



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:48 AM UTC

PDB ID : 1Z9H / pdb_00001z9h
Title : Microsomal prostaglandin E synthase type-2
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Deposited on : 2005-04-02
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

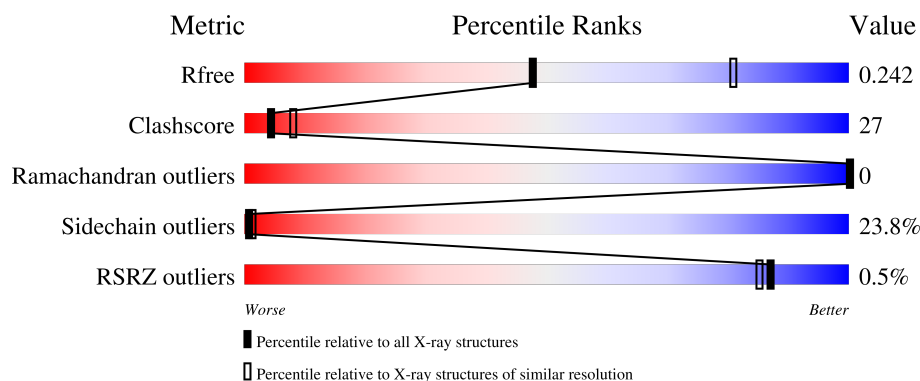
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	290	 47% 37% 10% • 6%
1	B	290	 45% 35% 14% • 6%
1	C	290	 44% 39% 10% • 6%
1	D	290	 46% 36% 12% • 6%

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
3	IMN	A	379	-	X	-	-
3	IMN	B	381	-	X	-	-
3	IMN	C	379	-	X	-	-
3	IMN	D	476	-	X	-	-

2 Entry composition [i](#)

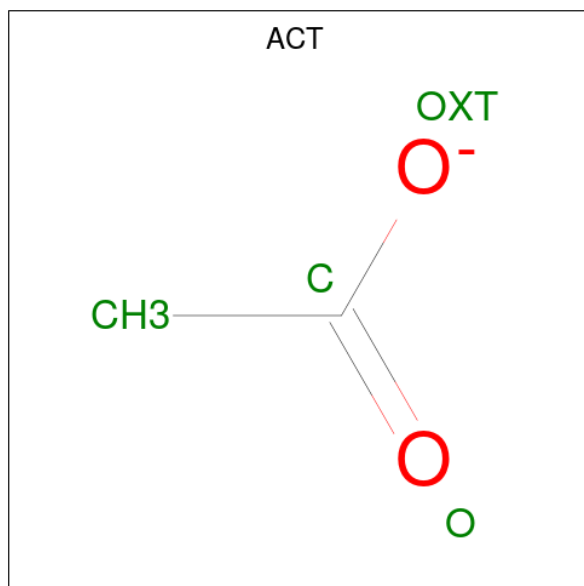
There are 5 unique types of molecules in this entry. The entry contains 9064 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 membrane-associated prostaglandin E synthase-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2214	1421	376	407	10			
1	B	274	Total	C	N	O	S	0	0	0
			2214	1421	376	407	10			
1	C	274	Total	C	N	O	S	0	0	0
			2214	1421	376	407	10			
1	D	274	Total	C	N	O	S	0	0	0
			2214	1421	376	407	10			

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



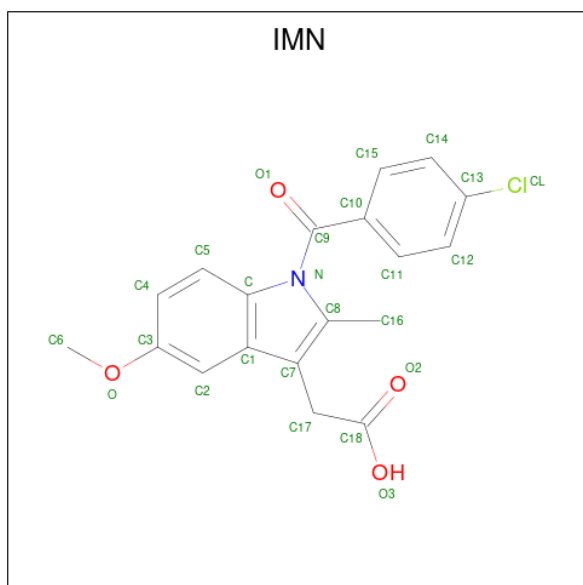
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is INDOMETHACIN (CCD ID: IMN) (formula: $C_{19}H_{16}ClNO_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			25	19	1	1	4		
3	B	1	Total	C	Cl	N	O	0	0
			25	19	1	1	4		
3	C	1	Total	C	Cl	N	O	0	0
			25	19	1	1	4		
3	D	1	Total	C	Cl	N	O	0	0
			25	19	1	1	4		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Cl	0	0
			2	2		
4	D	2	Total	Cl	0	0
			2	2		

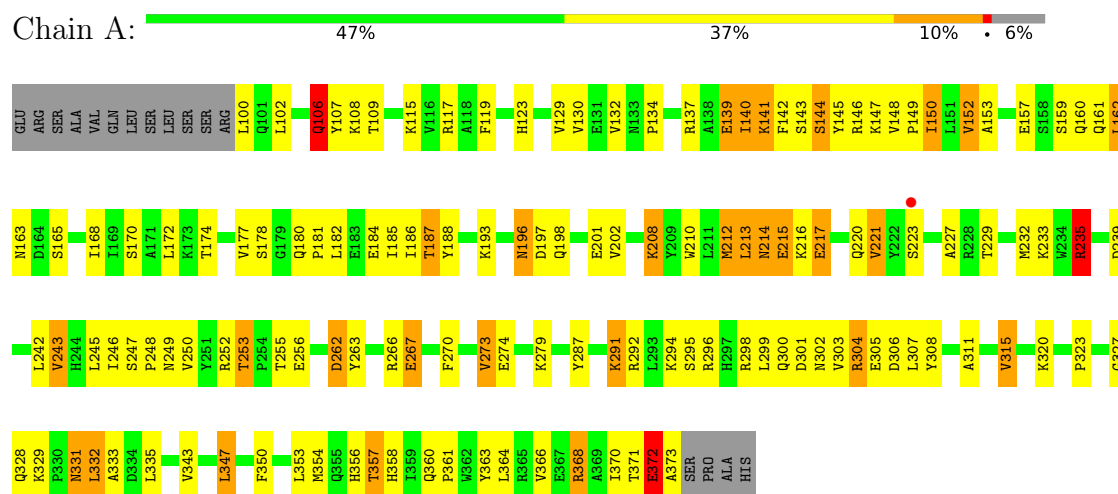
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	23	Total 23	O 23	0	0
5	B	26	Total 26	O 26	0	0
5	C	21	Total 21	O 21	0	0
5	D	18	Total 18	O 18	0	0

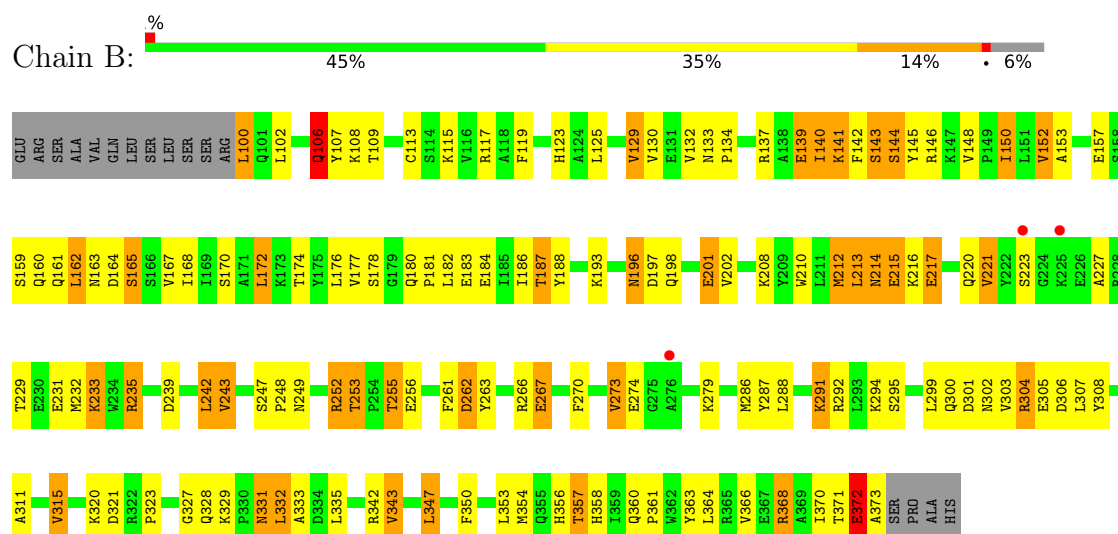
3 Residue-property plots

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: membrane-associated prostaglandin E synthase-2

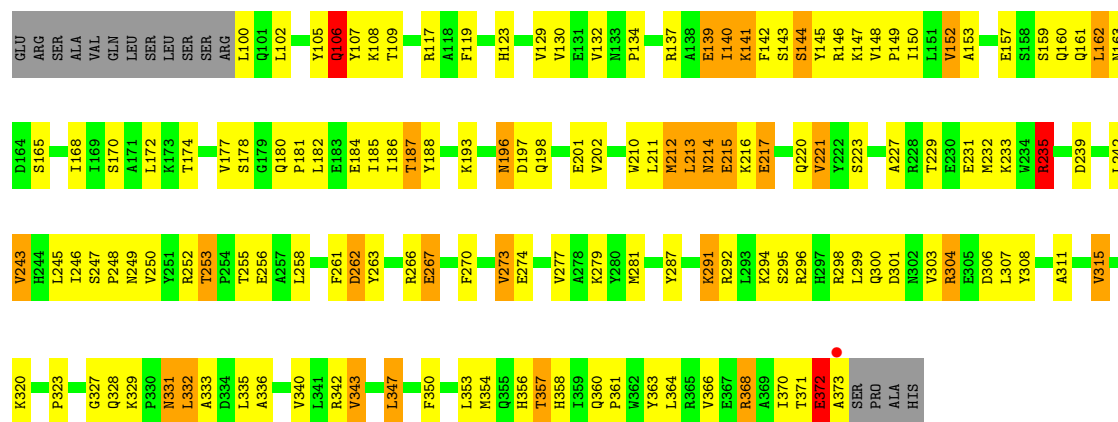


- Molecule 1: membrane-associated prostaglandin E synthase-2



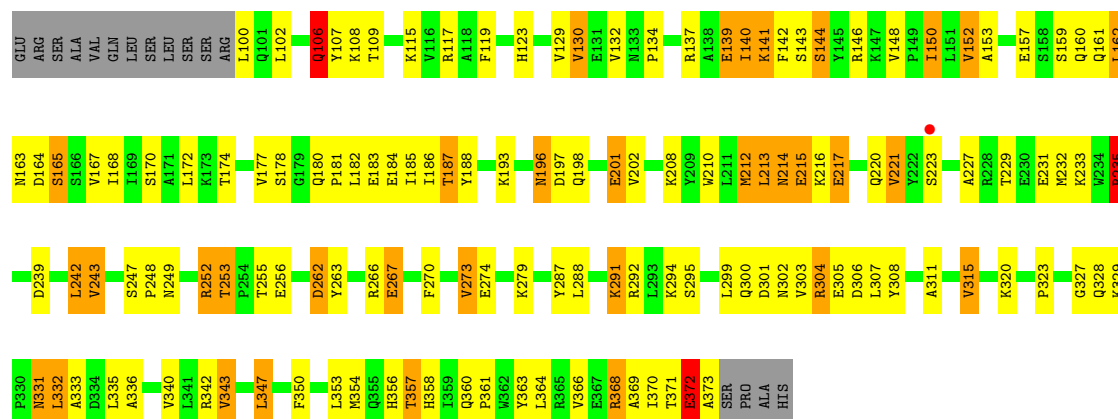
- Molecule 1: membrane-associated prostaglandin E synthase-2





- Molecule 1: membrane-associated prostaglandin E synthase-2

Chain D: 46% 36% 12% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.24Å 122.83Å 111.53Å 90.00° 110.60° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.60) 96.4 (20.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.51 (at 2.59Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.251 0.203 , 0.242	Depositor DCC
R_{free} test set	4812 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.13 , 25.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9064	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.76% 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: IMN, CL, ACT

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	0.45	0/2266	0.93	10/3070 (0.3%)
1	B	0.46	0/2266	0.94	9/3070 (0.3%)
1	C	0.43	0/2266	0.92	8/3070 (0.3%)
1	D	0.44	0/2266	0.93	11/3070 (0.4%)
All	All	0.45	0/9064	0.93	38/12280 (0.3%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	163	ASN	N-CA-C	7.86	123.59	111.56
1	D	163	ASN	N-CA-C	7.69	123.33	111.56
1	A	163	ASN	N-CA-C	7.26	122.67	111.56
1	C	163	ASN	N-CA-C	7.15	122.50	111.56
1	C	106	GLN	N-CA-C	6.89	118.25	108.74
1	B	107	TYR	N-CA-C	-6.50	96.64	108.02
1	A	106	GLN	N-CA-C	6.37	117.53	108.74
1	C	357	THR	N-CA-C	6.24	123.44	114.39
1	D	106	GLN	N-CA-C	6.21	117.32	108.74
1	A	357	THR	N-CA-C	6.16	123.32	114.39
1	B	106	GLN	N-CA-C	6.11	117.17	108.74
1	B	262	ASP	N-CA-C	-5.97	104.69	111.14
1	B	357	THR	N-CA-C	5.96	123.04	114.39
1	C	262	ASP	N-CA-C	-5.95	104.71	111.14
1	A	262	ASP	N-CA-C	-5.94	104.72	111.14
1	B	372	GLU	N-CA-C	-5.81	106.53	113.21
1	D	262	ASP	N-CA-C	-5.78	104.89	111.14
1	D	372	GLU	N-CA-C	-5.74	106.61	113.21
1	B	144	SER	N-CA-C	-5.69	105.83	112.89
1	D	357	THR	N-CA-C	5.68	122.62	114.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	372	GLU	N-CA-C	-5.67	106.69	113.21
1	C	372	GLU	N-CA-C	-5.65	106.71	113.21
1	D	144	SER	N-CA-C	-5.62	105.92	112.89
1	B	242	LEU	N-CA-C	5.54	117.00	111.07
1	A	235	ARG	N-CA-C	-5.46	105.41	111.36
1	C	107	TYR	N-CA-C	-5.41	96.82	107.69
1	D	107	TYR	N-CA-C	-5.37	96.89	107.69
1	B	150	ILE	N-CA-C	-5.36	100.51	108.45
1	A	208	LYS	N-CA-C	5.32	118.88	112.38
1	A	107	TYR	N-CA-C	-5.31	97.02	107.69
1	D	235	ARG	N-CA-C	-5.24	105.64	111.36
1	D	150	ILE	N-CA-C	-5.21	100.74	108.45
1	C	144	SER	N-CA-C	-5.18	106.47	112.89
1	A	144	SER	N-CA-C	-5.17	106.48	112.89
1	D	242	LEU	N-CA-C	5.08	116.51	111.07
1	C	235	ARG	N-CA-C	-5.07	105.84	111.36
1	A	150	ILE	N-CA-C	-5.07	100.95	108.45
1	D	369	ALA	N-CA-C	-5.04	105.97	111.82

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	2214	0	2197	117	0
1	B	2214	0	2197	131	1
1	C	2214	0	2197	127	0
1	D	2214	0	2197	123	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
2	C	4	0	3	0	0
2	D	4	0	3	0	0
3	A	25	0	15	2	0
3	B	25	0	15	2	0
3	C	25	0	15	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	25	0	15	2	0
4	B	2	0	0	0	0
4	D	2	0	0	0	0
5	A	23	0	0	2	0
5	B	26	0	0	3	0
5	C	21	0	0	6	0
5	D	18	0	0	2	0
All	All	9064	0	8860	476	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (476) 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:B:368:ARG:HD3	5:B:18:HOH:O	1.58	1.02
1:C:214:ASN:C	1:C:214:ASN:HD22	1.72	0.98
1:A:214:ASN:HD22	1:A:214:ASN:C	1.72	0.97
1:D:214:ASN:C	1:D:214:ASN:HD22	1.72	0.97
1:B:214:ASN:C	1:B:214:ASN:HD22	1.73	0.94
1:A:299:LEU:HD23	1:A:303:VAL:HG13	1.50	0.94
1:B:299:LEU:HD23	1:B:303:VAL:HG13	1.51	0.92
1:C:299:LEU:HD23	1:C:303:VAL:HG13	1.49	0.92
1:D:299:LEU:HD23	1:D:303:VAL:HG13	1.52	0.90
1:A:368:ARG:HD3	5:A:17:HOH:O	1.70	0.90
1:A:170:SER:O	1:A:174:THR:HG23	1.74	0.87
1:C:214:ASN:ND2	1:C:217:GLU:HG2	1.90	0.87
1:B:106:GLN:HE22	1:B:117:ARG:HE	1.23	0.86
1:C:170:SER:O	1:C:174:THR:HG23	1.74	0.86
1:B:214:ASN:ND2	1:B:217:GLU:HG2	1.91	0.84
1:B:170:SER:O	1:B:174:THR:HG23	1.78	0.84
1:D:170:SER:O	1:D:174:THR:HG23	1.78	0.83
1:C:106:GLN:HE22	1:C:117:ARG:HE	1.26	0.83
1:D:214:ASN:ND2	1:D:217:GLU:HG2	1.94	0.83
1:A:214:ASN:ND2	1:A:217:GLU:HG2	1.93	0.83
1:C:279:LYS:HD3	5:C:82:HOH:O	1.79	0.83
1:D:106:GLN:HE22	1:D:117:ARG:HE	1.26	0.81
1:C:364:LEU:O	1:C:368:ARG:HG2	1.81	0.81
1:A:364:LEU:O	1:A:368:ARG:HG2	1.81	0.81
1:C:140:ILE:HD12	1:C:150:ILE:HD12	1.63	0.80
1:A:106:GLN:HE22	1:A:117:ARG:HE	1.30	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ILE:HD12	1:A:150:ILE:HD12	1.64	0.79
1:B:364:LEU:O	1:B:368:ARG:HG2	1.82	0.79
1:D:364:LEU:O	1:D:368:ARG:HG2	1.82	0.79
1:B:132:VAL:HA	1:B:139:GLU:HG3	1.63	0.78
1:A:239:ASP:HA	1:A:243:VAL:HG13	1.64	0.78
1:D:140:ILE:HD12	1:D:150:ILE:HD12	1.66	0.78
1:D:141:LYS:HD2	1:D:146:ARG:HH12	1.49	0.78
1:C:132:VAL:HA	1:C:139:GLU:HG3	1.65	0.77
1:D:239:ASP:HA	1:D:243:VAL:HG13	1.65	0.77
1:C:239:ASP:HA	1:C:243:VAL:HG13	1.65	0.77
1:C:141:LYS:HD2	1:C:146:ARG:HH12	1.50	0.77
1:A:132:VAL:HA	1:A:139:GLU:HG3	1.66	0.76
1:A:141:LYS:HD2	1:A:146:ARG:HH12	1.50	0.76
1:B:229:THR:HA	1:B:232:MET:HE2	1.68	0.76
1:B:239:ASP:HA	1:B:243:VAL:HG13	1.68	0.76
1:B:140:ILE:HD12	1:B:150:ILE:HD12	1.67	0.76
1:D:132:VAL:HA	1:D:139:GLU:HG3	1.68	0.74
1:C:253:THR:HG22	1:C:256:GLU:HB2	1.69	0.74
1:C:368:ARG:HD3	5:C:19:HOH:O	1.89	0.73
1:D:235:ARG:HG2	1:D:235:ARG:HH21	1.53	0.73
1:B:141:LYS:HD2	1:B:146:ARG:HH12	1.54	0.72
1:D:253:THR:HG22	1:D:256:GLU:HB2	1.70	0.72
1:B:177:VAL:HG21	1:B:213:LEU:HD11	1.71	0.72
1:A:253:THR:HG22	1:A:256:GLU:HB2	1.72	0.72
1:A:214:ASN:HB2	1:B:215:GLU:OE1	1.89	0.71
1:A:253:THR:HG22	1:A:256:GLU:H	1.55	0.71
1:D:229:THR:HA	1:D:232:MET:HE2	1.72	0.71
1:D:235:ARG:HD2	1:D:332:LEU:HB3	1.73	0.71
1:D:235:ARG:HG2	1:D:235:ARG:NH2	2.06	0.71
1:A:235:ARG:HG2	1:A:235:ARG:HH21	1.56	0.70
1:B:253:THR:HG22	1:B:256:GLU:H	1.55	0.70
1:D:368:ARG:HD3	5:D:482:HOH:O	1.89	0.70
1:A:177:VAL:HG21	1:A:213:LEU:HD11	1.74	0.70
1:C:253:THR:HG22	1:C:256:GLU:H	1.56	0.70
1:B:182:LEU:O	1:B:186:ILE:HG23	1.91	0.70
1:D:177:VAL:HG21	1:D:213:LEU:HD11	1.73	0.70
1:D:165:SER:HB3	5:D:480:HOH:O	1.92	0.69
1:D:182:LEU:O	1:D:186:ILE:HG23	1.93	0.69
1:C:182:LEU:O	1:C:186:ILE:HG23	1.93	0.69
1:B:177:VAL:CG2	1:B:213:LEU:HD11	2.22	0.69
1:C:137:ARG:O	1:C:141:LYS:HD3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:THR:HA	1:C:232:MET:HE2	1.73	0.68
1:A:235:ARG:HD2	1:A:332:LEU:HB3	1.74	0.68
1:C:263:TYR:O	1:C:267:GLU:HB2	1.94	0.68
1:B:235:ARG:HG2	1:B:235:ARG:NH2	2.08	0.68
1:B:253:THR:HG22	1:B:256:GLU:HB2	1.75	0.68
1:B:249:ASN:ND2	1:B:303:VAL:HG12	2.09	0.68
1:B:235:ARG:HD2	1:B:332:LEU:HB3	1.76	0.68
1:D:249:ASN:ND2	1:D:303:VAL:HG12	2.09	0.68
1:B:235:ARG:HG2	1:B:235:ARG:HH21	1.58	0.68
1:A:177:VAL:CG2	1:A:213:LEU:HD11	2.24	0.68
1:A:182:LEU:O	1:A:186:ILE:HG23	1.93	0.68
1:C:258:LEU:HA	5:C:82:HOH:O	1.94	0.68
1:C:331:ASN:C	1:C:331:ASN:HD22	2.02	0.67
1:D:177:VAL:CG2	1:D:213:LEU:HD11	2.25	0.67
1:A:137:ARG:O	1:A:141:LYS:HD3	1.94	0.67
1:A:263:TYR:O	1:A:267:GLU:HB2	1.94	0.67
1:D:331:ASN:C	1:D:331:ASN:HD22	2.02	0.67
1:C:140:ILE:CD1	1:C:150:ILE:HD12	2.25	0.67
1:C:235:ARG:HD2	1:C:332:LEU:HB3	1.75	0.67
1:A:140:ILE:CD1	1:A:150:ILE:HD12	2.24	0.67
1:A:229:THR:HA	1:A:232:MET:HE2	1.75	0.67
1:C:214:ASN:C	1:C:214:ASN:ND2	2.46	0.67
1:B:331:ASN:C	1:B:331:ASN:HD22	2.02	0.67
1:A:331:ASN:HD22	1:A:331:ASN:C	2.02	0.66
1:C:214:ASN:HB2	1:D:215:GLU:OE1	1.95	0.66
1:C:174:THR:HG21	1:C:212:MET:H	1.60	0.66
1:D:311:ALA:O	1:D:315:VAL:HG13	1.95	0.66
1:D:253:THR:HG22	1:D:256:GLU:H	1.59	0.66
1:C:177:VAL:HG21	1:C:213:LEU:HD11	1.78	0.66
1:C:235:ARG:HG2	1:C:235:ARG:HH21	1.61	0.65
1:B:263:TYR:O	1:B:267:GLU:HB2	1.96	0.65
1:C:248:PRO:HB2	1:C:303:VAL:HG11	1.77	0.65
1:C:177:VAL:CG2	1:C:213:LEU:HD11	2.26	0.65
1:C:235:ARG:HG2	1:C:235:ARG:NH2	2.11	0.65
1:D:157:GLU:H	1:D:157:GLU:CD	2.05	0.65
1:A:235:ARG:HG2	1:A:235:ARG:NH2	2.09	0.65
1:B:140:ILE:CD1	1:B:150:ILE:HD12	2.27	0.65
1:B:157:GLU:H	1:B:157:GLU:CD	2.05	0.64
1:A:187:THR:HG23	1:B:229:THR:HG21	1.79	0.64
1:B:311:ALA:O	1:B:315:VAL:HG13	1.98	0.64
1:C:157:GLU:CD	1:C:157:GLU:H	2.06	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:THR:HG21	1:A:212:MET:H	1.62	0.64
1:C:214:ASN:HD21	1:C:217:GLU:H	1.46	0.64
1:A:214:ASN:C	1:A:214:ASN:ND2	2.46	0.63
1:A:366:VAL:O	1:A:370:ILE:HG13	1.99	0.63
1:C:249:ASN:ND2	1:C:303:VAL:HG12	2.14	0.63
1:D:140:ILE:CD1	1:D:150:ILE:HD12	2.28	0.63
1:D:263:TYR:O	1:D:267:GLU:HB2	1.98	0.63
1:C:304:ARG:HG3	1:C:308:TYR:CZ	2.34	0.63
1:B:137:ARG:O	1:B:141:LYS:HD3	1.99	0.62
1:B:174:THR:HG21	1:B:212:MET:H	1.64	0.62
1:B:214:ASN:HD21	1:B:217:GLU:H	1.47	0.62
1:C:187:THR:HG23	1:D:229:THR:HG21	1.82	0.62
1:A:180:GLN:HG3	1:A:181:PRO:HD2	1.82	0.62
1:A:249:ASN:ND2	1:A:303:VAL:HG12	2.15	0.62
1:D:174:THR:HG21	1:D:212:MET:H	1.66	0.61
1:A:273:VAL:HG13	1:A:274:GLU:H	1.65	0.61
1:B:214:ASN:ND2	1:B:217:GLU:H	1.99	0.61
1:D:137:ARG:O	1:D:141:LYS:HD3	2.01	0.61
1:A:157:GLU:CD	1:A:157:GLU:H	2.09	0.60
1:C:253:THR:CG2	1:C:256:GLU:H	2.15	0.60
1:C:273:VAL:HG13	1:C:274:GLU:H	1.66	0.60
1:A:304:ARG:HG3	1:A:308:TYR:CZ	2.37	0.60
1:C:217:GLU:O	1:C:221:VAL:HG13	2.01	0.60
1:A:217:GLU:O	1:A:221:VAL:HG13	2.01	0.60
1:D:273:VAL:HG13	1:D:274:GLU:H	1.67	0.60
1:D:214:ASN:HD21	1:D:217:GLU:H	1.49	0.59
1:C:311:ALA:O	1:C:315:VAL:HG13	2.01	0.59
1:B:366:VAL:O	1:B:370:ILE:HG13	2.01	0.59
1:D:214:ASN:ND2	1:D:217:GLU:H	2.00	0.59
1:A:311:ALA:O	1:A:315:VAL:HG13	2.02	0.59
1:B:262:ASP:HB2	1:B:279:LYS:HE2	1.85	0.59
1:B:273:VAL:HG13	1:B:274:GLU:H	1.68	0.59
1:D:304:ARG:HG3	1:D:308:TYR:CZ	2.37	0.59
1:D:357:THR:O	1:D:358:HIS:HB2	2.03	0.59
1:C:180:GLN:HG3	1:C:181:PRO:HD2	1.85	0.59
1:D:217:GLU:O	1:D:221:VAL:HG13	2.02	0.58
1:A:214:ASN:HD21	1:A:217:GLU:H	1.51	0.58
1:B:217:GLU:O	1:B:221:VAL:HG13	2.03	0.58
1:B:180:GLN:HG3	1:B:181:PRO:HD2	1.85	0.58
1:B:304:ARG:HG3	1:B:308:TYR:CZ	2.38	0.58
1:A:357:THR:O	1:A:358:HIS:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:LEU:HB2	1:C:168:ILE:HG12	1.85	0.58
1:A:210:TRP:CE2	1:B:212:MET:HE2	2.39	0.58
1:A:300:GLN:HG3	1:A:306:ASP:OD1	2.04	0.58
1:C:181:PRO:HG2	1:C:184:GLU:CD	2.28	0.58
1:A:248:PRO:HB2	1:A:303:VAL:HG11	1.84	0.58
1:A:253:THR:CG2	1:A:256:GLU:H	2.17	0.58
1:B:357:THR:O	1:B:358:HIS:HB2	2.04	0.58
1:D:235:ARG:HH21	1:D:235:ARG:CG	2.16	0.58
1:C:366:VAL:O	1:C:370:ILE:HG13	2.04	0.57
1:D:188:TYR:CD1	1:D:212:MET:HG2	2.39	0.57
1:B:235:ARG:HH21	1:B:235:ARG:CG	2.17	0.57
1:B:188:TYR:CD1	1:B:212:MET:HG2	2.40	0.57
1:C:262:ASP:HB2	1:C:279:LYS:HE2	1.85	0.57
1:D:248:PRO:HB2	1:D:303:VAL:HG11	1.85	0.57
1:A:350:PHE:CZ	1:A:354:MET:HE2	2.40	0.57
1:D:106:GLN:NE2	1:D:117:ARG:HE	1.99	0.57
1:A:214:ASN:ND2	1:A:217:GLU:H	2.03	0.57
1:B:106:GLN:NE2	1:B:117:ARG:HE	1.98	0.57
1:C:214:ASN:ND2	1:C:217:GLU:H	2.01	0.57
1:A:235:ARG:HH21	1:A:235:ARG:CG	2.18	0.56
1:D:180:GLN:HG3	1:D:181:PRO:HD2	1.87	0.56
1:B:170:SER:OG	1:B:235:ARG:NH1	2.39	0.56
1:D:253:THR:CG2	1:D:256:GLU:H	2.19	0.56
1:A:323:PRO:HG2	1:A:327:GLY:O	2.06	0.56
1:D:141:LYS:HD2	1:D:146:ARG:NH1	2.20	0.56
1:C:210:TRP:CE2	1:D:212:MET:HE2	2.41	0.56
1:B:248:PRO:HB2	1:B:303:VAL:HG11	1.86	0.55
1:D:262:ASP:HB2	1:D:279:LYS:HE2	1.87	0.55
1:A:170:SER:OG	1:A:235:ARG:NH1	2.40	0.55
1:C:357:THR:O	1:C:358:HIS:HB2	2.07	0.55
1:D:371:THR:C	1:D:373:ALA:H	2.13	0.55
1:D:366:VAL:O	1:D:370:ILE:HG13	2.06	0.55
1:A:298:ARG:NH1	1:B:201:GLU:HG3	2.21	0.55
1:B:371:THR:C	1:B:373:ALA:H	2.14	0.55
1:B:300:GLN:HG3	1:B:306:ASP:OD1	2.07	0.55
1:D:184:GLU:O	1:D:187:THR:HB	2.06	0.55
1:A:106:GLN:NE2	1:A:117:ARG:HE	2.03	0.55
1:B:184:GLU:O	1:B:187:THR:HB	2.06	0.55
1:C:235:ARG:HH21	1:C:235:ARG:CG	2.19	0.55
1:A:162:LEU:HB2	1:A:168:ILE:HG12	1.87	0.54
1:A:188:TYR:CD1	1:A:212:MET:HG2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ASP:HB2	1:A:279:LYS:HE2	1.88	0.54
1:C:188:TYR:CD1	1:C:212:MET:HG2	2.42	0.54
1:D:300:GLN:HG3	1:D:306:ASP:OD1	2.08	0.54
1:A:360:GLN:HB3	1:A:361:PRO:HD3	1.90	0.54
1:D:331:ASN:HD21	1:D:333:ALA:HB3	1.72	0.54
1:B:253:THR:CG2	1:B:256:GLU:H	2.19	0.54
1:B:350:PHE:CZ	1:B:354:MET:HE2	2.41	0.54
1:B:142:PHE:C	1:B:142:PHE:CD2	2.86	0.54
1:B:162:LEU:HB2	1:B:168:ILE:HG12	1.89	0.54
1:C:360:GLN:HB3	1:C:361:PRO:HD3	1.89	0.54
1:C:350:PHE:CZ	1:C:354:MET:HE2	2.43	0.54
1:C:106:GLN:NE2	1:C:117:ARG:HE	2.01	0.53
1:C:170:SER:OG	1:C:235:ARG:NH1	2.40	0.53
1:C:177:VAL:HG23	1:C:178:SER:N	2.23	0.53
1:A:119:PHE:O	1:A:123:HIS:HD2	1.92	0.53
1:A:177:VAL:HG23	1:A:178:SER:N	2.24	0.53
1:C:239:ASP:HA	1:C:243:VAL:CG1	2.35	0.53
1:B:132:VAL:HA	1:B:139:GLU:CG	2.34	0.53
1:A:132:VAL:HA	1:A:139:GLU:CG	2.38	0.52
1:B:214:ASN:C	1:B:214:ASN:ND2	2.48	0.52
1:C:300:GLN:HG3	1:C:306:ASP:OD1	2.09	0.52
1:B:119:PHE:O	1:B:123:HIS:HD2	1.91	0.52
1:D:239:ASP:HA	1:D:243:VAL:CG1	2.38	0.52
1:C:132:VAL:HA	1:C:139:GLU:CG	2.38	0.52
1:A:181:PRO:HG2	1:A:184:GLU:CD	2.33	0.52
1:C:323:PRO:HG2	1:C:327:GLY:O	2.09	0.52
1:C:371:THR:C	1:C:373:ALA:H	2.17	0.52
1:D:170:SER:OG	1:D:235:ARG:NH1	2.43	0.52
1:D:177:VAL:HG23	1:D:178:SER:N	2.23	0.52
1:D:142:PHE:C	1:D:142:PHE:CD2	2.87	0.52
1:B:181:PRO:HG2	1:B:184:GLU:CD	2.35	0.52
1:D:181:PRO:HG2	1:D:184:GLU:CD	2.35	0.52
1:D:294:LYS:HD2	1:D:303:VAL:HG22	1.91	0.52
1:A:210:TRP:NE1	1:B:212:MET:HE2	2.25	0.52
1:C:134:PRO:HG3	3:C:379:IMN:H61	1.91	0.52
1:C:153:ALA:O	1:C:159:SER:HA	2.09	0.51
1:A:371:THR:C	1:A:373:ALA:H	2.17	0.51
1:D:162:LEU:N	1:D:162:LEU:HD23	2.25	0.51
1:C:298:ARG:NH1	1:D:201:GLU:HG3	2.26	0.51
1:C:347:LEU:HD21	3:C:379:IMN:CL	2.48	0.51
1:D:162:LEU:HB2	1:D:168:ILE:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:LEU:HD23	1:B:162:LEU:N	2.25	0.51
1:D:350:PHE:CZ	1:D:354:MET:HE2	2.45	0.51
1:B:177:VAL:HG23	1:B:178:SER:N	2.25	0.51
1:B:233:LYS:HB2	5:B:51:HOH:O	2.10	0.51
1:C:141:LYS:HD2	1:C:146:ARG:NH1	2.22	0.51
1:C:162:LEU:N	1:C:162:LEU:HD23	2.25	0.51
1:B:141:LYS:HD2	1:B:146:ARG:NH1	2.22	0.51
1:C:196:ASN:ND2	1:C:197:ASP:H	2.08	0.51
1:C:212:MET:HE2	1:D:210:TRP:CE2	2.46	0.51
1:A:184:GLU:O	1:A:187:THR:HB	2.11	0.51
1:B:165:SER:HB3	5:B:10:HOH:O	2.10	0.51
1:B:294:LYS:HD2	1:B:303:VAL:HG22	1.91	0.51
1:D:132:VAL:HA	1:D:139:GLU:CG	2.38	0.51
1:A:141:LYS:HD2	1:A:146:ARG:NH1	2.22	0.50
1:A:347:LEU:HD21	3:A:379:IMN:CL	2.48	0.50
1:C:212:MET:HE2	1:D:210:TRP:NE1	2.27	0.50
1:A:153:ALA:O	1:A:159:SER:HA	2.11	0.50
1:C:258:LEU:CA	5:C:82:HOH:O	2.57	0.50
1:D:347:LEU:HD21	3:D:476:IMN:CL	2.48	0.50
1:D:134:PRO:HG2	1:D:270:PHE:CZ	2.47	0.50
1:A:162:LEU:N	1:A:162:LEU:HD23	2.26	0.50
1:C:368:ARG:O	1:C:372:GLU:HB2	2.11	0.50
1:C:331:ASN:C	1:C:331:ASN:ND2	2.69	0.50
1:D:140:ILE:HG23	1:D:140:ILE:O	2.11	0.50
1:C:196:ASN:HD22	1:C:197:ASP:H	1.59	0.50
1:B:132:VAL:HG13	1:B:139:GLU:HG2	1.93	0.50
1:B:140:ILE:O	1:B:140:ILE:CG2	2.60	0.50
1:B:140:ILE:O	1:B:140:ILE:HG23	2.10	0.50
1:A:214:ASN:HD21	1:A:216:LYS:HB2	1.77	0.49
1:A:239:ASP:HA	1:A:243:VAL:CG1	2.36	0.49
1:D:214:ASN:HD21	1:D:216:LYS:HB2	1.77	0.49
1:D:262:ASP:O	1:D:266:ARG:HD3	2.11	0.49
1:B:153:ALA:O	1:B:159:SER:HA	2.12	0.49
1:C:142:PHE:C	1:C:142:PHE:CD2	2.90	0.49
1:C:210:TRP:NE1	1:D:212:MET:HE2	2.26	0.49
1:B:331:ASN:HD21	1:B:333:ALA:HB3	1.77	0.49
1:D:153:ALA:O	1:D:159:SER:HA	2.12	0.49
1:A:196:ASN:ND2	1:A:197:ASP:H	2.09	0.49
1:B:196:ASN:ND2	1:B:197:ASP:H	2.10	0.49
1:D:187:THR:HG22	1:D:188:TYR:CD2	2.48	0.49
1:A:187:THR:CG2	1:B:229:THR:HG21	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ASN:C	1:A:331:ASN:ND2	2.69	0.49
1:B:214:ASN:HD21	1:B:216:LYS:HB2	1.77	0.49
1:B:347:LEU:HD21	3:B:381:IMN:CL	2.48	0.49
1:D:140:ILE:O	1:D:140:ILE:CG2	2.60	0.49
1:D:323:PRO:HG2	1:D:327:GLY:O	2.12	0.49
1:D:368:ARG:O	1:D:372:GLU:HB2	2.12	0.49
1:B:239:ASP:HA	1:B:243:VAL:CG1	2.41	0.49
1:C:140:ILE:HD13	1:C:140:ILE:HA	1.69	0.49
1:B:262:ASP:O	1:B:266:ARG:HD3	2.13	0.48
1:C:184:GLU:O	1:C:187:THR:HB	2.13	0.48
1:D:132:VAL:HG13	1:D:139:GLU:HG2	1.94	0.48
1:B:187:THR:HG22	1:B:188:TYR:CD2	2.48	0.48
1:D:108:LYS:HG2	1:D:267:GLU:HG3	1.96	0.48
1:D:119:PHE:O	1:D:123:HIS:HD2	1.96	0.48
1:A:134:PRO:HG3	3:A:379:IMN:H61	1.96	0.48
1:A:187:THR:HG22	1:A:188:TYR:CD2	2.49	0.48
1:A:273:VAL:HG13	1:A:274:GLU:N	2.28	0.48
1:A:294:LYS:HD2	1:A:303:VAL:HG22	1.95	0.48
1:B:302:ASN:ND2	1:B:305:GLU:HG2	2.29	0.48
1:B:140:ILE:HD13	1:B:140:ILE:HA	1.64	0.48
1:C:273:VAL:HG13	1:C:274:GLU:N	2.29	0.48
1:B:247:SER:HB2	1:B:248:PRO:CD	2.43	0.48
1:D:287:TYR:O	1:D:291:LYS:HG2	2.14	0.48
1:D:196:ASN:ND2	1:D:197:ASP:H	2.12	0.47
1:B:331:ASN:C	1:B:331:ASN:ND2	2.70	0.47
1:C:132:VAL:HG13	1:C:139:GLU:HG2	1.94	0.47
1:A:296:ARG:NH2	1:B:197:ASP:HA	2.29	0.47
1:C:262:ASP:O	1:C:266:ARG:HD3	2.15	0.47
1:C:331:ASN:HD21	1:C:333:ALA:HB3	1.79	0.47
1:B:125:LEU:HD11	1:B:176:LEU:HD11	1.96	0.47
1:B:287:TYR:O	1:B:291:LYS:HG2	2.14	0.47
1:C:294:LYS:HD2	1:C:303:VAL:HG22	1.95	0.47
1:C:304:ARG:HG3	1:C:308:TYR:OH	2.14	0.47
1:D:360:GLN:HB3	1:D:361:PRO:HD3	1.96	0.47
1:A:287:TYR:O	1:A:291:LYS:HG2	2.14	0.47
1:A:108:LYS:HG2	1:A:267:GLU:HG3	1.97	0.47
1:A:139:GLU:H	1:A:139:GLU:CD	2.22	0.47
1:A:140:ILE:HD13	1:A:140:ILE:HA	1.67	0.47
1:A:253:THR:HG22	1:A:256:GLU:CB	2.43	0.47
1:B:196:ASN:HD22	1:B:197:ASP:H	1.63	0.47
1:C:149:PRO:HD3	5:C:7:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:ASN:C	1:D:214:ASN:ND2	2.46	0.47
1:A:140:ILE:HG23	1:A:140:ILE:O	2.14	0.47
1:C:108:LYS:HG2	1:C:267:GLU:HG3	1.97	0.47
1:D:273:VAL:HG13	1:D:274:GLU:N	2.30	0.47
1:A:368:ARG:O	1:A:372:GLU:HB2	2.14	0.47
1:B:273:VAL:HG13	1:B:274:GLU:N	2.29	0.47
1:A:141:LYS:HA	1:A:146:ARG:HH22	1.81	0.46
1:C:253:THR:HG22	1:C:256:GLU:CB	2.41	0.46
1:D:115:LYS:HZ3	1:D:165:SER:HG	1.62	0.46
1:D:109:THR:O	1:D:343:VAL:HG22	2.14	0.46
1:D:302:ASN:ND2	1:D:305:GLU:HG2	2.30	0.46
1:A:212:MET:HE2	1:B:210:TRP:CE2	2.51	0.46
1:B:249:ASN:HD21	1:B:303:VAL:HG12	1.78	0.46
1:D:161:GLN:C	1:D:162:LEU:HD23	2.40	0.46
1:A:196:ASN:HD22	1:A:197:ASP:H	1.62	0.46
1:A:142:PHE:C	1:A:142:PHE:CD2	2.93	0.46
1:B:323:PRO:HG2	1:B:327:GLY:O	2.15	0.46
1:B:368:ARG:O	1:B:372:GLU:HB2	2.15	0.46
1:A:262:ASP:O	1:A:266:ARG:HD3	2.15	0.46
1:C:246:ILE:O	1:C:250:VAL:HG22	2.15	0.46
1:A:149:PRO:HD3	5:A:5:HOH:O	2.15	0.46
1:D:139:GLU:CD	1:D:139:GLU:H	2.24	0.46
1:A:140:ILE:O	1:A:140:ILE:CG2	2.64	0.46
1:A:246:ILE:O	1:A:250:VAL:HG22	2.15	0.46
1:B:134:PRO:HG2	1:B:270:PHE:CZ	2.51	0.46
1:B:161:GLN:C	1:B:162:LEU:HD23	2.41	0.46
1:A:331:ASN:HD21	1:A:333:ALA:HB3	1.81	0.46
1:B:187:THR:HG22	1:B:188:TYR:CE2	2.51	0.46
1:B:360:GLN:HB3	1:B:361:PRO:HD3	1.98	0.46
1:D:115:LYS:HB3	1:D:115:LYS:HE2	1.70	0.46
1:A:247:SER:HB2	1:A:248:PRO:CD	2.46	0.45
1:C:134:PRO:HG2	1:C:270:PHE:CZ	2.52	0.45
1:C:139:GLU:H	1:C:139:GLU:CD	2.23	0.45
1:A:212:MET:HE2	1:B:210:TRP:NE1	2.31	0.45
1:C:141:LYS:HA	1:C:146:ARG:HH22	1.81	0.45
1:C:247:SER:HB2	1:C:248:PRO:CD	2.46	0.45
1:D:134:PRO:HG3	3:D:476:IMN:H61	1.98	0.45
1:D:174:THR:OG1	1:D:185:ILE:HD13	2.17	0.45
1:D:187:THR:HG22	1:D:188:TYR:CE2	2.52	0.45
1:D:294:LYS:O	1:D:299:LEU:HB2	2.16	0.45
1:C:109:THR:HG22	1:C:263:TYR:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:LYS:HD2	1:D:303:VAL:CG2	2.46	0.45
1:B:108:LYS:O	1:B:117:ARG:NH2	2.50	0.45
1:C:287:TYR:O	1:C:291:LYS:HG2	2.17	0.45
1:D:152:VAL:HA	1:D:160:GLN:O	2.16	0.45
1:B:152:VAL:HA	1:B:160:GLN:O	2.16	0.45
1:A:296:ARG:HD2	1:B:197:ASP:C	2.42	0.45
1:B:223:SER:HB2	1:B:227:ALA:CB	2.46	0.45
1:D:331:ASN:C	1:D:331:ASN:ND2	2.69	0.45
1:B:342:ARG:HA	1:B:363:TYR:OH	2.17	0.45
1:C:187:THR:HG22	1:C:188:TYR:CD2	2.52	0.44
1:C:108:LYS:O	1:C:117:ARG:NH2	2.51	0.44
1:D:342:ARG:HA	1:D:363:TYR:OH	2.18	0.44
1:A:109:THR:HG22	1:A:263:TYR:CZ	2.53	0.44
1:C:294:LYS:O	1:C:299:LEU:HB2	2.17	0.44
1:D:130:VAL:O	1:D:130:VAL:HG22	2.17	0.44
1:B:108:LYS:HG2	1:B:267:GLU:HG3	1.99	0.44
1:B:143:SER:OG	1:B:145:TYR:O	2.36	0.44
1:B:368:ARG:HH21	1:B:368:ARG:HG3	1.83	0.44
1:C:181:PRO:O	1:C:185:ILE:HG13	2.17	0.44
1:C:217:GLU:O	1:C:220:GLN:HB3	2.18	0.44
1:B:141:LYS:HA	1:B:146:ARG:HH22	1.83	0.44
1:B:139:GLU:CD	1:B:139:GLU:H	2.25	0.44
1:B:223:SER:HB2	1:B:227:ALA:HB2	2.00	0.44
1:D:196:ASN:HD22	1:D:197:ASP:H	1.65	0.44
1:D:252:ARG:CG	1:D:252:ARG:HH11	2.31	0.44
1:A:294:LYS:O	1:A:299:LEU:HB2	2.17	0.43
1:C:119:PHE:O	1:C:123:HIS:HD2	2.00	0.43
1:D:331:ASN:ND2	1:D:333:ALA:H	2.16	0.43
1:C:140:ILE:O	1:C:140:ILE:CG2	2.66	0.43
1:C:187:THR:CG2	1:D:229:THR:HG21	2.48	0.43
1:D:253:THR:HG22	1:D:256:GLU:CB	2.45	0.43
1:A:181:PRO:O	1:A:185:ILE:HG13	2.19	0.43
1:A:253:THR:HB	1:A:256:GLU:OE2	2.18	0.43
1:C:140:ILE:O	1:C:140:ILE:HG23	2.18	0.43
1:C:217:GLU:HG2	1:C:217:GLU:H	1.59	0.43
1:C:253:THR:HB	1:C:256:GLU:OE2	2.19	0.43
1:D:137:ARG:HB2	1:D:141:LYS:HE3	2.01	0.43
1:D:164:ASP:HB3	1:D:167:VAL:HG23	2.00	0.43
1:D:217:GLU:O	1:D:220:GLN:HB3	2.18	0.43
1:D:247:SER:HB2	1:D:248:PRO:CD	2.48	0.43
1:A:152:VAL:HA	1:A:160:GLN:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:THR:HG22	1:A:188:TYR:CE2	2.53	0.43
1:D:108:LYS:O	1:D:117:ARG:NH2	2.52	0.43
1:A:323:PRO:HD2	1:A:327:GLY:O	2.18	0.43
1:A:354:MET:HE1	1:A:363:TYR:CG	2.54	0.43
1:B:134:PRO:HG3	3:B:381:IMN:H61	2.01	0.43
1:B:304:ARG:HG3	1:B:308:TYR:OH	2.19	0.43
1:C:258:LEU:HD23	5:C:82:HOH:O	2.18	0.43
1:D:141:LYS:HA	1:D:146:ARG:HH22	1.83	0.43
1:A:132:VAL:HG13	1:A:139:GLU:HG2	2.01	0.43
1:A:223:SER:HB2	1:A:227:ALA:HB2	2.00	0.43
1:B:115:LYS:HE2	1:B:115:LYS:HB3	1.71	0.43
1:D:141:LYS:HA	1:D:146:ARG:NH2	2.34	0.43
1:B:356:HIS:CD2	1:B:356:HIS:N	2.87	0.42
1:A:217:GLU:O	1:A:220:GLN:HB3	2.20	0.42
1:C:161:GLN:C	1:C:162:LEU:HD23	2.45	0.42
1:D:249:ASN:HD21	1:D:303:VAL:HG12	1.82	0.42
1:B:137:ARG:HB2	1:B:141:LYS:HE3	2.02	0.42
1:B:252:ARG:HH11	1:B:252:ARG:CG	2.31	0.42
1:B:294:LYS:O	1:B:299:LEU:HB2	2.18	0.42
1:C:296:ARG:NH2	1:D:197:ASP:HA	2.34	0.42
1:D:164:ASP:HB3	1:D:167:VAL:CG2	2.49	0.42
1:D:336:ALA:O	1:D:340:VAL:HG23	2.20	0.42
1:B:294:LYS:HD2	1:B:303:VAL:CG2	2.49	0.42
1:C:132:VAL:O	1:C:134:PRO:HD3	2.20	0.42
1:C:152:VAL:HA	1:C:160:GLN:O	2.20	0.42
1:B:261:PHE:HE2	1:B:286:MET:HG3	1.84	0.42
1:C:141:LYS:HA	1:C:146:ARG:NH2	2.35	0.42
1:C:223:SER:HB2	1:C:227:ALA:HB2	1.99	0.42
1:A:134:PRO:HG2	1:A:270:PHE:CZ	2.54	0.42
1:A:145:TYR:CZ	1:A:147:LYS:HB2	2.54	0.42
1:A:302:ASN:ND2	1:A:305:GLU:HG2	2.34	0.42
1:B:141:LYS:HA	1:B:146:ARG:NH2	2.34	0.42
1:C:187:THR:HG22	1:C:188:TYR:CE2	2.55	0.42
1:C:214:ASN:HD21	1:C:216:LYS:HB2	1.85	0.42
1:C:336:ALA:O	1:C:340:VAL:HG23	2.20	0.42
1:B:231:GLU:HG3	1:B:232:MET:N	2.35	0.42
1:C:215:GLU:OE1	1:D:214:ASN:HB2	2.20	0.41
1:D:356:HIS:N	1:D:356:HIS:CD2	2.88	0.41
1:A:108:LYS:O	1:A:117:ARG:NH2	2.53	0.41
1:A:115:LYS:HB3	1:A:115:LYS:HE2	1.71	0.41
1:B:177:VAL:HG21	1:B:213:LEU:CD1	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:THR:HG22	1:C:211:LEU:HB3	2.02	0.41
1:C:354:MET:HE1	1:C:363:TYR:CG	2.56	0.41
1:D:223:SER:HB2	1:D:227:ALA:HB2	2.02	0.41
1:C:109:THR:O	1:C:343:VAL:HG22	2.20	0.41
1:A:331:ASN:ND2	1:A:333:ALA:H	2.18	0.41
1:A:368:ARG:HH21	1:A:368:ARG:HG3	1.85	0.41
1:A:141:LYS:HA	1:A:146:ARG:NH2	2.35	0.41
1:D:231:GLU:HG3	1:D:232:MET:N	2.35	0.41
1:D:371:THR:C	1:D:373:ALA:N	2.79	0.41
1:A:245:LEU:O	1:A:249:ASN:HB2	2.20	0.41
1:C:342:ARG:HA	1:C:363:TYR:OH	2.20	0.41
1:A:215:GLU:OE1	1:B:214:ASN:HB2	2.20	0.41
1:C:294:LYS:HD2	1:C:303:VAL:CG2	2.50	0.41
1:B:100:LEU:HD21	1:B:153:ALA:HB1	2.03	0.41
1:B:129:VAL:O	1:B:129:VAL:CG2	2.69	0.41
1:B:217:GLU:O	1:B:220:GLN:HB3	2.21	0.41
1:B:368:ARG:HG2	1:B:368:ARG:H	1.55	0.41
1:C:231:GLU:HG3	1:C:232:MET:N	2.36	0.41
1:C:331:ASN:ND2	1:C:333:ALA:H	2.18	0.41
1:A:137:ARG:HB2	1:A:141:LYS:HE3	2.03	0.41
1:A:161:GLN:C	1:A:162:LEU:HD23	2.46	0.41
1:B:109:THR:O	1:B:343:VAL:HG22	2.21	0.41
1:C:356:HIS:CD2	1:C:356:HIS:N	2.89	0.41
1:A:356:HIS:CD2	1:A:356:HIS:N	2.88	0.40
1:C:145:TYR:CE1	1:C:147:LYS:HB2	2.57	0.40
1:B:288:LEU:O	1:B:291:LYS:HB2	2.21	0.40
1:B:331:ASN:ND2	1:B:333:ALA:H	2.19	0.40
1:C:245:LEU:O	1:C:249:ASN:HB2	2.21	0.40
1:C:277:VAL:HG13	1:C:281:MET:HG3	2.02	0.40
1:B:133:ASN:HA	1:B:134:PRO:HD2	1.96	0.40
1:D:109:THR:HG22	1:D:263:TYR:CZ	2.56	0.40
1:B:164:ASP:HB3	1:B:167:VAL:CG2	2.51	0.40
1:B:255:THR:HB	1:C:141:LYS:NZ	2.37	0.40
1:B:371:THR:C	1:B:373:ALA:N	2.79	0.40
1:D:288:LEU:O	1:D:291:LYS:HB2	2.21	0.40
1:D:368:ARG:HG2	1:D:368:ARG:H	1.57	0.40
1:B:106:GLN:HB2	1:B:113:CYS:SG	2.61	0.40
1:B:168:ILE:O	1:B:172:LEU:HB2	2.22	0.40
1:C:105:TYR:HE1	1:C:152:VAL:HG13	1.86	0.40
1:D:368:ARG:HH21	1:D:368:ARG:HG3	1.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:SER:OG	1:B:321:ASP:OD2[2_556]	2.19	0.01

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	272/290 (94%)	262 (96%)	10 (4%)	0	100	100
1	B	272/290 (94%)	264 (97%)	8 (3%)	0	100	100
1	C	272/290 (94%)	263 (97%)	9 (3%)	0	100	100
1	D	272/290 (94%)	263 (97%)	9 (3%)	0	100	100
All	All	1088/1160 (94%)	1052 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	233/247 (94%)	178 (76%)	55 (24%)	1	1
1	B	233/247 (94%)	177 (76%)	56 (24%)	1	1
1	C	233/247 (94%)	178 (76%)	55 (24%)	1	1
1	D	233/247 (94%)	177 (76%)	56 (24%)	1	1
All	All	932/988 (94%)	710 (76%)	222 (24%)	1	1

All (222) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	LEU
1	A	102	LEU
1	A	106	GLN
1	A	129	VAL
1	A	130	VAL
1	A	139	GLU
1	A	140	ILE
1	A	141	LYS
1	A	143	SER
1	A	144	SER
1	A	148	VAL
1	A	152	VAL
1	A	162	LEU
1	A	165	SER
1	A	172	LEU
1	A	187	THR
1	A	193	LYS
1	A	196	ASN
1	A	198	GLN
1	A	201	GLU
1	A	202	VAL
1	A	208	LYS
1	A	212	MET
1	A	213	LEU
1	A	214	ASN
1	A	215	GLU
1	A	217	GLU
1	A	221	VAL
1	A	233	LYS
1	A	235	ARG
1	A	242	LEU
1	A	243	VAL
1	A	252	ARG
1	A	253	THR
1	A	255	THR
1	A	267	GLU
1	A	273	VAL
1	A	291	LYS
1	A	292	ARG
1	A	295	SER
1	A	301	ASP
1	A	304	ARG

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Mol	Chain	Res	Type
1	A	307	LEU
1	A	315	VAL
1	A	320	LYS
1	A	328	GLN
1	A	329	LYS
1	A	331	ASN
1	A	332	LEU
1	A	335	LEU
1	A	343	VAL
1	A	347	LEU
1	A	353	LEU
1	A	368	ARG
1	A	372	GLU
1	B	100	LEU
1	B	102	LEU
1	B	106	GLN
1	B	129	VAL
1	B	130	VAL
1	B	139	GLU
1	B	140	ILE
1	B	141	LYS
1	B	143	SER
1	B	144	SER
1	B	148	VAL
1	B	152	VAL
1	B	162	LEU
1	B	165	SER
1	B	172	LEU
1	B	183	GLU
1	B	187	THR
1	B	193	LYS
1	B	196	ASN
1	B	198	GLN
1	B	201	GLU
1	B	202	VAL
1	B	208	LYS
1	B	212	MET
1	B	213	LEU
1	B	214	ASN
1	B	215	GLU
1	B	217	GLU
1	B	221	VAL

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Mol	Chain	Res	Type
1	B	233	LYS
1	B	235	ARG
1	B	242	LEU
1	B	243	VAL
1	B	252	ARG
1	B	253	THR
1	B	255	THR
1	B	267	GLU
1	B	273	VAL
1	B	291	LYS
1	B	292	ARG
1	B	295	SER
1	B	301	ASP
1	B	304	ARG
1	B	307	LEU
1	B	315	VAL
1	B	320	LYS
1	B	328	GLN
1	B	329	LYS
1	B	331	ASN
1	B	332	LEU
1	B	335	LEU
1	B	343	VAL
1	B	347	LEU
1	B	353	LEU
1	B	368	ARG
1	B	372	GLU
1	C	100	LEU
1	C	102	LEU
1	C	106	GLN
1	C	129	VAL
1	C	130	VAL
1	C	139	GLU
1	C	140	ILE
1	C	141	LYS
1	C	143	SER
1	C	144	SER
1	C	148	VAL
1	C	152	VAL
1	C	162	LEU
1	C	165	SER
1	C	172	LEU

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Mol	Chain	Res	Type
1	C	187	THR
1	C	193	LYS
1	C	196	ASN
1	C	198	GLN
1	C	201	GLU
1	C	202	VAL
1	C	212	MET
1	C	213	LEU
1	C	214	ASN
1	C	215	GLU
1	C	217	GLU
1	C	221	VAL
1	C	233	LYS
1	C	235	ARG
1	C	242	LEU
1	C	243	VAL
1	C	252	ARG
1	C	253	THR
1	C	255	THR
1	C	261	PHE
1	C	267	GLU
1	C	273	VAL
1	C	291	LYS
1	C	292	ARG
1	C	295	SER
1	C	301	ASP
1	C	304	ARG
1	C	307	LEU
1	C	315	VAL
1	C	320	LYS
1	C	328	GLN
1	C	329	LYS
1	C	331	ASN
1	C	332	LEU
1	C	335	LEU
1	C	343	VAL
1	C	347	LEU
1	C	353	LEU
1	C	368	ARG
1	C	372	GLU
1	D	100	LEU
1	D	102	LEU

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Mol	Chain	Res	Type
1	D	106	GLN
1	D	129	VAL
1	D	130	VAL
1	D	139	GLU
1	D	140	ILE
1	D	141	LYS
1	D	143	SER
1	D	144	SER
1	D	148	VAL
1	D	152	VAL
1	D	162	LEU
1	D	165	SER
1	D	172	LEU
1	D	183	GLU
1	D	187	THR
1	D	193	LYS
1	D	196	ASN
1	D	198	GLN
1	D	201	GLU
1	D	202	VAL
1	D	208	LYS
1	D	212	MET
1	D	213	LEU
1	D	214	ASN
1	D	215	GLU
1	D	217	GLU
1	D	221	VAL
1	D	233	LYS
1	D	235	ARG
1	D	242	LEU
1	D	243	VAL
1	D	252	ARG
1	D	253	THR
1	D	255	THR
1	D	267	GLU
1	D	273	VAL
1	D	291	LYS
1	D	292	ARG
1	D	295	SER
1	D	301	ASP
1	D	304	ARG
1	D	307	LEU

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Mol	Chain	Res	Type
1	D	315	VAL
1	D	320	LYS
1	D	328	GLN
1	D	329	LYS
1	D	331	ASN
1	D	332	LEU
1	D	335	LEU
1	D	343	VAL
1	D	347	LEU
1	D	353	LEU
1	D	368	ARG
1	D	372	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	123	HIS
1	A	160	GLN
1	A	196	ASN
1	A	214	ASN
1	A	219	GLN
1	A	236	GLN
1	A	244	HIS
1	A	302	ASN
1	A	331	ASN
1	A	356	HIS
1	B	106	GLN
1	B	123	HIS
1	B	160	GLN
1	B	196	ASN
1	B	214	ASN
1	B	219	GLN
1	B	236	GLN
1	B	244	HIS
1	B	302	ASN
1	B	331	ASN
1	B	356	HIS
1	C	106	GLN
1	C	123	HIS
1	C	160	GLN
1	C	161	GLN

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Mol	Chain	Res	Type
1	C	196	ASN
1	C	214	ASN
1	C	219	GLN
1	C	236	GLN
1	C	244	HIS
1	C	297	HIS
1	C	331	ASN
1	C	356	HIS
1	D	106	GLN
1	D	123	HIS
1	D	196	ASN
1	D	214	ASN
1	D	219	GLN
1	D	236	GLN
1	D	244	HIS
1	D	302	ASN
1	D	331	ASN
1	D	356	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\# Z > 2$
2	ACT	B	379	-	3,3,3	1.36	1 (33%)	3,3,3	0.67	0
3	IMN	B	381	-	27,27,27	3.43	17 (62%)	39,39,39	2.93	17 (43%)
3	IMN	C	379	-	27,27,27	3.43	17 (62%)	39,39,39	2.92	17 (43%)
2	ACT	C	378	-	3,3,3	1.23	1 (33%)	3,3,3	0.67	0
2	ACT	A	378	-	3,3,3	1.20	1 (33%)	3,3,3	0.65	0
3	IMN	D	476	-	27,27,27	3.36	18 (66%)	39,39,39	2.91	18 (46%)
3	IMN	A	379	-	27,27,27	3.45	17 (62%)	39,39,39	2.92	17 (43%)
2	ACT	D	477	-	3,3,3	1.40	1 (33%)	3,3,3	0.71	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
3	IMN	B	381	-	-	2/14/14/14	0/3/3/3
3	IMN	D	476	-	-	2/14/14/14	0/3/3/3
3	IMN	A	379	-	-	2/14/14/14	0/3/3/3
3	IMN	C	379	-	-	2/14/14/14	0/3/3/3

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	379	IMN	C1-C	7.65	1.51	1.41
3	C	379	IMN	C1-C	7.57	1.51	1.41
3	C	379	IMN	C8-C7	7.49	1.51	1.36
3	B	381	IMN	C1-C	7.49	1.51	1.41
3	B	381	IMN	C8-C7	7.40	1.51	1.36
3	D	476	IMN	C1-C	7.36	1.50	1.41
3	A	379	IMN	C8-C7	7.16	1.50	1.36
3	D	476	IMN	C8-C7	7.15	1.50	1.36
3	B	381	IMN	C10-C9	5.51	1.59	1.50
3	C	379	IMN	C10-C9	5.04	1.58	1.50
3	D	476	IMN	C10-C9	5.01	1.58	1.50
3	A	379	IMN	C5-C	4.95	1.47	1.39
3	A	379	IMN	C10-C9	4.75	1.58	1.50
3	C	379	IMN	C5-C	4.74	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	381	IMN	C5-C	4.72	1.46	1.39
3	D	476	IMN	C5-C	4.43	1.46	1.39
3	A	379	IMN	C2-C1	4.34	1.46	1.39
3	D	476	IMN	C15-C14	4.30	1.45	1.38
3	A	379	IMN	C11-C10	4.30	1.45	1.39
3	C	379	IMN	C2-C1	4.27	1.46	1.39
3	B	381	IMN	C15-C10	4.21	1.45	1.39
3	A	379	IMN	C12-C11	4.18	1.45	1.38
3	A	379	IMN	C15-C14	4.17	1.45	1.38
3	B	381	IMN	C11-C10	4.17	1.45	1.39
3	C	379	IMN	C9-N	4.15	1.51	1.41
3	C	379	IMN	C12-C11	4.12	1.45	1.38
3	C	379	IMN	C11-C10	4.11	1.45	1.39
3	D	476	IMN	C15-C10	4.05	1.45	1.39
3	D	476	IMN	C9-N	4.05	1.50	1.41
3	B	381	IMN	C15-C14	4.03	1.45	1.38
3	A	379	IMN	C9-N	4.03	1.50	1.41
3	B	381	IMN	C12-C11	3.99	1.45	1.38
3	D	476	IMN	C11-C10	3.96	1.45	1.39
3	A	379	IMN	C15-C10	3.92	1.45	1.39
3	B	381	IMN	C9-N	3.89	1.50	1.41
3	D	476	IMN	C12-C11	3.87	1.45	1.38
3	D	476	IMN	C2-C1	3.80	1.45	1.39
3	C	379	IMN	C15-C14	3.80	1.44	1.38
3	C	379	IMN	C15-C10	3.56	1.44	1.39
3	B	381	IMN	C2-C1	3.55	1.45	1.39
3	A	379	IMN	C1-C7	3.48	1.50	1.44
3	D	476	IMN	C1-C7	3.43	1.50	1.44
3	B	381	IMN	C1-C7	3.36	1.50	1.44
3	C	379	IMN	C1-C7	3.04	1.49	1.44
3	B	381	IMN	C17-C18	2.83	1.55	1.51
3	D	476	IMN	C12-C13	2.70	1.43	1.38
3	D	476	IMN	C2-C3	2.69	1.43	1.39
3	C	379	IMN	C5-C4	2.66	1.43	1.38
3	A	379	IMN	C12-C13	2.65	1.42	1.38
3	C	379	IMN	C2-C3	2.61	1.43	1.39
3	A	379	IMN	C4-C3	2.57	1.43	1.38
3	C	379	IMN	C12-C13	2.57	1.42	1.38
3	A	379	IMN	C5-C4	2.50	1.42	1.38
3	B	381	IMN	C2-C3	2.49	1.43	1.39
3	B	381	IMN	C12-C13	2.49	1.42	1.38
3	C	379	IMN	C17-C18	2.47	1.54	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	379	IMN	C4-C3	2.44	1.43	1.38
3	B	381	IMN	C16-C8	2.43	1.53	1.49
3	B	381	IMN	C14-C13	2.39	1.42	1.38
2	D	477	ACT	O-C	2.36	1.32	1.22
3	A	379	IMN	C14-C13	2.36	1.42	1.38
3	A	379	IMN	C16-C8	2.35	1.53	1.49
3	D	476	IMN	C17-C18	2.33	1.54	1.51
3	C	379	IMN	C16-C8	2.31	1.53	1.49
3	A	379	IMN	C2-C3	2.31	1.42	1.39
3	D	476	IMN	C16-C8	2.29	1.53	1.49
2	B	379	ACT	O-C	2.29	1.32	1.22
3	D	476	IMN	C14-C13	2.27	1.42	1.38
3	B	381	IMN	C5-C4	2.06	1.42	1.38
2	C	378	ACT	O-C	2.06	1.31	1.22
3	D	476	IMN	C4-C3	2.03	1.42	1.38
2	A	378	ACT	O-C	2.02	1.31	1.22
3	D	476	IMN	C5-C4	2.01	1.42	1.38

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	381	IMN	C-N-C8	8.18	114.47	107.80
3	D	476	IMN	C-N-C8	8.09	114.40	107.80
3	A	379	IMN	C-N-C8	8.07	114.38	107.80
3	C	379	IMN	C-N-C8	8.02	114.34	107.80
3	C	379	IMN	C17-C7-C8	5.77	135.54	126.86
3	C	379	IMN	C5-C-C1	-5.74	115.54	121.95
3	A	379	IMN	C5-C-C1	-5.72	115.57	121.95
3	B	381	IMN	C5-C-C1	-5.64	115.65	121.95
3	D	476	IMN	C5-C-C1	-5.56	115.74	121.95
3	B	381	IMN	C17-C7-C8	5.56	135.22	126.86
3	A	379	IMN	C17-C7-C8	5.53	135.18	126.86
3	D	476	IMN	C17-C7-C8	5.48	135.10	126.86
3	D	476	IMN	C10-C9-N	5.43	128.35	117.92
3	A	379	IMN	C10-C9-N	5.43	128.34	117.92
3	B	381	IMN	C10-C9-N	5.40	128.30	117.92
3	C	379	IMN	C10-C9-N	5.40	128.30	117.92
3	B	381	IMN	C16-C8-N	5.19	129.84	122.07
3	D	476	IMN	C16-C8-N	5.06	129.65	122.07
3	A	379	IMN	C16-C8-N	5.02	129.60	122.07
3	C	379	IMN	C16-C8-N	4.85	129.34	122.07
3	A	379	IMN	C5-C-N	4.34	139.23	130.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	379	IMN	C5-C-N	4.26	139.07	130.65
3	B	381	IMN	C5-C-N	4.22	139.00	130.65
3	D	476	IMN	C5-C-N	4.16	138.89	130.65
3	C	379	IMN	C18-C17-C7	4.14	124.74	113.73
3	D	476	IMN	C6-O-C3	4.09	126.27	117.50
3	A	379	IMN	C18-C17-C7	3.92	124.16	113.73
3	B	381	IMN	C18-C17-C7	3.91	124.13	113.73
3	B	381	IMN	C6-O-C3	3.85	125.75	117.50
3	A	379	IMN	O1-C9-C10	-3.84	112.67	120.29
3	D	476	IMN	C18-C17-C7	3.83	123.94	113.73
3	D	476	IMN	O1-C9-C10	-3.82	112.71	120.29
3	A	379	IMN	C6-O-C3	3.82	125.69	117.50
3	C	379	IMN	O1-C9-C10	-3.79	112.79	120.29
3	C	379	IMN	C6-O-C3	3.75	125.55	117.50
3	B	381	IMN	O1-C9-C10	-3.70	112.96	120.29
3	D	476	IMN	C1-C7-C8	-3.48	105.10	108.13
3	B	381	IMN	C1-C7-C8	-3.46	105.11	108.13
3	C	379	IMN	C1-C7-C8	-3.35	105.21	108.13
3	A	379	IMN	C1-C7-C8	-3.31	105.24	108.13
3	C	379	IMN	C17-C7-C1	-3.23	119.25	124.80
3	D	476	IMN	C15-C10-C9	3.18	128.44	120.28
3	A	379	IMN	C15-C10-C9	3.16	128.39	120.28
3	B	381	IMN	C15-C10-C9	3.14	128.33	120.28
3	C	379	IMN	C15-C10-C9	3.13	128.32	120.28
3	A	379	IMN	C17-C7-C1	-3.04	119.57	124.80
3	B	381	IMN	C17-C7-C1	-2.99	119.66	124.80
3	D	476	IMN	C16-C8-C7	-2.91	123.51	128.07
3	B	381	IMN	C16-C8-C7	-2.91	123.51	128.07
3	D	476	IMN	C17-C7-C1	-2.91	119.80	124.80
3	A	379	IMN	C16-C8-C7	-2.88	123.56	128.07
3	C	379	IMN	O3-C18-O2	-2.78	116.18	123.33
3	B	381	IMN	O3-C18-O2	-2.74	116.29	123.33
3	A	379	IMN	O3-C18-O2	-2.70	116.39	123.33
3	C	379	IMN	C16-C8-C7	-2.68	123.88	128.07
3	D	476	IMN	O3-C18-O2	-2.64	116.55	123.33
3	B	381	IMN	C7-C8-N	-2.32	106.64	108.85
3	D	476	IMN	C11-C10-C9	-2.26	114.47	120.28
3	A	379	IMN	C1-C-N	-2.23	105.20	107.69
3	A	379	IMN	C11-C10-C9	-2.22	114.59	120.28
3	C	379	IMN	C7-C8-N	-2.17	106.78	108.85
3	B	381	IMN	C11-C10-C9	-2.16	114.75	120.28
3	C	379	IMN	C11-C10-C9	-2.15	114.78	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	379	IMN	C7-C8-N	-2.11	106.84	108.85
3	D	476	IMN	C7-C8-N	-2.11	106.84	108.85
3	B	381	IMN	C1-C-N	-2.10	105.34	107.69
3	D	476	IMN	C1-C-N	-2.08	105.37	107.69
3	C	379	IMN	C1-C-N	-2.06	105.39	107.69
3	D	476	IMN	O2-C18-C17	2.04	127.94	122.11

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	379	IMN	C7-C17-C18-O3
3	C	379	IMN	C7-C17-C18-O3
3	D	476	IMN	C7-C17-C18-O3
3	B	381	IMN	C7-C17-C18-O3
3	A	379	IMN	C7-C17-C18-O2
3	B	381	IMN	C7-C17-C18-O2
3	C	379	IMN	C7-C17-C18-O2
3	D	476	IMN	C7-C17-C18-O2

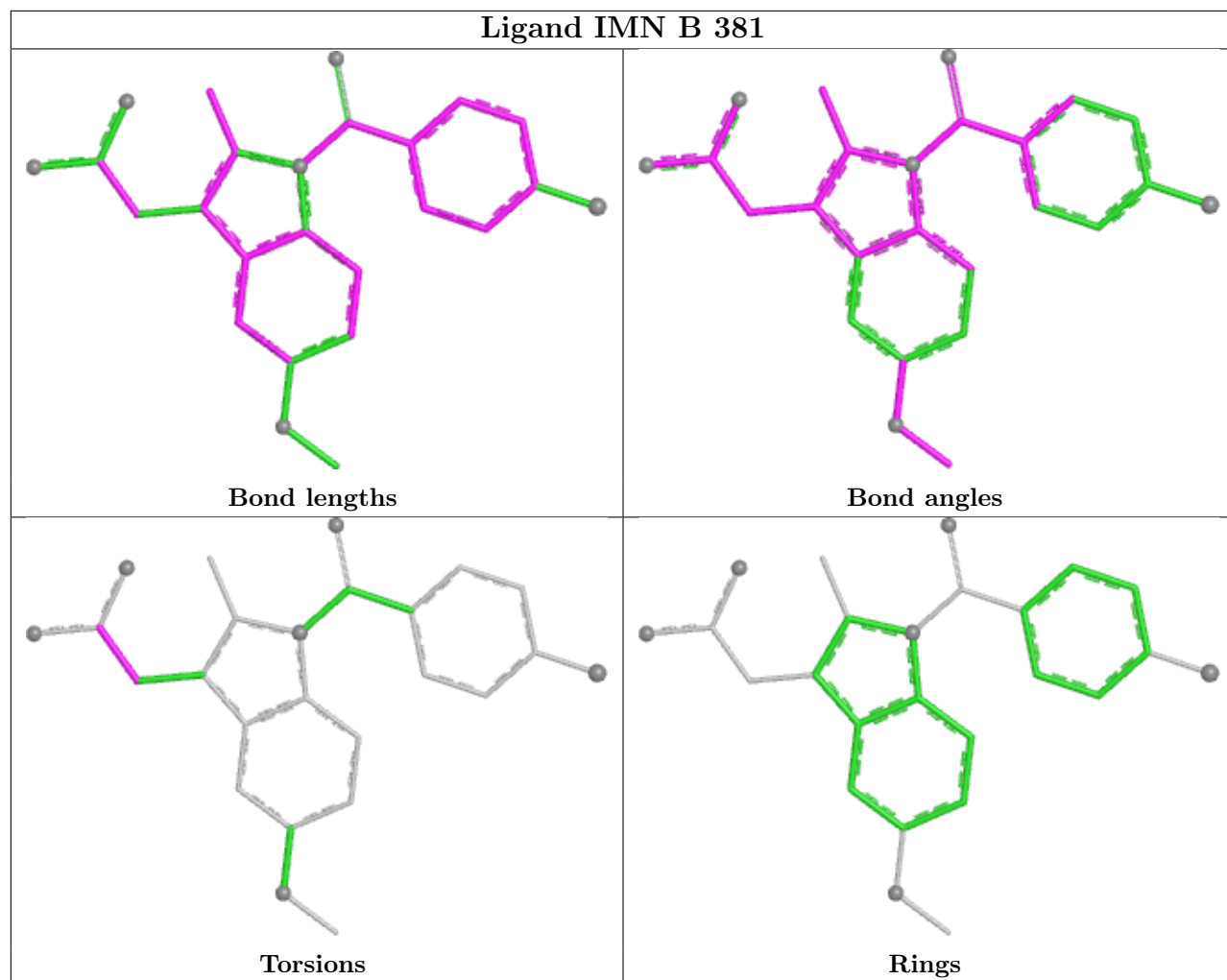
There are no ring outliers.

4 monomers are involved in 8 short contacts:

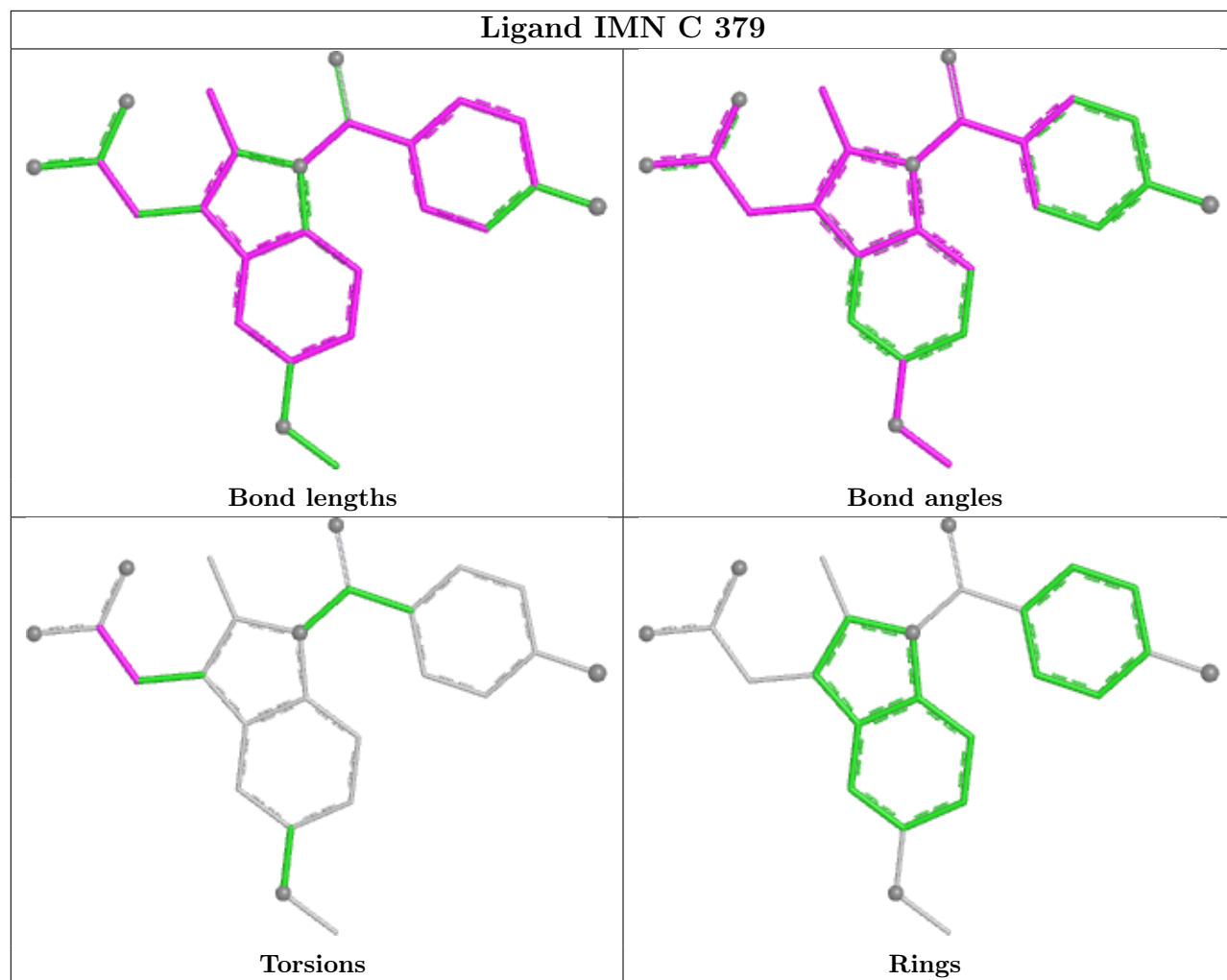
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	381	IMN	2	0
3	C	379	IMN	2	0
3	D	476	IMN	2	0
3	A	379	IMN	2	0

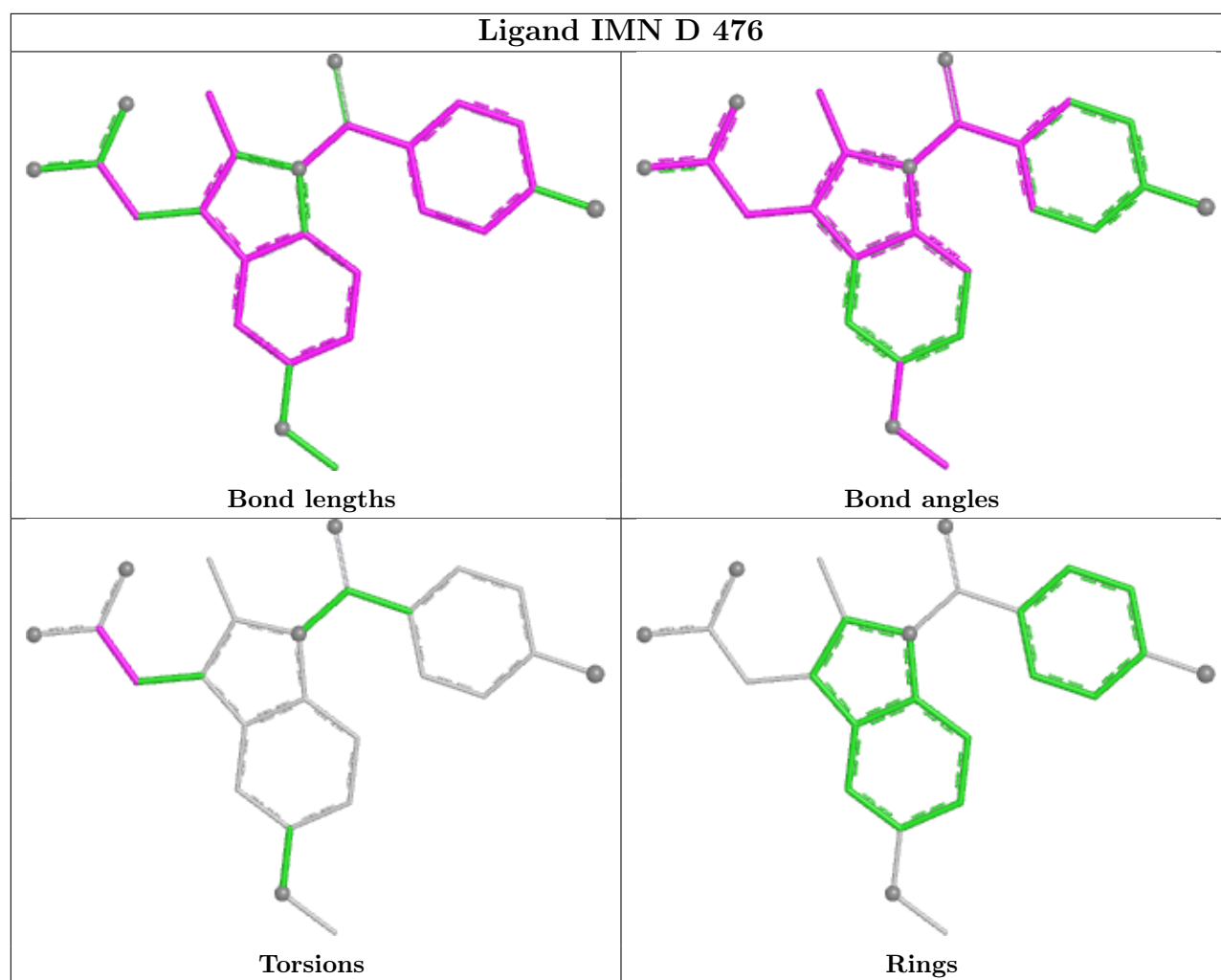
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

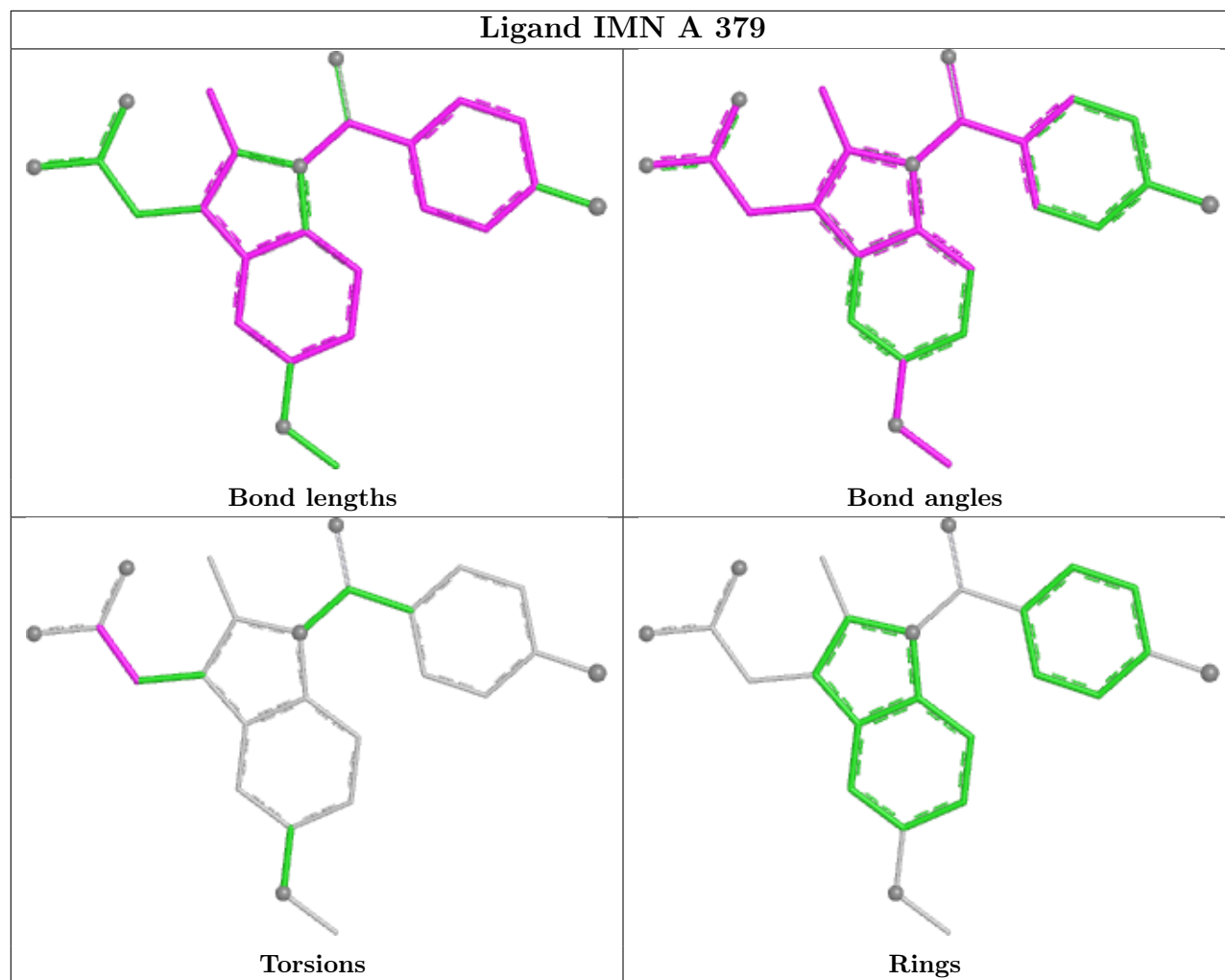
Ligand IMN B 381



Ligand IMN C 379







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	274/290 (94%)	-0.42	1 (0%) 88 86	4, 15, 45, 79	0
1	B	274/290 (94%)	-0.44	3 (1%) 78 74	3, 14, 49, 66	0
1	C	274/290 (94%)	-0.38	1 (0%) 88 86	4, 17, 47, 71	0
1	D	274/290 (94%)	-0.36	1 (0%) 88 86	3, 18, 52, 68	0
All	All	1096/1160 (94%)	-0.40	6 (0%) 87 85	3, 16, 50, 79	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	373	ALA	2.7
1	B	225	LYS	2.4
1	A	223	SER	2.4
1	D	223	SER	2.4
1	B	223	SER	2.3
1	B	276	ALA	2.1

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,

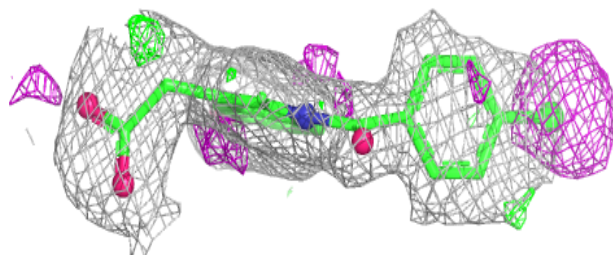
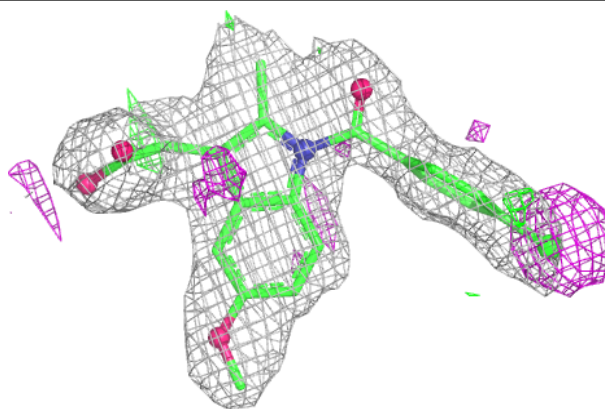
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ACT	B	379	4/4	0.78	0.17	27,30,31,32	0
3	IMN	B	381	25/25	0.79	0.12	10,13,20,20	0
2	ACT	D	477	4/4	0.80	0.14	10,12,16,18	0
3	IMN	D	476	25/25	0.80	0.11	10,13,16,17	0
3	IMN	A	379	25/25	0.83	0.10	5,11,17,22	0
3	IMN	C	379	25/25	0.85	0.09	7,9,17,19	0
2	ACT	C	378	4/4	0.86	0.13	13,14,14,16	0
2	ACT	A	378	4/4	0.93	0.09	6,8,10,11	0
4	CL	D	378	1/1	0.94	0.06	13,13,13,13	0
4	CL	D	475	1/1	0.97	0.09	15,15,15,15	0
4	CL	B	378	1/1	0.98	0.11	15,15,15,15	0
4	CL	B	380	1/1	0.99	0.06	10,10,10,10	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.

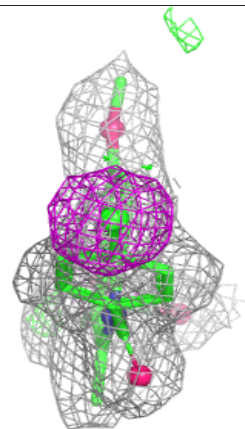
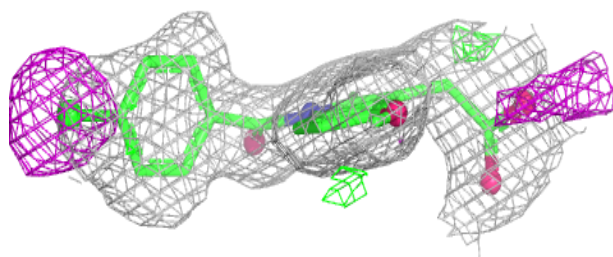
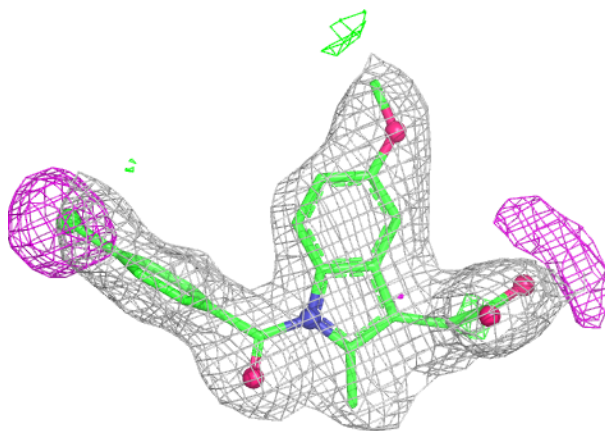
Electron density around IMN B 381:

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



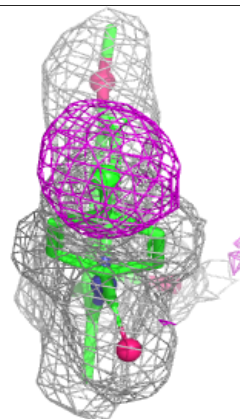
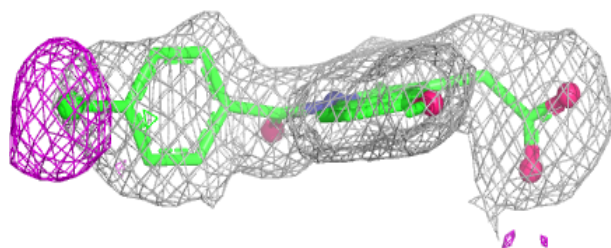
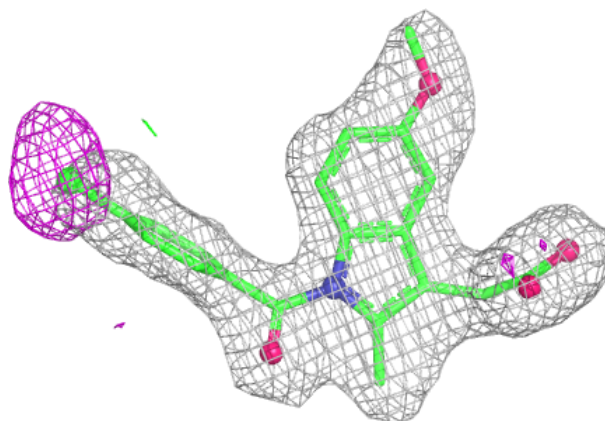
Electron density around IMN D 476:

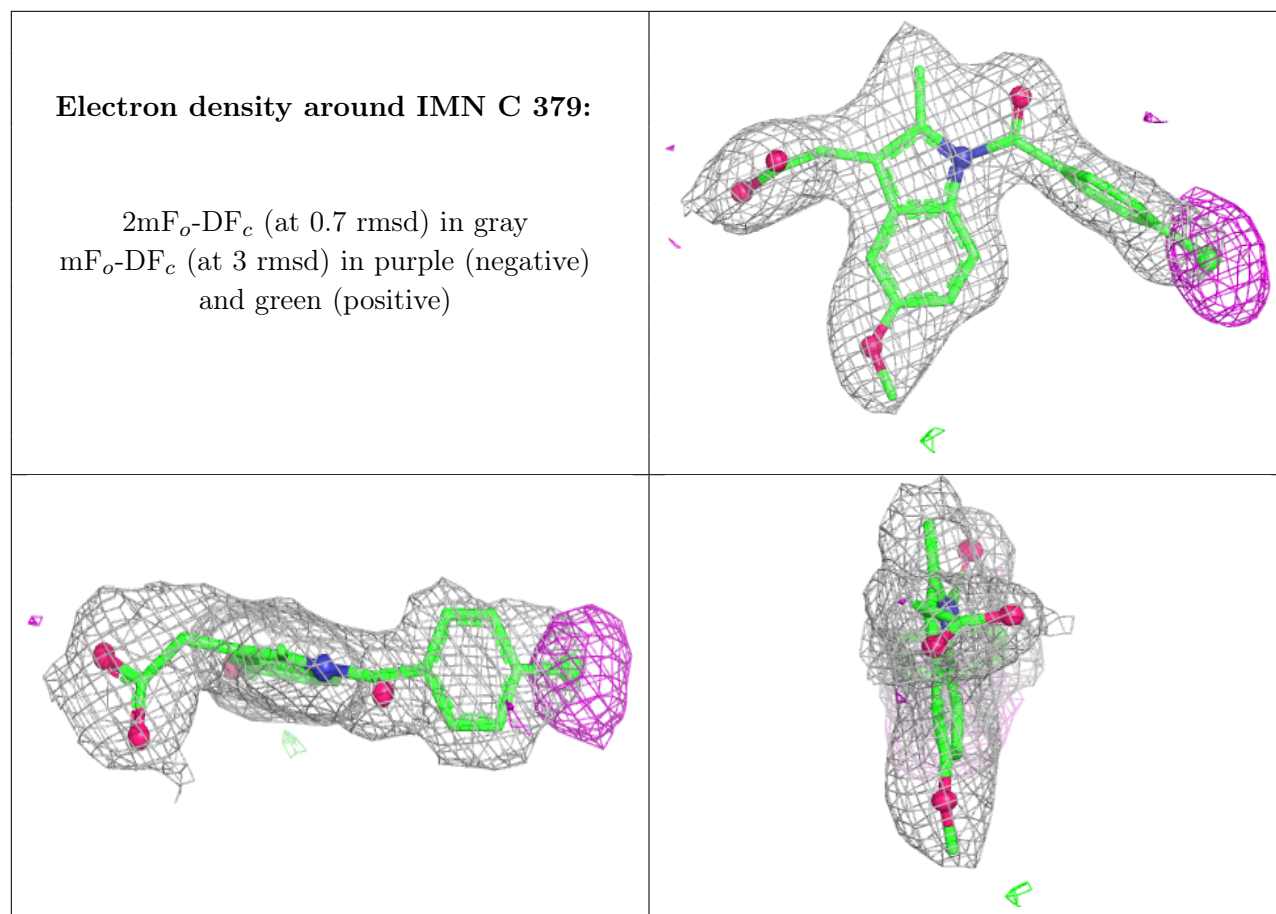
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around IMN A 379:

$2mF_o-DF_c$ (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.