



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:42 PM UTC

PDB ID : 8RDX / pdb_00008rdx
Title : PGGtase I in complex with probe BAY-6092
Authors : Steuber, H.
Deposited on : 2023-12-08
Resolution : 3.67 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:

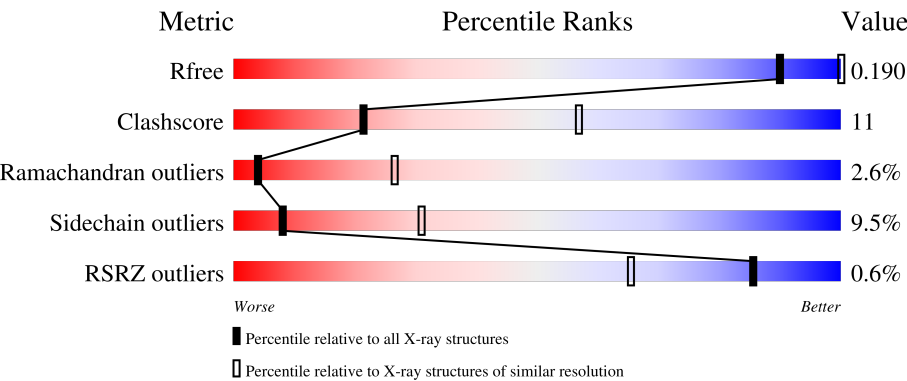
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 3.67 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	1263 (3.80-3.56)
Clashscore	190562	1305 (3.80-3.56)
Ramachandran outliers	187476	1259 (3.80-3.56)
Sidechain outliers	187428	1256 (3.80-3.56)
RSRZ outliers	180081	1262 (3.80-3.56)

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	314	68%29%..
1	C	314	64%32%. .
1	E	314	% 68%27%. .
1	G	314	% 63%32%. .
1	I	314	70%25%5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	314	 66%29%5%
2	B	346	%  71%23%6%
2	D	346	 65%29%6%
2	F	346	%  70%26%. .
2	H	346	 66%29%. .
2	J	346	 68%27%. .
2	L	346	%  59%34%7%

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	DPO	D	403	-	-	X	-
5	DPO	H	403	-	-	X	-
5	DPO	J	403	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 32241 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-1 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2629	1679	463	482	5			
1	C	314	Total	C	N	O	S	0	0	0
			2629	1679	463	482	5			
1	E	314	Total	C	N	O	S	0	0	0
			2632	1680	463	484	5			
1	G	314	Total	C	N	O	S	0	0	0
			2629	1679	463	482	5			
1	I	314	Total	C	N	O	S	0	0	0
			2629	1679	463	482	5			
1	K	314	Total	C	N	O	S	0	0	0
			2629	1679	463	482	5			

- Molecule 2 is a protein called Geranylgeranyl transferase type-1 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	346	Total	C	N	O	S	0	0	0
			2697	1707	467	499	24			
2	D	346	Total	C	N	O	S	0	0	0
			2697	1707	467	499	24			
2	F	346	Total	C	N	O	S	0	0	0
			2697	1707	467	499	24			
2	H	346	Total	C	N	O	S	0	0	0
			2697	1707	467	499	24			
2	J	346	Total	C	N	O	S	0	0	0
			2697	1707	467	499	24			
2	L	346	Total	C	N	O	S	0	0	0
			2697	1707	467	499	24			

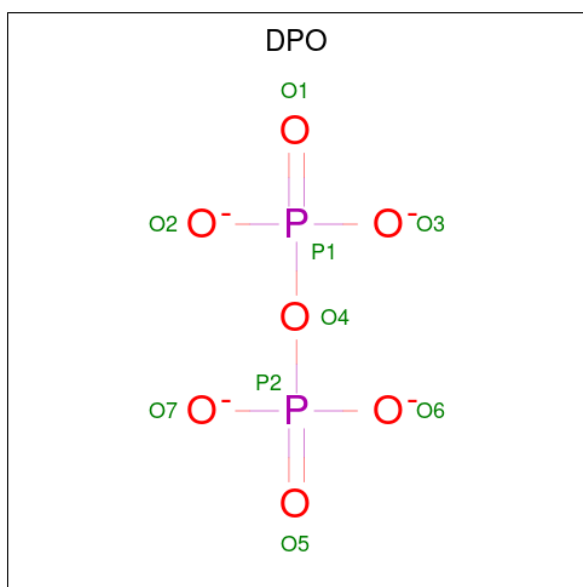
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

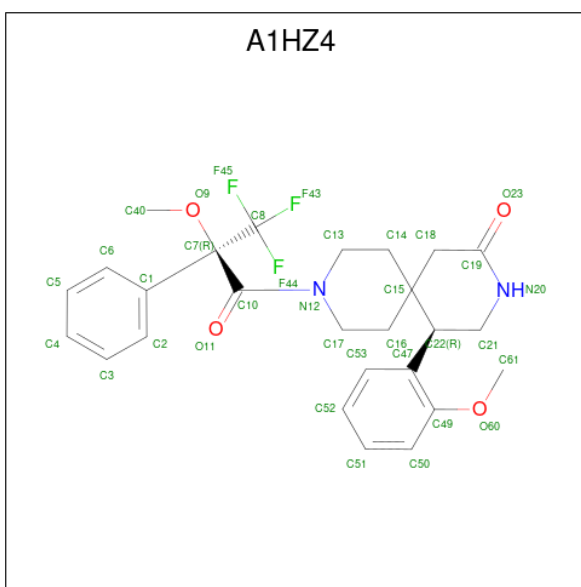
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Cl 1	0	0
4	D	1	Total 1	Cl 1	0	0
4	F	1	Total 1	Cl 1	0	0
4	H	1	Total 1	Cl 1	0	0
4	J	1	Total 1	Cl 1	0	0
4	L	1	Total 1	Cl 1	0	0

- Molecule 5 is DIPHOSPHATE (CCD ID: DPO) (formula: O₇P₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			9	7	2		
5	D	1	Total	O	P	0	0
			9	7	2		
5	F	1	Total	O	P	0	0
			9	7	2		
5	H	1	Total	O	P	0	0
			9	7	2		
5	J	1	Total	O	P	0	0
			9	7	2		
5	L	1	Total	O	P	0	0
			9	7	2		

- Molecule 6 is (5 {R})-5-(2-methoxyphenyl)-9-[(2 {R})-3,3,3-tris(fluoranyl)-2-methoxy-2-phenyl-propanoyl]-3,9-diazaspiro[5.5]undecan-2-one (CCD ID: A1HZ4) (formula: C₂₆H₂₉F₃N₂O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total 35	C 26	F 3	N 2	O 4	0	0
6	D	1	Total 35	C 26	F 3	N 2	O 4	0	0
6	F	1	Total 35	C 26	F 3	N 2	O 4	0	0
6	H	1	Total 35	C 26	F 3	N 2	O 4	0	0
6	J	1	Total 35	C 26	F 3	N 2	O 4	0	0
6	L	1	Total 35	C 26	F 3	N 2	O 4	0	0

- Molecule 7 is water.

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

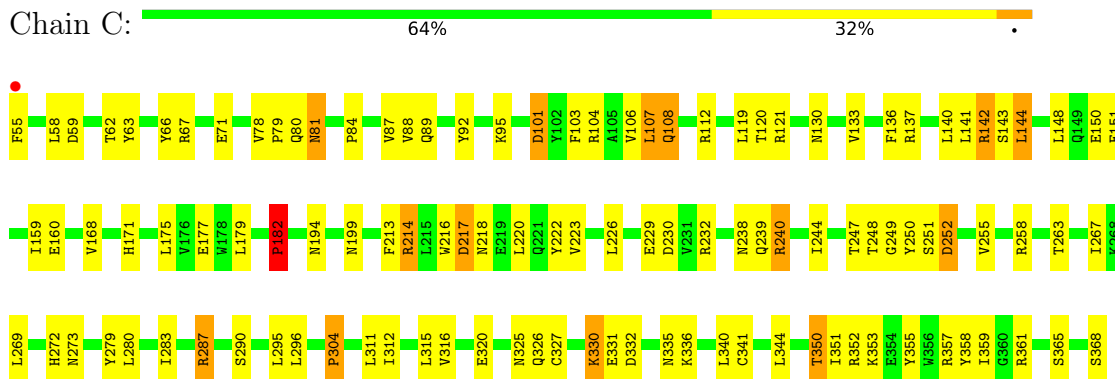
3 Residue-property plots

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

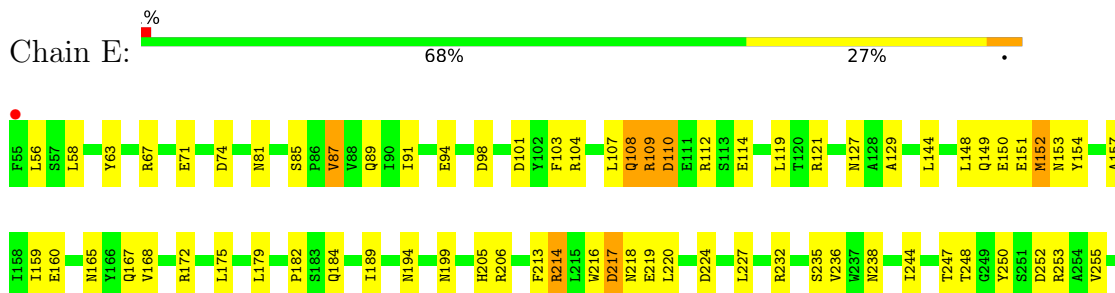
- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha

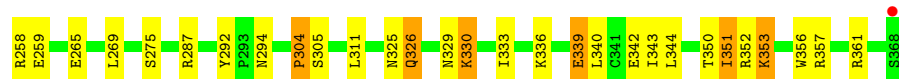


- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha

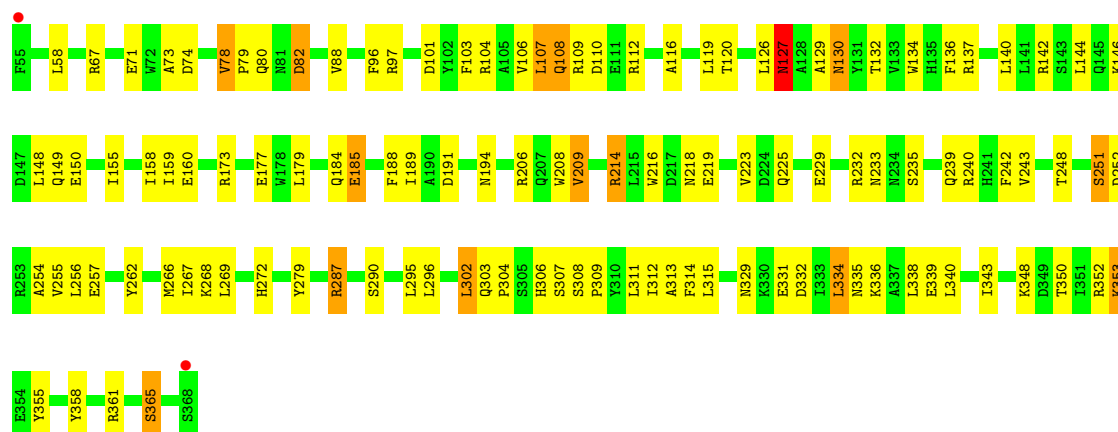


- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha

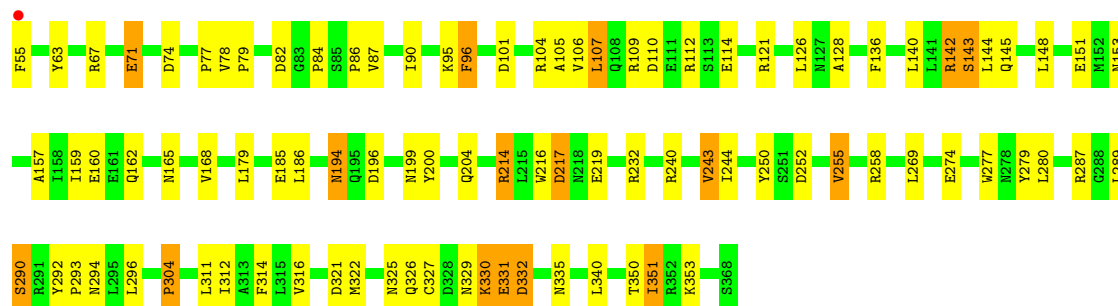




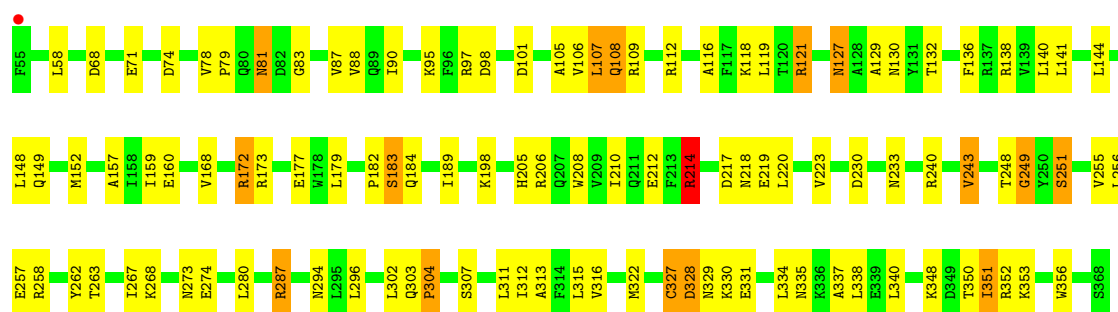
- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha



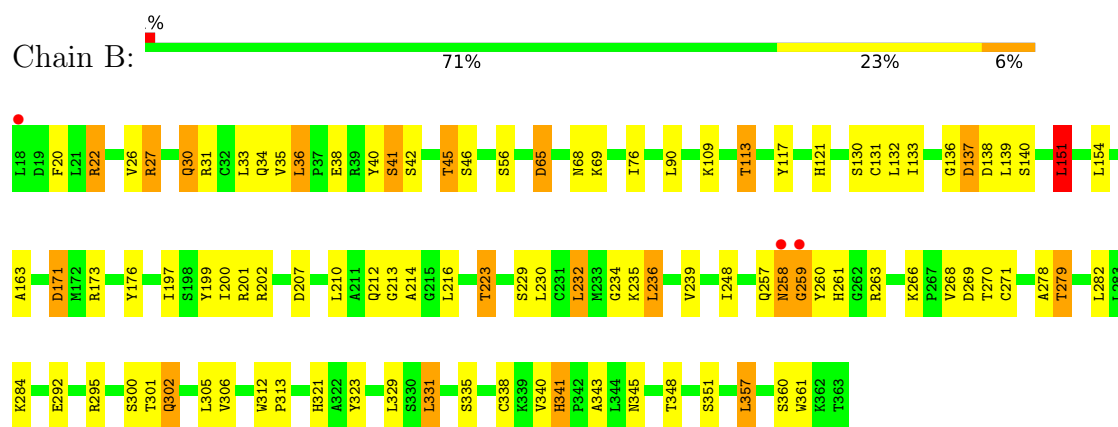
- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha



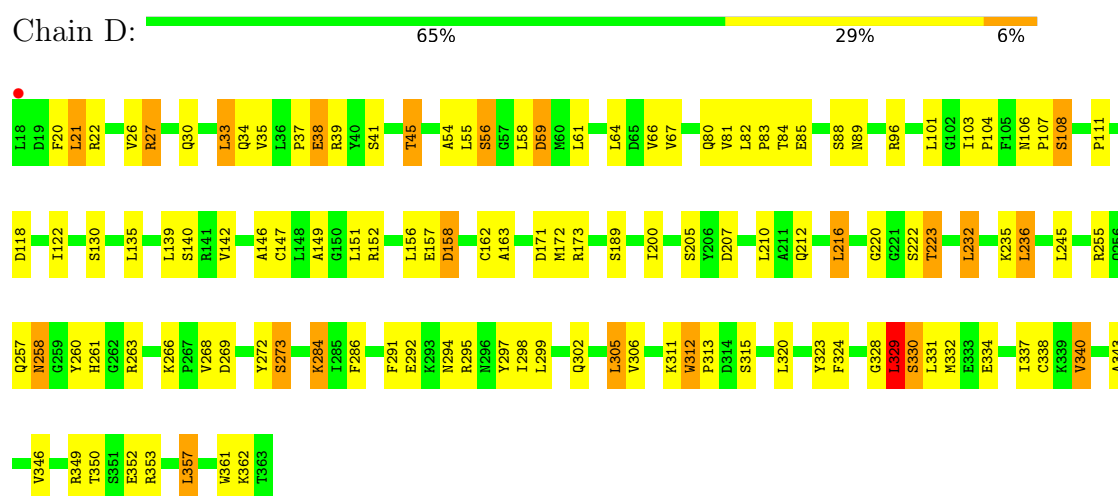
- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha



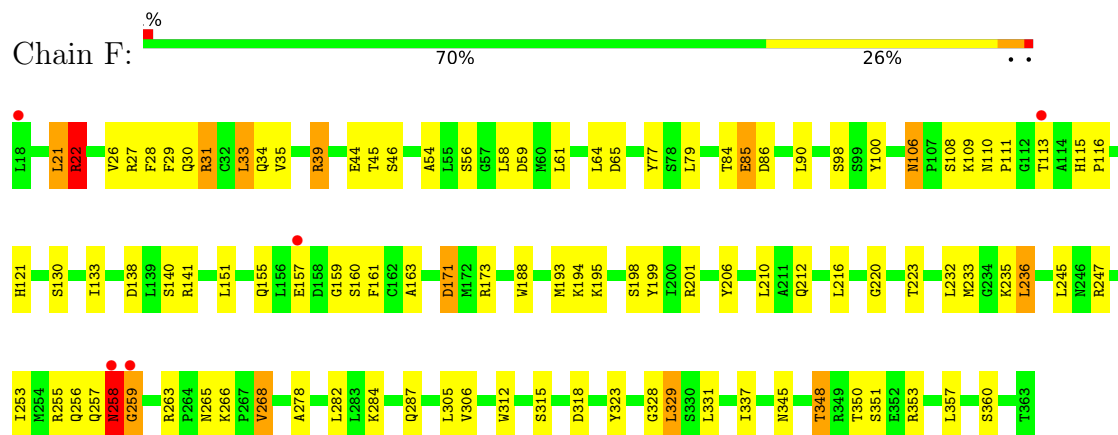
- Molecule 2: Geranylgeranyl transferase type-1 subunit beta



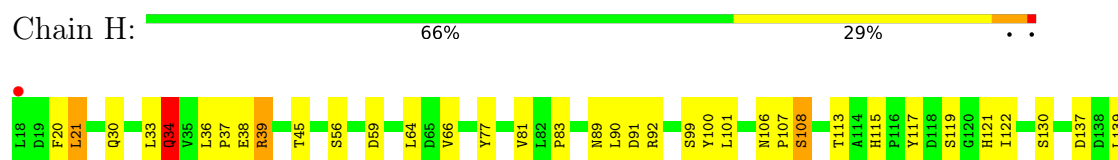
• Molecule 2: Geranylgeranyl transferase type-1 subunit beta



• Molecule 2: Geranylgeranyl transferase type-1 subunit beta



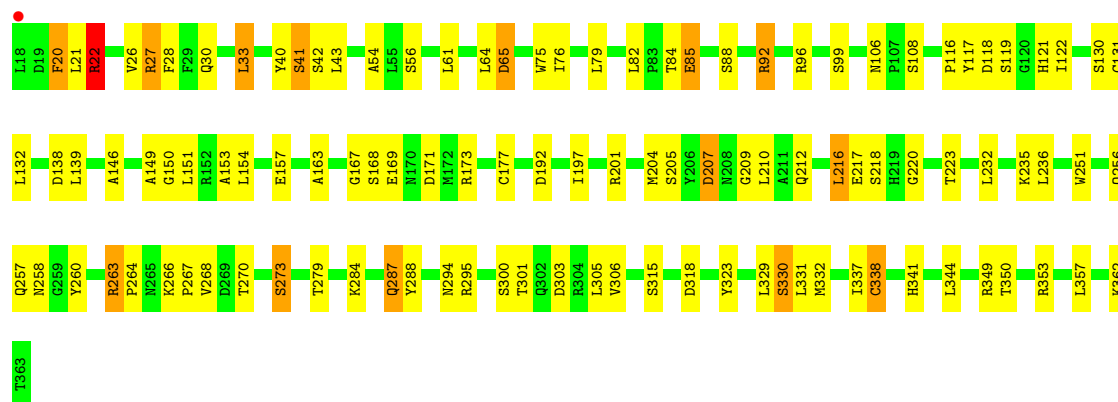
• Molecule 2: Geranylgeranyl transferase type-1 subunit beta





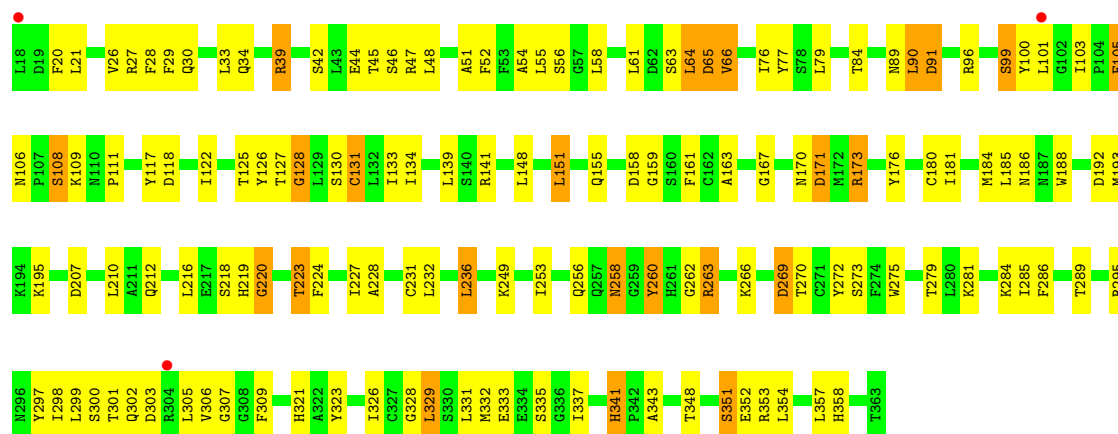
- Molecule 2: Geranylgeranyl transferase type-1 subunit beta

Chain J: 68% 27%



- Molecule 2: Geranylgeranyl transferase type-1 subunit beta

Chain L: 59% 34% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	270.89Å 269.26Å 185.25Å 90.00° 131.77° 90.00°	Depositor
Resolution (Å)	48.21 – 3.67 48.21 – 3.67	Depositor EDS
% Data completeness (in resolution range)	97.9 (48.21-3.67) 97.9 (48.21-3.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 3.67Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.137 , 0.189 0.147 , 0.190	Depositor DCC
R_{free} test set	2100 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	94.8	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 65.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.087 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32241	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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: DPO, A1HZ4, ZN, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.03	0/2695	1.59	16/3668 (0.4%)
1	C	1.03	0/2695	1.59	13/3668 (0.4%)
1	E	1.04	0/2698	1.60	7/3672 (0.2%)
1	G	1.04	0/2695	1.57	9/3668 (0.2%)
1	I	1.04	0/2695	1.58	10/3668 (0.3%)
1	K	1.03	0/2695	1.57	9/3668 (0.2%)
2	B	1.07	0/2759	1.63	20/3733 (0.5%)
2	D	1.09	2/2759 (0.1%)	1.60	14/3733 (0.4%)
2	F	1.09	0/2759	1.60	19/3733 (0.5%)
2	H	1.07	2/2759 (0.1%)	1.63	13/3733 (0.3%)
2	J	1.08	1/2759 (0.0%)	1.63	20/3733 (0.5%)
2	L	1.10	0/2759	1.60	15/3733 (0.4%)
All	All	1.06	5/32727 (0.0%)	1.60	165/44410 (0.4%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	273	SER	C-O	6.18	1.31	1.24
2	D	81	VAL	C-O	5.51	1.29	1.24
2	H	81	VAL	C-O	5.41	1.29	1.24
2	H	273	SER	C-O	5.20	1.30	1.24
2	J	273	SER	C-O	5.12	1.30	1.24

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	258	ASN	N-CA-C	-9.78	99.92	112.93
2	B	65	ASP	CA-CB-CG	8.16	120.76	112.60
2	J	258	ASN	N-CA-C	-7.98	102.07	112.68
1	K	68	ASP	CA-CB-CG	7.33	119.93	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	167	GLY	CA-C-O	-7.19	117.55	122.22
2	F	65	ASP	CA-CB-CG	7.05	119.65	112.60
2	L	167	GLY	CA-C-O	-7.03	117.65	122.22
2	J	207	ASP	CA-CB-CG	6.59	119.19	112.60
2	D	352	GLU	N-CA-C	-6.47	103.92	110.97
2	F	345	ASN	CA-C-N	6.42	129.30	122.11
2	F	345	ASN	C-N-CA	6.42	129.30	122.11
2	L	65	ASP	CA-CB-CG	6.41	119.01	112.60
2	J	65	ASP	CA-CB-CG	6.40	119.00	112.60
2	F	337	ILE	CA-C-O	-6.34	114.57	120.22
1	E	247	THR	CA-CB-OG1	6.28	119.02	109.60
1	C	95	LYS	CA-C-N	6.28	129.17	120.63
1	C	95	LYS	C-N-CA	6.28	129.17	120.63
2	F	220	GLY	O-C-N	6.20	128.21	122.19
2	B	207	ASP	CA-CB-CG	6.18	118.78	112.60
2	F	259	GLY	CA-C-N	-6.16	114.00	122.93
2	F	259	GLY	C-N-CA	-6.16	114.00	122.93
2	L	125	THR	CA-CB-OG1	6.11	118.76	109.60
2	L	236	LEU	CA-C-N	6.09	128.72	120.38
2	L	236	LEU	C-N-CA	6.09	128.72	120.38
2	H	328	GLY	O-C-N	6.08	128.90	122.28
2	D	220	GLY	CA-C-N	6.06	126.66	119.94
2	D	220	GLY	C-N-CA	6.06	126.66	119.94
2	H	279	THR	CA-CB-OG1	6.04	118.67	109.60
2	B	345	ASN	CA-C-N	6.04	128.88	122.11
2	B	345	ASN	C-N-CA	6.04	128.88	122.11
2	B	202	ARG	N-CA-C	-6.04	104.77	111.71
1	E	342	GLU	CB-CG-CD	6.02	122.84	112.60
2	J	220	GLY	CA-C-N	6.02	126.62	119.94
2	J	220	GLY	C-N-CA	6.02	126.62	119.94
1	A	255	VAL	N-CA-C	-6.01	104.64	110.72
2	J	92	ARG	CB-CA-C	6.00	119.46	109.38
1	G	130	ASN	CA-C-N	5.97	128.28	120.28
1	G	130	ASN	C-N-CA	5.97	128.28	120.28
1	A	339	GLU	N-CA-C	-5.96	104.12	111.33
2	B	236	LEU	N-CA-C	-5.86	104.80	111.07
2	J	205	SER	CA-C-N	5.86	128.40	120.38
2	J	205	SER	C-N-CA	5.86	128.40	120.38
1	A	336	LYS	CA-C-N	5.85	128.60	120.29
1	A	336	LYS	C-N-CA	5.85	128.60	120.29
2	D	260	TYR	CA-C-O	-5.82	114.58	121.16
1	C	150	GLU	N-CA-C	-5.80	104.86	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	328	GLY	CA-C-N	5.79	128.31	120.44
2	L	328	GLY	C-N-CA	5.79	128.31	120.44
1	I	95	LYS	O-C-N	5.76	128.22	122.12
2	J	177	CYS	N-CA-C	-5.71	104.96	111.07
1	I	157	ALA	CA-C-N	5.68	127.71	120.56
1	I	157	ALA	C-N-CA	5.68	127.71	120.56
1	E	157	ALA	CA-C-N	5.67	127.70	120.56
1	E	157	ALA	C-N-CA	5.67	127.70	120.56
2	F	258	ASN	N-CA-C	-5.66	104.58	112.45
2	B	279	THR	CA-CB-OG1	5.66	118.09	109.60
2	L	207	ASP	CA-CB-CG	5.66	118.26	112.60
1	A	355	TYR	N-CA-C	-5.66	105.03	111.14
2	L	269	ASP	CA-CB-CG	5.64	118.24	112.60
2	L	258	ASN	N-CA-C	-5.64	98.79	110.80
2	F	247	ARG	O-C-N	5.63	127.86	122.07
1	E	275	SER	CA-C-N	5.62	128.08	120.44
1	E	275	SER	C-N-CA	5.62	128.08	120.44
1	C	80	GLN	CA-C-O	-5.58	115.63	121.55
2	J	251	TRP	O-C-N	5.58	127.81	122.07
1	K	95	LYS	CA-C-N	5.57	129.90	120.88
1	K	95	LYS	C-N-CA	5.57	129.90	120.88
1	G	150	GLU	N-CA-C	-5.57	105.11	111.07
1	I	63	TYR	N-CA-CB	5.56	118.22	109.83
2	F	328	GLY	CA-C-N	5.55	128.18	120.29
2	F	328	GLY	C-N-CA	5.55	128.18	120.29
1	C	249	GLY	CA-C-O	-5.53	117.24	122.39
2	B	269	ASP	CB-CA-C	5.53	119.82	109.86
2	H	328	GLY	CA-C-N	5.53	127.96	120.44
2	H	328	GLY	C-N-CA	5.53	127.96	120.44
2	H	202	ARG	N-CA-C	-5.53	105.35	111.71
2	J	20	PHE	CA-C-O	-5.53	114.56	120.92
1	C	142	ARG	CA-C-O	-5.52	115.01	120.80
1	G	82	ASP	N-CA-C	-5.52	106.40	113.02
2	D	157	GLU	N-CA-C	-5.51	105.65	112.38
2	J	318	ASP	CA-CB-CG	5.51	118.11	112.60
1	C	182	PRO	N-CA-CB	-5.50	97.48	103.25
1	K	233	ASN	CA-C-O	-5.50	114.90	120.84
2	H	292	GLU	CB-CG-CD	5.48	121.91	112.60
2	H	236	LEU	CA-C-N	5.46	127.59	120.28
2	H	236	LEU	C-N-CA	5.46	127.59	120.28
1	K	218	ASN	CA-CB-CG	-5.46	107.14	112.60
1	K	267	ILE	N-CA-C	-5.46	105.80	111.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	142	ARG	CA-C-O	-5.44	115.17	120.89
2	F	201	ARG	O-C-N	5.44	127.67	122.07
2	B	113	THR	CB-CA-C	5.43	120.02	111.77
2	B	133	ILE	CA-C-N	5.43	127.60	120.60
2	B	133	ILE	C-N-CA	5.43	127.60	120.60
2	B	30	GLN	CB-CA-C	-5.42	101.74	110.74
1	A	336	LYS	O-C-N	5.39	127.83	122.12
1	C	101	ASP	CA-CB-CG	5.38	117.98	112.60
1	G	73	ALA	CA-C-N	5.38	127.93	120.29
1	G	73	ALA	C-N-CA	5.38	127.93	120.29
2	D	286	PHE	N-CA-C	-5.38	105.58	111.82
1	K	268	LYS	N-CA-C	-5.36	104.68	111.11
2	D	59	ASP	CA-CB-CG	5.34	117.94	112.60
2	J	201	ARG	O-C-N	5.32	127.62	122.09
2	L	220	GLY	O-C-N	5.32	127.30	122.19
2	L	236	LEU	O-C-N	5.31	127.56	122.03
1	A	150	GLU	N-CA-C	-5.31	105.49	111.28
1	A	247	THR	CA-CB-OG1	5.31	117.56	109.60
2	D	346	VAL	CA-C-O	-5.30	116.13	121.49
2	D	328	GLY	O-C-N	5.26	128.01	122.28
1	I	204	GLN	CA-C-N	5.24	127.61	120.54
1	I	204	GLN	C-N-CA	5.24	127.61	120.54
1	A	345	ALA	O-C-N	5.23	127.46	122.07
2	H	270	THR	CA-CB-OG1	-5.23	101.76	109.60
2	J	201	ARG	CA-C-N	5.22	127.80	120.28
2	J	201	ARG	C-N-CA	5.22	127.80	120.28
2	B	259	GLY	CA-C-N	-5.21	113.15	122.07
2	B	259	GLY	C-N-CA	-5.21	113.15	122.07
2	D	329	LEU	O-C-N	5.21	128.67	122.27
1	C	218	ASN	CA-CB-CG	-5.20	107.40	112.60
1	I	255	VAL	N-CA-C	-5.20	105.64	110.53
2	D	147	CYS	O-C-N	5.20	127.49	122.09
2	F	318	ASP	CA-CB-CG	5.19	117.79	112.60
2	J	330	SER	CA-C-N	5.19	127.75	120.28
2	J	330	SER	C-N-CA	5.19	127.75	120.28
2	D	216	LEU	CA-C-N	5.18	128.70	121.24
2	D	216	LEU	C-N-CA	5.18	128.70	121.24
1	A	68	ASP	CA-CB-CG	5.18	117.78	112.60
2	B	201	ARG	O-C-N	5.18	127.40	122.07
1	G	302	LEU	CA-C-N	5.17	127.41	120.58
1	G	302	LEU	C-N-CA	5.17	127.41	120.58
1	C	267	ILE	N-CA-C	-5.17	106.04	110.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	147	CYS	O-C-N	5.17	127.46	122.09
2	B	201	ARG	CA-C-N	5.16	127.72	120.28
2	B	201	ARG	C-N-CA	5.16	127.72	120.28
1	C	320	GLU	N-CA-C	-5.16	105.77	111.71
2	F	171	ASP	CA-C-N	5.16	127.45	120.38
2	F	171	ASP	C-N-CA	5.16	127.45	120.38
2	H	207	ASP	CA-CB-CG	5.14	117.74	112.60
2	F	157	GLU	N-CA-C	-5.13	104.95	111.11
2	L	328	GLY	O-C-N	5.13	127.87	122.28
2	L	352	GLU	CA-C-N	5.13	127.11	120.44
2	L	352	GLU	C-N-CA	5.13	127.11	120.44
1	C	229	GLU	CA-C-N	5.11	128.48	121.33
1	C	229	GLU	C-N-CA	5.11	128.48	121.33
2	B	257	GLN	N-CA-C	-5.09	107.13	113.55
2	B	151	LEU	O-C-N	5.08	127.31	122.03
1	I	96	PHE	CA-CB-CG	5.08	118.88	113.80
1	K	157	ALA	CA-C-N	5.07	126.95	120.56
1	K	157	ALA	C-N-CA	5.07	126.95	120.56
2	B	248	ILE	N-CA-C	-5.06	105.61	110.72
1	A	278	ASN	CA-C-N	5.06	127.32	120.44
1	A	278	ASN	C-N-CA	5.06	127.32	120.44
2	F	111	PRO	CA-C-N	5.05	124.89	120.10
2	F	111	PRO	C-N-CA	5.05	124.89	120.10
2	H	220	GLY	O-C-N	5.04	127.12	122.13
1	I	95	LYS	CA-C-N	5.04	131.02	121.81
1	I	95	LYS	C-N-CA	5.04	131.02	121.81
1	A	63	TYR	N-CA-CB	5.03	117.68	109.69
1	A	101	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	218	ASN	CA-CB-CG	-5.02	107.58	112.60
1	E	339	GLU	N-CA-C	-5.01	106.26	112.38
2	J	216	LEU	CA-C-N	5.01	127.97	120.95
2	J	216	LEU	C-N-CA	5.01	127.97	120.95
1	A	66	TYR	N-CA-C	-5.01	105.95	111.71
2	D	329	LEU	N-CA-C	-5.01	106.01	111.82
2	F	328	GLY	O-C-N	5.00	128.09	122.34

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	2629	0	2520	59	0
1	C	2629	0	2520	62	0
1	E	2632	0	2522	58	0
1	G	2629	0	2520	67	0
1	I	2629	0	2520	49	0
1	K	2629	0	2520	64	0
2	B	2697	0	2600	52	0
2	D	2697	0	2600	70	0
2	F	2697	0	2600	51	0
2	H	2697	0	2600	56	0
2	J	2697	0	2600	57	0
2	L	2697	0	2600	80	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	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
4	J	1	0	0	0	0
4	L	1	0	0	0	0
5	B	9	0	0	0	0
5	D	9	0	0	2	0
5	F	9	0	0	0	0
5	H	9	0	0	2	0
5	J	9	0	0	2	0
5	L	9	0	0	1	0
6	B	35	0	0	0	0
6	D	35	0	0	0	0
6	F	35	0	0	0	0
6	H	35	0	0	1	0
6	J	35	0	0	0	0
6	L	35	0	0	0	0
7	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	1	0	0	0	0
7	F	1	0	0	0	0
7	H	1	0	0	0	0
7	J	1	0	0	0	0
7	L	1	0	0	0	0
All	All	32241	0	30722	688	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 11.

All (688) 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)
6:H:404:A1HZ4:C40	6:H:404:A1HZ4:C2	2.31	1.08
2:F:258:ASN:OD1	2:F:268:VAL:HG21	1.72	0.90
2:B:259:GLY:O	2:B:268:VAL:CG1	2.21	0.89
1:I:296:LEU:HD22	1:I:322:MET:HE1	1.56	0.87
2:B:259:GLY:O	2:B:268:VAL:HG12	1.75	0.86
1:I:351:ILE:HD13	2:J:257:GLN:O	1.81	0.81
1:G:112:ARG:O	1:G:144:LEU:HD21	1.81	0.80
2:L:148:LEU:HD21	2:L:185:LEU:HD12	1.66	0.78
2:D:27:ARG:HA	2:D:30:GLN:HE21	1.49	0.78
1:C:59:ASP:HA	1:E:294:ASN:HD21	1.49	0.78
1:C:59:ASP:HA	1:E:294:ASN:ND2	2.00	0.77
2:H:284:LYS:HE3	2:H:284:LYS:HA	1.67	0.77
2:L:148:LEU:CD2	2:L:185:LEU:HD12	2.14	0.77
2:B:212:GLN:HE21	2:B:212:GLN:HA	1.53	0.74
2:D:266:LYS:HE2	5:D:403:DPO:O7	1.88	0.73
2:B:212:GLN:HA	2:B:212:GLN:NE2	2.04	0.73
1:E:214:ARG:HG2	1:E:214:ARG:HH11	1.52	0.73
2:L:212:GLN:HE21	2:L:212:GLN:HA	1.53	0.72
1:K:79:PRO:HA	1:K:101:ASP:OD1	1.90	0.71
1:I:280:LEU:HD23	1:I:314:PHE:CE2	2.25	0.71
2:B:27:ARG:NH1	2:D:292:GLU:OE1	2.23	0.71
2:D:212:GLN:HA	2:D:212:GLN:NE2	2.06	0.70
1:I:128:ALA:HB3	1:I:162:GLN:HE22	1.57	0.68
1:K:81:ASN:N	1:K:81:ASN:HD22	1.91	0.68
2:L:29:PHE:CD1	2:L:54:ALA:HA	2.28	0.68
2:B:259:GLY:O	2:B:268:VAL:HG11	1.91	0.68
1:E:351:ILE:HD11	2:F:256:GLN:HG2	1.76	0.67
1:K:112:ARG:O	1:K:144:LEU:HD21	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:ASP:HB3	1:E:255:VAL:HG23	1.77	0.66
1:E:149:GLN:HE22	1:E:184:GLN:HE22	1.43	0.65
1:G:96:PHE:CD2	1:G:126:LEU:HD22	2.31	0.65
2:F:22:ARG:O	2:F:26:VAL:HG23	1.95	0.65
2:B:171:ASP:OD1	2:B:173:ARG:HG3	1.96	0.65
1:C:232:ARG:NH2	1:C:272:HIS:O	2.30	0.65
1:I:79:PRO:HA	1:I:101:ASP:OD1	1.97	0.64
2:L:151:LEU:HD12	2:L:181:ILE:HG21	1.79	0.64
2:H:284:LYS:HA	2:H:284:LYS:CE	2.27	0.64
2:J:210:LEU:HB2	2:J:223:THR:HA	1.81	0.63
2:B:56:SER:HB3	2:B:323:TYR:CE1	2.33	0.63
1:K:182:PRO:O	1:K:184:GLN:N	2.32	0.63
1:A:311:LEU:C	1:A:311:LEU:HD23	2.24	0.62
2:D:330:SER:OG	2:D:340:VAL:HG12	1.99	0.62
1:A:107:LEU:HD22	2:B:117:TYR:CD2	2.34	0.62
1:C:182:PRO:HG3	1:C:213:PHE:CG	2.35	0.62
1:G:329:ASN:HB3	1:G:332:ASP:HB3	1.80	0.62
2:L:210:LEU:HB2	2:L:223:THR:HA	1.82	0.61
1:A:96:PHE:CE2	1:A:126:LEU:HB3	2.35	0.61
1:K:255:VAL:HG13	1:K:258:ARG:NH2	2.14	0.61
2:F:33:LEU:HD22	2:F:54:ALA:HB1	1.82	0.61
2:H:295:ARG:HB2	2:H:332:MET:HE1	1.82	0.61
1:G:331:GLU:O	1:G:335:ASN:ND2	2.32	0.61
1:K:322:MET:O	1:K:327:CYS:HB3	2.01	0.61
2:H:168:SER:OG	2:H:169:GLU:O	2.19	0.61
1:E:252:ASP:HB3	1:E:255:VAL:CG2	2.31	0.61
2:L:58:LEU:O	2:L:61:LEU:N	2.33	0.61
2:F:210:LEU:HB2	2:F:223:THR:HA	1.83	0.60
2:B:22:ARG:O	2:B:26:VAL:HG23	2.01	0.60
1:K:296:LEU:CD2	1:K:322:MET:HE1	2.32	0.60
1:C:331:GLU:O	1:C:335:ASN:ND2	2.34	0.60
2:J:22:ARG:O	2:J:26:VAL:HG23	2.01	0.60
1:E:148:LEU:HB2	1:E:179:LEU:HD21	1.84	0.60
1:G:132:THR:HG21	2:H:101:LEU:HD21	1.84	0.60
1:I:312:ILE:O	1:I:316:VAL:HG23	2.02	0.59
1:E:325:ASN:O	1:E:326:GLN:C	2.45	0.59
2:D:312:TRP:O	2:D:315:SER:HB3	2.03	0.59
1:E:244:ILE:HG21	1:E:250:TYR:CE1	2.38	0.59
1:C:89:GLN:HE21	2:D:35:VAL:HG22	1.67	0.58
2:F:258:ASN:OD1	2:F:268:VAL:CG2	2.49	0.58
1:I:107:LEU:HD22	2:J:117:TYR:CD2	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:210:LEU:HB2	2:H:223:THR:HA	1.86	0.58
2:J:171:ASP:OD1	2:J:173:ARG:HG3	2.04	0.58
2:L:212:GLN:HA	2:L:212:GLN:NE2	2.16	0.58
1:A:59:ASP:HA	1:K:294:ASN:ND2	2.18	0.58
2:B:210:LEU:HB2	2:B:223:THR:HA	1.85	0.58
2:D:122:ILE:HG22	2:D:163:ALA:HA	1.86	0.58
1:E:151:GLU:HG3	1:E:175:LEU:HD11	1.84	0.58
1:A:58:LEU:HD23	1:A:63:TYR:CE2	2.39	0.58
1:I:136:PHE:O	1:I:140:LEU:HG	2.03	0.58
1:E:357:ARG:O	1:E:361:ARG:HG3	2.04	0.57
2:H:59:ASP:OD1	2:H:349:ARG:NH1	2.36	0.57
1:C:263:THR:HG21	1:C:280:LEU:HB2	1.86	0.57
1:G:251:SER:HA	1:G:287:ARG:HH22	1.69	0.57
2:H:171:ASP:OD1	2:H:173:ARG:HB2	2.03	0.57
2:F:236:LEU:CD2	2:F:245:LEU:HD21	2.35	0.57
1:G:232:ARG:NH2	1:G:272:HIS:O	2.36	0.57
2:H:303:ASP:OD1	2:H:306:VAL:HG22	2.04	0.57
2:J:212:GLN:HA	2:J:212:GLN:NE2	2.19	0.57
1:K:312:ILE:HG23	1:K:340:LEU:HD22	1.87	0.57
1:E:159:ILE:HG12	1:E:168:VAL:HG23	1.86	0.57
1:A:173:ARG:HD2	1:A:208:TRP:CD2	2.40	0.56
2:B:68:ASN:O	2:B:69:LYS:C	2.48	0.56
2:D:80:GLN:HE22	2:D:142:VAL:HA	1.69	0.56
2:L:89:ASN:O	2:L:91:ASP:N	2.38	0.56
2:L:273:SER:HB3	2:L:298:ILE:HD11	1.87	0.56
1:A:101:ASP:OD1	1:A:104:ARG:NH1	2.38	0.56
2:L:27:ARG:HA	2:L:30:GLN:HE21	1.70	0.56
2:J:116:PRO:HB2	2:J:117:TYR:CD2	2.40	0.56
2:J:257:GLN:NE2	2:J:257:GLN:HA	2.20	0.56
1:G:130:ASN:HA	2:H:45:THR:HG21	1.87	0.56
2:D:21:LEU:N	2:D:21:LEU:CD1	2.68	0.56
2:D:96:ARG:HD3	2:D:101:LEU:HD12	1.87	0.56
2:F:212:GLN:NE2	2:F:212:GLN:HA	2.20	0.56
1:A:352:ARG:O	1:A:353:LYS:C	2.49	0.56
1:C:251:SER:HA	1:C:287:ARG:NH2	2.21	0.56
2:D:171:ASP:OD1	2:D:173:ARG:HG3	2.06	0.56
1:G:312:ILE:HG23	1:G:340:LEU:HD22	1.88	0.55
1:A:93:SER:HB3	2:B:38:GLU:OE2	2.05	0.55
1:E:189:ILE:HD11	1:E:205:HIS:CD2	2.41	0.55
2:B:76:ILE:HG21	2:B:132:LEU:HG	1.89	0.55
2:D:298:ILE:HG21	2:D:329:LEU:HD13	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:308:SER:HB2	1:G:309:PRO:HD2	1.88	0.55
2:H:77:TYR:HE2	2:H:137:ASP:OD2	1.88	0.55
2:L:48:LEU:O	2:L:51:ALA:HB3	2.06	0.55
1:C:78:VAL:O	1:C:104:ARG:HD2	2.06	0.54
2:L:171:ASP:OD1	2:L:173:ARG:HG3	2.07	0.54
1:A:189:ILE:HG21	1:A:206:ARG:HB2	1.89	0.54
1:A:103:PHE:HA	1:A:119:LEU:HD21	1.88	0.54
2:F:56:SER:HB3	2:F:323:TYR:CE1	2.43	0.54
2:F:77:TYR:CE1	2:F:141:ARG:HB2	2.42	0.54
2:F:195:LYS:HA	2:F:198:SER:HB3	1.90	0.54
1:K:351:ILE:HD11	2:L:256:GLN:HG2	1.88	0.54
1:I:331:GLU:O	1:I:335:ASN:ND2	2.40	0.54
2:D:82:LEU:HD11	2:D:108:SER:HA	1.88	0.54
2:H:77:TYR:CZ	2:H:141:ARG:HB2	2.42	0.54
1:K:350:THR:O	1:K:353:LYS:N	2.40	0.54
2:D:106:ASN:O	2:D:108:SER:N	2.41	0.54
1:K:130:ASN:HA	2:L:45:THR:HG21	1.88	0.54
2:H:360:SER:OG	2:H:361:TRP:N	2.39	0.54
1:E:311:LEU:C	1:E:311:LEU:HD23	2.33	0.54
1:G:110:ASP:OD1	1:G:112:ARG:NE	2.27	0.54
2:H:20:PHE:CZ	2:H:337:ILE:HD11	2.43	0.54
2:H:212:GLN:HA	2:H:212:GLN:NE2	2.22	0.54
1:G:97:ARG:HG2	1:G:101:ASP:OD2	2.07	0.53
2:D:56:SER:HB3	2:D:323:TYR:CE1	2.42	0.53
2:D:103:ILE:HD11	2:D:118:ASP:HB2	1.89	0.53
1:K:240:ARG:CZ	1:K:262:TYR:CE2	2.90	0.53
2:D:21:LEU:N	2:D:21:LEU:HD13	2.24	0.53
1:C:351:ILE:CD1	2:D:257:GLN:O	2.57	0.53
2:F:212:GLN:HA	2:F:212:GLN:HE21	1.74	0.53
1:E:91:ILE:O	1:E:91:ILE:HD12	2.07	0.53
2:B:223:THR:HG22	2:B:279:THR:HG21	1.89	0.53
1:E:87:VAL:CG1	2:F:33:LEU:HD12	2.39	0.53
2:J:84:THR:O	2:J:85:GLU:C	2.51	0.53
2:L:127:THR:O	2:L:131:CYS:HB2	2.08	0.53
1:A:223:VAL:HG11	1:A:240:ARG:HB2	1.90	0.53
2:D:172:MET:HE1	2:D:200:ILE:HA	1.91	0.53
2:F:236:LEU:HD22	2:F:245:LEU:HD21	1.90	0.53
2:H:56:SER:HB3	2:H:323:TYR:CE1	2.44	0.53
1:C:171:HIS:O	1:C:175:LEU:HG	2.09	0.53
2:D:27:ARG:HA	2:D:30:GLN:NE2	2.21	0.53
2:B:121:HIS:HA	2:B:163:ALA:O	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:197:ILE:HD11	2:B:235:LYS:HD3	1.89	0.53
1:E:352:ARG:O	1:E:353:LYS:C	2.52	0.53
1:G:148:LEU:HB2	1:G:179:LEU:HD21	1.91	0.53
2:H:269:ASP:HB3	2:H:272:TYR:HD2	1.74	0.53
2:L:219:HIS:CD2	2:L:263:ARG:HD3	2.44	0.53
1:G:127:ASN:OD1	1:G:129:ALA:HB3	2.09	0.52
2:H:188:TRP:CE3	2:H:193:MET:HE2	2.44	0.52
2:J:209:GLY:HA3	2:J:218:SER:HB2	1.92	0.52
2:D:210:LEU:HB2	2:D:223:THR:HA	1.91	0.52
2:D:268:VAL:HG23	2:D:297:TYR:CZ	2.45	0.52
1:E:265:GLU:HA	1:E:265:GLU:OE1	2.08	0.52
1:C:336:LYS:O	1:C:340:LEU:HG	2.10	0.52
1:G:350:THR:O	1:G:353:LYS:HB2	2.10	0.52
1:I:78:VAL:O	1:I:104:ARG:HD2	2.09	0.52
2:B:22:ARG:HB3	2:B:22:ARG:HH11	1.75	0.52
1:C:58:LEU:HD23	1:C:63:TYR:CE2	2.45	0.52
1:G:329:ASN:HB3	1:G:332:ASP:CB	2.40	0.52
2:J:121:HIS:HA	2:J:163:ALA:O	2.09	0.52
1:A:148:LEU:HB2	1:A:179:LEU:HD21	1.92	0.52
2:B:270:THR:OG1	2:B:301:THR:HG21	2.10	0.52
1:E:340:LEU:O	1:E:343:ILE:N	2.43	0.52
2:H:339:LYS:O	2:H:348:THR:OG1	2.26	0.52
1:I:112:ARG:O	1:I:144:LEU:HD21	2.09	0.52
1:E:165:ASN:OD1	1:E:167:GLN:HB2	2.11	0.51
1:I:159:ILE:HG12	1:I:168:VAL:HG23	1.92	0.51
2:B:136:GLY:O	2:B:137:ASP:O	2.28	0.51
2:H:223:THR:HG22	2:H:279:THR:HG21	1.93	0.51
1:K:87:VAL:O	2:L:47:ARG:NH2	2.42	0.51
1:A:189:ILE:HD11	1:A:205:HIS:CD2	2.46	0.51
1:I:128:ALA:HB3	1:I:162:GLN:NE2	2.23	0.51
2:J:287:GLN:HG2	2:J:288:TYR:N	2.24	0.51
1:K:97:ARG:HG2	1:K:101:ASP:OD2	2.10	0.51
2:D:212:GLN:HA	2:D:212:GLN:HE21	1.75	0.51
1:A:149:GLN:NE2	1:A:184:GLN:OE1	2.44	0.51
1:C:230:ASP:OD1	1:C:232:ARG:HB2	2.11	0.51
2:F:29:PHE:O	2:F:33:LEU:HD22	2.10	0.51
2:L:64:LEU:HD11	2:L:134:ILE:HG22	1.93	0.51
1:K:148:LEU:HB2	1:K:179:LEU:HD21	1.92	0.51
1:A:121:ARG:NH1	1:A:121:ARG:HG3	2.25	0.51
1:A:251:SER:HA	1:A:287:ARG:NH2	2.25	0.51
1:C:222:TYR:CE2	1:C:226:LEU:CD1	2.94	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:39:ARG:HB2	2:D:39:ARG:HH11	1.75	0.51
1:E:250:TYR:HE1	1:E:259:GLU:HG3	1.76	0.51
2:F:259:GLY:H	2:F:268:VAL:HG11	1.75	0.51
1:G:267:ILE:O	1:G:268:LYS:C	2.54	0.50
2:H:122:ILE:HG22	2:H:163:ALA:HA	1.93	0.50
2:F:278:ALA:O	2:F:282:LEU:HG	2.11	0.50
2:H:21:LEU:CD1	2:H:21:LEU:N	2.75	0.50
1:I:351:ILE:CD1	2:J:257:GLN:O	2.54	0.50
2:D:357:LEU:HD22	2:D:361:TRP:CZ2	2.46	0.50
1:I:289:LEU:N	1:I:321:ASP:OD2	2.44	0.50
2:J:303:ASP:CG	2:J:306:VAL:HG22	2.37	0.50
2:F:312:TRP:O	2:F:315:SER:HB3	2.12	0.50
1:G:74:ASP:OD1	1:G:74:ASP:N	2.43	0.50
1:K:78:VAL:HG23	1:K:105:ALA:HA	1.94	0.50
2:L:299:LEU:O	2:L:302:GLN:HB2	2.11	0.50
2:B:138:ASP:OD1	2:B:140:SER:HB3	2.11	0.50
1:C:87:VAL:HG12	1:C:88:VAL:HG23	1.94	0.50
2:D:20:PHE:CZ	2:D:337:ILE:HD11	2.46	0.50
2:H:92:ARG:HB3	2:H:119:SER:HB3	1.93	0.50
2:L:219:HIS:HD2	2:L:263:ARG:HD3	1.77	0.50
1:C:279:TYR:CE1	1:C:283:ILE:HD13	2.46	0.50
1:E:351:ILE:O	1:E:351:ILE:HG13	2.10	0.50
2:F:138:ASP:OD1	2:F:140:SER:HB3	2.12	0.50
1:I:78:VAL:HG23	1:I:105:ALA:HB2	1.93	0.50
2:L:28:PHE:CD1	2:L:28:PHE:C	2.90	0.50
2:B:200:ILE:HG21	2:B:230:LEU:HD11	1.94	0.50
1:G:248:THR:HB	1:G:255:VAL:HG21	1.94	0.49
2:H:92:ARG:HB3	2:H:119:SER:CB	2.42	0.49
2:J:168:SER:OG	2:J:169:GLU:O	2.27	0.49
1:A:251:SER:HA	1:A:287:ARG:HH22	1.77	0.49
2:D:156:LEU:HD21	2:D:162:CYS:SG	2.52	0.49
2:L:133:ILE:HG13	2:L:139:LEU:HD11	1.93	0.49
2:F:133:ILE:HG22	2:F:350:THR:CG2	2.42	0.49
1:G:252:ASP:HB3	1:G:255:VAL:HG23	1.94	0.49
1:E:214:ARG:HG2	1:E:214:ARG:NH1	2.25	0.49
2:J:197:ILE:HD11	2:J:235:LYS:HD3	1.93	0.49
2:D:55:LEU:HD22	2:D:135:LEU:HD21	1.95	0.49
1:G:329:ASN:CB	1:G:332:ASP:HB3	2.42	0.49
1:I:219:GLU:HB3	1:I:243:VAL:HG21	1.94	0.49
2:J:41:SER:OG	2:J:42:SER:N	2.45	0.49
2:J:76:ILE:HG21	2:J:132:LEU:HG	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:334:LEU:O	1:K:337:ALA:HB3	2.13	0.49
2:L:354:LEU:HG	2:L:358:HIS:CE1	2.48	0.49
2:L:44:GLU:C	2:L:46:SER:H	2.21	0.49
2:L:186:ASN:HB2	2:L:358:HIS:CD2	2.47	0.49
2:L:269:ASP:HB3	2:L:272:TYR:HD2	1.77	0.49
2:D:268:VAL:O	2:D:312:TRP:HD1	1.96	0.49
1:G:295:LEU:O	1:G:296:LEU:C	2.55	0.49
1:K:138:ARG:HA	1:K:141:LEU:HD12	1.95	0.49
2:L:170:ASN:O	2:L:171:ASP:HB3	2.13	0.49
1:A:172:ARG:NE	1:A:185:GLU:OE2	2.44	0.48
2:D:106:ASN:O	2:D:106:ASN:ND2	2.46	0.48
2:D:255:ARG:HD3	2:D:261:HIS:NE2	2.28	0.48
2:D:266:LYS:CE	5:D:403:DPO:O7	2.59	0.48
2:J:33:LEU:HD22	2:J:54:ALA:HB1	1.95	0.48
2:J:266:LYS:CE	5:J:403:DPO:O2	2.62	0.48
1:A:311:LEU:HD23	1:A:311:LEU:O	2.14	0.48
2:B:357:LEU:HD22	2:B:361:TRP:CZ2	2.48	0.48
1:E:127:ASN:OD1	1:E:129:ALA:HB3	2.13	0.48
1:G:233:ASN:OD1	1:G:235:SER:HB2	2.13	0.48
1:I:351:ILE:HD11	2:J:256:GLN:HG2	1.94	0.48
2:L:295:ARG:HB2	2:L:332:MET:HE1	1.95	0.48
2:D:156:LEU:C	2:D:158:ASP:H	2.21	0.48
1:I:240:ARG:HD3	1:I:279:TYR:CZ	2.48	0.48
2:J:138:ASP:O	2:J:139:LEU:HB2	2.13	0.48
2:L:309:PHE:HB2	2:L:321:HIS:O	2.13	0.48
2:B:271:CYS:HB3	2:B:321:HIS:CD2	2.49	0.48
1:C:355:TYR:CE1	1:C:359:ILE:HD11	2.48	0.48
1:G:252:ASP:C	1:G:254:ALA:H	2.21	0.48
2:L:155:GLN:HB2	2:L:161:PHE:CE2	2.48	0.48
1:I:82:ASP:HB2	1:I:86:PRO:HB3	1.96	0.48
1:I:148:LEU:HB2	1:I:179:LEU:HD21	1.96	0.48
1:E:189:ILE:HD11	1:E:205:HIS:HD2	1.78	0.48
1:G:107:LEU:O	1:G:108:GLN:C	2.56	0.48
2:H:266:LYS:HE2	5:H:403:DPO:O1	2.14	0.48
1:E:150:GLU:HA	1:E:153:ASN:HD22	1.77	0.48
1:E:216:TRP:O	1:E:217:ASP:C	2.57	0.48
1:G:107:LEU:HD22	2:H:117:TYR:CD2	2.49	0.48
1:G:173:ARG:HD2	1:G:208:TRP:CD2	2.49	0.48
1:K:159:ILE:HG12	1:K:168:VAL:HG23	1.95	0.48
2:F:84:THR:O	2:F:85:GLU:C	2.57	0.47
1:I:194:ASN:HD22	1:I:194:ASN:HA	1.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:136:PHE:O	1:G:140:LEU:HG	2.14	0.47
1:G:355:TYR:O	1:G:358:TYR:HB3	2.14	0.47
2:J:223:THR:HG22	2:J:279:THR:HG21	1.94	0.47
1:K:327:CYS:SG	1:K:328:ASP:N	2.87	0.47
2:F:106:ASN:O	2:F:108:SER:N	2.47	0.47
1:I:244:ILE:HG21	1:I:250:TYR:CZ	2.49	0.47
1:A:300:LEU:O	1:A:303:GLN:HB2	2.15	0.47
1:C:148:LEU:HB2	1:C:179:LEU:HD21	1.96	0.47
1:I:151:GLU:C	1:I:153:ASN:H	2.23	0.47
2:B:341:HIS:ND1	2:B:341:HIS:C	2.73	0.47
2:L:77:TYR:CZ	2:L:141:ARG:HB2	2.50	0.47
2:L:341:HIS:C	2:L:341:HIS:HD1	2.22	0.47
1:A:127:ASN:OD1	2:B:42:SER:HA	2.15	0.47
2:B:171:ASP:OD2	2:B:173:ARG:NH2	2.48	0.47
1:C:222:TYR:CZ	1:C:226:LEU:HD11	2.49	0.47
1:C:240:ARG:HD3	1:C:279:TYR:CZ	2.50	0.47
1:C:244:ILE:HG22	1:C:250:TYR:CE1	2.50	0.47
2:D:273:SER:HB3	2:D:294:ASN:OD1	2.14	0.47
1:G:252:ASP:HB3	1:G:255:VAL:CG2	2.45	0.47
2:J:122:ILE:HB	2:J:154:LEU:HD13	1.97	0.47
1:K:212:GLU:O	1:K:212:GLU:HG3	2.14	0.47
1:K:273:ASN:O	1:K:274:GLU:C	2.57	0.47
2:L:63:SER:O	2:L:66:VAL:HG22	2.15	0.47
2:L:158:ASP:C	2:L:158:ASP:OD1	2.58	0.47
2:H:291:PHE:HE2	2:H:332:MET:HA	1.80	0.47
2:L:224:PHE:CD1	2:L:224:PHE:C	2.93	0.47
1:C:103:PHE:CZ	1:C:133:VAL:HG22	2.49	0.47
1:A:148:LEU:HD11	1:A:178:TRP:HE3	1.81	0.46
1:A:151:GLU:CG	1:A:175:LEU:HD11	2.45	0.46
1:K:251:SER:HA	1:K:287:ARG:HH22	1.79	0.46
1:A:107:LEU:O	1:A:108:GLN:C	2.58	0.46
2:B:40:TYR:O	2:B:41:SER:C	2.58	0.46
1:C:79:PRO:HA	1:C:101:ASP:OD1	2.15	0.46
1:C:159:ILE:HG12	1:C:168:VAL:HG23	1.95	0.46
1:E:149:GLN:HE22	1:E:184:GLN:NE2	2.11	0.46
2:F:44:GLU:C	2:F:46:SER:H	2.23	0.46
1:I:71:GLU:H	1:I:71:GLU:CD	2.23	0.46
2:L:184:MET:C	2:L:186:ASN:H	2.23	0.46
1:C:251:SER:HA	1:C:287:ARG:HH22	1.81	0.46
1:G:240:ARG:HD3	1:G:279:TYR:CZ	2.50	0.46
1:G:336:LYS:O	1:G:340:LEU:HG	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:269:ASP:HB3	2:H:272:TYR:CD2	2.49	0.46
2:L:286:PHE:O	2:L:289:THR:HG23	2.15	0.46
1:A:130:ASN:HA	2:B:45:THR:HG21	1.97	0.46
2:D:236:LEU:HD22	2:D:245:LEU:HD21	1.97	0.46
2:F:86:ASP:C	2:F:86:ASP:OD1	2.58	0.46
1:G:223:VAL:HG11	1:G:240:ARG:HB2	1.98	0.46
2:D:84:THR:O	2:D:85:GLU:C	2.59	0.46
2:H:286:PHE:O	2:H:289:THR:HG23	2.16	0.46
2:J:266:LYS:HD2	2:J:267:PRO:HD2	1.96	0.46
2:L:269:ASP:HB3	2:L:272:TYR:CD2	2.51	0.46
1:C:62:THR:HA	1:E:292:TYR:HD2	1.79	0.46
2:D:320:LEU:HG	2:D:324:PHE:HD2	1.81	0.46
2:F:79:LEU:HD22	2:F:98:SER:HA	1.96	0.46
1:I:200:TYR:HE1	2:J:217:GLU:HB3	1.80	0.46
2:L:159:GLY:HA3	2:L:195:LYS:O	2.15	0.46
1:I:110:ASP:OD1	1:I:112:ARG:NE	2.44	0.46
2:J:76:ILE:O	2:J:79:LEU:HB2	2.16	0.46
1:K:263:THR:HG21	1:K:280:LEU:HB2	1.98	0.46
2:L:20:PHE:CE2	2:L:337:ILE:HD11	2.51	0.46
1:A:206:ARG:HE	1:A:219:GLU:CD	2.24	0.46
1:C:312:ILE:O	1:C:316:VAL:HG23	2.16	0.46
1:I:255:VAL:HG13	1:I:258:ARG:NH2	2.31	0.46
2:J:56:SER:HB3	2:J:323:TYR:CE1	2.50	0.46
2:L:89:ASN:O	2:L:90:LEU:C	2.59	0.46
1:A:311:LEU:C	1:A:311:LEU:CD2	2.89	0.46
2:D:88:SER:OG	2:D:89:ASN:N	2.49	0.46
1:E:344:LEU:HD13	1:E:356:TRP:CD2	2.50	0.46
2:F:29:PHE:CD1	2:F:54:ALA:HA	2.51	0.46
2:F:39:ARG:HH11	2:F:39:ARG:HB3	1.80	0.46
1:G:96:PHE:CE2	1:G:126:LEU:HB3	2.51	0.46
1:G:219:GLU:HA	1:G:219:GLU:OE1	2.16	0.46
2:J:150:GLY:O	2:J:153:ALA:HB3	2.15	0.46
1:K:136:PHE:CZ	1:K:140:LEU:HD21	2.51	0.46
1:K:172:ARG:HG3	1:K:172:ARG:HH11	1.81	0.46
1:K:189:ILE:HD11	1:K:205:HIS:CD2	2.50	0.46
1:A:239:GLN:HA	1:A:239:GLN:OE1	2.16	0.45
2:B:278:ALA:O	2:B:282:LEU:HG	2.16	0.45
2:D:22:ARG:O	2:D:26:VAL:HG23	2.16	0.45
2:F:155:GLN:HB2	2:F:161:PHE:CE2	2.51	0.45
2:H:290:ASN:OD1	2:H:293:LYS:HB2	2.16	0.45
1:K:313:ALA:O	1:K:316:VAL:HB	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:55:LEU:HD12	2:L:131:CYS:SG	2.55	0.45
2:L:65:ASP:OD1	2:L:66:VAL:HG13	2.16	0.45
1:A:238:ASN:O	1:A:239:GLN:C	2.60	0.45
1:A:302:LEU:HB3	1:A:306:HIS:HB2	1.98	0.45
1:C:81:ASN:HD21	2:D:104:PRO:HA	1.81	0.45
1:C:107:LEU:O	1:C:108:GLN:C	2.58	0.45
2:L:298:ILE:HG21	2:L:329:LEU:HD13	1.98	0.45
2:B:138:ASP:OD1	2:B:140:SER:CB	2.65	0.45
2:J:20:PHE:C	2:J:21:LEU:HD12	2.41	0.45
1:A:344:LEU:HD13	1:A:356:TRP:CD2	2.52	0.45
1:C:311:LEU:CD2	1:C:315:LEU:HD11	2.46	0.45
1:I:77:PRO:HB2	1:I:101:ASP:HB3	1.98	0.45
1:G:256:LEU:O	1:G:257:GLU:C	2.59	0.45
1:G:303:GLN:O	1:G:307:SER:HB2	2.16	0.45
1:A:252:ASP:HB3	1:A:255:VAL:HG23	1.98	0.45
1:G:149:GLN:NE2	1:G:184:GLN:OE1	2.49	0.45
2:H:121:HIS:NE2	2:H:163:ALA:HB1	2.31	0.45
2:H:283:LEU:O	2:H:284:LYS:HB2	2.17	0.45
2:H:341:HIS:ND1	2:H:341:HIS:C	2.75	0.45
2:L:348:THR:HA	2:L:351:SER:OG	2.15	0.45
1:C:182:PRO:HG3	1:C:213:PHE:CD2	2.52	0.45
2:D:334:GLU:HG2	2:D:337:ILE:HD12	1.98	0.45
1:E:238:ASN:HA	2:F:206:TYR:HE2	1.81	0.45
1:G:352:ARG:O	1:G:353:LYS:C	2.59	0.45
1:I:274:GLU:OE1	2:J:264:PRO:HB3	2.17	0.45
2:L:260:TYR:CD1	2:L:260:TYR:N	2.85	0.45
2:B:136:GLY:O	2:B:137:ASP:C	2.60	0.45
1:C:120:THR:OG1	1:C:137:ARG:NH1	2.50	0.45
1:E:182:PRO:HD3	1:E:213:PHE:CE1	2.52	0.45
2:F:33:LEU:CD2	2:F:54:ALA:HB1	2.46	0.45
1:E:311:LEU:HD23	1:E:311:LEU:O	2.16	0.45
1:I:216:TRP:O	1:I:217:ASP:C	2.59	0.45
2:J:22:ARG:NH2	2:J:61:LEU:O	2.50	0.45
1:K:136:PHE:O	1:K:140:LEU:HG	2.17	0.45
2:L:122:ILE:HG22	2:L:163:ALA:HA	1.98	0.45
2:B:295:ARG:NH1	2:B:295:ARG:HG2	2.31	0.45
1:G:134:TRP:CH2	1:G:155:ILE:CD1	2.99	0.45
1:K:107:LEU:HD22	2:L:117:TYR:CD2	2.51	0.45
1:A:151:GLU:C	1:A:153:ASN:H	2.23	0.44
2:B:35:VAL:CG1	2:B:36:LEU:N	2.80	0.44
2:D:146:ALA:O	2:D:149:ALA:HB3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:156:LEU:C	2:D:158:ASP:N	2.75	0.44
2:D:269:ASP:HB3	2:D:272:TYR:HD2	1.82	0.44
1:E:107:LEU:O	1:E:110:ASP:N	2.50	0.44
1:E:232:ARG:HD3	2:F:265:ASN:OD1	2.17	0.44
1:G:334:LEU:CD1	1:G:338:LEU:HD11	2.48	0.44
2:J:40:TYR:HB3	2:J:43:LEU:HD12	1.98	0.44
2:L:303:ASP:HB3	2:L:307:GLY:O	2.17	0.44
1:C:255:VAL:HG13	1:C:258:ARG:HH12	1.82	0.44
1:C:355:TYR:O	1:C:358:TYR:HB3	2.16	0.44
1:E:112:ARG:O	1:E:144:LEU:HD21	2.18	0.44
1:K:88:VAL:O	2:L:47:ARG:NE	2.44	0.44
2:B:230:LEU:O	2:B:234:GLY:N	2.48	0.44
1:C:66:TYR:CE2	1:C:119:LEU:HD13	2.51	0.44
2:D:295:ARG:HB2	2:D:332:MET:HE1	2.00	0.44
2:D:305:LEU:HD22	2:D:305:LEU:HA	1.88	0.44
1:G:313:ALA:O	1:G:314:PHE:C	2.61	0.44
2:H:201:ARG:HD2	2:H:239:VAL:O	2.17	0.44
1:I:350:THR:O	1:I:353:LYS:HB2	2.16	0.44
1:C:136:PHE:CE2	1:C:140:LEU:HD11	2.52	0.44
1:I:296:LEU:CD2	1:I:322:MET:HE1	2.35	0.44
1:K:182:PRO:O	1:K:183:SER:C	2.60	0.44
2:D:205:SER:HB3	2:D:207:ASP:OD1	2.18	0.44
1:E:107:LEU:O	1:E:109:ARG:N	2.50	0.44
2:F:115:HIS:ND1	2:F:116:PRO:HD2	2.32	0.44
2:H:271:CYS:HB3	2:H:321:HIS:CD2	2.53	0.44
2:J:106:ASN:O	2:J:108:SER:N	2.50	0.44
2:L:232:LEU:HD13	2:L:343:ALA:HB1	1.99	0.44
2:D:39:ARG:HB2	2:D:39:ARG:NH1	2.32	0.44
2:J:256:GLN:HB2	2:J:260:TYR:CE2	2.53	0.44
2:L:249:LYS:HD3	2:L:285:ILE:HG21	1.98	0.44
2:L:263:ARG:HG3	2:L:266:LYS:HG3	2.00	0.44
1:E:101:ASP:OD1	1:E:104:ARG:NH1	2.50	0.44
2:F:171:ASP:OD1	2:F:173:ARG:HB2	2.18	0.44
2:H:64:LEU:HD23	2:H:64:LEU:HA	1.77	0.44
1:C:223:VAL:HG11	1:C:240:ARG:HB2	1.99	0.44
1:G:262:TYR:OH	1:G:266:MET:HE3	2.18	0.44
1:K:220:LEU:HB2	1:K:243:VAL:HG11	2.00	0.44
1:A:230:ASP:OD1	1:A:230:ASP:C	2.61	0.44
1:G:144:LEU:N	1:G:144:LEU:HD23	2.33	0.44
2:L:56:SER:HB3	2:L:323:TYR:CE1	2.52	0.44
2:B:295:ARG:HG2	2:B:295:ARG:HH11	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:273:SER:HB3	2:D:298:ILE:HD11	1.99	0.43
2:F:188:TRP:CE3	2:F:193:MET:HE2	2.53	0.43
2:H:107:PRO:O	2:H:108:SER:C	2.61	0.43
2:L:52:PHE:CD1	2:L:52:PHE:C	2.96	0.43
2:B:199:TYR:OH	2:B:213:GLY:HA3	2.18	0.43
1:C:216:TRP:O	1:C:217:ASP:C	2.61	0.43
2:L:188:TRP:CE3	2:L:193:MET:HE2	2.53	0.43
2:L:297:TYR:O	2:L:300:SER:N	2.50	0.43
1:A:121:ARG:HH11	1:A:121:ARG:CG	2.30	0.43
1:C:92:TYR:HA	2:D:38:GLU:HG3	2.00	0.43
2:D:83:PRO:HA	2:D:89:ASN:OD1	2.17	0.43
2:D:212:GLN:NE2	2:D:222:SER:OG	2.51	0.43
1:E:216:TRP:O	1:E:218:ASN:N	2.51	0.43
2:F:121:HIS:CE1	2:F:163:ALA:HB1	2.53	0.43
2:H:219:HIS:NE2	5:H:403:DPO:O2	2.51	0.43
1:K:223:VAL:HG11	1:K:240:ARG:HB2	1.99	0.43
1:K:303:GLN:O	1:K:307:SER:HB2	2.19	0.43
1:A:159:ILE:HG21	1:A:188:PHE:HZ	1.82	0.43
1:C:238:ASN:O	1:C:239:GLN:C	2.61	0.43
2:D:64:LEU:HD23	2:D:64:LEU:HA	1.86	0.43
2:F:329:LEU:HD12	2:F:329:LEU:HA	1.88	0.43
2:J:27:ARG:O	2:J:30:GLN:HB2	2.19	0.43
2:J:131:CYS:O	2:J:132:LEU:C	2.62	0.43
1:E:244:ILE:HG21	1:E:250:TYR:CZ	2.52	0.43
2:F:58:LEU:O	2:F:61:LEU:N	2.52	0.43
1:I:330:LYS:C	1:I:332:ASP:H	2.27	0.43
1:K:116:ALA:O	1:K:119:LEU:HB3	2.19	0.43
2:L:96:ARG:HE	2:L:118:ASP:CG	2.26	0.43
1:A:227:LEU:HD12	1:A:262:TYR:OH	2.18	0.43
2:D:58:LEU:O	2:D:61:LEU:N	2.50	0.43
2:D:299:LEU:O	2:D:302:GLN:HB2	2.18	0.43
1:E:151:GLU:O	1:E:154:TYR:HB3	2.19	0.43
1:G:106:VAL:HG11	1:G:116:ALA:HB1	2.01	0.43
1:I:321:ASP:O	1:I:325:ASN:ND2	2.52	0.43
2:J:266:LYS:NZ	5:J:403:DPO:O2	2.52	0.43
2:L:227:ILE:HD13	2:L:227:ILE:HA	1.93	0.43
2:L:270:THR:OG1	2:L:301:THR:HG21	2.19	0.43
1:A:66:TYR:CE2	1:A:119:LEU:HD13	2.54	0.43
1:A:213:PHE:O	1:A:214:ARG:C	2.62	0.43
1:C:144:LEU:N	1:C:144:LEU:HD23	2.33	0.43
1:C:355:TYR:CZ	1:C:359:ILE:HD11	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:GLU:HA	1:E:144:LEU:CD1	2.49	0.43
1:E:199:ASN:OD1	1:E:199:ASN:C	2.62	0.43
1:G:251:SER:HA	1:G:287:ARG:NH2	2.33	0.43
2:H:217:GLU:OE1	2:H:263:ARG:NH1	2.51	0.43
1:I:332:ASP:C	1:I:332:ASP:OD1	2.60	0.43
2:J:146:ALA:O	2:J:149:ALA:HB3	2.18	0.43
2:B:76:ILE:CD1	2:B:131:CYS:HB3	2.49	0.43
2:B:230:LEU:HD22	2:B:239:VAL:HG21	2.01	0.43
2:D:291:PHE:HD2	2:D:332:MET:SD	2.42	0.43
2:F:21:LEU:N	2:F:21:LEU:CD1	2.82	0.43
1:I:165:ASN:O	1:I:168:VAL:HG22	2.19	0.43
2:J:207:ASP:OD1	2:J:218:SER:OG	2.33	0.43
1:K:127:ASN:OD1	2:L:42:SER:HA	2.18	0.43
2:L:210:LEU:O	2:L:218:SER:HA	2.19	0.43
1:C:312:ILE:HG23	1:C:340:LEU:HD22	2.01	0.43
1:E:56:LEU:HD21	1:E:63:TYR:HA	2.01	0.43
2:H:106:ASN:O	2:H:108:SER:N	2.52	0.43
1:C:357:ARG:O	1:C:361:ARG:HG3	2.18	0.43
2:F:34:GLN:HB3	2:F:35:VAL:HG23	2.01	0.43
1:G:106:VAL:HG11	1:G:116:ALA:CB	2.49	0.43
1:G:216:TRP:O	1:G:218:ASN:N	2.52	0.43
2:H:250:ARG:O	2:H:254:MET:HG2	2.18	0.43
1:K:337:ALA:O	1:K:340:LEU:HB2	2.19	0.43
2:L:39:ARG:NH1	2:L:39:ARG:HB3	2.34	0.43
2:L:192:ASP:OD2	2:L:195:LYS:HE3	2.19	0.43
1:A:313:ALA:O	1:A:314:PHE:C	2.61	0.42
1:A:329:ASN:O	1:A:330:LYS:C	2.62	0.42
2:B:331:LEU:HD13	2:B:340:VAL:CG1	2.49	0.42
1:C:130:ASN:HA	2:D:45:THR:HG21	2.01	0.42
2:D:152:ARG:HD3	2:D:189:SER:O	2.19	0.42
1:G:159:ILE:HG21	1:G:188:PHE:HZ	1.83	0.42
1:K:136:PHE:CE2	1:K:140:LEU:HD11	2.53	0.42
1:C:295:LEU:O	1:C:296:LEU:C	2.61	0.42
2:F:90:LEU:HD23	2:F:90:LEU:HA	1.87	0.42
1:I:277:TRP:CH2	1:I:311:LEU:HG	2.54	0.42
2:J:207:ASP:CG	2:J:218:SER:HG	2.26	0.42
1:K:118:LYS:O	1:K:121:ARG:HB3	2.18	0.42
2:B:261:HIS:ND1	2:B:266:LYS:O	2.52	0.42
1:C:330:LYS:O	1:C:332:ASP:N	2.52	0.42
1:K:206:ARG:HE	1:K:219:GLU:CD	2.25	0.42
1:K:296:LEU:HD22	1:K:322:MET:HE1	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:334:LEU:O	1:K:338:LEU:HG	2.19	0.42
2:L:106:ASN:O	2:L:108:SER:N	2.52	0.42
2:B:27:ARG:HE	2:B:30:GLN:HE21	1.68	0.42
1:G:189:ILE:HG21	1:G:206:ARG:HB2	2.00	0.42
2:L:151:LEU:HD12	2:L:181:ILE:CG2	2.47	0.42
2:L:224:PHE:HB2	2:L:275:TRP:O	2.20	0.42
2:B:20:PHE:HA	2:B:302:GLN:OE1	2.20	0.42
1:E:152:MET:CE	1:E:172:ARG:CZ	2.97	0.42
2:F:159:GLY:HA3	2:F:195:LYS:O	2.19	0.42
1:G:78:VAL:HG12	1:G:79:PRO:HD2	2.01	0.42
1:G:144:LEU:HB2	1:G:146:LYS:HG2	2.00	0.42
1:G:185:GLU:HG3	1:G:209:VAL:HG21	2.02	0.42
2:H:299:LEU:HD22	2:H:302:GLN:NE2	2.35	0.42
1:K:256:LEU:O	1:K:257:GLU:C	2.63	0.42
2:L:76:ILE:O	2:L:79:LEU:HB2	2.19	0.42
2:L:128:GLY:O	2:L:131:CYS:N	2.53	0.42
1:A:112:ARG:O	1:A:144:LEU:HD21	2.18	0.42
1:A:344:LEU:HD13	1:A:356:TRP:CE2	2.54	0.42
2:D:232:LEU:HD13	2:D:343:ALA:HB1	2.00	0.42
1:I:312:ILE:HG23	1:I:340:LEU:HD22	2.02	0.42
1:K:248:THR:C	1:K:249:GLY:O	2.63	0.42
2:L:228:ALA:HA	2:L:231:CYS:HB2	2.02	0.42
2:L:266:LYS:HE2	5:L:403:DPO:O2	2.19	0.42
2:B:40:TYR:O	2:B:42:SER:N	2.52	0.42
2:B:213:GLY:O	2:B:214:ALA:C	2.62	0.42
2:D:297:TYR:OH	2:D:312:TRP:HA	2.20	0.42
1:I:144:LEU:O	1:I:145:GLN:C	2.62	0.42
2:J:82:LEU:HD11	2:J:108:SER:HA	2.02	0.42
2:B:173:ARG:O	2:B:176:TYR:HB3	2.20	0.42
1:C:112:ARG:HA	1:C:140:LEU:CD2	2.50	0.42
1:C:232:ARG:HA	1:C:273:ASN:OD1	2.20	0.42
1:C:341:CYS:O	1:C:344:LEU:HB2	2.19	0.42
1:C:350:THR:O	1:C:353:LYS:HB2	2.19	0.42
2:D:329:LEU:HD12	2:D:329:LEU:HA	1.88	0.42
1:E:103:PHE:HA	1:E:119:LEU:HD21	2.01	0.42
1:G:155:ILE:HD12	1:G:155:ILE:HA	1.91	0.42
1:G:312:ILE:O	1:G:315:LEU:HB2	2.20	0.42
1:G:339:GLU:O	1:G:343:ILE:HD12	2.19	0.42
2:J:92:ARG:NH1	2:J:119:SER:HB3	2.34	0.42
2:J:204:MET:HB2	2:J:204:MET:HE2	1.75	0.42
1:K:219:GLU:OE1	1:K:219:GLU:HA	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:298:ILE:O	2:L:301:THR:OG1	2.36	0.42
1:C:141:LEU:HD11	1:C:151:GLU:HG2	2.00	0.42
1:C:222:TYR:CE2	1:C:226:LEU:HD11	2.55	0.42
2:D:37:PRO:C	2:D:39:ARG:N	2.78	0.42
1:G:80:GLN:NE2	2:H:100:TYR:HA	2.34	0.42
1:G:103:PHE:HA	1:G:119:LEU:HD21	2.01	0.42
1:G:120:THR:OG1	1:G:137:ARG:NH1	2.52	0.42
2:H:30:GLN:O	2:H:34:GLN:HG2	2.19	0.42
2:J:192:ASP:OD1	2:J:192:ASP:C	2.63	0.42
1:K:210:ILE:O	1:K:214:ARG:HA	2.19	0.42
1:K:331:GLU:O	1:K:335:ASN:ND2	2.53	0.42
2:B:260:TYR:N	2:B:260:TYR:CD1	2.88	0.42
2:F:58:LEU:O	2:F:59:ASP:C	2.63	0.42
2:F:64:LEU:HD23	2:F:64:LEU:HA	1.83	0.42
2:F:233:MET:O	2:F:235:LYS:HG3	2.20	0.42
1:G:340:LEU:O	1:G:343:ILE:N	2.53	0.42
2:J:28:PHE:CD1	2:J:28:PHE:C	2.98	0.42
1:K:87:VAL:HG12	1:K:88:VAL:HG23	2.01	0.42
1:K:348:LYS:HD3	1:K:348:LYS:HA	1.92	0.42
1:A:151:GLU:C	1:A:153:ASN:N	2.78	0.41
1:E:151:GLU:CG	1:E:175:LEU:HD11	2.50	0.41
2:F:263:ARG:HG3	2:F:266:LYS:HG3	2.01	0.41
2:H:197:ILE:CD1	2:H:235:LYS:HD3	2.49	0.41
2:H:298:ILE:HG21	2:H:329:LEU:HD13	2.01	0.41
2:J:273:SER:HB3	2:J:294:ASN:OD1	2.20	0.41
1:K:251:SER:HA	1:K:287:ARG:NH2	2.35	0.41
2:D:312:TRP:HB3	2:D:313:PRO:HD2	2.02	0.41
1:G:239:GLN:O	1:G:242:PHE:HB3	2.20	0.41
2:J:341:HIS:ND1	2:J:344:LEU:HB3	2.36	0.41
1:K:149:GLN:NE2	1:K:184:GLN:OE1	2.53	0.41
2:L:357:LEU:HD23	2:L:357:LEU:O	2.20	0.41
1:A:86:PRO:CG	1:A:89:GLN:NE2	2.84	0.41
1:C:252:ASP:OD2	1:C:255:VAL:HG23	2.20	0.41
2:D:171:ASP:OD2	2:D:173:ARG:NH1	2.54	0.41
1:E:74:ASP:OD1	1:E:74:ASP:N	2.44	0.41
1:E:227:LEU:HG	1:E:236:VAL:CG1	2.51	0.41
1:E:333:ILE:HA	1:E:336:LYS:HD2	2.02	0.41
1:G:302:LEU:HD22	1:G:306:HIS:HB2	2.01	0.41
1:I:110:ASP:CG	1:I:112:ARG:HE	2.27	0.41
1:A:121:ARG:NH1	1:A:121:ARG:CG	2.82	0.41
2:B:312:TRP:HB3	2:B:313:PRO:HD2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:ASN:O	1:C:326:GLN:C	2.63	0.41
1:G:361:ARG:O	1:G:365:SER:OG	2.37	0.41
2:H:256:GLN:HB2	2:H:260:TYR:CE2	2.56	0.41
2:H:284:LYS:O	2:H:286:PHE:N	2.53	0.41
1:I:142:ARG:O	1:I:143:SER:C	2.63	0.41
1:A:189:ILE:HD11	1:A:205:HIS:HD2	1.85	0.41
1:C:142:ARG:O	1:C:143:SER:C	2.63	0.41
2:D:268:VAL:O	2:D:312:TRP:CD1	2.74	0.41
1:E:107:LEU:HD23	1:E:107:LEU:HA	1.93	0.41
2:H:357:LEU:HD22	2:H:361:TRP:CZ2	2.55	0.41
1:I:74:ASP:OD1	1:I:74:ASP:N	2.53	0.41
1:I:96:PHE:CD2	1:I:126:LEU:HD22	2.55	0.41
2:J:263:ARG:O	2:J:266:LYS:HB2	2.21	0.41
1:K:127:ASN:OD1	1:K:129:ALA:HB3	2.20	0.41
1:A:107:LEU:O	1:A:109:ARG:N	2.53	0.41
1:C:247:THR:O	1:C:248:THR:C	2.63	0.41
2:F:160:SER:HB3	2:F:199:TYR:CE1	2.55	0.41
2:H:77:TYR:CE1	2:H:141:ARG:HB2	2.55	0.41
1:K:81:ASN:N	1:K:81:ASN:ND2	2.61	0.41
1:K:106:VAL:HG11	1:K:116:ALA:HB1	2.03	0.41
1:K:152:MET:HE3	1:K:152:MET:HB3	1.82	0.41
1:K:198:LYS:O	2:L:263:ARG:NH2	2.53	0.41
1:A:92:TYR:CE1	1:A:96:PHE:CE1	3.09	0.41
1:A:148:LEU:CD1	1:A:178:TRP:HE3	2.34	0.41
1:A:319:TYR:O	1:A:323:LEU:HG	2.21	0.41
2:D:258:ASN:ND2	2:D:258:ASN:N	2.69	0.41
1:E:333:ILE:O	1:E:336:LYS:N	2.53	0.41
2:H:37:PRO:C	2:H:39:ARG:H	2.28	0.41
2:H:236:LEU:HD22	2:H:245:LEU:HD21	2.03	0.41
1:K:107:LEU:O	1:K:108:GLN:C	2.63	0.41
2:L:99:SER:C	2:L:101:LEU:H	2.28	0.41
2:J:197:ILE:CD1	2:J:235:LYS:HD3	2.50	0.41
1:K:83:GLY:HA3	2:L:105:PHE:CE1	2.56	0.41
1:K:311:LEU:CD2	1:K:315:LEU:HD11	2.51	0.41
1:K:356:TRP:HA	1:K:356:TRP:CE3	2.54	0.41
1:A:103:PHE:CZ	1:A:133:VAL:HG22	2.56	0.41
1:A:206:ARG:NE	1:A:219:GLU:OE2	2.50	0.41
2:B:232:LEU:HD13	2:B:343:ALA:HB1	2.02	0.41
1:C:58:LEU:HD23	1:C:58:LEU:HA	1.87	0.41
1:E:255:VAL:HG13	1:E:258:ARG:NH2	2.35	0.41
1:G:214:ARG:O	1:G:214:ARG:HD3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:219:GLU:HB3	1:G:243:VAL:HG21	2.01	0.41
2:H:290:ASN:OD1	2:H:290:ASN:C	2.64	0.41
2:H:299:LEU:HD21	2:H:329:LEU:HD21	2.02	0.41
1:I:292:TYR:O	1:I:294:ASN:N	2.54	0.41
2:J:270:THR:OG1	2:J:301:THR:HG21	2.20	0.41
2:J:330:SER:OG	2:J:338:CYS:O	2.22	0.41
1:K:173:ARG:CZ	1:K:208:TRP:CD1	3.04	0.41
1:C:140:LEU:O	1:C:141:LEU:C	2.64	0.41
2:D:255:ARG:HD3	2:D:261:HIS:CD2	2.56	0.41
1:E:206:ARG:HE	1:E:219:GLU:CD	2.29	0.41
2:H:83:PRO:HA	2:H:89:ASN:OD1	2.21	0.41
1:I:112:ARG:HA	1:I:140:LEU:CD2	2.51	0.41
2:J:21:LEU:CD1	2:J:21:LEU:N	2.84	0.41
2:L:220:GLY:N	2:L:262:GLY:O	2.53	0.41
2:D:33:LEU:HD22	2:D:54:ALA:HB1	2.03	0.40
2:D:149:ALA:HA	2:D:152:ARG:NH2	2.35	0.40
1:G:311:LEU:C	1:G:311:LEU:HD23	2.47	0.40
2:J:64:LEU:HD23	2:J:64:LEU:HA	1.80	0.40
2:L:341:HIS:C	2:L:341:HIS:ND1	2.79	0.40
1:A:144:LEU:N	1:A:144:LEU:HD23	2.36	0.40
1:A:267:ILE:O	1:A:268:LYS:C	2.64	0.40
1:E:351:ILE:O	1:E:351:ILE:CG1	2.68	0.40
1:I:244:ILE:HG21	1:I:250:TYR:CE1	2.57	0.40
2:J:295:ARG:HB2	2:J:332:MET:HE1	2.03	0.40
1:K:74:ASP:OD1	1:K:74:ASP:N	2.55	0.40
1:A:89:GLN:HB3	2:B:35:VAL:HG22	2.04	0.40
1:C:352:ARG:O	1:C:353:LYS:C	2.64	0.40
1:E:159:ILE:HG12	1:E:168:VAL:CG2	2.51	0.40
2:F:133:ILE:HG22	2:F:350:THR:HG23	2.02	0.40
1:G:206:ARG:NE	1:G:219:GLU:OE2	2.41	0.40
2:H:311:LYS:HG3	2:H:312:TRP:CD2	2.56	0.40
1:I:87:VAL:HG23	2:J:75:TRP:CG	2.56	0.40
1:I:185:GLU:O	1:I:186:LEU:C	2.64	0.40
1:A:287:ARG:O	1:A:291:ARG:HD3	2.22	0.40
1:E:339:GLU:O	1:E:343:ILE:HG13	2.22	0.40
2:F:28:PHE:O	2:F:31:ARG:N	2.55	0.40
2:F:257:GLN:HB2	2:F:258:ASN:H	1.74	0.40
2:J:96:ARG:NE	2:J:118:ASP:OD1	2.48	0.40
2:L:176:TYR:CZ	2:L:180:CYS:SG	3.15	0.40
1:A:250:TYR:C	1:A:287:ARG:HH22	2.30	0.40
2:B:151:LEU:O	2:B:154:LEU:HB2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:TYR:HA	2:B:229:SER:OG	2.22	0.40
1:C:130:ASN:OD1	1:C:130:ASN:C	2.63	0.40
2:F:138:ASP:OD1	2:F:140:SER:CB	2.69	0.40
2:F:348:THR:HA	2:F:351:SER:OG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	312/314 (99%)	266 (85%)	40 (13%)	6 (2%)	6	32
1	C	312/314 (99%)	257 (82%)	47 (15%)	8 (3%)	4	26
1	E	312/314 (99%)	266 (85%)	37 (12%)	9 (3%)	3	25
1	G	312/314 (99%)	255 (82%)	52 (17%)	5 (2%)	7	34
1	I	312/314 (99%)	254 (81%)	42 (14%)	16 (5%)	1	16
1	K	312/314 (99%)	255 (82%)	48 (15%)	9 (3%)	3	25
2	B	344/346 (99%)	297 (86%)	39 (11%)	8 (2%)	5	29
2	D	344/346 (99%)	301 (88%)	34 (10%)	9 (3%)	4	26
2	F	344/346 (99%)	301 (88%)	38 (11%)	5 (2%)	8	35
2	H	344/346 (99%)	296 (86%)	37 (11%)	11 (3%)	3	24
2	J	344/346 (99%)	299 (87%)	40 (12%)	5 (2%)	8	35
2	L	344/346 (99%)	281 (82%)	50 (14%)	13 (4%)	2	20
All	All	3936/3960 (99%)	3328 (85%)	504 (13%)	104 (3%)	4	26

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	ASP
1	A	326	GLN
1	A	329	ASN
2	B	137	ASP
1	C	304	PRO
1	C	330	LYS
1	E	110	ASP
1	E	217	ASP
1	E	353	LYS
1	G	185	GLU
1	I	217	ASP
1	I	304	PRO
1	I	326	GLN
1	I	329	ASN
1	K	217	ASP
2	L	34	GLN
2	L	90	LEU
1	A	108	GLN
1	A	214	ARG
2	B	34	GLN
2	B	46	SER
2	B	171	ASP
1	C	214	ARG
1	C	217	ASP
1	E	108	GLN
1	E	253	ARG
1	E	304	PRO
1	E	326	GLN
1	E	329	ASN
1	E	330	LYS
2	F	22	ARG
2	F	109	LYS
1	G	127	ASN
2	H	284	LYS
2	H	285	ILE
2	H	333	GLU
2	H	362	LYS
1	I	214	ARG
1	I	252	ASP
2	J	41	SER
1	K	108	GLN
1	K	183	SER
1	K	214	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	230	ASP
1	K	249	GLY
2	L	91	ASP
2	L	105	PHE
2	L	109	LYS
2	L	333	GLU
2	B	41	SER
2	B	109	LYS
2	D	362	LYS
2	F	100	TYR
2	H	38	GLU
2	H	108	SER
1	I	84	PRO
1	I	199	ASN
1	I	290	SER
1	I	330	LYS
2	J	22	ARG
2	J	85	GLU
2	J	362	LYS
2	L	100	TYR
2	L	108	SER
2	L	126	TYR
1	A	180	LYS
1	C	252	ASP
2	D	41	SER
2	D	108	SER
1	G	108	GLN
2	H	34	GLN
2	H	171	ASP
1	I	327	CYS
1	I	331	GLU
2	J	157	GLU
1	K	304	PRO
2	L	111	PRO
1	C	84	PRO
1	C	199	ASN
2	D	59	ASP
2	D	107	PRO
2	D	284	LYS
2	F	85	GLU
2	F	110	ASN
1	G	353	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	66	VAL
1	I	142	ARG
1	I	196	ASP
1	K	127	ASN
1	K	329	ASN
2	B	258	ASN
2	B	302	GLN
2	D	34	GLN
2	D	38	GLU
2	H	91	ASP
2	L	171	ASP
2	L	128	GLY
1	C	182	PRO
2	L	66	VAL
2	H	115	HIS
1	I	293	PRO
1	I	351	ILE
2	D	111	PRO
1	G	304	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	280/293 (96%)	258 (92%)	22 (8%)	11	37
1	C	280/293 (96%)	257 (92%)	23 (8%)	10	35
1	E	281/293 (96%)	254 (90%)	27 (10%)	8	30
1	G	280/293 (96%)	254 (91%)	26 (9%)	8	31
1	I	280/293 (96%)	260 (93%)	20 (7%)	13	40
1	K	280/293 (96%)	257 (92%)	23 (8%)	10	35
2	B	289/301 (96%)	257 (89%)	32 (11%)	6	25
2	D	289/301 (96%)	256 (89%)	33 (11%)	5	24
2	F	289/301 (96%)	259 (90%)	30 (10%)	7	28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	289/301 (96%)	257 (89%)	32 (11%)	6	25
2	J	289/301 (96%)	263 (91%)	26 (9%)	9	32
2	L	289/301 (96%)	258 (89%)	31 (11%)	6	27
All	All	3415/3564 (96%)	3090 (90%)	325 (10%)	8	31

All (325) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	PHE
1	A	67	ARG
1	A	71	GLU
1	A	80	GLN
1	A	82	ASP
1	A	107	LEU
1	A	108	GLN
1	A	121	ARG
1	A	124	ILE
1	A	156	ILE
1	A	160	GLU
1	A	191	ASP
1	A	194	ASN
1	A	214	ARG
1	A	231	VAL
1	A	232	ARG
1	A	235	SER
1	A	243	VAL
1	A	275	SER
1	A	287	ARG
1	A	303	GLN
1	A	354	GLU
2	B	22	ARG
2	B	27	ARG
2	B	31	ARG
2	B	33	LEU
2	B	36	LEU
2	B	45	THR
2	B	65	ASP
2	B	90	LEU
2	B	113	THR
2	B	130	SER
2	B	139	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	151	LEU
2	B	216	LEU
2	B	223	THR
2	B	232	LEU
2	B	236	LEU
2	B	258	ASN
2	B	263	ARG
2	B	284	LYS
2	B	292	GLU
2	B	300	SER
2	B	305	LEU
2	B	306	VAL
2	B	329	LEU
2	B	331	LEU
2	B	335	SER
2	B	338	CYS
2	B	341	HIS
2	B	348	THR
2	B	351	SER
2	B	357	LEU
2	B	360	SER
1	C	55	PHE
1	C	67	ARG
1	C	71	GLU
1	C	81	ASN
1	C	106	VAL
1	C	107	LEU
1	C	108	GLN
1	C	121	ARG
1	C	144	LEU
1	C	160	GLU
1	C	177	GLU
1	C	194	ASN
1	C	214	ARG
1	C	220	LEU
1	C	240	ARG
1	C	269	LEU
1	C	287	ARG
1	C	290	SER
1	C	304	PRO
1	C	327	CYS
1	C	350	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	365	SER
1	C	368	SER
2	D	21	LEU
2	D	27	ARG
2	D	33	LEU
2	D	45	THR
2	D	56	SER
2	D	66	VAL
2	D	67	VAL
2	D	130	SER
2	D	139	LEU
2	D	140	SER
2	D	151	LEU
2	D	158	ASP
2	D	216	LEU
2	D	223	THR
2	D	232	LEU
2	D	235	LYS
2	D	236	LEU
2	D	258	ASN
2	D	263	ARG
2	D	284	LYS
2	D	305	LEU
2	D	306	VAL
2	D	311	LYS
2	D	312	TRP
2	D	329	LEU
2	D	330	SER
2	D	331	LEU
2	D	338	CYS
2	D	340	VAL
2	D	349	ARG
2	D	350	THR
2	D	353	ARG
2	D	357	LEU
1	E	58	LEU
1	E	67	ARG
1	E	71	GLU
1	E	81	ASN
1	E	85	SER
1	E	87	VAL
1	E	89	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	94	GLU
1	E	98	ASP
1	E	108	GLN
1	E	109	ARG
1	E	121	ARG
1	E	152	MET
1	E	160	GLU
1	E	194	ASN
1	E	214	ARG
1	E	220	LEU
1	E	224	ASP
1	E	235	SER
1	E	248	THR
1	E	269	LEU
1	E	287	ARG
1	E	304	PRO
1	E	305	SER
1	E	330	LYS
1	E	350	THR
1	E	351	ILE
2	F	21	LEU
2	F	22	ARG
2	F	27	ARG
2	F	30	GLN
2	F	31	ARG
2	F	33	LEU
2	F	39	ARG
2	F	45	THR
2	F	106	ASN
2	F	113	THR
2	F	130	SER
2	F	151	LEU
2	F	194	LYS
2	F	216	LEU
2	F	232	LEU
2	F	236	LEU
2	F	253	ILE
2	F	255	ARG
2	F	258	ASN
2	F	268	VAL
2	F	284	LYS
2	F	287	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	305	LEU
2	F	306	VAL
2	F	329	LEU
2	F	331	LEU
2	F	348	THR
2	F	353	ARG
2	F	357	LEU
2	F	360	SER
1	G	58	LEU
1	G	67	ARG
1	G	71	GLU
1	G	78	VAL
1	G	82	ASP
1	G	88	VAL
1	G	104	ARG
1	G	107	LEU
1	G	109	ARG
1	G	127	ASN
1	G	158	ILE
1	G	160	GLU
1	G	177	GLU
1	G	191	ASP
1	G	194	ASN
1	G	209	VAL
1	G	214	ARG
1	G	225	GLN
1	G	229	GLU
1	G	251	SER
1	G	269	LEU
1	G	287	ARG
1	G	290	SER
1	G	334	LEU
1	G	348	LYS
1	G	365	SER
2	H	21	LEU
2	H	33	LEU
2	H	34	GLN
2	H	36	LEU
2	H	39	ARG
2	H	90	LEU
2	H	99	SER
2	H	113	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	130	SER
2	H	139	LEU
2	H	151	LEU
2	H	205	SER
2	H	216	LEU
2	H	232	LEU
2	H	236	LEU
2	H	253	ILE
2	H	263	ARG
2	H	284	LYS
2	H	287	GLN
2	H	292	GLU
2	H	296	ASN
2	H	300	SER
2	H	302	GLN
2	H	305	LEU
2	H	329	LEU
2	H	331	LEU
2	H	335	SER
2	H	341	HIS
2	H	348	THR
2	H	353	ARG
2	H	357	LEU
2	H	360	SER
1	I	55	PHE
1	I	67	ARG
1	I	71	GLU
1	I	90	ILE
1	I	106	VAL
1	I	107	LEU
1	I	109	ARG
1	I	114	GLU
1	I	121	ARG
1	I	143	SER
1	I	160	GLU
1	I	194	ASN
1	I	214	ARG
1	I	232	ARG
1	I	243	VAL
1	I	269	LEU
1	I	287	ARG
1	I	290	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	304	PRO
1	I	332	ASP
2	J	22	ARG
2	J	27	ARG
2	J	33	LEU
2	J	65	ASP
2	J	88	SER
2	J	99	SER
2	J	130	SER
2	J	151	LEU
2	J	216	LEU
2	J	232	LEU
2	J	236	LEU
2	J	263	ARG
2	J	268	VAL
2	J	284	LYS
2	J	287	GLN
2	J	300	SER
2	J	305	LEU
2	J	315	SER
2	J	329	LEU
2	J	331	LEU
2	J	337	ILE
2	J	338	CYS
2	J	349	ARG
2	J	350	THR
2	J	353	ARG
2	J	357	LEU
1	K	58	LEU
1	K	71	GLU
1	K	81	ASN
1	K	90	ILE
1	K	98	ASP
1	K	107	LEU
1	K	109	ARG
1	K	121	ARG
1	K	132	THR
1	K	160	GLU
1	K	172	ARG
1	K	177	GLU
1	K	214	ARG
1	K	243	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	251	SER
1	K	287	ARG
1	K	302	LEU
1	K	304	PRO
1	K	327	CYS
1	K	328	ASP
1	K	330	LYS
1	K	351	ILE
1	K	352	ARG
2	L	21	LEU
2	L	26	VAL
2	L	33	LEU
2	L	39	ARG
2	L	64	LEU
2	L	84	THR
2	L	99	SER
2	L	103	ILE
2	L	130	SER
2	L	131	CYS
2	L	151	LEU
2	L	173	ARG
2	L	216	LEU
2	L	223	THR
2	L	236	LEU
2	L	253	ILE
2	L	258	ASN
2	L	260	TYR
2	L	263	ARG
2	L	279	THR
2	L	281	LYS
2	L	284	LYS
2	L	305	LEU
2	L	306	VAL
2	L	326	ILE
2	L	329	LEU
2	L	331	LEU
2	L	335	SER
2	L	341	HIS
2	L	351	SER
2	L	353	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	153	ASN
1	A	194	ASN
1	A	201	HIS
1	A	285	GLN
1	A	329	ASN
1	A	335	ASN
2	B	30	GLN
2	B	212	GLN
2	B	257	GLN
1	C	81	ASN
1	C	89	GLN
1	C	135	HIS
1	C	149	GLN
1	C	170	HIS
1	C	194	ASN
1	C	201	HIS
1	C	238	ASN
1	C	285	GLN
1	C	329	ASN
2	D	30	GLN
2	D	186	ASN
2	D	208	ASN
2	D	212	GLN
2	D	257	GLN
2	D	258	ASN
1	E	89	GLN
1	E	149	GLN
1	E	153	ASN
1	E	167	GLN
1	E	170	HIS
1	E	184	GLN
1	E	194	ASN
1	E	195	GLN
1	E	201	HIS
1	E	241	HIS
1	E	298	GLN
1	E	329	ASN
2	F	30	GLN
2	F	256	GLN
2	F	257	GLN
2	F	287	GLN
1	G	149	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	162	GLN
1	G	167	GLN
1	G	195	GLN
1	G	241	HIS
1	G	329	ASN
2	H	212	GLN
2	H	296	ASN
1	I	81	ASN
1	I	89	GLN
1	I	135	HIS
1	I	162	GLN
1	I	194	ASN
1	I	195	GLN
1	I	201	HIS
1	I	238	ASN
1	I	273	ASN
1	I	306	HIS
1	I	329	ASN
1	I	367	HIS
2	J	30	GLN
2	J	212	GLN
2	J	257	GLN
2	J	265	ASN
2	J	287	GLN
1	K	135	HIS
1	K	149	GLN
1	K	184	GLN
1	K	201	HIS
1	K	218	ASN
1	K	261	GLN
1	K	329	ASN
1	K	335	ASN
1	K	367	HIS
2	L	30	GLN
2	L	212	GLN
2	L	257	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 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$
6	A1HZ4	L	404	-	38,38,38	1.95	8 (21%)	49,57,57	2.72	20 (40%)
6	A1HZ4	B	404	-	38,38,38	1.81	8 (21%)	49,57,57	2.30	14 (28%)
6	A1HZ4	D	404	-	38,38,38	1.94	5 (13%)	49,57,57	2.55	16 (32%)
5	DPO	B	403	-	6,8,8	0.65	0	12,13,13	0.94	0
5	DPO	L	403	-	6,8,8	0.92	0	12,13,13	0.73	0
6	A1HZ4	F	404	-	38,38,38	1.86	9 (23%)	49,57,57	2.43	18 (36%)
6	A1HZ4	J	404	-	38,38,38	1.88	5 (13%)	49,57,57	2.50	18 (36%)
6	A1HZ4	H	404	-	38,38,38	2.00	5 (13%)	49,57,57	2.54	17 (34%)
5	DPO	F	403	-	6,8,8	1.07	1 (16%)	12,13,13	0.80	0
5	DPO	H	403	-	6,8,8	0.60	0	12,13,13	0.87	0
5	DPO	J	403	-	6,8,8	0.70	0	12,13,13	0.82	0
5	DPO	D	403	-	6,8,8	0.94	0	12,13,13	0.74	0

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
6	A1HZ4	L	404	-	-	0/34/62/62	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	A1HZ4	B	404	-	-	0/34/62/62	0/4/4/4
6	A1HZ4	D	404	-	-	5/34/62/62	0/4/4/4
5	DPO	B	403	-	-	2/6/6/6	-
5	DPO	L	403	-	-	0/6/6/6	-
6	A1HZ4	F	404	-	-	8/34/62/62	0/4/4/4
6	A1HZ4	J	404	-	-	1/34/62/62	0/4/4/4
6	A1HZ4	H	404	-	-	0/34/62/62	0/4/4/4
5	DPO	F	403	-	-	4/6/6/6	-
5	DPO	H	403	-	-	0/6/6/6	-
5	DPO	J	403	-	-	4/6/6/6	-
5	DPO	D	403	-	-	4/6/6/6	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	404	A1HZ4	C21-N20	6.80	1.53	1.46
6	B	404	A1HZ4	C21-N20	6.48	1.52	1.46
6	L	404	A1HZ4	C21-N20	6.24	1.52	1.46
6	F	404	A1HZ4	O9-C7	6.12	1.53	1.41
6	H	404	A1HZ4	C21-N20	6.10	1.52	1.46
6	J	404	A1HZ4	C47-C22	5.85	1.60	1.51
6	H	404	A1HZ4	C19-N20	5.55	1.44	1.33
6	D	404	A1HZ4	C19-N20	5.15	1.43	1.33
6	H	404	A1HZ4	C18-C19	5.07	1.55	1.50
6	J	404	A1HZ4	O9-C7	4.98	1.51	1.41
6	L	404	A1HZ4	O9-C7	4.97	1.51	1.41
6	L	404	A1HZ4	C19-N20	4.71	1.43	1.33
6	D	404	A1HZ4	C47-C22	4.36	1.58	1.51
6	D	404	A1HZ4	C18-C19	4.26	1.54	1.50
6	B	404	A1HZ4	C18-C19	4.22	1.54	1.50
6	J	404	A1HZ4	C21-N20	4.20	1.50	1.46
6	J	404	A1HZ4	C19-N20	4.13	1.41	1.33
6	H	404	A1HZ4	C13-N12	4.04	1.54	1.47
6	B	404	A1HZ4	C47-C22	3.92	1.57	1.51
6	L	404	A1HZ4	C18-C19	3.90	1.54	1.50
6	F	404	A1HZ4	C47-C22	3.87	1.57	1.51
6	F	404	A1HZ4	C19-N20	3.55	1.40	1.33
6	J	404	A1HZ4	C18-C19	3.44	1.54	1.50
6	B	404	A1HZ4	C19-N20	3.24	1.39	1.33
6	F	404	A1HZ4	C18-C19	3.18	1.53	1.50
6	F	404	A1HZ4	C21-N20	3.07	1.49	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	404	A1HZ4	C47-C22	2.90	1.56	1.51
6	F	404	A1HZ4	C7-C10	2.72	1.59	1.55
6	L	404	A1HZ4	C17-N12	2.64	1.51	1.47
6	L	404	A1HZ4	C47-C22	2.46	1.55	1.51
6	F	404	A1HZ4	C16-C15	2.39	1.57	1.53
6	B	404	A1HZ4	O60-C61	2.37	1.49	1.42
6	B	404	A1HZ4	C13-N12	2.36	1.51	1.47
6	F	404	A1HZ4	C17-N12	2.28	1.51	1.47
6	L	404	A1HZ4	C7-C10	2.23	1.58	1.55
6	B	404	A1HZ4	O9-C7	2.22	1.45	1.41
6	D	404	A1HZ4	C21-C22	2.18	1.57	1.53
6	B	404	A1HZ4	C14-C15	2.16	1.56	1.53
6	F	404	A1HZ4	C7-C1	2.12	1.56	1.52
6	L	404	A1HZ4	O9-C40	2.07	1.49	1.43
5	F	403	DPO	P2-O5	2.00	1.56	1.50

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	404	A1HZ4	C7-C10-N12	10.44	128.20	117.64
6	H	404	A1HZ4	C7-C10-N12	9.79	127.54	117.64
6	J	404	A1HZ4	C7-C10-N12	9.38	127.13	117.64
6	B	404	A1HZ4	O60-C49-C47	8.01	123.79	115.84
6	D	404	A1HZ4	C7-C10-N12	7.66	125.39	117.64
6	B	404	A1HZ4	C7-C10-N12	7.42	125.14	117.64
6	H	404	A1HZ4	O60-C49-C47	7.04	122.83	115.84
6	F	404	A1HZ4	C7-C10-N12	7.00	124.72	117.64
6	L	404	A1HZ4	O60-C49-C47	6.91	122.70	115.84
6	J	404	A1HZ4	O60-C49-C47	6.54	122.34	115.84
6	F	404	A1HZ4	O60-C49-C47	6.50	122.30	115.84
6	D	404	A1HZ4	O60-C49-C47	6.23	122.03	115.84
6	F	404	A1HZ4	C14-C15-C18	-6.06	103.44	110.16
6	D	404	A1HZ4	O60-C49-C50	-5.43	115.14	124.30
6	D	404	A1HZ4	C61-O60-C49	-5.25	109.82	117.51
6	D	404	A1HZ4	O9-C7-C10	-4.99	106.42	113.23
6	L	404	A1HZ4	C61-O60-C49	-4.86	110.38	117.51
6	H	404	A1HZ4	C14-C15-C18	-4.60	105.05	110.16
6	L	404	A1HZ4	O60-C49-C50	-4.49	116.72	124.30
6	J	404	A1HZ4	O60-C49-C50	-4.42	116.85	124.30
6	B	404	A1HZ4	O60-C49-C50	-4.41	116.86	124.30
6	D	404	A1HZ4	C14-C15-C18	-4.29	105.41	110.16
6	L	404	A1HZ4	C16-C15-C18	-4.10	105.61	110.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	404	A1HZ4	O60-C49-C50	-4.09	117.40	124.30
6	J	404	A1HZ4	C61-O60-C49	-4.05	111.57	117.51
6	H	404	A1HZ4	O60-C49-C50	-4.00	117.56	124.30
6	B	404	A1HZ4	F45-C8-C7	-3.97	104.36	112.02
6	L	404	A1HZ4	C16-C17-N12	3.91	118.12	110.82
6	L	404	A1HZ4	C8-C7-C1	-3.81	100.35	109.51
6	H	404	A1HZ4	C14-C13-N12	3.76	117.86	110.82
6	D	404	A1HZ4	O23-C19-C18	-3.76	116.61	122.56
6	F	404	A1HZ4	C4-C5-C6	-3.69	115.68	120.24
6	H	404	A1HZ4	C40-O9-C7	-3.64	111.67	117.97
6	L	404	A1HZ4	C3-C2-C1	-3.63	117.06	120.75
6	J	404	A1HZ4	C14-C13-N12	3.43	117.23	110.82
6	B	404	A1HZ4	C16-C15-C18	-3.42	106.37	110.16
6	F	404	A1HZ4	C3-C2-C1	-3.40	117.30	120.75
6	D	404	A1HZ4	C21-N20-C19	-3.32	121.13	126.22
6	L	404	A1HZ4	O11-C10-N12	-3.32	114.42	121.77
6	F	404	A1HZ4	C8-C7-C1	-3.23	101.76	109.51
6	J	404	A1HZ4	C2-C1-C6	3.16	122.74	118.03
6	B	404	A1HZ4	C21-N20-C19	-3.12	121.44	126.22
6	J	404	A1HZ4	C3-C4-C5	3.12	124.13	119.87
6	D	404	A1HZ4	C14-C13-N12	-3.10	105.04	110.82
6	H	404	A1HZ4	C2-C1-C6	3.07	122.61	118.03
6	L	404	A1HZ4	C8-C7-C10	3.00	112.18	109.33
6	L	404	A1HZ4	C4-C5-C6	-2.96	116.58	120.24
6	D	404	A1HZ4	O11-C10-N12	-2.93	115.27	121.77
6	B	404	A1HZ4	C49-C47-C22	2.93	123.78	119.76
6	F	404	A1HZ4	F43-C8-F45	2.90	116.35	107.54
6	J	404	A1HZ4	C16-C15-C18	-2.88	106.96	110.16
6	D	404	A1HZ4	C2-C1-C6	2.86	122.29	118.03
6	F	404	A1HZ4	C21-N20-C19	-2.81	121.92	126.22
6	J	404	A1HZ4	C14-C15-C22	-2.78	107.24	111.74
6	L	404	A1HZ4	C15-C22-C47	-2.73	110.91	117.53
6	J	404	A1HZ4	C1-C7-C10	-2.73	106.76	110.50
6	H	404	A1HZ4	C16-C17-N12	-2.71	105.76	110.82
6	D	404	A1HZ4	C49-C47-C22	2.65	123.40	119.76
6	F	404	A1HZ4	O23-C19-C18	-2.65	118.36	122.56
6	B	404	A1HZ4	C4-C3-C2	-2.64	116.98	120.24
6	F	404	A1HZ4	C3-C4-C5	2.63	123.47	119.87
6	F	404	A1HZ4	F43-C8-F44	-2.62	99.59	107.54
6	J	404	A1HZ4	C49-C47-C22	2.61	123.34	119.76
6	H	404	A1HZ4	C3-C4-C5	2.60	123.43	119.87
6	J	404	A1HZ4	C4-C3-C2	-2.60	117.04	120.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	404	A1HZ4	C14-C15-C18	-2.55	107.33	110.16
6	J	404	A1HZ4	C8-C7-C1	-2.51	103.48	109.51
6	J	404	A1HZ4	C5-C6-C1	-2.51	118.20	120.75
6	H	404	A1HZ4	O11-C10-C7	-2.48	116.02	119.72
6	H	404	A1HZ4	C15-C22-C47	-2.47	111.54	117.53
6	J	404	A1HZ4	O11-C10-N12	-2.45	116.35	121.77
6	L	404	A1HZ4	C2-C1-C6	2.45	121.68	118.03
6	H	404	A1HZ4	O9-C7-C10	-2.44	109.91	113.23
6	H	404	A1HZ4	O11-C10-N12	-2.40	116.44	121.77
6	L	404	A1HZ4	C1-C7-C10	-2.40	107.21	110.50
6	H	404	A1HZ4	O23-C19-C18	-2.39	118.78	122.56
6	L	404	A1HZ4	C3-C4-C5	2.37	123.11	119.87
6	B	404	A1HZ4	C8-C7-C1	-2.37	103.83	109.51
6	D	404	A1HZ4	C16-C15-C18	-2.35	107.55	110.16
6	F	404	A1HZ4	C16-C17-N12	2.33	115.19	110.82
6	L	404	A1HZ4	C14-C15-C18	-2.30	107.61	110.16
6	H	404	A1HZ4	C49-C47-C22	2.29	122.90	119.76
6	F	404	A1HZ4	C15-C22-C47	-2.27	112.02	117.53
6	B	404	A1HZ4	C5-C6-C1	-2.27	118.44	120.75
6	F	404	A1HZ4	C61-O60-C49	-2.26	114.20	117.51
6	L	404	A1HZ4	C21-N20-C19	-2.21	122.83	126.22
6	D	404	A1HZ4	C3-C4-C5	2.20	122.89	119.87
6	H	404	A1HZ4	C3-C2-C1	-2.20	118.52	120.75
6	B	404	A1HZ4	C3-C4-C5	2.20	122.88	119.87
6	J	404	A1HZ4	O11-C10-C7	-2.20	116.44	119.72
6	F	404	A1HZ4	F43-C8-C7	-2.15	107.87	112.02
6	B	404	A1HZ4	C14-C13-N12	2.13	114.80	110.82
6	J	404	A1HZ4	F45-C8-F44	2.12	113.97	107.54
6	L	404	A1HZ4	C14-C15-C22	-2.11	108.31	111.74
6	F	404	A1HZ4	C16-C15-C18	-2.08	107.85	110.16
6	F	404	A1HZ4	C2-C1-C6	2.07	121.11	118.03
6	B	404	A1HZ4	O11-C10-N12	-2.06	117.21	121.77
6	D	404	A1HZ4	F43-C8-F45	2.04	113.75	107.54
6	D	404	A1HZ4	C15-C22-C47	-2.04	112.59	117.53
6	H	404	A1HZ4	C21-N20-C19	-2.04	123.10	126.22
6	L	404	A1HZ4	O23-C19-C18	-2.03	119.35	122.56
6	B	404	A1HZ4	C2-C1-C6	2.02	121.05	118.03
6	L	404	A1HZ4	F44-C8-C7	-2.01	108.14	112.02

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	403	DPO	P1-O4-P2-O7
5	J	403	DPO	P2-O4-P1-O2
5	J	403	DPO	P1-O4-P2-O7
6	D	404	A1HZ4	C8-C7-O9-C40
6	F	404	A1HZ4	C10-C7-C8-F44
6	F	404	A1HZ4	C1-C7-C8-F44
6	F	404	A1HZ4	C1-C7-C8-F45
6	F	404	A1HZ4	O9-C7-C8-F44
6	F	404	A1HZ4	O9-C7-C8-F45
6	F	404	A1HZ4	C10-C7-C8-F45
6	D	404	A1HZ4	C1-C7-O9-C40
6	D	404	A1HZ4	C10-C7-O9-C40
5	B	403	DPO	P2-O4-P1-O1
6	F	404	A1HZ4	C50-C49-O60-C61
5	F	403	DPO	P2-O4-P1-O1
5	B	403	DPO	P2-O4-P1-O3
5	D	403	DPO	P2-O4-P1-O2
5	D	403	DPO	P2-O4-P1-O3
5	F	403	DPO	P1-O4-P2-O7
6	F	404	A1HZ4	C47-C49-O60-C61
6	D	404	A1HZ4	C50-C49-O60-C61
6	D	404	A1HZ4	C47-C49-O60-C61
5	J	403	DPO	P2-O4-P1-O1
5	D	403	DPO	P1-O4-P2-O6
5	F	403	DPO	P2-O4-P1-O2
5	F	403	DPO	P2-O4-P1-O3
6	J	404	A1HZ4	C1-C7-C8-F43
5	J	403	DPO	P1-O4-P2-O5

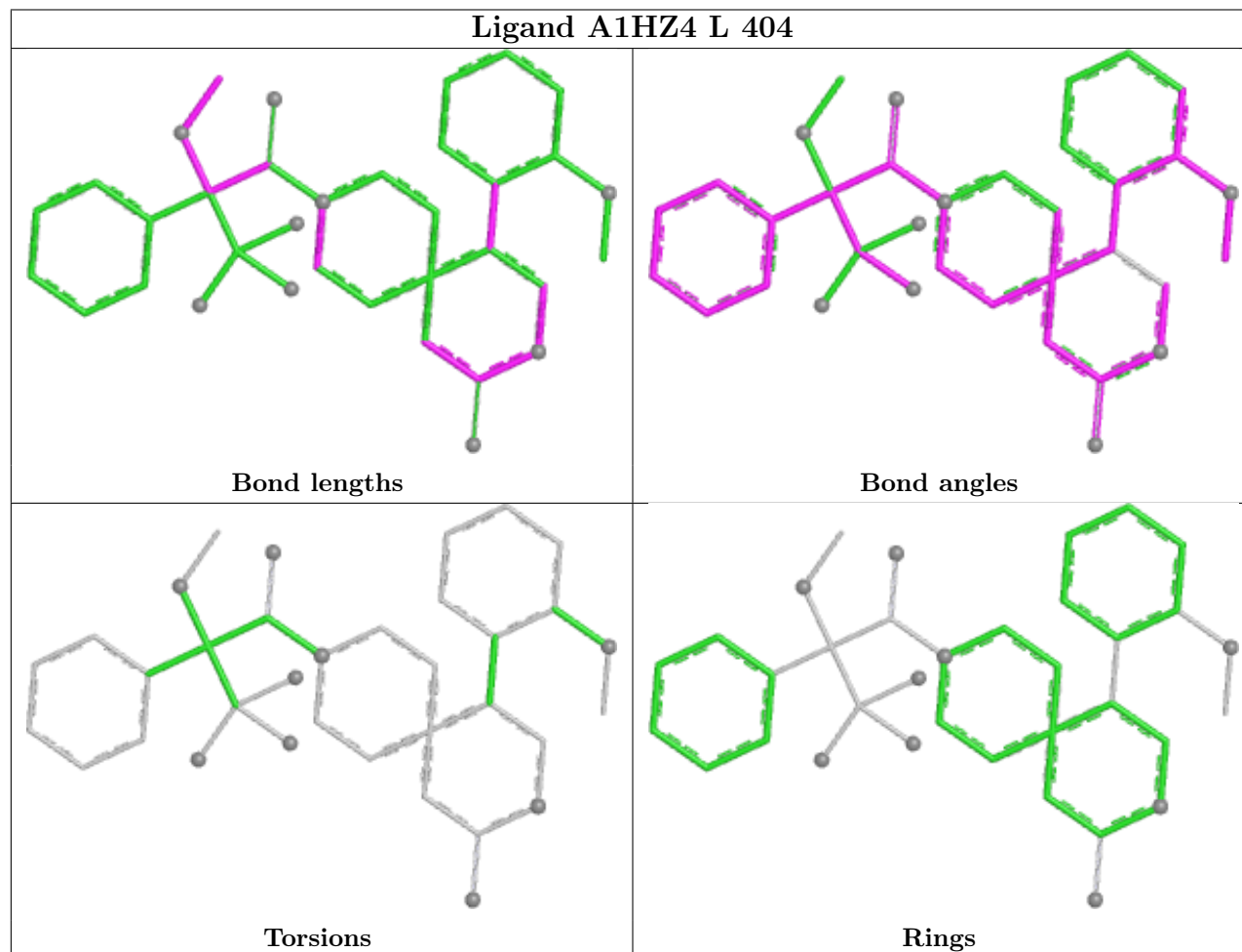
There are no ring outliers.

5 monomers are involved in 8 short contacts:

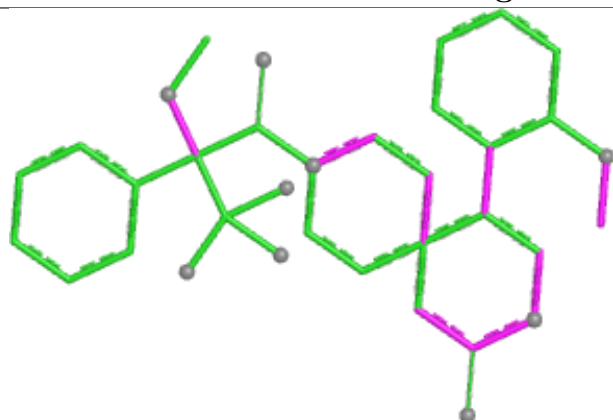
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	403	DPO	1	0
6	H	404	A1HZ4	1	0
5	H	403	DPO	2	0
5	J	403	DPO	2	0
5	D	403	DPO	2	0

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

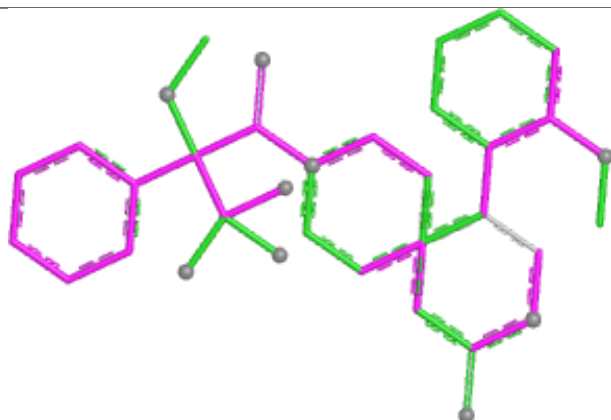
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.



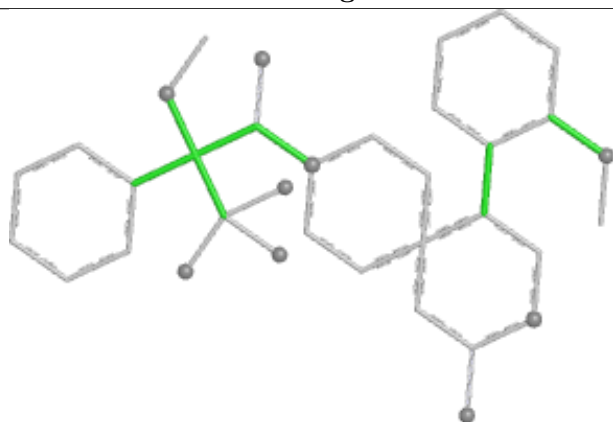
Ligand A1HZ4 B 404



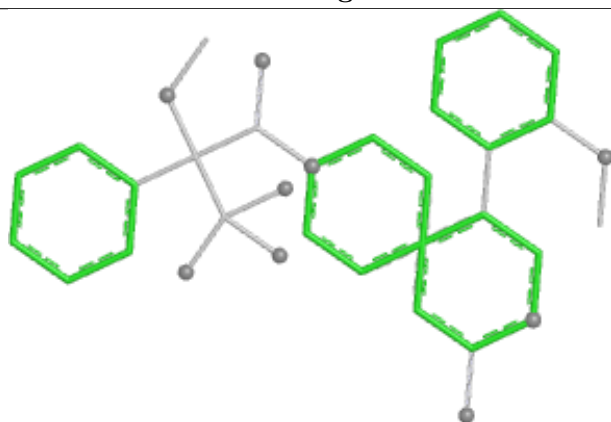
Bond lengths



Bond angles

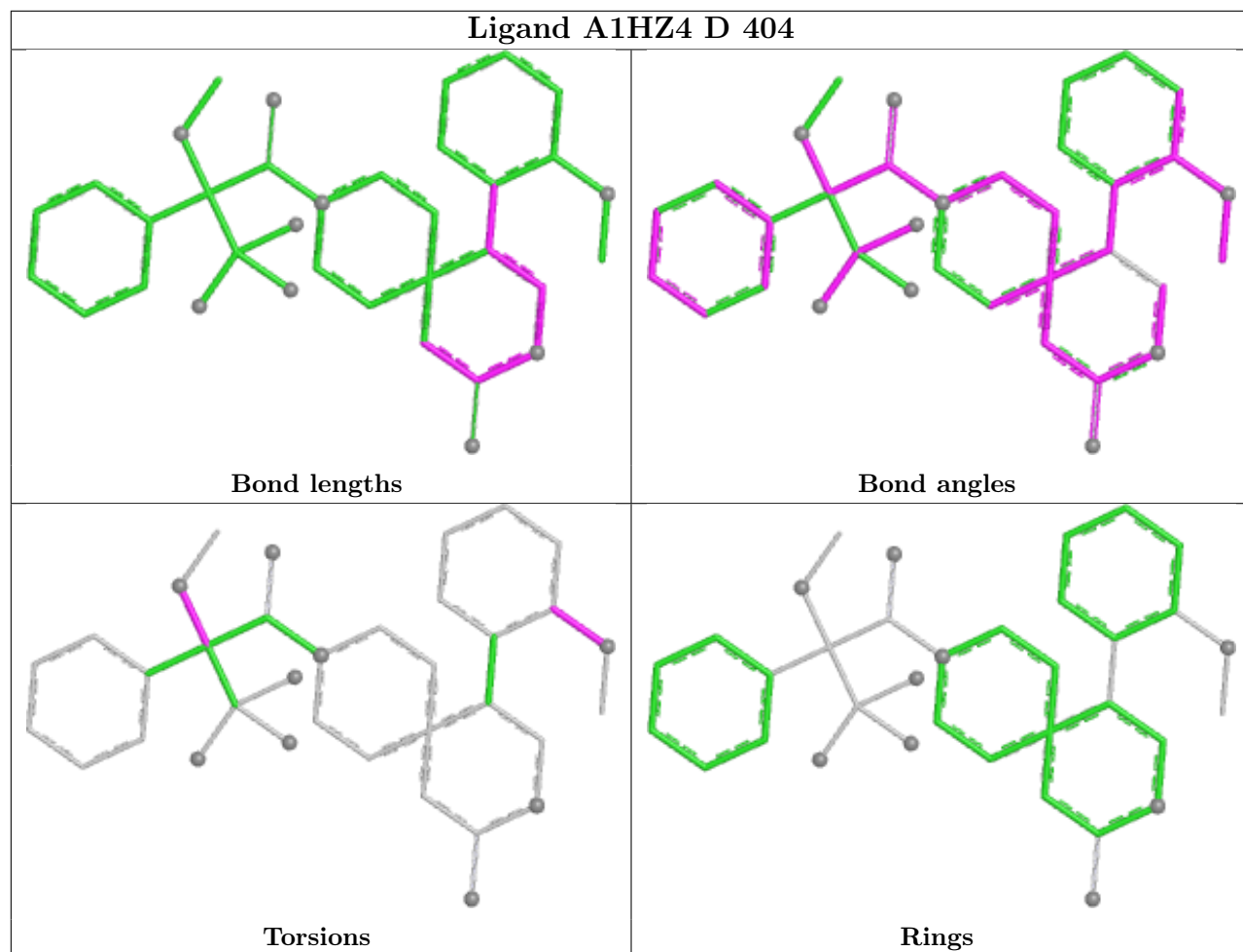


Torsions

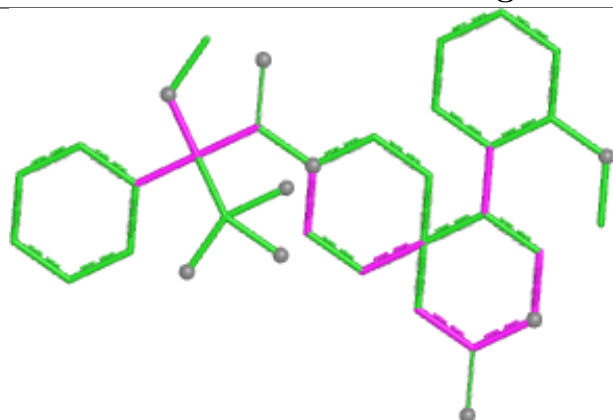


Rings

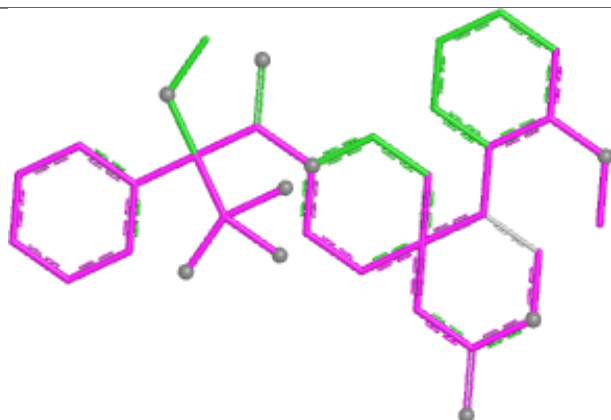
Ligand A1HZ4 D 404



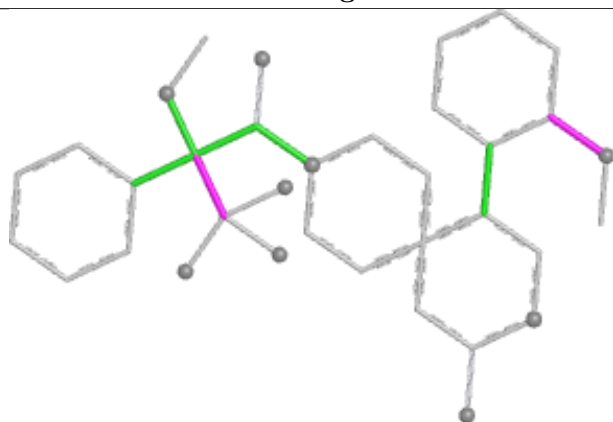
Ligand A1HZ4 F 404



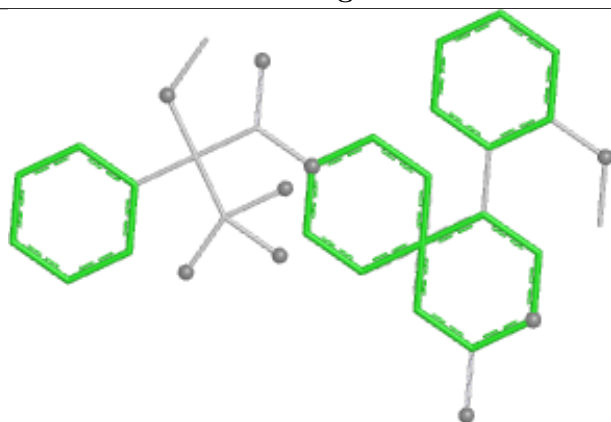
Bond lengths



Bond angles

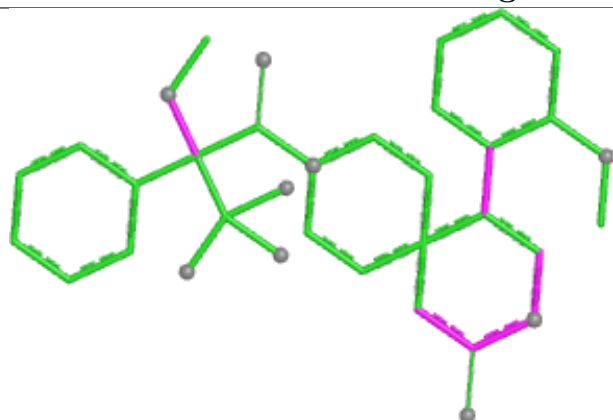


Torsions

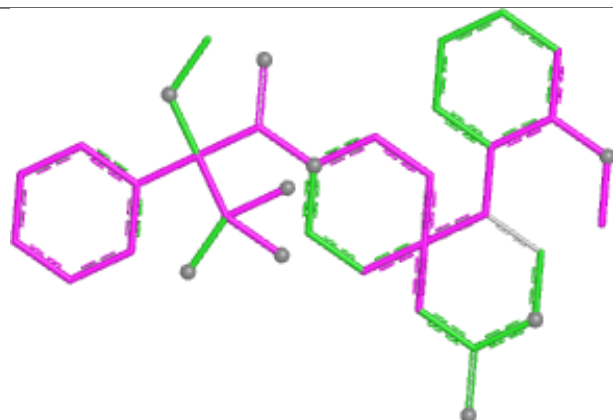


Rings

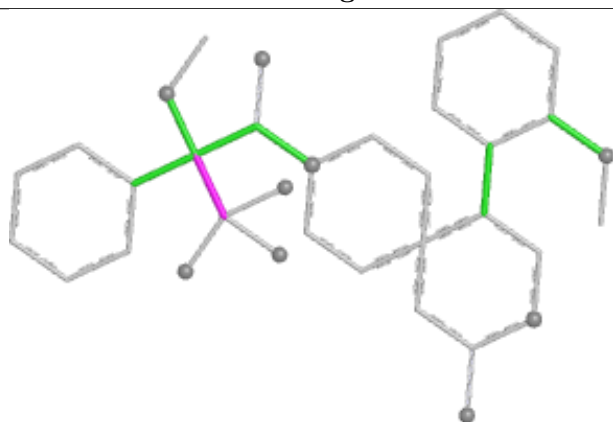
Ligand A1HZ4 J 404



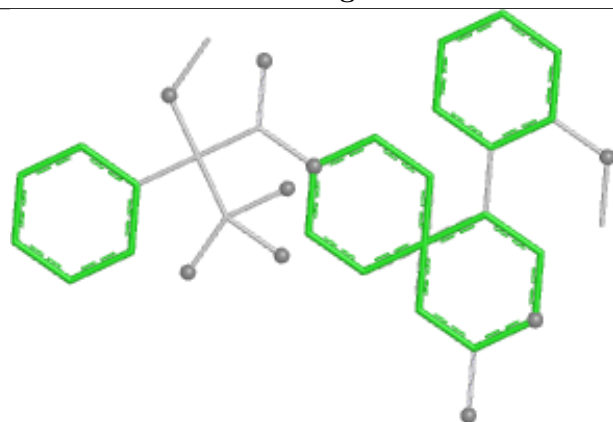
Bond lengths



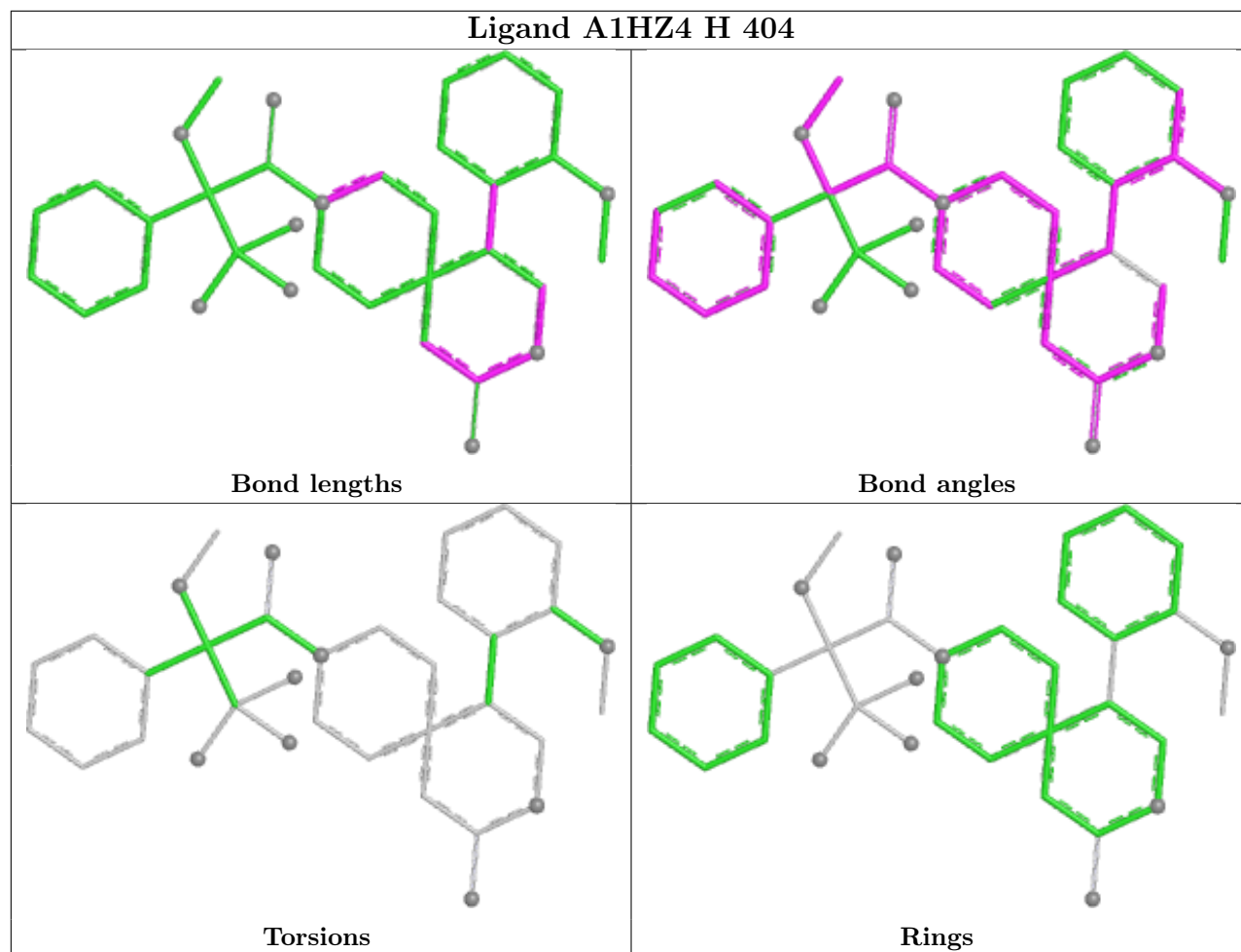
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	314/314 (100%)	-0.71	1 (0%) 90 76	52, 78, 111, 143	0
1	C	314/314 (100%)	-0.63	1 (0%) 90 76	58, 87, 122, 144	0
1	E	314/314 (100%)	-0.67	2 (0%) 85 65	56, 84, 123, 151	0
1	G	314/314 (100%)	-0.66	2 (0%) 85 65	60, 88, 125, 155	0
1	I	314/314 (100%)	-0.62	1 (0%) 90 76	62, 93, 135, 162	0
1	K	314/314 (100%)	-0.61	1 (0%) 90 76	62, 93, 131, 158	0
2	B	346/346 (100%)	-0.68	3 (0%) 81 57	50, 72, 108, 140	0
2	D	346/346 (100%)	-0.72	1 (0%) 90 76	50, 73, 109, 153	0
2	F	346/346 (100%)	-0.59	5 (1%) 73 47	58, 84, 126, 177	0
2	H	346/346 (100%)	-0.67	1 (0%) 90 76	57, 82, 120, 152	0
2	J	346/346 (100%)	-0.63	1 (0%) 90 76	62, 85, 119, 153	0
2	L	346/346 (100%)	-0.49	3 (0%) 81 57	62, 97, 140, 171	0
All	All	3960/3960 (100%)	-0.64	22 (0%) 85 65	50, 84, 126, 177	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	258	ASN	3.9
2	H	18	LEU	3.8
2	L	18	LEU	3.8
1	K	55	PHE	3.1
1	C	55	PHE	3.0
2	L	101	LEU	2.8
2	B	259	GLY	2.6
2	F	113	THR	2.6
2	F	157	GLU	2.4
1	G	55	PHE	2.4
1	A	55	PHE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	J	18	LEU	2.3
1	E	368	SER	2.3
2	F	18	LEU	2.3
2	L	304	ARG	2.3
2	B	258	ASN	2.2
2	B	18	LEU	2.2
2	D	18	LEU	2.1
1	I	55	PHE	2.0
2	F	259	GLY	2.0
1	E	55	PHE	2.0
1	G	368	SER	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.

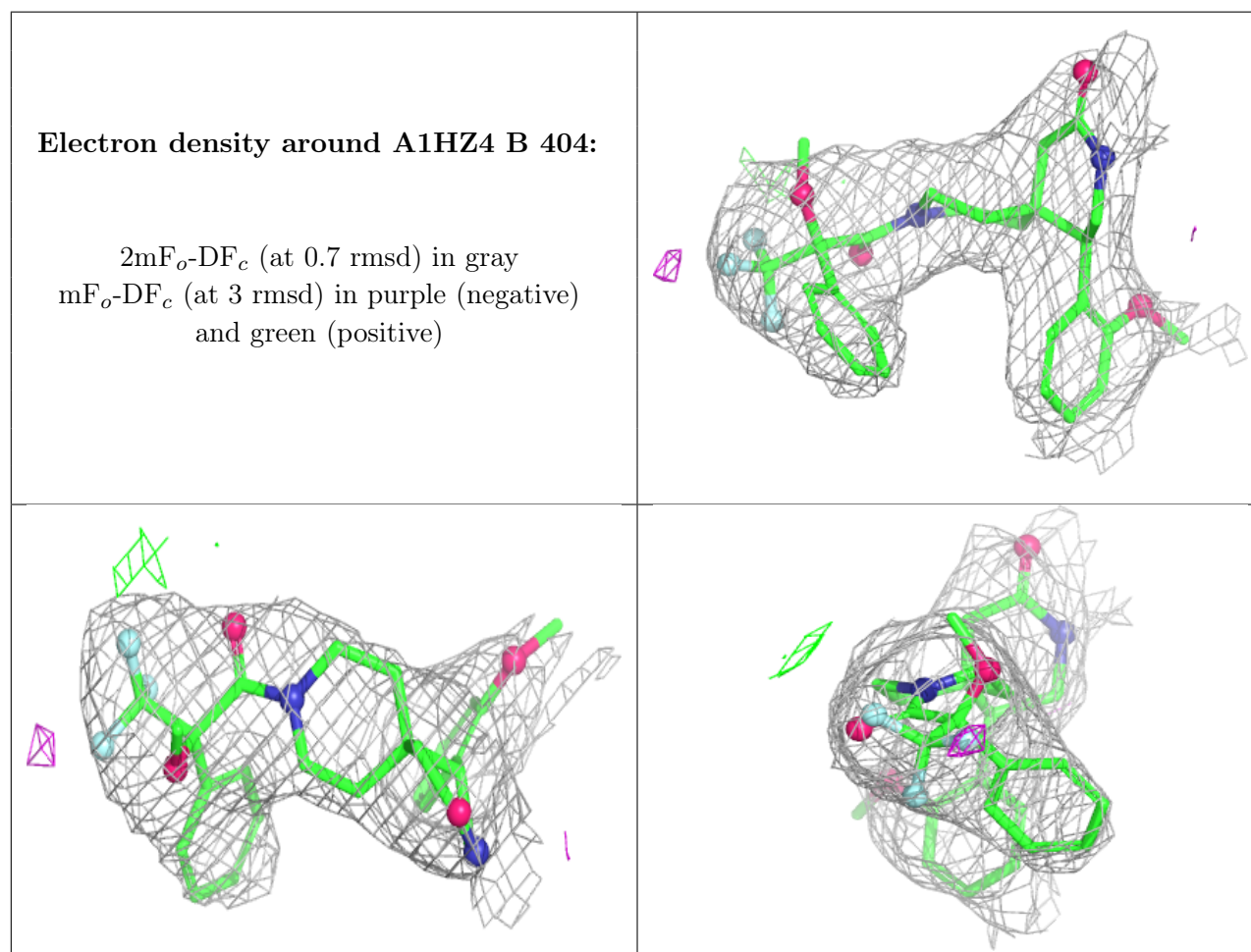
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	DPO	J	403	9/9	0.87	0.09	117,130,149,151	0
5	DPO	H	403	9/9	0.89	0.08	116,124,150,182	0
4	CL	B	402	1/1	0.89	0.13	81,81,81,81	0
4	CL	L	402	1/1	0.90	0.15	76,76,76,76	0
5	DPO	D	403	9/9	0.90	0.09	114,129,145,161	0
4	CL	J	402	1/1	0.91	0.19	91,91,91,91	0
4	CL	D	402	1/1	0.91	0.19	70,70,70,70	0
5	DPO	B	403	9/9	0.91	0.10	118,130,152,169	0
4	CL	H	402	1/1	0.94	0.10	76,76,76,76	0
5	DPO	L	403	9/9	0.94	0.16	112,126,140,142	0
5	DPO	F	403	9/9	0.95	0.16	98,124,148,161	0
4	CL	F	402	1/1	0.95	0.12	88,88,88,88	0

Continued on next page...

Continued from previous page...

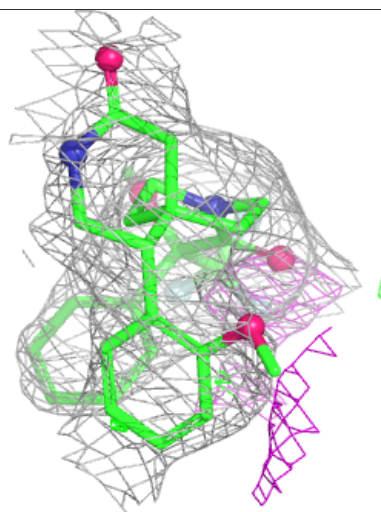
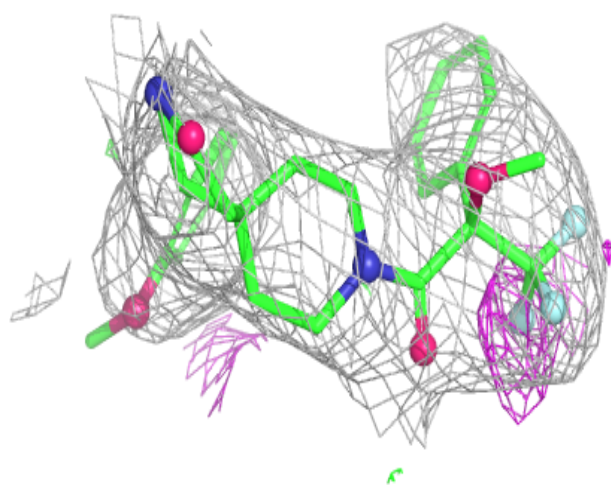
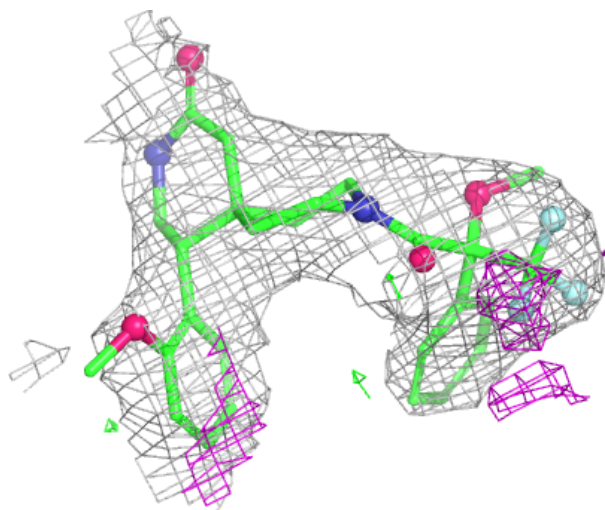
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	A1HZ4	B	404	35/35	0.98	0.08	58,75,101,113	0
6	A1HZ4	D	404	35/35	0.98	0.08	61,78,93,109	0
6	A1HZ4	F	404	35/35	0.98	0.08	67,79,97,103	0
6	A1HZ4	H	404	35/35	0.98	0.08	74,82,111,120	0
6	A1HZ4	J	404	35/35	0.98	0.08	71,82,103,109	0
6	A1HZ4	L	404	35/35	0.98	0.09	73,92,116,125	0
3	ZN	L	401	1/1	0.99	0.04	70,70,70,70	0
3	ZN	J	401	1/1	1.00	0.02	64,64,64,64	0
3	ZN	B	401	1/1	1.00	0.02	50,50,50,50	0
3	ZN	D	401	1/1	1.00	0.01	63,63,63,63	0
3	ZN	F	401	1/1	1.00	0.02	61,61,61,61	0
3	ZN	H	401	1/1	1.00	0.01	63,63,63,63	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.



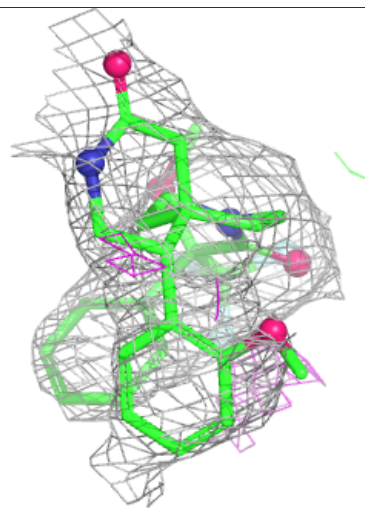
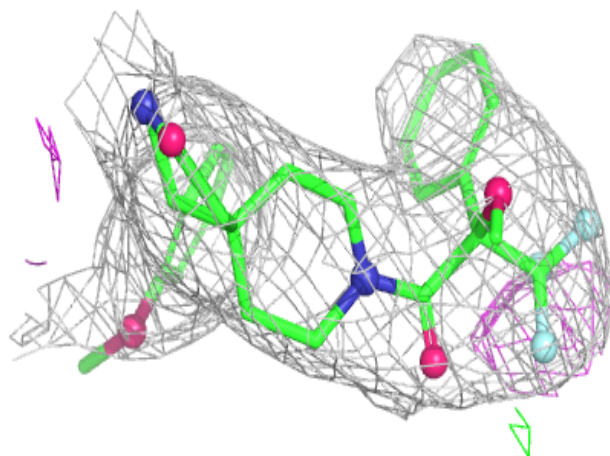
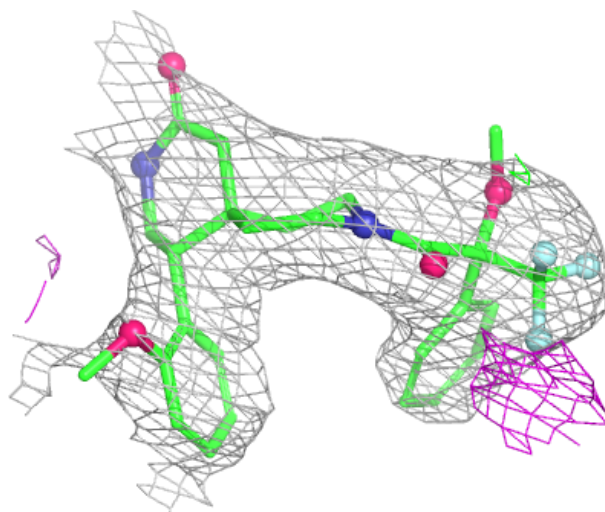
Electron density around A1HZ4 D 404:

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



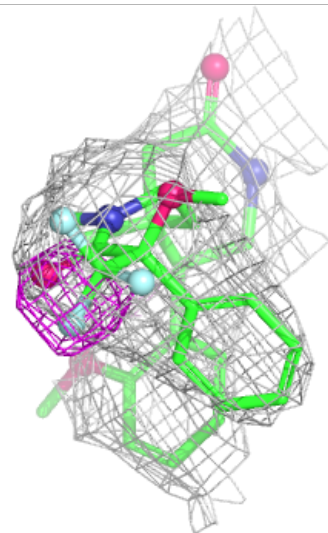
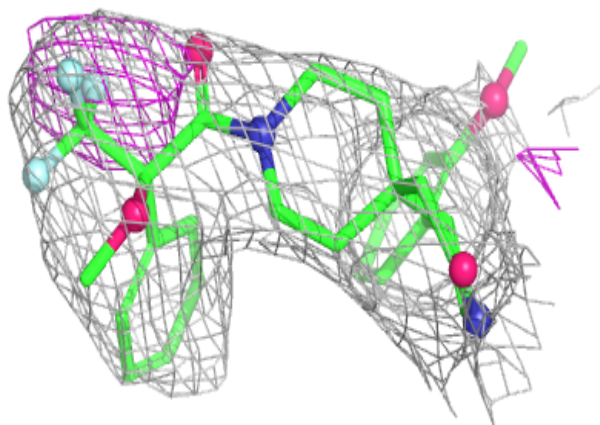
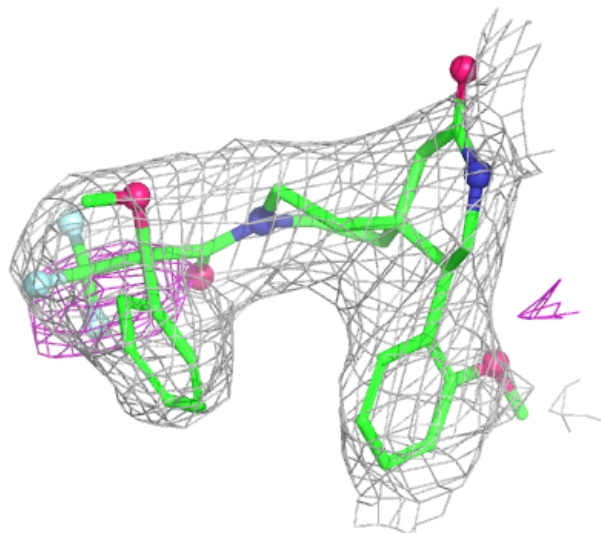
Electron density around A1HZ4 F 404:

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



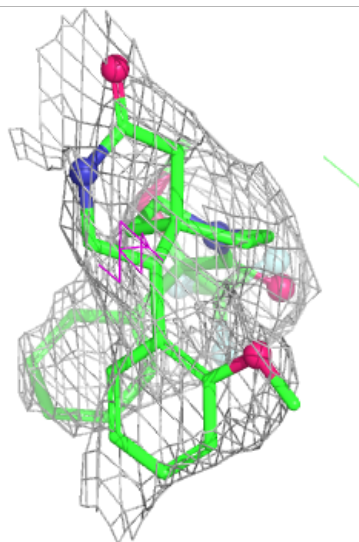
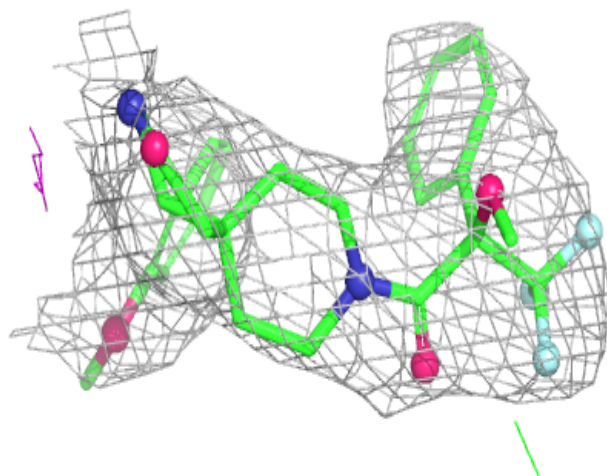
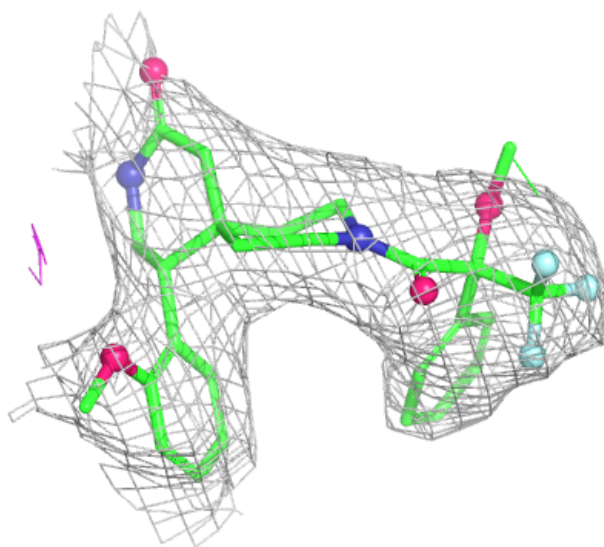
Electron density around A1HZ4 H 404:

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



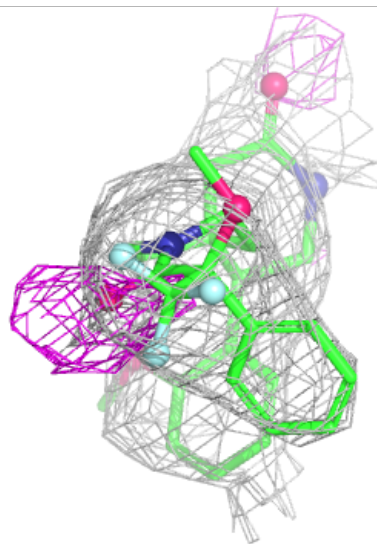
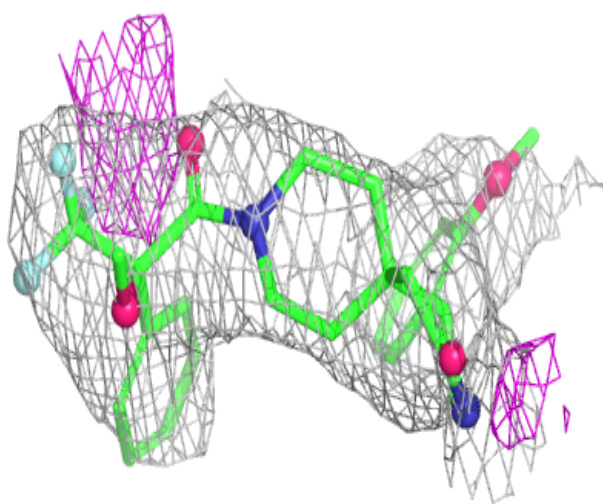
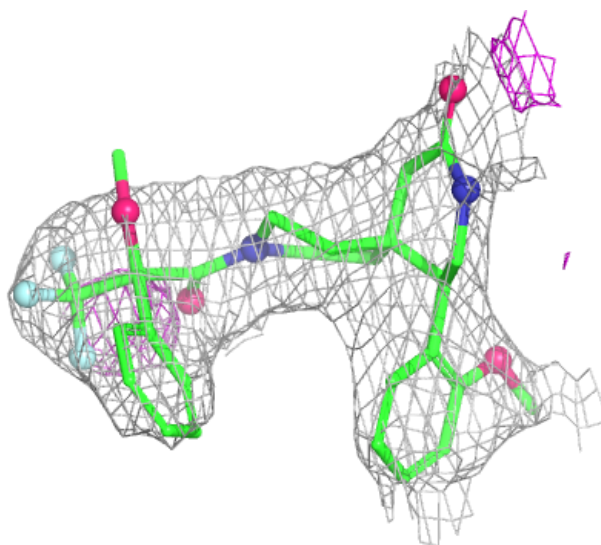
Electron density around A1HZ4 J 404:

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



Electron density around A1HZ4 L 404:

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.