



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:16 PM UTC

PDB ID : 5TV3 / pdb_00005tv3
Title : Crystal structure of the complex of Helicobacter pylori alpha-carbonic anhydrase with (E)-5-(((4-(tert-butyl)phenyl)sulfonyl)imino)-4-methyl-4,5-dihydro-1,3,4-thiadiazole-2-sulfonamide
Authors : Modak, J.K.; Roujeinikova, A.
Deposited on : 2016-11-07
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

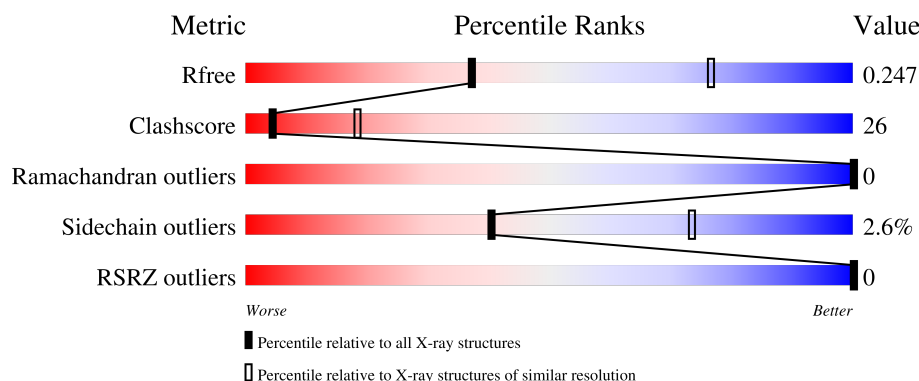
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



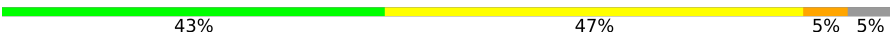
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	234	
1	B	234	
1	C	234	
1	D	234	

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Mol	Chain	Length	Quality of chain
1	E	234	
1	F	234	
1	G	234	
1	H	234	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CL	D	302	-	-	X	-
5	CL	G	302	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 14830 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 Alpha-carbonic anhydrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	2	0
			1857	1192	325	336	4			
1	B	218	Total	C	N	O	S	0	1	0
			1787	1147	312	324	4			
1	C	225	Total	C	N	O	S	0	2	0
			1848	1186	323	335	4			
1	D	220	Total	C	N	O	S	0	0	0
			1801	1157	316	324	4			
1	E	226	Total	C	N	O	S	0	1	0
			1853	1188	325	336	4			
1	F	222	Total	C	N	O	S	0	0	0
			1815	1164	318	329	4			
1	G	222	Total	C	N	O	S	0	1	0
			1820	1166	319	331	4			
1	H	225	Total	C	N	O	S	0	0	0
			1841	1180	323	334	4			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

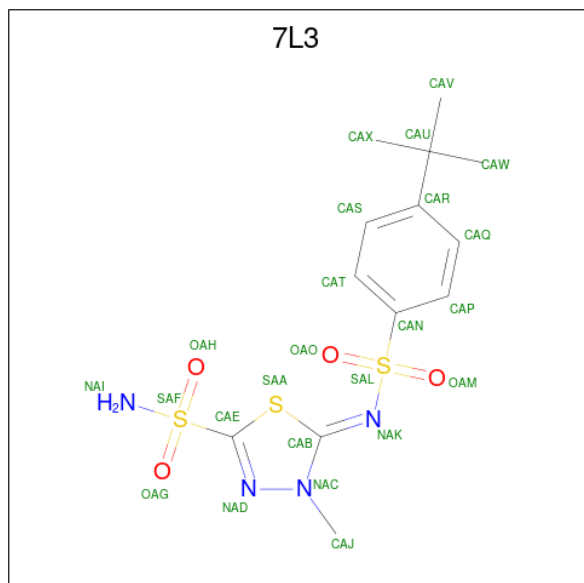
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

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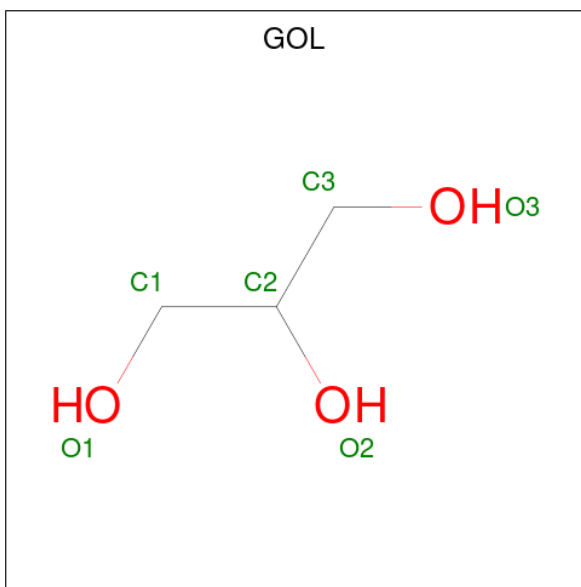
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Zn	0	0
			1	1		
2	H	1	Total	Zn	0	0
			1	1		

- Molecule 3 is (5Z)-5-[[[(4-tert-butylphenyl)sulfonyl]imino}-4-methyl-4,5-dihydro-1,3,4-thiadiazole-2-sulfonamide (CCD ID: 7L3) (formula: $C_{13}H_{18}N_4O_4S_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			24	13	4	4	3		
3	B	1	Total	C	N	O	S	0	0
			24	13	4	4	3		
3	C	1	Total	C	N	O	S	0	0
			24	13	4	4	3		
3	D	1	Total	C	N	O	S	0	0
			24	13	4	4	3		
3	E	1	Total	C	N	O	S	0	0
			24	13	4	4	3		
3	F	1	Total	C	N	O	S	0	0
			24	13	4	4	3		
3	G	1	Total	C	N	O	S	0	0
			24	13	4	4	3		
3	H	1	Total	C	N	O	S	0	0
			24	13	4	4	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		

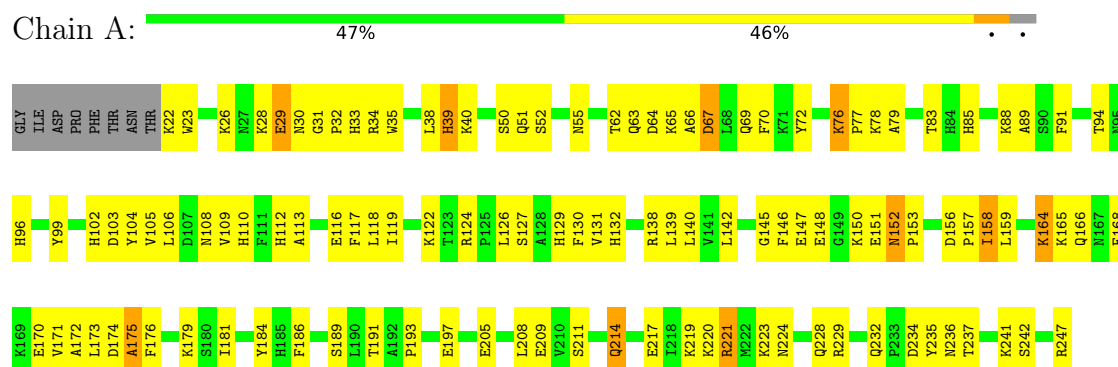
- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Cl	0	0
			1	1		
5	G	1	Total	Cl	0	0
			1	1		

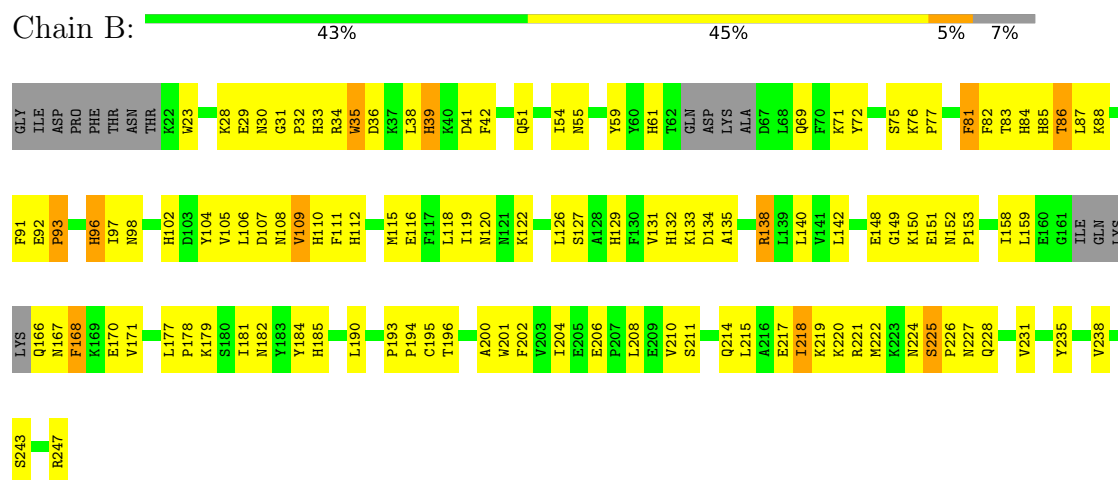
3 Residue-property plots

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

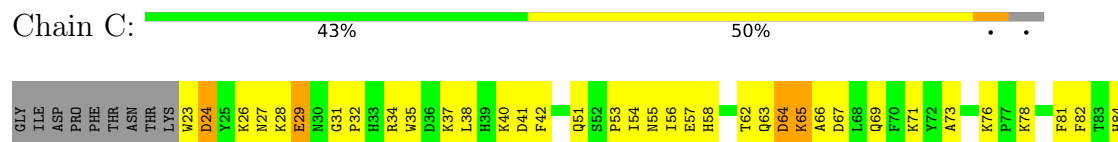
• Molecule 1: Alpha-carbonic anhydrase



• Molecule 1: Alpha-carbonic anhydrase



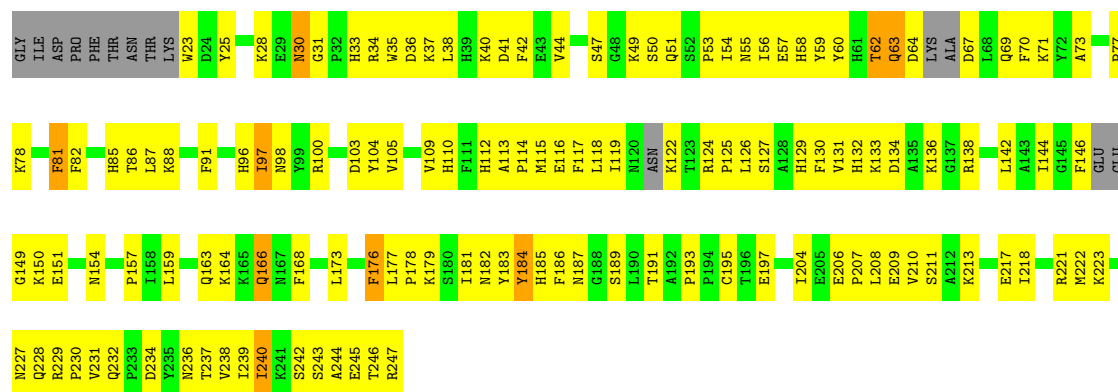
• Molecule 1: Alpha-carbonic anhydrase





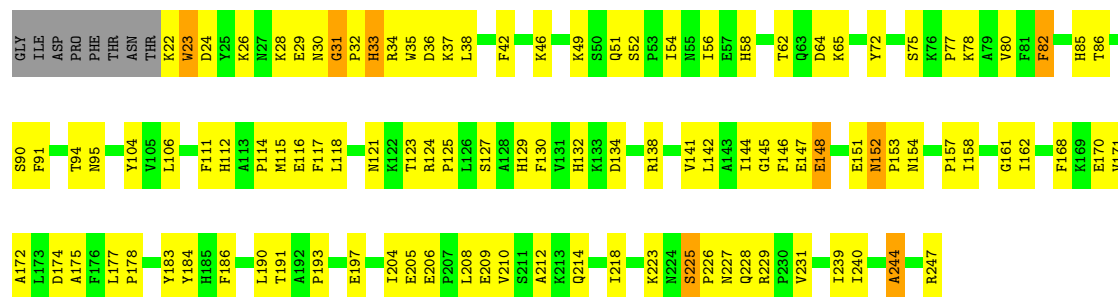
• Molecule 1: Alpha-carbonic anhydrase

Chain D: 36% 54% 6%



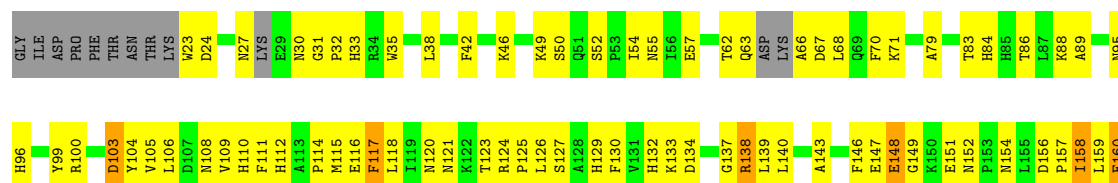
• Molecule 1: Alpha-carbonic anhydrase

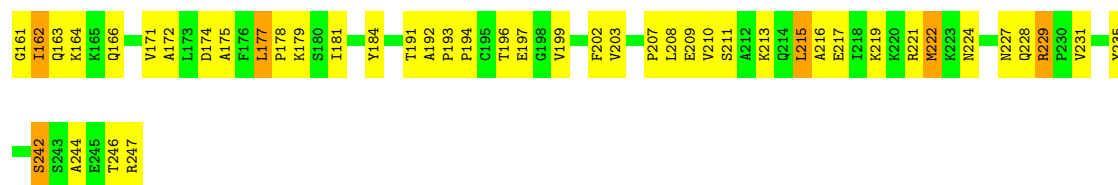
Chain E: 51% 42%



• Molecule 1: Alpha-carbonic anhydrase

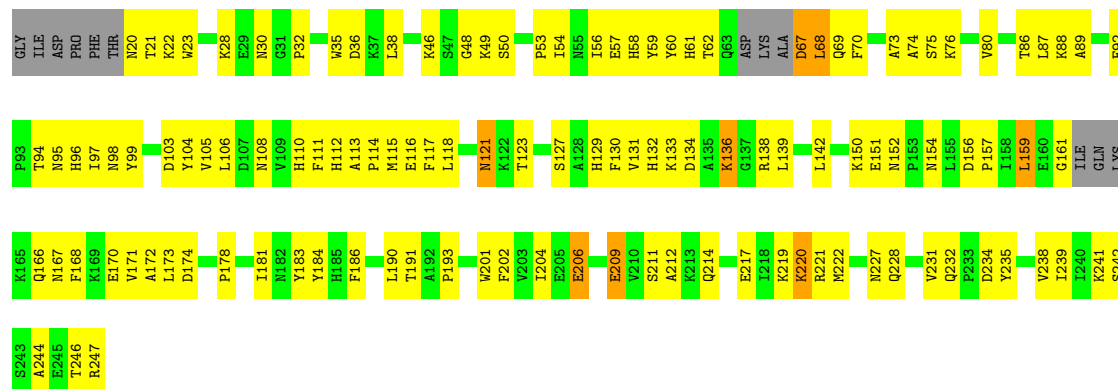
Chain F: 43% 47% 5% 5%





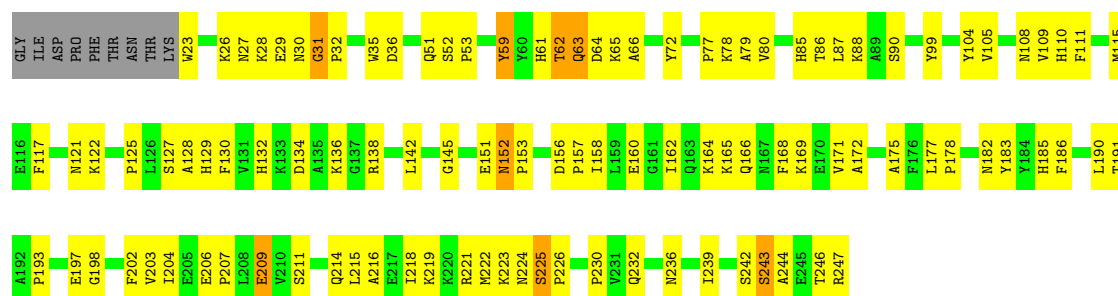
• Molecule 1: Alpha-carbonic anhydrase

Chain G: 44% 48% 5%



• Molecule 1: Alpha-carbonic anhydrase

Chain H: 51% 42%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.56Å 133.89Å 166.60Å 90.00° 90.30° 90.00°	Depositor
Resolution (Å)	29.94 – 2.90 29.94 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.94-2.90) 97.2 (29.94-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.187 , 0.243 0.183 , 0.247	Depositor DCC
R_{free} test set	2006 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 31.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.447 for h,-k,-l	Xtriage
Reported twinning fraction	0.500 for h,-k,-l	Depositor
Outliers	1 of 39903 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14830	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, GOL, CL, 7L3

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	0.67	0/1918	1.20	19/2594 (0.7%)
1	B	0.70	0/1843	1.17	12/2492 (0.5%)
1	C	0.75	0/1909	1.21	19/2583 (0.7%)
1	D	0.73	0/1853	1.12	10/2503 (0.4%)
1	E	0.75	0/1911	1.24	15/2584 (0.6%)
1	F	0.67	0/1868	1.21	19/2526 (0.8%)
1	G	0.67	0/1876	1.17	14/2536 (0.6%)
1	H	0.72	0/1896	1.19	16/2565 (0.6%)
All	All	0.71	0/15074	1.19	124/20383 (0.6%)

There are no bond length outliers.

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	62	THR	N-CA-C	-11.06	93.45	108.38
1	E	31	GLY	CA-C-N	10.02	130.30	119.28
1	E	31	GLY	C-N-CA	10.02	130.30	119.28
1	E	65	LYS	N-CA-C	-9.93	101.17	113.38
1	C	31	GLY	CA-C-N	9.26	130.21	119.47
1	C	31	GLY	C-N-CA	9.26	130.21	119.47
1	B	152	ASN	CA-C-N	9.20	129.44	119.87
1	B	152	ASN	C-N-CA	9.20	129.44	119.87
1	D	62	THR	N-CA-C	9.17	120.01	108.19
1	B	28	LYS	N-CA-C	9.04	116.20	108.78
1	E	23	TRP	N-CA-C	8.80	123.30	110.28
1	F	158	ILE	N-CA-C	-8.66	104.36	111.81
1	D	49	LYS	N-CA-C	-8.21	103.28	113.38
1	H	225	SER	CA-C-N	7.94	129.76	119.84
1	H	225	SER	C-N-CA	7.94	129.76	119.84
1	G	156	ASP	CA-C-N	-7.80	111.76	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	156	ASP	C-N-CA	-7.80	111.76	119.87
1	A	181	ILE	N-CA-C	7.80	119.55	108.17
1	C	170	GLU	N-CA-C	7.78	120.93	110.35
1	F	222	MET	N-CA-C	-7.70	102.40	112.41
1	E	152	ASN	CA-C-N	7.54	127.71	119.87
1	E	152	ASN	C-N-CA	7.54	127.71	119.87
1	A	39	HIS	N-CA-C	-7.32	98.17	109.52
1	G	28	LYS	N-CA-C	7.26	114.73	108.78
1	C	29	GLU	N-CA-C	-7.22	103.02	112.41
1	A	67	ASP	N-CA-C	7.17	119.77	111.02
1	C	40	LYS	N-CA-C	-7.11	104.61	113.28
1	F	162	ILE	N-CA-C	-7.03	103.06	113.39
1	F	161	GLY	N-CA-C	-6.99	106.16	115.32
1	F	242	SER	N-CA-C	6.93	117.18	108.45
1	F	160	GLU	N-CA-C	-6.89	104.90	113.38
1	H	62	THR	N-CA-C	6.85	118.19	108.74
1	G	244	ALA	N-CA-C	6.83	118.16	108.74
1	G	220	LYS	N-CA-C	-6.64	104.65	112.89
1	A	94	THR	N-CA-C	-6.62	105.11	113.72
1	H	31	GLY	CA-C-N	6.58	126.52	119.28
1	H	31	GLY	C-N-CA	6.58	126.52	119.28
1	A	29	GLU	N-CA-C	-6.57	104.74	112.89
1	D	30	ASN	N-CA-C	-6.53	104.89	112.92
1	C	124	ARG	N-CA-C	-6.45	100.58	110.32
1	G	48	GLY	N-CA-C	6.45	120.31	111.54
1	A	175	ALA	N-CA-C	-6.41	103.91	112.94
1	C	28	LYS	CA-C-O	6.41	121.66	117.94
1	E	94	THR	N-CA-C	-6.39	105.52	113.38
1	A	40	LYS	N-CA-C	-6.37	105.26	113.16
1	C	26	LYS	N-CA-C	6.21	118.72	110.53
1	C	131	VAL	N-CA-C	6.17	117.19	108.36
1	F	108	ASN	N-CA-C	6.16	116.69	108.38
1	B	31	GLY	CA-C-N	6.15	126.60	119.47
1	B	31	GLY	C-N-CA	6.15	126.60	119.47
1	D	166	GLN	N-CA-C	6.13	117.46	107.23
1	H	156	ASP	CA-C-N	-6.09	113.53	119.87
1	H	156	ASP	C-N-CA	-6.09	113.53	119.87
1	C	96	HIS	N-CA-C	6.09	118.96	109.52
1	E	225	SER	CA-C-N	6.05	127.00	119.98
1	E	225	SER	C-N-CA	6.05	127.00	119.98
1	G	28	LYS	CB-CA-C	-6.03	108.38	117.07
1	G	209	GLU	N-CA-C	6.03	119.72	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	PHE	N-CA-C	6.02	117.69	108.42
1	C	219	LYS	N-CA-C	-5.99	105.24	112.54
1	H	160	GLU	N-CA-C	-5.98	105.98	113.28
1	H	158	ILE	N-CA-C	5.98	117.35	111.67
1	C	225	SER	CA-C-N	5.96	127.29	119.84
1	C	225	SER	C-N-CA	5.96	127.29	119.84
1	C	158	ILE	N-CA-C	-5.93	106.71	111.81
1	A	164	LYS	N-CA-C	5.91	118.39	109.23
1	F	231	VAL	N-CA-C	5.88	117.31	109.37
1	G	28	LYS	CA-C-O	5.79	121.30	117.94
1	H	203	VAL	N-CA-C	5.79	116.20	107.75
1	G	121	ASN	CA-C-N	-5.79	114.73	122.72
1	G	121	ASN	C-N-CA	-5.79	114.73	122.72
1	A	221	ARG	N-CA-C	-5.79	106.20	113.20
1	F	151	GLU	N-CA-C	5.77	118.83	110.28
1	A	158	ILE	N-CA-C	5.73	116.74	111.81
1	G	212	ALA	N-CA-C	-5.70	105.58	112.54
1	B	96	HIS	N-CA-C	5.70	118.35	109.52
1	E	117	PHE	N-CA-C	5.64	119.43	109.96
1	A	65	LYS	N-CA-C	-5.62	106.01	112.92
1	B	35	TRP	N-CA-C	5.60	118.15	111.71
1	F	38	LEU	N-CA-C	-5.59	105.09	111.07
1	C	163	GLN	N-CA-C	-5.56	106.47	113.20
1	B	93	PRO	CA-C-O	-5.56	117.20	121.31
1	G	121	ASN	N-CA-C	5.51	119.83	113.38
1	A	152	ASN	CA-C-N	5.49	125.10	119.56
1	A	152	ASN	C-N-CA	5.49	125.10	119.56
1	A	33	HIS	N-CA-C	-5.48	105.33	112.23
1	F	177	LEU	CA-C-N	5.47	125.41	119.78
1	F	177	LEU	C-N-CA	5.47	125.41	119.78
1	H	152	ASN	CA-C-N	5.46	125.55	119.87
1	H	152	ASN	C-N-CA	5.46	125.55	119.87
1	E	174	ASP	N-CA-C	-5.45	106.61	113.20
1	A	76	LYS	CA-C-N	5.45	125.37	119.76
1	A	76	LYS	C-N-CA	5.45	125.37	119.76
1	H	72	TYR	N-CA-C	5.43	117.88	110.55
1	D	223	LYS	N-CA-C	5.42	119.19	112.58
1	C	24	ASP	N-CA-C	5.42	116.21	108.74
1	A	214	GLN	N-CA-C	-5.41	105.04	111.69
1	D	31	GLY	CA-C-N	5.39	125.21	119.28
1	D	31	GLY	C-N-CA	5.39	125.21	119.28
1	C	64	ASP	N-CA-C	5.39	117.49	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	144	ILE	N-CA-C	5.39	116.13	108.42
1	C	139	LEU	N-CA-C	5.36	118.48	109.95
1	H	121	ASN	N-CA-C	5.35	119.39	112.86
1	A	145	GLY	N-CA-C	5.32	121.29	112.89
1	B	225	SER	CA-C-N	5.31	126.14	119.98
1	B	225	SER	C-N-CA	5.31	126.14	119.98
1	D	78	LYS	N-CA-C	-5.29	105.69	111.82
1	F	31	GLY	CA-C-N	5.29	125.60	119.47
1	F	31	GLY	C-N-CA	5.29	125.60	119.47
1	H	244	ALA	N-CA-C	5.27	115.50	108.38
1	H	122	LYS	N-CA-C	5.25	117.80	109.24
1	E	33	HIS	N-CA-C	-5.23	106.00	112.38
1	G	68	LEU	N-CA-C	5.21	118.05	109.76
1	A	70	PHE	N-CA-C	5.18	116.85	108.41
1	C	37	LYS	N-CA-C	-5.16	106.74	112.57
1	B	158	ILE	N-CA-C	-5.15	107.38	111.81
1	F	216	ALA	N-CA-C	5.15	116.97	111.36
1	F	117	PHE	N-CA-C	5.14	118.60	109.96
1	D	63	GLN	N-CA-C	5.11	118.48	109.80
1	E	244	ALA	N-CA-C	5.09	115.25	108.38
1	F	229	ARG	CA-C-N	5.09	125.37	119.92
1	F	229	ARG	C-N-CA	5.09	125.37	119.92
1	E	148	GLU	N-CA-C	5.05	117.63	110.50
1	F	215	LEU	N-CA-C	5.05	117.44	111.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1857	0	1825	98	0
1	B	1787	0	1739	95	1
1	C	1848	0	1812	103	0
1	D	1801	0	1759	125	0
1	E	1853	0	1816	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1815	0	1766	98	0
1	G	1820	0	1773	107	0
1	H	1841	0	1798	79	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	24	0	0	3	0
3	B	24	0	0	3	0
3	C	24	0	0	3	0
3	D	24	0	0	3	0
3	E	24	0	0	2	0
3	F	24	0	0	4	0
3	G	24	0	0	2	0
3	H	24	0	0	2	0
4	C	6	0	8	1	0
5	D	1	0	0	2	0
5	G	1	0	0	2	0
All	All	14830	0	14296	768	1

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 26.

All (768) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:LEU:HD12	1:D:246:THR:CG2	1.68	1.21
1:D:177:LEU:HD12	1:D:246:THR:HG21	1.29	1.11
1:D:177:LEU:HD12	1:D:246:THR:HG23	1.47	0.97
1:A:102:HIS:HB3	1:A:138:ARG:HH22	1.31	0.96
1:B:41:ASP:HA	1:D:40:LYS:HE3	1.50	0.94
1:B:87:LEU:H	1:B:222:MET:HE2	1.34	0.93
1:D:177:LEU:CD1	1:D:246:THR:HG21	2.00	0.89
1:B:111:PHE:HB2	1:B:222:MET:HE1	1.55	0.89
1:B:72:TYR:OH	1:B:132:HIS:NE2	2.06	0.88
1:D:177:LEU:HB2	1:D:246:THR:HG21	1.54	0.88
1:H:130:PHE:HB2	1:H:142:LEU:HB3	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:23:TRP:HA	1:F:30:ASN:HB3	1.56	0.86
1:E:115:MET:O	1:E:228:GLN:NE2	2.09	0.84
1:C:71:LYS:NZ	1:C:103:ASP:OD2	2.12	0.83
1:C:219:LYS:O	1:C:224:ASN:N	2.10	0.83
1:G:157:PRO:HB2	1:G:171:VAL:HG22	1.61	0.83
1:A:219:LYS:O	1:A:224:ASN:N	2.11	0.82
1:B:177:LEU:O	1:B:247:ARG:NH1	2.12	0.82
1:E:191:THR:OG1	3:E:302:7L3:NAI	2.12	0.81
1:C:159:LEU:HD21	1:C:218:ILE:HG22	1.62	0.81
1:D:54:ILE:HA	1:D:231:VAL:HG13	1.61	0.80
1:G:115:MET:HG3	1:G:127:SER:HB3	1.63	0.80
1:D:149:GLY:N	1:D:210:VAL:O	2.15	0.79
1:B:71:LYS:HB2	1:B:96:HIS:H	1.47	0.78
1:F:104:TYR:HB3	1:F:132:HIS:HB3	1.65	0.78
1:G:136:LYS:HE3	1:G:138:ARG:HG3	1.66	0.77
1:C:32:PRO:HA	1:C:35:TRP:CG	2.19	0.77
1:E:157:PRO:HB2	1:E:171:VAL:HG22	1.66	0.77
1:G:118:LEU:HD23	1:G:121:ASN:HA	1.66	0.77
1:G:76:LYS:HB2	1:G:170:GLU:HG2	1.66	0.77
1:B:33:HIS:CD2	1:B:34:ARG:HG3	2.20	0.77
1:H:151:GLU:HG2	1:H:211:SER:HB3	1.66	0.77
1:D:204:ILE:HG22	1:D:206:GLU:H	1.49	0.76
1:D:23:TRP:HA	1:D:30:ASN:HB3	1.66	0.76
1:C:191:THR:OG1	3:C:303:7L3:NAI	2.18	0.76
1:A:119:ILE:HD13	1:A:205:GLU:HA	1.67	0.75
1:C:71:LYS:HD2	1:C:96:HIS:HB2	1.68	0.75
1:F:219:LYS:O	1:F:224:ASN:N	2.17	0.74
1:D:150:LYS:H	1:D:209:GLU:HG2	1.52	0.74
1:A:152:ASN:ND2	1:A:209:GLU:O	2.21	0.74
1:H:62:THR:OG1	1:H:63:GLN:N	2.19	0.73
1:H:204:ILE:HG22	1:H:206:GLU:H	1.53	0.73
1:D:36:ASP:OD2	1:D:37:LYS:NZ	2.21	0.73
1:E:23:TRP:HA	1:E:30:ASN:HB3	1.70	0.73
1:E:172:ALA:HB1	1:E:175:ALA:HB3	1.69	0.73
1:B:75:SER:O	1:B:171:VAL:N	2.20	0.73
1:C:178:PRO:O	1:C:246:THR:OG1	2.05	0.73
1:E:204:ILE:HG22	1:E:206:GLU:H	1.53	0.73
1:B:134:ASP:CG	1:B:135:ALA:H	1.97	0.72
1:B:102:HIS:HB3	1:B:134:ASP:OD1	1.89	0.72
1:C:24:ASP:O	1:C:35:TRP:NE1	2.19	0.72
1:G:178:PRO:HG2	1:G:206:GLU:HG3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:156:ASP:O	1:F:160:GLU:N	2.18	0.71
1:G:54:ILE:HA	1:G:231:VAL:HG13	1.71	0.71
1:D:28:LYS:O	1:D:33:HIS:NE2	2.24	0.71
1:C:115:MET:HG3	1:C:127:SER:HB3	1.70	0.71
1:F:160:GLU:HA	1:F:163:GLN:HB2	1.73	0.71
1:F:181:ILE:HD11	1:F:244:ALA:O	1.91	0.70
1:F:217:GLU:O	1:F:221:ARG:N	2.24	0.70
1:B:82:PHE:HA	1:B:87:LEU:HA	1.72	0.70
1:F:139:LEU:HB2	1:F:199:VAL:HG22	1.74	0.70
1:H:214:GLN:O	1:H:218:ILE:HG13	1.90	0.70
1:A:148:GLU:O	1:F:179:LYS:NZ	2.25	0.70
1:D:130:PHE:HB3	1:D:132:HIS:HE1	1.56	0.69
1:D:230:PRO:O	1:D:232:GLN:NE2	2.24	0.69
1:C:54:ILE:HA	1:C:231:VAL:HG13	1.75	0.69
1:G:234:ASP:O	1:H:138:ARG:NH2	2.25	0.69
1:A:39:HIS:ND1	1:C:41:ASP:OD2	2.23	0.69
1:H:177:LEU:O	1:H:247:ARG:NH1	2.26	0.69
1:C:118:LEU:HD22	1:C:123:THR:HA	1.75	0.68
1:C:104:TYR:HB3	1:C:132:HIS:HB3	1.74	0.68
1:F:184:TYR:N	1:F:203:VAL:O	2.22	0.68
1:B:23:TRP:O	1:B:85:HIS:NE2	2.27	0.67
1:D:71:LYS:HB2	1:D:96:HIS:HB2	1.76	0.67
1:D:62:THR:OG1	1:D:63:GLN:N	2.27	0.67
1:E:82:PHE:CE2	1:E:85:HIS:HA	2.28	0.67
1:G:74:ALA:HA	1:G:172:ALA:HA	1.76	0.67
1:A:72:TYR:OH	1:A:132:HIS:NE2	2.19	0.67
1:H:219:LYS:O	1:H:224:ASN:N	2.17	0.66
1:D:33:HIS:ND1	1:D:34:ARG:HG3	2.10	0.66
1:D:159:LEU:HD21	1:D:218:ILE:HG12	1.78	0.66
1:G:73:ALA:H	1:G:95:ASN:ND2	1.93	0.66
1:B:96:HIS:CD2	1:B:105:VAL:HG22	2.30	0.66
1:A:174:ASP:O	1:A:247:ARG:HD3	1.96	0.66
1:D:181:ILE:O	1:D:244:ALA:N	2.26	0.66
1:H:29:GLU:HG3	1:H:30:ASN:H	1.60	0.66
1:A:62:THR:OG1	1:A:63:GLN:OE1	2.14	0.65
1:A:116:GLU:HG2	1:A:228:GLN:HG3	1.78	0.65
1:E:54:ILE:HA	1:E:231:VAL:HG13	1.76	0.65
1:E:178:PRO:HD3	1:E:208:LEU:HD21	1.78	0.65
1:D:177:LEU:CB	1:D:246:THR:HG21	2.25	0.65
1:G:73:ALA:H	1:G:95:ASN:HD22	1.44	0.65
1:C:66:ALA:O	1:C:69:GLN:NE2	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:LEU:O	1:E:247:ARG:NH1	2.29	0.65
1:G:59:TYR:HB3	1:G:239:ILE:HB	1.79	0.65
1:C:186:PHE:HA	1:D:238:VAL:HG21	1.78	0.65
1:C:29:GLU:HA	1:C:34:ARG:HE	1.63	0.64
1:F:110:HIS:CE1	1:F:129:HIS:HB2	2.32	0.64
1:F:191:THR:OG1	3:F:302:7L3:NAI	2.31	0.64
1:A:28:LYS:O	1:A:34:ARG:NH1	2.30	0.64
1:D:177:LEU:CD1	1:D:246:THR:CG2	2.58	0.64
1:G:57:GLU:HG3	1:G:58:HIS:ND1	2.13	0.64
1:A:76:LYS:HG2	1:A:170:GLU:HG2	1.80	0.64
1:A:156:ASP:OD1	1:A:214:GLN:NE2	2.30	0.64
1:C:51:GLN:HB3	1:C:232:GLN:HG3	1.80	0.64
1:A:23:TRP:O	1:A:85:HIS:NE2	2.31	0.64
1:B:185:HIS:HA	1:B:201:TRP:O	1.97	0.64
1:A:96:HIS:ND1	1:A:105:VAL:HG22	2.13	0.63
1:G:150:LYS:HG3	1:G:151:GLU:H	1.63	0.63
1:A:151:GLU:HA	1:A:211:SER:HB3	1.81	0.63
1:C:96:HIS:ND1	1:C:105:VAL:HG22	2.14	0.63
1:F:49:LYS:N	1:F:197:GLU:OE2	2.31	0.63
1:A:130:PHE:HB2	1:A:142:LEU:HB3	1.79	0.63
1:C:64:ASP:H	1:H:65:LYS:HB2	1.62	0.63
1:G:32:PRO:HA	1:G:35:TRP:CD2	2.34	0.63
1:A:119:ILE:HG21	1:A:205:GLU:HG3	1.79	0.63
1:H:157:PRO:HB2	1:H:171:VAL:HG22	1.79	0.63
1:A:124:ARG:NH2	1:A:205:GLU:O	2.32	0.63
1:G:69:GLN:HG3	1:G:70:PHE:N	2.12	0.63
1:C:55:ASN:ND2	1:C:57:GLU:OE1	2.28	0.63
1:G:112:HIS:HA	1:G:227:ASN:ND2	2.14	0.63
1:B:30:ASN:HA	1:B:38:LEU:HD11	1.80	0.62
1:E:130:PHE:HB2	1:E:142:LEU:HB3	1.79	0.62
1:F:33:HIS:O	1:F:46:LYS:HE2	2.00	0.62
1:F:156:ASP:HA	1:F:159:LEU:HB2	1.79	0.62
1:F:146:PHE:CE1	1:F:208:LEU:HB2	2.34	0.62
1:F:177:LEU:HB2	1:F:247:ARG:HH22	1.64	0.62
1:E:32:PRO:HA	1:E:35:TRP:CG	2.35	0.62
1:G:159:LEU:HD11	1:G:217:GLU:HG2	1.81	0.62
1:E:104:TYR:HB3	1:E:132:HIS:HB3	1.81	0.62
1:G:112:HIS:HA	1:G:227:ASN:HD21	1.64	0.62
1:E:24:ASP:OD1	1:E:30:ASN:HB2	2.00	0.62
1:F:118:LEU:HD23	1:F:121:ASN:HA	1.81	0.62
1:G:53:PRO:HG3	1:G:116:GLU:HB3	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:PRO:HG2	1:B:196:THR:OG1	2.00	0.62
1:E:35:TRP:CH2	1:E:193:PRO:HD3	2.35	0.62
1:B:54:ILE:HA	1:B:231:VAL:HG13	1.81	0.61
1:H:152:ASN:HB2	1:H:209:GLU:O	1.99	0.61
1:D:62:THR:OG1	1:D:63:GLN:OE1	2.19	0.61
1:G:134:ASP:OD1	1:G:138:ARG:N	2.33	0.61
1:B:134:ASP:CG	1:B:135:ALA:N	2.55	0.61
1:E:86:THR:OG1	1:E:111:PHE:O	2.18	0.61
1:C:124:ARG:NH1	1:C:207:PRO:HB3	2.16	0.61
1:C:152:ASN:HB3	1:C:155:LEU:HG	1.83	0.61
1:D:113:ALA:HB2	1:D:126:LEU:HD13	1.83	0.61
1:A:191:THR:OG1	3:A:302:7L3:NAI	2.33	0.61
1:A:102:HIS:HB3	1:A:138:ARG:NH2	2.11	0.61
1:G:23:TRP:HA	1:G:30:ASN:HB3	1.83	0.60
1:H:86:THR:OG1	1:H:111:PHE:O	2.15	0.60
1:A:236:ASN:OD1	1:B:138:ARG:NH2	2.34	0.60
1:B:69:GLN:HB3	1:B:98:ASN:HB3	1.82	0.60
1:D:182:ASN:HA	1:D:243:SER:HA	1.84	0.60
1:G:80:VAL:HG12	1:G:87:LEU:HD11	1.83	0.60
1:B:87:LEU:N	1:B:222:MET:HE2	2.11	0.60
1:C:164:LYS:HE2	1:C:166:GLN:O	2.02	0.60
1:G:142:LEU:HD12	1:G:202:PHE:HB2	1.82	0.60
1:B:29:GLU:HA	1:B:34:ARG:HD3	1.82	0.60
1:D:189:SER:HA	1:D:197:GLU:HA	1.84	0.60
1:E:124:ARG:HG3	1:E:145:GLY:HA3	1.83	0.60
1:B:59:TYR:HE1	1:B:61:HIS:CE1	2.20	0.60
1:E:144:ILE:HB	1:E:204:ILE:HD12	1.84	0.60
1:F:124:ARG:CZ	1:F:207:PRO:HG3	2.31	0.60
1:G:105:VAL:O	1:G:132:HIS:HA	2.02	0.60
1:C:81:PHE:HA	1:C:162:ILE:HD13	1.84	0.59
1:G:21:THR:HG22	1:G:22:LYS:H	1.66	0.59
1:G:116:GLU:HA	1:G:228:GLN:HG3	1.83	0.59
1:A:29:GLU:HA	1:A:34:ARG:NH1	2.17	0.59
1:F:172:ALA:HB1	1:F:175:ALA:HB3	1.85	0.59
1:G:62:THR:OG1	1:H:61:HIS:O	2.06	0.59
1:H:87:LEU:H	1:H:222:MET:HE2	1.66	0.59
1:D:88:LYS:NZ	3:D:303:7L3:OAM	2.35	0.59
1:G:130:PHE:HB2	1:G:142:LEU:HB3	1.83	0.59
1:B:179:LYS:HE2	1:B:247:ARG:HE	1.68	0.59
1:H:164:LYS:NZ	1:H:166:GLN:HB3	2.17	0.59
1:A:91:PHE:HE2	1:A:109[B]:VAL:HG12	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:111:PHE:HD2	1:F:126:LEU:HD11	1.68	0.59
1:C:86:THR:OG1	1:C:111:PHE:O	2.21	0.59
1:F:177:LEU:HB2	1:F:247:ARG:NH2	2.17	0.59
1:G:49:LYS:HB3	1:H:198:GLY:HA3	1.85	0.58
1:E:134:ASP:OD1	1:E:138:ARG:N	2.36	0.58
1:A:126:LEU:HB3	1:A:146:PHE:HB2	1.85	0.58
1:C:157:PRO:HB2	1:C:171:VAL:HG22	1.85	0.58
1:G:87:LEU:HD22	1:G:221:ARG:HD2	1.84	0.58
1:G:97:ILE:HD11	1:G:142:LEU:HD22	1.85	0.58
1:C:148:GLU:HA	1:C:210:VAL:O	2.03	0.58
1:D:64:ASP:OD1	1:D:183:TYR:OH	2.16	0.58
1:F:63:GLN:N	1:F:63:GLN:OE1	2.36	0.58
1:G:219:LYS:HG2	1:G:222:MET:HE2	1.85	0.58
1:H:134:ASP:OD1	1:H:138:ARG:N	2.37	0.58
1:H:151:GLU:HG2	1:H:211:SER:CB	2.34	0.58
1:E:115:MET:HG3	1:E:127:SER:HB3	1.85	0.58
1:G:110:HIS:NE2	1:G:129:HIS:HB2	2.18	0.58
1:C:214:GLN:O	1:C:218:ILE:HG23	2.04	0.58
1:F:110:HIS:NE2	1:F:129:HIS:HB2	2.19	0.58
1:G:110:HIS:CE1	1:G:129:HIS:HB2	2.39	0.58
1:A:153:PRO:HA	1:A:156:ASP:OD2	2.04	0.57
1:B:149:GLY:N	1:B:210:VAL:O	2.31	0.57
1:A:104:TYR:HB3	1:A:132:HIS:HB3	1.87	0.57
1:F:95:ASN:HB2	1:F:106:LEU:HB3	1.86	0.57
1:A:165:LYS:HG3	1:A:166:GLN:H	1.68	0.57
1:G:150:LYS:O	1:G:209:GLU:HG2	2.04	0.57
1:H:23:TRP:HA	1:H:30:ASN:CB	2.34	0.57
1:A:173:LEU:HA	1:A:176:PHE:HB2	1.85	0.57
1:E:36:ASP:OD2	1:E:37:LYS:NZ	2.33	0.57
1:F:52:SER:O	1:F:229:ARG:NH1	2.38	0.57
1:B:166:GLN:HG3	1:B:167:ASN:H	1.70	0.57
1:H:183:TYR:CZ	1:H:242:SER:HB3	2.40	0.57
1:A:67:ASP:HB2	1:A:99:TYR:CE1	2.39	0.57
1:D:116:GLU:HG2	1:D:228:GLN:HG3	1.87	0.57
1:C:32:PRO:HA	1:C:35:TRP:CD2	2.39	0.56
1:C:133:LYS:HD3	3:C:303:7L3:CAV	2.35	0.56
1:E:191:THR:O	1:E:229:ARG:HD2	2.05	0.56
1:B:133:LYS:HD2	3:B:302:7L3:CAW	2.35	0.56
1:C:58:HIS:CB	1:D:100:ARG:HH12	2.17	0.56
1:G:130:PHE:HB3	1:G:132:HIS:HE1	1.70	0.56
1:A:62:THR:HG1	1:A:63:GLN:H	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:LEU:HB3	1:B:222:MET:HE2	1.87	0.56
1:B:109:VAL:HA	1:B:129:HIS:O	2.05	0.56
1:B:185:HIS:HE1	1:B:200:ALA:HB1	1.70	0.56
1:D:183:TYR:N	1:D:242:SER:O	2.33	0.56
1:A:159:LEU:HD23	1:A:217:GLU:OE1	2.05	0.56
1:H:80:VAL:HG12	1:H:162:ILE:HD13	1.87	0.56
1:A:172:ALA:HB1	1:A:175:ALA:HB3	1.87	0.56
1:B:76:LYS:HG3	1:B:170:GLU:HG2	1.86	0.56
1:C:218:ILE:O	1:C:222:MET:N	2.39	0.56
1:G:138:ARG:NH1	1:H:236:ASN:OD1	2.38	0.56
1:G:183:TYR:CZ	1:G:242:SER:HB3	2.41	0.56
1:A:219:LYS:HE3	1:A:224:ASN:HD22	1.71	0.56
1:D:115:MET:HG3	1:D:127:SER:HB3	1.86	0.56
1:G:235:TYR:HA	1:H:138:ARG:HH21	1.71	0.56
1:C:142:LEU:HD21	1:C:204:ILE:HD11	1.88	0.56
1:F:116:GLU:OE1	1:F:129:HIS:HE1	1.89	0.56
1:D:35:TRP:CH2	1:D:193:PRO:HD3	2.40	0.56
1:D:119:ILE:O	1:D:122:LYS:N	2.38	0.56
1:B:88:LYS:HE3	1:B:108:ASN:CG	2.31	0.55
1:B:91:PHE:N	1:B:107:ASP:O	2.39	0.55
1:D:146:PHE:HA	1:D:208:LEU:O	2.06	0.55
1:H:164:LYS:HZ2	1:H:166:GLN:HB3	1.71	0.55
3:H:302:7L3:SAA	3:H:302:7L3:OAO	2.64	0.55
1:A:132:HIS:HB2	1:A:140:LEU:HB3	1.88	0.55
1:B:217:GLU:O	1:B:221:ARG:HG2	2.07	0.55
1:C:110:HIS:CE1	1:C:129:HIS:HB2	2.41	0.55
1:F:32:PRO:HA	1:F:35:TRP:CD2	2.41	0.55
1:A:83:THR:HG21	1:A:88:LYS:HD3	1.88	0.55
1:C:236:ASN:O	1:D:187:ASN:ND2	2.30	0.55
1:D:179:LYS:NZ	1:D:245:GLU:OE2	2.39	0.55
1:B:102:HIS:HB3	1:B:134:ASP:CG	2.30	0.55
1:E:26:LYS:C	1:E:28:LYS:H	2.13	0.55
1:B:190:LEU:HD22	3:B:302:7L3:CAE	2.36	0.55
1:C:116:GLU:HG2	1:C:228:GLN:HG3	1.87	0.55
1:E:154:ASN:C	1:E:157:PRO:HD2	2.32	0.55
1:G:75:SER:O	1:G:171:VAL:N	2.25	0.55
1:C:97:ILE:O	1:C:104:TYR:N	2.24	0.55
1:F:116:GLU:HA	1:F:228:GLN:HG3	1.89	0.55
1:D:56:ILE:HG23	1:D:239:ILE:HD13	1.87	0.55
1:E:214:GLN:O	1:E:218:ILE:HG13	2.07	0.55
1:H:219:LYS:HB3	1:H:224:ASN:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:HIS:HE1	1:B:131:VAL:HG21	1.72	0.55
1:B:55:ASN:HB2	1:B:118:LEU:HD12	1.88	0.55
1:B:82:PHE:CE2	1:B:222:MET:HA	2.41	0.54
1:D:69:GLN:O	1:D:97:ILE:HG23	2.08	0.54
1:D:178:PRO:HD3	1:D:208:LEU:HD21	1.88	0.54
1:E:112:HIS:ND1	1:E:116:GLU:OE2	2.41	0.54
1:G:60:TYR:OH	1:H:99:TYR:OH	2.21	0.54
1:B:71:LYS:HD2	1:B:96:HIS:HB2	1.89	0.54
1:C:71:LYS:HB2	1:C:96:HIS:HB2	1.88	0.54
1:F:24:ASP:OD1	1:F:30:ASN:HB2	2.07	0.54
1:E:130:PHE:O	1:E:141:VAL:HA	2.07	0.54
1:F:99:TYR:CZ	1:F:202:PHE:HZ	2.25	0.54
1:A:158:ILE:HD11	1:A:171:VAL:HG22	1.90	0.54
1:C:182:ASN:HB3	1:C:241:LYS:NZ	2.23	0.54
1:F:132:HIS:HB2	1:F:140:LEU:HB3	1.90	0.54
1:G:69:GLN:HG3	1:G:70:PHE:H	1.73	0.54
1:C:187:ASN:ND2	1:D:236:ASN:O	2.39	0.54
1:D:154:ASN:O	1:D:157:PRO:HD2	2.08	0.54
1:A:112:HIS:O	1:A:126:LEU:HD12	2.07	0.54
1:B:82:PHE:CD2	1:B:222:MET:HA	2.43	0.54
1:G:111:PHE:O	1:G:227:ASN:ND2	2.40	0.54
1:G:161:GLY:HA2	1:G:168:PHE:CE1	2.43	0.54
1:A:234:ASP:OD1	1:A:235:TYR:N	2.40	0.54
1:B:116:GLU:HA	1:B:228:GLN:HG3	1.89	0.54
1:C:67:ASP:OD1	1:D:60:TYR:OH	2.25	0.54
1:C:164:LYS:NZ	1:C:167:ASN:O	2.23	0.54
1:B:182:ASN:N	1:B:206:GLU:OE1	2.34	0.53
1:B:215:LEU:O	1:B:219:LYS:HG3	2.08	0.53
1:D:130:PHE:HB3	1:D:132:HIS:CE1	2.38	0.53
1:H:191:THR:N	3:H:302:7L3:OAH	2.33	0.53
1:A:179:LYS:HG3	1:A:247:ARG:HB2	1.89	0.53
3:A:302:7L3:OAO	3:A:302:7L3:SAA	2.66	0.53
1:G:106:LEU:HD11	1:G:108:ASN:O	2.08	0.53
1:G:142:LEU:CD1	1:G:202:PHE:HB2	2.37	0.53
1:H:162:ILE:HG21	1:H:221:ARG:HE	1.72	0.53
1:A:55:ASN:HA	1:A:118:LEU:HB2	1.90	0.53
1:D:63:GLN:N	1:D:63:GLN:OE1	2.41	0.53
1:F:79:ALA:O	1:F:89:ALA:HA	2.08	0.53
1:G:152:ASN:HB2	1:G:209:GLU:O	2.07	0.53
1:A:67:ASP:HB2	1:A:99:TYR:HE1	1.73	0.53
1:G:56:ILE:HG23	1:G:239:ILE:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:TRP:CH2	1:C:193:PRO:HD3	2.43	0.53
1:D:63:GLN:O	1:D:242:SER:OG	2.15	0.53
1:D:182:ASN:H	1:D:206:GLU:CD	2.17	0.53
1:E:33:HIS:C	1:E:46:LYS:HZ1	2.16	0.53
1:E:186:PHE:HB3	1:E:239:ILE:HG12	1.91	0.53
1:F:148:GLU:HA	1:F:210:VAL:O	2.08	0.53
3:D:303:7L3:SAA	3:D:303:7L3:OAO	2.67	0.53
1:E:35:TRP:CZ3	1:E:193:PRO:HD3	2.43	0.53
1:E:151:GLU:O	1:E:153:PRO:HD3	2.09	0.53
1:A:179:LYS:N	1:A:247:ARG:HH21	2.06	0.53
1:B:110:HIS:CE1	1:B:131:VAL:HG21	2.44	0.53
1:A:119:ILE:O	1:A:122:LYS:HB2	2.09	0.53
1:B:115:MET:HG3	1:B:127:SER:HB3	1.91	0.53
1:C:238:VAL:HG21	1:D:186:PHE:HA	1.90	0.52
1:F:181:ILE:HD13	1:F:246:THR:HG23	1.90	0.52
1:G:67:ASP:HB2	1:G:99:TYR:CD1	2.44	0.52
1:H:219:LYS:O	1:H:223:LYS:N	2.43	0.52
1:H:105:VAL:O	1:H:132:HIS:HA	2.10	0.52
1:H:109:VAL:HA	1:H:129:HIS:O	2.09	0.52
1:H:115:MET:HG3	1:H:127:SER:HB3	1.92	0.52
1:B:77:PRO:HD3	1:B:171:VAL:HG23	1.91	0.52
1:D:191:THR:OG1	3:D:303:7L3:NAI	2.42	0.52
1:G:35:TRP:CZ3	1:G:193:PRO:HD3	2.45	0.52
1:C:112:HIS:HA	1:C:227:ASN:HD21	1.74	0.52
1:F:164:LYS:HE2	1:F:166:GLN:OE1	2.10	0.52
1:C:110:HIS:HD2	1:C:112:HIS:NE2	2.07	0.52
1:D:67:ASP:OD1	1:D:67:ASP:N	2.40	0.52
1:E:82:PHE:CD1	1:E:82:PHE:C	2.88	0.52
1:G:95:ASN:CG	1:G:173:LEU:HD12	2.35	0.52
1:G:68:LEU:HA	1:G:98:ASN:O	2.10	0.52
3:G:303:7L3:OAO	3:G:303:7L3:SAA	2.68	0.52
1:A:62:THR:OG1	1:A:63:GLN:N	2.40	0.51
1:D:124:ARG:CZ	1:D:207:PRO:HB3	2.40	0.51
1:B:204:ILE:HG22	1:B:206:GLU:H	1.75	0.51
1:C:76:LYS:HG3	1:C:170:GLU:HG2	1.91	0.51
1:C:128:ALA:O	1:C:143:ALA:HA	2.11	0.51
1:A:150:LYS:H	1:A:209:GLU:HG2	1.75	0.51
1:B:111:PHE:HB2	1:B:222:MET:CE	2.33	0.51
1:B:159:LEU:HD21	1:B:218:ILE:HG12	1.92	0.51
1:D:51:GLN:HB3	1:D:232:GLN:HG3	1.93	0.51
1:F:147:GLU:HG3	1:F:209:GLU:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:THR:N	1:B:86:THR:O	2.30	0.51
1:H:157:PRO:HA	1:H:169:LYS:HE3	1.92	0.51
1:B:88:LYS:HE3	1:B:108:ASN:CB	2.40	0.51
1:E:172:ALA:CB	1:E:175:ALA:HB3	2.40	0.51
1:F:146:PHE:HB3	1:F:210:VAL:HG12	1.93	0.51
1:E:51:GLN:OE1	1:E:229:ARG:NH2	2.38	0.51
1:F:35:TRP:CZ3	1:F:193:PRO:HD3	2.46	0.51
1:F:105:VAL:O	1:F:132:HIS:HA	2.10	0.51
1:G:30:ASN:O	1:G:35:TRP:NE1	2.44	0.51
1:H:52:SER:HB3	1:H:117:PHE:CZ	2.45	0.51
1:H:110:HIS:NE2	1:H:129:HIS:HB2	2.25	0.51
1:A:164:LYS:HG2	1:A:165:LYS:O	2.11	0.51
1:B:83:THR:OG1	1:B:84:HIS:ND1	2.43	0.51
1:D:64:ASP:HB2	1:D:242:SER:OG	2.11	0.51
1:G:115:MET:O	1:G:228:GLN:NE2	2.44	0.51
1:G:133:LYS:HG2	1:G:134:ASP:O	2.11	0.51
1:A:22:LYS:NZ	1:A:30:ASN:OD1	2.43	0.50
1:D:96:HIS:HB3	1:D:103:ASP:OD1	2.10	0.50
1:A:119:ILE:HD12	1:A:124:ARG:HH21	1.76	0.50
1:B:32:PRO:HA	1:B:35:TRP:CD2	2.46	0.50
1:C:63:GLN:OE1	1:G:61:HIS:ND1	2.44	0.50
1:F:217:GLU:OE2	1:F:221:ARG:NH1	2.44	0.50
1:H:26:LYS:C	1:H:28:LYS:H	2.19	0.50
1:A:152:ASN:HB2	1:A:209:GLU:O	2.11	0.50
1:D:183:TYR:CE1	1:D:242:SER:HB3	2.46	0.50
1:F:32:PRO:HA	1:F:35:TRP:CE2	2.47	0.50
1:A:220:LYS:C	1:A:223:LYS:H	2.20	0.50
3:F:302:7L3:OAO	3:F:302:7L3:SAA	2.70	0.50
1:G:104:TYR:HB3	1:G:132:HIS:HB3	1.92	0.50
1:C:58:HIS:HB2	1:D:100:ARG:HH12	1.76	0.50
1:E:146:PHE:HD2	1:E:210:VAL:HB	1.77	0.50
1:H:172:ALA:HB1	1:H:175:ALA:HB3	1.93	0.50
1:D:69:GLN:HB3	1:D:98:ASN:HB3	1.93	0.50
1:H:216:ALA:HA	1:H:219:LYS:HZ1	1.77	0.50
1:G:96:HIS:HB3	1:G:103:ASP:OD1	2.11	0.50
1:A:29:GLU:HA	1:A:34:ARG:HH12	1.75	0.49
1:H:78:LYS:HB2	1:H:90:SER:OG	2.11	0.49
1:A:147:GLU:HG3	1:A:148:GLU:HG2	1.94	0.49
1:D:179:LYS:O	1:D:246:THR:N	2.38	0.49
1:E:29:GLU:HA	1:E:34:ARG:NH2	2.28	0.49
1:E:138:ARG:HD2	1:F:235:TYR:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:GLU:OE2	1:E:212:ALA:HA	2.11	0.49
1:A:51:GLN:HB3	1:A:232:GLN:HG3	1.93	0.49
1:C:116:GLU:HA	1:C:228:GLN:HG3	1.94	0.49
1:C:182:ASN:HB3	1:C:241:LYS:HZ1	1.77	0.49
1:D:82:PHE:CE1	1:D:222:MET:HA	2.47	0.49
1:E:56:ILE:N	1:E:118:LEU:O	2.33	0.49
1:A:146:PHE:HA	1:A:208:LEU:O	2.13	0.49
1:G:30:ASN:HA	1:G:38:LEU:HD11	1.95	0.49
1:H:216:ALA:HA	1:H:219:LYS:NZ	2.27	0.49
1:D:133:LYS:NZ	1:D:134:ASP:O	2.44	0.49
1:H:104:TYR:HB3	1:H:132:HIS:HB3	1.94	0.49
1:C:183:TYR:CZ	1:C:242:SER:HB3	2.48	0.49
1:E:152:ASN:H	1:E:214:GLN:HE22	1.59	0.49
1:F:112:HIS:HA	1:F:227:ASN:ND2	2.28	0.49
1:A:130:PHE:HB3	1:A:132:HIS:CE1	2.48	0.49
1:B:115:MET:HE1	1:B:119:ILE:HD11	1.94	0.49
1:C:23:TRP:HB3	1:C:42:PHE:CE2	2.47	0.49
1:D:30:ASN:HA	1:D:38:LEU:HD11	1.95	0.49
1:D:70:PHE:CE2	1:D:246:THR:HG23	2.48	0.49
1:D:179:LYS:HG3	1:D:247:ARG:HB2	1.95	0.49
1:F:23:TRP:CZ2	1:F:84:HIS:HB3	2.48	0.49
1:F:71:LYS:HB2	1:F:96:HIS:HB2	1.95	0.49
1:B:104:TYR:HB3	1:B:132:HIS:HB3	1.95	0.49
1:E:77:PRO:HD2	1:E:168:PHE:HB3	1.95	0.49
1:F:125:PRO:HD2	1:F:146:PHE:O	2.13	0.49
1:G:106:LEU:HD12	1:G:131:VAL:O	2.13	0.49
1:H:23:TRP:HA	1:H:30:ASN:HB3	1.94	0.49
1:H:186:PHE:HD2	1:H:239:ILE:HG23	1.77	0.49
1:C:82:PHE:CD1	1:C:82:PHE:C	2.91	0.48
3:C:303:7L3:SAA	3:C:303:7L3:OAO	2.70	0.48
1:F:177:LEU:C	1:F:247:ARG:HH22	2.20	0.48
1:F:71:LYS:HD3	1:F:103:ASP:OD2	2.13	0.48
1:H:153:PRO:O	1:H:157:PRO:HD3	2.13	0.48
1:A:157:PRO:HB2	1:A:170:GLU:O	2.13	0.48
1:B:178:PRO:HD3	1:B:208:LEU:HD21	1.96	0.48
1:F:130:PHE:CD1	1:F:130:PHE:N	2.81	0.48
1:G:22:LYS:O	1:G:30:ASN:ND2	2.46	0.48
3:B:302:7L3:SAA	3:B:302:7L3:OAO	2.70	0.48
1:C:183:TYR:CE1	1:C:242:SER:HB3	2.47	0.48
1:D:116:GLU:HA	1:D:228:GLN:HG3	1.95	0.48
1:F:146:PHE:HA	1:F:208:LEU:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:54:ILE:HG22	1:G:232:GLN:O	2.13	0.48
1:H:36:ASP:OD1	1:H:36:ASP:N	2.43	0.48
1:A:79:ALA:HA	1:A:168:PHE:CE1	2.48	0.48
1:B:142:LEU:HD12	1:B:202:PHE:HB2	1.95	0.48
1:H:32:PRO:HA	1:H:35:TRP:CG	2.49	0.48
1:C:192:ALA:O	1:C:195:CYS:N	2.41	0.48
1:C:112:HIS:HA	1:C:227:ASN:ND2	2.29	0.48
1:E:78:LYS:HB2	1:E:90:SER:HB2	1.95	0.48
1:E:223:LYS:HD2	1:E:223:LYS:N	2.29	0.48
1:F:111:PHE:O	1:F:227:ASN:ND2	2.46	0.48
1:B:179:LYS:HG2	1:B:247:ARG:NE	2.29	0.48
1:E:23:TRP:CZ3	1:E:193:PRO:HD2	2.49	0.48
1:A:147:GLU:HG3	1:A:148:GLU:N	2.28	0.47
1:E:58:HIS:CD2	1:F:100:ARG:HH12	2.31	0.47
1:E:190:LEU:O	1:E:229:ARG:NH1	2.47	0.47
1:A:67:ASP:N	1:A:67:ASP:OD1	2.46	0.47
1:B:220:LYS:HA	1:B:224:ASN:H	1.79	0.47
1:C:35:TRP:CE3	1:C:193:PRO:HG3	2.48	0.47
1:C:102:HIS:HB2	1:C:104:TYR:CE1	2.49	0.47
1:D:28:LYS:O	1:D:33:HIS:CE1	2.67	0.47
1:F:147:GLU:O	1:F:209:GLU:HG3	2.15	0.47
1:H:23:TRP:O	1:H:85:HIS:NE2	2.35	0.47
1:A:156:ASP:N	1:A:157:PRO:HD2	2.29	0.47
1:C:53:PRO:HA	1:C:117:PHE:CE1	2.49	0.47
1:D:154:ASN:HB2	1:D:176:PHE:CE1	2.49	0.47
1:E:29:GLU:HA	1:E:34:ARG:HH22	1.79	0.47
1:E:118:LEU:CD2	1:E:123:THR:HG22	2.44	0.47
1:F:42:PHE:CD1	1:F:42:PHE:N	2.81	0.47
1:F:110:HIS:CE1	3:F:302:7L3:SAA	3.07	0.47
1:F:67:ASP:OD1	1:F:68:LEU:N	2.45	0.47
1:A:139:LEU:HD21	3:A:302:7L3:CAV	2.45	0.47
1:D:112:HIS:O	1:D:126:LEU:HD12	2.14	0.47
1:G:76:LYS:HA	1:G:170:GLU:HA	1.96	0.47
1:G:115:MET:HG3	5:G:302:CL:CL	2.51	0.47
1:H:115:MET:HA	1:H:127:SER:HB3	1.96	0.47
1:B:166:GLN:HG3	1:B:167:ASN:N	2.29	0.47
1:D:59:TYR:HB3	1:D:239:ILE:HB	1.96	0.47
1:D:82:PHE:HZ	1:D:85:HIS:HA	1.80	0.47
1:E:114:PRO:HD2	1:E:228:GLN:OE1	2.15	0.47
3:E:302:7L3:SAA	3:E:302:7L3:OAO	2.72	0.47
1:F:55:ASN:ND2	1:F:57:GLU:HG3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:GLN:O	1:F:242:SER:OG	2.32	0.47
1:G:181:ILE:HG13	1:G:181:ILE:O	2.14	0.47
1:A:220:LYS:NZ	1:A:224:ASN:OD1	2.36	0.47
1:D:53:PRO:O	1:D:232:GLN:N	2.30	0.47
1:D:109:VAL:HA	1:D:129:HIS:O	2.15	0.47
1:D:184:TYR:HA	1:D:240:ILE:O	2.15	0.47
1:G:59:TYR:CE2	1:G:184:TYR:HE2	2.33	0.47
1:G:113:ALA:HB3	1:G:222:MET:HE1	1.96	0.47
1:A:51:GLN:OE1	1:A:229:ARG:NH1	2.43	0.47
1:C:219:LYS:HB3	1:C:224:ASN:HA	1.97	0.47
1:F:178:PRO:HD3	1:F:208:LEU:HD21	1.97	0.47
1:B:140:LEU:HG	1:B:202:PHE:HE1	1.79	0.46
1:B:168:PHE:N	1:B:168:PHE:CD1	2.84	0.46
1:F:215:LEU:O	1:F:219:LYS:HG3	2.15	0.46
1:C:23:TRP:HB3	1:C:42:PHE:HE2	1.80	0.46
1:E:34:ARG:HA	1:E:36:ASP:OD1	2.15	0.46
1:E:112:HIS:ND1	1:E:116:GLU:CD	2.74	0.46
1:C:102:HIS:HB2	1:C:104:TYR:HE1	1.79	0.46
1:B:42:PHE:N	1:B:42:PHE:CD1	2.81	0.46
1:C:96:HIS:CE1	1:C:105:VAL:HG22	2.50	0.46
1:C:62:THR:OG1	1:C:63:GLN:N	2.48	0.46
1:D:77:PRO:HD2	1:D:168:PHE:HB2	1.98	0.46
1:E:116:GLU:HG2	1:E:228:GLN:HG3	1.96	0.46
1:E:184:TYR:OH	1:E:205:GLU:OE2	2.28	0.46
1:H:77:PRO:HD2	1:H:168:PHE:HB2	1.97	0.46
1:B:210:VAL:HG23	1:B:214:GLN:OE1	2.15	0.46
1:D:56:ILE:N	1:D:118:LEU:O	2.42	0.46
1:A:112:HIS:O	1:A:127:SER:N	2.35	0.46
1:E:72:TYR:OH	1:E:132:HIS:NE2	2.38	0.46
1:E:116:GLU:HA	1:E:228:GLN:HG3	1.97	0.46
1:G:183:TYR:CE1	1:G:242:SER:HB3	2.51	0.46
1:G:127:SER:OG	5:G:302:CL:CL	2.58	0.46
1:D:114:PRO:HA	1:D:125:PRO:O	2.16	0.46
1:D:204:ILE:HG22	1:D:206:GLU:N	2.26	0.46
1:E:52:SER:O	1:E:229:ARG:NH1	2.49	0.46
1:E:125:PRO:HD2	1:E:146:PHE:O	2.15	0.46
1:G:49:LYS:HB3	1:H:198:GLY:CA	2.45	0.46
1:G:238:VAL:HG21	1:H:186:PHE:HA	1.97	0.46
1:H:215:LEU:O	1:H:219:LYS:NZ	2.48	0.46
1:A:63:GLN:HG2	1:A:64:ASP:N	2.30	0.46
1:C:235:TYR:CD2	1:D:138:ARG:HG2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:54:ILE:HG12	1:F:117:PHE:HE1	1.79	0.46
1:G:89:ALA:O	1:G:108:ASN:HA	2.16	0.46
1:D:146:PHE:CE2	1:D:208:LEU:HB2	2.50	0.45
1:F:181:ILE:HG21	1:F:246:THR:HG21	1.98	0.45
1:G:56:ILE:HG23	1:G:239:ILE:HG21	1.99	0.45
1:G:151:GLU:HG2	1:G:211:SER:OG	2.16	0.45
1:D:42:PHE:N	1:D:42:PHE:CD1	2.83	0.45
1:D:44:VAL:HG13	1:D:195:CYS:HB2	1.98	0.45
1:D:151:GLU:OE2	1:D:213:LYS:NZ	2.39	0.45
1:G:74:ALA:HA	1:G:171:VAL:O	2.15	0.45
1:B:83:THR:O	1:B:84:HIS:C	2.59	0.45
1:B:92:GLU:OE1	1:B:93:PRO:HD2	2.17	0.45
1:H:190:LEU:HD23	1:H:190:LEU:HA	1.70	0.45
1:H:125:PRO:HB2	1:H:215:LEU:HD11	1.98	0.45
1:A:112:HIS:CD2	1:A:129:HIS:CE1	3.05	0.45
1:C:29:GLU:CA	1:C:34:ARG:HE	2.28	0.45
1:D:117:PHE:HD2	5:D:302:CL:CL	2.37	0.45
1:C:86:THR:HG21	4:C:302:GOL:H12	1.99	0.45
1:D:182:ASN:N	1:D:206:GLU:OE1	2.50	0.45
1:B:151:GLU:OE1	1:B:151:GLU:N	2.49	0.45
1:D:25:TYR:HE1	1:D:229:ARG:HA	1.81	0.45
1:G:118:LEU:HG	1:G:123:THR:HG22	1.99	0.45
1:H:178:PRO:O	1:H:246:THR:OG1	2.18	0.45
1:B:35:TRP:CZ3	1:B:193:PRO:HD3	2.52	0.45
1:D:35:TRP:CZ2	1:D:193:PRO:HD3	2.52	0.45
1:E:82:PHE:CE2	1:E:223:LYS:HD3	2.52	0.45
1:B:150:LYS:O	1:B:211:SER:N	2.50	0.45
1:C:132:HIS:HB2	1:C:140:LEU:HB3	1.99	0.45
1:A:26:LYS:HA	1:A:26:LYS:HD3	1.72	0.45
1:A:119:ILE:CD1	1:A:205:GLU:HA	2.42	0.45
1:D:133:LYS:HA	1:D:138:ARG:O	2.17	0.45
1:B:39:HIS:ND1	1:D:41:ASP:OD2	2.50	0.44
1:B:112:HIS:O	1:B:126:LEU:HD12	2.17	0.44
1:D:130:PHE:HB2	1:D:142:LEU:HB3	1.99	0.44
1:D:150:LYS:O	1:D:211:SER:N	2.49	0.44
1:D:181:ILE:O	1:D:181:ILE:HG13	2.16	0.44
1:E:26:LYS:C	1:E:28:LYS:N	2.74	0.44
1:F:83:THR:O	1:F:86:THR:HG22	2.18	0.44
1:G:211:SER:OG	1:G:214:GLN:N	2.47	0.44
1:C:217:GLU:O	1:C:220:LYS:HB3	2.17	0.44
1:D:23:TRP:CD1	1:D:42:PHE:HE2	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:HIS:CE1	1:D:129:HIS:HB2	2.52	0.44
1:F:70:PHE:HB2	1:F:247:ARG:HG3	2.00	0.44
1:F:115:MET:HG3	1:F:127:SER:HB3	1.99	0.44
1:H:51:GLN:HE21	1:H:197:GLU:CD	2.24	0.44
1:A:32:PRO:HA	1:A:35:TRP:CE2	2.52	0.44
1:B:227:ASN:OD1	1:B:227:ASN:N	2.51	0.44
1:A:76:LYS:HA	1:A:77:PRO:HD3	1.85	0.44
1:E:80:VAL:HB	1:E:161:GLY:O	2.17	0.44
1:F:88:LYS:HA	1:F:109:VAL:O	2.17	0.44
1:H:64:ASP:OD1	1:H:64:ASP:N	2.50	0.44
1:C:57:GLU:HG2	1:C:58:HIS:CE1	2.52	0.44
1:D:110:HIS:NE2	1:D:129:HIS:HB2	2.32	0.44
1:A:78:LYS:HE2	1:A:78:LYS:HB3	1.80	0.44
1:A:165:LYS:HA	1:A:168:PHE:CE2	2.53	0.44
1:B:87:LEU:HD12	1:B:88:LYS:H	1.83	0.44
1:B:184:TYR:O	1:B:202:PHE:HA	2.17	0.44
1:G:166:GLN:HB3	1:G:167:ASN:H	1.64	0.44
1:H:77:PRO:HA	1:H:90:SER:O	2.18	0.44
1:H:79:ALA:HB2	1:H:165:LYS:NZ	2.33	0.44
1:A:105:VAL:O	1:A:132:HIS:HA	2.18	0.44
1:B:105:VAL:O	1:B:132:HIS:HA	2.17	0.44
1:B:106:LEU:HD12	1:B:131:VAL:O	2.17	0.44
1:C:27:ASN:OD1	1:C:27:ASN:N	2.41	0.44
1:C:42:PHE:N	1:C:42:PHE:CD1	2.84	0.44
1:D:146:PHE:HB3	1:D:210:VAL:HG12	2.00	0.44
1:F:181:ILE:HD11	1:F:244:ALA:C	2.42	0.44
1:F:211:SER:HB2	1:F:213:LYS:NZ	2.33	0.44
1:C:184:TYR:HE1	1:C:205:GLU:HB2	1.82	0.44
1:D:82:PHE:CZ	1:D:85:HIS:HA	2.53	0.44
1:F:118:LEU:HG	1:F:123:THR:CG2	2.48	0.44
1:F:158:ILE:HD11	1:F:171:VAL:HG21	2.00	0.44
1:G:106:LEU:HA	1:G:131:VAL:O	2.18	0.44
1:G:139:LEU:HD13	1:G:190:LEU:HD21	2.00	0.44
1:B:51:GLN:OE1	1:B:195:CYS:HB3	2.17	0.44
1:D:116:GLU:HB2	5:D:302:CL:CL	2.54	0.44
1:D:177:LEU:CG	1:D:246:THR:HG21	2.48	0.44
1:G:36:ASP:CG	1:G:46:LYS:HB2	2.43	0.44
1:G:204:ILE:HG22	1:G:206:GLU:HG2	1.99	0.44
1:C:23:TRP:HZ2	1:C:84:HIS:HB3	1.82	0.43
1:C:66:ALA:O	1:C:67:ASP:C	2.61	0.43
1:D:44:VAL:HA	1:D:47:SER:OG	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:TYR:CE2	1:D:184:TYR:HE2	2.36	0.43
1:G:105:VAL:HG12	1:G:133:LYS:O	2.18	0.43
1:A:130:PHE:HB3	1:A:132:HIS:HE1	1.82	0.43
1:A:219:LYS:HE3	1:A:224:ASN:ND2	2.33	0.43
1:D:86:THR:HA	1:D:222:MET:SD	2.57	0.43
1:E:118:LEU:HD13	1:E:121:ASN:HA	1.99	0.43
1:E:147:GLU:O	1:E:209:GLU:HA	2.17	0.43
1:F:181:ILE:CD1	1:F:244:ALA:H	2.30	0.43
1:H:27:ASN:OD1	1:H:27:ASN:N	2.50	0.43
1:B:119:ILE:O	1:B:122:LYS:N	2.38	0.43
1:C:34:ARG:O	1:C:38:LEU:HG	2.17	0.43
1:C:104:TYR:HB3	1:C:132:HIS:CB	2.45	0.43
1:C:189:SER:HA	1:C:197:GLU:HA	2.00	0.43
1:D:104:TYR:CD2	1:D:134:ASP:HB3	2.52	0.43
1:G:184:TYR:CE2	1:G:241:LYS:HD2	2.54	0.43
1:H:64:ASP:O	1:H:66:ALA:N	2.51	0.43
1:D:227:ASN:OD1	1:D:227:ASN:N	2.43	0.43
1:A:64:ASP:OD1	1:A:242:SER:OG	2.36	0.43
1:A:113:ALA:HB2	1:A:126:LEU:HD13	1.99	0.43
1:D:133:LYS:HG2	1:D:134:ASP:O	2.18	0.43
1:F:66:ALA:HA	1:F:244:ALA:HB1	2.01	0.43
1:G:113:ALA:HA	1:G:114:PRO:HA	1.87	0.43
1:A:35:TRP:CH2	1:A:193:PRO:HD3	2.53	0.43
1:B:87:LEU:HB3	1:B:222:MET:CE	2.47	0.43
1:C:100:ARG:HD2	1:D:58:HIS:CE1	2.53	0.43
1:C:234:ASP:O	1:D:138:ARG:NE	2.52	0.43
1:E:42:PHE:N	1:E:42:PHE:CD1	2.87	0.43
1:G:30:ASN:O	1:G:35:TRP:CD1	2.72	0.43
1:G:174:ASP:OD1	1:G:174:ASP:N	2.46	0.43
1:H:182:ASN:OD1	1:H:243:SER:HB3	2.19	0.43
1:D:154:ASN:C	1:D:157:PRO:HD2	2.43	0.43
1:E:31:GLY:HA3	1:E:33:HIS:CE1	2.54	0.43
1:F:192:ALA:HB3	3:F:302:7L3:NAD	2.34	0.43
1:H:62:THR:HG1	1:H:63:GLN:N	2.16	0.43
1:A:189:SER:HA	1:A:197:GLU:HA	2.00	0.43
1:B:32:PRO:HA	1:B:35:TRP:CE2	2.54	0.43
1:B:112:HIS:CD2	1:B:129:HIS:CE1	3.06	0.43
1:C:65:LYS:C	1:C:67:ASP:H	2.27	0.43
1:C:105:VAL:O	1:C:132:HIS:HA	2.18	0.43
1:E:152:ASN:N	1:E:214:GLN:HE22	2.17	0.43
1:F:134:ASP:OD1	1:F:138:ARG:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:PHE:HD1	1:B:168:PHE:H	1.66	0.43
1:C:56:ILE:O	1:C:120:ASN:N	2.43	0.43
1:E:146:PHE:CD2	1:E:210:VAL:HB	2.54	0.43
1:F:114:PRO:O	1:F:228:GLN:HB2	2.19	0.43
1:H:59:TYR:CD1	1:H:59:TYR:N	2.87	0.43
1:E:30:ASN:HA	1:E:38:LEU:HD11	2.00	0.42
1:E:227:ASN:OD1	1:E:227:ASN:N	2.48	0.42
1:F:54:ILE:O	1:F:117:PHE:HD1	2.02	0.42
1:F:62:THR:OG1	1:F:63:GLN:N	2.51	0.42
1:F:105:VAL:HG12	1:F:133:LYS:O	2.19	0.42
1:H:186:PHE:HB3	1:H:239:ILE:HG12	2.01	0.42
1:A:102:HIS:CG	1:A:138:ARG:HH12	2.37	0.42
1:A:138:ARG:HG2	1:B:235:TYR:HD2	1.85	0.42
1:B:119:ILE:O	1:B:120:ASN:C	2.62	0.42
1:B:225:SER:HA	1:B:226:PRO:HD3	1.77	0.42
1:D:163:GLN:O	1:D:164:LYS:HD2	2.19	0.42
1:A:96:HIS:HB3	1:A:103:ASP:OD1	2.20	0.42
1:A:150:LYS:HG2	1:A:151:GLU:N	2.33	0.42
1:H:53:PRO:HA	1:H:117:PHE:CE1	2.54	0.42
1:H:88:LYS:HD2	1:H:108:ASN:CG	2.44	0.42
1:H:129:HIS:HA	1:H:142:LEU:O	2.20	0.42
1:A:217:GLU:O	1:A:221:ARG:HG2	2.19	0.42
1:C:99:TYR:CZ	1:C:100:ARG:HG3	2.53	0.42
1:F:194:PRO:HG2	1:F:196:THR:OG1	2.19	0.42
1:G:115:MET:HG2	1:G:117:PHE:O	2.19	0.42
1:C:115:MET:HB2	1:C:124:ARG:HB2	2.01	0.42
1:E:183:TYR:CD1	1:E:183:TYR:C	2.96	0.42
1:G:104:TYR:CB	1:G:132:HIS:HB3	2.50	0.42
1:G:183:TYR:O	1:G:241:LYS:HA	2.20	0.42
1:B:151:GLU:O	1:B:153:PRO:HD3	2.20	0.42
1:B:112:HIS:HA	1:B:227:ASN:ND2	2.35	0.42
1:C:67:ASP:O	1:C:99:TYR:HD1	2.02	0.42
1:C:128:ALA:HB2	1:C:146:PHE:HE1	1.84	0.42
1:D:81:PHE:N	1:D:81:PHE:CD1	2.87	0.42
1:D:105:VAL:O	1:D:132:HIS:HA	2.20	0.42
1:E:161:GLY:HA2	1:E:168:PHE:CD1	2.54	0.42
1:E:225:SER:HA	1:E:226:PRO:HD3	1.74	0.42
1:G:110:HIS:HE1	1:G:131:VAL:CG2	2.32	0.42
1:H:230:PRO:O	1:H:232:GLN:NE2	2.42	0.42
1:A:117:PHE:CE1	1:A:186:PHE:HZ	2.37	0.42
1:C:32:PRO:HA	1:C:35:TRP:CD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:LYS:HG3	1:F:197:GLU:C	2.44	0.42
1:E:158:ILE:HD11	1:E:171:VAL:HG21	2.02	0.42
1:F:55:ASN:HD21	1:F:57:GLU:HG3	1.85	0.42
1:F:174:ASP:HA	1:F:247:ARG:HH11	1.84	0.42
1:H:35:TRP:CZ3	1:H:193:PRO:HD3	2.54	0.42
1:A:51:GLN:OE1	1:A:229:ARG:NH2	2.52	0.42
1:A:110:HIS:CE1	1:A:129:HIS:HB2	2.55	0.42
1:C:32:PRO:HG3	1:C:35:TRP:CZ2	2.55	0.42
1:C:108:ASN:HD21	1:C:131:VAL:HG21	1.85	0.42
1:E:116:GLU:OE1	1:E:129:HIS:HE1	2.02	0.42
1:G:92:GLU:O	1:G:94:THR:N	2.50	0.42
1:H:165:LYS:O	1:H:165:LYS:HG2	2.20	0.42
1:A:66:ALA:O	1:A:69:GLN:NE2	2.52	0.42
1:C:58:HIS:HB2	1:D:100:ARG:NH1	2.35	0.42
1:C:73:ALA:O	1:C:173:LEU:HB2	2.20	0.42
1:C:190:LEU:HD23	1:C:190:LEU:HA	1.82	0.42
1:D:164:LYS:HG2	1:D:166:GLN:NE2	2.34	0.42
1:D:234:ASP:OD1	1:D:237:THR:N	2.42	0.42
1:E:191:THR:HA	1:E:229:ARG:HH11	1.83	0.42
1:F:129:HIS:CD2	1:F:143:ALA:HB2	2.55	0.42
1:B:181:ILE:HA	1:B:206:GLU:OE1	2.21	0.41
1:D:54:ILE:HG22	1:D:232:GLN:O	2.19	0.41
1:D:55:ASN:HD22	1:D:57:GLU:CD	2.27	0.41
1:H:185:HIS:CE1	1:H:202:PHE:CZ	3.08	0.41
1:D:182:ASN:CG	1:D:243:SER:HB3	2.44	0.41
1:F:57:GLU:HG2	1:F:120:ASN:OD1	2.21	0.41
1:G:130:PHE:HB3	1:G:132:HIS:CE1	2.53	0.41
1:A:38:LEU:HD23	1:A:38:LEU:HA	1.88	0.41
1:B:55:ASN:HA	1:B:118:LEU:HB2	2.02	0.41
1:C:165:LYS:HA	1:C:165:LYS:HD3	1.93	0.41
1:D:73:ALA:O	1:D:173:LEU:HD12	2.20	0.41
1:D:185:HIS:HB3	1:D:240:ILE:HG13	2.02	0.41
1:G:87:LEU:HD12	1:G:88:LYS:H	1.85	0.41
1:A:89:ALA:O	1:A:108:ASN:HB2	2.20	0.41
1:C:107:ASP:OD1	1:C:107:ASP:C	2.62	0.41
1:E:197:GLU:HB2	1:F:49:LYS:HG3	2.02	0.41
1:B:179:LYS:HG2	1:B:247:ARG:CZ	2.50	0.41
1:C:109[B]:VAL:HA	1:C:129:HIS:O	2.21	0.41
1:E:152:ASN:H	1:E:214:GLN:NE2	2.18	0.41
1:F:32:PRO:HA	1:F:35:TRP:CG	2.55	0.41
1:G:154:ASN:O	1:G:157:PRO:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:174:ASP:O	1:G:247:ARG:NH1	2.54	0.41
1:G:219:LYS:HB3	1:G:219:LYS:HE3	1.82	0.41
1:A:91:PHE:CE2	1:A:109[B]:VAL:HG12	2.52	0.41
1:A:234:ASP:OD1	1:A:237:THR:N	2.47	0.41
1:C:115:MET:HG3	1:C:127:SER:CB	2.46	0.41
1:E:129:HIS:HB3	1:E:141:VAL:HG11	2.02	0.41
1:E:204:ILE:HG22	1:E:206:GLU:N	2.27	0.41
1:H:79:ALA:HB2	1:H:165:LYS:HZ3	1.85	0.41
1:G:150:LYS:C	1:G:211:SER:HB3	2.46	0.41
1:A:228:GLN:HG2	1:A:229:ARG:O	2.20	0.41
1:D:87:LEU:HD12	1:D:88:LYS:H	1.86	0.41
1:E:138:ARG:HG2	1:F:235:TYR:CD2	2.56	0.41
1:F:149:GLY:HA3	1:F:209:GLU:OE2	2.21	0.41
1:A:31:GLY:O	1:A:34:ARG:HB2	2.21	0.41
1:A:52:SER:HB3	1:A:117:PHE:CZ	2.56	0.41
1:D:62:THR:HG1	1:D:63:GLN:H	1.63	0.41
1:D:217:GLU:O	1:D:221:ARG:HG2	2.21	0.41
1:E:29:GLU:H	1:E:29:GLU:CD	2.28	0.41
1:F:111:PHE:HB2	1:F:222:MET:SD	2.61	0.41
1:G:75:SER:N	1:G:171:VAL:O	2.45	0.41
1:H:31:GLY:HA2	1:H:32:PRO:HD3	1.87	0.41
1:H:225:SER:HA	1:H:226:PRO:HD3	1.68	0.41
1:A:106:LEU:HD12	1:A:131:VAL:O	2.21	0.41
1:B:71:LYS:N	1:B:96:HIS:O	2.27	0.41
1:C:115:MET:HB3	1:C:124:ARG:H	1.85	0.41
1:C:185:HIS:HA	1:C:201:TRP:O	2.21	0.41
1:E:115:MET:CG	1:E:127:SER:HB3	2.51	0.41
1:F:104:TYR:HA	1:F:134:ASP:HA	2.02	0.41
1:G:21:THR:HG22	1:G:22:LYS:N	2.34	0.41
1:H:111:PHE:HA	1:H:128:ALA:HA	2.03	0.41
1:B:81:PHE:O	1:B:88:LYS:N	2.52	0.40
1:D:191:THR:O	1:D:229:ARG:HB2	2.21	0.40
1:G:191:THR:OG1	3:G:303:7L3:NAI	2.54	0.40
1:C:71:LYS:HD2	1:C:96:HIS:CB	2.45	0.40
1:F:49:LYS:HD3	1:F:49:LYS:HA	1.80	0.40
1:G:70:PHE:CD1	1:G:246:THR:HA	2.56	0.40
1:A:184:TYR:CE2	1:A:241:LYS:HD2	2.57	0.40
1:E:22:LYS:O	1:E:30:ASN:ND2	2.54	0.40
1:E:64:ASP:OD1	1:E:244:ALA:HA	2.21	0.40
1:F:159:LEU:O	1:F:162:ILE:HG22	2.22	0.40
1:G:174:ASP:O	1:G:247:ARG:HD3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:ASP:HA	1:B:42:PHE:O	2.22	0.40
1:D:56:ILE:HG21	1:D:184:TYR:CD2	2.56	0.40
1:D:136:LYS:HD2	1:D:138:ARG:HH11	1.87	0.40
1:E:162:ILE:HD12	1:E:162:ILE:HA	1.90	0.40
1:F:174:ASP:OD1	1:F:174:ASP:N	2.49	0.40
1:F:181:ILE:HD11	1:F:244:ALA:H	1.87	0.40
1:G:32:PRO:HA	1:G:35:TRP:CE2	2.55	0.40
1:H:145:GLY:O	1:H:207:PRO:HA	2.21	0.40
1:B:76:LYS:HZ3	1:B:170:GLU:HG3	1.86	0.40
1:C:215:LEU:O	1:C:219:LYS:HG3	2.22	0.40
1:D:77:PRO:HG3	1:D:91:PHE:CZ	2.56	0.40
1:E:75:SER:HB2	1:E:91:PHE:CE1	2.56	0.40
1:E:95:ASN:HB2	1:E:106:LEU:HB3	2.03	0.40
1:F:63:GLN:H	1:F:63:GLN:CD	2.29	0.40
1:F:133:LYS:HD2	1:F:137:GLY:HA2	2.02	0.40
1:F:154:ASN:C	1:F:157:PRO:HD2	2.46	0.40
1:G:186:PHE:CE1	1:G:201:TRP:HB2	2.57	0.40
1:H:209:GLU:H	1:H:209:GLU:HG3	1.33	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:HIS:ND1	1:B:148:GLU:OE1[1_655]	2.14	0.06

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	226/234 (97%)	211 (93%)	15 (7%)	0	100	100
1	B	213/234 (91%)	200 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	225/234 (96%)	209 (93%)	16 (7%)	0	100	100
1	D	212/234 (91%)	198 (93%)	14 (7%)	0	100	100
1	E	225/234 (96%)	209 (93%)	16 (7%)	0	100	100
1	F	216/234 (92%)	202 (94%)	14 (6%)	0	100	100
1	G	217/234 (93%)	198 (91%)	19 (9%)	0	100	100
1	H	223/234 (95%)	208 (93%)	15 (7%)	0	100	100
All	All	1757/1872 (94%)	1635 (93%)	122 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	203/208 (98%)	201 (99%)	2 (1%)	68	89
1	B	195/208 (94%)	186 (95%)	9 (5%)	24	57
1	C	202/208 (97%)	198 (98%)	4 (2%)	48	78
1	D	196/208 (94%)	189 (96%)	7 (4%)	31	65
1	E	202/208 (97%)	199 (98%)	3 (2%)	57	84
1	F	197/208 (95%)	191 (97%)	6 (3%)	36	70
1	G	199/208 (96%)	192 (96%)	7 (4%)	32	66
1	H	200/208 (96%)	195 (98%)	5 (2%)	42	74
All	All	1594/1664 (96%)	1551 (97%)	43 (3%)	40	73

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50[A]	SER
1	A	50[B]	SER
1	B	39	HIS
1	B	86	THR

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Mol	Chain	Res	Type
1	B	97	ILE
1	B	109	VAL
1	B	138	ARG
1	B	168	PHE
1	B	218	ILE
1	B	238	VAL
1	B	243	SER
1	C	65	LYS
1	C	78	LYS
1	C	136	LYS
1	C	151	GLU
1	D	50	SER
1	D	81	PHE
1	D	97	ILE
1	D	131	VAL
1	D	176	PHE
1	D	184	TYR
1	D	240	ILE
1	E	82	PHE
1	E	170	GLU
1	E	240	ILE
1	F	27	ASN
1	F	50	SER
1	F	103	ASP
1	F	138	ARG
1	F	148	GLU
1	F	152	ASN
1	G	20	ASN
1	G	67	ASP
1	G	86	THR
1	G	136	LYS
1	G	159	LEU
1	G	206	GLU
1	G	220	LYS
1	H	59	TYR
1	H	63	GLN
1	H	136	LYS
1	H	209	GLU
1	H	243	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	120	ASN
1	A	154	ASN
1	B	185	HIS
1	C	69	GLN
1	C	108	ASN
1	C	121	ASN
1	C	232	GLN
1	D	30	ASN
1	D	85	HIS
1	D	96	HIS
1	D	154	ASN
1	E	30	ASN
1	E	84	HIS
1	E	95	ASN
1	F	55	ASN
1	F	102	HIS
1	G	95	ASN
1	G	96	HIS
1	G	120	ASN
1	G	232	GLN
1	H	185	HIS

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](#)

Of 19 ligands modelled in this entry, 10 are monoatomic - leaving 9 for Mogul analysis.

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
3	7L3	H	302	2	24,25,25	2.90	8 (33%)	33,40,40	2.19	8 (24%)
3	7L3	D	303	2	24,25,25	2.89	8 (33%)	33,40,40	2.18	8 (24%)
3	7L3	C	303	2	24,25,25	2.90	8 (33%)	33,40,40	2.19	8 (24%)
3	7L3	G	303	2	24,25,25	2.89	8 (33%)	33,40,40	2.19	8 (24%)
3	7L3	B	302	2	24,25,25	2.90	8 (33%)	33,40,40	2.18	8 (24%)
3	7L3	E	302	2	24,25,25	2.89	8 (33%)	33,40,40	2.18	8 (24%)
4	GOL	C	302	-	5,5,5	0.26	0	5,5,5	0.31	0
3	7L3	F	302	2	24,25,25	2.94	8 (33%)	33,40,40	2.21	7 (21%)
3	7L3	A	302	2	24,25,25	2.95	8 (33%)	33,40,40	2.21	7 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	7L3	H	302	2	-	11/23/23/23	0/2/2/2
3	7L3	D	303	2	-	11/23/23/23	0/2/2/2
3	7L3	C	303	2	-	11/23/23/23	0/2/2/2
3	7L3	G	303	2	-	13/23/23/23	0/2/2/2
3	7L3	B	302	2	-	9/23/23/23	0/2/2/2
3	7L3	E	302	2	-	11/23/23/23	0/2/2/2
4	GOL	C	302	-	-	2/4/4/4	-
3	7L3	F	302	2	-	9/23/23/23	0/2/2/2
3	7L3	A	302	2	-	7/23/23/23	0/2/2/2

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	7L3	OAO-SAL	7.26	1.52	1.44
3	H	302	7L3	OAO-SAL	7.25	1.52	1.44
3	C	303	7L3	OAO-SAL	7.22	1.52	1.44
3	E	302	7L3	OAO-SAL	7.22	1.52	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	303	7L3	OAO-SAL	7.22	1.52	1.44
3	G	303	7L3	OAO-SAL	7.18	1.52	1.44
3	A	302	7L3	OAO-SAL	6.42	1.51	1.44
3	F	302	7L3	OAO-SAL	6.39	1.51	1.44
3	F	302	7L3	OAG-SAF	6.33	1.53	1.43
3	A	302	7L3	OAG-SAF	6.31	1.53	1.43
3	G	303	7L3	OAG-SAF	5.88	1.52	1.43
3	H	302	7L3	OAG-SAF	5.85	1.52	1.43
3	C	303	7L3	OAG-SAF	5.83	1.52	1.43
3	E	302	7L3	OAG-SAF	5.80	1.52	1.43
3	B	302	7L3	OAG-SAF	5.78	1.52	1.43
3	D	303	7L3	OAG-SAF	5.77	1.52	1.43
3	H	302	7L3	OAM-SAL	5.55	1.50	1.44
3	B	302	7L3	OAM-SAL	5.51	1.50	1.44
3	C	303	7L3	OAM-SAL	5.49	1.50	1.44
3	D	303	7L3	OAM-SAL	5.49	1.50	1.44
3	G	303	7L3	OAM-SAL	5.48	1.50	1.44
3	E	302	7L3	OAM-SAL	5.47	1.50	1.44
3	A	302	7L3	OAM-SAL	5.26	1.50	1.44
3	F	302	7L3	OAM-SAL	5.14	1.50	1.44
3	H	302	7L3	OAH-SAF	4.95	1.51	1.43
3	D	303	7L3	OAH-SAF	4.90	1.51	1.43
3	B	302	7L3	OAH-SAF	4.90	1.51	1.43
3	C	303	7L3	OAH-SAF	4.88	1.51	1.43
3	E	302	7L3	OAH-SAF	4.88	1.51	1.43
3	G	303	7L3	OAH-SAF	4.85	1.50	1.43
3	F	302	7L3	CAN-SAL	4.64	1.83	1.76
3	A	302	7L3	CAN-SAL	4.60	1.83	1.76
3	A	302	7L3	SAF-NAI	4.52	1.68	1.58
3	F	302	7L3	SAF-NAI	4.46	1.68	1.58
3	A	302	7L3	CAB-NAK	4.31	1.44	1.33
3	F	302	7L3	CAB-NAK	4.28	1.44	1.33
3	G	303	7L3	CAB-NAK	4.07	1.44	1.33
3	C	303	7L3	CAB-NAK	4.07	1.44	1.33
3	D	303	7L3	CAB-NAK	4.06	1.44	1.33
3	B	302	7L3	CAB-NAK	4.05	1.44	1.33
3	H	302	7L3	CAB-NAK	4.05	1.44	1.33
3	E	302	7L3	CAB-NAK	4.04	1.44	1.33
3	A	302	7L3	OAH-SAF	3.80	1.49	1.43
3	F	302	7L3	OAH-SAF	3.76	1.49	1.43
3	C	303	7L3	CAE-SAF	3.52	1.80	1.78
3	B	302	7L3	CAE-SAF	3.51	1.80	1.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	302	7L3	CAE-SAF	3.48	1.80	1.78
3	G	303	7L3	CAE-SAF	3.44	1.80	1.78
3	H	302	7L3	CAE-SAF	3.36	1.80	1.78
3	D	303	7L3	CAE-SAF	3.36	1.80	1.78
3	E	302	7L3	CAN-SAL	3.10	1.81	1.76
3	H	302	7L3	CAN-SAL	3.08	1.81	1.76
3	C	303	7L3	CAN-SAL	3.08	1.81	1.76
3	B	302	7L3	CAN-SAL	3.05	1.81	1.76
3	D	303	7L3	CAN-SAL	3.04	1.81	1.76
3	G	303	7L3	CAN-SAL	3.03	1.81	1.76
3	E	302	7L3	SAF-NAI	2.86	1.65	1.58
3	B	302	7L3	SAF-NAI	2.86	1.65	1.58
3	D	303	7L3	SAF-NAI	2.84	1.65	1.58
3	G	303	7L3	SAF-NAI	2.81	1.64	1.58
3	H	302	7L3	SAF-NAI	2.81	1.64	1.58
3	C	303	7L3	SAF-NAI	2.79	1.64	1.58
3	A	302	7L3	CAP-CAN	2.35	1.42	1.38
3	F	302	7L3	CAP-CAN	2.31	1.42	1.38

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	302	7L3	OAH-SAF-OAG	-7.63	109.36	120.27
3	A	302	7L3	OAH-SAF-OAG	-7.62	109.37	120.27
3	G	303	7L3	OAH-SAF-OAG	-7.59	109.42	120.27
3	H	302	7L3	OAH-SAF-OAG	-7.58	109.43	120.27
3	C	303	7L3	OAH-SAF-OAG	-7.58	109.43	120.27
3	D	303	7L3	OAH-SAF-OAG	-7.56	109.46	120.27
3	E	302	7L3	OAH-SAF-OAG	-7.55	109.47	120.27
3	B	302	7L3	OAH-SAF-OAG	-7.55	109.47	120.27
3	E	302	7L3	OAQ-SAL-OAM	-5.52	109.45	117.25
3	B	302	7L3	OAQ-SAL-OAM	-5.51	109.47	117.25
3	G	303	7L3	OAQ-SAL-OAM	-5.50	109.48	117.25
3	H	302	7L3	OAQ-SAL-OAM	-5.50	109.48	117.25
3	C	303	7L3	OAQ-SAL-OAM	-5.49	109.50	117.25
3	D	303	7L3	OAQ-SAL-OAM	-5.49	109.50	117.25
3	A	302	7L3	OAQ-SAL-OAM	-5.45	109.56	117.25
3	F	302	7L3	OAQ-SAL-OAM	-5.40	109.62	117.25
3	F	302	7L3	SAA-CAE-SAF	5.09	128.38	121.62
3	A	302	7L3	SAA-CAE-SAF	5.08	128.36	121.62
3	C	303	7L3	SAA-CAE-SAF	4.96	128.20	121.62
3	G	303	7L3	SAA-CAE-SAF	4.95	128.19	121.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	302	7L3	SAA-CAE-SAF	4.95	128.19	121.62
3	B	302	7L3	SAA-CAE-SAF	4.94	128.18	121.62
3	D	303	7L3	SAA-CAE-SAF	4.93	128.16	121.62
3	E	302	7L3	SAA-CAE-SAF	4.92	128.15	121.62
3	B	302	7L3	CAJ-NAC-CAB	-3.15	122.35	128.94
3	H	302	7L3	CAJ-NAC-CAB	-3.14	122.37	128.94
3	C	303	7L3	CAJ-NAC-CAB	-3.13	122.39	128.94
3	G	303	7L3	CAJ-NAC-CAB	-3.13	122.39	128.94
3	D	303	7L3	CAJ-NAC-CAB	-3.13	122.40	128.94
3	E	302	7L3	CAJ-NAC-CAB	-3.12	122.41	128.94
3	F	302	7L3	CAJ-NAC-CAB	-3.09	122.47	128.94
3	A	302	7L3	CAJ-NAC-CAB	-3.08	122.49	128.94
3	A	302	7L3	OAG-SAF-CAE	2.63	109.57	105.65
3	F	302	7L3	OAH-SAF-CAE	2.62	109.55	105.65
3	A	302	7L3	OAH-SAF-CAE	2.61	109.54	105.65
3	F	302	7L3	OAG-SAF-CAE	2.61	109.53	105.65
3	E	302	7L3	OAH-SAF-CAE	2.60	109.53	105.65
3	D	303	7L3	OAG-SAF-CAE	2.60	109.52	105.65
3	E	302	7L3	OAG-SAF-CAE	2.60	109.52	105.65
3	G	303	7L3	OAH-SAF-CAE	2.59	109.51	105.65
3	D	303	7L3	OAH-SAF-CAE	2.59	109.50	105.65
3	G	303	7L3	OAG-SAF-CAE	2.58	109.50	105.65
3	B	302	7L3	OAH-SAF-CAE	2.58	109.50	105.65
3	C	303	7L3	OAH-SAF-CAE	2.57	109.47	105.65
3	C	303	7L3	OAG-SAF-CAE	2.57	109.47	105.65
3	H	302	7L3	OAG-SAF-CAE	2.57	109.47	105.65
3	B	302	7L3	OAG-SAF-CAE	2.56	109.47	105.65
3	H	302	7L3	OAH-SAF-CAE	2.56	109.47	105.65
3	H	302	7L3	CAE-SAF-NAI	2.10	109.50	107.40
3	A	302	7L3	CAE-SAF-NAI	2.08	109.47	107.40
3	F	302	7L3	CAE-SAF-NAI	2.07	109.46	107.40
3	G	303	7L3	CAE-SAF-NAI	2.07	109.46	107.40
3	C	303	7L3	CAE-SAF-NAI	2.07	109.46	107.40
3	D	303	7L3	CAE-SAF-NAI	2.05	109.45	107.40
3	B	302	7L3	CAE-SAF-NAI	2.05	109.44	107.40
3	B	302	7L3	CAJ-NAC-NAD	2.04	122.35	119.29
3	C	303	7L3	CAJ-NAC-NAD	2.04	122.34	119.29
3	E	302	7L3	CAE-SAF-NAI	2.04	109.43	107.40
3	H	302	7L3	CAJ-NAC-NAD	2.04	122.34	119.29
3	E	302	7L3	CAJ-NAC-NAD	2.03	122.32	119.29
3	G	303	7L3	CAJ-NAC-NAD	2.03	122.32	119.29
3	D	303	7L3	CAJ-NAC-NAD	2.01	122.30	119.29

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	302	GOL	C1-C2-C3-O3
3	B	302	7L3	CAP-CAN-SAL-NAK
3	A	302	7L3	CAP-CAN-SAL-NAK
3	F	302	7L3	CAP-CAN-SAL-NAK
3	B	302	7L3	CAT-CAN-SAL-NAK
3	A	302	7L3	CAT-CAN-SAL-NAK
3	C	303	7L3	CAP-CAN-SAL-NAK
3	F	302	7L3	CAT-CAN-SAL-NAK
4	C	302	GOL	O2-C2-C3-O3
3	E	302	7L3	CAP-CAN-SAL-NAK
3	C	303	7L3	CAT-CAN-SAL-NAK
3	E	302	7L3	CAT-CAN-SAL-NAK
3	G	303	7L3	CAP-CAN-SAL-NAK
3	D	303	7L3	CAP-CAN-SAL-NAK
3	B	302	7L3	CAB-NAK-SAL-OAM
3	H	302	7L3	CAB-NAK-SAL-OAM
3	G	303	7L3	CAB-NAK-SAL-OAM
3	D	303	7L3	CAT-CAN-SAL-NAK
3	G	303	7L3	CAT-CAN-SAL-NAK
3	D	303	7L3	CAB-NAK-SAL-OAM
3	E	302	7L3	CAB-NAK-SAL-OAM
3	H	302	7L3	CAP-CAN-SAL-NAK
3	A	302	7L3	CAB-NAK-SAL-OAM
3	H	302	7L3	CAT-CAN-SAL-OAO
3	H	302	7L3	CAP-CAN-SAL-OAO
3	G	303	7L3	CAT-CAN-SAL-OAO
3	D	303	7L3	CAT-CAN-SAL-OAO
3	G	303	7L3	CAP-CAN-SAL-OAO
3	D	303	7L3	CAP-CAN-SAL-OAO
3	G	303	7L3	SAA-CAE-SAF-OAH
3	H	302	7L3	CAT-CAN-SAL-NAK
3	B	302	7L3	CAQ-CAR-CAU-CAX
3	C	303	7L3	CAQ-CAR-CAU-CAV
3	E	302	7L3	CAS-CAR-CAU-CAX
3	H	302	7L3	CAS-CAR-CAU-CAW
3	D	303	7L3	CAQ-CAR-CAU-CAX
3	C	303	7L3	CAS-CAR-CAU-CAV
3	H	302	7L3	CAQ-CAR-CAU-CAW
3	G	303	7L3	CAS-CAR-CAU-CAX
3	B	302	7L3	CAS-CAR-CAU-CAX

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Mol	Chain	Res	Type	Atoms
3	F	302	7L3	CAQ-CAR-CAU-CAW
3	D	303	7L3	CAS-CAR-CAU-CAX
3	E	302	7L3	CAQ-CAR-CAU-CAX
3	E	302	7L3	CAT-CAN-SAL-OAM
3	G	303	7L3	CAQ-CAR-CAU-CAX
3	F	302	7L3	CAS-CAR-CAU-CAW
3	E	302	7L3	CAP-CAN-SAL-OAM
3	G	303	7L3	NAD-CAE-SAF-OAH
3	A	302	7L3	CAQ-CAR-CAU-CAV
3	B	302	7L3	CAQ-CAR-CAU-CAV
3	D	303	7L3	CAS-CAR-CAU-CAW
3	C	303	7L3	CAQ-CAR-CAU-CAX
3	C	303	7L3	CAS-CAR-CAU-CAW
3	D	303	7L3	CAQ-CAR-CAU-CAV
3	B	302	7L3	CAS-CAR-CAU-CAW
3	E	302	7L3	CAQ-CAR-CAU-CAW
3	H	302	7L3	CAS-CAR-CAU-CAX
3	E	302	7L3	CAS-CAR-CAU-CAW
3	G	303	7L3	CAS-CAR-CAU-CAV
3	H	302	7L3	CAQ-CAR-CAU-CAV
3	D	303	7L3	CAQ-CAR-CAU-CAW
3	E	302	7L3	CAS-CAR-CAU-CAV
3	B	302	7L3	CAQ-CAR-CAU-CAW
3	C	303	7L3	CAQ-CAR-CAU-CAW
3	F	302	7L3	CAQ-CAR-CAU-CAV
3	G	303	7L3	CAS-CAR-CAU-CAW
3	H	302	7L3	CAS-CAR-CAU-CAV
3	G	303	7L3	CAQ-CAR-CAU-CAW
3	H	302	7L3	CAQ-CAR-CAU-CAX
3	B	302	7L3	CAS-CAR-CAU-CAV
3	F	302	7L3	CAQ-CAR-CAU-CAX
3	C	303	7L3	CAS-CAR-CAU-CAX
3	D	303	7L3	CAS-CAR-CAU-CAV
3	E	302	7L3	CAQ-CAR-CAU-CAV
3	G	303	7L3	CAQ-CAR-CAU-CAV
3	F	302	7L3	CAS-CAR-CAU-CAV
3	F	302	7L3	CAS-CAR-CAU-CAX
3	C	303	7L3	CAB-NAK-SAL-OAM
3	F	302	7L3	CAB-NAK-SAL-OAM
3	A	302	7L3	CAQ-CAR-CAU-CAW
3	A	302	7L3	CAS-CAR-CAU-CAV
3	A	302	7L3	CAQ-CAR-CAU-CAX

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Mol	Chain	Res	Type	Atoms
3	C	303	7L3	CAP-CAN-SAL-OAO
3	C	303	7L3	CAT-CAN-SAL-OAO

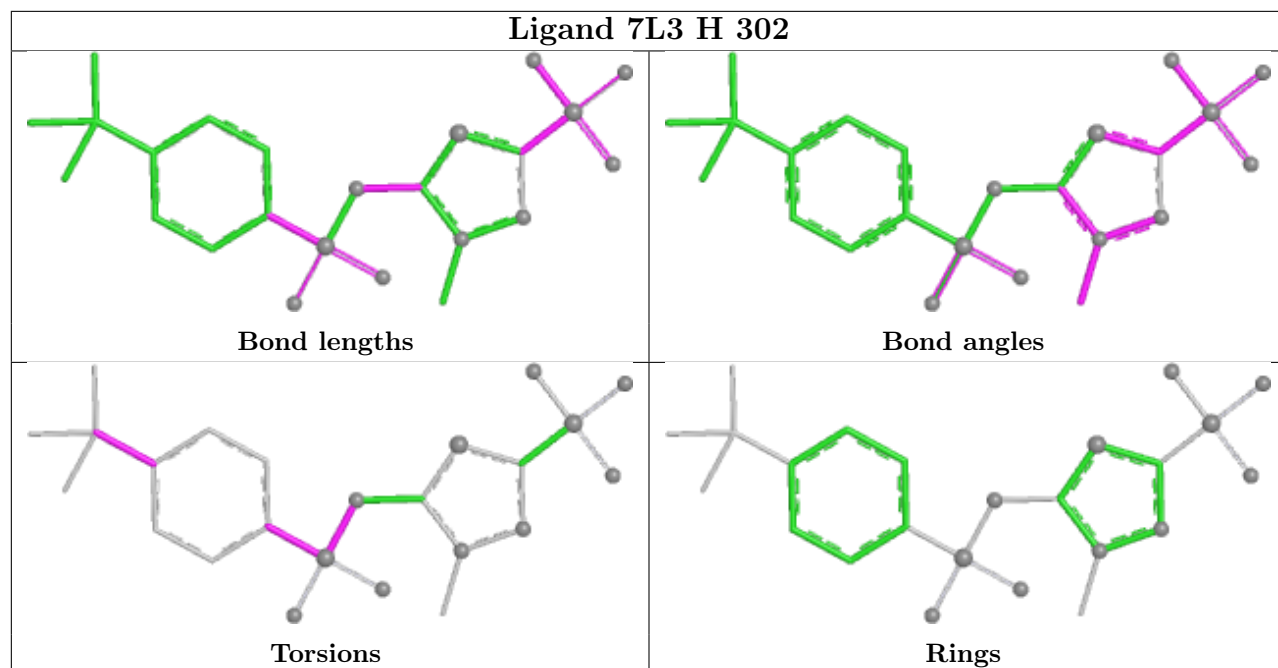
There are no ring outliers.

9 monomers are involved in 23 short contacts:

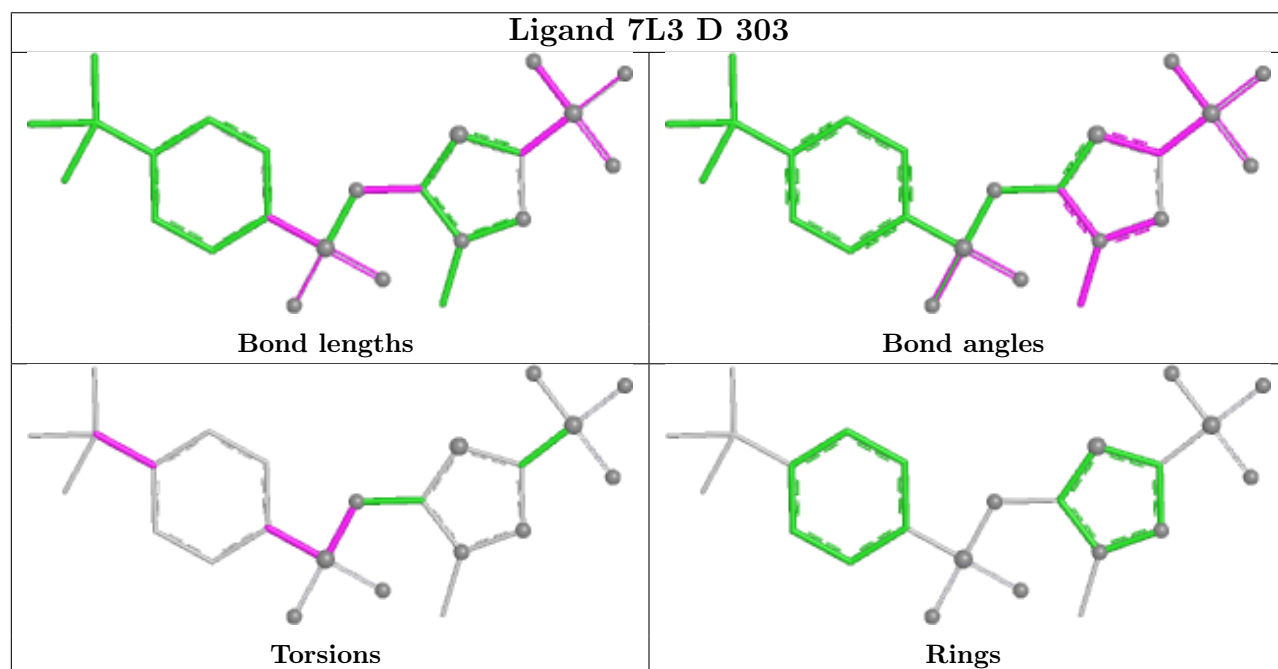
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	302	7L3	2	0
3	D	303	7L3	3	0
3	C	303	7L3	3	0
3	G	303	7L3	2	0
3	B	302	7L3	3	0
3	E	302	7L3	2	0
4	C	302	GOL	1	0
3	F	302	7L3	4	0
3	A	302	7L3	3	0

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.

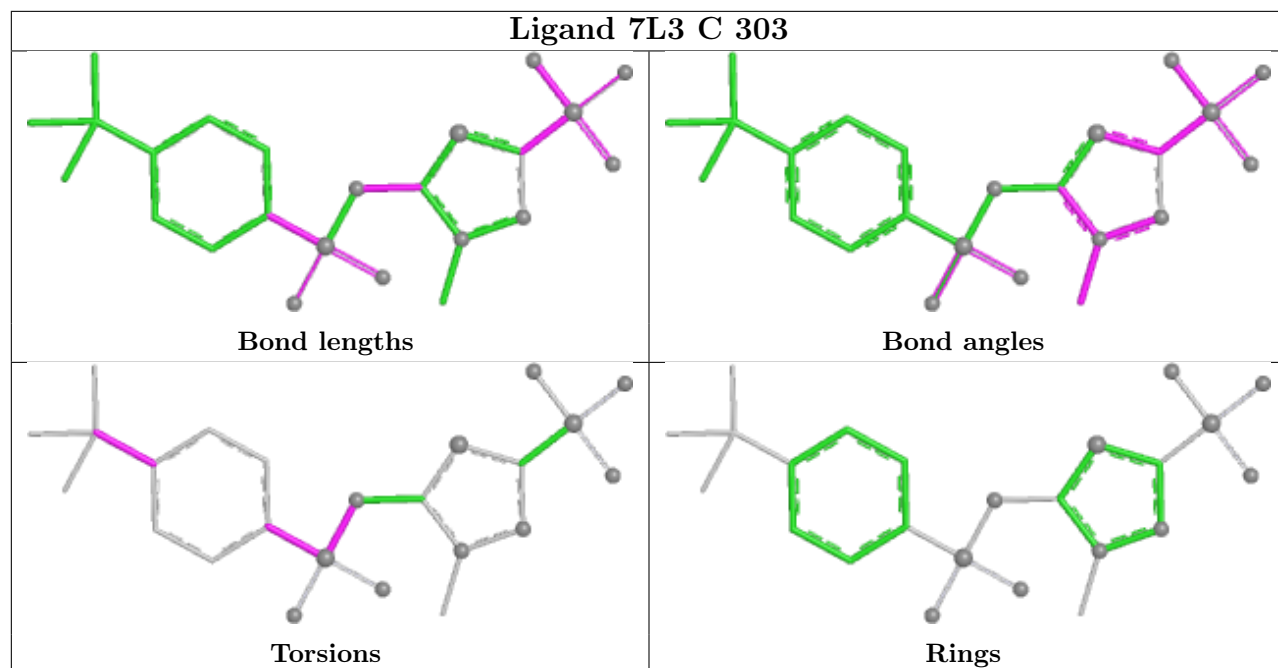
Ligand 7L3 H 302



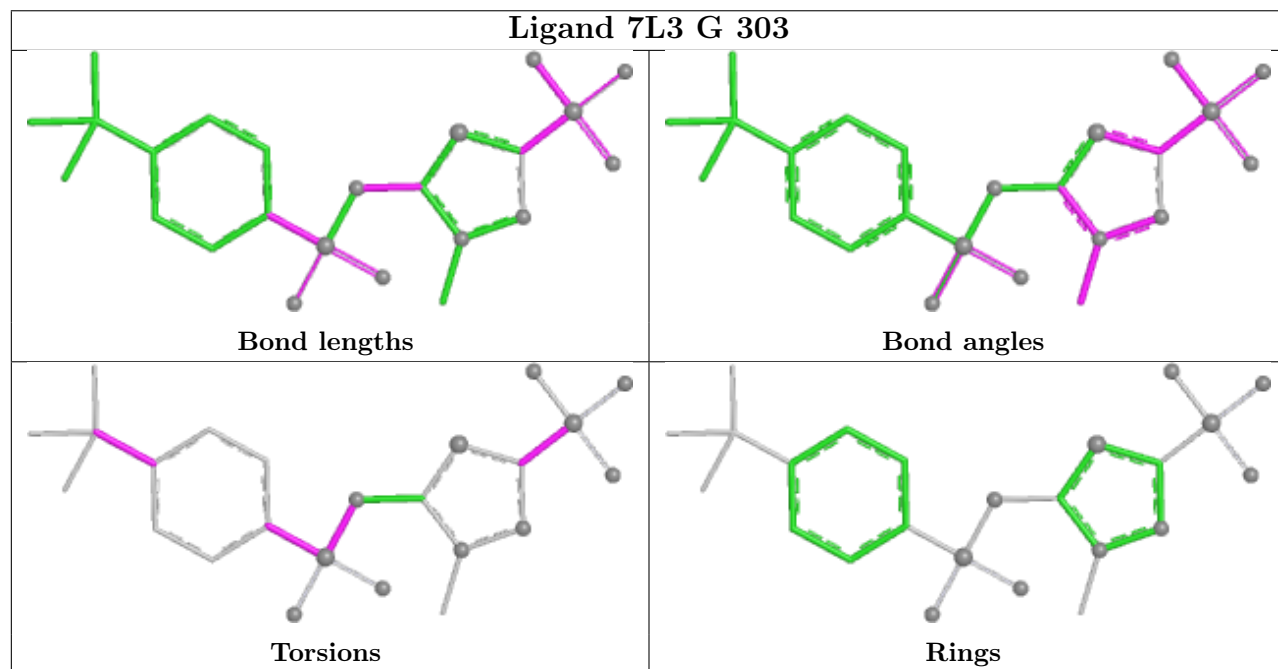
Ligand 7L3 D 303



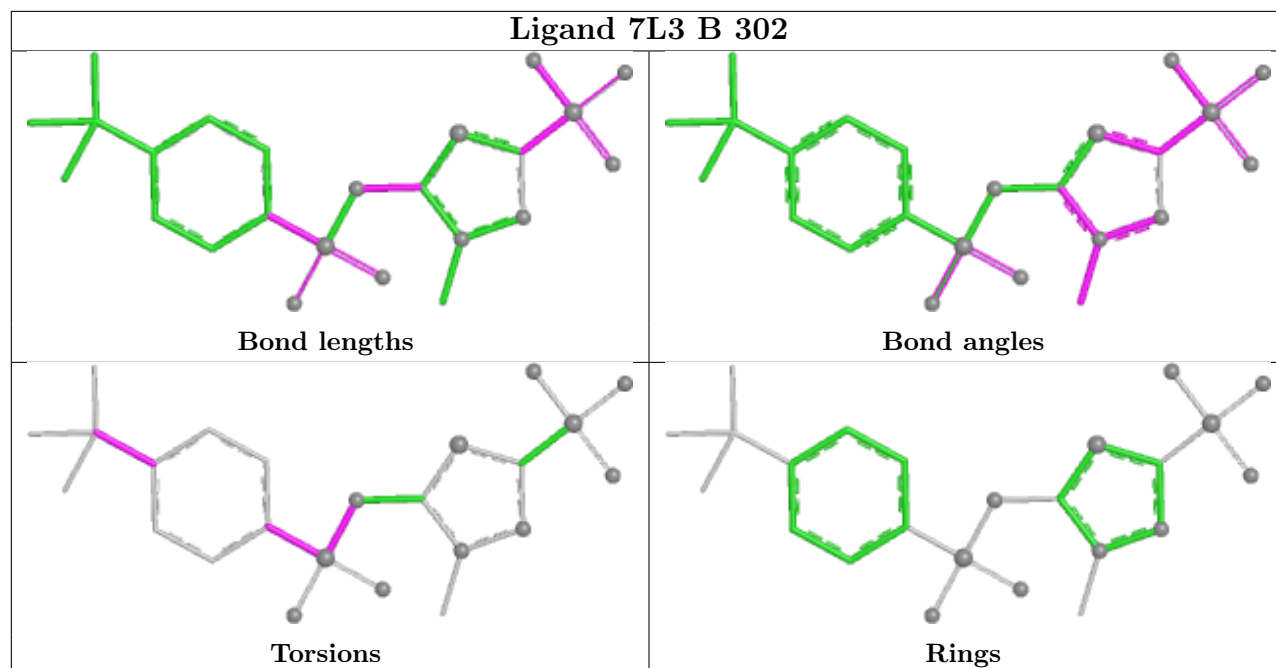
Ligand 7L3 C 303



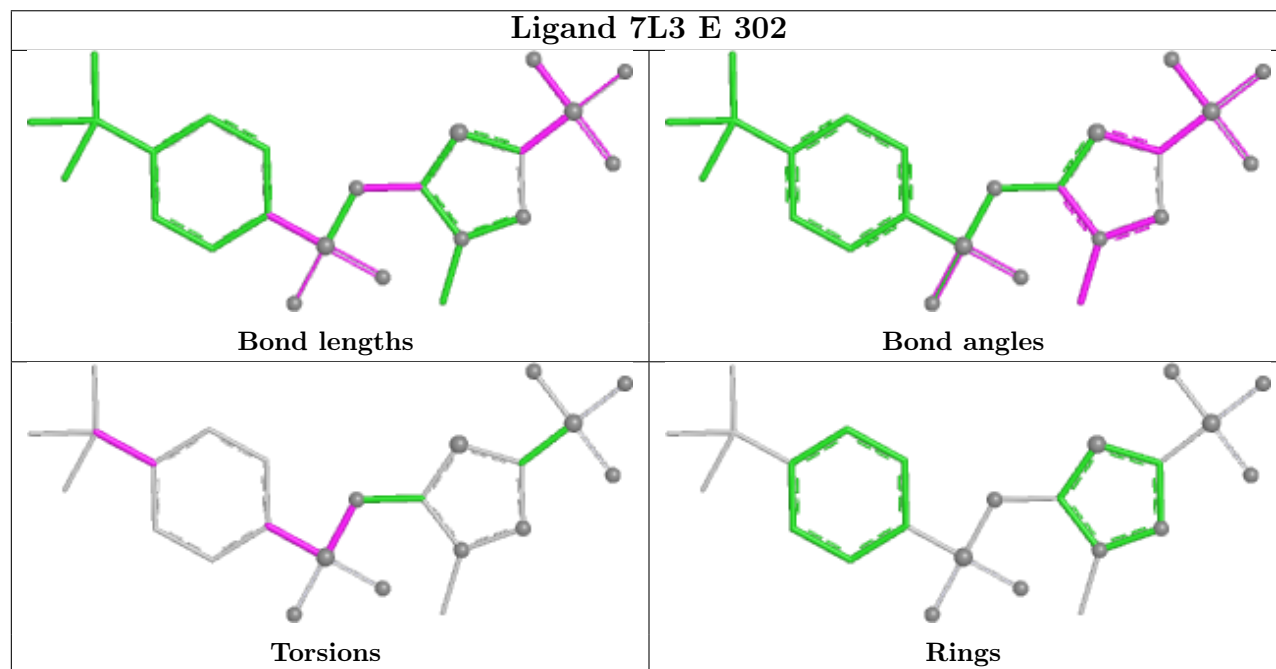
Ligand 7L3 G 303

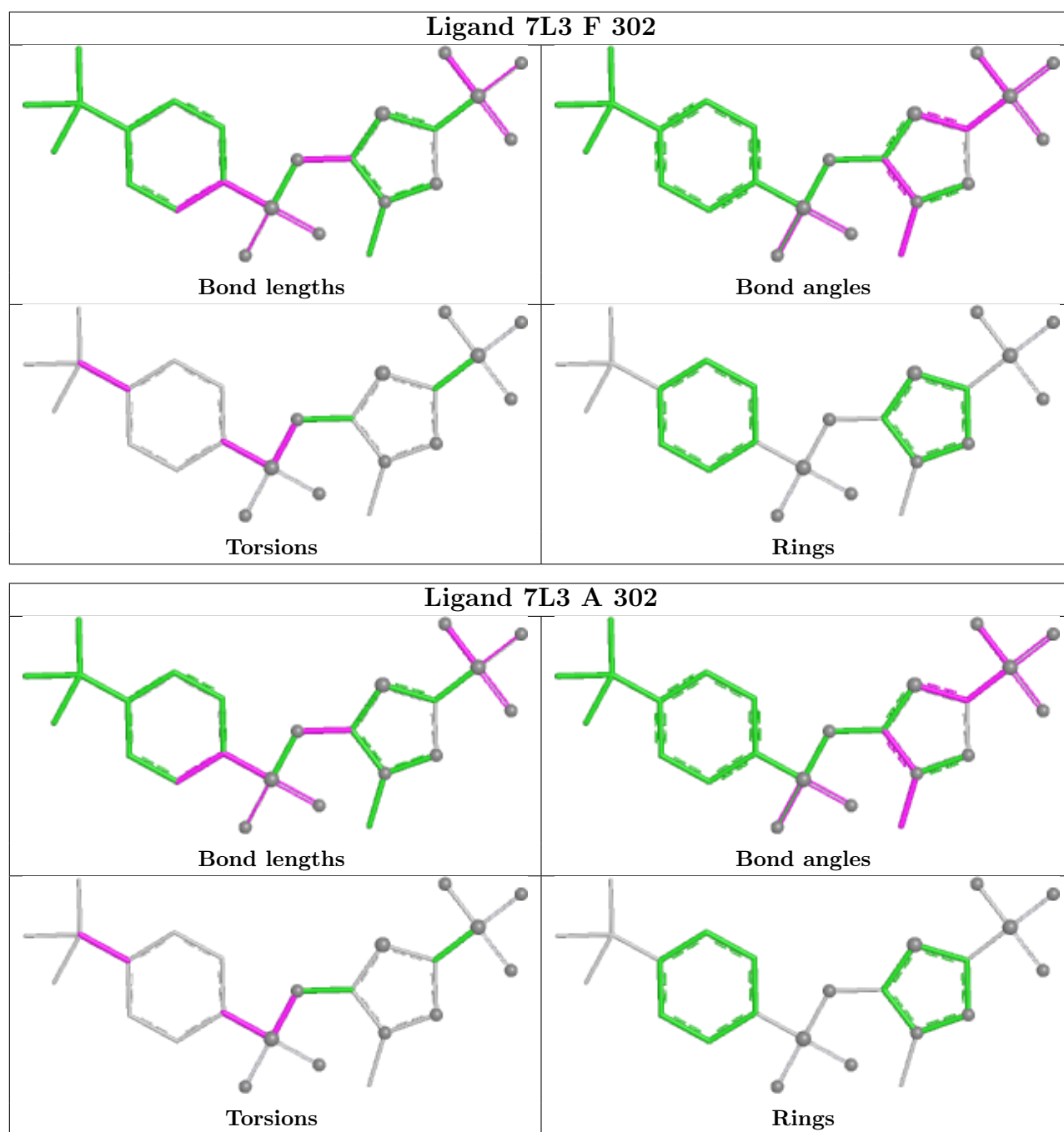


Ligand 7L3 B 302



Ligand 7L3 E 302





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	226/234 (96%)	-1.69	0 100 100	22, 50, 76, 95	2 (0%)
1	B	218/234 (93%)	-1.73	0 100 100	21, 38, 60, 83	1 (0%)
1	C	225/234 (96%)	-1.75	0 100 100	18, 37, 56, 88	2 (0%)
1	D	220/234 (94%)	-1.67	0 100 100	25, 48, 74, 86	0
1	E	226/234 (96%)	-1.75	0 100 100	17, 36, 61, 81	1 (0%)
1	F	222/234 (94%)	-1.68	0 100 100	22, 49, 72, 89	0
1	G	222/234 (94%)	-1.69	0 100 100	19, 50, 79, 86	1 (0%)
1	H	225/234 (96%)	-1.74	0 100 100	20, 40, 62, 78	0
All	All	1784/1872 (95%)	-1.71	0 100 100	17, 43, 72, 95	7 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

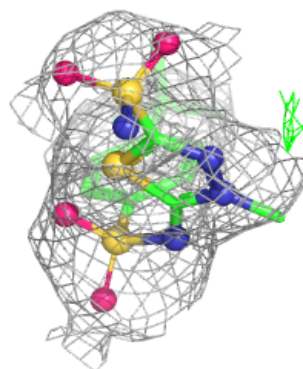
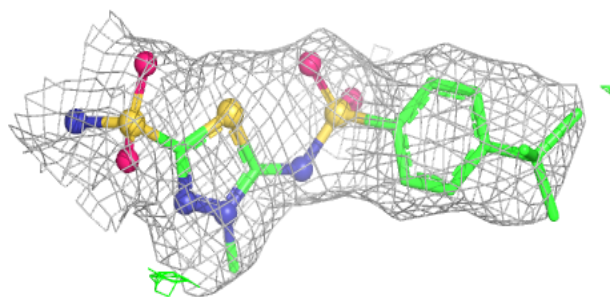
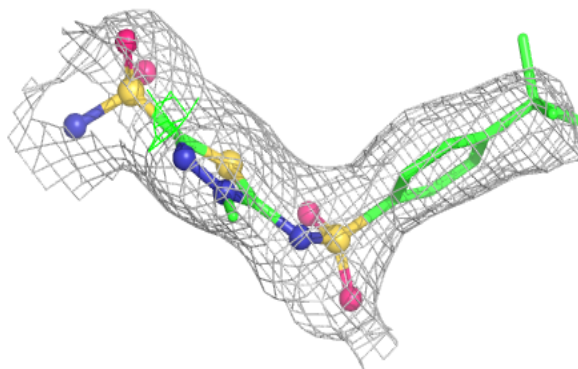
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	7L3	A	302	24/24	0.99	0.03	32,35,49,57	0
3	7L3	C	303	24/24	0.99	0.03	32,42,50,53	24
3	7L3	F	302	24/24	0.99	0.03	32,40,50,60	24
5	CL	D	302	1/1	0.99	0.04	59,59,59,59	0
5	CL	G	302	1/1	0.99	0.06	70,70,70,70	0
2	ZN	F	301	1/1	1.00	0.01	33,33,33,33	1
2	ZN	G	301	1/1	1.00	0.01	32,32,32,32	0
2	ZN	H	301	1/1	1.00	0.01	32,32,32,32	0
2	ZN	A	301	1/1	1.00	0.01	30,30,30,30	1
3	7L3	B	302	24/24	1.00	0.03	32,38,50,59	24
2	ZN	B	301	1/1	1.00	0.01	33,33,33,33	0
3	7L3	D	303	24/24	1.00	0.03	32,42,51,51	0
3	7L3	E	302	24/24	1.00	0.03	21,33,41,48	0
2	ZN	C	301	1/1	1.00	0.01	31,31,31,31	0
3	7L3	G	303	24/24	1.00	0.03	32,37,47,51	0
3	7L3	H	302	24/24	1.00	0.03	32,39,49,52	0
4	GOL	C	302	6/6	1.00	0.04	42,45,54,64	0
2	ZN	D	301	1/1	1.00	0.01	50,50,50,50	0
2	ZN	E	301	1/1	1.00	0.01	32,32,32,32	0

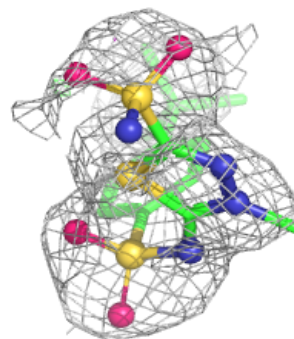
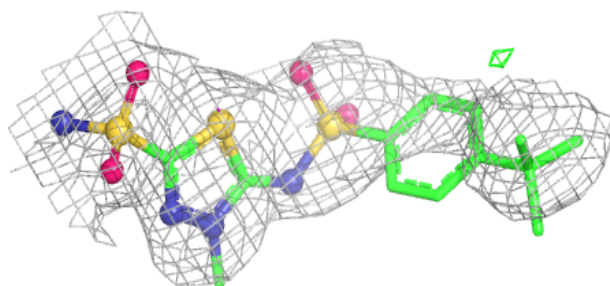
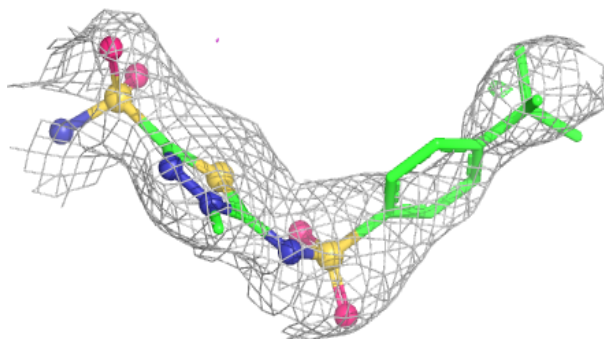
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 7L3 A 302:

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

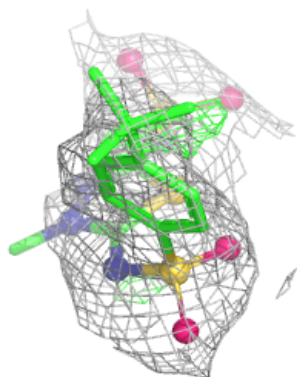
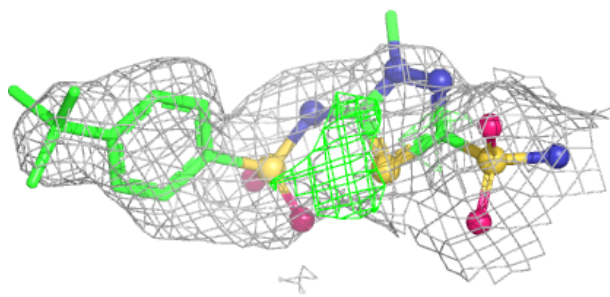
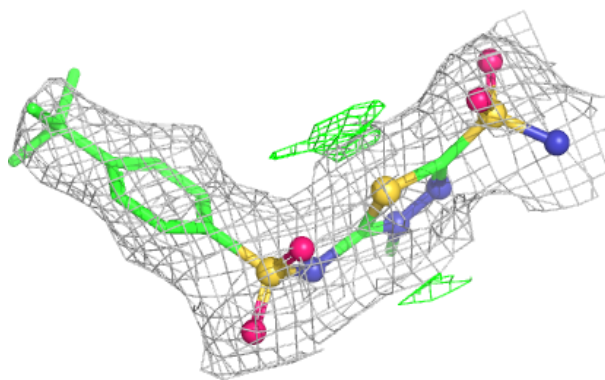
**Electron density around 7L3 C 303:**

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

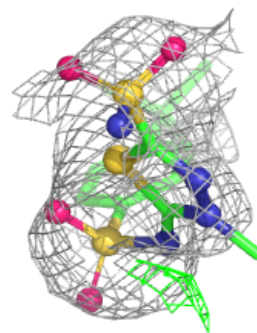
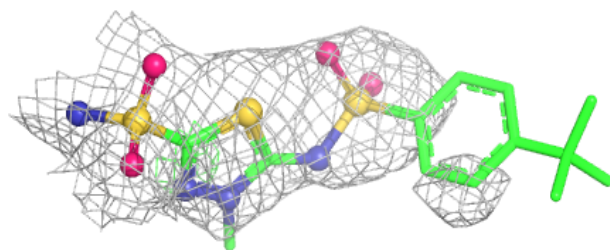
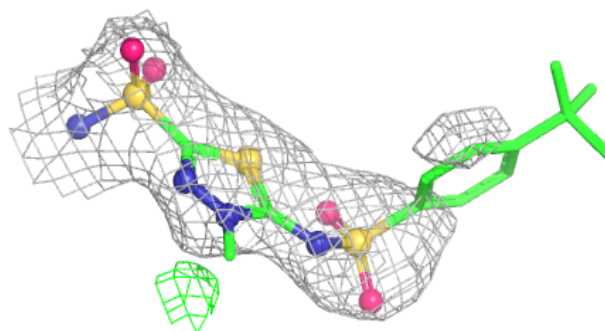


Electron density around 7L3 F 302:

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

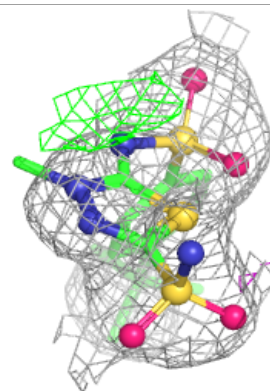
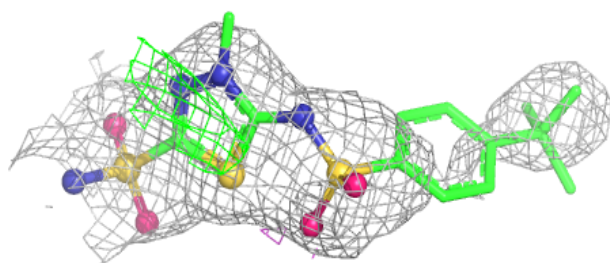
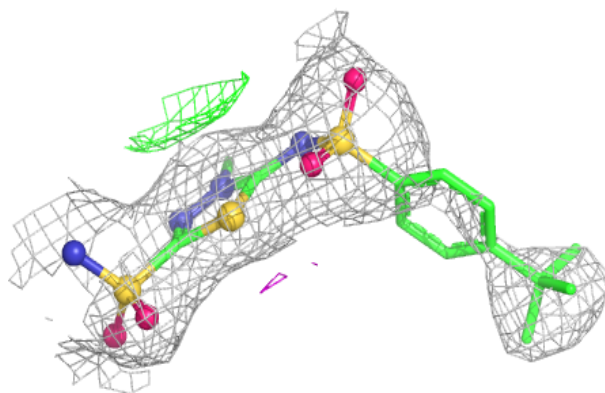
**Electron density around 7L3 B 302:**

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

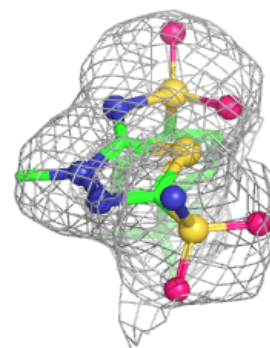
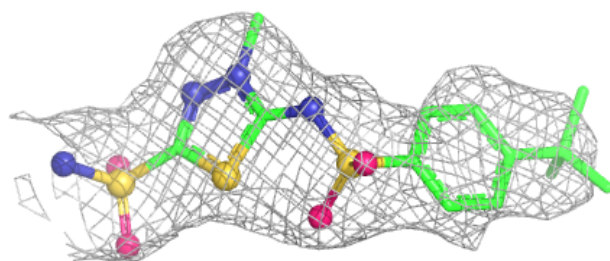
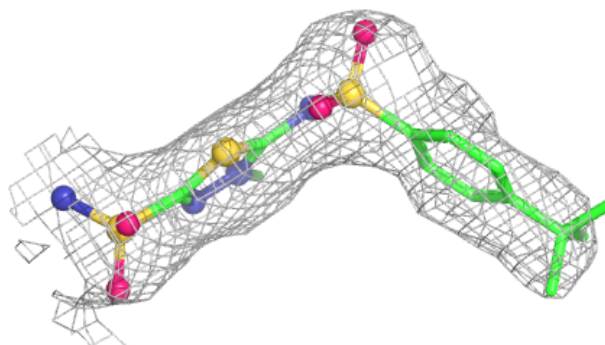


Electron density around 7L3 D 303:

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

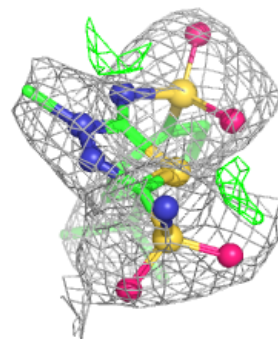
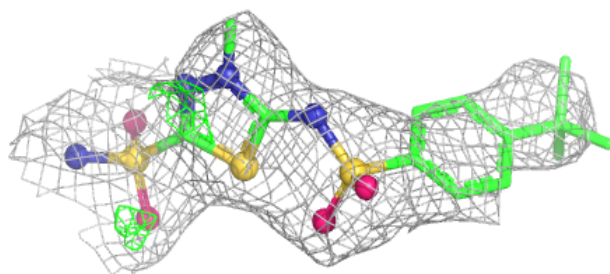
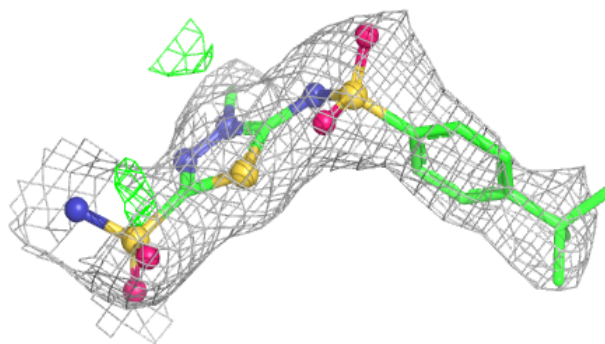
**Electron density around 7L3 E 302:**

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

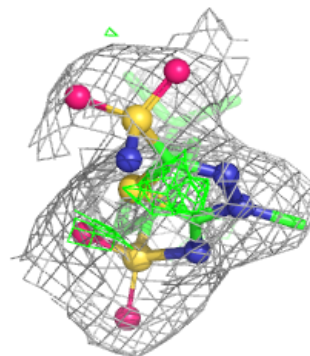
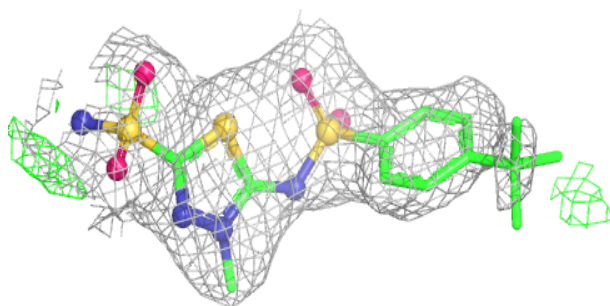
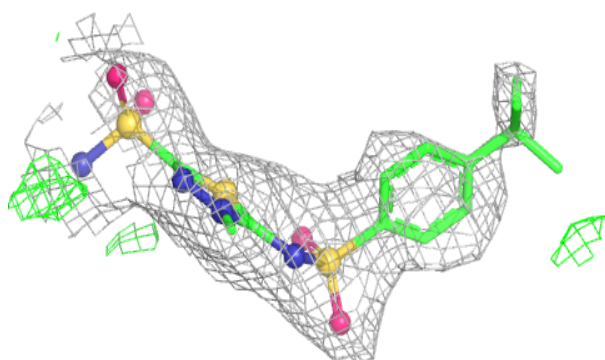


Electron density around 7L3 G 303:

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

**Electron density around 7L3 H 302:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.