



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:50 PM UTC

PDB ID : 1QPN / pdb_00001qpn
Title : Quinolate Phosphoribosyl Transferase from Mycobacterium Tuberculosis in Complex with NCNN
Authors : Sharma, V.; Grubmeyer, C.; Sacchettini, J.C.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 1998-11-20
Resolution : 2.60 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

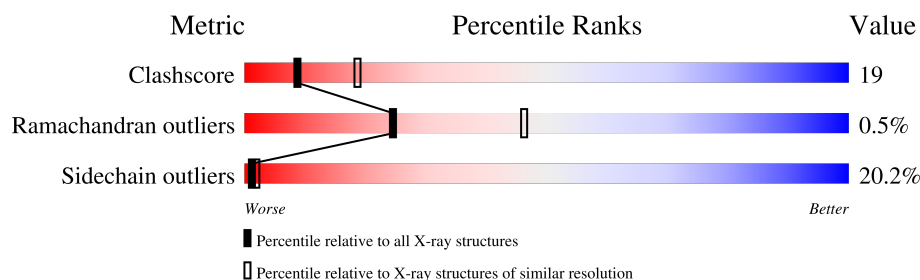
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	284	
1	B	284	
1	C	284	
1	D	284	
1	E	284	
1	F	284	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NCN	C	2905	-	-	X	-
2	NCN	F	2906	-	-	X	-

2 Entry composition [i](#)

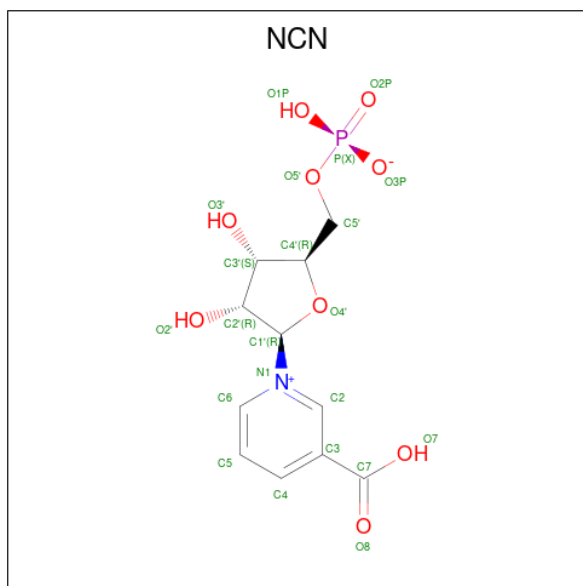
There are 3 unique types of molecules in this entry. The entry contains 12965 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (QUINOLINATE PHOSPHORIBOSYL TRANSFERASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2095	1301	378	411	5			
1	B	284	Total	C	N	O	S	0	0	0
			2095	1301	378	411	5			
1	C	284	Total	C	N	O	S	0	0	0
			2095	1301	378	411	5			
1	D	284	Total	C	N	O	S	0	0	0
			2095	1301	378	411	5			
1	E	284	Total	C	N	O	S	0	0	0
			2095	1301	378	411	5			
1	F	284	Total	C	N	O	S	0	0	0
			2095	1301	378	411	5			

- Molecule 2 is NICOTINATE MONONUCLEOTIDE (CCD ID: NCN) (formula: $C_{11}H_{14}NO_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	11	1	9	1		
2	B	1	Total	C	N	O	P	0	0
			22	11	1	9	1		
2	C	1	Total	C	N	O	P	0	0
			22	11	1	9	1		
2	D	1	Total	C	N	O	P	0	0
			22	11	1	9	1		
2	E	1	Total	C	N	O	P	0	0
			22	11	1	9	1		
2	F	1	Total	C	N	O	P	0	0
			22	11	1	9	1		

- Molecule 3 is water.

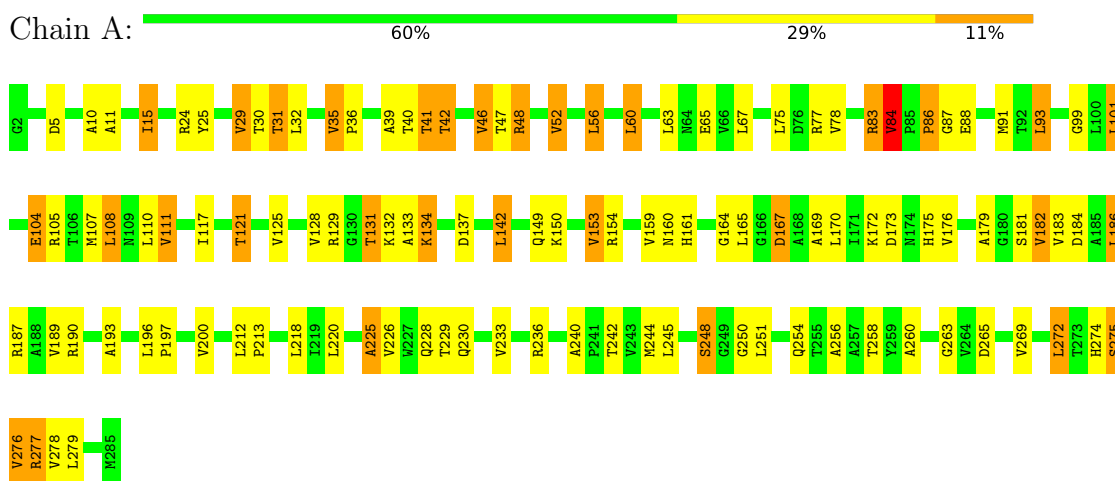
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	46	Total	O	0	0
			46	46		
3	B	48	Total	O	0	0
			48	48		
3	C	54	Total	O	0	0
			54	54		
3	D	40	Total	O	0	0
			40	40		
3	E	45	Total	O	0	0
			45	45		
3	F	30	Total	O	0	0
			30	30		

3 Residue-property plots

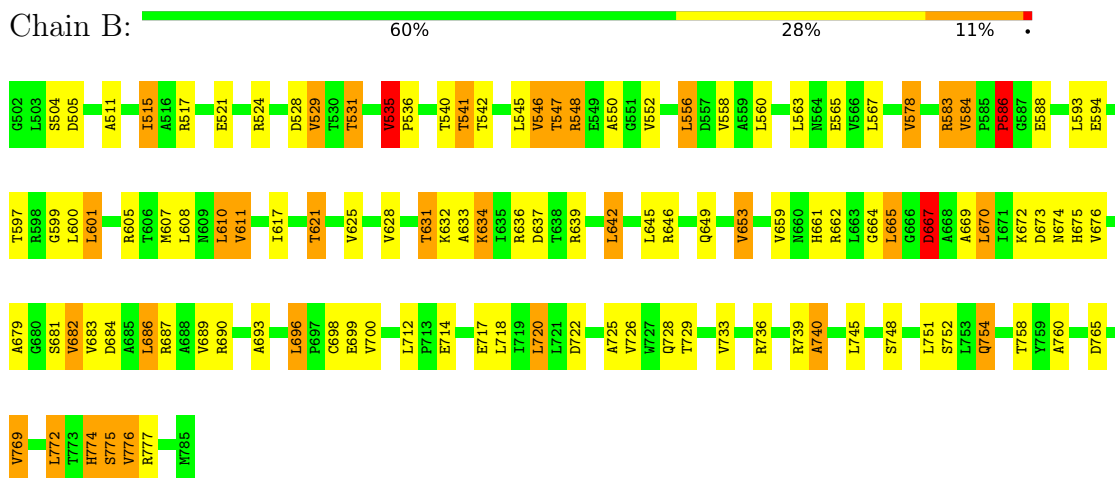
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: PROTEIN (QUINOLINATE PHOSPHORIBOSYL TRANSFERASE)

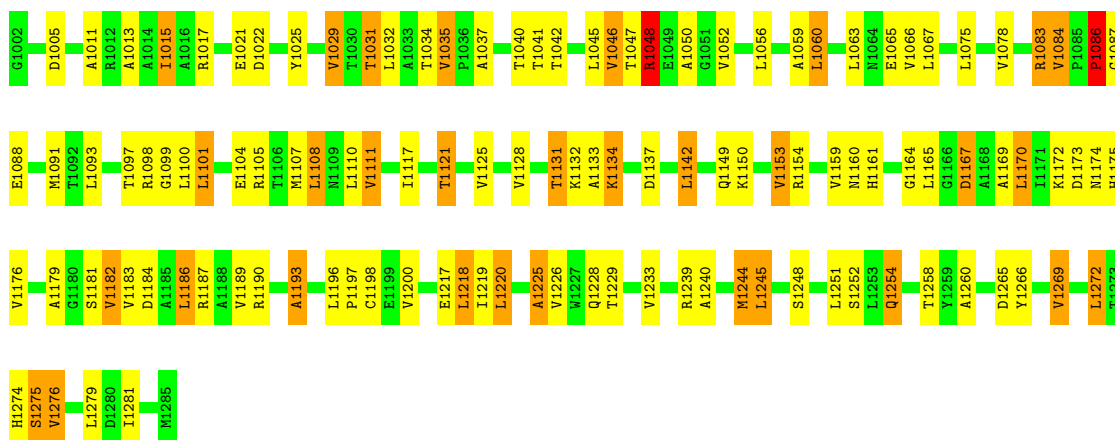


• Molecule 1: PROTEIN (QUINOLINATE PHOSPHORIBOSYL TRANSFERASE)



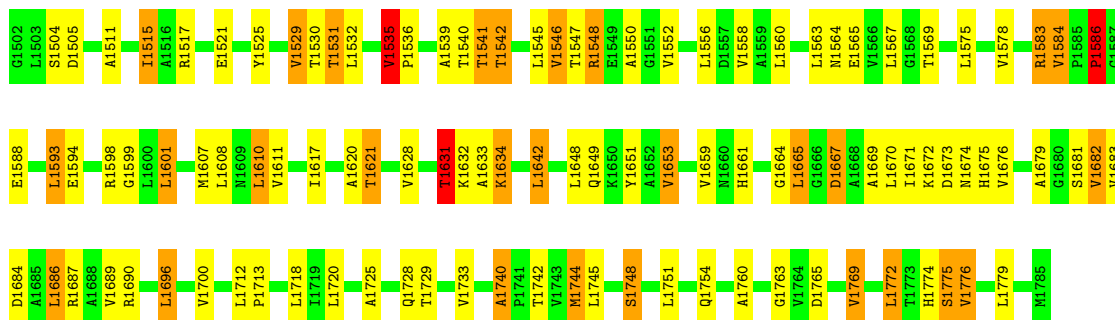
• Molecule 1: PROTEIN (QUINOLINATE PHOSPHORIBOSYL TRANSFERASE)





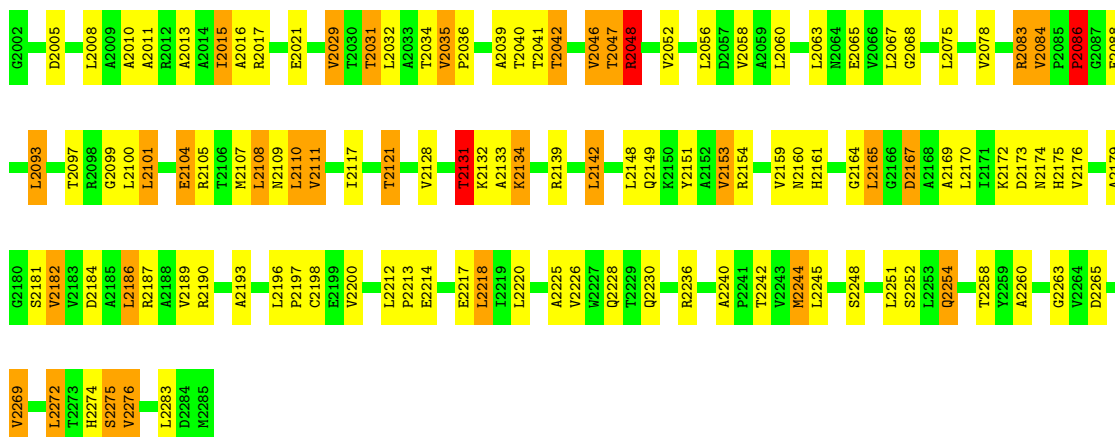
• Molecule 1: PROTEIN (QUINOLINATE PHOSPHORIBOSYL TRANSFERASE)

Chain D: 62% 27% 10%



• Molecule 1: PROTEIN (QUINOLINATE PHOSPHORIBOSYL TRANSFERASE)

Chain E: 59% 30% 11%



• Molecule 1: PROTEIN (QUINOLINATE PHOSPHORIBOSYL TRANSFERASE)

Chain F: 56% 33% 10%

K2672	D2673	N2674	H2675	V2676	K2679	D2680	S2681	V2682	D2683	D2684	A2685	L2686	R2687	A2688	V2689	R2690	A2693	L2696	E2699	V2700	E2706	L2712	P2713	E2714	L2718	L2719	L2720	A2725	V2726	Q2727	Q2728	T2729	V2733	R2736	A2740	P2741	T2742	V2743	H2744	L2745	S2748	L2751	Q2754	T2758																				
Y2759	A2760	D2765	A2768	V2769	L2772	T2773	H2774	S2775	V2776	R2777	V2778	L2779	H2785	G2587	E2588	L2593	G2599	L2600	L2601	E2604	R2605	T2606	M2607	L2608	N2609	L2610	V2611	L2617	T2621	V2628	T2631	K2632	A2633	K2634	I2635	R2636	D2637	T2638	R2639	K2640	T2641	L2642	L2645	R2646	A2647	L2648	Q2649	K2650	Y2651	A2652	V2653	V2659	N2660	H2661	R2662	L2663	G2664	L2665	G2666	D2667	A2668	A2669	L2670	I2671
L2502	L2503	S2504	D2505	L2508	A2511	R2512	A2513	A2514	I2515	A2516	R2517	E2521	D2522	L2523	R2524	Y2525	D2528	V2529	T2530	T2531	L2532	V2535	T2540	T2541	T2542	L2545	V2546	T2547	R2548	E2549	A2550	L2556	D2557	V2558	A2559	L2560	L2563	N2564	E2565	V2566	L2567	G2568	T2569	V2578	R2583	V2584	P2585	P2586																

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	100.38Å 100.38Å 144.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.60	Depositor
% Data completeness (in resolution range)	96.3 (8.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.185 , 0.269	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12965	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

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: NCN

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	0.95	1/2120 (0.0%)	1.25	20/2891 (0.7%)
1	B	0.96	2/2120 (0.1%)	1.24	24/2891 (0.8%)
1	C	0.97	2/2120 (0.1%)	1.23	18/2891 (0.6%)
1	D	0.93	2/2120 (0.1%)	1.23	15/2891 (0.5%)
1	E	0.91	1/2120 (0.0%)	1.23	19/2891 (0.7%)
1	F	0.94	1/2120 (0.0%)	1.23	15/2891 (0.5%)
All	All	0.94	9/12720 (0.1%)	1.23	111/17346 (0.6%)

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	D	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1035	VAL	CA-CB	10.25	1.62	1.54
1	B	535	VAL	CA-CB	7.86	1.61	1.54
1	F	2535	VAL	CA-CB	7.30	1.59	1.54
1	A	35	VAL	CA-CB	6.07	1.59	1.54
1	C	1091	MET	SD-CE	-5.68	1.65	1.79
1	D	1620	ALA	CA-CB	-5.64	1.44	1.53
1	D	1607	MET	SD-CE	-5.61	1.65	1.79
1	E	2035	VAL	CA-CB	5.58	1.58	1.54
1	B	636	ARG	CA-C	-5.10	1.46	1.52

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	HIS	N-CA-C	-8.58	97.76	110.46
1	D	1774	HIS	N-CA-C	-8.31	98.55	110.59
1	C	1274	HIS	N-CA-C	-8.19	98.72	110.59
1	D	1545	LEU	N-CA-C	-8.05	96.17	108.96
1	B	774	HIS	N-CA-C	-8.01	98.97	110.59
1	D	1665	LEU	N-CA-C	7.97	119.97	111.28
1	F	2774	HIS	N-CA-C	-7.74	99.37	110.59
1	F	2769	VAL	N-CA-C	7.53	117.55	106.85
1	A	240	ALA	CA-C-N	7.41	128.06	119.47
1	A	240	ALA	C-N-CA	7.41	128.06	119.47
1	B	583	ARG	N-CA-C	-7.38	98.03	109.76
1	E	2274	HIS	N-CA-C	-7.36	99.56	110.46
1	D	1583	ARG	N-CA-C	-7.29	98.18	109.76
1	C	1275	SER	N-CA-C	7.15	121.26	111.39
1	F	2583	ARG	N-CA-C	-7.00	97.84	109.46
1	C	1083	ARG	N-CA-C	-6.99	98.65	109.76
1	E	2240	ALA	CA-C-N	6.96	127.54	119.47
1	E	2240	ALA	C-N-CA	6.96	127.54	119.47
1	A	35	VAL	N-CA-C	6.91	115.84	107.61
1	F	2531	THR	N-CA-C	-6.91	103.68	111.14
1	A	83	ARG	N-CA-C	-6.85	98.87	109.76
1	E	2083	ARG	N-CA-C	-6.82	98.91	109.76
1	C	1240	ALA	CA-C-N	6.78	127.34	119.47
1	C	1240	ALA	C-N-CA	6.78	127.34	119.47
1	A	42	THR	N-CA-C	-6.75	97.51	108.52
1	F	2725	ALA	N-CA-C	-6.71	102.16	110.41
1	D	1542	THR	N-CA-C	-6.70	98.28	109.07
1	F	2542	THR	N-CA-C	-6.68	98.02	108.90
1	D	1740	ALA	CA-C-N	6.41	126.91	119.47
1	D	1740	ALA	C-N-CA	6.41	126.91	119.47
1	D	1769	VAL	N-CA-C	6.41	115.95	106.85
1	F	2740	ALA	CA-C-N	6.39	126.88	119.47
1	F	2740	ALA	C-N-CA	6.39	126.88	119.47
1	B	740	ALA	CA-C-N	6.37	126.86	119.47
1	B	740	ALA	C-N-CA	6.37	126.86	119.47
1	B	775	SER	N-CA-C	6.34	119.92	111.30
1	F	2548	ARG	N-CA-C	-6.31	105.62	113.38
1	D	1775	SER	N-CA-C	6.31	120.09	111.39
1	B	531	THR	N-CA-C	-6.26	104.38	111.14
1	E	2275	SER	N-CA-C	6.21	119.95	111.39
1	E	2052	VAL	N-CA-C	-6.17	99.48	108.11
1	C	1269	VAL	N-CA-C	6.17	116.49	107.37
1	B	665	LEU	N-CA-C	6.15	117.98	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	2035	VAL	N-CA-C	6.13	114.90	107.61
1	C	1048	ARG	N-CA-C	-6.12	105.81	113.28
1	E	2274	HIS	CA-C-N	-6.06	113.75	122.36
1	E	2274	HIS	C-N-CA	-6.06	113.75	122.36
1	B	542	THR	N-CA-C	-6.03	98.59	108.41
1	C	1042	THR	N-CA-C	-6.03	99.07	108.90
1	B	696	LEU	N-CA-C	6.02	117.65	110.07
1	C	1031	THR	N-CA-C	-6.01	104.81	111.36
1	C	1225	ALA	N-CA-C	-5.99	102.62	110.53
1	E	2068	GLY	N-CA-C	-5.97	104.18	112.18
1	D	1535	VAL	N-CA-C	5.91	114.33	107.89
1	D	1696	LEU	N-CA-C	5.89	117.49	110.07
1	E	2193	ALA	CA-C-N	5.85	125.53	119.56
1	E	2193	ALA	C-N-CA	5.85	125.53	119.56
1	E	2048	ARG	N-CA-C	-5.82	106.18	113.28
1	B	639	ARG	N-CA-C	-5.81	105.77	112.92
1	C	1097	THR	N-CA-C	5.78	118.05	111.11
1	E	2269	VAL	N-CA-C	5.76	115.03	106.85
1	B	545	LEU	N-CA-C	-5.72	99.87	108.96
1	A	256	ALA	N-CA-C	5.70	117.95	111.11
1	E	2042	THR	N-CA-C	-5.69	99.14	108.41
1	A	274	HIS	CA-C-N	-5.65	114.34	122.36
1	A	274	HIS	C-N-CA	-5.65	114.34	122.36
1	F	2696	LEU	N-CA-C	5.62	116.91	109.93
1	A	84	VAL	N-CA-CB	-5.62	103.34	111.21
1	B	739	ARG	N-CA-C	5.59	120.23	112.90
1	A	52	VAL	N-CA-C	-5.55	100.35	108.11
1	B	774	HIS	CA-C-N	-5.54	114.65	122.46
1	B	774	HIS	C-N-CA	-5.54	114.65	122.46
1	A	31	THR	N-CA-C	-5.45	105.42	111.36
1	A	193	ALA	CA-C-N	5.43	125.10	119.56
1	A	193	ALA	C-N-CA	5.43	125.10	119.56
1	B	693	ALA	CA-C-N	5.42	125.25	119.28
1	B	693	ALA	C-N-CA	5.42	125.25	119.28
1	E	2034	THR	N-CA-C	5.42	120.00	112.90
1	E	2031	THR	N-CA-C	-5.40	105.47	111.36
1	A	275	SER	N-CA-C	5.40	118.84	111.39
1	A	279	LEU	N-CA-C	-5.40	100.38	108.96
1	E	2097	THR	N-CA-C	5.38	117.56	111.11
1	D	1779	LEU	N-CA-C	-5.37	100.42	108.96
1	C	1034	THR	N-CA-C	5.36	119.94	113.41
1	D	1531	THR	N-CA-C	-5.35	105.36	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	667	ASP	N-CA-C	5.35	116.79	111.07
1	A	278	VAL	N-CA-C	5.32	117.29	109.63
1	C	1274	HIS	CA-C-N	-5.31	114.82	122.36
1	C	1274	HIS	C-N-CA	-5.31	114.82	122.36
1	B	769	VAL	N-CA-C	5.28	114.35	106.85
1	B	535	VAL	CA-C-N	5.28	125.22	119.78
1	B	535	VAL	C-N-CA	5.28	125.22	119.78
1	F	2545	LEU	N-CA-C	-5.23	99.99	108.41
1	B	597	THR	N-CA-C	5.23	117.66	111.33
1	C	1066	VAL	N-CA-C	5.21	117.11	111.58
1	D	1631	THR	N-CA-C	-5.19	101.52	109.41
1	F	2706	GLU	N-CA-C	-5.19	105.52	111.07
1	C	1193	ALA	CA-C-N	5.18	124.84	119.56
1	C	1193	ALA	C-N-CA	5.18	124.84	119.56
1	B	722	ASP	N-CA-C	5.16	116.67	108.67
1	B	667	ASP	CB-CA-C	-5.13	102.82	110.88
1	D	1504	SER	N-CA-C	-5.13	103.92	110.53
1	E	2131	THR	N-CA-C	-5.08	102.67	110.14
1	A	225	ALA	N-CA-C	-5.07	104.17	110.41
1	F	2774	HIS	CA-C-N	-5.07	115.16	122.36
1	F	2774	HIS	C-N-CA	-5.07	115.16	122.36
1	A	10	ALA	N-CA-C	-5.07	105.76	111.28
1	C	1045	LEU	N-CA-C	-5.06	100.26	108.41
1	A	41	THR	CB-CA-C	-5.05	100.30	110.30
1	F	2588	GLU	N-CA-C	5.02	117.51	110.23
1	B	504	SER	N-CA-C	-5.00	103.80	110.55

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	1525	TYR	Sidechain

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	2095	0	2135	84	0
1	B	2095	0	2135	81	0
1	C	2095	0	2135	87	0
1	D	2095	0	2135	71	0
1	E	2095	0	2135	89	0
1	F	2095	0	2135	89	0
2	A	22	0	12	5	0
2	B	22	0	12	6	0
2	C	22	0	12	8	0
2	D	22	0	12	6	0
2	E	22	0	12	5	0
2	F	22	0	12	7	0
3	A	46	0	0	5	0
3	B	48	0	0	2	0
3	C	54	0	0	5	0
3	D	40	0	0	1	0
3	E	45	0	0	3	0
3	F	30	0	0	2	0
All	All	12965	0	12882	478	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 19.

All (478) 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)
2:E:2903:NCN:H2	3:E:3006:HOH:O	1.57	1.04
1:F:2661:HIS:ND1	2:F:2906:NCN:H4	1.75	1.01
1:D:1748:SER:OG	2:D:2904:NCN:H3'	1.62	0.97
1:A:248:SER:OG	2:A:2901:NCN:H3'	1.65	0.96
1:E:2248:SER:OG	2:E:2903:NCN:H3'	1.66	0.94
1:A:67:LEU:HD21	1:A:99:GLY:HA3	1.50	0.93
1:A:131:THR:HG21	1:A:260:ALA:HB1	1.50	0.93
2:C:2905:NCN:H2	3:C:3005:HOH:O	1.68	0.92
1:E:2131:THR:HG21	1:E:2260:ALA:HB1	1.53	0.91
1:A:225:ALA:H	1:A:228:GLN:HE21	1.18	0.89
1:C:1248:SER:OG	2:C:2905:NCN:H3'	1.72	0.89
2:A:2901:NCN:H2	3:A:3014:HOH:O	1.71	0.89
1:D:1631:THR:HG21	1:D:1760:ALA:HB1	1.52	0.89
2:B:2902:NCN:H2	3:B:3031:HOH:O	1.72	0.89
1:D:1567:LEU:HD21	1:D:1599:GLY:HA3	1.51	0.88
1:B:631:THR:HG21	1:B:760:ALA:HB1	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:725:ALA:H	1:B:728:GLN:HE21	1.17	0.88
1:F:2748:SER:OG	2:F:2906:NCN:H3'	1.73	0.87
1:F:2725:ALA:H	1:F:2728:GLN:HE21	1.18	0.87
1:A:84:VAL:HG22	1:A:88:GLU:HG2	1.56	0.85
1:B:567:LEU:HD21	1:B:599:GLY:HA3	1.57	0.84
1:C:1225:ALA:H	1:C:1228:GLN:HE21	1.25	0.84
1:E:2067:LEU:HD21	1:E:2099:GLY:HA3	1.60	0.83
1:B:748:SER:OG	2:B:2902:NCN:H3'	1.78	0.83
1:D:1621:THR:HG21	1:D:1653:VAL:HA	1.61	0.83
1:B:584:VAL:HG22	1:B:588:GLU:HG2	1.62	0.82
1:B:725:ALA:H	1:B:728:GLN:NE2	1.77	0.82
1:C:1276:VAL:O	1:D:1775:SER:HA	1.79	0.82
1:D:1748:SER:HG	2:D:2904:NCN:H6	1.45	0.80
1:A:225:ALA:H	1:A:228:GLN:NE2	1.79	0.80
2:D:2904:NCN:H2	3:D:3008:HOH:O	1.83	0.79
1:F:2725:ALA:H	1:F:2728:GLN:NE2	1.80	0.78
1:E:2248:SER:OG	2:E:2903:NCN:H6	1.82	0.78
1:B:632:LYS:O	1:B:634:LYS:HE2	1.83	0.78
1:A:276:VAL:O	1:B:775:SER:HA	1.83	0.78
1:D:1725:ALA:H	1:D:1728:GLN:HE21	1.29	0.78
1:C:1132:LYS:O	1:C:1134:LYS:HE2	1.85	0.77
1:A:161:HIS:ND1	2:A:2901:NCN:H4	1.99	0.77
1:A:186:LEU:HD22	1:A:187:ARG:HH21	1.51	0.76
1:D:1661:HIS:ND1	2:D:2904:NCN:H4	2.02	0.75
1:F:2531:THR:HG22	1:F:2601:LEU:HD23	1.69	0.75
1:C:1161:HIS:ND1	2:C:2905:NCN:H4	2.03	0.74
1:F:2515:ILE:HD11	1:F:2565:GLU:HG2	1.69	0.74
1:A:269:VAL:HB	1:A:272:LEU:HD22	1.68	0.74
1:B:686:LEU:HD22	1:B:687:ARG:HH21	1.53	0.74
1:C:1161:HIS:HD1	2:C:2905:NCN:H4	1.52	0.74
1:D:1672:LYS:H	1:D:1675:HIS:HD2	1.36	0.74
1:D:1515:ILE:HD11	1:D:1565:GLU:HG2	1.70	0.73
1:E:2225:ALA:H	1:E:2228:GLN:NE2	1.85	0.73
1:C:1186:LEU:HD22	1:C:1187:ARG:HH21	1.52	0.73
1:E:2121:THR:HG21	1:E:2153:VAL:HA	1.70	0.73
1:E:2275:SER:HA	1:F:2776:VAL:O	1.89	0.73
1:E:2132:LYS:O	1:E:2134:LYS:HE2	1.88	0.73
1:D:1748:SER:OG	2:D:2904:NCN:H6	1.89	0.72
1:C:1117:ILE:O	1:C:1121:THR:HG23	1.89	0.72
1:F:2503:LEU:HB2	1:F:2508:LEU:HD13	1.71	0.72
1:D:1725:ALA:H	1:D:1728:GLN:NE2	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1634:LYS:HE3	1:D:1765:ASP:O	1.90	0.71
1:B:672:LYS:H	1:B:675:HIS:CD2	2.08	0.71
1:D:1632:LYS:O	1:D:1634:LYS:HE2	1.89	0.71
1:F:2632:LYS:O	1:F:2634:LYS:HE2	1.91	0.71
1:D:1672:LYS:H	1:D:1675:HIS:CD2	2.07	0.71
1:E:2128:VAL:O	1:E:2131:THR:HB	1.90	0.71
1:E:2134:LYS:HE3	1:E:2265:ASP:O	1.90	0.71
1:E:2225:ALA:H	1:E:2228:GLN:HE21	1.37	0.70
1:D:1661:HIS:CE1	2:D:2904:NCN:H4	2.26	0.70
1:A:186:LEU:HD22	1:A:187:ARG:NH2	2.05	0.70
1:E:2084:VAL:HG22	1:E:2088:GLU:HG2	1.74	0.70
1:E:2031:THR:HG22	1:E:2101:LEU:HD23	1.72	0.70
1:C:1218:LEU:HD23	1:C:1244:MET:HB2	1.74	0.70
1:C:1186:LEU:HD22	1:C:1187:ARG:NH2	2.06	0.70
1:F:2567:LEU:HD21	1:F:2599:GLY:HA3	1.74	0.70
1:C:1225:ALA:H	1:C:1228:GLN:NE2	1.90	0.69
1:D:1584:VAL:HG22	1:D:1588:GLU:HG2	1.74	0.69
1:C:1196:LEU:CD2	1:D:1529:VAL:HG11	2.22	0.69
1:F:2628:VAL:O	1:F:2631:THR:HB	1.93	0.68
1:E:2015:ILE:HD11	1:E:2065:GLU:HG2	1.74	0.68
1:B:672:LYS:H	1:B:675:HIS:HD2	1.39	0.68
1:F:2686:LEU:HD22	1:F:2687:ARG:NH2	2.09	0.68
1:D:1558:VAL:HG11	1:D:1610:LEU:HG	1.76	0.67
1:F:2686:LEU:HD22	1:F:2687:ARG:HH21	1.58	0.67
1:F:2631:THR:HG21	1:F:2760:ALA:HB1	1.76	0.67
1:B:686:LEU:HD22	1:B:687:ARG:NH2	2.10	0.67
1:E:2161:HIS:ND1	2:E:2903:NCN:H4	2.10	0.67
1:B:546:VAL:HG22	1:B:548:ARG:HH21	1.59	0.67
1:F:2676:VAL:HG22	1:F:2682:VAL:HA	1.76	0.67
1:A:132:LYS:O	1:A:134:LYS:HE2	1.94	0.67
1:C:1067:LEU:HD21	1:C:1099:GLY:HA3	1.77	0.66
1:B:676:VAL:HG13	1:B:682:VAL:N	2.10	0.66
1:A:31:THR:HG22	1:A:101:LEU:HD23	1.78	0.66
1:A:196:LEU:CD2	1:B:529:VAL:HG11	2.26	0.66
1:E:2029:VAL:HG11	1:F:2696:LEU:HD21	1.77	0.66
1:E:2196:LEU:CD2	1:F:2529:VAL:HG11	2.26	0.66
1:E:2276:VAL:O	1:F:2775:SER:HA	1.96	0.65
1:E:2029:VAL:HG11	1:F:2696:LEU:CD2	2.26	0.65
1:C:1186:LEU:O	1:C:1190:ARG:HG2	1.97	0.65
1:F:2621:THR:HG21	1:F:2653:VAL:HA	1.77	0.65
1:A:46:VAL:HG22	1:A:48:ARG:HH21	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1187:ARG:HH22	1:C:1190:ARG:HE	1.44	0.64
1:A:83:ARG:HD3	3:A:3082:HOH:O	1.96	0.64
1:C:1029:VAL:HG11	1:D:1696:LEU:CD2	2.27	0.64
1:C:1084:VAL:HG22	1:C:1088:GLU:HG2	1.79	0.64
1:C:1050:ALA:HB2	1:C:1086:PRO:HD3	1.78	0.64
1:F:2661:HIS:CE1	2:F:2906:NCN:H4	2.33	0.64
1:B:531:THR:HG22	1:B:601:LEU:HD23	1.79	0.63
1:B:725:ALA:N	1:B:728:GLN:HE21	1.95	0.63
1:B:748:SER:OG	2:B:2902:NCN:H6	1.99	0.63
1:C:1011:ALA:O	1:C:1015:ILE:HG23	1.98	0.63
1:A:172:LYS:H	1:A:175:HIS:HD2	1.45	0.63
1:C:1015:ILE:HD11	1:C:1065:GLU:HG2	1.78	0.63
1:C:1121:THR:HG22	1:C:1272:LEU:HG	1.80	0.63
1:C:1275:SER:HA	1:D:1776:VAL:O	1.98	0.63
1:A:87:GLY:HA3	1:E:2230:GLN:HB3	1.81	0.63
1:C:1017:ARG:NH1	1:D:1517:ARG:HD3	2.14	0.63
1:D:1676:VAL:HG22	1:D:1682:VAL:HA	1.80	0.63
1:F:2676:VAL:HG13	1:F:2682:VAL:N	2.14	0.63
1:E:2104:GLU:HG3	1:E:2283:LEU:HD23	1.81	0.62
1:C:1131:THR:HG23	1:C:1133:ALA:H	1.65	0.62
1:A:15:ILE:HD11	1:A:65:GLU:HG2	1.81	0.62
1:A:275:SER:HA	1:B:776:VAL:O	1.99	0.62
1:D:1686:LEU:HD22	1:D:1687:ARG:HH21	1.64	0.62
1:E:2132:LYS:HE2	1:E:2263:GLY:O	2.00	0.62
2:F:2906:NCN:H2	3:F:3101:HOH:O	1.97	0.62
1:C:1269:VAL:HB	1:C:1272:LEU:HD22	1.81	0.61
1:A:176:VAL:HG13	1:A:182:VAL:N	2.15	0.61
1:C:1134:LYS:HE3	1:C:1265:ASP:O	2.01	0.61
1:F:2617:ILE:O	1:F:2621:THR:HG23	2.00	0.61
1:B:621:THR:HG21	1:B:653:VAL:HA	1.82	0.61
1:B:515:ILE:HD11	1:B:565:GLU:HG2	1.82	0.61
1:B:634:LYS:HE3	1:B:765:ASP:O	2.01	0.60
1:A:172:LYS:H	1:A:175:HIS:CD2	2.18	0.60
1:C:1172:LYS:H	1:C:1175:HIS:CD2	2.19	0.60
1:E:2187:ARG:NH2	1:E:2214:GLU:HB3	2.17	0.60
1:C:1046:VAL:HG22	1:C:1048:ARG:HH21	1.66	0.60
1:C:1196:LEU:HD21	1:D:1529:VAL:HG11	1.83	0.60
1:D:1632:LYS:HE2	1:D:1763:GLY:O	2.01	0.60
1:E:2104:GLU:HG3	1:E:2283:LEU:CD2	2.32	0.60
1:A:67:LEU:CD2	1:A:99:GLY:HA3	2.30	0.59
1:E:2186:LEU:HD22	1:E:2187:ARG:HH21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2631:THR:HG23	1:F:2633:ALA:H	1.66	0.59
1:E:2036:PRO:HG2	1:E:2039:ALA:HB2	1.84	0.59
1:F:2584:VAL:HG22	1:F:2588:GLU:HG2	1.85	0.59
1:C:1176:VAL:HG13	1:C:1182:VAL:N	2.17	0.59
1:E:2046:VAL:HG22	1:E:2048:ARG:HH21	1.67	0.59
1:E:2172:LYS:H	1:E:2175:HIS:HD2	1.50	0.59
1:A:121:THR:HG21	1:A:153:VAL:HA	1.84	0.59
1:F:2607:MET:O	1:F:2611:VAL:HG13	2.01	0.59
1:F:2693:ALA:HB1	1:F:2696:LEU:HB2	1.84	0.59
1:C:1239:ARG:NH1	3:C:3047:HOH:O	2.35	0.59
1:A:161:HIS:CE1	2:A:2901:NCN:H4	2.37	0.59
1:C:1161:HIS:CE1	2:C:2905:NCN:H4	2.38	0.58
1:B:687:ARG:HH22	1:B:690:ARG:HE	1.49	0.58
1:F:2546:VAL:HG22	1:F:2548:ARG:HH21	1.67	0.58
1:E:2172:LYS:H	1:E:2175:HIS:CD2	2.20	0.58
1:B:769:VAL:HB	1:B:772:LEU:HD22	1.84	0.58
1:B:720:LEU:HD21	2:B:2902:NCN:C5	2.33	0.58
1:D:1686:LEU:HD22	1:D:1687:ARG:NH2	2.19	0.58
1:F:2558:VAL:HG11	1:F:2610:LEU:HG	1.83	0.58
1:F:2769:VAL:HB	1:F:2772:LEU:HD22	1.85	0.58
1:A:176:VAL:HG13	1:A:181:SER:C	2.28	0.58
1:A:179:ALA:HB1	1:A:184:ASP:HB3	1.85	0.57
1:C:1052:VAL:HG22	1:C:1083:ARG:HD2	1.84	0.57
1:C:1172:LYS:H	1:C:1175:HIS:HD2	1.51	0.57
1:A:142:LEU:H	1:A:149:GLN:HE22	1.52	0.57
1:B:676:VAL:HG22	1:B:682:VAL:HA	1.86	0.57
1:C:1131:THR:HG21	1:C:1260:ALA:HB1	1.87	0.57
1:E:2161:HIS:CE1	2:E:2903:NCN:H4	2.39	0.57
1:B:607:MET:O	1:B:611:VAL:HG13	2.03	0.57
1:C:1252:SER:OG	1:C:1254:GLN:HG2	2.05	0.57
1:C:1046:VAL:CG2	1:C:1048:ARG:HH21	2.18	0.57
1:D:1511:ALA:O	1:D:1515:ILE:HG23	2.04	0.57
1:E:2142:LEU:H	1:E:2149:GLN:HE22	1.51	0.57
1:F:2687:ARG:CZ	1:F:2690:ARG:HG3	2.36	0.56
1:D:1718:LEU:HD23	1:D:1744:MET:HB2	1.87	0.56
1:E:2225:ALA:N	1:E:2228:GLN:HE21	2.03	0.56
1:F:2725:ALA:N	1:F:2728:GLN:HE21	1.97	0.56
1:E:2187:ARG:HH22	1:E:2190:ARG:HE	1.52	0.56
1:E:2218:LEU:HD23	1:E:2244:MET:HB2	1.86	0.56
1:E:2186:LEU:HD22	1:E:2187:ARG:NH2	2.20	0.56
1:F:2672:LYS:H	1:F:2675:HIS:CD2	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2511:ALA:O	1:F:2515:ILE:HG23	2.05	0.56
1:C:1031:THR:HG22	1:C:1101:LEU:HD23	1.88	0.55
1:C:1142:LEU:H	1:C:1149:GLN:HE22	1.52	0.55
1:F:2638:THR:OG1	1:F:2640:LYS:HG3	2.06	0.55
1:A:117:ILE:O	1:A:121:THR:HG23	2.06	0.55
1:A:169:ALA:HB1	1:A:189:VAL:HG11	1.88	0.55
1:B:712:LEU:HD22	1:B:740:ALA:HB3	1.87	0.55
1:D:1546:VAL:HG22	1:D:1548:ARG:HH21	1.71	0.55
1:C:1183:VAL:O	1:C:1187:ARG:HG2	2.07	0.55
1:C:1187:ARG:NH2	1:C:1190:ARG:HE	2.04	0.55
1:A:128:VAL:O	1:A:131:THR:HB	2.07	0.54
1:E:2187:ARG:CZ	1:E:2190:ARG:HG3	2.37	0.54
1:F:2634:LYS:HE3	1:F:2765:ASP:O	2.07	0.54
1:F:2687:ARG:HH22	1:F:2690:ARG:HE	1.55	0.54
1:A:11:ALA:O	1:A:15:ILE:HG23	2.07	0.54
1:C:1017:ARG:O	1:C:1021:GLU:HG3	2.08	0.54
1:E:2083:ARG:HB3	3:E:3033:HOH:O	2.07	0.54
1:A:134:LYS:HE3	1:A:265:ASP:O	2.07	0.54
1:D:1628:VAL:O	1:D:1631:THR:HB	2.07	0.54
1:D:1729:THR:O	1:D:1733:VAL:HG23	2.07	0.54
1:B:686:LEU:O	1:B:690:ARG:HG2	2.06	0.54
1:D:1676:VAL:HG13	1:D:1682:VAL:N	2.23	0.54
1:C:1121:THR:HG21	1:C:1153:VAL:HA	1.91	0.53
1:D:1515:ILE:C	1:D:1515:ILE:HD12	2.32	0.53
1:A:248:SER:OG	2:A:2901:NCN:H6	2.08	0.53
1:B:642:LEU:H	1:B:649:GLN:HE22	1.55	0.53
1:E:2107:MET:O	1:E:2111:VAL:HG13	2.08	0.53
1:D:1550:ALA:HB2	1:D:1586:PRO:HD3	1.90	0.53
1:A:31:THR:CG2	1:A:101:LEU:HD23	2.37	0.53
1:A:52:VAL:HG22	1:A:83:ARG:HD2	1.90	0.53
1:E:2176:VAL:HG13	1:E:2182:VAL:N	2.23	0.53
1:C:1107:MET:O	1:C:1111:VAL:HG13	2.09	0.53
1:B:676:VAL:HG13	1:B:681:SER:C	2.33	0.53
1:D:1536:PRO:HG2	1:D:1539:ALA:HB2	1.90	0.53
1:B:617:ILE:O	1:B:621:THR:HG23	2.09	0.53
1:B:669:ALA:HB1	1:B:689:VAL:HG11	1.90	0.53
1:B:670:LEU:HD13	1:B:672:LYS:HG3	1.90	0.53
1:C:1193:ALA:HB1	1:C:1196:LEU:HB2	1.91	0.53
1:D:1542:THR:HA	1:D:1593:LEU:O	2.09	0.53
1:B:687:ARG:NH2	1:B:690:ARG:HE	2.06	0.53
1:C:1187:ARG:CZ	1:C:1190:ARG:HG3	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2169:ALA:HB1	1:E:2189:VAL:HG11	1.90	0.52
1:C:1176:VAL:HG22	1:C:1182:VAL:HA	1.92	0.52
1:A:131:THR:HG23	1:A:133:ALA:H	1.73	0.52
1:A:176:VAL:HG22	1:A:182:VAL:HA	1.92	0.52
1:A:187:ARG:HH22	1:A:190:ARG:HE	1.57	0.52
1:A:218:LEU:HD23	1:A:244:MET:HB2	1.92	0.52
1:D:1531:THR:HG22	1:D:1601:LEU:HD23	1.92	0.52
1:D:1683:VAL:O	1:D:1687:ARG:HG2	2.10	0.52
1:B:541:THR:O	1:B:594:GLU:HA	2.10	0.52
1:A:131:THR:CG2	1:A:133:ALA:H	2.23	0.52
1:B:631:THR:CG2	1:B:633:ALA:H	2.23	0.52
1:C:1029:VAL:HG11	1:D:1696:LEU:HD21	1.92	0.52
1:F:2664:GLY:N	1:F:2667:ASP:OD1	2.43	0.52
1:A:105:ARG:HD3	1:A:105:ARG:O	2.09	0.51
1:B:550:ALA:HB2	1:B:586:PRO:HD3	1.92	0.51
1:E:2269:VAL:HB	1:E:2272:LEU:HD22	1.90	0.51
1:F:2768:ALA:HB1	2:F:2906:NCN:H5	1.92	0.51
1:D:1712:LEU:N	1:D:1713:PRO:HD2	2.26	0.51
1:D:1687:ARG:HH22	1:D:1690:ARG:HE	1.58	0.51
1:F:2637:ASP:OD2	1:F:2653:VAL:HG21	2.09	0.51
1:F:2672:LYS:H	1:F:2675:HIS:HD2	1.59	0.51
1:E:2154:ARG:HE	1:E:2160:ASN:ND2	2.08	0.51
1:A:186:LEU:O	1:A:190:ARG:HG2	2.09	0.51
1:D:1642:LEU:H	1:D:1649:GLN:HE22	1.59	0.50
1:F:2712:LEU:N	1:F:2713:PRO:HD2	2.26	0.50
1:B:679:ALA:HB1	1:B:684:ASP:HB3	1.92	0.50
1:B:662:ARG:HG3	2:B:2902:NCN:O7	2.12	0.50
1:D:1769:VAL:HB	1:D:1772:LEU:HD22	1.92	0.50
1:F:2531:THR:CG2	1:F:2601:LEU:HD23	2.40	0.50
1:A:196:LEU:HD21	1:B:529:VAL:HG11	1.94	0.50
1:A:212:LEU:N	1:A:213:PRO:HD2	2.27	0.50
1:B:552:VAL:HG22	1:B:583:ARG:HD2	1.93	0.50
1:B:584:VAL:CG2	1:B:588:GLU:HG2	2.38	0.50
1:B:729:THR:O	1:B:733:VAL:HG23	2.12	0.50
1:C:1176:VAL:HG13	1:C:1181:SER:C	2.37	0.50
1:C:1170:LEU:HD13	1:C:1172:LYS:HG3	1.94	0.50
1:D:1670:LEU:HD13	1:D:1672:LYS:HG3	1.94	0.50
1:E:2131:THR:HG23	1:E:2133:ALA:H	1.76	0.50
1:E:2179:ALA:HB1	1:E:2184:ASP:HB3	1.93	0.50
1:A:225:ALA:N	1:A:228:GLN:HE21	1.97	0.50
1:C:1229:THR:O	1:C:1233:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1679:ALA:HB1	1:D:1684:ASP:HB3	1.94	0.49
1:E:2176:VAL:HG22	1:E:2182:VAL:HA	1.94	0.49
1:C:1161:HIS:ND1	3:C:3177:HOH:O	2.33	0.49
1:B:661:HIS:CE1	2:B:2902:NCN:H4	2.47	0.49
1:C:1037:ALA:HA	1:C:1098:ARG:HD2	1.94	0.49
1:F:2676:VAL:HG13	1:F:2681:SER:C	2.37	0.49
1:A:132:LYS:HE2	1:A:263:GLY:O	2.12	0.49
1:C:1279:LEU:O	1:C:1281:ILE:HG13	2.13	0.49
1:C:1179:ALA:HB1	1:C:1184:ASP:HB3	1.95	0.49
1:D:1517:ARG:O	1:D:1521:GLU:HG3	2.13	0.49
1:E:2011:ALA:O	1:E:2015:ILE:HG23	2.12	0.49
1:E:2117:ILE:O	1:E:2121:THR:HG23	2.13	0.49
1:A:104:GLU:O	1:A:108:LEU:HD22	2.13	0.49
1:C:1142:LEU:H	1:C:1149:GLN:NE2	2.09	0.49
1:A:170:LEU:CD1	1:A:172:LYS:HG3	2.43	0.49
1:A:226:VAL:HG11	1:A:258:THR:HG22	1.95	0.49
1:A:170:LEU:HD13	1:A:172:LYS:HG3	1.94	0.48
1:E:2236:ARG:HD2	1:E:2236:ARG:C	2.38	0.48
1:B:605:ARG:O	1:B:605:ARG:HD3	2.13	0.48
1:F:2515:ILE:HD11	1:F:2565:GLU:CG	2.39	0.48
1:C:1226:VAL:HG11	1:C:1258:THR:HG22	1.95	0.48
1:E:2226:VAL:HG11	1:E:2258:THR:HG22	1.95	0.48
1:E:2047:THR:O	1:E:2086:PRO:O	2.32	0.48
1:E:2058:VAL:HG11	1:E:2110:LEU:HG	1.95	0.48
1:A:244:MET:HE2	1:A:244:MET:HA	1.95	0.48
1:D:1669:ALA:HB1	1:D:1689:VAL:HG11	1.95	0.48
1:F:2669:ALA:HB1	1:F:2689:VAL:HG11	1.96	0.48
1:F:2631:THR:CG2	1:F:2633:ALA:H	2.25	0.48
1:A:154:ARG:HH21	1:A:160:ASN:HD21	1.62	0.47
1:C:1154:ARG:HE	1:C:1160:ASN:ND2	2.12	0.47
2:C:2905:NCN:C4	3:C:3177:HOH:O	2.61	0.47
1:F:2686:LEU:O	1:F:2690:ARG:HG2	2.14	0.47
1:A:137:ASP:OD1	1:A:150:LYS:NZ	2.47	0.47
1:E:2186:LEU:O	1:E:2190:ARG:HG2	2.13	0.47
1:A:24:ARG:HD2	1:A:25:TYR:CZ	2.50	0.47
1:B:628:VAL:O	1:B:631:THR:HB	2.15	0.47
1:E:2100:LEU:HA	1:E:2100:LEU:HD23	1.72	0.47
1:F:2524:ARG:HD2	1:F:2525:TYR:CZ	2.50	0.47
1:C:1219:ILE:HB	1:C:1245:LEU:HD12	1.97	0.47
1:E:2031:THR:CG2	1:E:2101:LEU:HD23	2.44	0.47
1:B:556:LEU:HD23	1:B:578:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:718:LEU:CD1	1:B:720:LEU:HD12	2.45	0.47
1:C:1117:ILE:O	1:C:1121:THR:CG2	2.62	0.47
1:E:2164:GLY:N	1:E:2167:ASP:OD1	2.47	0.47
1:F:2687:ARG:NH2	1:F:2690:ARG:HE	2.12	0.47
1:B:687:ARG:CZ	1:B:690:ARG:HG3	2.45	0.47
1:A:46:VAL:CG2	1:A:48:ARG:HH21	2.28	0.47
1:A:129:ARG:HA	3:A:3088:HOH:O	2.13	0.47
1:E:2187:ARG:NH2	1:E:2190:ARG:HE	2.11	0.47
1:D:1564:ASN:OD1	1:D:1569:THR:HA	2.15	0.47
1:D:1671:ILE:HG23	1:D:1675:HIS:HB2	1.96	0.47
1:E:2142:LEU:H	1:E:2149:GLN:NE2	2.11	0.46
1:F:2642:LEU:H	1:F:2649:GLN:HE22	1.63	0.46
1:A:229:THR:O	1:A:233:VAL:HG23	2.15	0.46
1:C:1013:ALA:O	1:C:1017:ARG:HG3	2.15	0.46
1:C:1181:SER:H	1:C:1184:ASP:HB2	1.81	0.46
1:F:2617:ILE:O	1:F:2621:THR:CG2	2.62	0.46
1:A:29:VAL:HG11	1:B:696:LEU:CD2	2.45	0.46
1:E:2154:ARG:HE	1:E:2160:ASN:HD21	1.63	0.46
1:A:121:THR:O	1:A:125:VAL:HG23	2.16	0.46
1:D:1617:ILE:O	1:D:1621:THR:HG23	2.15	0.46
1:A:36:PRO:HG2	1:A:39:ALA:HB2	1.96	0.46
1:C:1031:THR:HG22	1:D:1675:HIS:HE1	1.80	0.46
1:D:1712:LEU:HD22	1:D:1740:ALA:HB3	1.97	0.46
1:E:2046:VAL:CG2	1:E:2048:ARG:HH21	2.28	0.46
1:C:1031:THR:CG2	1:C:1101:LEU:HD23	2.46	0.46
1:C:1060:LEU:HD12	1:C:1060:LEU:HA	1.81	0.46
1:C:1198:CYS:O	1:C:1217:GLU:HB2	2.16	0.46
1:B:670:LEU:HA	1:B:699:GLU:O	2.16	0.46
1:F:2768:ALA:HB1	2:F:2906:NCN:C5	2.46	0.46
1:F:2633:ALA:HA	1:F:2765:ASP:O	2.16	0.46
1:F:2768:ALA:CB	2:F:2906:NCN:H5	2.46	0.46
1:C:1128:VAL:HG23	1:C:1128:VAL:O	2.14	0.45
1:E:2017:ARG:O	1:E:2021:GLU:HG3	2.16	0.45
1:B:683:VAL:O	1:B:687:ARG:HG2	2.16	0.45
1:B:774:HIS:O	1:B:775:SER:C	2.59	0.45
1:E:2170:LEU:CD1	1:E:2172:LYS:HG3	2.45	0.45
1:C:1225:ALA:N	1:C:1228:GLN:HE21	2.04	0.45
1:E:2196:LEU:HD21	1:F:2529:VAL:HG11	1.96	0.45
1:F:2564:ASN:OD1	1:F:2569:THR:HA	2.16	0.45
1:E:2244:MET:HA	1:E:2244:MET:HE2	1.99	0.45
1:A:164:GLY:N	1:A:167:ASP:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ARG:CZ	1:A:190:ARG:HG3	2.47	0.45
1:B:621:THR:O	1:B:625:VAL:HG23	2.16	0.45
2:C:2905:NCN:C5	3:C:3177:HOH:O	2.64	0.45
1:F:2779:LEU:HD12	1:F:2779:LEU:HA	1.79	0.45
1:B:528:ASP:OD2	1:B:531:THR:HG23	2.17	0.45
1:B:547:THR:O	1:B:586:PRO:O	2.35	0.45
1:B:698:CYS:O	1:B:717:GLU:HB2	2.17	0.45
1:E:2117:ILE:O	1:E:2121:THR:CG2	2.65	0.45
1:E:2017:ARG:NH1	1:F:2517:ARG:HD3	2.31	0.44
1:E:2131:THR:CG2	1:E:2133:ALA:H	2.29	0.44
1:F:2726:VAL:HG11	1:F:2758:THR:HG22	1.99	0.44
1:A:107:MET:O	1:A:111:VAL:HG13	2.17	0.44
1:B:670:LEU:CD1	1:B:672:LYS:HG3	2.47	0.44
1:A:183:VAL:O	1:A:187:ARG:HG2	2.17	0.44
1:D:1687:ARG:CZ	1:D:1690:ARG:HG3	2.47	0.44
1:A:236:ARG:HD2	1:A:236:ARG:C	2.43	0.44
1:D:1687:ARG:NH2	1:D:1690:ARG:HE	2.15	0.44
1:A:154:ARG:HE	1:A:160:ASN:ND2	2.16	0.44
1:C:1164:GLY:N	1:C:1167:ASP:OD1	2.50	0.44
1:D:1686:LEU:O	1:D:1690:ARG:HG2	2.17	0.43
1:E:2015:ILE:HG13	1:E:2016:ALA:N	2.33	0.43
1:E:2029:VAL:HG21	1:F:2693:ALA:HB2	2.00	0.43
1:E:2187:ARG:HH21	1:E:2214:GLU:HB3	1.82	0.43
1:A:154:ARG:NH2	3:A:3224:HOH:O	2.50	0.43
1:B:645:LEU:O	1:B:646:ARG:C	2.60	0.43
1:D:1676:VAL:HG13	1:D:1681:SER:C	2.43	0.43
1:E:2010:ALA:HB1	3:E:3140:HOH:O	2.18	0.43
1:A:175:HIS:HE1	1:B:531:THR:CG2	2.31	0.43
1:B:642:LEU:H	1:B:649:GLN:NE2	2.15	0.43
1:E:2013:ALA:O	1:E:2017:ARG:HG3	2.17	0.43
1:F:2513:ALA:O	1:F:2517:ARG:HG3	2.17	0.43
1:A:77:ARG:HA	1:A:91:MET:HA	2.00	0.43
1:B:546:VAL:CG2	1:B:548:ARG:HH21	2.29	0.43
1:D:1648:LEU:O	1:D:1651:TYR:HB3	2.17	0.43
1:F:2670:LEU:HD23	1:F:2699:GLU:HB2	2.00	0.43
1:F:2777:ARG:HH11	1:F:2777:ARG:CG	2.31	0.43
1:C:1105:ARG:O	1:C:1105:ARG:HD3	2.17	0.43
1:D:1535:VAL:HG22	1:D:1598:ARG:HG3	2.00	0.43
1:F:2671:ILE:HG23	1:F:2675:HIS:HB2	2.00	0.43
1:B:726:VAL:HG21	1:B:758:THR:CG2	2.48	0.43
1:D:1649:GLN:O	1:D:1653:VAL:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1670:LEU:CD1	1:D:1672:LYS:HG3	2.48	0.43
1:E:2165:LEU:HG	1:F:2528:ASP:HB2	2.01	0.43
1:F:2639:ARG:NH2	3:F:3060:HOH:O	2.49	0.43
1:B:535:VAL:HA	1:B:536:PRO:HD2	1.79	0.43
1:B:726:VAL:HG21	1:B:758:THR:HG21	2.01	0.43
1:A:117:ILE:O	1:A:121:THR:CG2	2.66	0.43
1:B:631:THR:HG23	1:B:633:ALA:H	1.83	0.43
1:A:42:THR:HA	1:A:93:LEU:O	2.19	0.43
1:B:664:GLY:N	1:B:667:ASP:OD1	2.52	0.43
1:F:2604:GLU:HA	1:F:2607:MET:HE2	2.01	0.43
1:C:1031:THR:CG2	1:D:1675:HIS:HE1	2.31	0.43
1:D:1664:GLY:N	1:D:1667:ASP:OD1	2.51	0.43
1:E:2031:THR:HG22	1:F:2675:HIS:HE1	1.84	0.43
1:E:2212:LEU:N	1:E:2213:PRO:HD2	2.34	0.43
1:A:277:ARG:HH11	1:A:277:ARG:CG	2.32	0.42
1:B:752:SER:OG	1:B:754:GLN:HG2	2.19	0.42
1:D:1541:THR:O	1:D:1594:GLU:HA	2.19	0.42
1:E:2252:SER:OG	1:E:2254:GLN:HG2	2.18	0.42
1:B:600:LEU:HD23	1:B:600:LEU:HA	1.89	0.42
1:E:2017:ARG:HD3	1:F:2517:ARG:NH1	2.35	0.42
1:E:2104:GLU:O	1:E:2108:LEU:HD22	2.18	0.42
1:E:2196:LEU:HA	1:E:2197:PRO:HD3	1.87	0.42
1:F:2641:THR:HB	1:F:2649:GLN:NE2	2.33	0.42
1:F:2663:LEU:H	1:F:2667:ASP:CG	2.27	0.42
1:F:2683:VAL:HG13	1:F:2714:GLU:HG3	2.01	0.42
1:A:56:LEU:HD12	1:A:56:LEU:HA	1.84	0.42
1:B:511:ALA:O	1:B:515:ILE:HG23	2.19	0.42
1:E:2139:ARG:NH1	1:F:2522:ASP:OD2	2.52	0.42
1:A:25:TYR:CD1	1:A:25:TYR:N	2.88	0.42
1:A:25:TYR:HE1	3:B:3093:HOH:O	2.01	0.42
1:F:2636:ARG:CD	1:F:2659:VAL:HG22	2.50	0.42
1:A:142:LEU:H	1:A:149:GLN:NE2	2.17	0.42
1:A:172:LYS:O	1:A:176:VAL:HG23	2.19	0.42
1:C:1196:LEU:HA	1:C:1197:PRO:HD3	1.80	0.42
1:E:2015:ILE:HD12	1:E:2015:ILE:C	2.44	0.42
1:E:2031:THR:CG2	1:F:2675:HIS:HE1	2.32	0.42
1:F:2679:ALA:HB1	1:F:2684:ASP:HB3	2.02	0.42
1:B:736:ARG:HD2	1:B:736:ARG:C	2.45	0.41
1:C:1121:THR:O	1:C:1125:VAL:HG23	2.19	0.41
1:C:1142:LEU:HD13	1:C:1142:LEU:HA	1.88	0.41
1:E:2148:LEU:O	1:E:2151:TYR:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2508:LEU:HD12	1:F:2508:LEU:HA	1.95	0.41
1:C:1025:TYR:CD1	1:C:1025:TYR:N	2.88	0.41
1:C:1059:ALA:HA	1:C:1107:MET:HG3	2.02	0.41
1:C:1220:LEU:HD21	2:C:2905:NCN:C5	2.50	0.41
1:E:2181:SER:H	1:E:2184:ASP:HB2	1.85	0.41
1:F:2517:ARG:O	1:F:2521:GLU:HG3	2.19	0.41
1:F:2736:ARG:HD2	1:F:2736:ARG:C	2.45	0.41
1:D:1676:VAL:CG2	1:D:1682:VAL:HG13	2.51	0.41
1:F:2729:THR:O	1:F:2733:VAL:HG23	2.20	0.41
1:C:1108:LEU:HD12	1:C:1108:LEU:HA	1.93	0.41
1:C:1137:ASP:OD1	1:C:1150:LYS:NZ	2.53	0.41
1:B:517:ARG:O	1:B:521:GLU:HG3	2.20	0.41
1:E:2105:ARG:HD3	1:E:2109:ASN:OD1	2.20	0.41
1:E:2176:VAL:HG13	1:E:2181:SER:C	2.45	0.41
1:F:2515:ILE:HD12	1:F:2515:ILE:C	2.46	0.41
1:C:1181:SER:O	1:C:1184:ASP:HB2	2.20	0.41
1:D:1552:VAL:HG22	1:D:1583:ARG:HD2	2.01	0.41
1:B:601:LEU:HD12	1:B:601:LEU:HA	1.86	0.41
1:B:686:LEU:HD13	1:B:714:GLU:CB	2.50	0.41
1:A:60:LEU:HD12	1:A:60:LEU:HA	1.92	0.41
1:C:1170:LEU:CD1	1:C:1172:LYS:HG3	2.51	0.41
1:D:1515:ILE:HD11	1:D:1565:GLU:CG	2.45	0.41
1:B:558:VAL:HG11	1:B:610:LEU:HG	2.03	0.41
1:B:621:THR:HG22	1:B:772:LEU:HG	2.03	0.41
1:C:1134:LYS:HD2	1:C:1266:TYR:HE1	1.86	0.41
1:D:1672:LYS:N	1:D:1675:HIS:HD2	2.13	0.41
1:E:2131:THR:CG2	1:E:2260:ALA:HB1	2.36	0.41
1:A:230:GLN:HB3	1:C:1087:GLY:HA3	2.02	0.41
1:C:1031:THR:HG22	1:D:1675:HIS:CE1	2.56	0.41
1:E:2008:LEU:HD12	1:E:2008:LEU:HA	1.89	0.41
1:F:2648:LEU:O	1:F:2651:TYR:HB3	2.20	0.41
1:F:2740:ALA:N	1:F:2741:PRO:HD3	2.36	0.40
1:B:681:SER:H	1:B:684:ASP:HB2	1.85	0.40
1:D:1631:THR:CG2	1:D:1633:ALA:H	2.34	0.40
1:F:2645:LEU:O	1:F:2646:ARG:C	2.61	0.40
1:A:187:ARG:NH2	1:A:190:ARG:HE	2.17	0.40
1:B:524:ARG:HH11	1:B:524:ARG:HG3	1.86	0.40
1:C:1169:ALA:HB1	1:C:1189:VAL:HG11	2.02	0.40
1:A:196:LEU:HA	1:A:197:PRO:HD3	1.81	0.40
1:A:250:GLY:N	3:A:3051:HOH:O	2.50	0.40
1:B:637:ASP:OD2	1:B:653:VAL:HG21	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1100:LEU:HD23	1:C:1100:LEU:HA	1.73	0.40
1:D:1531:THR:HG21	1:D:1601:LEU:HB3	2.03	0.40
1:F:2515:ILE:HD11	1:F:2565:GLU:CB	2.50	0.40
1:F:2718:LEU:HD23	1:F:2744:MET:HB2	2.03	0.40
1:A:104:GLU:HA	1:A:107:MET:HE2	2.03	0.40
1:B:696:LEU:HD12	1:B:696:LEU:HA	1.90	0.40
1:C:1128:VAL:O	1:C:1131:THR:HB	2.22	0.40
1:E:2042:THR:HA	1:E:2093:LEU:O	2.21	0.40
1:E:2198:CYS:O	1:E:2217:GLU:HB2	2.21	0.40
1:F:2550:ALA:HB2	1:F:2586:PRO:HD3	2.02	0.40
1:F:2605:ARG:O	1:F:2605:ARG:HD3	2.21	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	282/284 (99%)	274 (97%)	6 (2%)	2 (1%)	18	38
1	B	282/284 (99%)	273 (97%)	8 (3%)	1 (0%)	30	51
1	C	282/284 (99%)	272 (96%)	8 (3%)	2 (1%)	18	38
1	D	282/284 (99%)	273 (97%)	8 (3%)	1 (0%)	30	51
1	E	282/284 (99%)	273 (97%)	7 (2%)	2 (1%)	18	38
1	F	282/284 (99%)	273 (97%)	8 (3%)	1 (0%)	30	51
All	All	1692/1704 (99%)	1638 (97%)	45 (3%)	9 (0%)	24	46

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	586	PRO

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Mol	Chain	Res	Type
1	A	86	PRO
1	C	1086	PRO
1	D	1586	PRO
1	F	2586	PRO
1	E	2086	PRO
1	E	2104	GLU
1	A	104	GLU
1	C	1104	GLU

5.3.2 Protein sidechains [i](#)

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	216/216 (100%)	172 (80%)	44 (20%)	1	2
1	B	216/216 (100%)	175 (81%)	41 (19%)	1	2
1	C	216/216 (100%)	171 (79%)	45 (21%)	1	2
1	D	216/216 (100%)	171 (79%)	45 (21%)	1	2
1	E	216/216 (100%)	172 (80%)	44 (20%)	1	2
1	F	216/216 (100%)	173 (80%)	43 (20%)	1	2
All	All	1296/1296 (100%)	1034 (80%)	262 (20%)	1	2

All (262) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
1	A	15	ILE
1	A	29	VAL
1	A	30	THR
1	A	32	LEU
1	A	35	VAL
1	A	40	THR
1	A	41	THR
1	A	46	VAL
1	A	47	THR

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Mol	Chain	Res	Type
1	A	48	ARG
1	A	56	LEU
1	A	60	LEU
1	A	63	LEU
1	A	75	LEU
1	A	78	VAL
1	A	84	VAL
1	A	86	PRO
1	A	93	LEU
1	A	101	LEU
1	A	108	LEU
1	A	110	LEU
1	A	111	VAL
1	A	121	THR
1	A	131	THR
1	A	134	LYS
1	A	142	LEU
1	A	153	VAL
1	A	159	VAL
1	A	165	LEU
1	A	167	ASP
1	A	173	ASP
1	A	182	VAL
1	A	186	LEU
1	A	200	VAL
1	A	220	LEU
1	A	242	THR
1	A	245	LEU
1	A	248	SER
1	A	251	LEU
1	A	254	GLN
1	A	272	LEU
1	A	276	VAL
1	A	277	ARG
1	B	505	ASP
1	B	515	ILE
1	B	529	VAL
1	B	535	VAL
1	B	540	THR
1	B	541	THR
1	B	546	VAL
1	B	547	THR

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Mol	Chain	Res	Type
1	B	548	ARG
1	B	556	LEU
1	B	560	LEU
1	B	563	LEU
1	B	578	VAL
1	B	584	VAL
1	B	586	PRO
1	B	593	LEU
1	B	601	LEU
1	B	608	LEU
1	B	610	LEU
1	B	611	VAL
1	B	621	THR
1	B	631	THR
1	B	634	LYS
1	B	642	LEU
1	B	653	VAL
1	B	659	VAL
1	B	665	LEU
1	B	667	ASP
1	B	670	LEU
1	B	673	ASP
1	B	674	ASN
1	B	682	VAL
1	B	686	LEU
1	B	700	VAL
1	B	720	LEU
1	B	745	LEU
1	B	751	LEU
1	B	754	GLN
1	B	772	LEU
1	B	776	VAL
1	B	777	ARG
1	C	1005	ASP
1	C	1015	ILE
1	C	1022	ASP
1	C	1029	VAL
1	C	1032	LEU
1	C	1035	VAL
1	C	1040	THR
1	C	1041	THR
1	C	1046	VAL

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Mol	Chain	Res	Type
1	C	1047	THR
1	C	1048	ARG
1	C	1056	LEU
1	C	1060	LEU
1	C	1063	LEU
1	C	1075	LEU
1	C	1078	VAL
1	C	1084	VAL
1	C	1086	PRO
1	C	1093	LEU
1	C	1101	LEU
1	C	1108	LEU
1	C	1110	LEU
1	C	1111	VAL
1	C	1121	THR
1	C	1131	THR
1	C	1134	LYS
1	C	1142	LEU
1	C	1153	VAL
1	C	1159	VAL
1	C	1165	LEU
1	C	1167	ASP
1	C	1170	LEU
1	C	1173	ASP
1	C	1174	ASN
1	C	1182	VAL
1	C	1186	LEU
1	C	1200	VAL
1	C	1218	LEU
1	C	1220	LEU
1	C	1244	MET
1	C	1245	LEU
1	C	1251	LEU
1	C	1254	GLN
1	C	1272	LEU
1	C	1276	VAL
1	D	1505	ASP
1	D	1515	ILE
1	D	1529	VAL
1	D	1530	THR
1	D	1532	LEU
1	D	1535	VAL

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Mol	Chain	Res	Type
1	D	1540	THR
1	D	1541	THR
1	D	1546	VAL
1	D	1547	THR
1	D	1548	ARG
1	D	1556	LEU
1	D	1560	LEU
1	D	1563	LEU
1	D	1575	LEU
1	D	1578	VAL
1	D	1584	VAL
1	D	1586	PRO
1	D	1593	LEU
1	D	1601	LEU
1	D	1608	LEU
1	D	1610	LEU
1	D	1611	VAL
1	D	1621	THR
1	D	1631	THR
1	D	1634	LYS
1	D	1642	LEU
1	D	1653	VAL
1	D	1659	VAL
1	D	1665	LEU
1	D	1667	ASP
1	D	1673	ASP
1	D	1674	ASN
1	D	1682	VAL
1	D	1686	LEU
1	D	1700	VAL
1	D	1720	LEU
1	D	1742	THR
1	D	1744	MET
1	D	1745	LEU
1	D	1748	SER
1	D	1751	LEU
1	D	1754	GLN
1	D	1772	LEU
1	D	1776	VAL
1	E	2005	ASP
1	E	2015	ILE
1	E	2029	VAL

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Mol	Chain	Res	Type
1	E	2032	LEU
1	E	2035	VAL
1	E	2040	THR
1	E	2041	THR
1	E	2046	VAL
1	E	2047	THR
1	E	2048	ARG
1	E	2056	LEU
1	E	2060	LEU
1	E	2063	LEU
1	E	2075	LEU
1	E	2078	VAL
1	E	2084	VAL
1	E	2086	PRO
1	E	2093	LEU
1	E	2101	LEU
1	E	2108	LEU
1	E	2110	LEU
1	E	2111	VAL
1	E	2121	THR
1	E	2131	THR
1	E	2134	LYS
1	E	2142	LEU
1	E	2153	VAL
1	E	2159	VAL
1	E	2165	LEU
1	E	2167	ASP
1	E	2173	ASP
1	E	2174	ASN
1	E	2182	VAL
1	E	2186	LEU
1	E	2200	VAL
1	E	2218	LEU
1	E	2220	LEU
1	E	2242	THR
1	E	2244	MET
1	E	2245	LEU
1	E	2251	LEU
1	E	2254	GLN
1	E	2272	LEU
1	E	2276	VAL
1	F	2505	ASP

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Mol	Chain	Res	Type
1	F	2515	ILE
1	F	2529	VAL
1	F	2532	LEU
1	F	2535	VAL
1	F	2540	THR
1	F	2541	THR
1	F	2546	VAL
1	F	2547	THR
1	F	2548	ARG
1	F	2556	LEU
1	F	2560	LEU
1	F	2563	LEU
1	F	2578	VAL
1	F	2584	VAL
1	F	2586	PRO
1	F	2593	LEU
1	F	2601	LEU
1	F	2608	LEU
1	F	2610	LEU
1	F	2611	VAL
1	F	2621	THR
1	F	2631	THR
1	F	2634	LYS
1	F	2642	LEU
1	F	2653	VAL
1	F	2659	VAL
1	F	2665	LEU
1	F	2667	ASP
1	F	2673	ASP
1	F	2674	ASN
1	F	2682	VAL
1	F	2686	LEU
1	F	2700	VAL
1	F	2720	LEU
1	F	2742	THR
1	F	2744	MET
1	F	2745	LEU
1	F	2748	SER
1	F	2751	LEU
1	F	2754	GLN
1	F	2772	LEU
1	F	2776	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	160	ASN
1	A	175	HIS
1	A	228	GLN
1	B	649	GLN
1	B	675	HIS
1	B	728	GLN
1	C	1149	GLN
1	C	1160	ASN
1	C	1174	ASN
1	C	1175	HIS
1	C	1228	GLN
1	D	1649	GLN
1	D	1660	ASN
1	D	1675	HIS
1	D	1728	GLN
1	E	2149	GLN
1	E	2160	ASN
1	E	2175	HIS
1	E	2228	GLN
1	F	2649	GLN
1	F	2660	ASN
1	F	2675	HIS
1	F	2728	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

6 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	NCN	B	2902	-	21,23,23	3.68	12 (57%)	27,34,34	2.07	8 (29%)
2	NCN	E	2903	-	21,23,23	3.32	10 (47%)	27,34,34	2.17	8 (29%)
2	NCN	C	2905	-	21,23,23	3.38	11 (52%)	27,34,34	2.08	9 (33%)
2	NCN	F	2906	-	21,23,23	3.47	9 (42%)	27,34,34	2.06	8 (29%)
2	NCN	D	2904	-	21,23,23	3.65	14 (66%)	27,34,34	2.00	7 (25%)
2	NCN	A	2901	-	21,23,23	3.64	12 (57%)	27,34,34	2.04	7 (25%)

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	NCN	B	2902	-	-	6/14/30/30	0/2/2/2
2	NCN	E	2903	-	-	8/14/30/30	0/2/2/2
2	NCN	C	2905	-	-	8/14/30/30	0/2/2/2
2	NCN	F	2906	-	-	8/14/30/30	0/2/2/2
2	NCN	D	2904	-	-	8/14/30/30	0/2/2/2
2	NCN	A	2901	-	-	7/14/30/30	0/2/2/2

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2904	NCN	O4'-C1'	10.29	1.54	1.40
2	B	2902	NCN	O4'-C1'	10.25	1.54	1.40
2	A	2901	NCN	O4'-C1'	9.57	1.53	1.40
2	F	2906	NCN	O4'-C1'	9.45	1.53	1.40
2	E	2903	NCN	O4'-C1'	9.41	1.53	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2905	NCN	O4'-C1'	9.28	1.53	1.40
2	B	2902	NCN	C2-N1	9.08	1.45	1.35
2	A	2901	NCN	C2-N1	8.96	1.44	1.35
2	F	2906	NCN	C2-N1	8.71	1.44	1.35
2	C	2905	NCN	C2-N1	8.26	1.44	1.35
2	D	2904	NCN	C2-N1	8.20	1.44	1.35
2	E	2903	NCN	C2-N1	7.93	1.43	1.35
2	F	2906	NCN	C6-N1	4.71	1.46	1.35
2	A	2901	NCN	C6-N1	4.48	1.45	1.35
2	B	2902	NCN	C6-N1	4.46	1.45	1.35
2	D	2904	NCN	C6-N1	4.29	1.45	1.35
2	E	2903	NCN	C6-N1	3.83	1.44	1.35
2	D	2904	NCN	P-O5'	3.81	1.72	1.60
2	C	2905	NCN	C6-N1	3.76	1.43	1.35
2	B	2902	NCN	O3'-C3'	3.51	1.51	1.43
2	A	2901	NCN	O3'-C3'	3.41	1.51	1.43
2	C	2905	NCN	O3'-C3'	3.41	1.51	1.43
2	F	2906	NCN	O3'-C3'	3.34	1.51	1.43
2	B	2902	NCN	C3-C7	3.31	1.56	1.49
2	E	2903	NCN	P-O5'	3.29	1.70	1.60
2	D	2904	NCN	C3'-C4'	3.28	1.61	1.53
2	E	2903	NCN	O3'-C3'	3.22	1.50	1.43
2	A	2901	NCN	C3'-C4'	3.16	1.61	1.53
2	A	2901	NCN	O8-C7	3.14	1.31	1.22
2	C	2905	NCN	O8-C7	3.13	1.31	1.22
2	E	2903	NCN	O2'-C2'	3.12	1.50	1.43
2	C	2905	NCN	P-O5'	3.10	1.70	1.60
2	E	2903	NCN	C3'-C4'	3.10	1.60	1.53
2	C	2905	NCN	P-O2P	3.06	1.60	1.50
2	A	2901	NCN	O2'-C2'	3.04	1.50	1.43
2	B	2902	NCN	C3'-C4'	3.03	1.60	1.53
2	D	2904	NCN	C6-C5	3.02	1.44	1.38
2	F	2906	NCN	C3'-C4'	2.98	1.60	1.53
2	B	2902	NCN	O2'-C2'	2.97	1.50	1.43
2	A	2901	NCN	P-O5'	2.90	1.69	1.60
2	A	2901	NCN	C4-C3	2.89	1.43	1.39
2	A	2901	NCN	C6-C5	2.88	1.44	1.38
2	F	2906	NCN	P-O5'	2.83	1.69	1.60
2	D	2904	NCN	O3'-C3'	2.83	1.50	1.43
2	C	2905	NCN	O2'-C2'	2.82	1.49	1.43
2	D	2904	NCN	P-O2P	2.79	1.59	1.50
2	A	2901	NCN	C3-C7	2.78	1.55	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2904	NCN	O8-C7	2.76	1.30	1.22
2	C	2905	NCN	C3'-C4'	2.76	1.60	1.53
2	F	2906	NCN	C5'-C4'	2.66	1.59	1.51
2	F	2906	NCN	O2'-C2'	2.63	1.49	1.43
2	D	2904	NCN	O2'-C2'	2.60	1.49	1.43
2	E	2903	NCN	C6-C5	2.58	1.44	1.38
2	F	2906	NCN	O8-C7	2.57	1.30	1.22
2	B	2902	NCN	P-O5'	2.56	1.68	1.60
2	E	2903	NCN	O8-C7	2.50	1.30	1.22
2	D	2904	NCN	C5'-C4'	2.49	1.59	1.51
2	B	2902	NCN	C4-C3	2.41	1.43	1.39
2	B	2902	NCN	O8-C7	2.38	1.29	1.22
2	B	2902	NCN	C6-C5	2.37	1.43	1.38
2	B	2902	NCN	P-O2P	2.32	1.57	1.50
2	D	2904	NCN	C4-C3	2.30	1.42	1.39
2	E	2903	NCN	C5'-C4'	2.29	1.58	1.51
2	D	2904	NCN	C2-C3	2.21	1.42	1.39
2	D	2904	NCN	C3-C7	2.20	1.54	1.49
2	A	2901	NCN	C5'-C4'	2.08	1.57	1.51
2	C	2905	NCN	C5'-C4'	2.04	1.57	1.51
2	C	2905	NCN	C3-C7	2.02	1.53	1.49

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2903	NCN	C4'-O4'-C1'	-5.76	104.65	109.92
2	E	2903	NCN	C6-N1-C2	-5.26	117.40	121.88
2	B	2902	NCN	C4'-O4'-C1'	-5.14	105.22	109.92
2	D	2904	NCN	C4'-O4'-C1'	-5.00	105.35	109.92
2	A	2901	NCN	C4'-O4'-C1'	-4.85	105.49	109.92
2	C	2905	NCN	C4'-O4'-C1'	-4.68	105.64	109.92
2	C	2905	NCN	C6-N1-C2	-4.59	117.97	121.88
2	B	2902	NCN	C6-N1-C2	-4.52	118.03	121.88
2	A	2901	NCN	C6-N1-C2	-4.49	118.06	121.88
2	F	2906	NCN	C6-N1-C2	-4.46	118.08	121.88
2	F	2906	NCN	C4'-O4'-C1'	-4.44	105.86	109.92
2	D	2904	NCN	C6-N1-C2	-4.35	118.18	121.88
2	C	2905	NCN	C2-C3-C7	4.29	127.14	119.78
2	B	2902	NCN	C2-C3-C7	4.19	126.97	119.78
2	F	2906	NCN	C2-C3-C7	3.98	126.61	119.78
2	F	2906	NCN	C5-C4-C3	3.73	124.03	120.36
2	A	2901	NCN	C2-C3-C7	3.70	126.13	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2903	NCN	C2-C3-C7	3.68	126.10	119.78
2	D	2904	NCN	C2-C3-C7	3.61	125.97	119.78
2	E	2903	NCN	O3'-C3'-C4'	3.35	120.69	111.08
2	F	2906	NCN	O5'-C5'-C4'	3.12	119.61	108.99
2	A	2901	NCN	O5'-C5'-C4'	3.08	119.49	108.99
2	B	2902	NCN	C5-C4-C3	3.08	123.39	120.36
2	A	2901	NCN	O3'-C3'-C4'	3.08	119.92	111.08
2	D	2904	NCN	O3'-C3'-C4'	3.04	119.82	111.08
2	C	2905	NCN	O3'-C3'-C4'	3.03	119.78	111.08
2	D	2904	NCN	O5'-C5'-C4'	2.98	119.13	108.99
2	C	2905	NCN	C4-C3-C7	-2.94	114.56	120.37
2	F	2906	NCN	O3'-C3'-C4'	2.93	119.50	111.08
2	B	2902	NCN	O3'-C3'-C4'	2.82	119.18	111.08
2	B	2902	NCN	O5'-C5'-C4'	2.78	118.44	108.99
2	A	2901	NCN	C5-C4-C3	2.75	123.07	120.36
2	F	2906	NCN	C4-C3-C7	-2.75	114.93	120.37
2	E	2903	NCN	O5'-C5'-C4'	2.70	118.19	108.99
2	D	2904	NCN	C5-C4-C3	2.63	122.95	120.36
2	C	2905	NCN	O5'-C5'-C4'	2.63	117.94	108.99
2	D	2904	NCN	C4-C3-C7	-2.49	115.44	120.37
2	B	2902	NCN	C4-C3-C7	-2.45	115.53	120.37
2	C	2905	NCN	C2-N1-C1'	2.44	124.52	119.13
2	C	2905	NCN	C5-C4-C3	2.44	122.76	120.36
2	E	2903	NCN	C5-C4-C3	2.43	122.76	120.36
2	E	2903	NCN	C4-C3-C7	-2.41	115.61	120.37
2	A	2901	NCN	C4-C3-C7	-2.36	115.71	120.37
2	E	2903	NCN	C2-N1-C1'	2.28	124.18	119.13
2	F	2906	NCN	C2-N1-C1'	2.17	123.92	119.13
2	C	2905	NCN	O8-C7-C3	-2.10	115.97	121.46
2	B	2902	NCN	C2-N1-C1'	2.09	123.74	119.13

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2905	NCN	C5'-O5'-P-O1P
2	D	2904	NCN	C5'-O5'-P-O1P
2	E	2903	NCN	C5'-O5'-P-O1P
2	F	2906	NCN	C5'-O5'-P-O1P
2	F	2906	NCN	C5'-O5'-P-O3P
2	B	2902	NCN	C4'-C5'-O5'-P
2	A	2901	NCN	C4-C3-C7-O7

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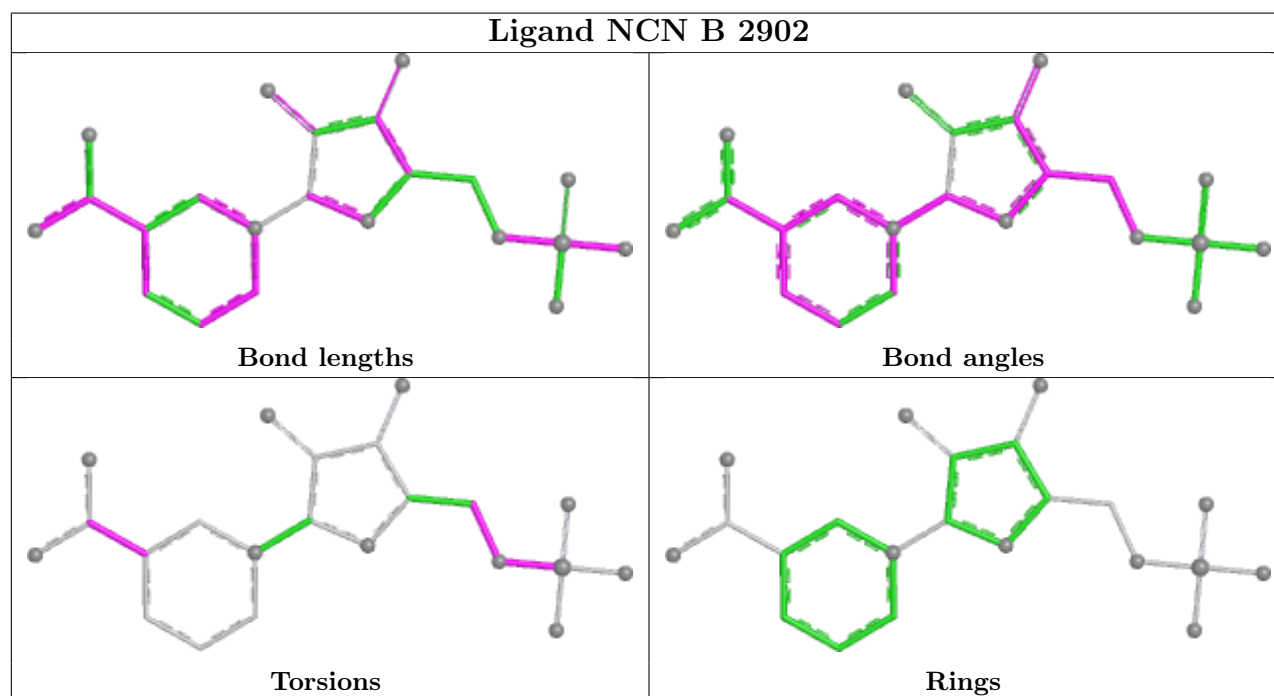
Mol	Chain	Res	Type	Atoms
2	C	2905	NCN	C4-C3-C7-O7
2	C	2905	NCN	C4-C3-C7-O8
2	A	2901	NCN	C4-C3-C7-O8
2	C	2905	NCN	C2-C3-C7-O7
2	E	2903	NCN	C4-C3-C7-O7
2	A	2901	NCN	C2-C3-C7-O7
2	E	2903	NCN	C4-C3-C7-O8
2	F	2906	NCN	C4-C3-C7-O7
2	B	2902	NCN	C4-C3-C7-O7
2	C	2905	NCN	C2-C3-C7-O8
2	F	2906	NCN	C4-C3-C7-O8
2	A	2901	NCN	C4'-C5'-O5'-P
2	D	2904	NCN	C4-C3-C7-O7
2	A	2901	NCN	C2-C3-C7-O8
2	E	2903	NCN	C2-C3-C7-O7
2	E	2903	NCN	C2-C3-C7-O8
2	F	2906	NCN	C4'-C5'-O5'-P
2	B	2902	NCN	C4-C3-C7-O8
2	E	2903	NCN	C5'-O5'-P-O2P
2	F	2906	NCN	C5'-O5'-P-O2P
2	C	2905	NCN	C4'-C5'-O5'-P
2	D	2904	NCN	C4'-C5'-O5'-P
2	E	2903	NCN	C4'-C5'-O5'-P
2	D	2904	NCN	C4-C3-C7-O8
2	D	2904	NCN	C2-C3-C7-O7
2	F	2906	NCN	C2-C3-C7-O7
2	F	2906	NCN	C2-C3-C7-O8
2	C	2905	NCN	C5'-O5'-P-O3P
2	D	2904	NCN	C5'-O5'-P-O3P
2	E	2903	NCN	C5'-O5'-P-O3P
2	B	2902	NCN	C2-C3-C7-O7
2	B	2902	NCN	C2-C3-C7-O8
2	D	2904	NCN	C2-C3-C7-O8
2	A	2901	NCN	C5'-O5'-P-O2P
2	C	2905	NCN	C5'-O5'-P-O2P
2	D	2904	NCN	C5'-O5'-P-O2P
2	A	2901	NCN	C5'-O5'-P-O3P
2	B	2902	NCN	C5'-O5'-P-O3P

There are no ring outliers.

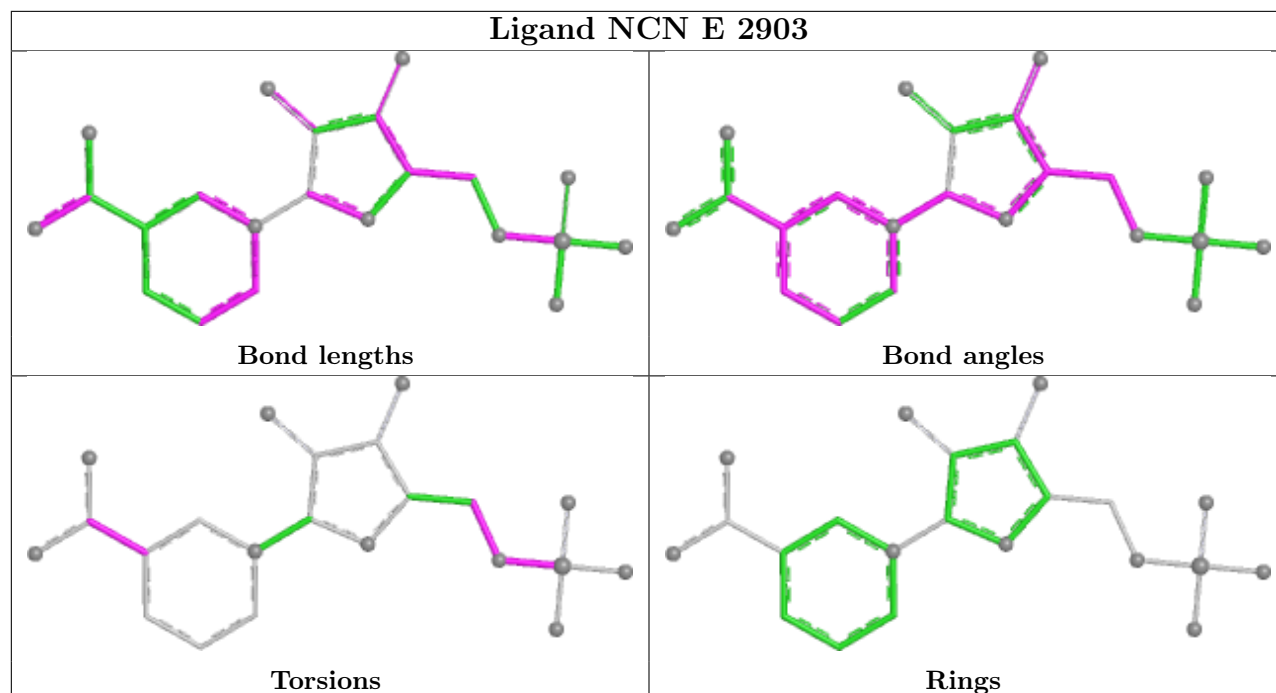
6 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2902	NCN	6	0
2	E	2903	NCN	5	0
2	C	2905	NCN	8	0
2	F	2906	NCN	7	0
2	D	2904	NCN	6	0
2	A	2901	NCN	5	0

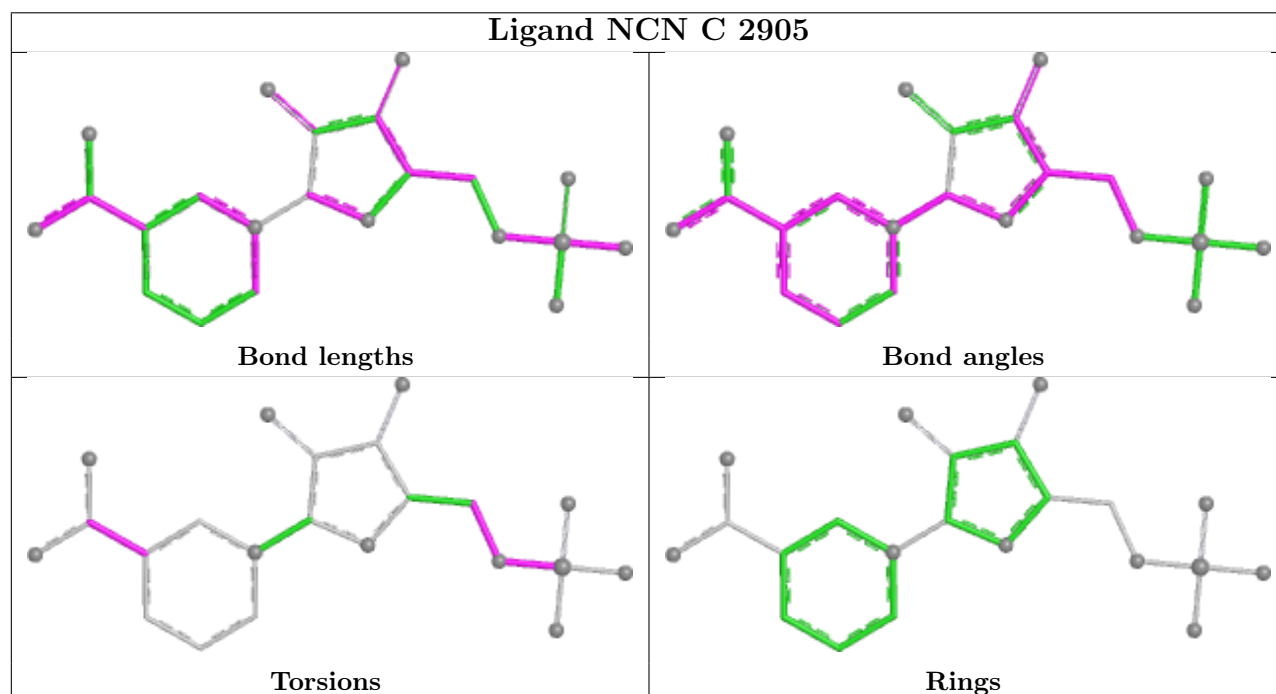
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



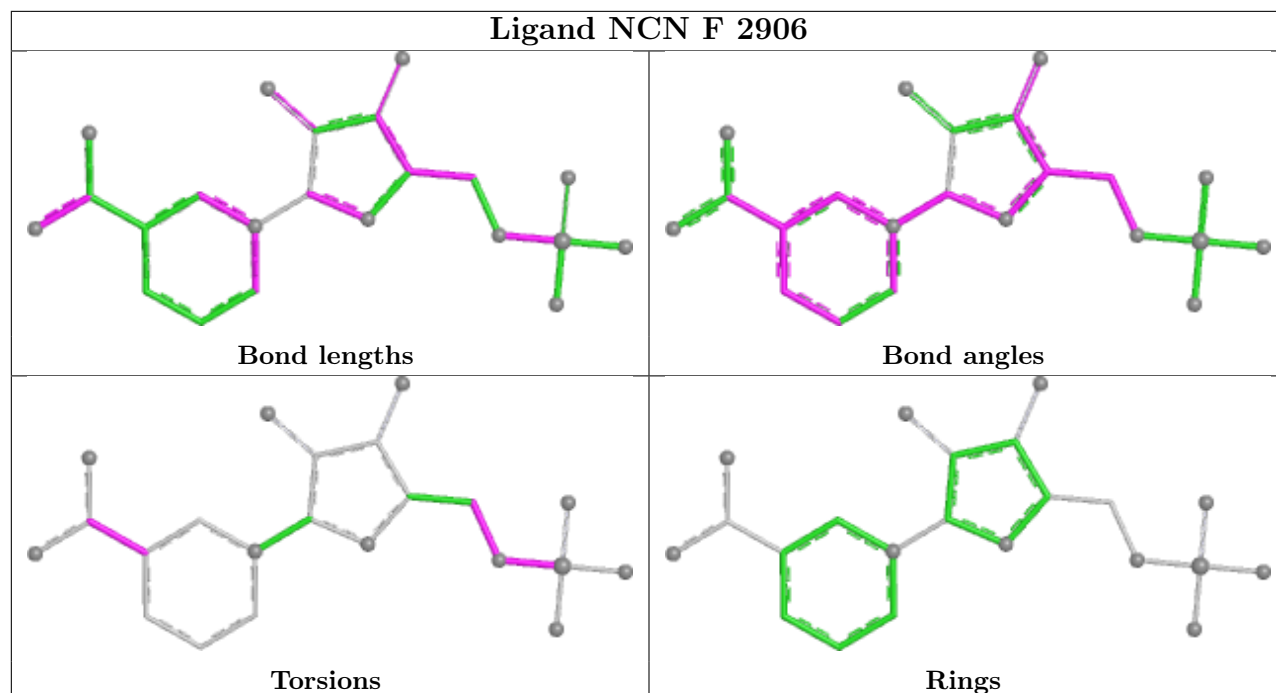
Ligand NCN E 2903



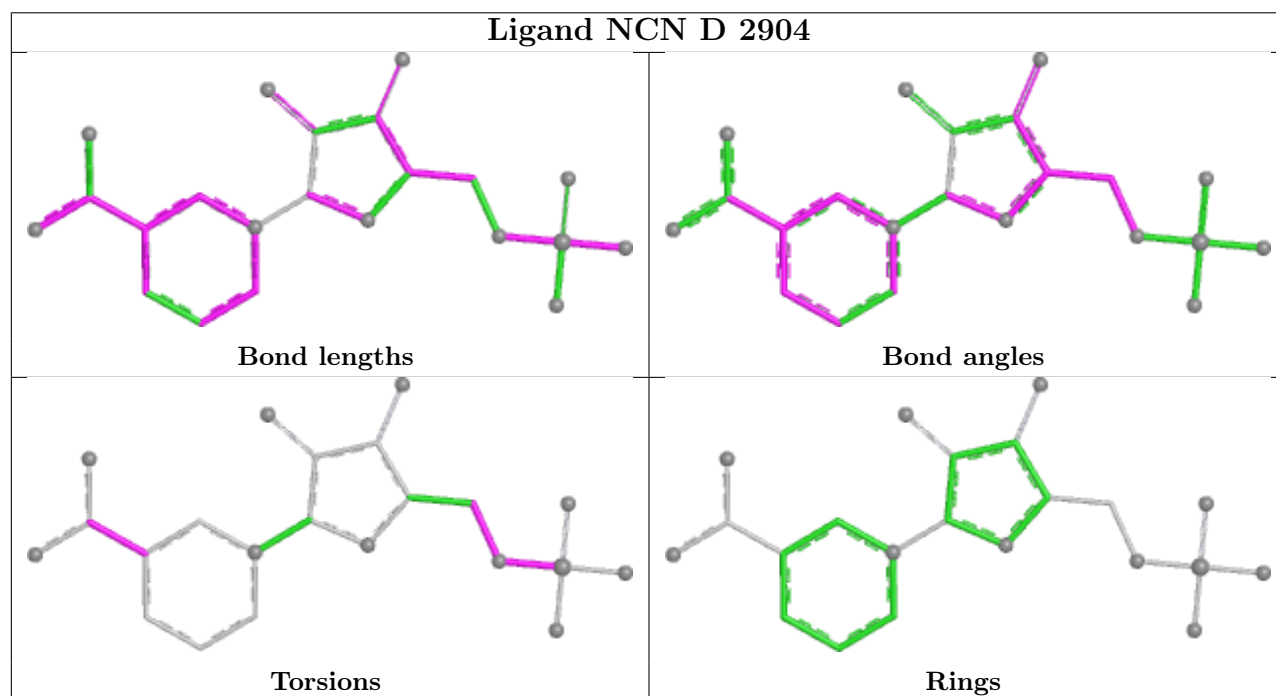
Ligand NCN C 2905

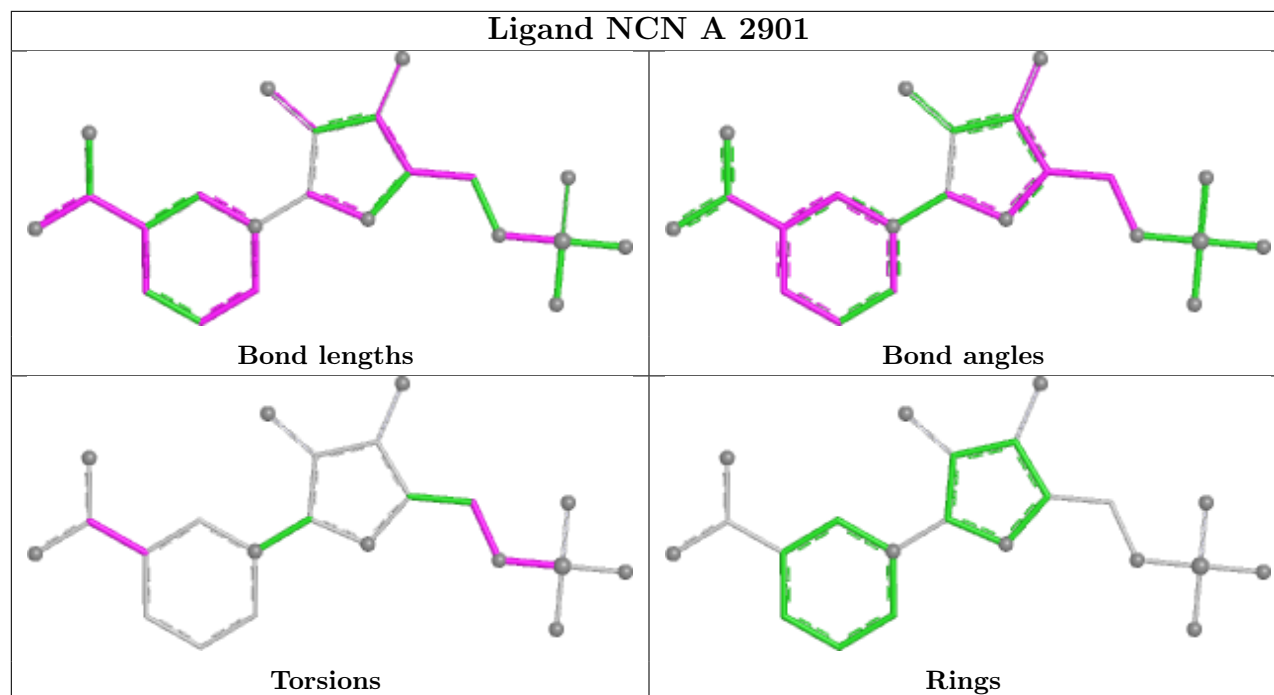


Ligand NCN F 2906



Ligand NCN D 2904





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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.