



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:34 PM UTC

PDB ID : 1S64 / pdb_00001s64
Title : Rat protein geranylgeranyltransferase type-I complexed with L-778,123 and a sulfate anion
Authors : Reid, T.S.; Long, S.B.; Beese, L.S.
Deposited on : 2004-01-22
Resolution : 2.55 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

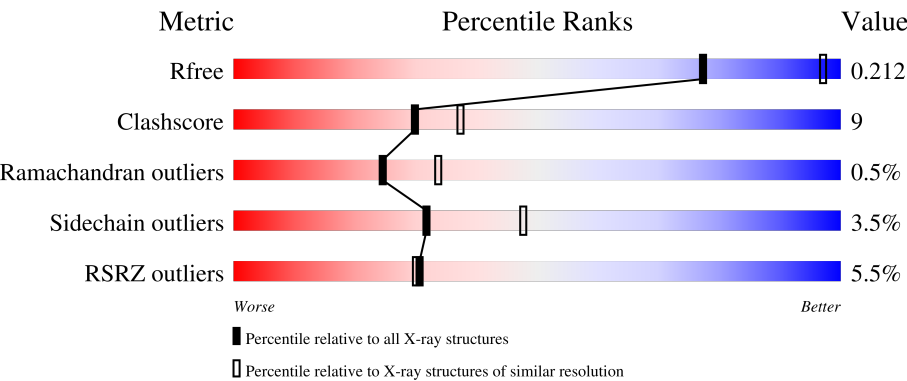
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	377	7% 67% 15% • 17%
1	C	377	3% 68% 15% • 17%
1	E	377	4% 63% 20% • 17%
1	G	377	8% 64% 19% • 17%
1	I	377	3% 66% 16% • 17%

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Mol	Chain	Length	Quality of chain
1	K	377	2% 67% 15% • 17%
2	B	377	2% 68% 21% • 8%
2	D	377	4% 72% 19% • 8%
2	F	377	3% 72% 18% • 8%
2	H	377	11% 67% 23% • 8%
2	J	377	5% 72% 18% • 8%
2	L	377	3% 75% 15% • 8%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 33735 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protein farnesyltransferase/geranylgeranyltransferase type I alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2626	1678	463	480	5			
1	C	314	Total	C	N	O	S	0	0	0
			2637	1686	458	488	5			
1	E	314	Total	C	N	O	S	0	0	0
			2642	1686	461	490	5			
1	G	314	Total	C	N	O	S	0	0	0
			2633	1683	459	486	5			
1	I	314	Total	C	N	O	S	0	0	0
			2651	1692	462	492	5			
1	K	314	Total	C	N	O	S	0	0	0
			2667	1700	466	496	5			

- Molecule 2 is a protein called Geranylgeranyl transferase type I beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	346	Total	C	N	O	S	0	0	0
			2693	1704	467	498	24			
2	D	346	Total	C	N	O	S	0	0	0
			2690	1705	463	498	24			
2	F	346	Total	C	N	O	S	0	0	0
			2714	1714	474	502	24			
2	H	346	Total	C	N	O	S	0	0	0
			2688	1701	463	500	24			
2	J	346	Total	C	N	O	S	0	0	0
			2709	1711	471	503	24			
2	L	346	Total	C	N	O	S	0	0	0
			2719	1717	473	505	24			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

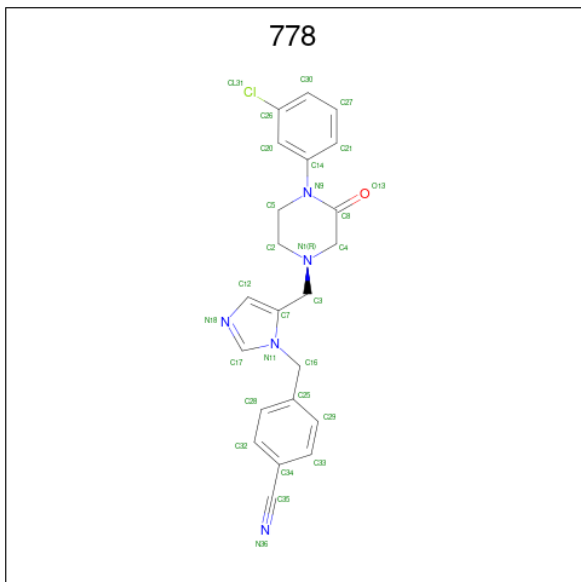
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		
3	H	1	Total	Zn	0	0
			1	1		
3	J	1	Total	Zn	0	0
			1	1		
3	L	1	Total	Zn	0	0
			1	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 4-[(5-{[4-(3-CHLOROPHENYL)-3-OXOPIPERAZIN-1-YL]METHYL}-1H-1-MIDAZOL-1-YL)METHYL]BENZONITRILE (CCD ID: 778) (formula: $C_{22}H_{20}ClN_5O$).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	J	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	L	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Cl	0	0
			1	1		
7	D	1	Total	Cl	0	0
			1	1		
7	F	1	Total	Cl	0	0
			1	1		
7	G	1	Total	Cl	0	0
			1	1		
7	H	1	Total	Cl	0	0
			1	1		
7	I	1	Total	Cl	0	0
			1	1		

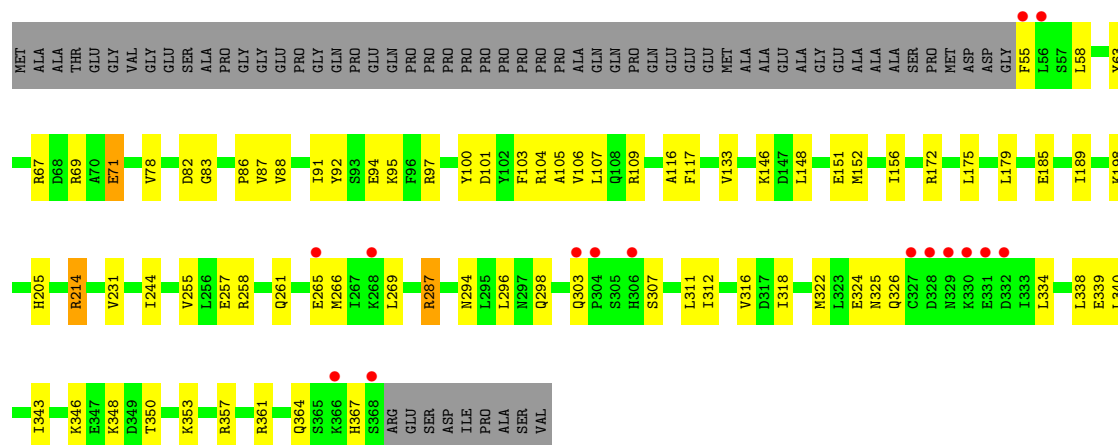
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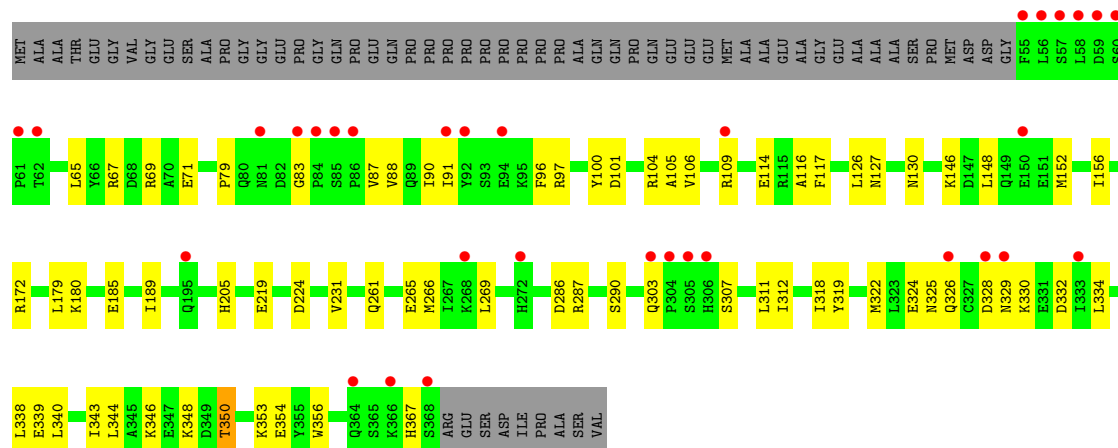
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	1	Total 1	Cl 1	0	0
7	K	1	Total 1	Cl 1	0	0
7	L	1	Total 1	Cl 1	0	0

- Molecule 8 is water.

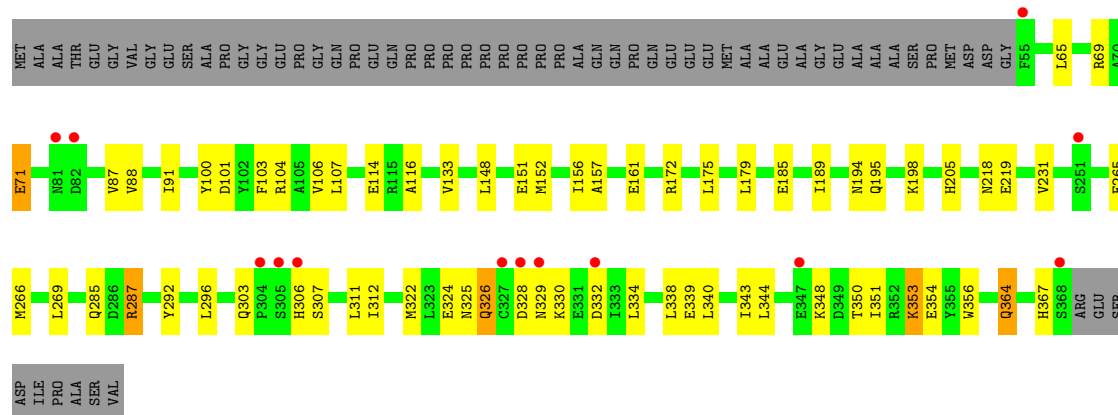
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	95	Total 95	O 95	0	0
8	B	74	Total 74	O 74	0	0
8	C	102	Total 102	O 102	0	0
8	D	123	Total 123	O 123	0	0
8	E	97	Total 97	O 97	0	0
8	F	114	Total 114	O 114	0	0
8	G	96	Total 96	O 96	0	0
8	H	65	Total 65	O 65	0	0
8	I	134	Total 134	O 134	0	0
8	J	102	Total 102	O 102	0	0
8	K	207	Total 207	O 207	0	0
8	L	166	Total 166	O 166	0	0



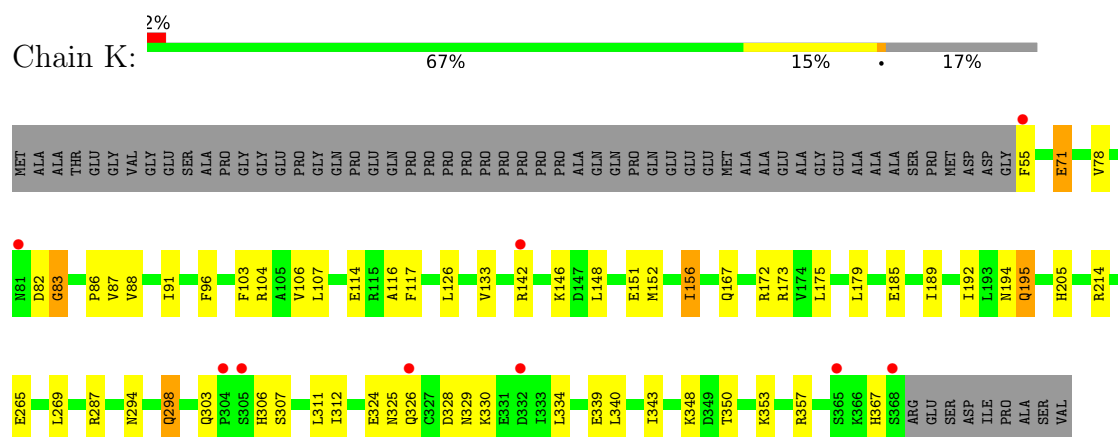
- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type I alpha subunit



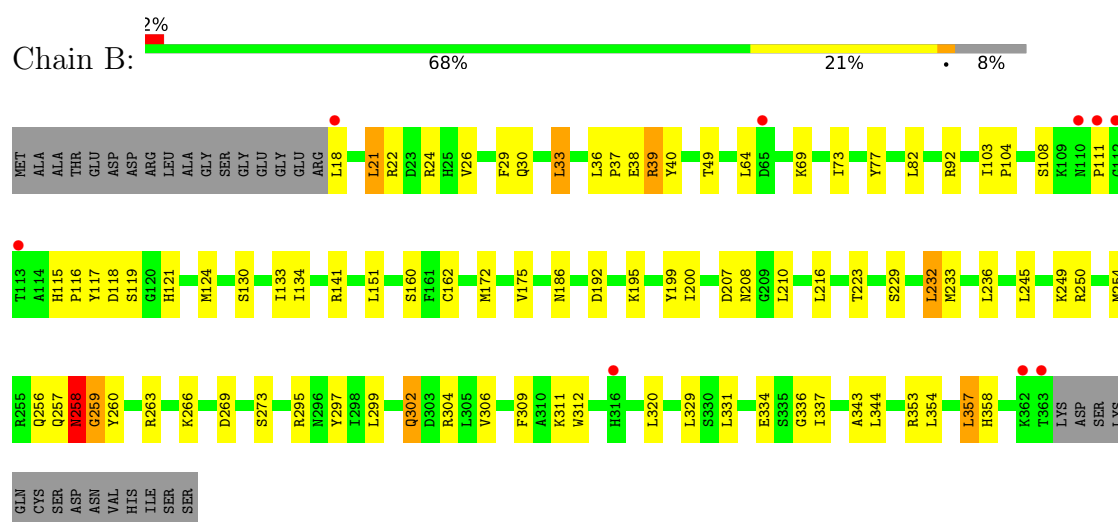
- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type I alpha subunit



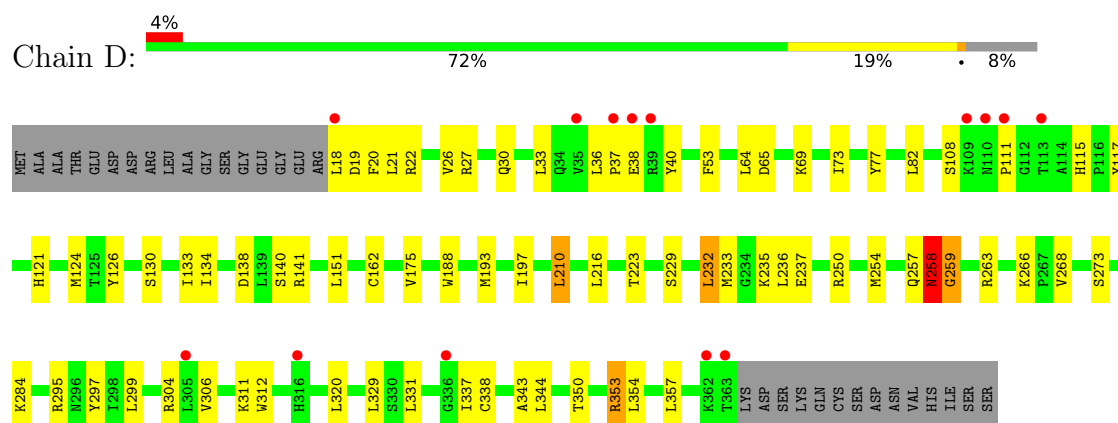
- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type I alpha subunit



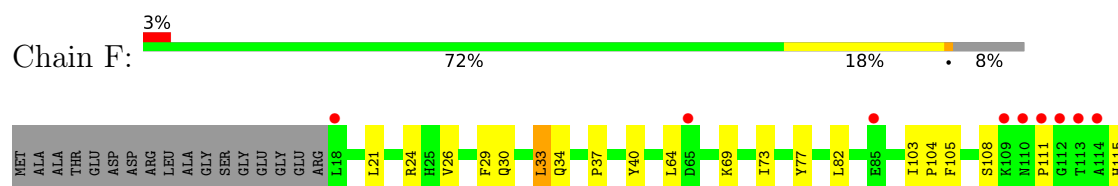
- Molecule 2: Geranylgeranyl transferase type I beta subunit

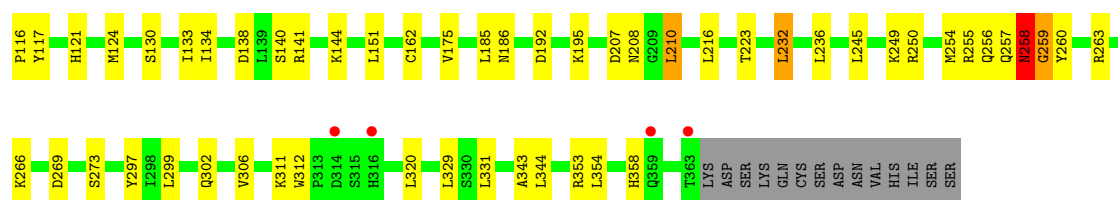


- Molecule 2: Geranylgeranyl transferase type I beta subunit

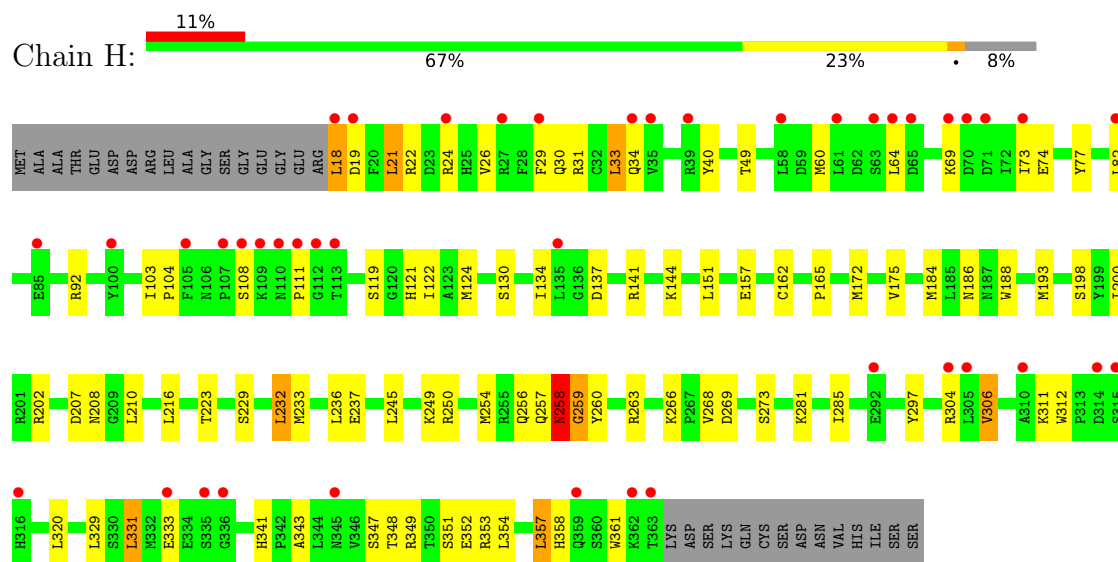


- Molecule 2: Geranylgeranyl transferase type I beta subunit

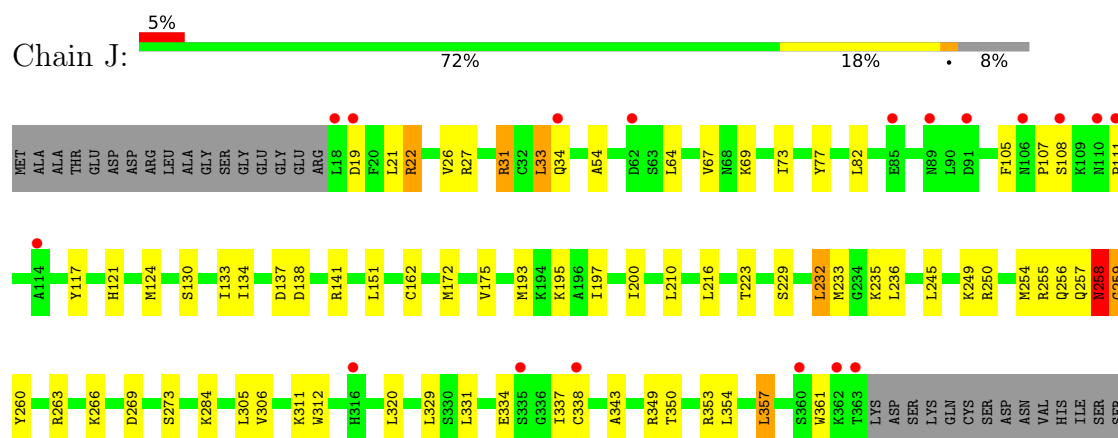




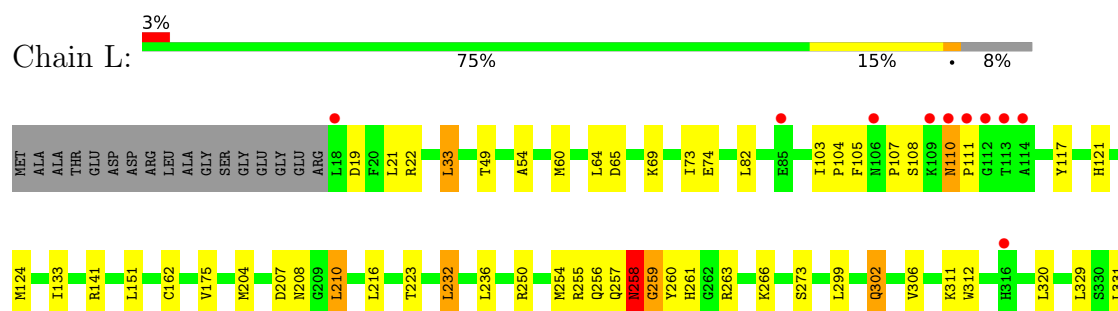
• Molecule 2: Geranylgeranyl transferase type I beta subunit

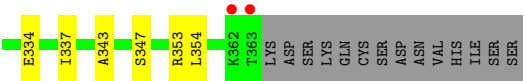


• Molecule 2: Geranylgeranyl transferase type I beta subunit



• Molecule 2: Geranylgeranyl transferase type I beta subunit





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	271.15Å 268.68Å 184.62Å 90.00° 131.55° 90.00°	Depositor
Resolution (Å)	30.00 – 2.55 30.00 – 2.55	Depositor EDS
% Data completeness (in resolution range)	93.4 (30.00-2.55) 93.3 (30.00-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.54Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.192 , 0.213 0.195 , 0.212	Depositor DCC
R_{free} test set	15041 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.086 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33735	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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: CL, MES, ZN, SO4, 778

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	0.40	0/2692	0.82	2/3664 (0.1%)
1	C	0.41	0/2703	0.84	5/3677 (0.1%)
1	E	0.40	0/2708	0.83	4/3684 (0.1%)
1	G	0.41	0/2699	0.83	5/3672 (0.1%)
1	I	0.41	0/2717	0.83	4/3694 (0.1%)
1	K	0.46	0/2733	0.84	5/3713 (0.1%)
2	B	0.40	0/2754	0.91	6/3725 (0.2%)
2	D	0.42	0/2751	0.91	10/3720 (0.3%)
2	F	0.42	0/2775	0.91	6/3750 (0.2%)
2	H	0.39	0/2749	0.91	9/3720 (0.2%)
2	J	0.41	0/2770	0.90	7/3745 (0.2%)
2	L	0.46	1/2780 (0.0%)	0.91	6/3756 (0.2%)
All	All	0.42	1/32831 (0.0%)	0.87	69/44520 (0.2%)

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
2	B	0	1
2	F	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	204	MET	SD-CE	5.63	1.93	1.79

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	259	GLY	N-CA-C	-10.25	97.95	112.60
2	H	259	GLY	N-CA-C	-10.06	98.21	112.60
2	F	259	GLY	N-CA-C	-9.97	98.34	112.60
2	D	259	GLY	N-CA-C	-9.90	98.44	112.60
2	L	259	GLY	N-CA-C	-9.86	98.50	112.60
2	B	259	GLY	N-CA-C	-9.67	98.77	112.60
1	E	185	GLU	N-CA-C	9.04	122.04	111.02
1	K	185	GLU	N-CA-C	8.82	121.78	111.02
1	A	185	GLU	N-CA-C	8.79	121.74	111.02
1	I	185	GLU	N-CA-C	8.77	121.72	111.02
1	C	185	GLU	N-CA-C	8.76	121.70	111.02
1	G	185	GLU	N-CA-C	8.49	121.38	111.02
1	K	348	LYS	N-CA-C	7.17	121.78	112.89
2	J	258	ASN	N-CA-C	-7.02	95.85	110.80
2	B	258	ASN	N-CA-C	-6.85	96.21	110.80
2	D	258	ASN	N-CA-C	-6.79	96.33	110.80
2	F	258	ASN	N-CA-C	-6.79	96.35	110.80
2	L	258	ASN	N-CA-C	-6.73	96.46	110.80
2	H	258	ASN	N-CA-C	-6.69	96.54	110.80
2	F	257	GLN	N-CA-C	-6.38	105.52	113.55
2	J	257	GLN	N-CA-C	-6.32	105.59	113.55
2	D	353	ARG	N-CA-C	-6.25	104.47	111.28
2	H	257	GLN	N-CA-C	-6.17	105.78	113.55
1	C	83	GLY	CA-C-N	6.17	125.65	119.24
1	C	83	GLY	C-N-CA	6.17	125.65	119.24
2	D	257	GLN	N-CA-C	-5.96	106.04	113.55
1	C	347	GLU	N-CA-C	5.95	121.41	114.62
1	K	83	GLY	CA-C-N	5.91	125.39	119.24
1	K	83	GLY	C-N-CA	5.91	125.39	119.24
2	L	257	GLN	N-CA-C	-5.85	106.17	113.55
1	C	350	THR	N-CA-C	5.84	118.43	111.71
2	B	257	GLN	N-CA-C	-5.84	106.19	113.55
2	H	175	VAL	N-CA-C	-5.74	104.93	110.72
2	J	22	ARG	N-CA-C	5.69	117.94	111.11
2	B	175	VAL	N-CA-C	-5.66	105.01	110.72
1	E	244	ILE	N-CA-C	5.64	115.84	110.42
2	J	175	VAL	N-CA-C	-5.64	105.02	110.72
2	F	175	VAL	N-CA-C	-5.64	105.03	110.72
2	D	162	CYS	N-CA-C	-5.52	102.29	110.46
2	B	273	SER	N-CA-C	-5.51	105.66	112.38
2	L	162	CYS	N-CA-C	-5.46	102.37	110.46
2	D	273	SER	N-CA-C	-5.45	105.44	111.71
1	K	350	THR	N-CA-C	5.42	118.69	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	273	SER	N-CA-C	-5.42	105.77	112.38
2	L	273	SER	N-CA-C	-5.39	105.51	111.71
1	A	217	ASP	N-CA-C	5.32	120.15	111.37
2	B	162	CYS	N-CA-C	-5.31	102.60	110.46
2	F	273	SER	N-CA-C	-5.30	105.62	111.71
2	D	175	VAL	N-CA-C	-5.29	105.38	110.72
2	J	162	CYS	N-CA-C	-5.27	102.67	110.46
1	I	292	TYR	CA-C-N	5.26	125.32	119.32
1	I	292	TYR	C-N-CA	5.26	125.32	119.32
1	G	350	THR	N-CA-C	5.21	117.64	111.33
2	F	162	CYS	N-CA-C	-5.19	102.78	110.46
2	J	273	SER	N-CA-C	-5.18	106.05	112.38
1	G	83	GLY	CA-C-N	5.16	124.61	119.24
1	G	83	GLY	C-N-CA	5.16	124.61	119.24
2	L	175	VAL	N-CA-C	-5.12	105.55	110.72
2	H	341	HIS	CA-C-N	5.11	125.40	119.47
2	H	341	HIS	C-N-CA	5.11	125.40	119.47
2	D	284	LYS	N-CA-C	5.10	118.77	112.24
1	E	346	LYS	N-CA-C	5.09	118.64	112.23
1	I	285	GLN	N-CA-C	5.07	117.47	111.33
2	D	115	HIS	CA-C-N	5.07	125.35	119.47
2	D	115	HIS	C-N-CA	5.07	125.35	119.47
2	H	122	ILE	N-CA-C	5.04	116.36	110.62
1	E	350	THR	N-CA-C	5.03	118.19	111.75
2	H	162	CYS	N-CA-C	-5.00	103.05	110.46
1	G	346	LYS	N-CA-C	5.00	117.84	111.69

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	297	TYR	Sidechain
2	F	297	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2626	0	2518	43	0
1	C	2637	0	2529	38	0
1	E	2642	0	2534	53	0
1	G	2633	0	2524	52	0
1	I	2651	0	2551	45	0
1	K	2667	0	2577	38	0
2	B	2693	0	2589	61	0
2	D	2690	0	2588	42	0
2	F	2714	0	2624	44	0
2	H	2688	0	2573	63	0
2	J	2709	0	2610	44	0
2	L	2719	0	2632	34	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
3	J	1	0	0	0	0
3	L	1	0	0	0	0
4	B	5	0	0	0	0
4	D	5	0	0	0	0
4	F	5	0	0	0	0
4	H	5	0	0	0	0
4	J	5	0	0	0	0
4	L	5	0	0	0	0
5	B	29	0	20	0	0
5	D	29	0	20	0	0
5	F	29	0	20	0	0
5	H	29	0	20	0	0
5	J	29	0	20	0	0
5	L	29	0	20	0	0
6	B	12	0	13	0	0
6	D	12	0	13	2	0
6	F	12	0	13	0	0
6	H	12	0	13	0	0
6	J	12	0	13	0	0
6	L	12	0	13	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
7	G	1	0	0	1	0
7	H	1	0	0	0	0
7	I	1	0	0	1	0
7	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	K	1	0	0	1	0
7	L	1	0	0	0	0
8	A	95	0	0	2	0
8	B	74	0	0	2	0
8	C	102	0	0	2	0
8	D	123	0	0	3	0
8	E	97	0	0	1	0
8	F	114	0	0	1	0
8	G	96	0	0	3	0
8	H	65	0	0	3	0
8	I	134	0	0	3	0
8	J	102	0	0	2	0
8	K	207	0	0	5	0
8	L	166	0	0	0	0
All	All	33735	0	31047	541	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 9.

All (541) 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:E:156:ILE:HG12	1:E:172:ARG:HH12	1.10	1.13
1:A:156:ILE:HG12	1:A:172:ARG:HH12	0.97	1.12
1:I:156:ILE:HG12	1:I:172:ARG:HH12	1.05	1.11
1:K:156:ILE:HG12	1:K:172:ARG:HH12	0.99	1.07
1:G:156:ILE:HG12	1:G:172:ARG:HH12	1.20	1.05
1:C:156:ILE:HG12	1:C:172:ARG:HH12	1.22	1.01
1:K:156:ILE:HG12	1:K:172:ARG:NH1	1.83	0.93
1:A:156:ILE:HG12	1:A:172:ARG:NH1	1.83	0.92
2:B:39:ARG:HB3	2:B:39:ARG:HH11	1.33	0.90
7:G:378:CL:CL	8:G:385:HOH:O	2.31	0.86
1:I:156:ILE:HG12	1:I:172:ARG:NH1	1.91	0.86
2:H:18:LEU:HA	2:H:304:ARG:NH2	1.93	0.83
1:E:156:ILE:HG12	1:E:172:ARG:NH1	1.94	0.82
1:G:231:VAL:HG23	1:G:266:MET:HE3	1.60	0.81
1:K:156:ILE:CG1	1:K:172:ARG:HH12	1.88	0.81
1:E:231:VAL:HG23	1:E:266:MET:HE3	1.63	0.81
2:H:348:THR:O	2:H:352:GLU:HG2	1.80	0.80
1:A:152:MET:O	1:A:156:ILE:HG13	1.81	0.80
1:G:152:MET:O	1:G:156:ILE:HG13	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:152:MET:O	1:K:156:ILE:HG13	1.83	0.78
1:I:152:MET:O	1:I:156:ILE:HG13	1.87	0.75
1:I:91:ILE:HD12	1:I:91:ILE:O	1.86	0.74
1:E:156:ILE:CG1	1:E:172:ARG:HH12	1.96	0.74
1:E:189:ILE:HD11	1:E:205:HIS:HD2	1.53	0.74
2:H:229:SER:O	2:H:233:MET:HG3	1.86	0.74
1:E:152:MET:O	1:E:156:ILE:HG13	1.87	0.74
1:A:214:ARG:HG2	1:G:180:LYS:HB2	1.69	0.73
1:G:91:ILE:HD12	1:G:91:ILE:O	1.89	0.72
1:K:189:ILE:HD11	1:K:205:HIS:HD2	1.54	0.72
1:C:189:ILE:HD11	1:C:205:HIS:HD2	1.55	0.72
2:B:69:LYS:O	2:B:73:ILE:HG13	1.89	0.72
1:E:353:LYS:HE2	1:E:357:ARG:HH12	1.55	0.71
1:E:214:ARG:O	1:E:214:ARG:HG3	1.91	0.71
1:K:298:GLN:HG2	8:K:529:HOH:O	1.90	0.71
1:G:189:ILE:HD11	1:G:205:HIS:HD2	1.56	0.71
1:C:152:MET:O	1:C:156:ILE:HG13	1.88	0.70
1:E:318:ILE:HG22	1:E:322:MET:HE3	1.73	0.70
1:A:189:ILE:HD11	1:A:205:HIS:HD2	1.57	0.70
2:H:92:ARG:HG2	2:H:165:PRO:HG3	1.74	0.69
1:G:100:TYR:O	1:G:104:ARG:HG3	1.91	0.69
1:A:91:ILE:HD12	1:A:91:ILE:O	1.92	0.69
1:E:353:LYS:HE3	1:E:357:ARG:HH22	1.58	0.69
1:G:97:ARG:HG2	1:G:101:ASP:OD2	1.92	0.69
2:B:353:ARG:HG2	2:B:353:ARG:HH11	1.57	0.69
2:B:133:ILE:HD13	2:B:354:LEU:HD13	1.75	0.68
1:I:189:ILE:HD11	1:I:205:HIS:HD2	1.58	0.68
2:F:69:LYS:O	2:F:73:ILE:HG13	1.93	0.68
1:E:91:ILE:O	1:E:91:ILE:HD12	1.94	0.68
1:K:91:ILE:HD12	1:K:91:ILE:O	1.94	0.68
1:A:339:GLU:O	1:A:343:ILE:HG13	1.95	0.67
2:H:18:LEU:HD22	2:H:18:LEU:N	2.09	0.67
2:D:69:LYS:O	2:D:73:ILE:HG13	1.95	0.67
2:F:133:ILE:HD13	2:F:354:LEU:HD13	1.77	0.66
1:C:91:ILE:O	1:C:91:ILE:HD12	1.95	0.66
2:J:232:LEU:HD13	2:J:343:ALA:HB1	1.76	0.66
2:H:18:LEU:HA	2:H:304:ARG:HH22	1.61	0.66
1:G:318:ILE:HG22	1:G:322:MET:HE2	1.76	0.66
1:G:87:VAL:HG12	1:G:88:VAL:HG23	1.76	0.66
1:G:231:VAL:CG2	1:G:266:MET:HE3	2.26	0.65
2:D:353:ARG:HH11	2:D:357:LEU:HG	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:378:CL:CL	8:K:389:HOH:O	2.51	0.65
2:D:65:ASP:HA	8:D:457:HOH:O	1.96	0.65
2:H:21:LEU:HD21	2:H:304:ARG:HG2	1.77	0.65
2:H:69:LYS:O	2:H:73:ILE:HG13	1.96	0.65
2:F:37:PRO:HD2	2:F:40:TYR:CD1	2.32	0.65
2:H:21:LEU:HD23	2:H:24:ARG:HE	1.63	0.64
1:I:231:VAL:HG23	1:I:266:MET:HE3	1.77	0.64
1:E:231:VAL:CG2	1:E:266:MET:HE3	2.27	0.64
1:E:198:LYS:HD3	2:F:266:LYS:HD3	1.80	0.64
2:L:232:LEU:HD13	2:L:343:ALA:HB1	1.80	0.64
1:K:87:VAL:HG12	1:K:88:VAL:HG23	1.80	0.64
1:G:334:LEU:HD22	1:G:367:HIS:O	1.97	0.63
1:I:156:ILE:CG1	1:I:172:ARG:HH12	1.96	0.63
1:G:343:ILE:HG22	1:G:348:LYS:HG3	1.81	0.63
1:A:214:ARG:HG3	1:A:214:ARG:O	1.98	0.62
2:J:133:ILE:HD13	2:J:354:LEU:HD13	1.79	0.62
2:L:133:ILE:HD13	2:L:354:LEU:HD13	1.82	0.62
1:C:334:LEU:HD22	1:C:367:HIS:O	1.99	0.61
1:E:255:VAL:HG13	1:E:258:ARG:NH2	2.16	0.61
2:H:26:VAL:O	2:H:30:GLN:HG3	2.01	0.60
2:H:92:ARG:HD2	2:H:119:SER:HB3	1.82	0.60
1:E:312:ILE:HG23	1:E:340:LEU:HD22	1.84	0.60
2:H:245:LEU:O	2:H:249:LYS:HG3	2.01	0.60
1:G:101:ASP:HA	1:G:104:ARG:NH1	2.17	0.60
1:E:87:VAL:HG12	1:E:88:VAL:HG23	1.84	0.59
1:A:87:VAL:HG12	1:A:88:VAL:HG23	1.82	0.59
1:C:303:GLN:O	1:C:307:SER:HB2	2.01	0.59
1:E:92:TYR:O	1:E:97:ARG:NH2	2.35	0.59
2:B:258:ASN:OD1	2:B:259:GLY:N	2.33	0.59
2:F:37:PRO:HD2	2:F:40:TYR:CE1	2.37	0.59
2:H:263:ARG:HG3	2:H:266:LYS:HG3	1.85	0.59
2:B:92:ARG:NH1	2:B:119:SER:HB3	2.17	0.59
2:F:26:VAL:O	2:F:30:GLN:HG3	2.03	0.58
2:H:144:LYS:HE2	8:H:439:HOH:O	2.02	0.58
2:H:210:LEU:HB2	2:H:223:THR:HA	1.85	0.58
2:F:263:ARG:HG3	2:F:266:LYS:HG3	1.84	0.58
2:F:353:ARG:HG3	8:F:406:HOH:O	2.03	0.58
1:E:353:LYS:CE	1:E:357:ARG:HH12	2.15	0.58
2:H:232:LEU:HD13	2:H:343:ALA:HB1	1.83	0.58
2:J:210:LEU:HB2	2:J:223:THR:HA	1.84	0.58
1:C:69:ARG:HB3	1:C:71:GLU:OE1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:VAL:HG12	1:C:88:VAL:HG23	1.85	0.58
2:L:210:LEU:HB2	2:L:223:THR:HA	1.85	0.58
2:B:186:ASN:HB2	2:B:358:HIS:CE1	2.39	0.58
2:D:263:ARG:HG3	2:D:266:LYS:HG3	1.86	0.58
2:B:210:LEU:HB2	2:B:223:THR:HA	1.85	0.58
1:A:334:LEU:HD22	1:A:367:HIS:O	2.04	0.57
1:C:328:ASP:O	1:C:329:ASN:HB2	2.04	0.57
1:I:334:LEU:HD22	1:I:367:HIS:O	2.03	0.57
2:B:295:ARG:HD3	8:B:438:HOH:O	2.05	0.57
1:C:231:VAL:HG23	1:C:266:MET:HE3	1.87	0.57
1:G:101:ASP:HA	1:G:104:ARG:HH11	1.68	0.57
1:I:311:LEU:HD23	1:I:311:LEU:C	2.29	0.57
2:B:26:VAL:O	2:B:30:GLN:HG3	2.04	0.57
1:A:303:GLN:O	1:A:307:SER:HB2	2.04	0.57
2:F:210:LEU:HB2	2:F:223:THR:HA	1.86	0.57
2:J:263:ARG:HG3	2:J:266:LYS:HG3	1.87	0.57
2:B:258:ASN:CG	2:B:259:GLY:H	2.12	0.57
1:I:69:ARG:HB3	1:I:71:GLU:OE1	2.04	0.57
1:K:107:LEU:HD22	2:L:117:TYR:CD2	2.40	0.57
2:B:39:ARG:HH11	2:B:39:ARG:CB	2.12	0.57
1:E:82:ASP:HB2	1:E:86:PRO:HB3	1.87	0.56
1:E:296:LEU:HD22	1:E:322:MET:HE1	1.87	0.56
1:A:78:VAL:O	1:A:104:ARG:HD2	2.05	0.56
2:D:210:LEU:HB2	2:D:223:THR:HA	1.86	0.56
2:L:263:ARG:HG3	2:L:266:LYS:HG3	1.87	0.56
2:B:334:GLU:HB3	2:B:337:ILE:HD12	1.88	0.56
2:B:353:ARG:HG2	2:B:353:ARG:NH1	2.17	0.56
1:C:339:GLU:O	1:C:343:ILE:HG13	2.05	0.56
2:H:60:MET:HE1	2:H:347:SER:N	2.20	0.56
2:J:22:ARG:O	2:J:26:VAL:HG23	2.05	0.56
1:G:303:GLN:O	1:G:307:SER:HB2	2.06	0.56
1:A:329:ASN:HB3	1:A:332:ASP:HB3	1.86	0.56
1:I:87:VAL:HG12	1:I:88:VAL:HG23	1.87	0.56
1:G:328:ASP:O	1:G:329:ASN:HB2	2.06	0.55
1:K:334:LEU:HD22	1:K:367:HIS:O	2.06	0.55
2:B:263:ARG:HG3	2:B:266:LYS:HG3	1.87	0.55
1:I:107:LEU:HD22	2:J:117:TYR:CD2	2.41	0.55
2:B:353:ARG:HH12	2:B:357:LEU:HG	1.72	0.55
1:C:156:ILE:HG12	1:C:172:ARG:NH1	2.06	0.55
2:D:295:ARG:CZ	2:D:299:LEU:HD11	2.37	0.55
1:E:339:GLU:O	1:E:343:ILE:HG13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:SER:HA	1:A:287:ARG:HH22	1.70	0.55
1:G:261:GLN:O	1:G:265:GLU:HG2	2.07	0.55
1:E:78:VAL:O	1:E:104:ARG:HD2	2.06	0.55
1:A:156:ILE:CG1	1:A:172:ARG:HH12	1.92	0.54
1:K:303:GLN:O	1:K:307:SER:HB2	2.08	0.54
2:D:133:ILE:HD13	2:D:354:LEU:HD13	1.89	0.54
2:D:26:VAL:O	2:D:30:GLN:HG3	2.08	0.54
1:G:97:ARG:HH11	1:G:97:ARG:HB3	1.73	0.54
1:I:348:LYS:HD2	8:I:473:HOH:O	2.07	0.54
1:K:189:ILE:HD11	1:K:205:HIS:CD2	2.41	0.54
1:G:339:GLU:O	1:G:343:ILE:HG13	2.07	0.54
1:I:303:GLN:O	1:I:307:SER:HB2	2.08	0.54
1:E:303:GLN:O	1:E:307:SER:HB2	2.07	0.54
1:C:156:ILE:HD12	8:C:433:HOH:O	2.07	0.54
2:H:349:ARG:O	2:H:352:GLU:HB2	2.08	0.54
1:E:261:GLN:O	1:E:265:GLU:HG2	2.07	0.53
2:J:197:ILE:HD11	2:J:235:LYS:HD3	1.91	0.53
7:I:378:CL:CL	8:I:512:HOH:O	2.56	0.53
1:K:265:GLU:O	1:K:269:LEU:HD13	2.09	0.53
1:C:261:GLN:O	1:C:265:GLU:HG2	2.08	0.53
1:G:318:ILE:HG22	1:G:322:MET:CE	2.39	0.53
2:H:202:ARG:HD2	8:H:440:HOH:O	2.08	0.53
2:B:18:LEU:HD12	2:B:304:ARG:CZ	2.38	0.53
2:D:27:ARG:HA	2:D:30:GLN:HE21	1.73	0.53
1:G:79:PRO:HA	1:G:101:ASP:OD1	2.09	0.53
1:E:318:ILE:HG22	1:E:322:MET:CE	2.38	0.53
2:D:338:CYS:HB3	8:D:402:HOH:O	2.08	0.53
2:H:22:ARG:HH11	2:H:22:ARG:HG2	1.73	0.53
2:J:138:ASP:HA	2:J:357:LEU:HD11	1.91	0.53
2:L:60:MET:CE	2:L:347:SER:HB3	2.38	0.53
2:B:229:SER:O	2:B:233:MET:HG3	2.08	0.53
1:C:311:LEU:C	1:C:311:LEU:HD23	2.34	0.53
1:K:311:LEU:C	1:K:311:LEU:HD23	2.34	0.53
2:H:74:GLU:CD	2:H:141:ARG:HH22	2.16	0.53
2:L:74:GLU:CD	2:L:141:ARG:HH22	2.16	0.53
2:J:69:LYS:O	2:J:73:ILE:HG13	2.08	0.52
2:F:232:LEU:HD13	2:F:343:ALA:HB1	1.91	0.52
1:A:71:GLU:CD	1:A:71:GLU:H	2.16	0.52
2:B:245:LEU:O	2:B:249:LYS:HG3	2.09	0.52
2:H:186:ASN:HB2	2:H:358:HIS:CE1	2.44	0.52
2:B:37:PRO:HD2	2:B:40:TYR:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:353:ARG:NH1	2:D:357:LEU:HG	2.22	0.52
2:B:37:PRO:HD2	2:B:40:TYR:CD1	2.44	0.52
1:G:156:ILE:HD12	8:G:459:HOH:O	2.08	0.52
1:A:328:ASP:O	1:A:329:ASN:HB2	2.10	0.52
1:I:189:ILE:HD11	1:I:205:HIS:CD2	2.43	0.52
1:I:218:ASN:HB3	8:I:510:HOH:O	2.10	0.52
1:E:255:VAL:HG13	1:E:258:ARG:HH21	1.75	0.52
1:C:198:LYS:HD3	2:D:266:LYS:HD3	1.91	0.52
1:E:214:ARG:O	1:E:214:ARG:CG	2.57	0.52
1:C:312:ILE:HG23	1:C:340:LEU:HD22	1.92	0.51
1:E:156:ILE:HD11	1:E:172:ARG:HH22	1.76	0.51
2:D:229:SER:O	2:D:233:MET:HG3	2.11	0.51
2:D:232:LEU:HD13	2:D:343:ALA:HB1	1.92	0.51
1:G:156:ILE:HG12	1:G:172:ARG:NH1	2.05	0.51
2:H:64:LEU:HD11	2:H:134:ILE:HG22	1.93	0.51
1:I:157:ALA:O	1:I:161:GLU:HG3	2.10	0.51
2:D:311:LYS:HG3	2:D:312:TRP:CD2	2.46	0.51
1:G:311:LEU:HD23	1:G:311:LEU:C	2.36	0.51
2:L:69:LYS:O	2:L:73:ILE:HG13	2.12	0.51
1:G:312:ILE:HG23	1:G:340:LEU:HD22	1.93	0.50
1:A:265:GLU:O	1:A:269:LEU:HD13	2.11	0.50
2:B:92:ARG:HH11	2:B:119:SER:HB3	1.75	0.50
1:C:156:ILE:CG1	1:C:172:ARG:HH12	2.08	0.50
1:E:265:GLU:O	1:E:269:LEU:HD13	2.11	0.50
1:C:189:ILE:HD11	1:C:205:HIS:CD2	2.42	0.50
2:D:18:LEU:HD12	2:D:304:ARG:NH1	2.26	0.50
2:H:202:ARG:HG3	2:H:202:ARG:HH11	1.76	0.50
2:F:311:LYS:HG3	2:F:312:TRP:CD2	2.47	0.50
2:D:138:ASP:OD1	2:D:140:SER:HB3	2.12	0.50
1:A:311:LEU:C	1:A:311:LEU:HD23	2.37	0.50
1:E:189:ILE:HD11	1:E:205:HIS:CD2	2.40	0.50
1:A:189:ILE:HD11	1:A:205:HIS:CD2	2.43	0.49
2:F:30:GLN:O	2:F:34:GLN:HG3	2.12	0.49
2:B:29:PHE:O	2:B:33:LEU:HD22	2.12	0.49
1:C:148:LEU:HB2	1:C:179:LEU:HD21	1.93	0.49
1:G:286:ASP:HB2	8:G:426:HOH:O	2.13	0.49
2:H:77:TYR:CZ	2:H:141:ARG:HB2	2.47	0.49
2:J:284:LYS:HE3	8:J:461:HOH:O	2.10	0.49
2:L:353:ARG:HD3	2:L:353:ARG:O	2.12	0.49
1:E:117:PHE:CE2	1:E:146:LYS:HE2	2.48	0.49
1:I:106:VAL:HG11	1:I:116:ALA:HB1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:133:ILE:CD1	2:J:354:LEU:HD13	2.42	0.49
2:L:133:ILE:CD1	2:L:354:LEU:HD13	2.42	0.49
1:C:82:ASP:HB2	1:C:86:PRO:HB3	1.94	0.49
2:D:77:TYR:CZ	2:D:141:ARG:HB2	2.48	0.49
1:K:214:ARG:HG3	1:K:214:ARG:HH11	1.78	0.49
1:K:312:ILE:HG23	1:K:340:LEU:HD22	1.94	0.49
2:L:103:ILE:HG23	2:L:104:PRO:HD2	1.93	0.49
1:I:296:LEU:CD2	1:I:322:MET:HE1	2.43	0.49
1:I:325:ASN:O	1:I:326:GLN:C	2.55	0.49
2:J:258:ASN:OD1	2:J:259:GLY:N	2.38	0.49
2:L:110:ASN:H	2:L:110:ASN:ND2	2.11	0.49
2:B:336:GLY:HA2	2:J:305:LEU:CD1	2.43	0.49
2:F:121:HIS:HB3	2:F:124:MET:HG2	1.95	0.49
2:H:311:LYS:HG3	2:H:312:TRP:CD2	2.48	0.49
1:A:92:TYR:O	1:A:97:ARG:NH2	2.46	0.48
2:B:77:TYR:CZ	2:B:141:ARG:HB2	2.48	0.48
1:E:334:LEU:HD22	1:E:367:HIS:O	2.12	0.48
1:K:104:ARG:NH2	8:K:393:HOH:O	2.46	0.48
1:G:325:ASN:O	1:G:326:GLN:C	2.56	0.48
1:E:107:LEU:HD22	2:F:117:TYR:CD2	2.48	0.48
2:F:245:LEU:O	2:F:249:LYS:HG3	2.13	0.48
1:E:58:LEU:HD22	1:E:95:LYS:HD3	1.95	0.48
1:E:338:LEU:HD11	1:E:364:GLN:HG3	1.95	0.48
1:G:189:ILE:HD11	1:G:205:HIS:CD2	2.42	0.48
2:H:29:PHE:O	2:H:33:LEU:HD22	2.12	0.48
1:A:325:ASN:O	1:A:326:GLN:C	2.56	0.48
1:E:97:ARG:HG2	1:E:101:ASP:OD2	2.14	0.48
1:E:148:LEU:HB2	1:E:179:LEU:HD21	1.94	0.48
1:K:192:ILE:O	1:K:195:GLN:HG3	2.14	0.48
2:L:311:LYS:HG3	2:L:312:TRP:CD2	2.48	0.48
2:B:64:LEU:HD11	2:B:134:ILE:HG22	1.94	0.48
2:H:21:LEU:CD1	2:H:21:LEU:N	2.75	0.48
2:B:299:LEU:O	2:B:302:GLN:HB2	2.14	0.48
1:C:286:ASP:HB2	8:C:437:HOH:O	2.14	0.48
2:F:186:ASN:HB2	2:F:358:HIS:NE2	2.29	0.48
1:G:148:LEU:HB2	1:G:179:LEU:HD21	1.95	0.48
1:A:287:ARG:O	1:A:291:ARG:HD3	2.14	0.48
2:B:311:LYS:HG3	2:B:312:TRP:CD2	2.47	0.48
1:C:265:GLU:O	1:C:269:LEU:HD13	2.14	0.48
1:C:329:ASN:HB3	1:C:332:ASP:HB3	1.96	0.48
1:K:71:GLU:H	1:K:71:GLU:CD	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:ILE:HG22	1:C:322:MET:HE3	1.96	0.48
2:F:37:PRO:HD2	2:F:40:TYR:HD1	1.79	0.48
1:G:344:LEU:HD13	1:G:356:TRP:CE2	2.49	0.48
1:E:58:LEU:HD23	1:E:63:TYR:CE2	2.49	0.47
1:I:329:ASN:HB3	1:I:332:ASP:HB3	1.96	0.47
1:E:106:VAL:HG11	1:E:116:ALA:HB1	1.96	0.47
1:G:319:TYR:HA	1:G:322:MET:HE3	1.96	0.47
1:G:330:LYS:HE2	1:G:367:HIS:HB3	1.94	0.47
2:H:130:SER:O	2:H:134:ILE:HG13	2.14	0.47
1:I:88:VAL:HG12	1:I:88:VAL:O	2.14	0.47
1:I:148:LEU:HB2	1:I:179:LEU:HD21	1.96	0.47
1:I:328:ASP:O	1:I:329:ASN:HB2	2.13	0.47
1:A:214:ARG:O	1:A:214:ARG:CG	2.58	0.47
1:K:311:LEU:HD23	1:K:311:LEU:O	2.14	0.47
2:D:121:HIS:HB3	2:D:124:MET:HG2	1.96	0.47
1:G:350:THR:O	1:G:353:LYS:HB3	2.14	0.47
1:C:106:VAL:HG11	1:C:116:ALA:HB1	1.96	0.47
2:J:334:GLU:HB3	2:J:337:ILE:HD12	1.96	0.47
2:L:60:MET:HE1	2:L:347:SER:N	2.29	0.47
1:E:103:PHE:CZ	1:E:133:VAL:HG22	2.50	0.47
1:G:265:GLU:O	1:G:269:LEU:HD13	2.15	0.47
1:A:97:ARG:HD3	8:A:437:HOH:O	2.14	0.47
2:B:250:ARG:O	2:B:254:MET:HG2	2.13	0.47
1:E:105:ALA:O	1:E:109:ARG:HG3	2.15	0.47
2:F:103:ILE:HG23	2:F:104:PRO:HD2	1.96	0.47
2:H:281:LYS:HE3	2:H:331:LEU:HD12	1.97	0.47
1:I:344:LEU:HD13	1:I:356:TRP:CE2	2.50	0.47
2:J:121:HIS:HB3	2:J:124:MET:HG2	1.96	0.47
2:J:311:LYS:HG3	2:J:312:TRP:CD2	2.50	0.47
2:D:82:LEU:HD11	2:D:108:SER:HA	1.97	0.47
2:F:29:PHE:O	2:F:33:LEU:HD22	2.14	0.47
2:F:192:ASP:CG	2:F:195:LYS:HG3	2.40	0.47
1:E:100:TYR:O	1:E:104:ARG:HG3	2.15	0.46
1:E:294:ASN:O	1:E:298:GLN:HG3	2.15	0.46
2:F:130:SER:O	2:F:134:ILE:HG13	2.15	0.46
1:I:350:THR:O	1:I:353:LYS:HB3	2.16	0.46
2:J:245:LEU:O	2:J:249:LYS:HG3	2.16	0.46
2:L:299:LEU:O	2:L:302:GLN:HB2	2.14	0.46
1:G:65:LEU:O	1:G:69:ARG:HG3	2.16	0.46
1:A:117:PHE:CE2	1:A:146:LYS:HE2	2.51	0.46
2:B:172:MET:HE1	2:B:200:ILE:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:22:ARG:HG2	2:H:22:ARG:NH1	2.29	0.46
2:J:77:TYR:CE1	2:J:141:ARG:HB2	2.50	0.46
1:I:100:TYR:O	1:I:104:ARG:HG3	2.16	0.46
2:J:105:PHE:CE2	2:J:107:PRO:HD3	2.51	0.46
2:B:22:ARG:HG2	2:B:22:ARG:HH11	1.81	0.46
1:C:91:ILE:HG13	2:D:36:LEU:O	2.15	0.46
1:G:106:VAL:HG11	1:G:116:ALA:HB1	1.97	0.46
2:H:207:ASP:O	2:H:208:ASN:HB2	2.16	0.46
1:A:106:VAL:HG11	1:A:116:ALA:HB1	1.97	0.46
2:D:188:TRP:CE3	2:D:193:MET:HE2	2.50	0.46
2:F:299:LEU:O	2:F:302:GLN:HB2	2.16	0.46
2:L:121:HIS:HB3	2:L:124:MET:HG2	1.98	0.46
2:B:192:ASP:OD1	2:B:195:LYS:HE3	2.16	0.46
2:B:207:ASP:O	2:B:208:ASN:HB2	2.16	0.46
1:K:151:GLU:HG3	1:K:175:LEU:HD11	1.97	0.46
2:L:60:MET:HE1	2:L:347:SER:HB3	1.98	0.46
2:B:232:LEU:HD13	2:B:343:ALA:HB1	1.98	0.45
2:B:336:GLY:HA2	2:J:305:LEU:HD13	1.98	0.45
1:C:97:ARG:HG2	1:C:101:ASP:OD2	2.15	0.45
1:E:325:ASN:O	1:E:326:GLN:C	2.58	0.45
1:I:231:VAL:CG2	1:I:266:MET:HE3	2.46	0.45
1:I:265:GLU:O	1:I:269:LEU:HD13	2.16	0.45
1:K:106:VAL:HG11	1:K:116:ALA:HB1	1.98	0.45
2:D:258:ASN:OD1	2:D:259:GLY:N	2.37	0.45
1:A:114:GLU:HB2	8:A:459:HOH:O	2.16	0.45
1:A:318:ILE:O	1:A:322:MET:HG3	2.16	0.45
1:E:71:GLU:H	1:E:71:GLU:CD	2.24	0.45
2:H:121:HIS:HB3	2:H:124:MET:HG2	1.98	0.45
2:H:188:TRP:CE3	2:H:193:MET:HE2	2.51	0.45
1:K:328:ASP:O	1:K:329:ASN:HB2	2.16	0.45
2:L:22:ARG:HG2	2:L:22:ARG:HH11	1.81	0.45
2:L:320:LEU:C	2:L:320:LEU:HD23	2.42	0.45
1:A:107:LEU:HD22	2:B:117:TYR:CD2	2.51	0.45
2:D:250:ARG:O	2:D:254:MET:HG2	2.17	0.45
2:F:353:ARG:O	2:F:353:ARG:HD3	2.17	0.45
2:H:357:LEU:HD22	2:H:361:TRP:CZ2	2.51	0.45
2:H:258:ASN:OD1	2:H:259:GLY:N	2.44	0.45
2:B:82:LEU:HD11	2:B:108:SER:HA	1.98	0.45
2:B:311:LYS:HG3	2:B:312:TRP:CE2	2.51	0.45
2:F:77:TYR:CZ	2:F:141:ARG:HB2	2.52	0.45
2:H:82:LEU:HD11	2:H:108:SER:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:65:LEU:O	1:I:69:ARG:HG3	2.16	0.45
2:L:250:ARG:O	2:L:254:MET:HG2	2.17	0.45
2:J:229:SER:O	2:J:233:MET:HG3	2.17	0.45
2:L:311:LYS:HG3	2:L:312:TRP:CE2	2.52	0.45
1:G:90:ILE:HD13	2:H:40:TYR:O	2.17	0.44
1:I:353:LYS:HG2	1:I:354:GLU:N	2.31	0.44
1:A:261:GLN:O	1:A:265:GLU:HG2	2.17	0.44
2:F:64:LEU:HA	2:F:64:LEU:HD23	1.86	0.44
1:K:82:ASP:HB2	1:K:86:PRO:HB3	1.99	0.44
1:A:91:ILE:HG13	2:B:36:LEU:O	2.18	0.44
1:A:67:ARG:NH2	1:A:94:GLU:OE1	2.51	0.44
2:B:121:HIS:HB3	2:B:124:MET:HG2	2.00	0.44
2:B:320:LEU:C	2:B:320:LEU:HD23	2.42	0.44
2:D:197:ILE:HD11	2:D:235:LYS:HD3	1.98	0.44
2:F:82:LEU:HD11	2:F:108:SER:HA	1.99	0.44
1:I:339:GLU:O	1:I:343:ILE:HG13	2.17	0.44
2:J:77:TYR:CZ	2:J:141:ARG:HB2	2.52	0.44
1:K:173:ARG:HD2	8:K:461:HOH:O	2.17	0.44
2:L:22:ARG:HG2	2:L:22:ARG:NH1	2.32	0.44
2:B:103:ILE:HG23	2:B:104:PRO:HD2	1.98	0.44
2:B:344:LEU:HD12	2:B:344:LEU:HA	1.84	0.44
2:H:31:ARG:HH22	2:H:306:VAL:HB	1.83	0.44
2:H:237:GLU:HG2	8:H:415:HOH:O	2.17	0.44
2:H:354:LEU:HD11	2:H:358:HIS:NE2	2.33	0.44
1:I:151:GLU:HG3	1:I:175:LEU:HD11	2.00	0.44
2:J:77:TYR:HE2	2:J:137:ASP:OD2	2.01	0.44
2:L:82:LEU:HD11	2:L:108:SER:HA	1.99	0.44
2:B:38:GLU:O	2:B:38:GLU:HG2	2.18	0.44
1:C:325:ASN:O	1:C:326:GLN:C	2.60	0.44
2:D:130:SER:O	2:D:134:ILE:HG13	2.18	0.44
1:G:290:SER:HB2	1:G:322:MET:HG2	2.00	0.44
1:I:311:LEU:HD23	1:I:311:LEU:O	2.17	0.44
1:E:311:LEU:C	1:E:311:LEU:HD23	2.43	0.44
2:H:21:LEU:CD2	2:H:304:ARG:HG2	2.45	0.44
1:A:156:ILE:HD11	1:A:172:ARG:HH22	1.83	0.44
2:H:18:LEU:N	2:H:18:LEU:CD2	2.79	0.44
2:H:353:ARG:O	2:H:357:LEU:HB2	2.18	0.44
1:A:148:LEU:HB2	1:A:179:LEU:HD21	2.00	0.44
2:F:311:LYS:HG3	2:F:312:TRP:CE2	2.53	0.44
1:G:65:LEU:HD12	1:G:67:ARG:HH11	1.83	0.44
2:H:103:ILE:HG23	2:H:104:PRO:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:105:PHE:CE2	2:L:107:PRO:HD3	2.52	0.43
2:D:311:LYS:HG3	2:D:312:TRP:CE2	2.53	0.43
1:G:219:GLU:HA	1:G:219:GLU:OE1	2.18	0.43
2:H:198:SER:OG	2:H:202:ARG:NH1	2.51	0.43
2:H:250:ARG:O	2:H:254:MET:HG2	2.18	0.43
2:J:64:LEU:O	2:J:67:VAL:HG22	2.17	0.43
1:K:83:GLY:HA3	2:L:105:PHE:CD1	2.53	0.43
1:C:287:ARG:H	1:C:287:ARG:HG2	1.59	0.43
1:G:329:ASN:HB3	1:G:332:ASP:HB3	1.99	0.43
2:H:311:LYS:HG3	2:H:312:TRP:CE2	2.53	0.43
2:J:19:ASP:OD2	2:J:19:ASP:N	2.51	0.43
2:B:115:HIS:HA	2:B:116:PRO:HD3	1.90	0.43
1:C:78:VAL:O	1:C:104:ARG:HD2	2.17	0.43
2:F:138:ASP:OD1	2:F:140:SER:HB3	2.18	0.43
2:F:207:ASP:O	2:F:208:ASN:HB2	2.18	0.43
2:B:269:ASP:OD1	2:B:269:ASP:C	2.62	0.43
8:B:441:HOH:O	2:J:31:ARG:HD3	2.18	0.43
2:H:22:ARG:O	2:H:26:VAL:HG23	2.18	0.43
1:A:103:PHE:CZ	1:A:133:VAL:HG22	2.54	0.43
2:B:36:LEU:HA	2:B:37:PRO:HD3	1.86	0.43
2:D:19:ASP:OD2	2:D:19:ASP:N	2.43	0.43
2:H:77:TYR:HE2	2:H:137:ASP:OD2	2.02	0.43
1:C:318:ILE:HG22	1:C:322:MET:CE	2.48	0.43
2:J:311:LYS:HG3	2:J:312:TRP:CE2	2.53	0.43
2:F:250:ARG:O	2:F:254:MET:HG2	2.18	0.43
2:H:92:ARG:HG2	2:H:165:PRO:CG	2.46	0.43
2:H:249:LYS:HB3	2:H:285:ILE:HD13	2.00	0.43
2:J:82:LEU:HD11	2:J:108:SER:HA	1.99	0.43
2:J:133:ILE:HG22	2:J:350:THR:HG23	1.99	0.43
2:L:334:GLU:HB3	2:L:337:ILE:HD12	2.00	0.43
1:C:107:LEU:HD22	2:D:117:TYR:CD2	2.54	0.43
1:G:105:ALA:O	1:G:109:ARG:HG3	2.18	0.43
2:H:30:GLN:O	2:H:34:GLN:HG3	2.19	0.43
2:H:269:ASP:OD1	2:H:269:ASP:C	2.62	0.43
1:G:353:LYS:CG	1:G:354:GLU:N	2.81	0.42
1:I:296:LEU:HD22	1:I:322:MET:HE1	2.00	0.42
2:J:320:LEU:C	2:J:320:LEU:HD23	2.44	0.42
1:E:83:GLY:HA3	2:F:105:PHE:CD1	2.55	0.42
2:F:133:ILE:CD1	2:F:354:LEU:HD13	2.48	0.42
2:H:320:LEU:C	2:H:320:LEU:HD23	2.44	0.42
2:F:256:GLN:HB2	2:F:260:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:64:LEU:HB3	2:J:69:LYS:HE2	2.01	0.42
2:L:33:LEU:HD22	2:L:54:ALA:HB1	2.02	0.42
2:D:320:LEU:HD23	2:D:320:LEU:C	2.44	0.42
1:E:312:ILE:O	1:E:316:VAL:HG23	2.20	0.42
2:J:130:SER:O	2:J:134:ILE:HG13	2.19	0.42
2:J:338:CYS:SG	2:J:349:ARG:NH2	2.92	0.42
1:K:148:LEU:HB2	1:K:179:LEU:HD21	2.00	0.42
2:L:64:LEU:HB3	2:L:69:LYS:HE2	2.02	0.42
1:C:311:LEU:HD23	1:C:311:LEU:O	2.18	0.42
2:B:22:ARG:HG2	2:B:22:ARG:NH1	2.34	0.42
2:B:77:TYR:CE1	2:B:141:ARG:HB2	2.54	0.42
2:B:133:ILE:CD1	2:B:354:LEU:HD13	2.47	0.42
2:L:256:GLN:HB2	2:L:260:TYR:CE2	2.55	0.42
2:B:256:GLN:HB2	2:B:260:TYR:CE2	2.55	0.42
2:D:37:PRO:HD2	2:D:40:TYR:CE1	2.54	0.42
1:I:338:LEU:HD11	1:I:364:GLN:HG2	2.00	0.42
1:K:330:LYS:HE2	1:K:367:HIS:HB3	2.02	0.42
2:L:49:THR:HG23	2:L:124:MET:SD	2.59	0.42
2:B:21:LEU:CD1	2:B:21:LEU:N	2.81	0.42
2:B:22:ARG:O	2:B:26:VAL:HG23	2.19	0.42
2:B:258:ASN:CG	2:B:259:GLY:N	2.76	0.42
1:K:167:GLN:NE2	8:K:569:HOH:O	2.52	0.42
1:A:274:GLU:HG3	1:A:310:TYR:CE2	2.55	0.42
1:E:151:GLU:HG3	1:E:175:LEU:HD11	2.02	0.42
1:E:361:ARG:HD3	8:E:456:HOH:O	2.20	0.42
1:I:198:LYS:HD3	2:J:266:LYS:HD3	2.02	0.42
1:I:351:ILE:CD1	2:J:256:GLN:HG2	2.50	0.42
1:K:96:PHE:CE1	1:K:126:LEU:HB3	2.55	0.42
1:A:151:GLU:HG3	1:A:175:LEU:HD11	2.02	0.42
2:B:64:LEU:HA	2:B:64:LEU:HD23	1.85	0.42
2:F:269:ASP:OD1	2:F:269:ASP:C	2.63	0.42
2:F:320:LEU:HD23	2:F:320:LEU:C	2.44	0.42
2:H:19:ASP:O	2:H:21:LEU:HD13	2.19	0.42
2:H:268:VAL:HG23	2:H:297:TYR:CZ	2.55	0.42
2:D:22:ARG:HG2	2:D:22:ARG:HH11	1.86	0.41
2:D:53:PHE:HZ	6:D:382:MES:H71	1.85	0.41
1:E:69:ARG:HB3	1:E:71:GLU:OE1	2.20	0.41
1:C:91:ILE:HD11	2:D:38:GLU:H	1.85	0.41
2:J:172:MET:HE1	2:J:200:ILE:HA	2.02	0.41
1:K:339:GLU:O	1:K:343:ILE:HG13	2.20	0.41
2:B:192:ASP:OD1	2:B:195:LYS:CE	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:258:ASN:OD1	2:L:259:GLY:N	2.43	0.41
2:B:130:SER:O	2:B:134:ILE:HG13	2.19	0.41
1:C:103:PHE:CZ	1:C:133:VAL:HG22	2.55	0.41
2:F:77:TYR:CE1	2:F:141:ARG:HB2	2.55	0.41
2:F:344:LEU:HD12	2:F:344:LEU:HA	1.73	0.41
1:K:325:ASN:O	1:K:326:GLN:C	2.63	0.41
2:B:92:ARG:NH1	2:B:118:ASP:O	2.54	0.41
1:G:334:LEU:O	1:G:338:LEU:HG	2.20	0.41
2:H:256:GLN:HB2	2:H:260:TYR:CE2	2.56	0.41
1:A:344:LEU:HD13	1:A:356:TRP:CE2	2.55	0.41
1:C:74:ASP:OD2	1:C:74:ASP:N	2.52	0.41
1:E:287:ARG:H	1:E:287:ARG:HG2	1.48	0.41
2:F:144:LYS:HG2	2:F:185:LEU:HD22	2.03	0.41
2:F:353:ARG:HD3	2:F:353:ARG:C	2.45	0.41
1:G:87:VAL:O	1:G:88:VAL:C	2.63	0.41
1:I:330:LYS:HE2	1:I:367:HIS:HB3	2.01	0.41
1:K:117:PHE:CE2	1:K:146:LYS:HE2	2.55	0.41
1:K:353:LYS:HE3	1:K:353:LYS:HB2	1.78	0.41
2:B:160:SER:HB3	2:B:199:TYR:CE1	2.56	0.41
2:B:302:GLN:HG3	2:B:309:PHE:CE2	2.55	0.41
2:F:207:ASP:OD2	2:F:207:ASP:C	2.63	0.41
1:G:97:ARG:NH1	1:G:97:ARG:CB	2.83	0.41
1:G:117:PHE:CE2	1:G:146:LYS:HE2	2.56	0.41
2:L:19:ASP:OD2	2:L:19:ASP:N	2.51	0.41
2:D:20:PHE:CZ	2:D:337:ILE:HD11	2.56	0.41
2:D:237:GLU:HG2	8:D:418:HOH:O	2.21	0.41
2:F:115:HIS:HA	2:F:116:PRO:HD3	1.92	0.41
1:I:91:ILE:HD12	1:I:91:ILE:C	2.46	0.41
1:I:101:ASP:HA	1:I:104:ARG:HH11	1.86	0.41
1:K:78:VAL:O	1:K:104:ARG:HD2	2.21	0.41
2:L:255:ARG:HD3	2:L:261:HIS:CD2	2.56	0.41
2:D:258:ASN:CG	2:D:259:GLY:H	2.26	0.41
1:E:348:LYS:HD3	1:E:348:LYS:HA	1.89	0.41
2:F:186:ASN:HB2	2:F:358:HIS:CE1	2.56	0.41
2:F:258:ASN:CG	2:F:259:GLY:H	2.27	0.41
1:A:212:GLU:O	1:G:180:LYS:HE3	2.21	0.41
1:C:96:PHE:CE1	1:C:126:LEU:HB3	2.56	0.41
2:D:133:ILE:HG22	2:D:350:THR:HG23	2.02	0.41
1:G:127:ASN:ND2	1:G:130:ASN:HB2	2.36	0.41
2:H:184:MET:HA	2:H:354:LEU:HD21	2.03	0.41
1:I:219:GLU:HA	1:I:219:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:195:LYS:NZ	8:J:415:HOH:O	2.54	0.41
1:A:355:TYR:O	1:A:358:TYR:HB3	2.21	0.40
1:I:103:PHE:CZ	1:I:133:VAL:HG22	2.56	0.40
2:J:250:ARG:O	2:J:254:MET:HG2	2.21	0.40
2:J:269:ASP:C	2:J:269:ASP:OD1	2.63	0.40
2:D:126:TYR:HE2	6:D:382:MES:C6	2.34	0.40
2:D:268:VAL:HG23	2:D:297:TYR:CZ	2.57	0.40
1:G:156:ILE:HD11	1:G:172:ARG:HH22	1.87	0.40
1:I:312:ILE:HG23	1:I:340:LEU:HD22	2.03	0.40
2:J:357:LEU:HD22	2:J:361:TRP:CZ2	2.57	0.40
1:K:103:PHE:CZ	1:K:133:VAL:HG22	2.56	0.40
1:K:294:ASN:O	1:K:298:GLN:HB2	2.21	0.40
1:A:267:ILE:HD13	1:A:277:TRP:CE2	2.57	0.40
1:A:348:LYS:HD3	1:A:348:LYS:HA	1.82	0.40
2:B:49:THR:HG23	2:B:124:MET:SD	2.62	0.40
2:D:64:LEU:HD11	2:D:134:ILE:HG22	2.03	0.40
2:D:344:LEU:HA	2:D:344:LEU:HD12	1.84	0.40
2:F:192:ASP:OD1	2:F:195:LYS:HG3	2.22	0.40
2:H:172:MET:HE1	2:H:200:ILE:HA	2.02	0.40
2:J:33:LEU:HD22	2:J:54:ALA:HB1	2.02	0.40
2:J:193:MET:HE3	2:J:193:MET:HB2	1.97	0.40
2:H:348:THR:HA	2:H:351:SER:OG	2.21	0.40
2:H:357:LEU:HD22	2:H:361:TRP:CE2	2.57	0.40
1:I:287:ARG:H	1:I:287:ARG:HG2	1.57	0.40
2:J:256:GLN:HB2	2:J:260:TYR:CE2	2.57	0.40
2:J:353:ARG:HG2	2:J:353:ARG:HH11	1.87	0.40
2:L:207:ASP:O	2:L:208:ASN:HB2	2.22	0.40
1:G:96:PHE:CE1	1:G:126:LEU:HB3	2.56	0.40
2:H:49:THR:HG23	2:H:124:MET:SD	2.62	0.40
1:K:156:ILE:HD11	1:K:172:ARG:HH22	1.87	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	312/377 (83%)	289 (93%)	22 (7%)	1 (0%)	36	45
1	C	312/377 (83%)	294 (94%)	17 (5%)	1 (0%)	36	45
1	E	312/377 (83%)	288 (92%)	24 (8%)	0	100	100
1	G	312/377 (83%)	291 (93%)	21 (7%)	0	100	100
1	I	312/377 (83%)	292 (94%)	18 (6%)	2 (1%)	21	29
1	K	312/377 (83%)	294 (94%)	17 (5%)	1 (0%)	36	45
2	B	344/377 (91%)	325 (94%)	17 (5%)	2 (1%)	21	29
2	D	344/377 (91%)	329 (96%)	13 (4%)	2 (1%)	21	29
2	F	344/377 (91%)	327 (95%)	15 (4%)	2 (1%)	21	29
2	H	344/377 (91%)	326 (95%)	15 (4%)	3 (1%)	14	20
2	J	344/377 (91%)	329 (96%)	12 (4%)	3 (1%)	14	20
2	L	344/377 (91%)	332 (96%)	10 (3%)	2 (1%)	21	29
All	All	3936/4524 (87%)	3716 (94%)	201 (5%)	19 (0%)	24	34

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	326	GLN
2	B	258	ASN
1	C	326	GLN
2	D	258	ASN
2	H	258	ASN
2	H	333	GLU
1	I	306	HIS
2	J	258	ASN
2	L	258	ASN
2	F	258	ASN
1	I	326	GLN
2	J	34	GLN
1	K	306	HIS
2	H	111	PRO
2	F	111	PRO
2	J	111	PRO
2	B	111	PRO
2	D	111	PRO
2	L	111	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	279/338 (82%)	273 (98%)	6 (2%)	45	64
1	C	282/338 (83%)	275 (98%)	7 (2%)	42	60
1	E	284/338 (84%)	276 (97%)	8 (3%)	38	57
1	G	281/338 (83%)	276 (98%)	5 (2%)	51	70
1	I	286/338 (85%)	278 (97%)	8 (3%)	38	57
1	K	290/338 (86%)	279 (96%)	11 (4%)	29	44
2	B	287/326 (88%)	274 (96%)	13 (4%)	24	38
2	D	286/326 (88%)	276 (96%)	10 (4%)	32	48
2	F	292/326 (90%)	279 (96%)	13 (4%)	24	38
2	H	286/326 (88%)	273 (96%)	13 (4%)	24	38
2	J	291/326 (89%)	278 (96%)	13 (4%)	24	38
2	L	294/326 (90%)	281 (96%)	13 (4%)	25	38
All	All	3438/3984 (86%)	3318 (96%)	120 (4%)	32	48

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
1	A	71	GLU
1	A	81	ASN
1	A	114	GLU
1	A	214	ARG
1	A	287	ARG
2	B	21	LEU
2	B	24	ARG
2	B	33	LEU
2	B	39	ARG
2	B	151	LEU
2	B	216	LEU
2	B	232	LEU
2	B	236	LEU

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Mol	Chain	Res	Type
2	B	302	GLN
2	B	306	VAL
2	B	329	LEU
2	B	331	LEU
2	B	357	LEU
1	C	59	ASP
1	C	71	GLU
1	C	76	ASP
1	C	182	PRO
1	C	287	ARG
1	C	324	GLU
1	C	364	GLN
2	D	21	LEU
2	D	33	LEU
2	D	151	LEU
2	D	210	LEU
2	D	216	LEU
2	D	232	LEU
2	D	236	LEU
2	D	306	VAL
2	D	329	LEU
2	D	331	LEU
1	E	55	PHE
1	E	67	ARG
1	E	71	GLU
1	E	94	GLU
1	E	214	ARG
1	E	257	GLU
1	E	287	ARG
1	E	324	GLU
2	F	21	LEU
2	F	24	ARG
2	F	33	LEU
2	F	151	LEU
2	F	210	LEU
2	F	216	LEU
2	F	232	LEU
2	F	236	LEU
2	F	255	ARG
2	F	258	ASN
2	F	306	VAL
2	F	329	LEU

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Mol	Chain	Res	Type
2	F	331	LEU
1	G	71	GLU
1	G	114	GLU
1	G	224	ASP
1	G	287	ARG
1	G	324	GLU
2	H	18	LEU
2	H	21	LEU
2	H	33	LEU
2	H	151	LEU
2	H	157	GLU
2	H	216	LEU
2	H	232	LEU
2	H	236	LEU
2	H	258	ASN
2	H	306	VAL
2	H	329	LEU
2	H	331	LEU
2	H	357	LEU
1	I	71	GLU
1	I	114	GLU
1	I	194	ASN
1	I	195	GLN
1	I	287	ARG
1	I	324	GLU
1	I	353	LYS
1	I	364	GLN
2	J	21	LEU
2	J	27	ARG
2	J	31	ARG
2	J	33	LEU
2	J	151	LEU
2	J	216	LEU
2	J	232	LEU
2	J	236	LEU
2	J	255	ARG
2	J	306	VAL
2	J	329	LEU
2	J	331	LEU
2	J	357	LEU
1	K	55	PHE
1	K	71	GLU

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Mol	Chain	Res	Type
1	K	114	GLU
1	K	142	ARG
1	K	156	ILE
1	K	194	ASN
1	K	195	GLN
1	K	287	ARG
1	K	298	GLN
1	K	324	GLU
1	K	357	ARG
2	L	21	LEU
2	L	33	LEU
2	L	65	ASP
2	L	110	ASN
2	L	151	LEU
2	L	210	LEU
2	L	216	LEU
2	L	232	LEU
2	L	236	LEU
2	L	302	GLN
2	L	306	VAL
2	L	329	LEU
2	L	331	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	135	HIS
1	A	184	GLN
1	A	285	GLN
1	A	329	ASN
2	B	30	GLN
2	B	208	ASN
2	B	257	GLN
1	C	81	ASN
1	C	108	GLN
1	C	135	HIS
1	C	218	ASN
1	C	285	GLN
1	C	298	GLN
1	C	303	GLN
1	C	364	GLN

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Mol	Chain	Res	Type
2	D	30	GLN
2	D	208	ASN
2	D	246	ASN
2	D	257	GLN
2	D	345	ASN
1	E	81	ASN
1	E	135	HIS
1	E	184	GLN
1	E	298	GLN
2	F	30	GLN
2	F	208	ASN
2	F	246	ASN
1	G	80	GLN
1	G	81	ASN
1	G	89	GLN
1	G	135	HIS
1	G	162	GLN
1	G	184	GLN
1	G	194	ASN
1	G	297	ASN
1	G	303	GLN
1	G	325	ASN
1	G	367	HIS
2	H	30	GLN
2	H	246	ASN
2	H	257	GLN
1	I	89	GLN
1	I	135	HIS
1	I	285	GLN
1	I	364	GLN
2	J	30	GLN
2	J	208	ASN
2	J	246	ASN
1	K	81	ASN
1	K	89	GLN
1	K	135	HIS
1	K	205	HIS
1	K	218	ASN
1	K	234	ASN
1	K	285	GLN
1	K	367	HIS
2	L	110	ASN

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Mol	Chain	Res	Type
2	L	208	ASN
2	L	257	GLN
2	L	345	ASN

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 33 ligands modelled in this entry, 15 are monoatomic - leaving 18 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	$\# Z > 2$
4	SO4	H	380	-	4,4,4	0.38	0	6,6,6	0.20	0
4	SO4	F	380	-	4,4,4	0.34	0	6,6,6	0.20	0
5	778	H	381	3	32,32,32	2.50	18 (56%)	39,44,44	2.67	12 (30%)
5	778	J	381	3	32,32,32	2.51	18 (56%)	39,44,44	2.64	12 (30%)
5	778	B	380	3	32,32,32	2.61	19 (59%)	39,44,44	2.65	11 (28%)
6	MES	D	382	-	12,12,12	9.71	8 (66%)	15,16,16	2.18	6 (40%)
4	SO4	J	380	-	4,4,4	0.34	0	6,6,6	0.24	0
6	MES	H	382	-	12,12,12	9.70	8 (66%)	15,16,16	2.09	6 (40%)
4	SO4	L	380	-	4,4,4	0.33	0	6,6,6	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MES	J	382	-	12,12,12	9.64	8 (66%)	15,16,16	2.24	7 (46%)
5	778	F	381	3	32,32,32	2.57	17 (53%)	39,44,44	2.69	12 (30%)
5	778	L	381	3	32,32,32	2.55	17 (53%)	39,44,44	2.63	12 (30%)
6	MES	L	382	-	12,12,12	9.88	9 (75%)	15,16,16	2.29	7 (46%)
4	SO4	B	379	-	4,4,4	0.37	0	6,6,6	0.08	0
5	778	D	381	3	32,32,32	2.52	19 (59%)	39,44,44	2.67	12 (30%)
6	MES	F	382	-	12,12,12	9.46	8 (66%)	15,16,16	2.25	7 (46%)
4	SO4	D	380	-	4,4,4	0.37	0	6,6,6	0.12	0
6	MES	B	381	-	12,12,12	9.55	8 (66%)	15,16,16	2.23	7 (46%)

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
5	778	H	381	3	-	0/14/27/27	0/4/4/4
5	778	J	381	3	-	0/14/27/27	0/4/4/4
5	778	B	380	3	-	0/14/27/27	0/4/4/4
6	MES	D	382	-	-	0/6/14/14	0/1/1/1
6	MES	H	382	-	-	0/6/14/14	0/1/1/1
6	MES	J	382	-	-	0/6/14/14	0/1/1/1
5	778	F	381	3	-	1/14/27/27	0/4/4/4
5	778	L	381	3	-	0/14/27/27	0/4/4/4
6	MES	L	382	-	-	0/6/14/14	0/1/1/1
5	778	D	381	3	-	0/14/27/27	0/4/4/4
6	MES	F	382	-	-	0/6/14/14	0/1/1/1
6	MES	B	381	-	-	0/6/14/14	0/1/1/1

All (157) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	382	MES	C8-S	-25.82	1.41	1.77
6	D	382	MES	C8-S	-25.25	1.42	1.77
6	H	382	MES	C8-S	-25.14	1.42	1.77
6	J	382	MES	C8-S	-24.87	1.42	1.77
6	B	381	MES	C8-S	-24.37	1.43	1.77
6	F	382	MES	C8-S	-23.87	1.44	1.77
6	F	382	MES	O1S-S	13.42	1.83	1.45
6	J	382	MES	O2S-S	13.32	1.82	1.45
6	F	382	MES	O2S-S	13.31	1.82	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	381	MES	O2S-S	13.30	1.82	1.45
6	L	382	MES	O2S-S	13.26	1.82	1.45
6	H	382	MES	O2S-S	13.18	1.82	1.45
6	D	382	MES	O1S-S	13.16	1.82	1.45
6	D	382	MES	O2S-S	13.08	1.82	1.45
6	J	382	MES	O1S-S	13.06	1.81	1.45
6	B	381	MES	O1S-S	13.04	1.81	1.45
6	L	382	MES	O1S-S	13.02	1.81	1.45
6	H	382	MES	O1S-S	13.02	1.81	1.45
6	B	381	MES	O3S-S	9.32	1.82	1.47
6	H	382	MES	O3S-S	9.30	1.82	1.47
6	F	382	MES	O3S-S	9.25	1.82	1.47
6	L	382	MES	O3S-S	9.20	1.81	1.47
6	J	382	MES	O3S-S	9.13	1.81	1.47
6	D	382	MES	O3S-S	9.06	1.81	1.47
5	B	380	778	C34-C35	-6.05	1.31	1.44
5	F	381	778	C34-C35	-6.03	1.31	1.44
6	L	382	MES	C7-C8	-5.94	1.36	1.52
5	D	381	778	C34-C35	-5.91	1.32	1.44
5	H	381	778	C34-C35	-5.83	1.32	1.44
6	H	382	MES	C7-C8	-5.78	1.37	1.52
6	D	382	MES	C7-C8	-5.71	1.37	1.52
5	J	381	778	C34-C35	-5.71	1.32	1.44
6	B	381	MES	C7-C8	-5.68	1.37	1.52
5	L	381	778	C34-C35	-5.66	1.32	1.44
6	J	382	MES	C7-C8	-5.60	1.37	1.52
6	F	382	MES	C7-C8	-5.48	1.38	1.52
5	F	381	778	C12-N18	4.82	1.46	1.37
5	B	380	778	C12-N18	4.73	1.45	1.37
5	D	381	778	C12-N18	4.62	1.45	1.37
5	L	381	778	C12-N18	4.57	1.45	1.37
5	H	381	778	C12-N18	4.55	1.45	1.37
5	F	381	778	C8-N9	4.54	1.44	1.36
5	J	381	778	C12-N18	4.45	1.45	1.37
5	J	381	778	C8-N9	4.30	1.44	1.36
5	B	380	778	C8-N9	4.26	1.44	1.36
5	H	381	778	C8-N9	4.23	1.44	1.36
5	D	381	778	C8-N9	4.22	1.44	1.36
5	L	381	778	C8-N9	4.07	1.43	1.36
5	F	381	778	C21-C14	3.79	1.46	1.39
5	F	381	778	C4-C8	3.75	1.58	1.51
5	B	380	778	C4-C8	3.75	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	381	778	C21-C14	3.70	1.46	1.39
6	L	382	MES	C7-N4	-3.63	1.39	1.47
5	J	381	778	C21-C14	3.62	1.46	1.39
5	L	381	778	C4-C8	3.58	1.58	1.51
5	B	380	778	C21-C14	3.47	1.45	1.39
5	H	381	778	C21-C14	3.45	1.45	1.39
5	D	381	778	C21-C14	3.44	1.45	1.39
5	J	381	778	C30-C26	3.42	1.44	1.38
6	D	382	MES	C7-N4	-3.40	1.39	1.47
6	H	382	MES	C7-N4	-3.34	1.39	1.47
5	L	381	778	C30-C26	3.32	1.44	1.38
6	J	382	MES	C7-N4	-3.28	1.40	1.47
5	D	381	778	C30-C26	3.26	1.44	1.38
5	B	380	778	C32-C28	3.26	1.44	1.38
5	L	381	778	C4-N1	3.26	1.49	1.46
5	D	381	778	C4-C8	3.23	1.57	1.51
6	B	381	MES	C7-N4	-3.18	1.40	1.47
5	H	381	778	C4-C8	3.17	1.57	1.51
5	F	381	778	C32-C28	3.12	1.43	1.38
5	L	381	778	C20-C26	3.10	1.43	1.38
5	F	381	778	C30-C26	3.10	1.43	1.38
5	J	381	778	C27-C21	3.10	1.44	1.38
5	F	381	778	C27-C21	3.09	1.44	1.38
6	L	382	MES	C3-C2	-3.05	1.39	1.50
5	H	381	778	C17-N18	3.01	1.40	1.32
5	L	381	778	C27-C21	3.00	1.44	1.38
6	J	382	MES	C3-C2	-2.99	1.39	1.50
5	H	381	778	C20-C26	2.98	1.43	1.38
5	B	380	778	C30-C26	2.98	1.43	1.38
5	D	381	778	C32-C28	2.97	1.43	1.38
5	J	381	778	C20-C26	2.95	1.43	1.38
6	D	382	MES	C3-C2	-2.94	1.39	1.50
5	B	380	778	C17-N18	2.93	1.39	1.32
5	J	381	778	C4-C8	2.93	1.56	1.51
6	F	382	MES	C3-C2	-2.93	1.39	1.50
6	B	381	MES	C3-C2	-2.89	1.39	1.50
5	H	381	778	C32-C28	2.89	1.43	1.38
6	H	382	MES	C3-C2	-2.87	1.39	1.50
5	J	381	778	C32-C28	2.87	1.43	1.38
5	B	380	778	C27-C21	2.87	1.43	1.38
5	B	380	778	C20-C26	2.86	1.42	1.38
5	H	381	778	C30-C26	2.85	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	380	778	C28-C25	2.80	1.44	1.38
6	L	382	MES	C5-C6	-2.79	1.40	1.50
5	D	381	778	C17-N18	2.78	1.39	1.32
5	L	381	778	C17-N18	2.77	1.39	1.32
5	D	381	778	C28-C25	2.76	1.44	1.38
6	F	382	MES	C7-N4	-2.74	1.41	1.47
5	D	381	778	C20-C26	2.71	1.42	1.38
5	L	381	778	C32-C28	2.71	1.43	1.38
5	H	381	778	C29-C25	2.71	1.44	1.38
5	J	381	778	C3-C7	2.71	1.53	1.50
5	B	380	778	C20-C14	2.70	1.44	1.39
6	J	382	MES	C5-C6	-2.70	1.40	1.50
5	D	381	778	C29-C25	2.69	1.44	1.38
5	B	380	778	C29-C25	2.69	1.44	1.38
5	B	380	778	C3-C7	2.69	1.53	1.50
5	H	381	778	C27-C21	2.68	1.43	1.38
6	D	382	MES	C5-C6	-2.68	1.40	1.50
6	H	382	MES	C5-C6	-2.66	1.40	1.50
5	F	381	778	C17-N18	2.66	1.39	1.32
5	L	381	778	C28-C25	2.65	1.44	1.38
6	F	382	MES	C5-C6	-2.63	1.40	1.50
6	B	381	MES	C5-C6	-2.63	1.40	1.50
5	J	381	778	C17-N18	2.59	1.38	1.32
5	D	381	778	C27-C21	2.56	1.43	1.38
5	F	381	778	C28-C25	2.56	1.44	1.38
5	D	381	778	C20-C14	2.55	1.44	1.39
5	B	380	778	C33-C29	2.54	1.42	1.38
5	J	381	778	C29-C25	2.54	1.43	1.38
5	B	380	778	C16-C25	2.52	1.56	1.51
5	F	381	778	C3-C7	2.52	1.53	1.50
5	L	381	778	C3-C7	2.52	1.53	1.50
5	B	380	778	C33-C34	2.49	1.44	1.39
5	B	380	778	C27-C30	2.48	1.43	1.38
5	H	381	778	C20-C14	2.47	1.43	1.39
5	F	381	778	C20-C26	2.47	1.42	1.38
5	J	381	778	C28-C25	2.46	1.43	1.38
5	L	381	778	C29-C25	2.44	1.43	1.38
5	F	381	778	C29-C25	2.44	1.43	1.38
5	H	381	778	C27-C30	2.43	1.43	1.38
5	H	381	778	C33-C29	2.43	1.42	1.38
5	D	381	778	C33-C34	2.41	1.44	1.39
5	L	381	778	C33-C34	2.40	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	381	778	C3-C7	2.38	1.53	1.50
5	J	381	778	C20-C14	2.38	1.43	1.39
5	F	381	778	C27-C30	2.37	1.43	1.38
5	H	381	778	C16-C25	2.34	1.55	1.51
5	D	381	778	C27-C30	2.33	1.42	1.38
5	L	381	778	C16-C25	2.33	1.55	1.51
5	J	381	778	C33-C34	2.32	1.44	1.39
5	D	381	778	C3-C7	2.32	1.53	1.50
5	F	381	778	C4-N1	2.25	1.48	1.46
5	D	381	778	C4-N1	2.24	1.48	1.46
5	D	381	778	C33-C29	2.24	1.42	1.38
5	D	381	778	C16-C25	2.23	1.55	1.51
5	F	381	778	C33-C29	2.23	1.42	1.38
5	B	380	778	C16-N11	2.21	1.51	1.47
5	L	381	778	C20-C14	2.21	1.43	1.39
5	F	381	778	C20-C14	2.17	1.43	1.39
5	H	381	778	C28-C25	2.17	1.43	1.38
6	L	382	MES	C5-N4	-2.15	1.41	1.46
5	J	381	778	C33-C29	2.14	1.42	1.38
5	J	381	778	C27-C30	2.12	1.42	1.38
5	J	381	778	C16-C25	2.11	1.55	1.51
5	H	381	778	C4-N1	2.10	1.48	1.46

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	381	778	C12-C7-N11	9.56	110.81	105.08
5	H	381	778	C12-C7-N11	9.46	110.75	105.08
5	F	381	778	C12-C7-N11	9.17	110.57	105.08
5	B	380	778	C12-C7-N11	9.12	110.55	105.08
5	J	381	778	C12-C7-N11	8.98	110.46	105.08
5	L	381	778	C12-C7-N11	8.95	110.44	105.08
5	F	381	778	C3-N1-C2	6.06	120.57	111.14
5	B	380	778	C3-N1-C2	5.95	120.40	111.14
5	L	381	778	C3-N1-C2	5.87	120.27	111.14
5	H	381	778	C3-N1-C2	5.85	120.25	111.14
5	J	381	778	C3-N1-C2	5.79	120.15	111.14
5	D	381	778	C3-N1-C2	5.76	120.10	111.14
5	L	381	778	C2-C5-N9	5.50	120.66	110.66
6	L	382	MES	O3S-S-C8	5.27	116.31	106.00
5	F	381	778	C2-C5-N9	5.22	120.14	110.66
5	D	381	778	C2-C5-N9	5.21	120.12	110.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	381	778	C2-C5-N9	5.12	119.96	110.66
5	B	380	778	C2-C5-N9	5.04	119.82	110.66
5	J	381	778	C14-N9-C8	5.00	126.31	120.48
5	B	380	778	C5-N9-C8	-5.00	116.11	122.50
5	H	381	778	C2-C5-N9	4.99	119.73	110.66
5	L	381	778	C5-N9-C8	-4.91	116.22	122.50
5	F	381	778	C5-N9-C8	-4.89	116.24	122.50
5	J	381	778	C5-N9-C8	-4.88	116.25	122.50
6	J	382	MES	O3S-S-C8	4.87	115.53	106.00
5	H	381	778	C5-N9-C8	-4.84	116.31	122.50
6	D	382	MES	O3S-S-C8	4.80	115.39	106.00
5	F	381	778	C14-N9-C8	4.80	126.07	120.48
6	B	381	MES	O3S-S-C8	4.76	115.31	106.00
5	B	380	778	C14-N9-C8	4.75	126.01	120.48
5	D	381	778	C5-N9-C8	-4.74	116.44	122.50
5	H	381	778	C14-N9-C8	4.72	125.98	120.48
5	H	381	778	C5-C2-N1	-4.70	101.17	110.65
5	D	381	778	C14-N9-C8	4.69	125.94	120.48
6	H	382	MES	O3S-S-C8	4.68	115.15	106.00
5	L	381	778	C14-N9-C8	4.65	125.90	120.48
5	D	381	778	C5-C2-N1	-4.57	101.42	110.65
5	B	380	778	C5-C2-N1	-4.47	101.64	110.65
5	J	381	778	C5-C2-N1	-4.45	101.68	110.65
6	F	382	MES	O3S-S-C8	4.39	114.59	106.00
5	F	381	778	C5-C2-N1	-4.35	101.88	110.65
5	L	381	778	C5-C2-N1	-4.29	101.99	110.65
6	F	382	MES	O1S-S-C8	4.00	112.77	106.73
5	D	381	778	C3-N1-C4	-3.68	103.68	112.41
5	H	381	778	C3-N1-C4	-3.66	103.72	112.41
5	B	380	778	C3-N1-C4	-3.64	103.77	112.41
6	B	381	MES	O1S-S-C8	3.63	112.22	106.73
5	L	381	778	C3-N1-C4	-3.61	103.84	112.41
5	J	381	778	C3-N1-C4	-3.55	103.98	112.41
5	F	381	778	C3-N1-C4	-3.47	104.17	112.41
6	F	382	MES	O2S-S-C8	3.46	111.95	106.73
6	L	382	MES	O1S-S-C8	3.44	111.92	106.73
6	H	382	MES	O1S-S-C8	3.34	111.77	106.73
6	J	382	MES	O1S-S-C8	3.27	111.67	106.73
6	J	382	MES	O2S-S-C8	3.27	111.66	106.73
6	D	382	MES	O2S-S-C8	3.24	111.62	106.73
6	B	381	MES	O2S-S-C8	3.16	111.51	106.73
5	H	381	778	C4-N1-C2	3.15	114.63	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	381	778	C4-N1-C2	3.11	114.57	110.10
5	B	380	778	C4-N1-C2	3.10	114.55	110.10
5	L	381	778	C4-N1-C2	3.07	114.51	110.10
5	F	381	778	C21-C14-N9	3.01	124.51	120.18
6	D	382	MES	O1S-S-C8	2.96	111.21	106.73
5	D	381	778	C4-N1-C2	2.96	114.36	110.10
5	F	381	778	C4-N1-C2	2.93	114.31	110.10
6	L	382	MES	O2S-S-C8	2.85	111.03	106.73
5	F	381	778	C16-N11-C17	-2.76	122.68	126.32
5	J	381	778	C21-C14-N9	2.75	124.13	120.18
5	L	381	778	C21-C14-N9	2.75	124.13	120.18
5	H	381	778	C16-N11-C17	-2.70	122.75	126.32
5	B	380	778	C16-N11-C17	-2.69	122.78	126.32
6	H	382	MES	O2S-S-C8	2.68	110.78	106.73
5	J	381	778	C16-N11-C17	-2.65	122.83	126.32
5	L	381	778	C16-N11-C17	-2.60	122.89	126.32
6	F	382	MES	O2S-S-O1S	-2.59	105.41	113.82
5	B	380	778	C21-C14-N9	2.58	123.89	120.18
5	D	381	778	C21-C14-N9	2.58	123.89	120.18
6	L	382	MES	O2S-S-O1S	-2.54	105.56	113.82
6	J	382	MES	O3S-S-O2S	-2.54	105.05	111.40
6	B	381	MES	O2S-S-O1S	-2.52	105.62	113.82
5	D	381	778	C16-N11-C17	-2.49	123.03	126.32
6	L	382	MES	O3S-S-O2S	-2.47	105.22	111.40
5	H	381	778	C21-C14-N9	2.46	123.72	120.18
6	D	382	MES	O2S-S-O1S	-2.43	105.92	113.82
6	H	382	MES	O2S-S-O1S	-2.40	106.02	113.82
6	J	382	MES	O2S-S-O1S	-2.40	106.02	113.82
6	D	382	MES	O3S-S-O2S	-2.37	105.46	111.40
6	B	381	MES	O3S-S-O2S	-2.37	105.48	111.40
5	D	381	778	C7-C12-N18	-2.36	104.78	109.79
6	F	382	MES	O3S-S-O1S	-2.36	105.50	111.40
5	H	381	778	C7-C12-N18	-2.31	104.89	109.79
5	F	381	778	C7-C12-N18	-2.29	104.93	109.79
5	B	380	778	C7-C12-N18	-2.23	105.05	109.79
5	J	381	778	C7-C12-N18	-2.23	105.06	109.79
6	L	382	MES	O1-C2-C3	-2.22	106.99	111.77
5	L	381	778	C7-C12-N18	-2.21	105.11	109.79
6	F	382	MES	O3S-S-O2S	-2.20	105.90	111.40
5	J	381	778	C17-N11-C7	2.19	109.06	106.30
6	J	382	MES	O1-C2-C3	-2.18	107.08	111.77
6	B	381	MES	O3S-S-O1S	-2.16	105.99	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	382	MES	O1-C2-C3	-2.15	107.14	111.77
6	L	382	MES	O3S-S-O1S	-2.15	106.02	111.40
5	F	381	778	C17-N11-C7	2.14	109.00	106.30
6	D	382	MES	O1-C2-C3	-2.13	107.18	111.77
6	H	382	MES	O3S-S-O2S	-2.12	106.09	111.40
5	D	381	778	C17-N11-C7	2.10	108.95	106.30
6	J	382	MES	O3S-S-O1S	-2.07	106.22	111.40
6	H	382	MES	O1-C2-C3	-2.05	107.36	111.77
6	B	381	MES	O1-C2-C3	-2.04	107.39	111.77
5	L	381	778	C17-N11-C7	2.02	108.85	106.30
5	H	381	778	C17-N11-C7	2.00	108.82	106.30

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	381	778	C32-C34-C35-N36

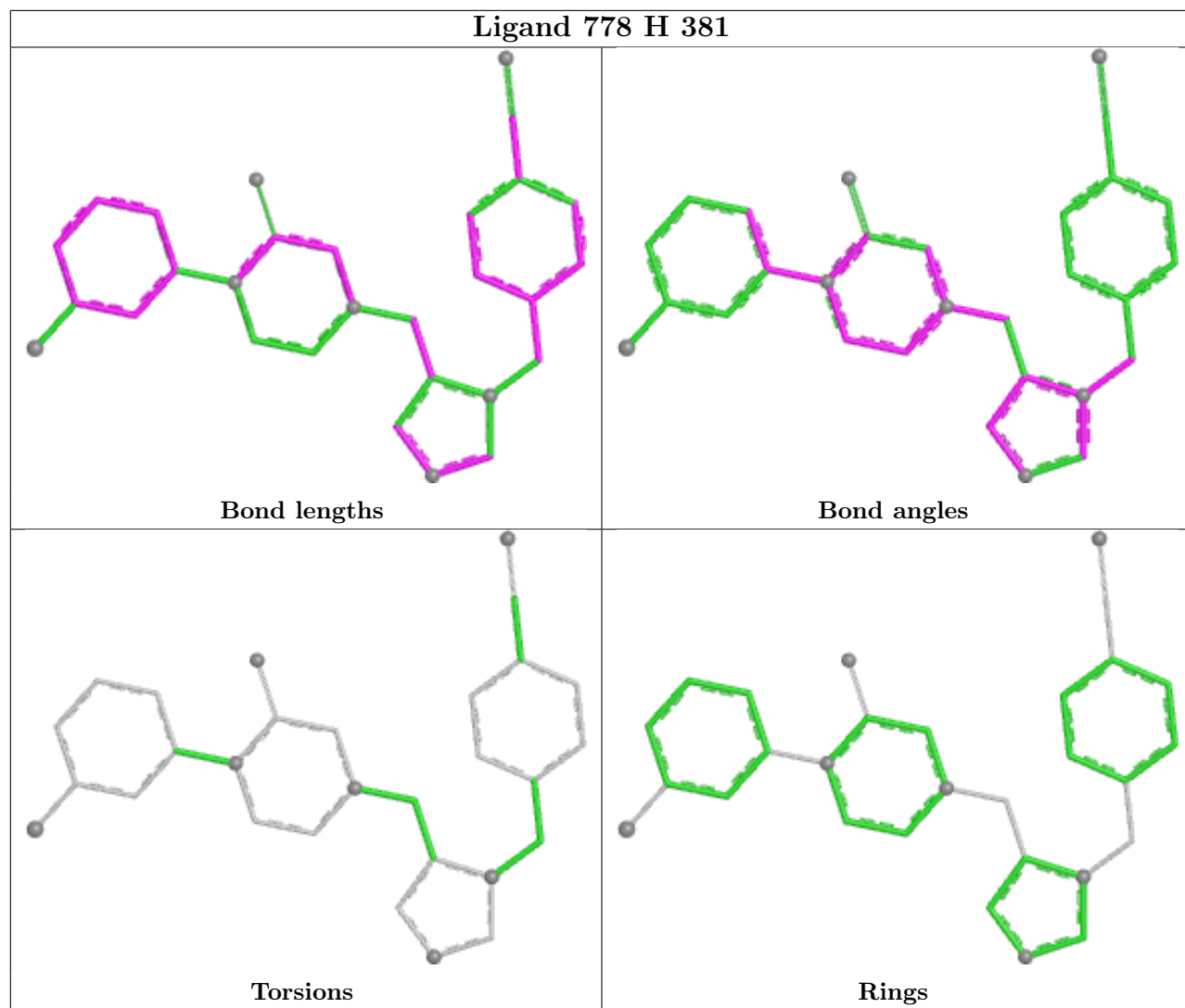
There are no ring outliers.

1 monomer is involved in 2 short contacts:

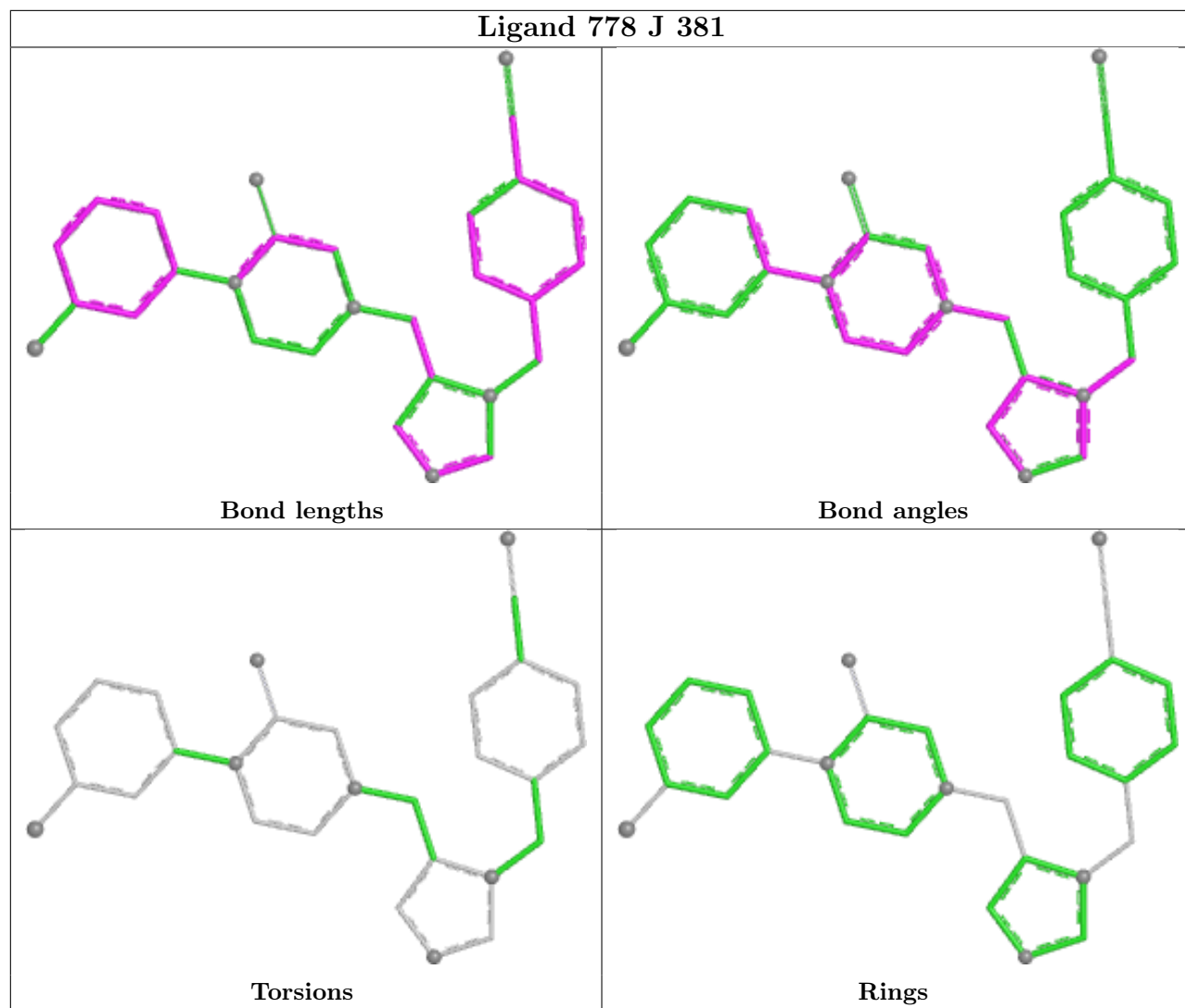
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	382	MES	2	0

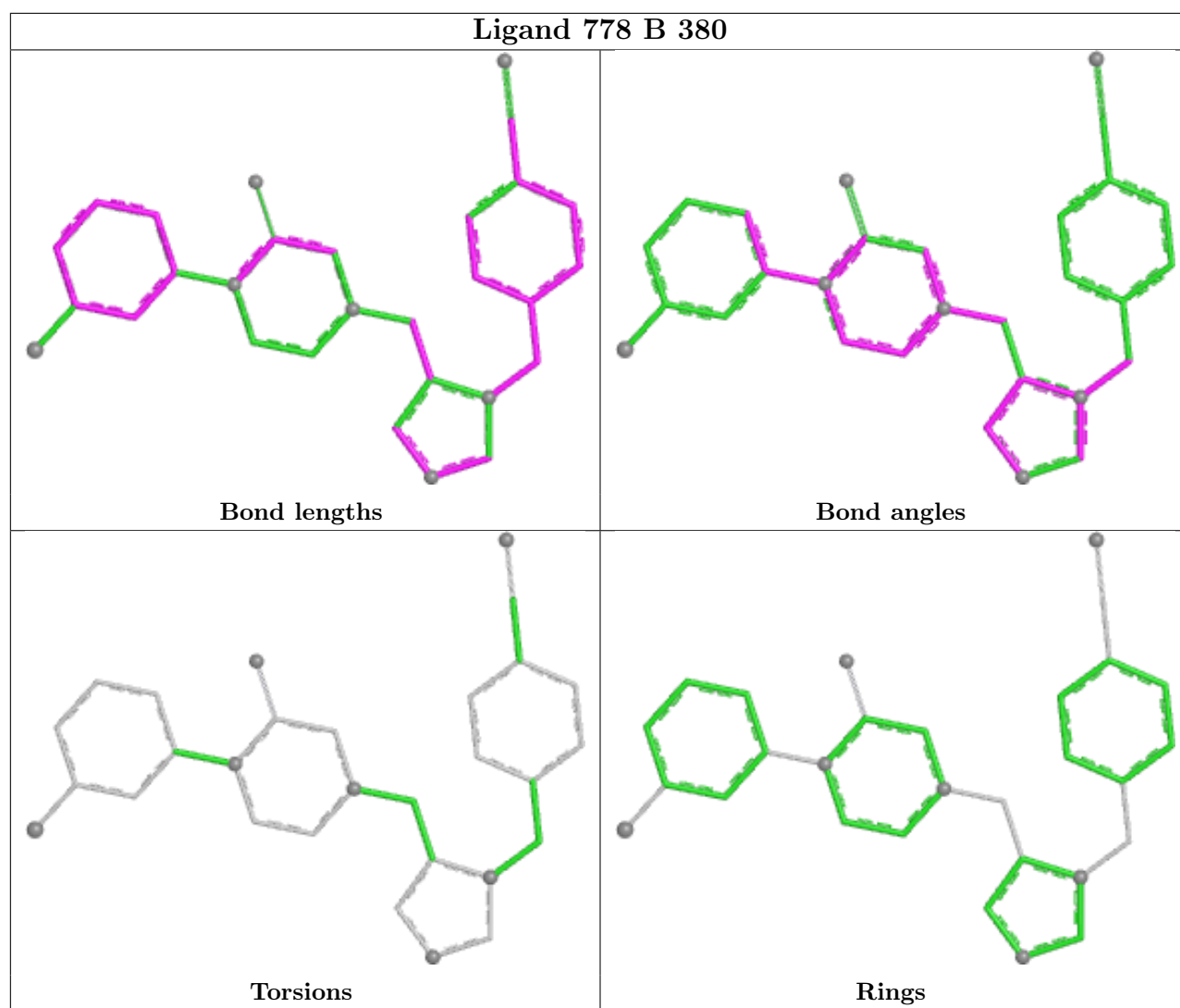
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand 778 H 381

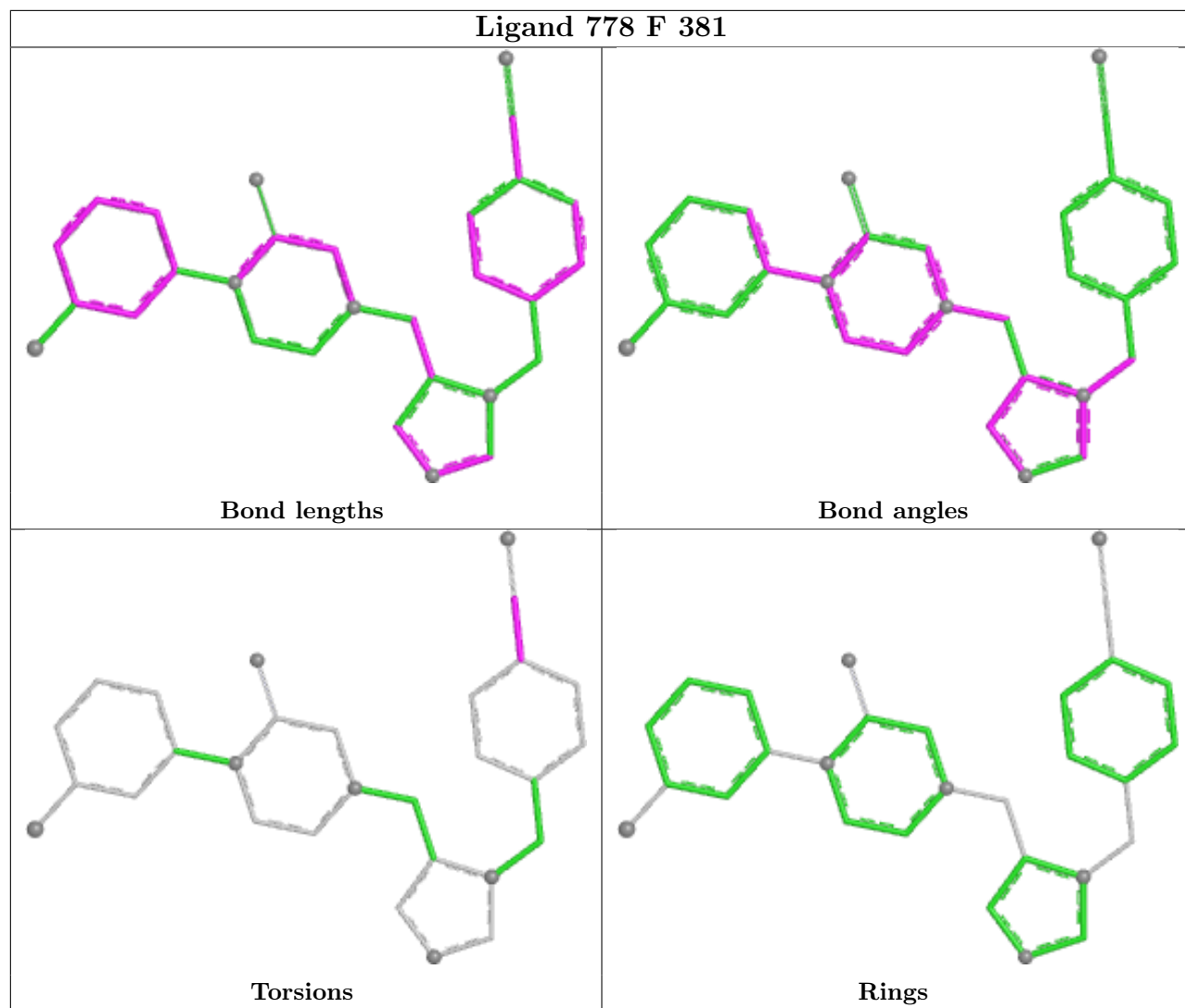


Ligand 778 J 381

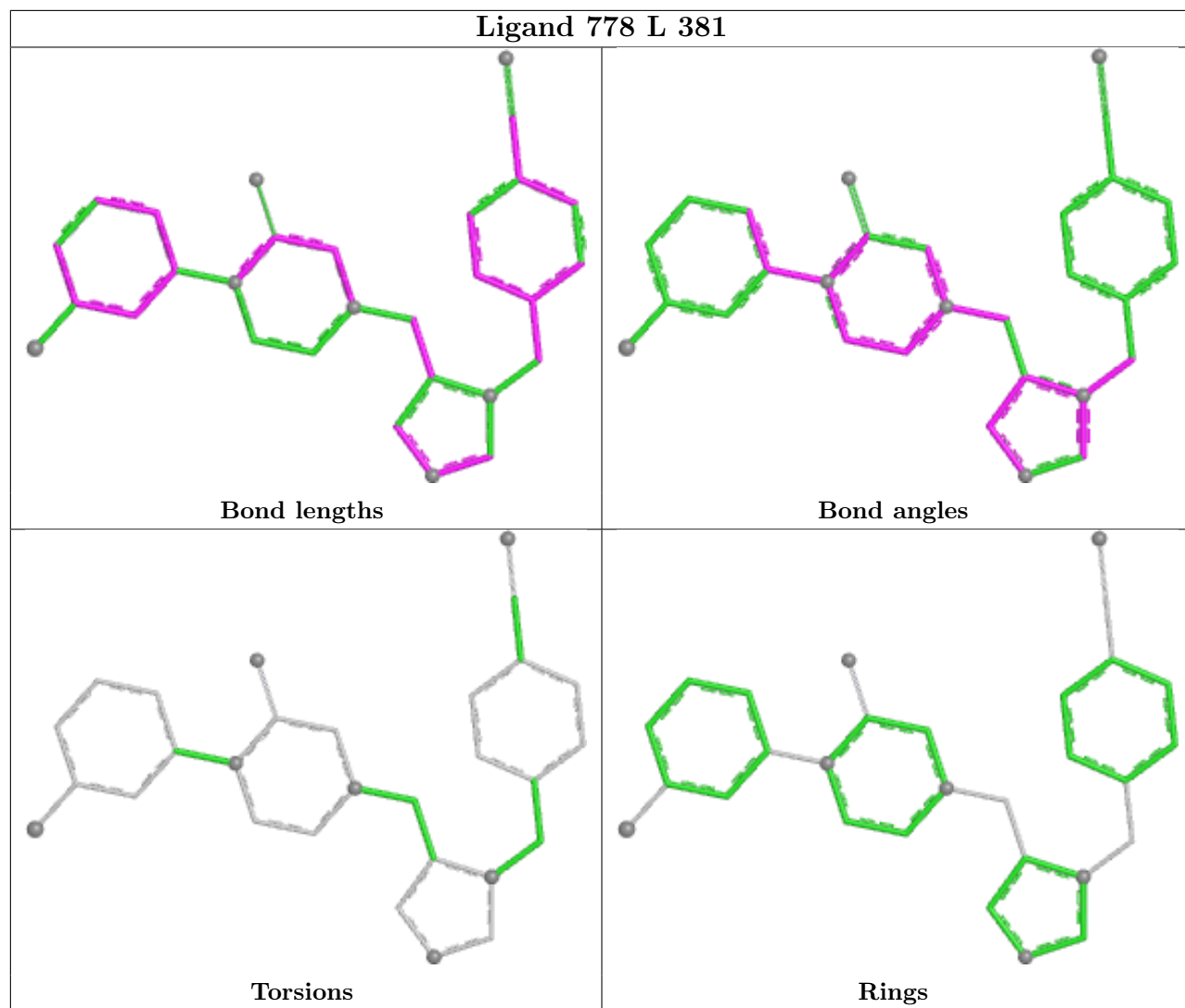


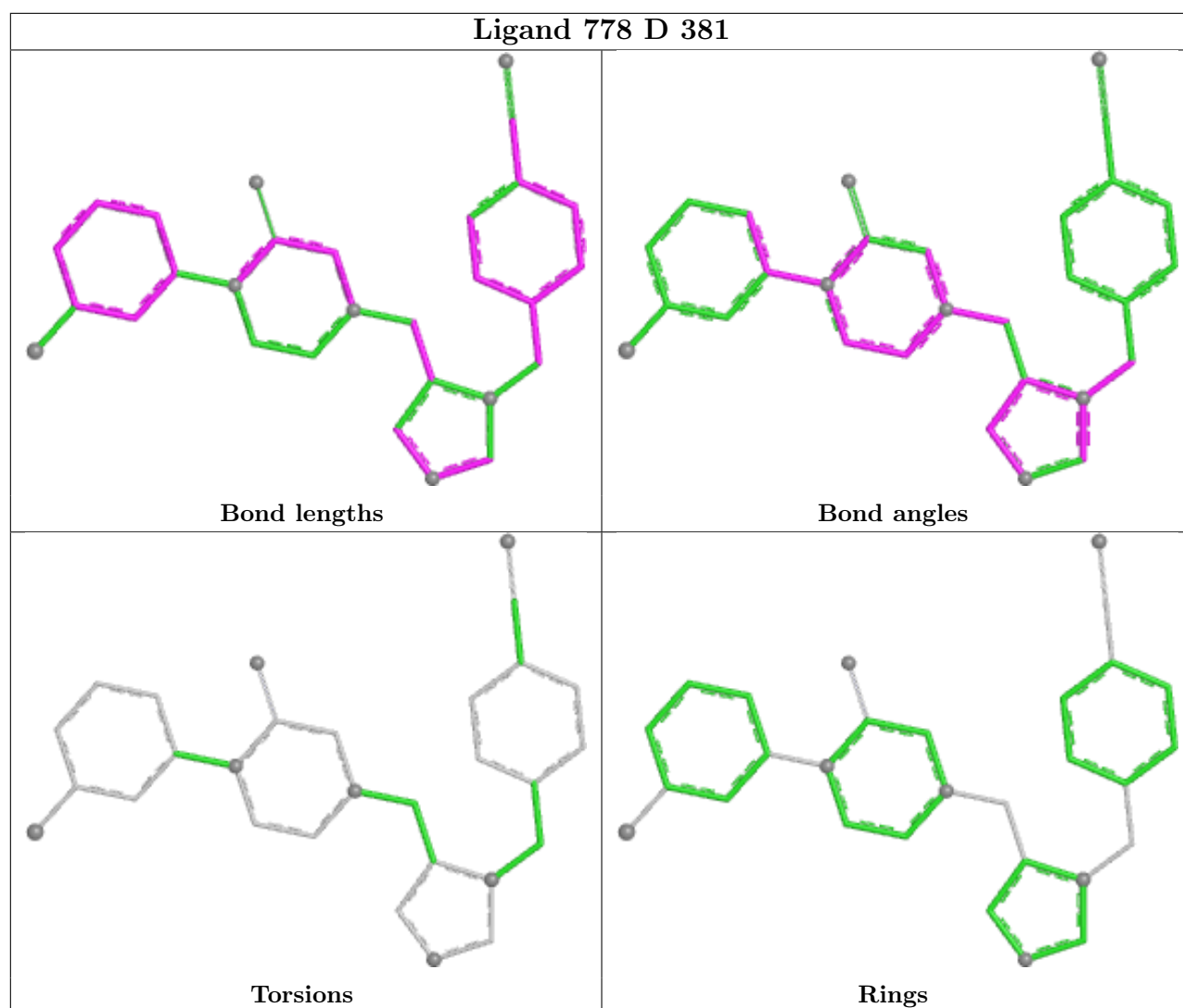


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Ligand 778 L 381





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	314/377 (83%)	0.50	27 (8%)	16 15	41, 63, 97, 108	0
1	C	314/377 (83%)	0.39	13 (4%)	41 42	41, 59, 87, 108	0
1	E	314/377 (83%)	0.53	15 (4%)	35 35	44, 63, 91, 106	0
1	G	314/377 (83%)	0.63	32 (10%)	12 11	41, 64, 94, 110	0
1	I	314/377 (83%)	0.28	13 (4%)	41 42	34, 57, 87, 96	0
1	K	314/377 (83%)	-0.08	9 (2%)	53 55	31, 47, 72, 87	0
2	B	346/377 (91%)	0.22	9 (2%)	57 58	42, 57, 82, 102	0
2	D	346/377 (91%)	-0.02	14 (4%)	42 43	35, 51, 77, 91	0
2	F	346/377 (91%)	0.05	13 (3%)	44 45	36, 51, 77, 101	0
2	H	346/377 (91%)	0.94	43 (12%)	8 7	40, 71, 97, 114	0
2	J	346/377 (91%)	0.20	18 (5%)	33 32	35, 55, 84, 104	0
2	L	346/377 (91%)	-0.18	12 (3%)	47 48	29, 44, 71, 95	0
All	All	3960/4524 (87%)	0.28	218 (5%)	30 30	29, 57, 88, 114	0

All (218) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	55	PHE	8.4
1	C	55	PHE	8.1
2	H	18	LEU	7.0
2	F	18	LEU	6.9
1	E	55	PHE	6.2
2	B	18	LEU	5.6
2	J	363	THR	5.6
1	I	55	PHE	5.3
2	L	111	PRO	5.3
2	J	18	LEU	5.2
2	D	363	THR	5.1

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Mol	Chain	Res	Type	RSRZ
2	L	363	THR	4.9
2	H	85	GLU	4.9
1	A	328	ASP	4.8
2	B	111	PRO	4.7
2	B	113	THR	4.7
2	B	363	THR	4.7
2	F	363	THR	4.7
2	H	363	THR	4.7
1	A	368	SER	4.7
2	H	362	LYS	4.6
2	L	362	LYS	4.6
2	J	110	ASN	4.6
1	G	328	ASP	4.5
1	I	368	SER	4.4
2	F	110	ASN	4.4
2	D	18	LEU	4.3
1	A	364	GLN	4.2
1	G	57	SER	4.1
2	H	113	THR	4.1
2	D	113	THR	4.1
1	E	332	ASP	4.1
2	F	316	HIS	3.9
2	L	18	LEU	3.9
2	F	85	GLU	3.9
1	G	368	SER	3.8
2	H	39	ARG	3.8
1	K	55	PHE	3.8
2	B	65	ASP	3.8
2	D	316	HIS	3.7
1	E	368	SER	3.7
2	H	111	PRO	3.7
1	A	268	LYS	3.7
2	B	362	LYS	3.5
2	H	58	LEU	3.5
2	H	110	ASN	3.5
2	B	316	HIS	3.5
2	J	362	LYS	3.5
1	C	368	SER	3.5
2	L	113	THR	3.5
1	A	55	PHE	3.5
2	H	316	HIS	3.5
2	F	111	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
2	H	65	ASP	3.4
1	G	364	GLN	3.4
2	B	110	ASN	3.4
2	H	305	LEU	3.3
2	J	111	PRO	3.3
1	C	306	HIS	3.3
2	H	335	SER	3.3
1	A	326	GLN	3.3
1	C	328	ASP	3.3
2	F	113	THR	3.3
2	J	360	SER	3.2
1	G	326	GLN	3.2
2	H	108	SER	3.2
1	G	85	SER	3.2
1	I	304	PRO	3.1
1	G	56	LEU	3.1
2	H	304	ARG	3.1
2	H	19	ASP	3.0
1	G	61	PRO	3.0
2	J	108	SER	3.0
1	C	307	SER	3.0
2	F	109	LYS	3.0
1	G	83	GLY	3.0
2	D	110	ASN	3.0
2	H	112	GLY	3.0
1	E	306	HIS	2.9
2	H	35	VAL	2.9
1	C	336	LYS	2.9
1	G	303	GLN	2.9
2	J	85	GLU	2.9
2	H	69	LYS	2.8
1	E	328	ASP	2.8
1	G	58	LEU	2.8
1	A	331	GLU	2.8
1	G	59	ASP	2.8
2	H	63	SER	2.8
1	G	366	LYS	2.8
2	L	316	HIS	2.8
1	A	304	PRO	2.7
1	C	304	PRO	2.7
1	E	268	LYS	2.7
2	L	85	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	327	CYS	2.7
1	G	91	ILE	2.7
1	C	62	THR	2.7
1	I	328	ASP	2.6
2	H	70	ASP	2.6
2	D	109	LYS	2.6
1	E	327	CYS	2.6
2	H	315	SER	2.6
2	H	109	LYS	2.6
1	A	59	ASP	2.6
2	F	65	ASP	2.6
2	D	305	LEU	2.6
2	J	106	ASN	2.6
1	C	326	GLN	2.6
1	K	365	SER	2.6
2	J	316	HIS	2.6
1	K	332	ASP	2.6
2	H	135	LEU	2.6
2	L	109	LYS	2.6
1	A	265	GLU	2.5
2	H	82	LEU	2.5
1	A	261	GLN	2.5
1	A	330	LYS	2.5
1	G	195	GLN	2.5
2	F	359	GLN	2.5
1	G	306	HIS	2.5
2	J	114	ALA	2.5
2	J	338	CYS	2.5
1	G	304	PRO	2.5
2	B	112	GLY	2.5
2	L	110	ASN	2.5
1	A	327	CYS	2.5
1	A	288	GLY	2.5
2	J	19	ASP	2.5
2	H	24	ARG	2.4
1	G	81	ASN	2.4
1	A	251	SER	2.4
1	A	366	LYS	2.4
1	E	366	LYS	2.4
2	D	362	LYS	2.4
1	I	332	ASP	2.4
2	H	314	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	359	GLN	2.4
2	H	310	ALA	2.4
1	A	332	ASP	2.4
1	A	300	LEU	2.4
1	I	306	HIS	2.4
1	G	329	ASN	2.4
1	G	86	PRO	2.4
2	F	314	ASP	2.4
2	H	100	TYR	2.4
1	K	81	ASN	2.4
2	L	114	ALA	2.4
2	H	292	GLU	2.4
1	E	303	GLN	2.3
2	H	71	ASP	2.3
1	G	62	THR	2.3
1	C	305	SER	2.3
1	K	368	SER	2.3
2	J	62	ASP	2.3
1	E	304	PRO	2.3
1	G	109	ARG	2.3
1	A	217	ASP	2.3
2	F	114	ALA	2.3
1	G	272	HIS	2.3
2	J	34	GLN	2.3
1	E	56	LEU	2.3
1	A	339	GLU	2.3
1	E	331	GLU	2.3
2	L	106	ASN	2.2
1	K	326	GLN	2.2
1	E	329	ASN	2.2
2	J	335	SER	2.2
1	G	92	TYR	2.2
1	G	268	LYS	2.2
1	I	251	SER	2.2
1	I	81	ASN	2.2
1	A	302	LEU	2.2
1	A	301	ASP	2.2
1	G	94	GLU	2.2
1	K	142	ARG	2.2
2	H	27	ARG	2.2
2	H	29	PHE	2.2
2	D	35	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	329	ASN	2.1
2	H	64	LEU	2.1
1	G	333	ILE	2.1
1	C	347	GLU	2.1
2	H	333	GLU	2.1
1	G	305	SER	2.1
1	E	330	LYS	2.1
2	H	34	GLN	2.1
1	A	294	ASN	2.1
2	J	89	ASN	2.1
1	I	82	ASP	2.1
1	K	304	PRO	2.1
2	H	107	PRO	2.1
2	H	105	PHE	2.1
1	C	94	GLU	2.1
1	G	150	GLU	2.1
1	G	60	SER	2.1
1	A	329	ASN	2.1
2	H	61	LEU	2.1
2	D	336	GLY	2.1
2	H	73	ILE	2.1
2	J	91	ASP	2.1
1	I	305	SER	2.1
1	K	305	SER	2.1
2	D	37	PRO	2.1
2	D	111	PRO	2.1
1	A	306	HIS	2.1
2	D	39	ARG	2.0
1	E	265	GLU	2.0
1	I	347	GLU	2.0
2	D	38	GLU	2.0
2	H	336	GLY	2.0
1	A	303	GLN	2.0
1	A	291	ARG	2.0
1	C	366	LYS	2.0
2	F	112	GLY	2.0
2	H	345	ASN	2.0
2	L	112	GLY	2.0
1	G	84	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	778	B	380	29/29	0.85	0.12	39,46,53,56	0
5	778	J	381	29/29	0.85	0.11	29,39,42,42	0
5	778	L	381	29/29	0.85	0.10	27,33,36,39	0
5	778	F	381	29/29	0.87	0.12	36,45,52,52	0
5	778	D	381	29/29	0.88	0.12	35,45,47,51	0
5	778	H	381	29/29	0.88	0.12	42,48,51,54	0
6	MES	H	382	12/12	0.90	0.14	74,75,84,84	0
6	MES	L	382	12/12	0.90	0.16	69,71,76,77	0
6	MES	B	381	12/12	0.93	0.13	69,71,81,83	0
6	MES	J	382	12/12	0.93	0.13	70,72,81,81	0
6	MES	F	382	12/12	0.93	0.12	72,73,85,86	0
6	MES	D	382	12/12	0.94	0.12	71,72,78,78	0
7	CL	I	378	1/1	0.94	0.23	75,75,75,75	0
7	CL	C	378	1/1	0.96	0.22	61,61,61,61	0
7	CL	H	379	1/1	0.97	0.07	68,68,68,68	0
7	CL	G	378	1/1	0.97	0.18	61,61,61,61	0
7	CL	J	379	1/1	0.97	0.08	63,63,63,63	0
7	CL	K	378	1/1	0.97	0.16	67,67,67,67	0
4	SO4	D	380	5/5	0.98	0.07	51,52,54,55	0
4	SO4	F	380	5/5	0.98	0.08	53,54,58,58	0
4	SO4	H	380	5/5	0.98	0.06	60,61,62,62	0
7	CL	F	379	1/1	0.99	0.10	53,53,53,53	0
3	ZN	H	378	1/1	0.99	0.03	55,55,55,55	0
4	SO4	J	380	5/5	0.99	0.05	45,45,47,48	0
4	SO4	L	380	5/5	0.99	0.05	41,44,45,47	0
4	SO4	B	379	5/5	0.99	0.06	56,56,58,59	0
7	CL	D	379	1/1	0.99	0.06	52,52,52,52	0

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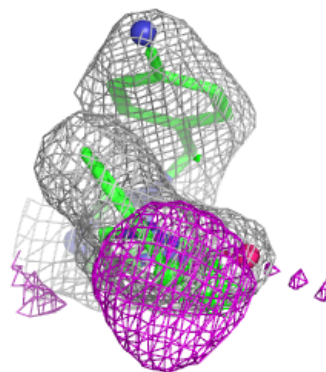
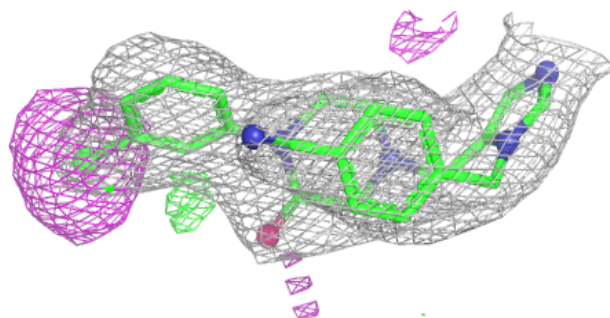
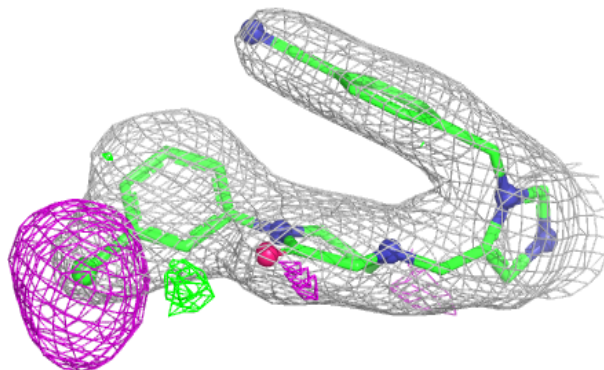
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	CL	L	379	1/1	0.99	0.06	53,53,53,53	0
3	ZN	B	378	1/1	1.00	0.01	45,45,45,45	0
3	ZN	J	378	1/1	1.00	0.02	39,39,39,39	0
3	ZN	L	378	1/1	1.00	0.02	35,35,35,35	0
3	ZN	D	378	1/1	1.00	0.03	43,43,43,43	0
3	ZN	F	378	1/1	1.00	0.01	45,45,45,45	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.

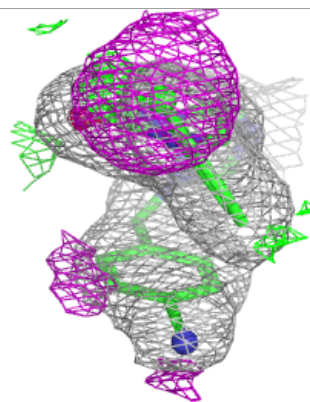
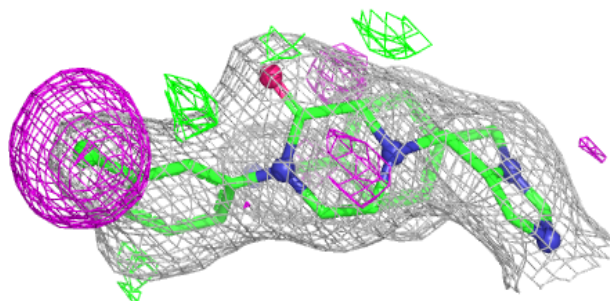
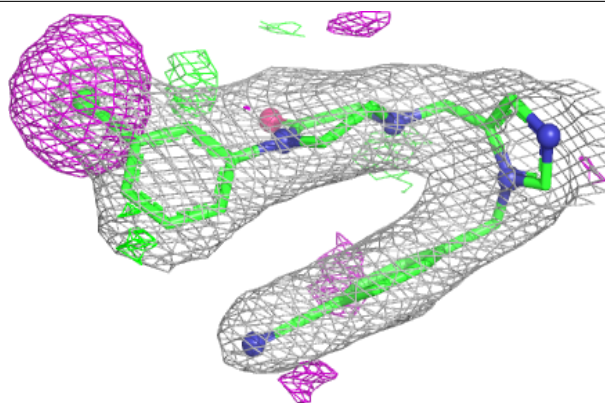
Electron density around 778 B 380:

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

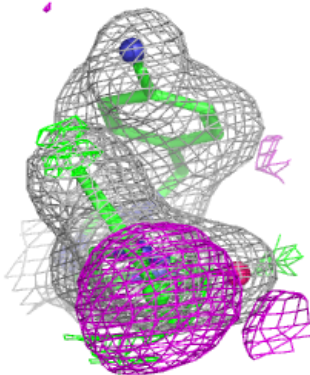
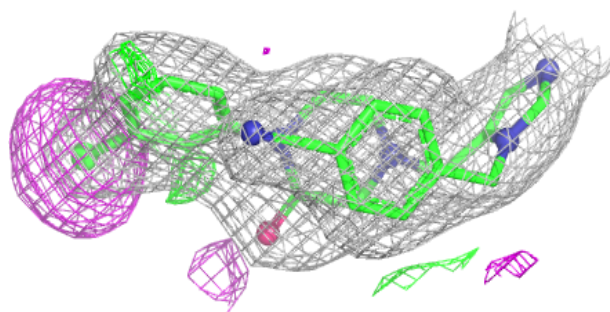
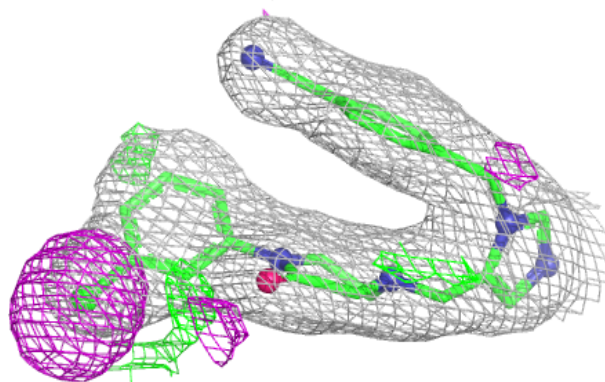


Electron density around 778 J 381:

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

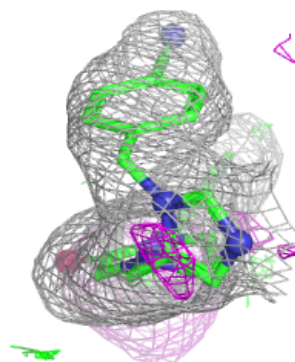
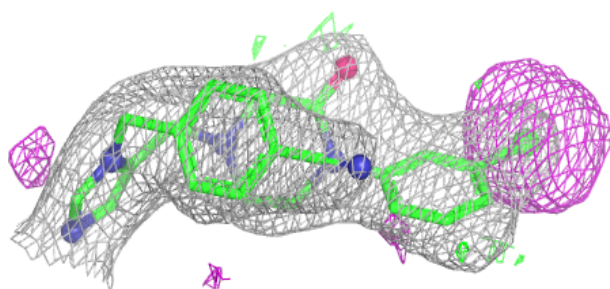
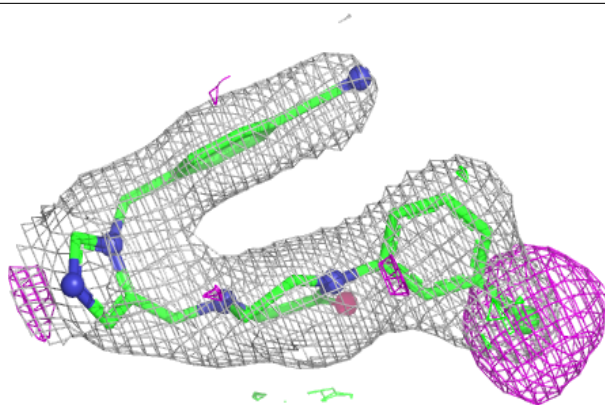
**Electron density around 778 L 381:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

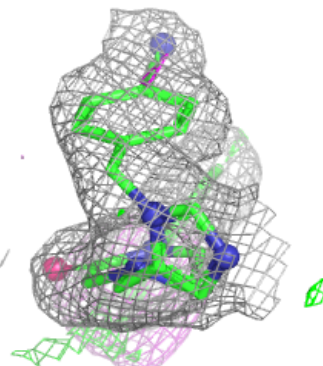
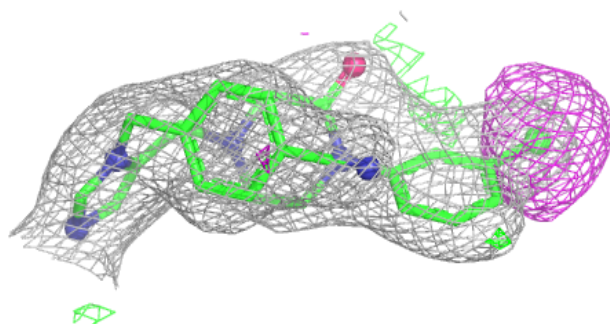
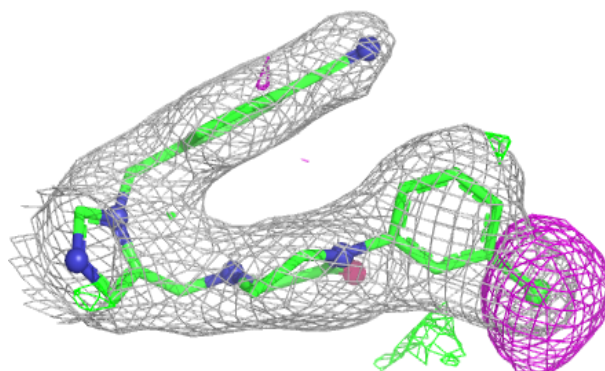


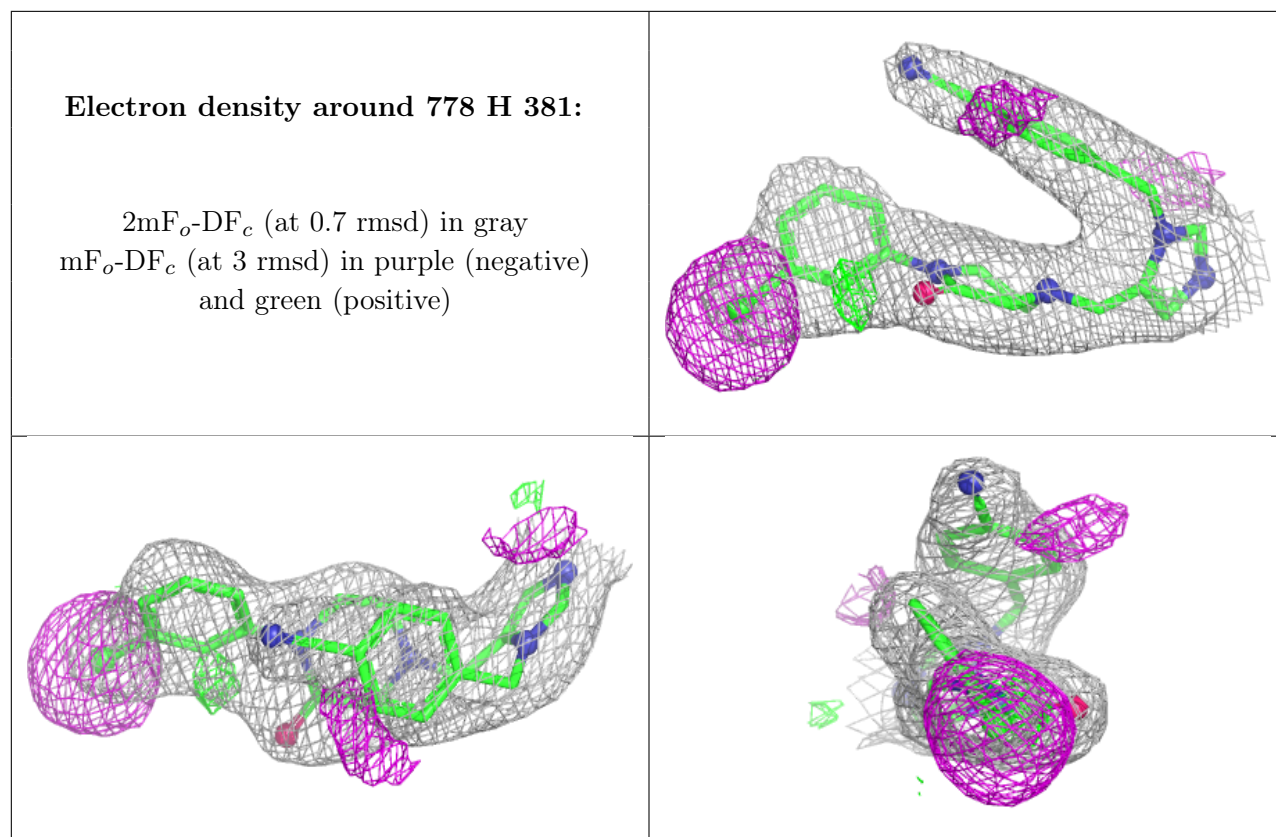
Electron density around 778 F 381:

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

**Electron density around 778 D 381:**

$2mF_o-DF_c$ (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.