



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:34 AM UTC

PDB ID : 1NXK / pdb_00001nxk
Title : Crystal structure of staurosporine bound to MAP KAP kinase 2
Authors : Underwood, K.W.; Parris, K.D.; Federico, E.; Mosyak, L.; Czerwinski, R.M.; Shane, T.; Taylor, M.; Svenson, K.; Liu, Y.; Hsiao, C.L.; Wolfrom, S.; Malakian, K.; Telliez, J.B.; Lin, L.L.; Kriz, R.W.; Seehra, J.; Somers, W.S.; Stahl, M.L.
Deposited on : 2003-02-10
Resolution : 2.70 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

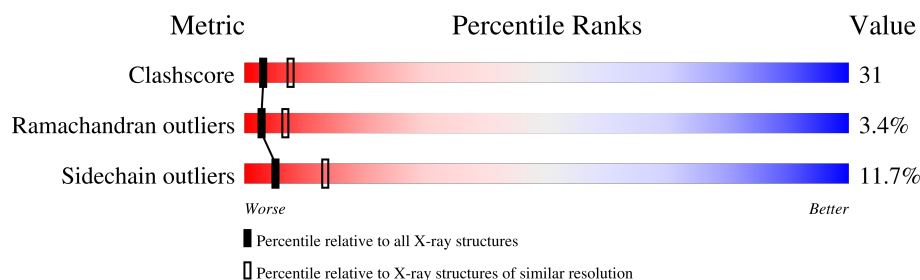
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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	400	33% 30% 8% 28%
1	B	400	30% 32% 8% 29%
1	C	400	30% 38% 8% 24%
1	D	400	34% 31% 8% 28%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9405 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 MAP kinase-activated protein kinase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	Se	0	0	0
			2289	1471	388	413	6	11			
1	B	283	Total	C	N	O	S	Se	0	0	0
			2234	1425	382	410	6	11			
1	C	306	Total	C	N	O	S	Se	0	0	0
			2438	1557	421	442	6	12			
1	D	288	Total	C	N	O	S	Se	0	0	0
			2252	1452	373	410	6	11			

There are 48 discrepancies between the modelled and reference sequences:

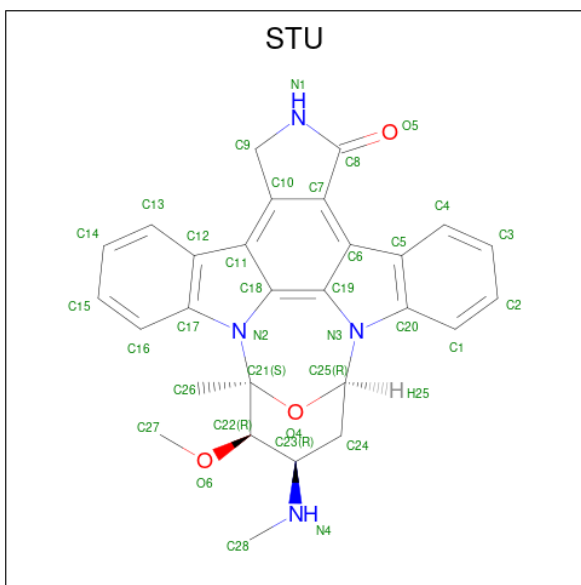
Chain	Residue	Modelled	Actual	Comment	Reference
A	94	MSE	MET	modified residue	UNP P49137
A	138	MSE	MET	modified residue	UNP P49137
A	167	MSE	MET	modified residue	UNP P49137
A	246	MSE	MET	modified residue	UNP P49137
A	253	MSE	MET	modified residue	UNP P49137
A	275	MSE	MET	modified residue	UNP P49137
A	281	MSE	MET	modified residue	UNP P49137
A	300	MSE	MET	modified residue	UNP P49137
A	314	MSE	MET	modified residue	UNP P49137
A	320	MSE	MET	modified residue	UNP P49137
A	326	MSE	MET	modified residue	UNP P49137
A	356	MSE	MET	modified residue	UNP P49137
B	94	MSE	MET	modified residue	UNP P49137
B	138	MSE	MET	modified residue	UNP P49137
B	167	MSE	MET	modified residue	UNP P49137
B	246	MSE	MET	modified residue	UNP P49137
B	253	MSE	MET	modified residue	UNP P49137
B	275	MSE	MET	modified residue	UNP P49137
B	281	MSE	MET	modified residue	UNP P49137
B	300	MSE	MET	modified residue	UNP P49137
B	314	MSE	MET	modified residue	UNP P49137

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Chain	Residue	Modelled	Actual	Comment	Reference
B	320	MSE	MET	modified residue	UNP P49137
B	326	MSE	MET	modified residue	UNP P49137
B	356	MSE	MET	modified residue	UNP P49137
C	94	MSE	MET	modified residue	UNP P49137
C	138	MSE	MET	modified residue	UNP P49137
C	167	MSE	MET	modified residue	UNP P49137
C	246	MSE	MET	modified residue	UNP P49137
C	253	MSE	MET	modified residue	UNP P49137
C	275	MSE	MET	modified residue	UNP P49137
C	281	MSE	MET	modified residue	UNP P49137
C	300	MSE	MET	modified residue	UNP P49137
C	314	MSE	MET	modified residue	UNP P49137
C	320	MSE	MET	modified residue	UNP P49137
C	326	MSE	MET	modified residue	UNP P49137
C	356	MSE	MET	modified residue	UNP P49137
D	94	MSE	MET	modified residue	UNP P49137
D	138	MSE	MET	modified residue	UNP P49137
D	167	MSE	MET	modified residue	UNP P49137
D	246	MSE	MET	modified residue	UNP P49137
D	253	MSE	MET	modified residue	UNP P49137
D	275	MSE	MET	modified residue	UNP P49137
D	281	MSE	MET	modified residue	UNP P49137
D	300	MSE	MET	modified residue	UNP P49137
D	314	MSE	MET	modified residue	UNP P49137
D	320	MSE	MET	modified residue	UNP P49137
D	326	MSE	MET	modified residue	UNP P49137
D	356	MSE	MET	modified residue	UNP P49137

- Molecule 2 is STAUROSPORINE (CCD ID: STU) (formula: $C_{28}H_{26}N_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			35	28	4	3		
2	B	1	Total	C	N	O	0	0
			35	28	4	3		
2	C	1	Total	C	N	O	0	0
			35	28	4	3		
2	D	1	Total	C	N	O	0	0
			35	28	4	3		

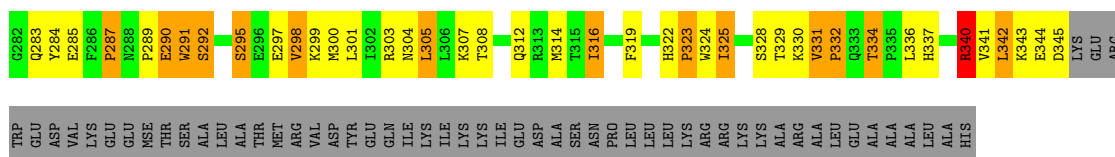
- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



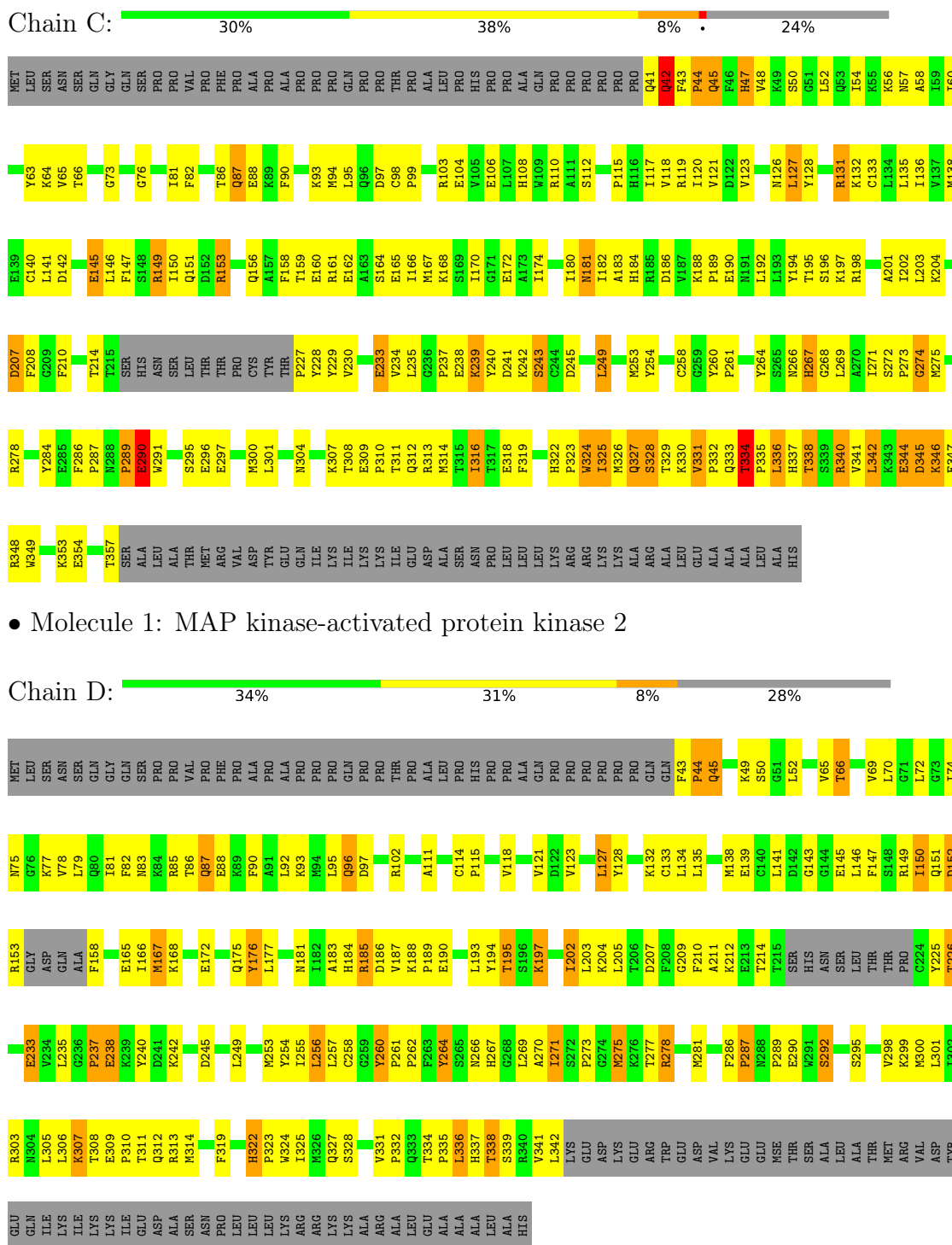
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	B	16	Total	O	0	0
			16	16		
4	C	9	Total	O	0	0
			9	9		
4	D	7	Total	O	0	0
			7	7		



- Molecule 1: MAP kinase-activated protein kinase 2



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	160.20Å 160.20Å 133.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	98.0 (20.00-2.70)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.239 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9405	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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: STU, SO4

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	0.94	4/2331 (0.2%)	1.38	31/3140 (1.0%)
1	B	0.99	4/2271 (0.2%)	1.32	17/3057 (0.6%)
1	C	0.96	3/2481 (0.1%)	1.32	28/3337 (0.8%)
1	D	0.84	3/2295 (0.1%)	1.23	15/3100 (0.5%)
All	All	0.94	14/9378 (0.1%)	1.31	91/12634 (0.7%)

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	3
1	B	0	2
1	C	0	1
1	D	0	2
All	All	0	8

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	291	TRP	NE1-CE2	10.45	1.49	1.37
1	C	324	TRP	NE1-CE2	10.32	1.48	1.37
1	A	109	TRP	NE1-CE2	10.31	1.48	1.37
1	A	291	TRP	NE1-CE2	10.30	1.48	1.37
1	B	247	TRP	NE1-CE2	10.30	1.48	1.37
1	A	281	MSE	CG-SE	-5.12	1.80	1.95
1	A	281	MSE	SE-CE	-5.10	1.80	1.95
1	B	281	MSE	CG-SE	-5.09	1.80	1.95
1	D	275	MSE	CG-SE	-5.07	1.80	1.95
1	D	167	MSE	CG-SE	-5.06	1.80	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	326	MSE	SE-CE	-5.06	1.80	1.95
1	B	281	MSE	SE-CE	-5.03	1.80	1.95
1	D	167	MSE	SE-CE	-5.03	1.80	1.95
1	C	326	MSE	CG-SE	-5.02	1.80	1.95

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	158	PHE	O-C-N	-10.12	110.39	123.13
1	B	257	LEU	N-CA-C	8.95	124.03	113.20
1	A	245	ASP	N-CA-C	-8.90	101.66	111.36
1	D	286	PHE	CA-C-N	8.38	128.44	119.89
1	D	286	PHE	C-N-CA	8.38	128.44	119.89
1	A	330	LYS	N-CA-C	-8.06	102.23	114.16
1	A	262	PRO	CA-C-N	-8.01	111.32	122.93
1	A	262	PRO	C-N-CA	-8.01	111.32	122.93
1	C	338	THR	N-CA-C	7.79	120.52	111.02
1	C	170	ILE	N-CA-C	-7.71	102.94	110.72
1	A	331	VAL	CA-C-N	7.65	128.11	119.93
1	A	331	VAL	C-N-CA	7.65	128.11	119.93
1	B	181	ASN	N-CA-C	7.64	121.93	111.54
1	C	334	THR	CA-C-N	7.64	128.85	119.98
1	C	334	THR	C-N-CA	7.64	128.85	119.98
1	A	242	LYS	O-C-N	7.58	130.79	122.15
1	C	183	ALA	N-CA-C	-7.48	96.70	108.90
1	C	64	LYS	N-CA-C	-7.46	97.06	109.07
1	A	64	LYS	N-CA-C	-7.24	97.45	109.24
1	C	295	SER	N-CA-C	6.86	119.42	110.43
1	D	322	HIS	CA-C-N	6.70	128.21	119.84
1	D	322	HIS	C-N-CA	6.70	128.21	119.84
1	C	328	SER	N-CA-C	-6.60	103.34	111.33
1	C	284	TYR	N-CA-C	-6.54	100.27	109.69
1	A	44	PRO	N-CA-CB	6.53	107.10	102.79
1	A	296	GLU	N-CA-C	-6.49	104.20	111.28
1	A	334	THR	CA-C-N	6.43	126.19	119.76
1	A	334	THR	C-N-CA	6.43	126.19	119.76
1	B	298	VAL	N-CA-C	-6.39	104.81	111.58
1	B	156	GLN	CB-CA-C	-6.32	109.27	116.54
1	B	89	LYS	N-CA-C	6.31	120.11	109.76
1	D	245	ASP	N-CA-C	-6.21	104.60	111.36
1	D	44	PRO	N-CA-CB	6.19	106.88	102.79
1	A	148	SER	N-CA-C	-6.08	104.57	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	ALA	N-CA-C	-6.07	99.30	109.07
1	B	147	PHE	N-CA-C	6.01	118.62	111.71
1	D	260	TYR	CA-C-N	5.97	126.53	120.38
1	D	260	TYR	C-N-CA	5.97	126.53	120.38
1	D	270	ALA	N-CA-C	-5.95	104.76	112.68
1	B	148	SER	N-CA-C	-5.94	104.71	111.07
1	C	188	LYS	CA-C-N	5.91	127.23	119.84
1	C	188	LYS	C-N-CA	5.91	127.23	119.84
1	A	282	GLY	N-CA-C	-5.88	99.25	113.18
1	A	305	LEU	N-CA-C	-5.87	105.79	113.12
1	C	44	PRO	N-CA-CB	5.82	106.63	102.79
1	D	287	PRO	N-CA-C	5.74	120.23	111.11
1	C	286	PHE	CA-C-N	5.72	126.20	120.14
1	C	286	PHE	C-N-CA	5.72	126.20	120.14
1	C	210	PHE	N-CA-C	-5.70	105.26	114.09
1	C	290	GLU	N-CA-C	5.57	122.66	110.80
1	A	46	PHE	N-CA-C	-5.53	106.38	113.01
1	D	181	ASN	N-CA-C	5.49	119.27	111.92
1	C	274	GLY	N-CA-C	5.39	119.92	112.37
1	A	181	ASN	N-CA-C	5.38	119.13	111.92
1	C	313	ARG	N-CA-C	5.36	118.01	110.23
1	A	247	TRP	N-CA-C	-5.36	105.33	111.07
1	C	181	ASN	N-CA-C	5.36	118.64	111.24
1	B	163	ALA	N-CA-C	-5.36	105.34	111.07
1	B	96	GLN	N-CA-C	-5.34	101.76	110.20
1	A	322	HIS	CA-C-N	5.33	124.97	119.05
1	A	322	HIS	C-N-CA	5.33	124.97	119.05
1	A	102	ARG	CD-NE-CZ	-5.30	116.98	124.40
1	D	307	LYS	N-CA-C	-5.28	102.47	110.28
1	B	85	ARG	CD-NE-CZ	-5.26	117.03	124.40
1	B	188	LYS	CA-C-N	5.26	124.71	119.24
1	B	188	LYS	C-N-CA	5.26	124.71	119.24
1	A	110	ARG	CD-NE-CZ	-5.25	117.05	124.40
1	D	185	ARG	N-CA-CB	-5.25	108.19	114.17
1	A	103	ARG	CD-NE-CZ	-5.24	117.06	124.40
1	C	318	GLU	N-CA-C	-5.24	105.48	111.14
1	A	179	SER	CA-C-N	-5.23	115.77	122.26
1	A	179	SER	C-N-CA	-5.23	115.77	122.26
1	A	162	GLU	N-CA-C	-5.21	105.25	111.03
1	C	347	GLU	N-CA-C	-5.21	105.29	111.69
1	B	305	LEU	N-CA-C	-5.20	105.22	112.45
1	B	153	ARG	CD-NE-CZ	-5.20	117.12	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	278	ARG	CD-NE-CZ	-5.19	117.14	124.40
1	D	197	LYS	N-CA-C	-5.16	106.83	113.02
1	A	280	ARG	CD-NE-CZ	-5.15	117.19	124.40
1	C	331	VAL	CA-C-N	5.15	125.06	119.76
1	C	331	VAL	C-N-CA	5.15	125.06	119.76
1	C	103	ARG	CD-NE-CZ	-5.12	117.23	124.40
1	B	287	PRO	N-CA-CB	5.09	108.17	103.39
1	A	261	PRO	CA-C-N	5.08	126.19	119.84
1	A	261	PRO	C-N-CA	5.08	126.19	119.84
1	C	334	THR	N-CA-C	5.07	116.08	109.64
1	B	340	ARG	CD-NE-CZ	-5.07	117.30	124.40
1	A	119	ARG	CD-NE-CZ	-5.06	117.31	124.40
1	C	258	CYS	N-CA-C	-5.05	108.14	114.56
1	C	119	ARG	CD-NE-CZ	-5.01	117.38	124.40
1	C	268	GLY	N-CA-C	-5.01	106.66	113.37

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ARG	Sidechain
1	A	103	ARG	Sidechain
1	A	119	ARG	Sidechain
1	B	158	PHE	Mainchain
1	B	176	TYR	Sidechain
1	C	340	ARG	Sidechain
1	D	102	ARG	Sidechain
1	D	176	TYR	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2289	0	2258	152	0
1	B	2234	0	2197	142	0
1	C	2438	0	2414	157	0
1	D	2252	0	2194	165	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	35	0	26	3	0
2	B	35	0	26	2	0
2	C	35	0	26	1	0
2	D	35	0	26	7	0
3	B	10	0	0	0	0
4	A	10	0	0	0	0
4	B	16	0	0	0	0
4	C	9	0	0	0	0
4	D	7	0	0	0	0
All	All	9405	0	9167	582	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 31.

All (582) 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:A:266:ASN:HD22	1:A:269:LEU:HG	1.30	0.96
1:A:158:PHE:CE1	1:A:162:GLU:HB3	2.00	0.95
1:A:260:TYR:HE2	1:A:290:GLU:HG2	1.30	0.94
1:C:328:SER:O	1:C:331:VAL:HG12	1.66	0.94
1:D:167:MSE:HG3	1:D:253:MSE:HG3	1.47	0.94
1:C:266:ASN:ND2	1:C:269:LEU:HG	1.81	0.94
1:D:314:MSE:HE3	1:D:319:PHE:HD1	1.32	0.94
1:C:332:PRO:HB2	1:C:334:THR:HG22	1.47	0.94
1:A:74:ILE:O	1:A:75:ASN:HB2	1.66	0.93
1:A:257:LEU:HA	1:A:336:LEU:HD13	1.51	0.92
1:D:300:MSE:HE3	1:D:303:ARG:HB2	1.49	0.92
1:B:278:ARG:HG2	1:B:283:GLN:HG3	1.49	0.92
1:D:266:ASN:HD22	1:D:269:LEU:HG	1.34	0.91
1:C:174:ILE:HG22	1:C:316:ILE:HG12	1.52	0.91
1:B:161:ARG:HG2	1:B:331:VAL:HG13	1.52	0.91
1:C:115:PRO:O	1:C:204:LYS:HE2	1.72	0.90
1:A:44:PRO:HG2	1:C:128:TYR:OH	1.71	0.90
1:A:198:ARG:HG2	1:A:199:PRO:CD	2.02	0.88
1:C:167:MSE:HG3	1:C:253:MSE:HE2	1.55	0.87
1:A:214:THR:O	1:A:215:THR:HG23	1.74	0.87
1:D:115:PRO:O	1:D:204:LYS:HE2	1.74	0.86
1:A:198:ARG:HG2	1:A:199:PRO:HD2	1.58	0.86
1:B:146:LEU:HD13	1:B:203:LEU:HD21	1.56	0.86
1:B:285:GLU:O	1:B:287:PRO:HD3	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:SER:HB2	1:A:283:GLN:HE22	1.40	0.84
1:A:285:GLU:HG2	1:A:287:PRO:HD3	1.60	0.84
1:B:301:LEU:HD13	1:B:322:HIS:CD2	2.13	0.83
1:A:179:SER:HB3	1:D:281:MSE:HE2	1.58	0.83
1:C:149:ARG:HB3	1:C:149:ARG:HH11	1.44	0.82
1:B:60:ILE:HG21	1:C:45:GLN:HG2	1.62	0.82
1:B:198:ARG:HB2	1:B:199:PRO:HD2	1.61	0.81
1:D:314:MSE:HE3	1:D:319:PHE:CD1	2.16	0.80
1:D:277:THR:O	1:D:281:MSE:HG2	1.82	0.80
1:A:233:GLU:HG2	1:D:310:PRO:HG3	1.63	0.80
1:B:46:PHE:C	1:B:48:VAL:H	1.88	0.80
1:A:45:GLN:HG2	1:C:60:ILE:HG21	1.63	0.79
1:D:314:MSE:CE	1:D:319:PHE:HD1	1.95	0.79
1:A:198:ARG:HD2	1:A:200:ASN:H	1.48	0.79
1:A:44:PRO:HG3	1:D:267:HIS:HB3	1.64	0.79
1:D:225:TYR:O	1:D:226:THR:HB	1.83	0.78
1:A:198:ARG:HG2	1:A:199:PRO:N	1.99	0.77
1:C:65:VAL:HA	1:C:81:ILE:HG22	1.65	0.77
1:B:98:CYS:HB2	1:B:99:PRO:HD2	1.66	0.77
1:D:301:LEU:HD13	1:D:322:HIS:CD2	2.20	0.77
1:B:74:ILE:HG22	1:B:75:ASN:ND2	2.00	0.76
1:B:151:GLN:NE2	1:B:343:LYS:HA	2.00	0.76
1:C:275:MSE:HA	1:C:278:ARG:HG3	1.68	0.76
1:B:67:SER:HB2	1:C:42:GLN:HB3	1.67	0.75
1:B:86:THR:O	1:B:87:GLN:HB3	1.85	0.75
1:D:83:ASN:O	1:D:87:GLN:HA	1.87	0.75
1:A:272:SER:OG	1:A:277:THR:HG22	1.87	0.75
1:D:300:MSE:SE	1:D:303:ARG:HH11	2.19	0.75
1:A:192:LEU:HB3	1:A:203:LEU:HD11	1.69	0.74
1:B:344:GLU:O	1:B:345:ASP:CB	2.33	0.74
1:A:227:PRO:HB3	1:A:229:TYR:CE2	2.23	0.74
1:D:78:VAL:HG21	2:D:401:STU:C17	2.16	0.74
1:B:86:THR:O	1:B:87:GLN:CB	2.35	0.73
1:A:295:SER:OG	1:A:298:VAL:HG23	1.88	0.73
1:B:305:LEU:HD21	1:B:314:MSE:CE	2.18	0.73
1:A:227:PRO:O	1:A:230:VAL:HG12	1.89	0.72
1:A:42:GLN:O	1:A:42:GLN:HG3	1.89	0.72
1:B:198:ARG:HB2	1:B:199:PRO:CD	2.19	0.72
1:D:74:ILE:HB	1:D:209:GLY:HA3	1.72	0.71
1:B:227:PRO:O	1:B:230:VAL:HG12	1.89	0.71
1:C:43:PHE:CB	1:C:44:PRO:CD	2.68	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:PHE:HE2	1:D:256:LEU:HD23	1.54	0.71
1:C:190:GLU:CD	1:C:190:GLU:H	1.98	0.71
1:C:149:ARG:HB3	1:C:153:ARG:HH12	1.54	0.71
1:D:277:THR:O	1:D:281:MSE:CG	2.37	0.71
1:B:253:MSE:HE1	1:B:319:PHE:HE1	1.54	0.71
1:D:267:HIS:HA	1:D:273:PRO:HB3	1.72	0.71
1:D:260:TYR:OH	1:D:287:PRO:HG2	1.92	0.70
1:B:305:LEU:HD21	1:B:314:MSE:HE3	1.74	0.70
1:D:138:MSE:SE	2:D:401:STU:H13	2.42	0.70
1:A:309:GLU:O	1:A:310:PRO:C	2.33	0.70
1:B:151:GLN:HE21	1:B:343:LYS:HA	1.57	0.70
1:A:233:GLU:HG2	1:D:310:PRO:CG	2.22	0.69
1:C:301:LEU:HD13	1:C:322:HIS:CD2	2.28	0.69
1:D:269:LEU:HD12	1:D:278:ARG:NH1	2.07	0.69
1:C:127:LEU:HA	1:C:131:ARG:O	1.92	0.69
1:B:332:PRO:HB2	1:B:334:THR:HG22	1.73	0.69
1:C:167:MSE:HE2	1:C:253:MSE:HE3	1.73	0.68
1:D:184:HIS:CD2	1:D:205:LEU:HD21	2.28	0.68
1:C:128:TYR:O	1:C:131:ARG:HB2	1.92	0.68
1:C:344:GLU:O	1:C:345:ASP:HB2	1.92	0.68
1:B:344:GLU:O	1:B:345:ASP:HB3	1.93	0.68
1:C:184:HIS:CD2	1:C:186:ASP:H	2.12	0.68
1:C:184:HIS:HD2	1:C:186:ASP:H	1.40	0.68
1:B:328:SER:O	1:B:331:VAL:HG12	1.94	0.68
1:B:90:PHE:CE2	1:B:121:VAL:HG21	2.28	0.67
1:D:307:LYS:HD2	1:D:312:GLN:HB3	1.76	0.67
1:D:266:ASN:ND2	1:D:269:LEU:HG	2.09	0.67
1:B:289:PRO:HA	1:B:292:SER:OG	1.94	0.67
1:A:337:HIS:O	1:A:341:VAL:HG23	1.94	0.67
1:C:150:ILE:O	1:C:153:ARG:HB2	1.94	0.67
1:A:272:SER:HB2	1:A:283:GLN:NE2	2.09	0.67
1:A:43:PHE:CD1	1:A:44:PRO:HD2	2.29	0.67
1:A:198:ARG:HD2	1:A:200:ASN:N	2.09	0.67
1:C:324:TRP:HE3	1:C:325:ILE:HD12	1.59	0.66
1:D:188:LYS:HB2	1:D:190:GLU:OE1	1.96	0.66
1:A:260:TYR:OH	1:A:287:PRO:HG2	1.96	0.66
1:B:295:SER:HB2	1:B:298:VAL:HG23	1.78	0.66
1:C:357:THR:HG22	1:C:357:THR:O	1.94	0.66
1:C:149:ARG:HB3	1:C:153:ARG:NH1	2.09	0.66
1:B:162:GLU:O	1:B:166:ILE:HG13	1.96	0.66
1:D:150:ILE:CG2	1:D:342:LEU:HD23	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ASN:ND2	1:A:269:LEU:HG	2.07	0.66
1:C:160:GLU:HB3	1:C:334:THR:HG23	1.77	0.66
1:B:253:MSE:HE1	1:B:319:PHE:CE1	2.31	0.65
1:C:264:TYR:CE1	1:C:348:ARG:NE	2.64	0.65
1:B:74:ILE:HD13	1:B:210:PHE:CD2	2.31	0.65
1:C:43:PHE:CB	1:C:44:PRO:HD2	2.27	0.65
1:B:337:HIS:HA	1:B:340:ARG:HE	1.62	0.65
1:A:186:ASP:HB2	1:A:210:PHE:HD2	1.62	0.65
1:D:264:TYR:O	1:D:278:ARG:NH2	2.30	0.65
1:D:300:MSE:CE	1:D:303:ARG:HB2	2.25	0.65
1:D:149:ARG:HH21	1:D:197:LYS:HA	1.61	0.65
1:D:150:ILE:HG22	1:D:342:LEU:HD23	1.78	0.65
1:D:150:ILE:HG21	1:D:338:THR:HG22	1.79	0.64
1:D:184:HIS:O	1:D:185:ARG:HB2	1.96	0.64
1:B:107:LEU:HD21	1:B:213:GLU:HG3	1.78	0.64
1:A:344:GLU:O	1:A:345:ASP:HB2	1.96	0.64
1:D:254:TYR:CG	1:D:262:PRO:HG3	2.33	0.64
1:B:289:PRO:O	1:B:292:SER:OG	2.17	0.63
1:D:86:THR:OG1	1:D:88:GLU:HG2	1.98	0.63
1:A:95:LEU:O	1:A:133:CYS:HB2	1.99	0.63
1:C:289:PRO:HG2	1:C:290:GLU:H	1.63	0.63
1:C:146:LEU:HD11	1:C:166:ILE:HD13	1.80	0.63
1:D:186:ASP:HB2	1:D:210:PHE:HD2	1.64	0.63
1:C:160:GLU:CB	1:C:334:THR:HG23	2.28	0.62
1:D:74:ILE:HG22	1:D:75:ASN:ND2	2.14	0.62
1:D:300:MSE:SE	1:D:303:ARG:HD2	2.48	0.62
1:D:225:TYR:O	1:D:226:THR:CB	2.45	0.62
1:B:69:VAL:HG22	1:B:79:LEU:CD2	2.29	0.62
1:B:331:VAL:HG23	1:B:332:PRO:HD2	1.81	0.62
1:D:141:LEU:HD13	1:D:193:LEU:HB2	1.81	0.62
1:D:264:TYR:O	1:D:275:MSE:HB2	2.00	0.62
1:A:332:PRO:HB2	1:A:334:THR:HG22	1.82	0.62
1:C:345:ASP:O	1:C:346:LYS:O	2.16	0.62
1:A:260:TYR:CE2	1:A:290:GLU:HG2	2.22	0.62
1:D:190:GLU:H	1:D:190:GLU:CD	2.08	0.61
1:C:151:GLN:C	1:C:153:ARG:H	2.09	0.61
1:A:47:HIS:NE2	1:D:269:LEU:O	2.33	0.61
1:A:258:CYS:HB2	1:A:290:GLU:HB3	1.83	0.61
1:D:93:LYS:HE2	1:D:95:LEU:HD21	1.83	0.61
1:B:289:PRO:O	1:B:290:GLU:C	2.42	0.61
1:B:274:GLY:C	1:B:278:ARG:HH21	2.08	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:ARG:O	1:C:156:GLN:NE2	2.34	0.60
1:C:174:ILE:CG2	1:C:316:ILE:HG12	2.29	0.60
1:D:337:HIS:HB3	1:D:341:VAL:HG23	1.83	0.60
1:C:264:TYR:CZ	1:C:348:ARG:NE	2.68	0.60
1:C:322:HIS:ND1	1:C:323:PRO:HD2	2.16	0.60
1:A:305:LEU:CD2	1:A:314:MSE:HE3	2.31	0.60
1:B:146:LEU:HD13	1:B:203:LEU:CD2	2.27	0.60
1:A:272:SER:CB	1:A:277:THR:HG22	2.32	0.60
1:D:90:PHE:CE2	1:D:121:VAL:HG21	2.37	0.60
1:A:264:TYR:CD1	1:A:264:TYR:N	2.70	0.60
1:D:305:LEU:HD21	1:D:314:MSE:HE2	1.83	0.60
1:D:290:GLU:CD	1:D:290:GLU:H	2.09	0.60
1:B:46:PHE:C	1:B:48:VAL:N	2.60	0.60
1:C:94:MSE:HE3	1:C:135:LEU:HD21	1.83	0.60
1:A:150:ILE:HG22	1:A:342:LEU:HD23	1.84	0.60
1:B:305:LEU:CD2	1:B:314:MSE:CE	2.79	0.60
1:A:298:VAL:HG22	1:A:324:TRP:NE1	2.16	0.59
1:A:164:SER:HA	1:A:324:TRP:CZ3	2.37	0.59
1:C:44:PRO:O	1:C:47:HIS:HB2	2.01	0.59
1:A:305:LEU:HG	1:A:314:MSE:CE	2.32	0.59
1:B:167:MSE:HE2	1:B:253:MSE:HE3	1.85	0.59
1:B:178:HIS:CE1	1:B:242:LYS:HB3	2.37	0.59
1:C:149:ARG:HH11	1:C:149:ARG:CB	2.12	0.59
1:B:92:LEU:HD11	1:B:135:LEU:HB3	1.84	0.59
1:B:299:LYS:O	1:B:303:ARG:HG3	2.02	0.59
1:C:337:HIS:HA	1:C:340:ARG:CZ	2.32	0.59
1:B:167:MSE:HG3	1:B:253:MSE:HE2	1.83	0.59
1:B:186:ASP:HB2	1:B:210:PHE:HD2	1.67	0.59
1:B:56:LYS:HD3	1:B:125:GLU:HB3	1.85	0.58
1:D:289:PRO:HA	1:D:292:SER:OG	2.03	0.58
1:A:111:ALA:HB1	1:A:177:LEU:HD21	1.85	0.58
1:A:271:ILE:O	1:A:272:SER:C	2.46	0.58
2:B:403:STU:H261	2:B:403:STU:H16	1.85	0.58
1:C:158:PHE:O	1:C:336:LEU:HB2	2.03	0.58
1:C:140:CYS:O	1:C:141:LEU:HD23	2.04	0.58
1:A:233:GLU:OE2	1:D:313:ARG:NH1	2.37	0.58
1:C:260:TYR:HB2	1:C:261:PRO:HD2	1.86	0.58
1:A:179:SER:HA	1:D:281:MSE:SE	2.54	0.58
1:D:337:HIS:O	1:D:338:THR:C	2.46	0.58
1:C:41:GLN:O	1:C:42:GLN:HB2	2.04	0.58
1:D:141:LEU:CD1	1:D:193:LEU:HB2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ARG:HD2	1:A:200:ASN:CA	2.34	0.57
1:B:285:GLU:C	1:B:287:PRO:HD3	2.28	0.57
1:C:266:ASN:HD22	1:C:269:LEU:HG	1.66	0.57
1:B:234:VAL:HG12	1:B:234:VAL:O	2.03	0.57
1:C:332:PRO:HB2	1:C:334:THR:CG2	2.31	0.57
1:A:149:ARG:HD3	1:A:194:TYR:CD2	2.40	0.57
1:B:67:SER:CB	1:C:42:GLN:HB3	2.35	0.57
1:D:74:ILE:HD12	1:D:209:GLY:HA3	1.86	0.57
1:D:300:MSE:HE3	1:D:303:ARG:CB	2.29	0.56
1:B:93:LYS:HE2	1:B:95:LEU:HD21	1.87	0.56
1:A:227:PRO:CB	1:A:229:TYR:CE2	2.87	0.56
1:B:232:PRO:O	1:B:235:LEU:HB2	2.06	0.56
1:C:260:TYR:CE1	1:C:348:ARG:NH1	2.74	0.56
1:C:357:THR:HG23	1:D:72:LEU:CD1	2.36	0.56
1:B:98:CYS:HB2	1:B:99:PRO:CD	2.35	0.56
1:D:66:THR:HG21	1:D:82:PHE:HE1	1.69	0.56
1:D:88:GLU:HG3	1:D:90:PHE:CE1	2.40	0.56
1:D:168:LYS:O	1:D:172:GLU:HG3	2.06	0.56
1:B:109:TRP:O	1:B:112:SER:HB3	2.06	0.56
1:B:147:PHE:HE2	1:B:256:LEU:HD23	1.71	0.56
1:A:45:GLN:HG2	1:C:60:ILE:CG2	2.35	0.56
1:B:69:VAL:HG22	1:B:79:LEU:HD23	1.86	0.56
1:B:264:TYR:HA	1:B:275:MSE:SE	2.56	0.56
1:A:115:PRO:O	1:A:202:ILE:HD11	2.06	0.55
1:A:272:SER:OG	1:A:277:THR:CG2	2.54	0.55
1:B:258:CYS:HB2	1:B:290:GLU:HB3	1.87	0.55
1:D:264:TYR:N	1:D:264:TYR:CD1	2.74	0.55
1:B:284:TYR:O	1:B:285:GLU:HB3	2.05	0.55
1:B:130:GLY:O	1:C:110:ARG:HD2	2.07	0.55
1:C:349:TRP:O	1:C:353:LYS:HG3	2.07	0.55
1:A:327:GLN:C	1:A:329:THR:H	2.14	0.55
1:D:118:VAL:O	1:D:118:VAL:HG13	2.05	0.55
1:C:153:ARG:NE	1:C:153:ARG:HA	2.22	0.55
1:C:117:ILE:HD13	1:C:208:PHE:HZ	1.72	0.55
1:D:189:PRO:HG2	1:D:190:GLU:OE2	2.07	0.55
1:A:149:ARG:HG2	1:A:149:ARG:HH11	1.72	0.54
1:C:86:THR:OG1	1:C:88:GLU:HG3	2.07	0.54
1:B:115:PRO:O	1:B:202:ILE:HD11	2.07	0.54
1:A:198:ARG:CD	1:A:200:ASN:H	2.19	0.54
1:A:288:ASN:HB3	1:A:289:PRO:HA	1.90	0.54
1:B:65:VAL:HA	1:B:81:ILE:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:ARG:CG	1:B:283:GLN:HG3	2.32	0.54
1:B:328:SER:C	1:B:330:LYS:N	2.64	0.54
1:C:253:MSE:HE1	1:C:319:PHE:HE1	1.73	0.54
1:A:230:VAL:HG21	1:A:235:LEU:CD2	2.38	0.54
1:B:90:PHE:CD2	1:B:121:VAL:HG21	2.43	0.54
1:C:184:HIS:CE1	1:C:207:ASP:O	2.61	0.54
2:C:401:STU:H16	2:C:401:STU:H261	1.90	0.54
1:B:46:PHE:O	1:B:48:VAL:N	2.39	0.53
1:A:124:TYR:HB2	1:A:135:LEU:HB2	1.91	0.53
1:B:324:TRP:CE3	1:B:325:ILE:HD12	2.43	0.53
1:C:108:HIS:CG	1:C:120:ILE:HD11	2.43	0.53
1:A:233:GLU:CG	1:D:310:PRO:HG3	2.36	0.53
1:B:83:ASN:O	1:B:87:GLN:N	2.41	0.53
1:B:305:LEU:CD2	1:B:314:MSE:HE2	2.38	0.53
1:D:305:LEU:CG	1:D:314:MSE:HE2	2.39	0.53
1:A:305:LEU:HD21	1:A:314:MSE:HE3	1.89	0.53
1:A:288:ASN:CB	1:A:289:PRO:HA	2.39	0.53
1:C:97:ASP:O	1:C:98:CYS:HB3	2.09	0.53
1:D:158:PHE:O	1:D:336:LEU:HB2	2.08	0.53
1:A:147:PHE:CE1	1:A:255:ILE:HG21	2.43	0.53
1:B:115:PRO:O	1:B:204:LYS:HE2	2.09	0.53
1:C:93:LYS:NZ	1:C:104:GLU:OE1	2.34	0.53
1:D:85:ARG:O	1:D:86:THR:C	2.51	0.52
1:A:301:LEU:HD13	1:A:322:HIS:CD2	2.45	0.52
1:C:149:ARG:HG3	1:C:194:TYR:CD2	2.44	0.52
1:C:266:ASN:ND2	1:C:269:LEU:CG	2.63	0.52
1:C:142:ASP:OD1	1:C:196:SER:HA	2.08	0.52
1:C:264:TYR:CE1	1:C:348:ARG:CZ	2.92	0.52
1:D:118:VAL:HG23	1:D:139:GLU:HG2	1.92	0.52
1:A:230:VAL:HG21	1:A:235:LEU:HD21	1.92	0.52
1:B:287:PRO:O	1:B:291:TRP:HD1	1.92	0.52
1:B:322:HIS:ND1	1:B:323:PRO:N	2.57	0.52
1:D:78:VAL:HA	1:D:92:LEU:O	2.10	0.52
1:D:267:HIS:HA	1:D:273:PRO:CB	2.40	0.52
2:A:401:STU:H261	2:A:401:STU:H16	1.91	0.52
1:C:195:THR:OG1	1:C:201:ALA:HB1	2.09	0.52
1:B:82:PHE:CE2	1:B:89:LYS:HB3	2.45	0.52
1:C:190:GLU:CD	1:C:190:GLU:N	2.66	0.52
1:D:277:THR:O	1:D:281:MSE:CB	2.58	0.52
1:A:44:PRO:HG3	1:D:267:HIS:CB	2.36	0.52
1:C:149:ARG:HH11	1:C:153:ARG:HH12	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:LEU:CD2	1:D:314:MSE:HE2	2.40	0.52
1:A:70:LEU:O	2:A:401:STU:H25	2.09	0.52
1:D:66:THR:HG21	1:D:82:PHE:CE1	2.45	0.52
1:D:184:HIS:HB3	1:D:187:VAL:HG23	1.91	0.51
1:A:167:MSE:HE2	1:A:253:MSE:HE3	1.91	0.51
1:A:179:SER:CB	1:D:281:MSE:HE2	2.34	0.51
1:C:242:LYS:O	1:C:245:ASP:HB2	2.10	0.51
1:B:298:VAL:HG22	1:B:324:TRP:CD1	2.46	0.51
1:B:307:LYS:HD3	1:B:312:GLN:HG2	1.92	0.51
1:D:70:LEU:HD22	2:D:401:STU:C3	2.40	0.51
1:A:52:LEU:HD21	1:A:123:VAL:HG21	1.93	0.51
1:D:70:LEU:C	2:D:401:STU:H25	2.35	0.51
1:A:188:LYS:HB2	1:A:189:PRO:HD2	1.93	0.51
1:B:328:SER:C	1:B:330:LYS:H	2.17	0.51
1:A:80:GLN:CD	1:A:89:LYS:HD2	2.36	0.51
1:D:240:TYR:CE2	1:D:311:THR:HG22	2.46	0.51
1:B:150:ILE:O	1:B:153:ARG:HB3	2.11	0.51
1:C:181:ASN:HB3	1:C:214:THR:OG1	2.10	0.51
1:A:138:MSE:SE	2:A:401:STU:H13	2.61	0.51
1:C:196:SER:H	1:C:201:ALA:HB1	1.76	0.51
1:D:254:TYR:CD1	1:D:262:PRO:HG3	2.46	0.51
1:A:286:PHE:HB3	1:A:291:TRP:CG	2.46	0.51
1:B:278:ARG:HG2	1:B:283:GLN:CG	2.32	0.51
1:C:332:PRO:C	1:C:334:THR:H	2.19	0.51
1:D:138:MSE:SE	2:D:401:STU:C13	3.07	0.51
1:A:50:SER:HB2	1:C:56:LYS:O	2.10	0.50
1:D:88:GLU:HG3	1:D:90:PHE:HE1	1.76	0.50
1:A:338:THR:O	1:A:342:LEU:HB2	2.11	0.50
1:B:128:TYR:HD1	1:C:48:VAL:CG2	2.25	0.50
1:B:214:THR:HG22	1:B:241:ASP:HB2	1.94	0.50
1:D:328:SER:O	1:D:331:VAL:HG12	2.11	0.50
1:D:128:TYR:C	1:D:128:TYR:CD2	2.89	0.50
1:B:67:SER:HB3	1:C:42:GLN:HG2	1.92	0.50
1:A:49:LYS:HD2	1:A:113:GLN:OE1	2.10	0.50
1:D:158:PHE:HZ	1:D:166:ILE:CD1	2.25	0.50
1:D:92:LEU:HD11	1:D:135:LEU:HB3	1.93	0.50
1:B:80:GLN:NE2	1:B:89:LYS:HD2	2.27	0.50
1:B:328:SER:O	1:B:330:LYS:N	2.44	0.50
1:A:258:CYS:SG	1:A:260:TYR:CE2	2.98	0.49
1:B:324:TRP:HE3	1:B:325:ILE:HD12	1.77	0.49
1:D:300:MSE:CE	1:D:303:ARG:HD2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:THR:O	1:D:339:SER:C	2.55	0.49
1:A:332:PRO:CB	1:A:334:THR:HG22	2.42	0.49
1:C:146:LEU:O	1:C:150:ILE:HD13	2.13	0.49
1:C:272:SER:N	1:C:273:PRO:HD3	2.28	0.49
1:C:324:TRP:CE3	1:C:325:ILE:HD12	2.44	0.49
1:D:300:MSE:CE	1:D:303:ARG:CB	2.87	0.49
1:A:97:ASP:H	1:A:133:CYS:HA	1.77	0.49
1:D:49:LYS:HG2	1:D:50:SER:N	2.27	0.49
1:D:266:ASN:O	1:D:273:PRO:HA	2.13	0.49
1:C:337:HIS:O	1:C:341:VAL:HG23	2.12	0.49
1:A:264:TYR:N	1:A:264:TYR:HD1	2.09	0.49
1:A:278:ARG:HE	1:A:283:GLN:HE21	1.59	0.49
1:D:69:VAL:HG22	1:D:79:LEU:HD23	1.94	0.49
1:A:327:GLN:O	1:A:329:THR:N	2.46	0.49
1:B:190:GLU:H	1:B:190:GLU:CD	2.21	0.49
1:C:90:PHE:CE2	1:C:121:VAL:HG21	2.48	0.49
1:C:329:THR:HG23	1:C:330:LYS:N	2.28	0.49
1:D:86:THR:O	1:D:87:GLN:HB3	2.12	0.49
1:D:257:LEU:CD1	1:D:298:VAL:HG11	2.43	0.49
1:D:335:PRO:O	1:D:336:LEU:HD12	2.12	0.49
1:A:168:LYS:HG3	1:A:325:ILE:HG23	1.95	0.49
1:A:288:ASN:ND2	1:A:292:SER:OG	2.45	0.49
1:B:341:VAL:O	1:B:344:GLU:HB2	2.12	0.49
1:C:66:THR:HG21	1:C:82:PHE:HE2	1.78	0.49
1:C:357:THR:HG23	1:D:72:LEU:HD11	1.94	0.49
1:D:158:PHE:HZ	1:D:166:ILE:HD12	1.77	0.49
1:D:257:LEU:HD11	1:D:298:VAL:HG11	1.95	0.48
1:B:255:ILE:O	1:B:256:LEU:C	2.54	0.48
1:D:324:TRP:HE3	1:D:325:ILE:HD12	1.78	0.48
1:A:245:ASP:O	1:A:248:SER:HB2	2.13	0.48
1:B:198:ARG:CB	1:B:199:PRO:CD	2.88	0.48
1:D:301:LEU:HD11	1:D:314:MSE:HE1	1.95	0.48
1:C:93:LYS:HE2	1:C:95:LEU:HD21	1.94	0.48
1:D:214:THR:HG21	1:D:242:LYS:CE	2.43	0.48
1:D:305:LEU:HG	1:D:314:MSE:HE2	1.94	0.48
1:A:274:GLY:O	1:A:278:ARG:HG3	2.14	0.48
1:B:69:VAL:HG22	1:B:79:LEU:HD21	1.94	0.48
1:C:149:ARG:NH1	1:C:153:ARG:HH12	2.11	0.48
1:B:149:ARG:NH2	1:B:196:SER:O	2.44	0.48
1:C:331:VAL:HG23	1:C:332:PRO:HD2	1.95	0.48
1:D:74:ILE:CB	1:D:209:GLY:HA3	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:CYS:HB2	1:D:176:TYR:CD2	2.48	0.48
1:A:337:HIS:N	1:A:337:HIS:CD2	2.82	0.48
1:B:57:ASN:HA	1:C:50:SER:HB2	1.96	0.48
1:B:89:LYS:O	1:B:140:CYS:HB2	2.14	0.48
1:D:74:ILE:CD1	1:D:209:GLY:HA3	2.42	0.48
1:A:247:TRP:HB2	1:A:313:ARG:NH1	2.29	0.48
1:B:69:VAL:HA	1:B:79:LEU:HD23	1.95	0.48
1:B:80:GLN:CD	1:B:89:LYS:HD2	2.38	0.48
1:D:127:LEU:HD12	1:D:132:LYS:HA	1.95	0.48
1:A:69:VAL:HA	1:A:79:LEU:HD23	1.96	0.48
1:A:253:MSE:HE1	1:A:325:ILE:HD11	1.96	0.48
1:C:52:LEU:HD21	1:C:123:VAL:HG21	1.95	0.48
1:C:145:GLU:O	1:C:146:LEU:C	2.57	0.48
1:C:180:ILE:HD11	1:C:182:ILE:HD12	1.95	0.48
1:C:230:VAL:HG22	1:C:234:VAL:HB	1.96	0.48
1:A:289:PRO:O	1:A:290:GLU:C	2.56	0.47
1:D:202:ILE:HG13	1:D:203:LEU:N	2.27	0.47
1:A:127:LEU:HD11	1:B:110:ARG:HD3	1.95	0.47
1:A:214:THR:O	1:A:215:THR:CG2	2.55	0.47
1:B:290:GLU:H	1:B:290:GLU:CD	2.22	0.47
1:C:151:GLN:C	1:C:153:ARG:N	2.70	0.47
1:C:264:TYR:OH	1:C:348:ARG:NH2	2.46	0.47
1:D:150:ILE:HG21	1:D:338:THR:CG2	2.44	0.47
1:C:267:HIS:HA	1:C:273:PRO:HB3	1.96	0.47
1:C:336:LEU:C	1:C:338:THR:H	2.20	0.47
1:A:44:PRO:CG	1:C:128:TYR:OH	2.53	0.47
1:B:56:LYS:HE3	1:B:125:GLU:CD	2.40	0.47
1:C:241:ASP:C	1:C:243:SER:N	2.70	0.47
1:D:225:TYR:CG	1:D:226:THR:N	2.81	0.47
1:C:233:GLU:H	1:C:233:GLU:HG3	1.22	0.47
1:A:50:SER:HB3	1:C:58:ALA:N	2.28	0.47
1:A:338:THR:HG22	1:A:342:LEU:HD22	1.97	0.47
1:A:90:PHE:CE2	1:A:121:VAL:HG21	2.50	0.47
1:B:138:MSE:SE	2:B:403:STU:H13	2.65	0.47
1:B:300:MSE:SE	1:B:303:ARG:HH11	2.48	0.47
1:C:41:GLN:O	1:C:42:GLN:NE2	2.48	0.47
1:C:90:PHE:HE2	1:C:121:VAL:HG21	1.80	0.47
1:C:274:GLY:O	1:C:278:ARG:HG2	2.14	0.47
1:A:281:MSE:HB2	1:A:283:GLN:HG3	1.97	0.47
1:D:187:VAL:O	1:D:187:VAL:HG12	2.15	0.47
1:A:111:ALA:HB1	1:A:117:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ILE:CD1	1:B:210:PHE:CD2	2.98	0.47
1:B:151:GLN:O	1:B:152:ASP:C	2.58	0.47
1:C:160:GLU:HA	1:C:336:LEU:HD21	1.97	0.47
1:B:289:PRO:CA	1:B:292:SER:OG	2.63	0.46
1:B:94:MSE:HE3	1:B:135:LEU:HD21	1.97	0.46
1:A:150:ILE:CG2	1:A:342:LEU:HD23	2.45	0.46
1:B:74:ILE:HB	1:B:209:GLY:HA3	1.96	0.46
1:B:143:GLY:HA3	1:B:196:SER:O	2.15	0.46
1:B:168:LYS:O	1:B:172:GLU:HG3	2.15	0.46
1:B:342:LEU:HD12	1:B:342:LEU:HA	1.70	0.46
1:D:260:TYR:HB2	1:D:261:PRO:HD2	1.97	0.46
1:C:254:TYR:CD1	1:C:254:TYR:C	2.92	0.46
1:D:52:LEU:HD21	1:D:123:VAL:HG21	1.97	0.46
1:D:233:GLU:H	1:D:233:GLU:HG3	1.24	0.46
1:C:98:CYS:HB2	1:C:99:PRO:CD	2.45	0.46
1:D:324:TRP:HE3	1:D:325:ILE:CD1	2.29	0.46
1:A:56:LYS:O	1:B:50:SER:HB2	2.15	0.46
1:A:253:MSE:O	1:A:254:TYR:C	2.59	0.46
1:B:52:LEU:HB2	1:B:109:TRP:CD2	2.50	0.46
1:B:60:ILE:HG21	1:C:45:GLN:CG	2.40	0.46
1:A:43:PHE:CG	1:A:44:PRO:HD2	2.51	0.46
1:B:128:TYR:CD2	1:B:128:TYR:C	2.94	0.46
1:C:127:LEU:HD12	1:C:132:LYS:HA	1.96	0.46
1:D:43:PHE:CD2	1:D:45:GLN:N	2.84	0.46
1:D:83:ASN:OD1	1:D:85:ARG:N	2.49	0.46
1:B:331:VAL:HG23	1:B:332:PRO:CD	2.46	0.46
1:D:143:GLY:HA3	1:D:194:TYR:CB	2.46	0.46
1:A:167:MSE:SE	1:A:256:LEU:HD12	2.67	0.45
1:B:289:PRO:HD2	1:B:290:GLU:OE2	2.16	0.45
1:C:159:THR:C	1:C:336:LEU:HD22	2.41	0.45
1:B:149:ARG:HH21	1:B:197:LYS:HA	1.81	0.45
1:C:266:ASN:HD22	1:C:269:LEU:CG	2.29	0.45
1:D:190:GLU:CD	1:D:190:GLU:N	2.74	0.45
1:D:72:LEU:HA	1:D:77:LYS:HA	1.97	0.45
1:D:183:ALA:O	1:D:211:ALA:HA	2.17	0.45
1:A:150:ILE:HG22	1:A:151:GLN:N	2.32	0.45
1:C:153:ARG:HA	1:C:153:ARG:HE	1.80	0.45
1:A:227:PRO:C	1:A:229:TYR:H	2.25	0.45
1:A:253:MSE:CE	1:A:325:ILE:HD11	2.47	0.45
1:D:306:LEU:HD23	1:D:306:LEU:HA	1.69	0.45
1:A:332:PRO:C	1:A:334:THR:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:PHE:CE2	1:D:256:LEU:HD23	2.42	0.45
1:D:331:VAL:HA	1:D:332:PRO:HD3	1.89	0.45
1:D:86:THR:O	1:D:87:GLN:CB	2.64	0.45
1:A:146:LEU:HG	1:A:147:PHE:CD2	2.52	0.45
1:A:158:PHE:CZ	1:A:166:ILE:HD12	2.51	0.45
1:B:289:PRO:O	1:B:292:SER:N	2.45	0.45
1:B:316:ILE:HD12	1:B:316:ILE:HA	1.78	0.45
1:D:96:GLN:HE21	1:D:96:GLN:HB2	1.61	0.45
1:D:150:ILE:O	1:D:153:ARG:HB2	2.17	0.45
1:D:264:TYR:C	1:D:275:MSE:HB2	2.42	0.45
1:A:81:ILE:HG21	1:A:92:LEU:HD22	1.98	0.45
1:B:124:TYR:HB2	1:B:135:LEU:HB2	1.98	0.45
1:C:296:GLU:O	1:C:300:MSE:HB2	2.16	0.45
1:D:299:LYS:O	1:D:303:ARG:HG3	2.16	0.45
1:A:305:LEU:HG	1:A:314:MSE:HE1	1.99	0.44
1:B:202:ILE:HD11	1:B:204:LYS:HE2	2.00	0.44
1:C:42:GLN:HB2	1:C:42:GLN:HE21	1.29	0.44
1:D:278:ARG:NH1	1:D:278:ARG:HG3	2.32	0.44
1:D:289:PRO:O	1:D:290:GLU:C	2.59	0.44
1:D:111:ALA:HB1	1:D:177:LEU:HD21	1.99	0.44
1:B:46:PHE:C	1:B:48:VAL:HG23	2.43	0.44
1:C:301:LEU:HD12	1:C:314:MSE:HE1	1.98	0.44
1:A:257:LEU:O	1:A:336:LEU:HD22	2.18	0.44
1:B:111:ALA:HB1	1:B:117:ILE:HD13	2.00	0.44
1:C:342:LEU:HD12	1:C:342:LEU:HA	1.83	0.44
1:A:49:LYS:O	1:C:126:ASN:HB3	2.17	0.44
1:A:90:PHE:HE2	1:A:121:VAL:HG21	1.81	0.44
1:A:240:TYR:HE2	1:D:309:GLU:CD	2.25	0.44
1:A:342:LEU:HD12	1:A:342:LEU:HA	1.81	0.44
1:B:83:ASN:HB3	1:B:86:THR:OG1	2.18	0.44
1:C:73:GLY:N	1:C:76:GLY:O	2.49	0.44
1:A:44:PRO:CG	1:D:267:HIS:HB3	2.42	0.44
1:C:86:THR:O	1:C:87:GLN:CB	2.65	0.44
1:C:160:GLU:HB2	1:C:334:THR:HG23	1.98	0.44
1:C:357:THR:CG2	1:D:72:LEU:HD13	2.47	0.44
1:D:43:PHE:CG	1:D:44:PRO:HD2	2.53	0.44
1:D:277:THR:O	1:D:281:MSE:HB2	2.17	0.44
1:A:149:ARG:HG2	1:A:149:ARG:NH1	2.31	0.44
1:A:189:PRO:HG2	1:A:190:GLU:CD	2.42	0.44
1:C:94:MSE:HG2	1:C:135:LEU:CD2	2.48	0.44
1:A:80:GLN:NE2	1:A:89:LYS:HD2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:HIS:ND1	1:A:323:PRO:HD2	2.32	0.44
1:C:136:ILE:HG22	1:C:138:MSE:HG3	2.00	0.44
1:C:164:SER:O	1:C:165:GLU:C	2.61	0.44
1:C:301:LEU:CD1	1:C:314:MSE:HE1	2.48	0.44
1:D:255:ILE:O	1:D:255:ILE:HG22	2.18	0.44
1:A:198:ARG:HD2	1:A:200:ASN:CB	2.48	0.44
1:B:145:GLU:O	1:B:146:LEU:C	2.61	0.44
1:B:289:PRO:O	1:B:291:TRP:N	2.50	0.44
1:C:227:PRO:C	1:C:229:TYR:H	2.26	0.44
1:C:249:LEU:HD12	1:C:249:LEU:HA	1.72	0.44
1:D:185:ARG:HH11	1:D:212:LYS:HB2	1.83	0.44
1:A:110:ARG:HH11	1:A:110:ARG:HD2	1.60	0.43
1:C:161:ARG:O	1:C:165:GLU:HG3	2.17	0.43
1:C:357:THR:HG23	1:D:72:LEU:HD13	1.99	0.43
1:B:97:ASP:OD2	1:B:102:ARG:NH2	2.50	0.43
1:B:275:MSE:O	1:B:279:ILE:HG13	2.18	0.43
1:C:118:VAL:O	1:C:118:VAL:HG13	2.17	0.43
1:D:87:GLN:HE21	1:D:87:GLN:HB2	1.43	0.43
1:B:284:TYR:CD1	1:B:284:TYR:N	2.86	0.43
1:C:327:GLN:O	1:C:328:SER:C	2.60	0.43
1:A:260:TYR:HB2	1:A:261:PRO:HD2	1.99	0.43
1:A:295:SER:HG	1:A:298:VAL:HG23	1.81	0.43
1:D:69:VAL:HG22	1:D:79:LEU:CD2	2.49	0.43
1:D:152:ASP:O	1:D:153:ARG:C	2.61	0.43
1:D:301:LEU:CD1	1:D:314:MSE:HE1	2.48	0.43
1:B:236:GLY:O	1:B:237:PRO:C	2.60	0.43
1:A:127:LEU:HD12	1:A:127:LEU:HA	1.90	0.43
1:B:100:LYS:O	1:B:103:ARG:HB3	2.19	0.43
1:C:57:ASN:H	1:C:57:ASN:HD22	1.67	0.43
1:A:98:CYS:O	1:A:101:ALA:HB3	2.19	0.43
1:B:56:LYS:O	1:C:50:SER:HB2	2.18	0.43
1:B:279:ILE:O	1:B:280:ARG:C	2.61	0.43
1:B:63:TYR:HA	1:B:82:PHE:O	2.18	0.42
1:C:159:THR:HA	1:C:334:THR:O	2.18	0.42
1:C:227:PRO:O	1:C:230:VAL:HG12	2.19	0.42
1:C:309:GLU:O	1:C:310:PRO:C	2.62	0.42
1:D:145:GLU:O	1:D:146:LEU:C	2.62	0.42
2:D:401:STU:H261	2:D:401:STU:H16	2.00	0.42
1:B:87:GLN:HE21	1:B:87:GLN:HB2	1.30	0.42
1:C:108:HIS:HB3	1:C:120:ILE:HD11	2.01	0.42
1:D:149:ARG:O	1:D:150:ILE:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:GLU:O	1:D:166:ILE:C	2.63	0.42
1:A:198:ARG:CG	1:A:199:PRO:HD2	2.40	0.42
1:A:257:LEU:HD12	1:A:291:TRP:CH2	2.54	0.42
1:D:65:VAL:HA	1:D:81:ILE:HG22	2.01	0.42
1:A:77:LYS:H	1:A:77:LYS:HG3	1.62	0.42
1:B:305:LEU:HD23	1:B:305:LEU:HA	1.60	0.42
1:D:74:ILE:HD12	1:D:209:GLY:CA	2.49	0.42
1:D:118:VAL:O	1:D:118:VAL:CG1	2.67	0.42
1:D:235:LEU:HD23	1:D:235:LEU:HA	1.62	0.42
1:A:229:TYR:CD1	1:A:229:TYR:C	2.97	0.42
1:C:334:THR:HA	1:C:335:PRO:HD3	1.63	0.42
1:D:43:PHE:HA	1:D:44:PRO:HD3	1.91	0.42
1:D:83:ASN:OD1	1:D:83:ASN:C	2.62	0.42
1:C:94:MSE:HA	1:C:135:LEU:HD23	2.01	0.42
1:C:253:MSE:HE1	1:C:319:PHE:CE1	2.54	0.42
1:C:238:GLU:O	1:C:239:LYS:O	2.37	0.42
1:D:225:TYR:CD1	1:D:225:TYR:C	2.93	0.42
1:A:50:SER:HB3	1:C:58:ALA:H	1.84	0.42
1:C:192:LEU:HB3	1:C:203:LEU:HD11	2.02	0.42
1:A:98:CYS:H	1:A:101:ALA:HB3	1.84	0.41
1:B:175:GLN:HA	1:B:316:ILE:HG21	2.02	0.41
1:C:147:PHE:O	1:C:151:GLN:HG2	2.20	0.41
1:C:180:ILE:CD1	1:C:182:ILE:HD12	2.50	0.41
1:D:237:PRO:HB2	1:D:238:GLU:H	1.62	0.41
1:C:304:ASN:HD22	1:C:304:ASN:HA	1.68	0.41
1:C:307:LYS:HD3	1:C:312:GLN:HB3	2.02	0.41
1:B:95:LEU:O	1:B:133:CYS:HB2	2.21	0.41
1:C:82:PHE:HA	1:C:88:GLU:O	2.20	0.41
1:C:63:TYR:CD1	1:C:81:ILE:HD12	2.55	0.41
1:D:97:ASP:H	1:D:133:CYS:HA	1.85	0.41
1:A:228:TYR:OH	1:D:190:GLU:OE2	2.33	0.41
1:A:331:VAL:HA	1:A:332:PRO:HD3	1.88	0.41
1:B:322:HIS:ND1	1:B:323:PRO:HD2	2.35	0.41
1:C:240:TYR:O	1:C:243:SER:HB2	2.20	0.41
1:C:289:PRO:O	1:C:291:TRP:N	2.52	0.41
1:D:95:LEU:O	1:D:133:CYS:HB2	2.20	0.41
1:A:67:SER:O	1:A:67:SER:OG	2.31	0.41
1:A:110:ARG:HG2	1:C:127:LEU:HD21	2.03	0.41
1:A:240:TYR:HE2	1:D:309:GLU:OE2	2.03	0.41
1:B:74:ILE:O	1:B:75:ASN:HB2	2.21	0.41
1:D:258:CYS:SG	1:D:260:TYR:CE2	3.13	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:LEU:C	1:C:338:THR:N	2.79	0.41
1:A:56:LYS:NZ	1:A:125:GLU:OE2	2.53	0.41
1:A:111:ALA:CB	1:A:177:LEU:HD21	2.51	0.41
1:A:310:PRO:O	1:A:313:ARG:HB2	2.21	0.41
1:B:183:ALA:O	1:B:211:ALA:HA	2.21	0.41
1:C:94:MSE:HE2	1:C:94:MSE:HB3	1.98	0.41
1:A:117:ILE:O	1:A:118:VAL:C	2.63	0.41
1:B:337:HIS:CD2	1:B:337:HIS:N	2.89	0.41
1:C:168:LYS:HD2	1:C:325:ILE:O	2.21	0.41
1:C:168:LYS:O	1:C:172:GLU:HG3	2.20	0.41
1:D:271:ILE:HD13	1:D:271:ILE:HA	1.77	0.41
1:A:152:ASP:O	1:A:153:ARG:HG3	2.21	0.41
1:B:151:GLN:C	1:B:153:ARG:N	2.78	0.41
1:D:70:LEU:HB3	2:D:401:STU:C20	2.51	0.41
1:A:305:LEU:O	1:A:313:ARG:HD3	2.20	0.40
1:A:334:THR:HA	1:A:335:PRO:HD3	1.79	0.40
1:B:289:PRO:HG2	1:B:337:HIS:CE1	2.56	0.40
1:A:138:MSE:HE3	1:A:138:MSE:HB2	2.00	0.40
1:D:264:TYR:N	1:D:264:TYR:HD1	2.15	0.40
1:A:167:MSE:HG3	1:A:253:MSE:HG3	2.04	0.40
1:D:43:PHE:HD2	1:D:45:GLN:N	2.18	0.40
1:A:272:SER:HA	1:A:277:THR:HG21	2.03	0.40
1:C:264:TYR:OH	1:C:348:ARG:NE	2.55	0.40
1:B:149:ARG:NH2	1:B:197:LYS:HA	2.37	0.40
1:D:185:ARG:NH1	1:D:212:LYS:HD2	2.37	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	284/400 (71%)	250 (88%)	25 (9%)	9 (3%)	3 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	277/400 (69%)	241 (87%)	26 (9%)	10 (4%)	2	6
1	C	302/400 (76%)	261 (86%)	30 (10%)	11 (4%)	2	6
1	D	282/400 (70%)	241 (86%)	32 (11%)	9 (3%)	3	7
All	All	1145/1600 (72%)	993 (87%)	113 (10%)	39 (3%)	3	7

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	ASP
1	B	66	THR
1	B	239	LYS
1	C	42	GLN
1	C	237	PRO
1	C	239	LYS
1	C	289	PRO
1	C	290	GLU
1	C	346	LYS
1	A	237	PRO
1	A	239	LYS
1	A	328	SER
1	B	146	LEU
1	B	207	ASP
1	B	238	GLU
1	D	152	ASP
1	D	195	THR
1	D	237	PRO
1	D	292	SER
1	D	338	THR
1	B	237	PRO
1	B	329	THR
1	C	345	ASP
1	D	151	GLN
1	D	238	GLU
1	B	47	HIS
1	B	290	GLU
1	C	207	ASP
1	C	228	TYR
1	C	267	HIS
1	D	207	ASP
1	A	238	GLU
1	A	310	PRO

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Mol	Chain	Res	Type
1	C	112	SER
1	D	226	THR
1	A	273	PRO
1	A	287	PRO
1	A	309	GLU
1	B	332	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	246/345 (71%)	221 (90%)	25 (10%)	7	18
1	B	241/345 (70%)	207 (86%)	34 (14%)	3	9
1	C	263/345 (76%)	227 (86%)	36 (14%)	3	9
1	D	241/345 (70%)	220 (91%)	21 (9%)	9	24
All	All	991/1380 (72%)	875 (88%)	116 (12%)	5	13

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	45	GLN
1	A	77	LYS
1	A	80	GLN
1	A	106	GLU
1	A	127	LEU
1	A	134	LEU
1	A	142	ASP
1	A	149	ARG
1	A	150	ILE
1	A	198	ARG
1	A	202	ILE
1	A	205	LEU
1	A	215	THR
1	A	233	GLU

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Mol	Chain	Res	Type
1	A	235	LEU
1	A	249	LEU
1	A	271	ILE
1	A	285	GLU
1	A	297	GLU
1	A	304	ASN
1	A	325	ILE
1	A	331	VAL
1	A	334	THR
1	A	342	LEU
1	B	45	GLN
1	B	47	HIS
1	B	52	LEU
1	B	66	THR
1	B	87	GLN
1	B	100	LYS
1	B	102	ARG
1	B	119	ARG
1	B	134	LEU
1	B	153	ARG
1	B	156	GLN
1	B	161	ARG
1	B	162	GLU
1	B	198	ARG
1	B	202	ILE
1	B	212	LYS
1	B	233	GLU
1	B	235	LEU
1	B	243	SER
1	B	249	LEU
1	B	256	LEU
1	B	292	SER
1	B	295	SER
1	B	297	GLU
1	B	304	ASN
1	B	308	THR
1	B	316	ILE
1	B	323	PRO
1	B	325	ILE
1	B	331	VAL
1	B	334	THR
1	B	336	LEU

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Mol	Chain	Res	Type
1	B	340	ARG
1	B	342	LEU
1	C	42	GLN
1	C	45	GLN
1	C	47	HIS
1	C	54	ILE
1	C	87	GLN
1	C	106	GLU
1	C	127	LEU
1	C	131	ARG
1	C	133	CYS
1	C	145	GLU
1	C	149	ARG
1	C	153	ARG
1	C	162	GLU
1	C	189	PRO
1	C	197	LYS
1	C	198	ARG
1	C	202	ILE
1	C	233	GLU
1	C	235	LEU
1	C	243	SER
1	C	249	LEU
1	C	271	ILE
1	C	287	PRO
1	C	290	GLU
1	C	297	GLU
1	C	308	THR
1	C	311	THR
1	C	316	ILE
1	C	325	ILE
1	C	327	GLN
1	C	333	GLN
1	C	334	THR
1	C	336	LEU
1	C	342	LEU
1	C	344	GLU
1	C	354	GLU
1	D	45	GLN
1	D	66	THR
1	D	87	GLN
1	D	96	GLN

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Mol	Chain	Res	Type
1	D	127	LEU
1	D	134	LEU
1	D	150	ILE
1	D	175	GLN
1	D	195	THR
1	D	202	ILE
1	D	233	GLU
1	D	249	LEU
1	D	256	LEU
1	D	264	TYR
1	D	271	ILE
1	D	295	SER
1	D	308	THR
1	D	323	PRO
1	D	327	GLN
1	D	334	THR
1	D	336	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	68	GLN
1	A	175	GLN
1	A	181	ASN
1	A	266	ASN
1	A	283	GLN
1	A	288	ASN
1	A	304	ASN
1	A	337	HIS
1	B	68	GLN
1	B	75	ASN
1	B	87	GLN
1	B	151	GLN
1	B	156	GLN
1	B	283	GLN
1	B	288	ASN
1	B	337	HIS
1	C	42	GLN
1	C	57	ASN
1	C	87	GLN
1	C	151	GLN

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Mol	Chain	Res	Type
1	C	184	HIS
1	C	266	ASN
1	C	283	GLN
1	C	288	ASN
1	C	304	ASN
1	C	327	GLN
1	C	333	GLN
1	D	45	GLN
1	D	68	GLN
1	D	75	ASN
1	D	87	GLN
1	D	96	GLN
1	D	175	GLN
1	D	181	ASN
1	D	266	ASN
1	D	304	ASN
1	D	333	GLN

5.3.3 RNA [i](#)

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](#)

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	STU	A	401	-	39,42,42	2.83	20 (51%)	50,68,68	2.05	20 (40%)
2	STU	B	403	-	39,42,42	2.96	18 (46%)	50,68,68	1.59	11 (22%)
3	SO4	B	402	-	4,4,4	0.60	0	6,6,6	0.97	0
2	STU	C	401	-	39,42,42	2.71	20 (51%)	50,68,68	2.00	20 (40%)
3	SO4	B	401	-	4,4,4	0.58	0	6,6,6	0.97	0
2	STU	D	401	-	39,42,42	3.05	20 (51%)	50,68,68	1.88	19 (38%)

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	STU	D	401	-	-	2/4/42/42	-
2	STU	A	401	-	-	2/4/42/42	-
2	STU	B	403	-	-	0/4/42/42	-
2	STU	C	401	-	-	1/4/42/42	-

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	403	STU	C23-N4	9.44	1.58	1.47
2	D	401	STU	C23-N4	9.42	1.58	1.47
2	A	401	STU	C23-N4	9.39	1.58	1.47
2	C	401	STU	C23-N4	7.69	1.56	1.47
2	D	401	STU	C22-C23	6.65	1.59	1.53
2	D	401	STU	C25-N3	5.69	1.50	1.45
2	B	403	STU	C6-C7	5.43	1.50	1.40
2	B	403	STU	C9-C10	5.41	1.55	1.50
2	B	403	STU	C25-N3	5.40	1.50	1.45
2	D	401	STU	C6-C7	5.25	1.50	1.40
2	C	401	STU	C6-C7	5.03	1.49	1.40
2	A	401	STU	C7-C10	-4.72	1.31	1.39
2	B	403	STU	C7-C10	-4.69	1.31	1.39
2	D	401	STU	C18-N2	4.67	1.45	1.40
2	C	401	STU	C22-C23	4.62	1.57	1.53
2	C	401	STU	C7-C10	-4.43	1.32	1.39
2	A	401	STU	C18-N2	4.36	1.44	1.40
2	D	401	STU	C9-C10	4.25	1.54	1.50
2	D	401	STU	C7-C10	-4.23	1.32	1.39
2	A	401	STU	C8-N1	-4.13	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	STU	C25-N3	4.09	1.49	1.45
2	A	401	STU	C22-C23	4.00	1.57	1.53
2	B	403	STU	C5-C20	3.99	1.47	1.41
2	C	401	STU	C3-C2	3.82	1.46	1.38
2	A	401	STU	C6-C7	3.81	1.47	1.40
2	A	401	STU	C12-C17	3.67	1.46	1.41
2	A	401	STU	C14-C15	3.50	1.45	1.38
2	A	401	STU	C5-C6	-3.48	1.38	1.46
2	B	403	STU	C5-C6	-3.45	1.38	1.46
2	C	401	STU	C5-C20	3.44	1.46	1.41
2	C	401	STU	C18-N2	3.43	1.43	1.40
2	D	401	STU	C1-C20	3.42	1.44	1.39
2	C	401	STU	C1-C20	3.34	1.44	1.39
2	D	401	STU	C12-C17	3.31	1.46	1.41
2	D	401	STU	C11-C18	3.28	1.47	1.41
2	B	403	STU	C19-N3	3.28	1.44	1.39
2	B	403	STU	C11-C10	3.25	1.46	1.40
2	C	401	STU	C20-N3	-3.23	1.35	1.40
2	C	401	STU	C25-N3	3.19	1.48	1.45
2	B	403	STU	C6-C19	3.17	1.47	1.41
2	C	401	STU	C9-C10	3.13	1.53	1.50
2	A	401	STU	C24-C25	3.01	1.57	1.51
2	B	403	STU	C22-C23	2.99	1.56	1.53
2	A	401	STU	C11-C18	2.97	1.47	1.41
2	C	401	STU	C12-C11	-2.94	1.39	1.46
2	D	401	STU	C5-C6	-2.93	1.39	1.46
2	B	403	STU	C12-C11	-2.87	1.40	1.46
2	D	401	STU	C14-C15	2.84	1.44	1.38
2	C	401	STU	C5-C6	-2.83	1.40	1.46
2	C	401	STU	C24-C23	2.81	1.57	1.53
2	C	401	STU	C19-N3	2.78	1.43	1.39
2	C	401	STU	C14-C15	2.71	1.44	1.38
2	D	401	STU	C3-C2	2.60	1.44	1.38
2	A	401	STU	C3-C2	2.60	1.43	1.38
2	D	401	STU	C24-C25	2.58	1.56	1.51
2	B	403	STU	C14-C15	2.58	1.43	1.38
2	B	403	STU	C3-C2	2.57	1.43	1.38
2	B	403	STU	C20-N3	-2.52	1.36	1.40
2	C	401	STU	C24-C25	2.51	1.56	1.51
2	C	401	STU	C11-C18	2.49	1.46	1.41
2	B	403	STU	C24-C25	2.47	1.56	1.51
2	A	401	STU	C1-C20	2.46	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	STU	C5-C20	2.45	1.44	1.41
2	D	401	STU	C6-C19	2.42	1.46	1.41
2	A	401	STU	C20-N3	-2.42	1.36	1.40
2	D	401	STU	C12-C11	-2.40	1.41	1.46
2	B	403	STU	C18-N2	2.37	1.42	1.40
2	A	401	STU	C12-C11	-2.34	1.41	1.46
2	D	401	STU	C5-C20	2.30	1.44	1.41
2	D	401	STU	C17-N2	2.30	1.43	1.40
2	D	401	STU	C11-C10	2.29	1.45	1.40
2	C	401	STU	C12-C17	2.23	1.44	1.41
2	A	401	STU	C28-N4	2.22	1.52	1.46
2	A	401	STU	C26-C21	2.16	1.54	1.51
2	D	401	STU	C20-N3	-2.16	1.37	1.40
2	B	403	STU	C19-C18	-2.12	1.35	1.40
2	A	401	STU	O6-C22	2.06	1.46	1.42
2	C	401	STU	C8-N1	-2.03	1.33	1.35

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	STU	C28-N4-C23	-3.97	109.64	114.39
2	D	401	STU	C9-N1-C8	3.94	117.45	113.86
2	C	401	STU	C9-N1-C8	3.89	117.40	113.86
2	A	401	STU	C28-N4-C23	-3.89	109.74	114.39
2	A	401	STU	C6-C7-C10	3.82	123.43	120.76
2	A	401	STU	C12-C17-N2	-3.79	106.45	108.94
2	D	401	STU	C7-C8-N1	-3.64	102.90	106.38
2	A	401	STU	C10-C7-C8	3.63	111.12	108.09
2	A	401	STU	C6-C7-C8	-3.60	125.45	130.53
2	A	401	STU	C9-N1-C8	3.57	117.11	113.86
2	C	401	STU	C11-C18-N2	-3.56	105.53	109.38
2	C	401	STU	C12-C17-N2	-3.51	106.64	108.94
2	A	401	STU	C7-C8-N1	-3.50	103.04	106.38
2	A	401	STU	C11-C18-N2	-3.38	105.72	109.38
2	B	403	STU	C12-C17-N2	-3.37	106.72	108.94
2	C	401	STU	C10-C9-N1	-3.36	98.48	101.75
2	C	401	STU	C7-C8-N1	-3.27	103.26	106.38
2	D	401	STU	C10-C9-N1	-3.26	98.57	101.75
2	A	401	STU	C18-C19-N3	3.25	132.18	129.42
2	C	401	STU	C6-C7-C10	3.24	123.02	120.76
2	A	401	STU	C10-C9-N1	-3.20	98.63	101.75
2	B	403	STU	C9-N1-C8	3.17	116.74	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	403	STU	C11-C18-N2	-3.14	105.99	109.38
2	C	401	STU	C10-C7-C8	3.01	110.61	108.09
2	C	401	STU	C18-C19-N3	2.99	131.96	129.42
2	A	401	STU	C18-C11-C10	-2.98	116.26	119.77
2	C	401	STU	C6-C7-C8	-2.95	126.37	130.53
2	D	401	STU	C12-C17-N2	-2.93	107.02	108.94
2	D	401	STU	C11-C18-N2	-2.92	106.22	109.38
2	D	401	STU	C10-C7-C8	2.92	110.53	108.09
2	C	401	STU	C18-C11-C10	-2.90	116.36	119.77
2	D	401	STU	C16-C17-N2	2.83	134.47	130.22
2	D	401	STU	C18-C19-N3	2.75	131.76	129.42
2	B	403	STU	C7-C8-N1	-2.73	103.78	106.38
2	B	403	STU	C11-C12-C17	2.71	109.22	106.49
2	B	403	STU	C18-C19-N3	2.66	131.68	129.42
2	C	401	STU	C11-C12-C17	2.64	109.15	106.49
2	D	401	STU	C16-C17-C12	-2.63	118.51	121.59
2	A	401	STU	O5-C8-N1	2.62	128.26	125.35
2	A	401	STU	C18-N2-C17	2.62	110.53	107.37
2	C	401	STU	C16-C17-N2	2.62	134.15	130.22
2	B	403	STU	C10-C7-C8	2.60	110.27	108.09
2	A	401	STU	C6-C19-N3	-2.46	105.50	109.61
2	B	403	STU	C16-C17-N2	2.45	133.90	130.22
2	A	401	STU	C16-C17-N2	2.43	133.87	130.22
2	D	401	STU	C6-C7-C8	-2.40	127.14	130.53
2	D	401	STU	C11-C12-C17	2.40	108.90	106.49
2	D	401	STU	C6-C19-N3	-2.40	105.61	109.61
2	A	401	STU	C11-C12-C17	2.39	108.89	106.49
2	C	401	STU	C18-N2-C17	2.38	110.24	107.37
2	A	401	STU	C19-C18-N2	2.33	133.36	131.38
2	B	403	STU	C10-C9-N1	-2.31	99.50	101.75
2	C	401	STU	C6-C19-N3	-2.27	105.82	109.61
2	D	401	STU	C18-C11-C10	-2.26	117.10	119.77
2	D	401	STU	C15-C14-C13	-2.26	117.45	120.24
2	A	401	STU	C5-C6-C19	2.26	109.60	106.44
2	D	401	STU	C6-C7-C10	2.25	122.33	120.76
2	C	401	STU	O5-C8-N1	2.17	127.76	125.35
2	D	401	STU	C9-C10-C11	-2.15	127.09	128.73
2	D	401	STU	O5-C8-N1	2.13	127.72	125.35
2	D	401	STU	C19-C18-N2	2.12	133.18	131.38
2	C	401	STU	C7-C6-C19	-2.11	114.50	118.04
2	D	401	STU	C28-N4-C23	-2.10	111.87	114.39
2	A	401	STU	C7-C6-C19	-2.10	114.51	118.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	403	STU	C6-C19-N3	-2.09	106.11	109.61
2	B	403	STU	C18-N2-C17	2.07	109.87	107.37
2	C	401	STU	C19-C18-N2	2.05	133.12	131.38
2	C	401	STU	C16-C17-C12	-2.03	119.22	121.59
2	C	401	STU	C9-C10-C11	-2.03	127.19	128.73
2	A	401	STU	C11-C10-C7	2.02	122.57	121.25

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	STU	C24-C23-N4-C28
2	C	401	STU	C24-C23-N4-C28
2	D	401	STU	C24-C23-N4-C28
2	A	401	STU	C22-C23-N4-C28
2	D	401	STU	C22-C23-N4-C28

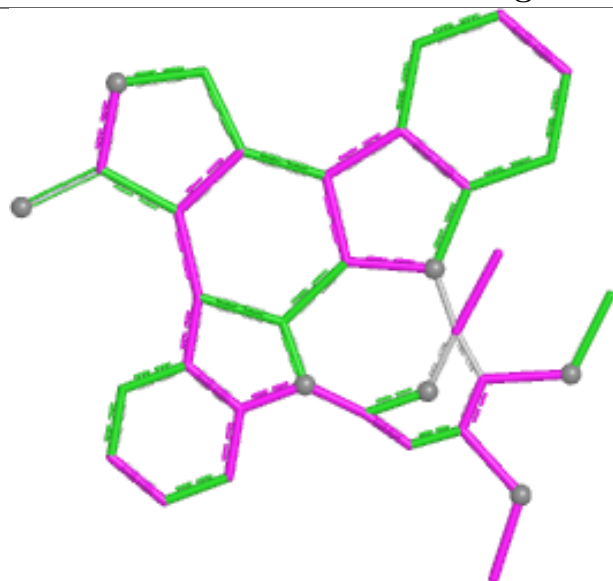
There are no ring outliers.

4 monomers are involved in 13 short contacts:

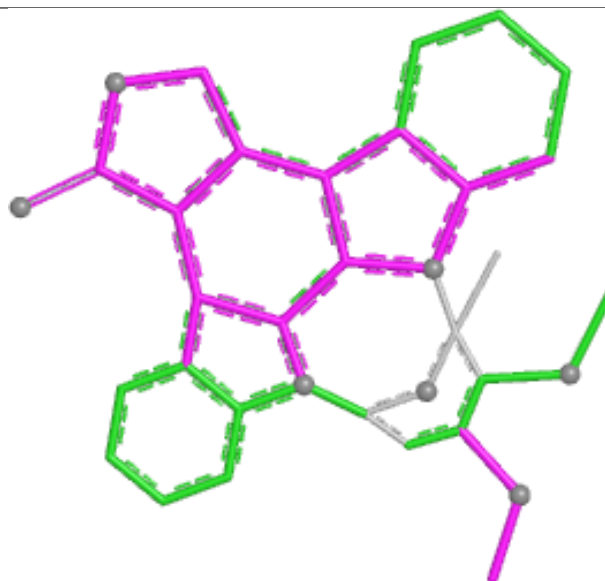
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	STU	3	0
2	B	403	STU	2	0
2	C	401	STU	1	0
2	D	401	STU	7	0

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.

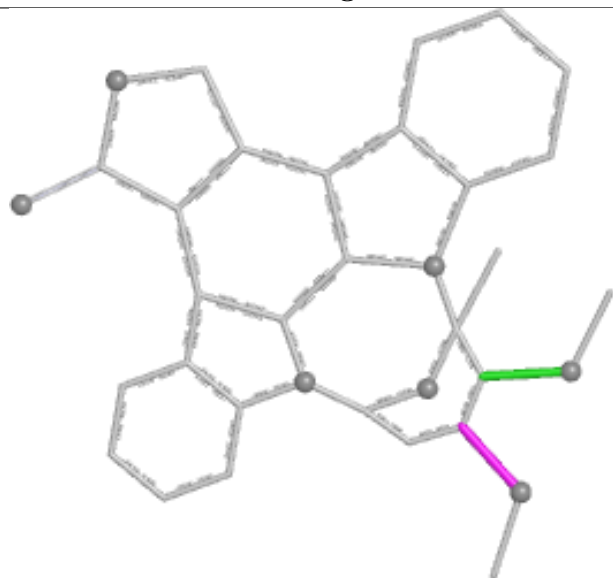
Ligand STU A 401



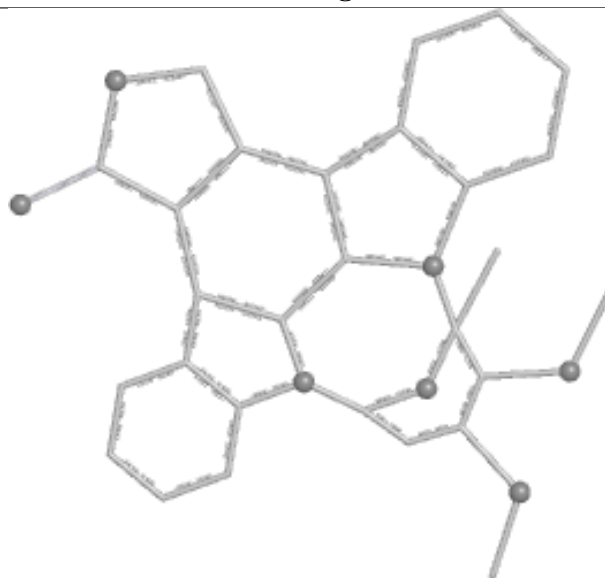
Bond lengths



Bond angles

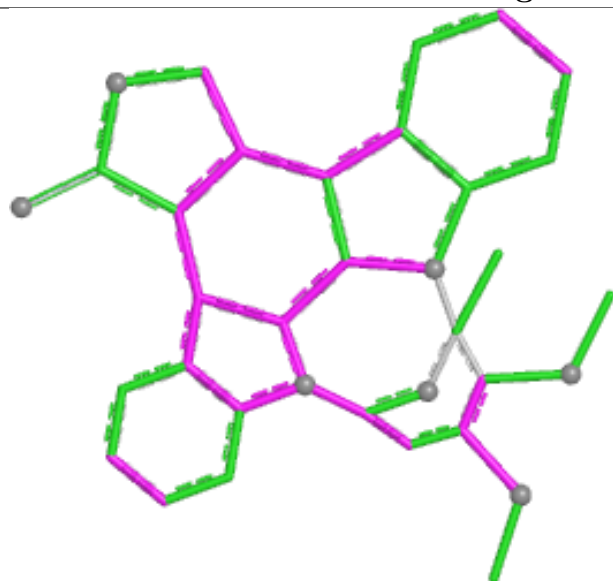


Torsions

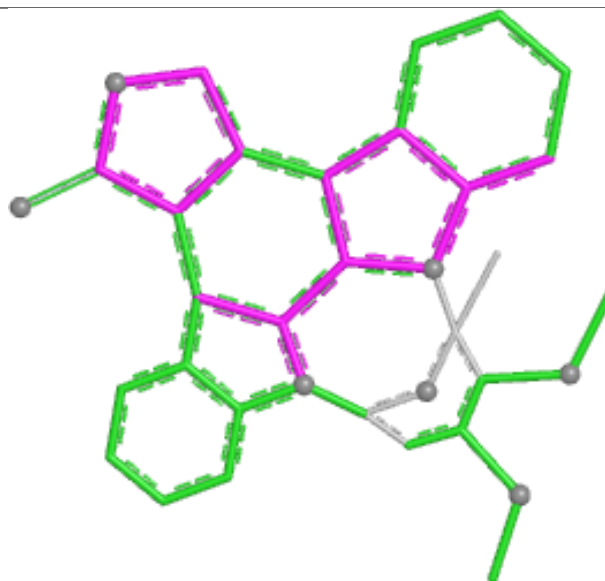


Rings

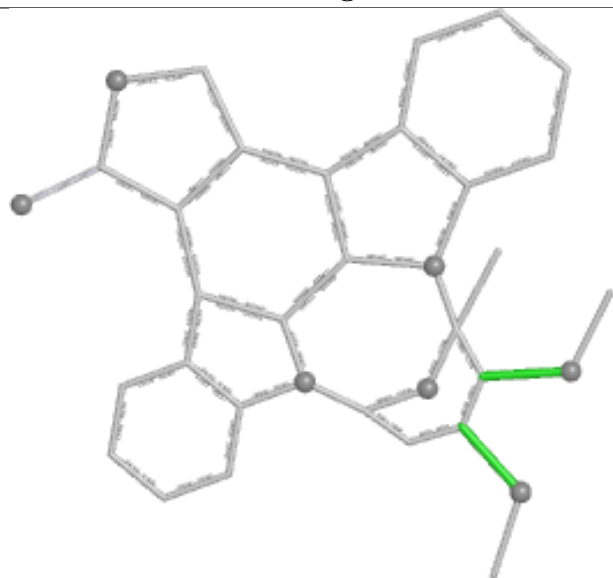
Ligand STU B 403



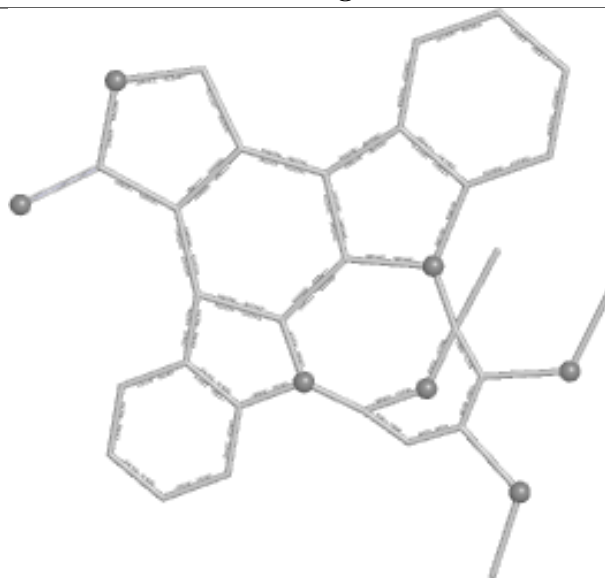
Bond lengths



Bond angles

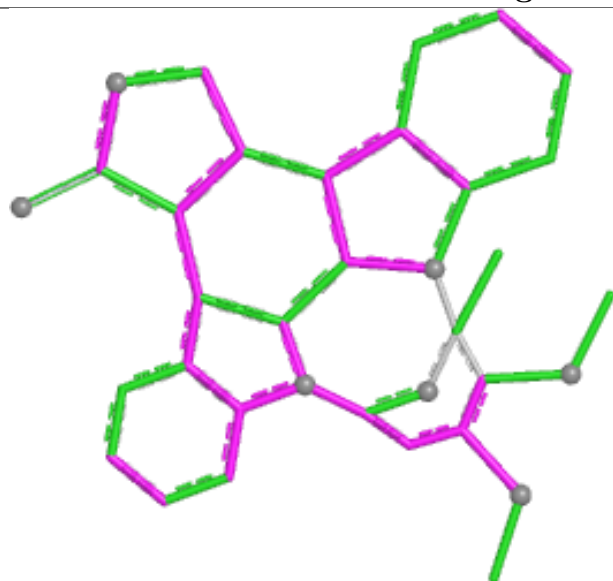


Torsions

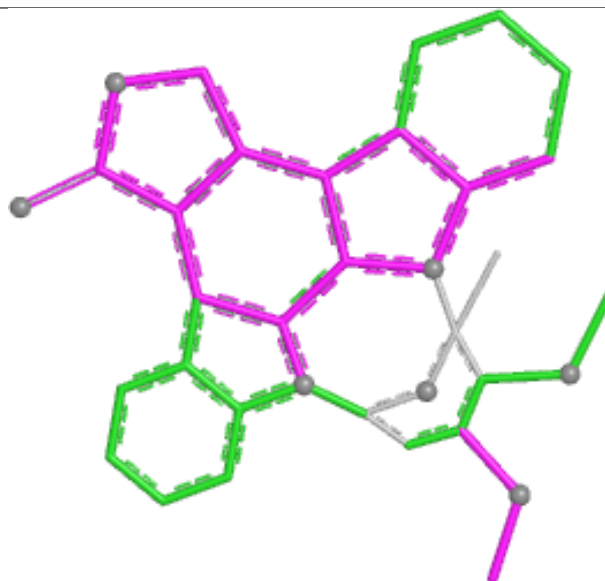


Rings

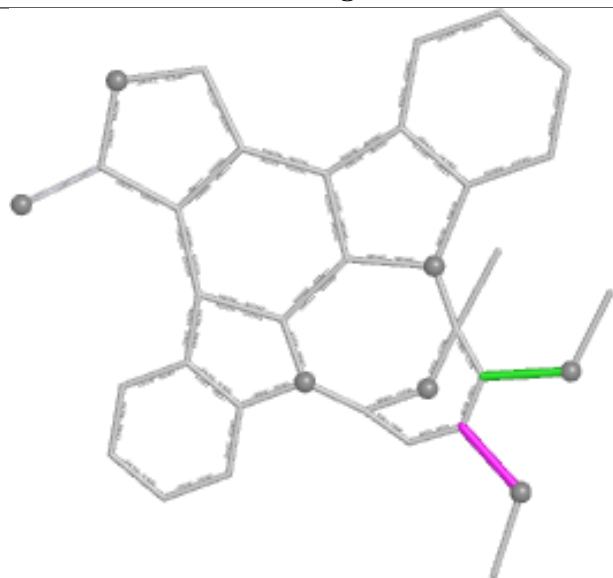
Ligand STU C 401



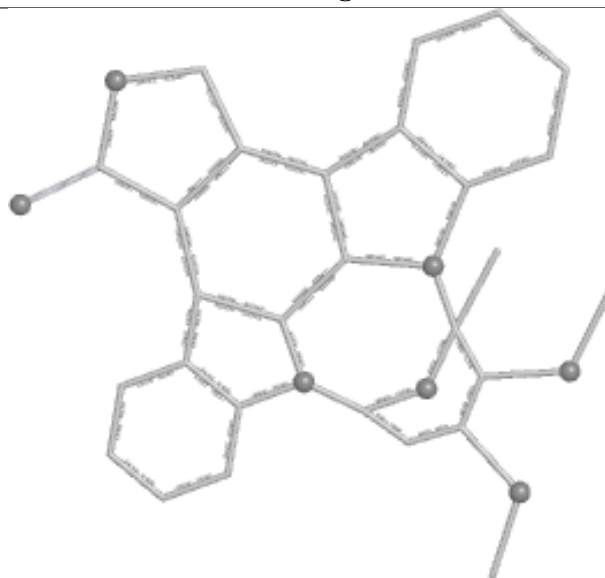
Bond lengths



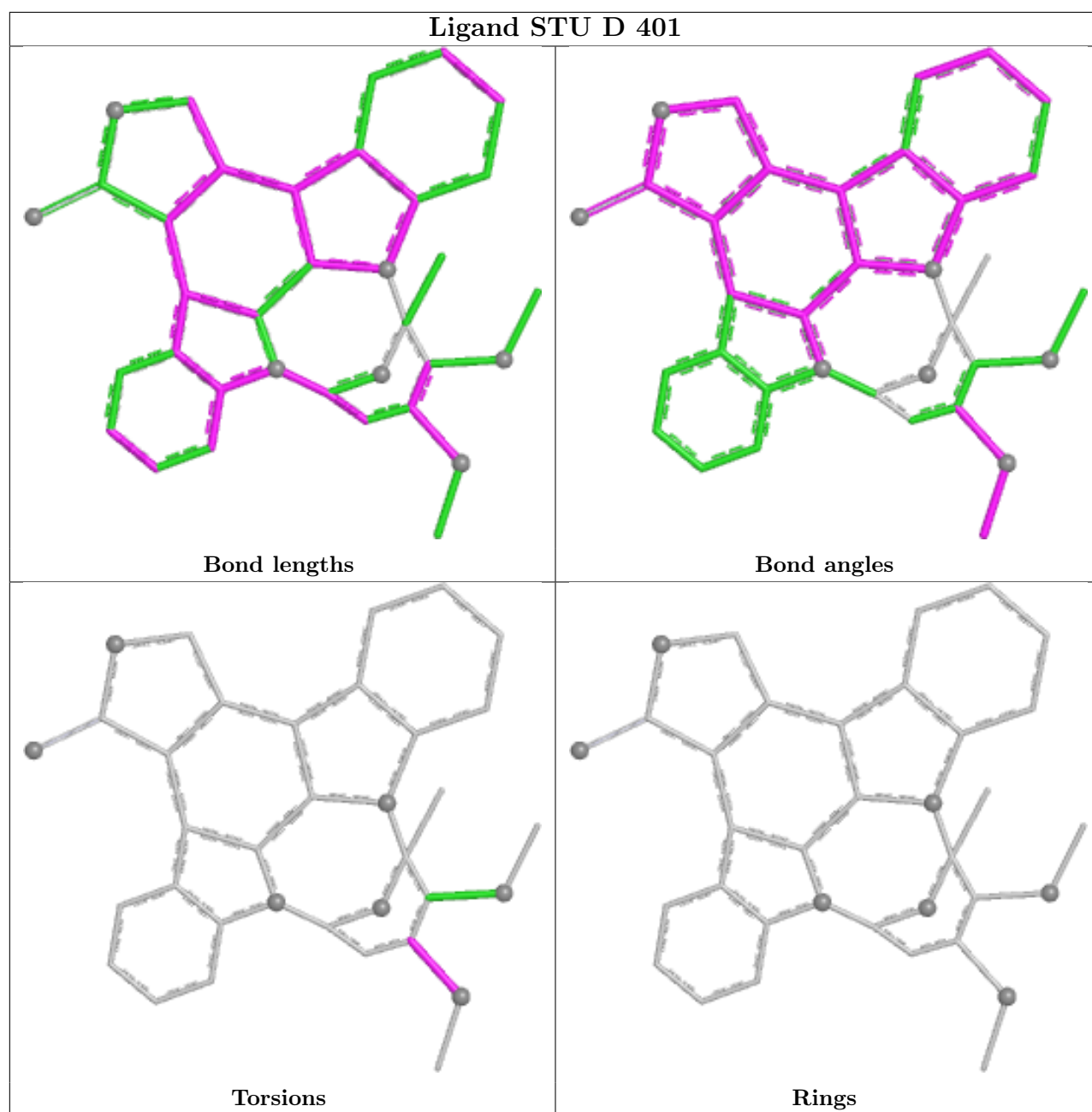
Bond angles



Torsions



Rings



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.