	B	737	TYR	CA-C-N	-6.37	111.24	120.29
1	B	737	TYR	C-N-CA	-6.37	111.24	120.29
1	A	909	HIS	CA-C-O	6.37	128.98	121.40
1	A	946	HIS	CA-C-O	6.36	126.14	119.14
1	A	724	SER	N-CA-C	6.34	124.30	110.80
1	B	833	VAL	N-CA-C	6.34	116.99	107.80
1	B	951	LEU	N-CA-C	6.33	119.03	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	858	ARG	CD-NE-CZ	-6.33	115.55	124.40
1	A	733	SER	CA-C-N	-6.32	110.70	120.31
1	A	733	SER	C-N-CA	-6.32	110.70	120.31
1	B	779	ARG	CD-NE-CZ	-6.30	115.58	124.40
1	A	931	GLU	N-CA-C	6.30	119.77	109.76
1	A	768	LEU	N-CA-C	6.29	118.94	111.33
1	B	945	LYS	N-CA-C	6.29	119.50	109.24
1	B	849	LYS	N-CA-C	6.29	123.71	109.81
1	B	912	GLN	CA-C-N	6.29	133.01	121.70
1	B	912	GLN	C-N-CA	6.29	133.01	121.70
1	A	679	VAL	N-CA-C	6.28	122.40	109.34
1	B	847	ARG	CD-NE-CZ	-6.28	115.61	124.40
1	B	879	ILE	CB-CG1-CD1	6.27	126.97	113.80
1	B	825	THR	CA-C-N	6.26	133.49	121.54
1	B	825	THR	C-N-CA	6.26	133.49	121.54
1	B	899	ASP	N-CA-C	6.25	120.51	112.26
1	A	816	LYS	N-CA-C	6.24	118.88	111.33
1	B	705	GLN	CB-CA-C	-6.24	98.00	110.42
1	A	933	LYS	N-CA-C	6.22	121.05	112.90
1	A	844	GLU	CA-C-N	-6.21	112.36	120.44
1	A	844	GLU	C-N-CA	-6.21	112.36	120.44
1	B	1001	TYR	CA-C-N	-6.21	111.98	121.66
1	B	1001	TYR	C-N-CA	-6.21	111.98	121.66
1	A	824	THR	N-CA-C	6.20	124.01	110.80
1	B	983	SER	CA-C-N	-6.20	114.24	122.99
1	B	983	SER	C-N-CA	-6.20	114.24	122.99
1	A	777	LEU	N-CA-C	6.20	117.71	111.07
1	B	780	GLY	N-CA-C	6.20	127.88	113.18
1	A	727	SER	N-CA-C	6.20	118.84	111.71
1	A	803	VAL	N-CA-C	6.19	116.42	108.12
1	A	847	ARG	N-CA-C	6.19	120.39	112.34
1	A	881	PRO	N-CA-C	6.14	118.19	110.70
1	A	729	ILE	CA-CB-CG1	-6.14	99.97	110.40
1	A	940	LYS	N-CA-C	6.14	118.41	108.41
1	A	736	PHE	N-CA-C	6.13	118.47	111.11
1	B	985	LEU	CD1-CG-CD2	-6.12	97.34	110.80
1	B	981	ASP	CA-CB-CG	6.12	118.72	112.60
1	B	867	THR	N-CA-C	6.12	118.74	111.71
1	B	920	LEU	N-CA-C	6.10	118.65	110.35
1	B	845	CYS	CA-CB-SG	-6.10	100.38	114.40
1	A	730	LEU	N-CA-C	6.09	119.91	112.23
1	B	938	ILE	CA-CB-CG2	6.08	120.83	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	808	SER	CB-CA-C	-6.07	100.74	109.84
1	B	869	PHE	N-CA-C	6.05	119.50	111.75
1	A	714	SER	N-CA-C	6.03	117.66	111.14
1	B	847	ARG	N-CA-C	6.03	119.74	112.38
1	A	704	ARG	CB-CG-CD	6.03	125.17	111.30
1	A	867	THR	N-CA-C	6.02	120.10	112.87
1	B	797	LEU	N-CA-C	6.02	123.62	110.80
1	A	898	ALA	N-CA-C	6.01	119.51	109.95
1	B	965	ASP	CA-C-O	6.01	125.08	118.65
1	B	1001	TYR	N-CA-C	6.01	118.54	108.02
1	A	994	ILE	N-CA-C	6.00	118.55	111.05
1	B	978	GLY	CA-C-O	5.99	126.92	120.75
1	B	903	LYS	CA-C-N	-5.98	110.73	120.72
1	B	903	LYS	C-N-CA	-5.98	110.73	120.72
1	A	861	TRP	N-CA-C	5.97	119.98	109.96
1	B	767	ASN	N-CA-C	5.97	121.16	111.37
1	B	720	VAL	N-CA-C	5.96	119.40	111.17
1	B	711	SER	N-CA-C	5.96	118.73	111.82
1	B	918	LEU	N-CA-C	5.95	118.60	108.90
1	A	945	LYS	N-CA-C	5.94	118.09	108.41
1	A	700	LYS	N-CA-C	5.93	118.99	111.69
1	B	860	LEU	CA-C-N	-5.92	112.96	121.42
1	B	860	LEU	C-N-CA	-5.92	112.96	121.42
1	B	981	ASP	N-CA-C	5.91	123.39	110.80
1	B	732	LEU	N-CA-C	5.91	117.40	111.07
1	A	949	LYS	N-CA-C	5.91	119.26	107.62
1	B	820	ASN	N-CA-C	5.90	120.09	113.01
1	B	983	SER	CB-CA-C	-5.89	99.41	110.01
1	A	917	GLY	CA-C-N	-5.89	115.19	122.84
1	A	917	GLY	C-N-CA	-5.89	115.19	122.84
1	A	858	ARG	N-CA-C	5.89	118.36	109.23
1	A	698	LEU	CB-CA-C	5.88	121.24	110.36
1	A	731	ASP	CA-CB-CG	-5.88	106.72	112.60
1	A	927	GLY	CA-C-N	-5.88	114.89	123.00
1	A	927	GLY	C-N-CA	-5.88	114.89	123.00
1	A	907	TYR	CA-C-N	-5.87	110.87	121.14
1	A	907	TYR	C-N-CA	-5.87	110.87	121.14
1	A	899	ASP	CA-CB-CG	5.86	118.46	112.60
1	B	857	ARG	CD-NE-CZ	-5.85	116.21	124.40
1	B	956	PRO	CA-C-N	-5.85	112.70	120.65
1	B	956	PRO	C-N-CA	-5.85	112.70	120.65
1	B	983	SER	N-CA-CB	5.84	119.38	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	813	ILE	N-CA-C	5.84	116.49	110.36
1	A	1010	LYS	CA-C-N	5.83	132.20	121.70
1	A	1010	LYS	C-N-CA	5.83	132.20	121.70
1	B	917	GLY	N-CA-C	5.83	122.72	112.10
1	B	928	ASN	CB-CA-C	5.83	119.96	110.22
1	A	814	ILE	N-CA-C	5.83	116.48	110.36
1	A	742	HIS	N-CA-C	5.83	118.73	109.24
1	A	961	ASN	N-CA-C	5.82	117.92	109.71
1	B	957	ASP	CA-C-O	5.81	125.21	119.75
1	A	747	LYS	N-CA-C	5.81	117.48	109.29
1	B	808	SER	N-CA-C	5.79	118.36	110.55
1	A	862	HIS	CA-C-N	-5.78	114.17	120.71
1	A	862	HIS	C-N-CA	-5.78	114.17	120.71
1	B	866	THR	N-CA-C	5.78	118.33	111.33
1	B	734	ASN	CA-CB-CG	-5.77	106.83	112.60
1	A	911	SER	N-CA-C	5.77	118.95	110.59
1	B	937	HIS	CA-CB-CG	-5.77	108.03	113.80
1	B	768	LEU	N-CA-C	5.75	118.32	111.71
1	B	688	GLU	N-CA-C	5.74	119.76	112.87
1	B	785	SER	N-CA-C	5.74	123.02	110.80
1	B	703	LYS	N-CA-C	5.73	120.83	111.37
1	B	938	ILE	N-CA-C	5.73	116.96	108.65
1	A	896	TYR	N-CA-C	5.73	118.81	109.59
1	B	924	VAL	CA-C-O	5.72	126.34	120.39
1	B	818	VAL	N-CA-C	5.72	115.91	110.42
1	B	724	SER	N-CA-C	5.71	117.89	110.53
1	B	823	ALA	N-CA-C	5.71	118.36	109.52
1	B	936	SER	CB-CA-C	-5.70	102.36	110.34
1	A	676	ILE	CA-CB-CG1	5.68	120.06	110.40
1	B	757	SER	CA-C-N	-5.68	112.35	120.42
1	B	757	SER	C-N-CA	-5.68	112.35	120.42
1	A	718	GLN	N-CA-CB	5.68	118.21	109.98
1	B	975	ILE	N-CA-C	5.67	121.13	109.34
1	A	836	ILE	N-CA-C	5.67	114.90	106.85
1	B	674	LYS	CA-C-N	-5.67	112.32	120.82
1	B	674	LYS	C-N-CA	-5.67	112.32	120.82
1	B	970	PRO	CA-C-N	-5.67	111.10	121.52
1	B	970	PRO	C-N-CA	-5.67	111.10	121.52
1	A	709	ALA	N-CA-C	5.66	120.03	113.18
1	A	726	ASP	CA-C-O	5.66	127.25	120.92
1	A	972	GLY	CA-C-N	-5.65	112.22	120.75
1	A	972	GLY	C-N-CA	-5.65	112.22	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	722	GLN	N-CA-C	5.65	119.93	112.25
1	B	921	LEU	CA-C-N	-5.64	117.33	122.80
1	B	921	LEU	C-N-CA	-5.64	117.33	122.80
1	A	805	ASP	N-CA-C	5.64	119.44	110.70
1	B	815	ARG	N-CA-C	5.64	118.19	111.71
1	B	880	ALA	N-CA-C	5.64	118.47	110.24
1	A	753	ASN	CA-C-N	-5.62	114.09	122.74
1	A	753	ASN	C-N-CA	-5.62	114.09	122.74
1	A	943	LYS	CA-C-N	-5.62	113.27	122.20
1	A	943	LYS	C-N-CA	-5.62	113.27	122.20
1	A	791	ASP	CA-CB-CG	-5.61	106.99	112.60
1	A	809	GLU	N-CA-C	5.60	122.73	110.80
1	A	750	PRO	CA-C-O	5.60	127.16	121.11
1	B	896	TYR	N-CA-C	5.59	118.35	109.24
1	A	839	ILE	CA-C-O	5.56	126.25	120.36
1	A	915	PRO	CA-C-N	-5.55	115.90	123.12
1	A	915	PRO	C-N-CA	-5.55	115.90	123.12
1	A	758	VAL	CA-C-N	-5.55	111.87	120.31
1	A	758	VAL	C-N-CA	-5.55	111.87	120.31
1	A	858	ARG	CA-C-N	-5.55	115.03	122.42
1	A	858	ARG	C-N-CA	-5.55	115.03	122.42
1	A	713	LEU	N-CA-C	5.55	118.05	111.33
1	A	854	LEU	CA-C-N	-5.54	110.89	120.97
1	A	854	LEU	C-N-CA	-5.54	110.89	120.97
1	A	666	PRO	CA-C-N	-5.54	113.17	120.09
1	A	666	PRO	C-N-CA	-5.54	113.17	120.09
1	B	921	LEU	CB-CA-C	-5.54	100.14	109.72
1	B	677	PHE	N-CA-C	5.53	119.77	113.19
1	B	864	SER	N-CA-C	5.52	116.66	108.60
1	A	682	MET	CA-C-N	-5.52	112.89	120.28
1	A	682	MET	C-N-CA	-5.52	112.89	120.28
1	B	830	ASP	CA-C-N	-5.51	112.88	122.64
1	B	830	ASP	C-N-CA	-5.51	112.88	122.64
1	A	955	THR	N-CA-C	5.51	117.90	110.29
1	B	742	HIS	N-CA-C	5.51	118.58	110.59
1	B	913	GLY	CA-C-N	5.50	131.61	121.70
1	B	913	GLY	C-N-CA	5.50	131.61	121.70
1	A	782	SER	N-CA-C	5.50	118.32	107.98
1	A	738	THR	CA-C-O	5.49	126.56	120.63
1	B	1008	ASN	N-CA-C	5.48	117.64	107.99
1	A	954	THR	N-CA-C	5.48	117.69	107.99
1	B	928	ASN	N-CA-CB	-5.48	100.97	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	936	SER	CA-C-N	-5.48	115.24	122.85
1	B	936	SER	C-N-CA	-5.48	115.24	122.85
1	B	798	LYS	CB-CG-CD	5.47	123.89	111.30
1	B	683	LYS	N-CA-C	5.46	117.99	111.71
1	B	912	GLN	N-CA-C	5.45	118.04	108.56
1	A	735	ARG	CD-NE-CZ	-5.45	116.77	124.40
1	B	1003	LEU	N-CA-C	5.44	119.10	109.96
1	B	1010	LYS	CA-CB-CG	5.43	124.96	114.10
1	B	762	VAL	N-CA-CB	5.41	118.70	110.58
1	A	999	LEU	N-CA-C	5.40	118.06	109.96
1	A	763	GLU	N-CA-C	5.40	116.97	111.14
1	B	829	TYR	N-CA-CB	5.40	119.61	110.49
1	B	1007	PHE	CA-C-N	-5.39	114.48	122.41
1	B	1007	PHE	C-N-CA	-5.39	114.48	122.41
1	B	997	VAL	N-CA-C	5.39	117.15	108.85
1	B	786	SER	N-CA-C	5.38	120.52	112.94
1	A	716	VAL	CA-C-N	-5.38	113.71	122.26
1	A	716	VAL	C-N-CA	-5.38	113.71	122.26
1	B	802	LYS	N-CA-C	5.38	117.62	110.53
1	B	916	ILE	N-CA-C	5.37	114.33	106.55
1	B	811	ALA	N-CA-C	5.37	119.45	113.01
1	A	810	GLU	CA-C-N	-5.36	113.09	120.28
1	A	810	GLU	C-N-CA	-5.36	113.09	120.28
1	A	901	VAL	N-CA-C	5.36	120.48	109.34
1	A	998	ASN	N-CA-C	5.36	118.19	109.24
1	B	680	GLU	CA-C-N	-5.36	112.50	122.09
1	B	680	GLU	C-N-CA	-5.36	112.50	122.09
1	B	678	ASP	CA-CB-CG	5.36	117.96	112.60
1	B	836	ILE	CA-C-N	-5.36	114.25	122.87
1	B	836	ILE	C-N-CA	-5.36	114.25	122.87
1	A	843	GLY	CA-C-N	-5.35	111.24	121.94
1	A	843	GLY	C-N-CA	-5.35	111.24	121.94
1	A	737	TYR	N-CA-C	5.35	117.19	111.36
1	A	749	PRO	N-CA-C	5.34	116.29	110.58
1	B	888	GLY	CA-C-N	5.33	131.73	121.54
1	B	888	GLY	C-N-CA	5.33	131.73	121.54
1	A	832	GLU	CA-C-N	-5.33	114.31	121.66
1	A	832	GLU	C-N-CA	-5.33	114.31	121.66
1	B	873	LEU	CA-C-N	-5.33	113.75	122.54
1	B	873	LEU	C-N-CA	-5.33	113.75	122.54
1	A	905	ALA	N-CA-C	5.32	117.83	111.71
1	B	854	LEU	N-CA-C	5.32	118.25	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	924	VAL	CA-CB-CG2	5.31	119.42	110.40
1	A	739	LEU	N-CA-C	5.30	118.92	112.23
1	A	793	ASN	N-CA-C	5.29	117.46	111.11
1	B	855	HIS	ND1-CG-CD2	5.29	111.39	106.10
1	B	822	HIS	N-CA-C	5.29	117.91	110.23
1	A	844	GLU	N-CA-C	5.29	119.60	113.20
1	B	957	ASP	N-CA-C	5.29	117.09	109.48
1	A	872	ILE	N-CA-C	5.29	117.66	111.05
1	A	937	HIS	CA-C-N	-5.29	116.13	122.90
1	A	937	HIS	C-N-CA	-5.29	116.13	122.90
1	A	675	MET	N-CA-C	5.28	118.89	112.23
1	A	953	LYS	N-CA-C	5.28	119.57	113.18
1	B	873	LEU	N-CA-C	5.28	117.95	111.82
1	A	865	ARG	NE-CZ-NH1	-5.28	116.22	121.50
1	B	743	ASP	CA-C-N	-5.28	113.48	122.56
1	B	743	ASP	C-N-CA	-5.28	113.48	122.56
1	A	928	ASN	CA-C-N	-5.27	115.76	122.77
1	A	928	ASN	C-N-CA	-5.27	115.76	122.77
1	B	897	PHE	CA-C-N	-5.27	114.05	122.53
1	B	897	PHE	C-N-CA	-5.27	114.05	122.53
1	B	868	ASN	CA-C-O	5.27	126.13	120.70
1	A	690	GLU	CA-C-N	-5.26	113.59	120.91
1	A	690	GLU	C-N-CA	-5.26	113.59	120.91
1	B	761	LYS	N-CA-C	5.25	120.34	113.30
1	B	1008	ASN	CA-C-N	-5.25	113.68	122.92
1	B	1008	ASN	C-N-CA	-5.25	113.68	122.92
1	B	939	SER	CA-C-N	5.25	130.91	123.14
1	B	939	SER	C-N-CA	5.25	130.91	123.14
1	B	985	LEU	CA-C-O	5.23	127.99	120.51
1	A	685	ALA	N-CA-C	5.23	117.39	111.11
1	A	981	ASP	CA-CB-CG	5.23	117.83	112.60
1	B	984	LEU	CA-C-O	5.23	126.00	120.36
1	B	908	CYS	N-CA-C	5.22	116.78	111.14
1	A	939	SER	N-CA-CB	-5.22	102.16	109.94
1	B	734	ASN	N-CA-C	5.21	116.96	111.28
1	A	1009	PHE	CA-C-N	-5.21	112.74	121.75
1	A	1009	PHE	C-N-CA	-5.21	112.74	121.75
1	B	832	GLU	CA-C-O	5.18	126.55	120.43
1	B	841	ARG	CA-C-N	-5.18	113.20	120.82
1	B	841	ARG	C-N-CA	-5.18	113.20	120.82
1	A	746	MET	CA-C-N	-5.18	113.21	123.99
1	A	746	MET	C-N-CA	-5.18	113.21	123.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	716	VAL	N-CA-C	5.18	119.34	112.76
1	A	759	GLN	N-CA-CB	5.18	118.31	110.28
1	B	798	LYS	N-CA-C	5.18	121.83	110.80
1	B	965	ASP	N-CA-C	5.18	122.04	113.50
1	B	702	SER	N-CA-C	5.17	117.88	109.24
1	A	1000	LYS	N-CA-C	5.17	119.25	111.96
1	B	767	ASN	CA-C-N	-5.17	112.83	120.28
1	B	767	ASN	C-N-CA	-5.17	112.83	120.28
1	B	968	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	708	ALA	CA-C-N	-5.17	111.51	121.58
1	A	708	ALA	C-N-CA	-5.17	111.51	121.58
1	B	698	LEU	CB-CA-C	-5.16	102.28	110.84
1	B	717	GLN	CA-C-N	-5.15	111.92	120.68
1	B	717	GLN	C-N-CA	-5.15	111.92	120.68
1	B	978	GLY	N-CA-C	5.15	118.91	112.73
1	A	806	ARG	CA-C-N	-5.15	112.13	120.72
1	A	806	ARG	C-N-CA	-5.15	112.13	120.72
1	A	689	TYR	CA-CB-CG	-5.14	104.64	113.90
1	B	916	ILE	CB-CA-C	-5.14	106.82	112.68
1	B	669	VAL	CA-CB-CG2	5.13	119.12	110.40
1	A	903	LYS	CA-CB-CG	5.13	124.35	114.10
1	B	974	GLY	N-CA-C	5.12	125.32	113.18
1	A	807	ASP	CA-CB-CG	-5.12	107.48	112.60
1	A	784	ASP	N-CA-C	5.12	117.76	109.06
1	A	918	LEU	N-CA-C	5.12	116.95	108.20
1	A	806	ARG	N-CA-C	5.11	121.69	110.80
1	B	772	GLU	CA-C-N	-5.10	113.18	120.42
1	B	772	GLU	C-N-CA	-5.10	113.18	120.42
1	A	757	SER	CA-C-N	-5.10	114.04	120.56
1	A	757	SER	C-N-CA	-5.10	114.04	120.56
1	A	778	LEU	CB-CA-C	5.09	120.55	110.42
1	A	790	ILE	CA-C-O	5.08	126.56	121.17
1	B	704	ARG	N-CA-C	5.08	116.63	111.14
1	B	687	VAL	N-CA-C	5.08	115.69	110.36
1	B	912	GLN	CB-CA-C	-5.08	104.11	112.03
1	A	853	GLN	CB-CA-C	5.07	119.59	111.73
1	A	942	PRO	CA-C-N	-5.07	113.52	120.71
1	A	942	PRO	C-N-CA	-5.07	113.52	120.71
1	A	667	LYS	N-CA-C	5.05	120.34	113.16
1	B	730	LEU	N-CA-C	5.04	116.47	111.07
1	B	803	VAL	CA-C-O	5.04	125.97	120.57
1	A	875	GLN	CA-C-O	5.04	124.72	119.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	945	LYS	CA-C-O	5.03	125.91	120.43
1	A	812	GLU	CA-C-N	-5.02	114.12	120.60
1	A	812	GLU	C-N-CA	-5.02	114.12	120.60
1	A	717	GLN	N-CA-C	5.02	120.25	113.72
1	A	846	GLN	N-CA-C	5.02	116.44	110.97
1	B	962	ILE	N-CA-C	5.01	119.77	109.34
1	A	935	ALA	N-CA-C	5.01	117.90	110.48
1	B	690	GLU	N-CA-CB	5.01	119.52	111.91
1	A	807	ASP	N-CA-C	5.00	118.65	112.54
1	A	894	GLY	N-CA-C	5.00	121.47	112.77
1	B	927	GLY	CA-C-N	-5.00	115.55	122.30
1	B	927	GLY	C-N-CA	-5.00	115.55	122.30
1	B	927	GLY	N-CA-C	5.00	120.20	111.50

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	663	SER	Peptide
1	A	694	GLN	Peptide
1	A	703	LYS	Peptide
1	A	744	PHE	Sidechain
1	A	745	GLY	Peptide
1	A	746	MET	Peptide
1	A	782	SER	Peptide
1	A	784	ASP	Peptide
1	A	786	SER	Peptide
1	A	794	TYR	Sidechain
1	A	805	ASP	Peptide
1	A	823	ALA	Peptide
1	A	938	ILE	Peptide
1	A	986	TYR	Sidechain
1	B	1009	PHE	Peptide
1	B	671	ASP	Peptide
1	B	680	GLU	Peptide
1	B	718	GLN	Peptide
1	B	743	ASP	Peptide
1	B	775	TYR	Sidechain
1	B	778	LEU	Peptide
1	B	779	ARG	Sidechain
1	B	783	ASP	Peptide
1	B	787	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	B	797	LEU	Peptide
1	B	798	LYS	Peptide
1	B	806	ARG	Sidechain
1	B	828	ALA	Peptide
1	B	837	PHE	Sidechain
1	B	841	ARG	Sidechain
1	B	854	LEU	Peptide
1	B	857	ARG	Sidechain
1	B	865	ARG	Sidechain
1	B	878	ARG	Sidechain
1	B	882	PRO	Peptide
1	B	920	LEU	Peptide
1	B	940	LYS	Peptide
1	B	963	SER	Peptide
1	B	964	LEU	Peptide
1	B	966	GLY	Peptide
1	B	981	ASP	Peptide
1	B	984	LEU	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	2754	0	2795	104	0
1	B	2754	0	2795	137	0
2	A	29	0	24	1	0
2	B	29	0	24	2	0
3	A	101	0	0	3	0
3	B	90	0	0	2	0
All	All	5757	0	5638	241	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 22.

All (241) 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:B:831:LEU:HG	1:B:1005:LEU:HD21	1.57	0.87
1:B:822:HIS:HE2	1:B:831:LEU:HD22	1.40	0.86
1:B:692:ASP:HB3	1:B:743:ASP:HB2	1.58	0.83
1:B:665:LEU:HB3	1:B:669:VAL:HG13	1.65	0.78
1:A:923:GLU:HG3	1:A:967:VAL:HG11	1.66	0.78
1:B:863:GLY:HA3	1:B:904:SER:O	1.83	0.77
1:B:857:ARG:H	1:B:926:LEU:HB2	1.50	0.76
1:B:686:MET:HB2	1:B:693:LEU:HD11	1.70	0.74
1:B:930:TYR:HB3	1:B:948:VAL:HG22	1.70	0.73
1:A:784:ASP:HA	1:A:785:SER:HB2	1.72	0.72
1:A:684:LYS:O	1:A:688:GLU:HG3	1.92	0.70
1:B:822:HIS:HE1	1:B:831:LEU:HD13	1.56	0.70
1:A:716:VAL:O	1:A:720:VAL:HG23	1.91	0.69
1:B:702:SER:O	1:B:706:ILE:HG12	1.91	0.69
1:B:822:HIS:CE1	1:B:831:LEU:HD13	2.27	0.69
1:B:770:ASP:HA	1:B:773:VAL:HG12	1.73	0.69
1:B:941:LEU:HD22	1:B:992:TYR:CD1	2.29	0.68
1:B:798:LYS:HG3	1:B:842:GLU:CD	2.18	0.68
1:A:941:LEU:HD22	1:A:992:TYR:CD1	2.29	0.67
1:B:834:ILE:HD11	1:B:1006:LYS:HB2	1.75	0.67
1:B:822:HIS:NE2	1:B:831:LEU:HD22	2.10	0.67
1:B:879:ILE:HG13	1:B:994:ILE:HG21	1.77	0.66
1:B:829:TYR:HD1	1:B:1007:PHE:HB3	1.61	0.65
1:B:770:ASP:HB2	1:B:868:ASN:OD1	1.94	0.65
1:B:829:TYR:CE1	1:B:1007:PHE:HD2	2.14	0.65
1:A:701:LEU:HD21	1:A:768:LEU:HD13	1.78	0.65
1:A:682:MET:O	1:A:686:MET:HG3	1.96	0.64
1:A:941:LEU:HD22	1:A:992:TYR:HD1	1.62	0.64
1:A:710:TYR:CE2	1:A:881:PRO:HG2	2.33	0.63
1:B:672:LEU:HA	1:B:675:MET:HB3	1.81	0.63
1:B:770:ASP:HB3	1:B:868:ASN:HA	1.81	0.63
1:B:679:VAL:HG13	1:B:682:MET:HE3	1.81	0.62
1:B:941:LEU:HD12	1:B:942:PRO:HD2	1.81	0.62
1:B:685:ALA:HA	1:B:688:GLU:OE2	1.99	0.62
1:B:925:ALA:HB3	1:B:996:GLN:HG2	1.80	0.61
1:B:666:PRO:HB2	1:B:668:PRO:HD2	1.82	0.61
1:B:829:TYR:CD1	1:B:831:LEU:HD11	2.35	0.61
1:A:849:LYS:O	1:A:852:LYS:HB2	2.01	0.61
1:A:872:ILE:HG21	1:A:920:LEU:HD11	1.84	0.60
1:A:954:THR:HB	1:A:986:TYR:CD1	2.36	0.60
1:B:897:PHE:HZ	1:B:997:VAL:HG11	1.65	0.60
1:B:911:SER:O	1:B:913:GLY:HA2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:ILE:HG23	1:A:765:LEU:HD22	1.84	0.60
1:A:777:LEU:HD13	1:A:796:LYS:HG3	1.84	0.60
1:B:712:ILE:HG21	1:B:736:PHE:HB2	1.85	0.58
1:B:857:ARG:HD2	1:B:967:VAL:HG22	1.85	0.58
1:B:936:SER:HB3	1:B:938:ILE:HD12	1.86	0.58
1:B:917:GLY:HA3	1:B:1007:PHE:CE1	2.38	0.58
1:B:837:PHE:HD2	1:B:1002:LEU:O	1.87	0.57
1:B:856:ASN:HA	1:B:857:ARG:CB	2.34	0.57
1:A:918:LEU:HD13	1:A:1002:LEU:HD11	1.86	0.57
1:B:914:ASP:HB2	1:B:916:ILE:HG12	1.86	0.57
1:A:910:THR:HG21	1:A:1007:PHE:CD1	2.39	0.56
1:A:826:HIS:CD2	1:A:902:SER:HB2	2.41	0.56
1:A:875:GLN:HB2	1:A:878:ARG:HD3	1.88	0.56
1:B:810:GLU:O	1:B:814:ILE:HG13	2.06	0.56
1:B:829:TYR:CD1	1:B:1007:PHE:HD2	2.23	0.56
1:B:834:ILE:HD11	1:B:1006:LYS:CB	2.35	0.56
1:A:863:GLY:H	1:A:904:SER:HB3	1.72	0.55
1:B:699:GLY:O	1:B:700:LYS:HG2	2.06	0.55
1:B:852:LYS:HD2	1:B:857:ARG:HH12	1.70	0.55
1:B:728:GLN:HB3	3:B:2:HOH:O	2.07	0.55
1:B:1007:PHE:CD1	1:B:1007:PHE:N	2.73	0.55
1:B:843:GLY:O	1:B:846:GLN:HB2	2.07	0.54
1:A:941:LEU:HD12	1:A:942:PRO:HD2	1.90	0.54
1:B:855:HIS:HB3	1:B:927:GLY:HA2	1.88	0.54
1:A:882:PRO:O	1:A:883:GLU:HG3	2.08	0.54
1:B:798:LYS:O	1:B:842:GLU:HG2	2.07	0.54
1:B:673:ILE:CD1	1:B:794:TYR:HD1	2.21	0.54
1:B:693:LEU:HA	1:B:696:MET:O	2.08	0.54
1:A:720:VAL:HG21	1:A:753:ASN:HA	1.89	0.53
1:B:829:TYR:CE1	1:B:831:LEU:HD11	2.44	0.53
1:A:931:GLU:HB3	1:A:951:LEU:HD11	1.89	0.53
1:B:770:ASP:CB	1:B:868:ASN:HA	2.38	0.53
1:A:859:LEU:HG	1:A:921:LEU:HD22	1.91	0.53
1:A:869:PHE:HE2	1:A:920:LEU:HG	1.74	0.53
1:B:685:ALA:O	1:B:688:GLU:HG2	2.09	0.53
1:A:822:HIS:CD2	1:A:831:LEU:HB2	2.44	0.53
1:A:702:SER:OG	1:A:705:GLN:HB3	2.08	0.52
1:B:831:LEU:CG	1:B:1005:LEU:HD21	2.34	0.52
1:B:880:ALA:HB3	1:B:893:LYS:HG2	1.91	0.52
1:A:846:GLN:O	1:A:849:LYS:HB2	2.08	0.52
1:A:948:VAL:HG23	1:A:992:TYR:HE1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:SER:HB2	1:A:665:LEU:HB2	1.91	0.52
1:B:689:TYR:CG	1:B:764:MET:HG2	2.44	0.52
1:B:835:ASP:H	1:B:1004:LYS:HB3	1.74	0.52
1:B:860:LEU:HD12	1:B:924:VAL:CG1	2.40	0.51
1:B:832:GLU:O	1:B:1005:LEU:HA	2.10	0.51
1:A:919:ILE:HG22	1:A:1003:LEU:HB2	1.92	0.51
1:B:851:PHE:CD1	1:B:996:GLN:HG3	2.46	0.51
1:B:835:ASP:HB2	1:B:837:PHE:CE2	2.45	0.51
1:B:926:LEU:HB3	1:B:929:MET:CE	2.41	0.51
1:B:704:ARG:H	1:B:704:ARG:HD3	1.75	0.51
1:B:917:GLY:HA3	1:B:1007:PHE:HE1	1.77	0.50
1:A:954:THR:HB	1:A:986:TYR:CE1	2.46	0.50
1:B:696:MET:HG3	1:B:741:PRO:HD2	1.94	0.50
1:B:801:ILE:HG22	1:B:837:PHE:CD1	2.46	0.50
1:A:702:SER:HB2	1:A:704:ARG:HB2	1.93	0.50
1:B:860:LEU:HD12	1:B:924:VAL:HG13	1.94	0.50
1:A:809:GLU:HA	1:A:812:GLU:HG2	1.92	0.49
1:B:841:ARG:HD2	1:B:999:LEU:HD12	1.94	0.49
1:B:839:ILE:HD12	1:B:999:LEU:HB3	1.94	0.49
1:A:915:PRO:O	1:A:916:ILE:HD13	2.12	0.49
1:B:897:PHE:CZ	1:B:997:VAL:HG11	2.47	0.49
1:A:822:HIS:HD2	1:A:831:LEU:HB2	1.77	0.49
1:A:903:LYS:O	1:A:907:TYR:CE2	2.66	0.49
1:B:864:SER:O	1:B:908:CYS:HA	2.13	0.48
1:A:665:LEU:HD21	1:A:794:TYR:CD1	2.48	0.48
1:B:662:LYS:HA	1:B:788:ASP:OD1	2.13	0.48
1:B:818:VAL:O	1:B:901:VAL:HG11	2.14	0.48
1:B:797:LEU:HD22	1:B:873:LEU:HB2	1.96	0.48
1:A:953:LYS:HB3	1:A:979:VAL:O	2.12	0.48
1:A:903:LYS:HD3	1:A:986:TYR:HD2	1.78	0.48
1:B:839:ILE:HG13	1:B:1000:LYS:O	2.14	0.48
1:A:886:VAL:HA	1:A:893:LYS:HD3	1.96	0.48
1:B:903:LYS:HZ2	2:B:502:FRQ:H6	1.78	0.47
1:B:926:LEU:HD13	1:B:929:MET:HE1	1.95	0.47
1:B:706:ILE:HG23	1:B:765:LEU:HD22	1.95	0.47
1:A:663:SER:HA	1:A:664:LYS:HZ2	1.80	0.47
1:A:702:SER:O	1:A:706:ILE:HG13	2.15	0.47
1:B:697:PRO:O	1:B:698:LEU:C	2.56	0.47
1:B:795:GLU:O	1:B:798:LYS:HB3	2.15	0.47
1:B:950:GLY:O	1:B:987:ASN:HA	2.14	0.47
1:A:948:VAL:HB	1:A:990:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:891:PHE:HA	1:B:936:SER:O	2.15	0.47
1:B:910:THR:O	1:B:1009:PHE:HZ	1.98	0.47
1:A:859:LEU:HD12	1:A:859:LEU:HA	1.75	0.46
1:A:805:ASP:OD1	1:A:806:ARG:HD2	2.15	0.46
1:B:852:LYS:HD2	1:B:857:ARG:NH1	2.30	0.46
1:B:673:ILE:HD11	1:B:794:TYR:HD1	1.81	0.46
1:B:788:ASP:O	1:B:789:PRO:C	2.59	0.46
1:A:663:SER:CB	1:A:665:LEU:HB2	2.46	0.46
1:A:762:VAL:HG11	1:A:888:GLY:HA3	1.98	0.46
1:A:952:GLY:H	1:A:987:ASN:HD22	1.62	0.46
1:B:776:SER:O	1:B:779:ARG:HG3	2.16	0.46
1:B:921:LEU:HD12	1:B:1001:TYR:HB2	1.98	0.46
1:A:858:ARG:HD2	1:A:860:LEU:HD21	1.98	0.46
1:A:874:SER:C	1:A:875:GLN:HG2	2.41	0.46
1:A:895:ILE:HG22	1:A:897:PHE:CE1	2.51	0.46
1:A:864:SER:HB3	1:A:869:PHE:CE1	2.51	0.45
1:A:904:SER:HB3	2:A:501:FRQ:O14	2.17	0.45
1:B:744:PHE:HD1	1:B:744:PHE:O	1.99	0.45
1:B:905:ALA:HB1	1:B:1007:PHE:HE2	1.80	0.45
1:A:703:LYS:O	1:A:707:GLN:HG3	2.16	0.45
1:A:749:PRO:O	1:A:751:LEU:HD22	2.16	0.45
1:A:749:PRO:HA	1:A:750:PRO:HD3	1.80	0.45
1:A:841:ARG:HD2	1:A:873:LEU:O	2.17	0.45
1:B:962:ILE:HG23	1:B:963:SER:H	1.81	0.45
1:A:677:PHE:HB3	1:A:778:LEU:HD12	1.99	0.45
1:B:963:SER:OG	1:B:966:GLY:N	2.49	0.45
1:A:748:LYS:HA	1:A:749:PRO:HD3	1.74	0.45
1:A:769:LEU:O	1:A:773:VAL:HG23	2.16	0.45
1:A:969:VAL:HA	1:A:970:PRO:HD3	1.79	0.45
1:A:696:MET:HA	1:A:697:PRO:HD3	1.82	0.45
1:B:879:ILE:CG1	1:B:994:ILE:HG21	2.46	0.45
1:B:889:TYR:HA	3:B:24:HOH:O	2.17	0.44
1:A:739:LEU:HA	1:A:739:LEU:HD12	1.57	0.44
1:B:695:LYS:HE3	1:B:695:LYS:HB3	1.75	0.44
1:A:928:ASN:HD21	1:A:946:HIS:CE1	2.36	0.44
1:B:777:LEU:HD12	1:B:796:LYS:HB3	2.00	0.44
1:A:809:GLU:HA	1:A:812:GLU:CG	2.47	0.44
1:B:809:GLU:HA	1:B:812:GLU:HG3	1.99	0.44
1:B:931:GLU:HB3	1:B:951:LEU:HD11	2.00	0.44
1:B:703:LYS:HB2	1:B:704:ARG:HH11	1.82	0.44
1:A:703:LYS:H	1:A:703:LYS:HD3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:MET:SD	1:A:746:MET:N	2.90	0.44
1:A:973:THR:O	1:A:975:ILE:HG12	2.18	0.44
1:B:696:MET:HB3	1:B:696:MET:HE3	1.80	0.44
1:B:755:ALA:HA	1:B:758:VAL:HG22	1.99	0.44
1:B:821:THR:O	1:B:900:MET:HG3	2.17	0.44
1:B:957:ASP:HA	1:B:958:PRO:HD3	1.70	0.44
1:A:679:VAL:HG13	1:A:682:MET:HE3	1.99	0.43
1:B:665:LEU:HD23	1:B:669:VAL:HG22	2.01	0.43
1:A:754:ASN:HB3	3:A:190:HOH:O	2.17	0.43
1:A:808:SER:HA	3:A:157:HOH:O	2.18	0.43
1:A:686:MET:HE3	1:A:768:LEU:HD22	2.00	0.43
1:A:745:GLY:O	1:A:746:MET:SD	2.76	0.43
1:A:1002:LEU:C	1:A:1003:LEU:HD12	2.43	0.43
1:B:822:HIS:CD2	1:B:901:VAL:HG13	2.53	0.43
1:A:696:MET:O	1:A:696:MET:HG3	2.17	0.43
1:A:852:LYS:O	1:A:857:ARG:CZ	2.66	0.43
1:B:829:TYR:CE1	1:B:1007:PHE:CD2	3.02	0.43
1:B:972:GLY:O	1:B:973:THR:C	2.62	0.43
1:A:769:LEU:HD11	1:A:881:PRO:HG3	2.00	0.43
1:A:915:PRO:HB2	1:A:1007:PHE:O	2.19	0.43
1:A:948:VAL:HG23	1:A:992:TYR:CE1	2.52	0.43
1:B:816:LYS:HA	1:B:816:LYS:HD3	1.82	0.43
1:B:817:TYR:OH	1:B:970:PRO:HD2	2.19	0.43
1:B:814:ILE:HG22	1:B:1003:LEU:HD21	2.01	0.43
1:B:840:GLU:HG3	1:B:845:CYS:SG	2.59	0.43
1:A:663:SER:HA	1:A:664:LYS:NZ	2.33	0.42
1:A:713:LEU:O	1:A:716:VAL:HG12	2.20	0.42
1:B:754:ASN:HB3	1:B:757:SER:H	1.84	0.42
1:B:713:LEU:HD12	1:B:765:LEU:HD12	2.00	0.42
1:A:811:ALA:O	1:A:815:ARG:HG3	2.19	0.42
1:A:928:ASN:ND2	1:A:946:HIS:CE1	2.88	0.42
1:B:673:ILE:HG21	1:B:790:ILE:O	2.20	0.42
1:B:666:PRO:O	1:B:667:LYS:C	2.62	0.42
1:B:672:LEU:HD11	1:B:918:LEU:HD21	2.02	0.42
1:A:700:LYS:O	1:A:701:LEU:C	2.62	0.42
1:B:912:GLN:HG3	1:B:1009:PHE:CD2	2.55	0.42
1:A:679:VAL:O	1:A:680:GLU:C	2.63	0.42
1:A:844:GLU:OE2	1:A:998:ASN:HB2	2.20	0.42
1:A:1010:LYS:HA	1:A:1010:LYS:HD2	1.82	0.42
1:B:689:TYR:O	1:B:690:GLU:HG2	2.19	0.42
1:B:804:VAL:O	1:B:805:ASP:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:895:ILE:HG22	1:A:897:PHE:CZ	2.55	0.42
1:B:813:ILE:HD12	1:B:964:LEU:HD13	2.01	0.42
1:A:728:GLN:O	1:A:729:ILE:C	2.62	0.41
1:A:781:GLY:H	1:A:796:LYS:NZ	2.19	0.41
1:A:823:ALA:O	1:A:825:THR:N	2.54	0.41
1:A:860:LEU:HD13	1:A:989:TYR:CD1	2.55	0.41
1:A:670:GLN:HG2	1:A:790:ILE:HG21	2.02	0.41
1:B:769:LEU:HD23	1:B:769:LEU:HA	1.89	0.41
1:A:679:VAL:HA	1:A:682:MET:HE3	2.02	0.41
1:B:877:LEU:HD23	1:B:877:LEU:HA	1.81	0.41
1:B:889:TYR:HE2	2:B:502:FRQ:H292	1.86	0.41
1:A:938:ILE:HB	1:A:940:LYS:H	1.85	0.41
1:B:674:LYS:HB3	1:B:790:ILE:HD11	2.02	0.41
1:B:829:TYR:HE1	1:B:1007:PHE:HD2	1.63	0.41
1:B:797:LEU:HD23	1:B:797:LEU:HA	1.86	0.41
1:B:823:ALA:HB3	1:B:826:HIS:HE1	1.85	0.41
1:B:917:GLY:O	1:B:918:LEU:HD12	2.21	0.41
1:A:849:LYS:O	1:A:850:PRO:C	2.62	0.41
1:A:928:ASN:ND2	1:A:946:HIS:ND1	2.68	0.41
1:B:716:VAL:O	1:B:719:ALA:HB3	2.21	0.41
1:B:903:LYS:HE2	1:B:985:LEU:HD13	2.02	0.41
1:B:962:ILE:HG23	1:B:963:SER:N	2.35	0.41
1:A:854:LEU:HD22	1:A:854:LEU:HA	1.91	0.41
1:A:902:SER:HA	1:A:905:ALA:HB3	2.01	0.41
1:B:674:LYS:O	1:B:675:MET:C	2.62	0.41
1:A:961:ASN:O	1:A:962:ILE:C	2.62	0.40
1:B:752:LEU:CD2	1:B:757:SER:HB3	2.51	0.40
1:B:814:ILE:HD13	1:B:814:ILE:HG21	1.90	0.40
1:B:841:ARG:CZ	1:B:841:ARG:HB3	2.50	0.40
1:A:811:ALA:HB1	1:A:836:ILE:HD13	2.03	0.40
1:A:824:THR:HA	3:A:169:HOH:O	2.20	0.40
1:B:805:ASP:O	1:B:807:ASP:N	2.54	0.40
1:B:941:LEU:HD22	1:B:992:TYR:HD1	1.80	0.40
1:A:802:LYS:HB3	1:A:838:LYS:HG2	2.03	0.40
1:B:829:TYR:HE1	1:B:1007:PHE:CD2	2.39	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	348/350 (99%)	271 (78%)	56 (16%)	21 (6%)	1	7
1	B	348/350 (99%)	259 (74%)	57 (16%)	32 (9%)	0	2
All	All	696/700 (99%)	530 (76%)	113 (16%)	53 (8%)	1	4

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	664	LYS
1	A	690	GLU
1	A	809	GLU
1	A	824	THR
1	A	829	TYR
1	A	981	ASP
1	A	1009	PHE
1	B	747	LYS
1	B	789	PRO
1	B	797	LEU
1	B	829	TYR
1	B	855	HIS
1	B	883	GLU
1	B	943	LYS
1	B	964	LEU
1	A	701	LEU
1	A	704	ARG
1	A	725	SER
1	A	806	ARG
1	A	883	GLU
1	A	962	ILE
1	A	974	GLY
1	B	671	ASP
1	B	699	GLY
1	B	723	GLY

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Mol	Chain	Res	Type
1	B	778	LEU
1	B	785	SER
1	B	805	ASP
1	B	806	ARG
1	B	826	HIS
1	B	857	ARG
1	B	877	LEU
1	B	974	GLY
1	B	987	ASN
1	A	780	GLY
1	B	722	GLN
1	B	788	ASP
1	B	973	THR
1	B	985	LEU
1	A	729	ILE
1	A	798	LYS
1	A	912	GLN
1	A	914	ASP
1	B	819	LYS
1	A	881	PRO
1	B	962	ILE
1	B	967	VAL
1	A	959	SER
1	B	846	GLN
1	B	882	PRO
1	B	970	PRO
1	B	667	LYS
1	B	780	GLY

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	308/308 (100%)	239 (78%)	69 (22%)	1	5
1	B	308/308 (100%)	237 (77%)	71 (23%)	1	5
All	All	616/616 (100%)	476 (77%)	140 (23%)	1	5

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	663	SER
1	A	664	LYS
1	A	665	LEU
1	A	667	LYS
1	A	672	LEU
1	A	679	VAL
1	A	690	GLU
1	A	693	LEU
1	A	696	MET
1	A	698	LEU
1	A	703	LYS
1	A	705	GLN
1	A	707	GLN
1	A	711	SER
1	A	715	GLU
1	A	716	VAL
1	A	720	VAL
1	A	722	GLN
1	A	726	ASP
1	A	727	SER
1	A	744	PHE
1	A	753	ASN
1	A	756	ASP
1	A	758	VAL
1	A	761	LYS
1	A	762	VAL
1	A	771	ILE
1	A	777	LEU
1	A	778	LEU
1	A	779	ARG
1	A	783	ASP
1	A	800	ASP
1	A	801	ILE
1	A	806	ARG
1	A	809	GLU
1	A	812	GLU
1	A	814	ILE
1	A	824	THR
1	A	831	LEU
1	A	841	ARG
1	A	844	GLU
1	A	849	LYS

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Mol	Chain	Res	Type
1	A	854	LEU
1	A	857	ARG
1	A	875	GLN
1	A	879	ILE
1	A	886	VAL
1	A	887	THR
1	A	893	LYS
1	A	904	SER
1	A	908	CYS
1	A	911	SER
1	A	912	GLN
1	A	924	VAL
1	A	928	ASN
1	A	940	LYS
1	A	943	LYS
1	A	955	THR
1	A	964	LEU
1	A	967	VAL
1	A	971	LEU
1	A	973	THR
1	A	976	SER
1	A	980	ASN
1	A	981	ASP
1	A	990	ILE
1	A	997	VAL
1	A	998	ASN
1	A	1002	LEU
1	B	665	LEU
1	B	669	VAL
1	B	672	LEU
1	B	674	LYS
1	B	675	MET
1	B	676	ILE
1	B	677	PHE
1	B	683	LYS
1	B	688	GLU
1	B	690	GLU
1	B	702	SER
1	B	704	ARG
1	B	714	SER
1	B	731	ASP
1	B	744	PHE

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Mol	Chain	Res	Type
1	B	747	LYS
1	B	748	LYS
1	B	751	LEU
1	B	754	ASN
1	B	756	ASP
1	B	759	GLN
1	B	761	LYS
1	B	767	ASN
1	B	778	LEU
1	B	779	ARG
1	B	783	ASP
1	B	784	ASP
1	B	785	SER
1	B	798	LYS
1	B	801	ILE
1	B	807	ASP
1	B	817	TYR
1	B	819	LYS
1	B	820	ASN
1	B	822	HIS
1	B	824	THR
1	B	826	HIS
1	B	829	TYR
1	B	833	VAL
1	B	834	ILE
1	B	835	ASP
1	B	838	LYS
1	B	839	ILE
1	B	847	ARG
1	B	852	LYS
1	B	879	ILE
1	B	887	THR
1	B	893	LYS
1	B	900	MET
1	B	903	LYS
1	B	904	SER
1	B	924	VAL
1	B	934	HIS
1	B	938	ILE
1	B	939	SER
1	B	941	LEU
1	B	955	THR

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Mol	Chain	Res	Type
1	B	962	ILE
1	B	965	ASP
1	B	981	ASP
1	B	982	THR
1	B	985	LEU
1	B	991	VAL
1	B	994	ILE
1	B	996	GLN
1	B	997	VAL
1	B	1004	LYS
1	B	1006	LYS
1	B	1007	PHE
1	B	1009	PHE
1	B	1010	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	718	GLN
1	A	722	GLN
1	A	820	ASN
1	A	928	ASN
1	A	934	HIS
1	A	937	HIS
1	A	961	ASN
1	B	670	GLN
1	B	717	GLN
1	B	728	GLN
1	B	820	ASN
1	B	826	HIS
1	B	827	ASN
1	B	855	HIS
1	B	928	ASN
1	B	961	ASN
1	B	996	GLN
1	B	1008	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](#)

2 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	FRQ	B	502	-	32,32,32	1.82	8 (25%)	41,44,44	1.84	10 (24%)
2	FRQ	A	501	-	32,32,32	2.15	7 (21%)	41,44,44	2.10	9 (21%)

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	FRQ	B	502	-	-	4/11/21/21	0/4/4/4
2	FRQ	A	501	-	-	2/11/21/21	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FRQ	C11-N12	-5.31	1.28	1.38
2	A	501	FRQ	C30-C31	-5.22	1.34	1.50
2	A	501	FRQ	C11-N10	-4.91	1.32	1.37
2	A	501	FRQ	C13-N12	-4.50	1.30	1.37
2	B	502	FRQ	C30-C31	-4.25	1.37	1.50
2	B	502	FRQ	C11-N12	-3.99	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	FRQ	C32-C31	3.97	1.50	1.35
2	A	501	FRQ	C32-C31	3.91	1.50	1.35
2	B	502	FRQ	C13-N12	-3.91	1.31	1.37
2	A	501	FRQ	C3-N10	-3.01	1.35	1.41
2	B	502	FRQ	C3-N10	-2.87	1.36	1.41
2	B	502	FRQ	C4-C3	-2.28	1.37	1.41
2	B	502	FRQ	C33-N26	-2.21	1.44	1.46
2	A	501	FRQ	C4-C3	-2.09	1.37	1.41
2	B	502	FRQ	C11-N10	-2.03	1.35	1.37

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FRQ	C33-N26-C29	7.51	117.23	109.78
2	B	502	FRQ	C33-N26-C29	5.78	115.52	109.78
2	A	501	FRQ	C29-C30-C31	5.16	126.16	112.38
2	A	501	FRQ	C33-C32-C31	-4.69	110.55	123.88
2	A	501	FRQ	C32-C33-N26	-4.47	109.36	112.89
2	B	502	FRQ	C29-C30-C31	4.47	124.31	112.38
2	B	502	FRQ	C13-N12-C11	-3.61	123.99	127.38
2	B	502	FRQ	C33-C32-C31	-3.37	114.30	123.88
2	A	501	FRQ	C23-N26-C29	3.08	119.45	111.24
2	B	502	FRQ	C23-N26-C29	3.04	119.33	111.24
2	A	501	FRQ	N12-C11-N10	2.70	120.44	115.53
2	A	501	FRQ	C13-N12-C11	-2.55	124.98	127.38
2	A	501	FRQ	C4-C3-N10	-2.49	116.76	120.31
2	B	502	FRQ	C3-C4-C5	2.45	120.23	117.13
2	B	502	FRQ	C32-C33-N26	-2.19	111.16	112.89
2	A	501	FRQ	C3-C4-C5	2.11	119.80	117.13
2	B	502	FRQ	C30-C31-C32	-2.09	118.89	120.63
2	B	502	FRQ	C4-C13-N12	2.05	117.34	115.05
2	B	502	FRQ	N12-C11-N10	2.01	119.19	115.53

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FRQ	C20-C23-N26-C29
2	B	502	FRQ	N10-C16-C17-C20
2	A	501	FRQ	C20-C23-N26-C33
2	B	502	FRQ	C17-C20-C23-N26
2	B	502	FRQ	C16-C17-C20-C23

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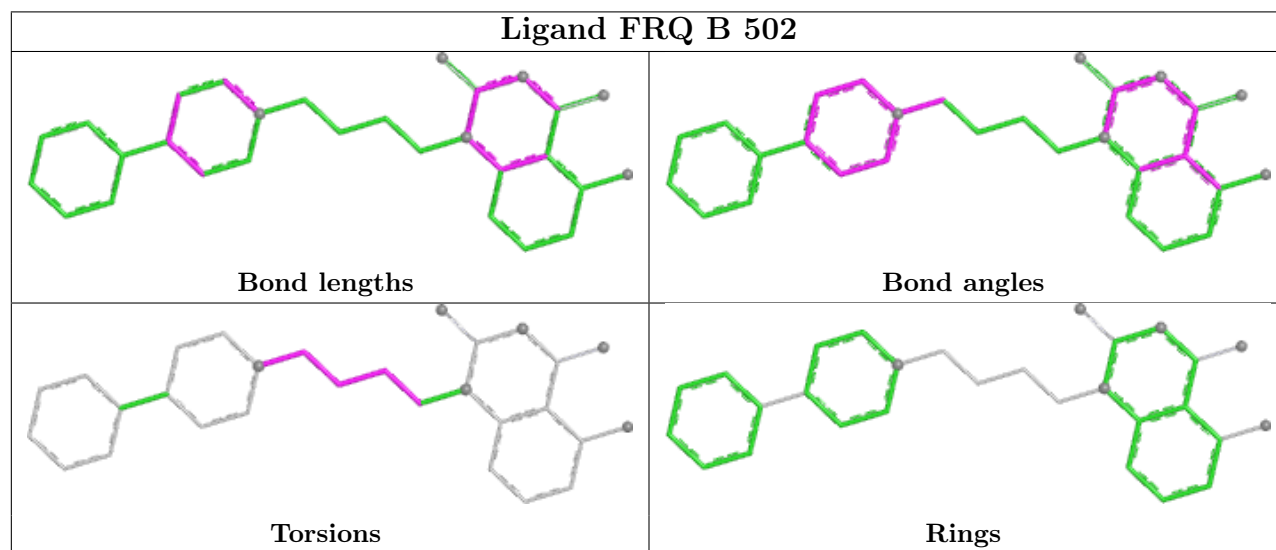
Mol	Chain	Res	Type	Atoms
2	B	502	FRQ	C20-C23-N26-C29

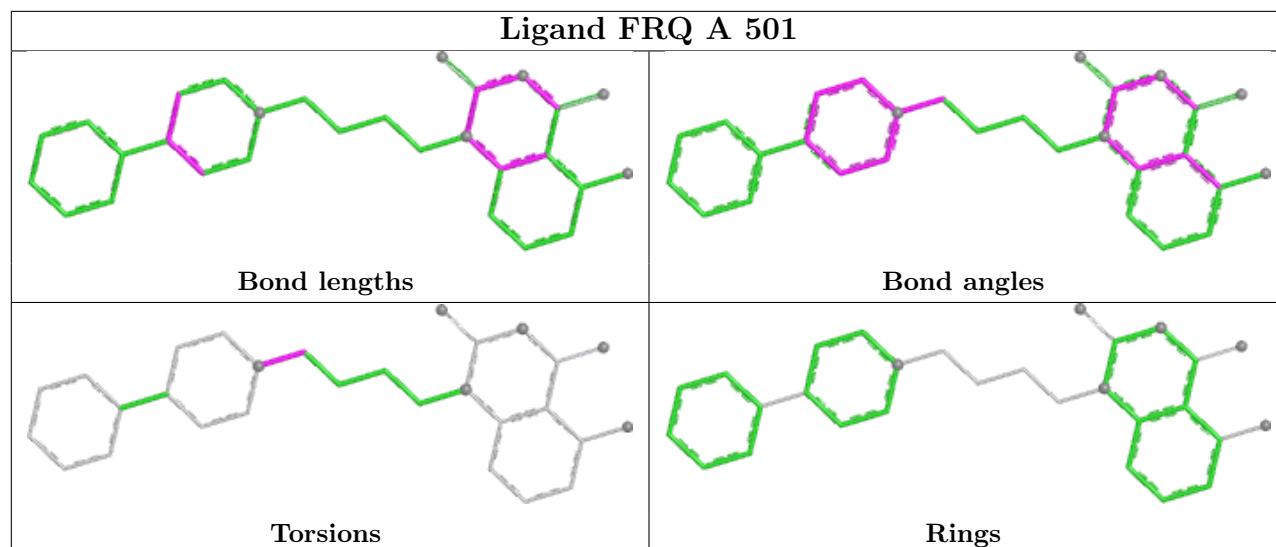
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	FRQ	2	0
2	A	501	FRQ	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	350/350 (100%)	0.40	12 (3%)	48	27	2, 15, 31, 42	0
1	B	350/350 (100%)	0.38	12 (3%)	48	27	2, 17, 33, 44	0
All	All	700/700 (100%)	0.39	24 (3%)	48	27	2, 16, 32, 44	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	783	ASP	3.5
1	B	963	SER	3.4
1	A	722	GLN	3.1
1	B	775	TYR	2.9
1	A	882	PRO	2.8
1	A	827	ASN	2.7
1	B	785	SER	2.7
1	B	680	GLU	2.6
1	B	902	SER	2.5
1	B	744	PHE	2.4
1	B	964	LEU	2.3
1	A	790	ILE	2.3
1	B	825	THR	2.3
1	A	807	ASP	2.3
1	B	728	GLN	2.3
1	B	784	ASP	2.2
1	A	784	ASP	2.2
1	A	826	HIS	2.2
1	A	782	SER	2.1
1	A	959	SER	2.1
1	B	965	ASP	2.1
1	A	823	ALA	2.1
1	A	745	GLY	2.1
1	A	824	THR	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](#)

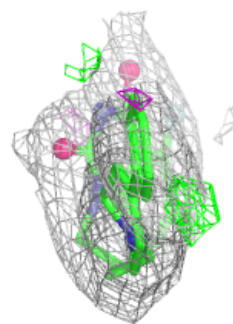
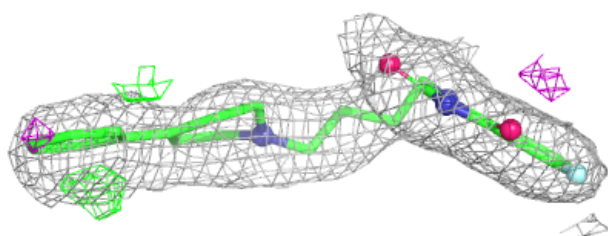
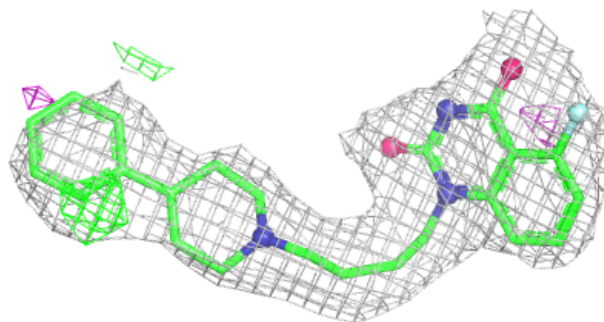
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FRQ	B	502	29/29	0.88	0.12	2,10,16,17	0
2	FRQ	A	501	29/29	0.89	0.14	3,11,19,20	0

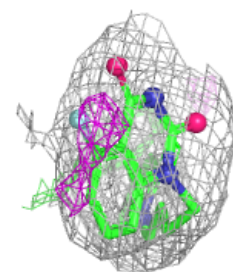
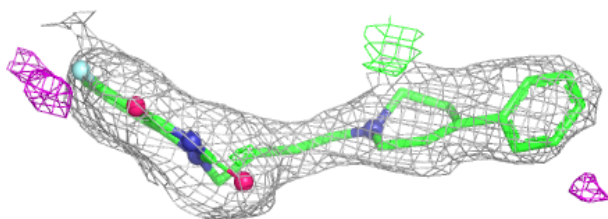
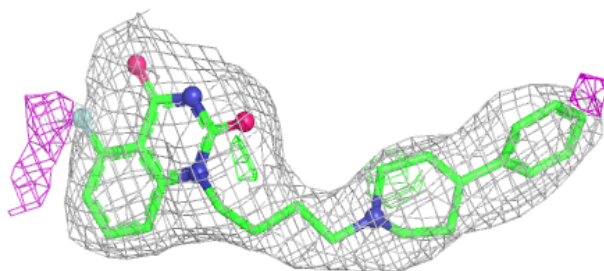
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FRQ B 502:

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

**Electron density around FRQ A 501:**

$2mF_o-DF_c$ (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.