



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:21 AM UTC

PDB ID : 2QE2 / pdb_00002qe2
Title : Structure of HCV NS5B Bound to an Anthranilic Acid Inhibitor
Authors : Chopra, R.; Svenson, K.; Bard, J.
Deposited on : 2007-06-22
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

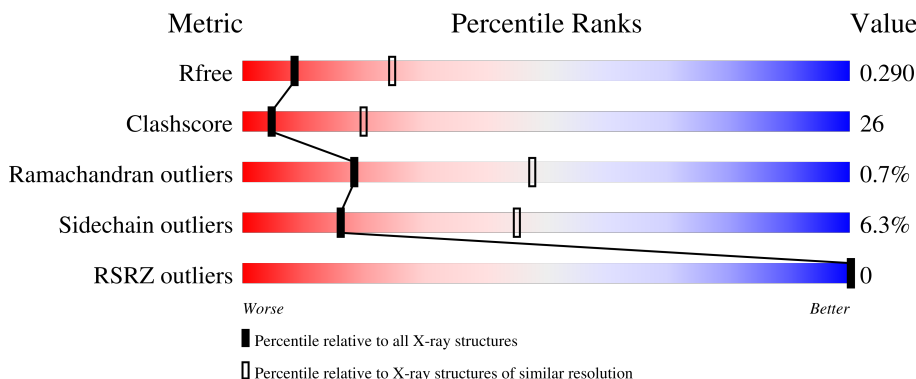
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	578	 49% 35% 6% 10%
1	B	578	 49% 33% 7% 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8193 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.

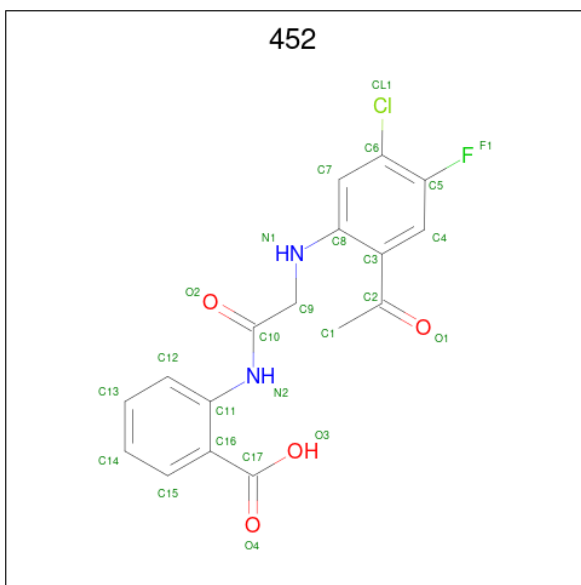
- Molecule 1 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	521	Total	C	N	O	S	0	0	0
			4065	2567	721	748	29			
1	B	523	Total	C	N	O	S	0	0	0
			4078	2573	725	751	29			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	571	GLY	-	expression tag	UNP Q99AU2
A	572	SER	-	expression tag	UNP Q99AU2
A	573	HIS	-	expression tag	UNP Q99AU2
A	574	HIS	-	expression tag	UNP Q99AU2
A	575	HIS	-	expression tag	UNP Q99AU2
A	576	HIS	-	expression tag	UNP Q99AU2
A	577	HIS	-	expression tag	UNP Q99AU2
A	578	HIS	-	expression tag	UNP Q99AU2
B	571	GLY	-	expression tag	UNP Q99AU2
B	572	SER	-	expression tag	UNP Q99AU2
B	573	HIS	-	expression tag	UNP Q99AU2
B	574	HIS	-	expression tag	UNP Q99AU2
B	575	HIS	-	expression tag	UNP Q99AU2
B	576	HIS	-	expression tag	UNP Q99AU2
B	577	HIS	-	expression tag	UNP Q99AU2
B	578	HIS	-	expression tag	UNP Q99AU2

- Molecule 2 is 2-[N-(2-ACETYL-5-CHLORO-4-FLUOROPHENYL)GLYCYL]AMINO}BE NZOIC ACID (CCD ID: 452) (formula: C₁₇H₁₄ClFN₂O₄).

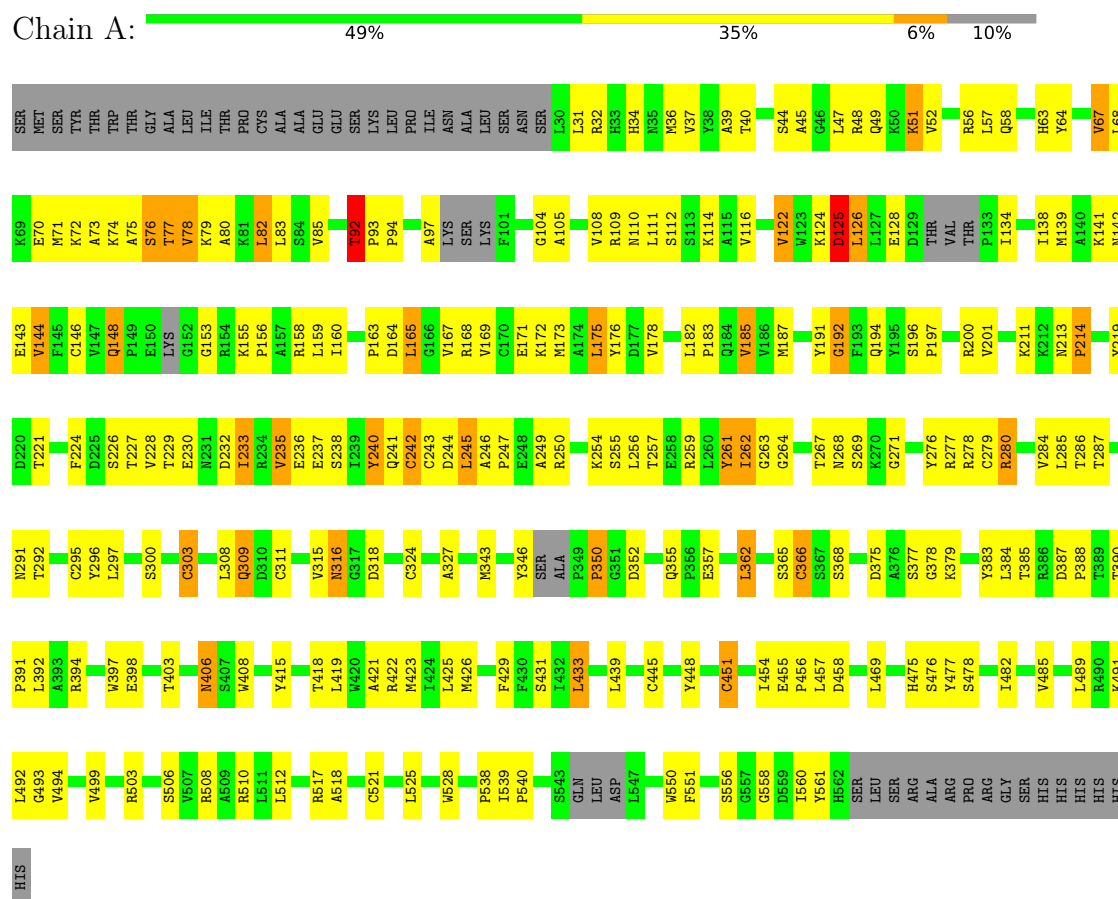


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0	0
			25	17	1	1	2	4		
2	B	1	Total	C	Cl	F	N	O	0	0
			25	17	1	1	2	4		

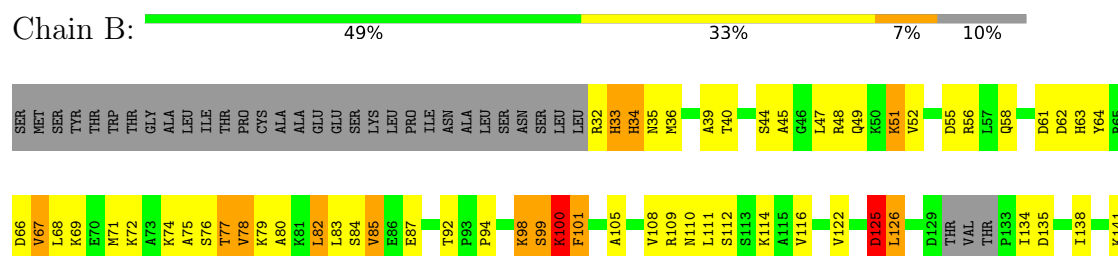
3 Residue-property plots

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: RNA-directed RNA polymerase



• Molecule 1: RNA-directed RNA polymerase



N142	E143	V144	F145	C146	V147	Q148	P149	E150	K151	G152	G153	R154	K155	P156	R157	R158	L159	I160		P163	D164	L165	G166	V167	R168	V169	C170	E171	K172	M173	A174	L175	Y176	D177	V178	V179	S180	T181	L182	P183	Q184	V185	V186	M187		S190	Y191	G192	F193	Q194	Y195	S196	P197		R200	V201		K211																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.83Å 70.88Å 251.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.77 – 2.90 19.77 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.77-2.90) 99.8 (19.77-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.279 , 0.296 0.270 , 0.290	Depositor DCC
R_{free} test set	2495 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.707	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 30.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.488 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8193	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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: 452

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	0.59	0/4151	1.18	36/5622 (0.6%)
1	B	0.64	3/4166 (0.1%)	1.23	45/5643 (0.8%)
All	All	0.62	3/8317 (0.0%)	1.21	81/11265 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	100	LYS	C-O	-10.62	1.10	1.24
1	B	100	LYS	C-N	6.88	1.44	1.33
1	B	99	SER	C-N	5.54	1.41	1.33

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	LYS	N-CA-C	12.99	128.42	112.58
1	B	101	PHE	N-CA-C	10.91	126.17	113.19
1	B	148	GLN	N-CA-C	10.46	125.18	110.01
1	A	558	GLY	N-CA-C	-10.25	98.66	112.81
1	A	78	VAL	N-CA-C	10.06	123.63	108.23
1	B	78	VAL	N-CA-C	9.76	122.31	108.36
1	A	148	GLN	N-CA-C	9.34	123.56	110.01
1	B	261	TYR	N-CA-C	9.12	122.91	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	196	SER	N-CA-C	-8.75	98.64	110.36
1	B	558	GLY	N-CA-C	-8.65	98.92	112.58
1	B	150	GLU	N-CA-C	-8.63	101.57	113.56
1	B	366	CYS	N-CA-C	-8.20	102.58	112.58
1	B	125	ASP	N-CA-C	-8.19	102.30	111.71
1	A	192	GLY	N-CA-C	7.92	122.24	112.73
1	A	196	SER	N-CA-C	-7.88	98.56	110.07
1	A	125	ASP	N-CA-C	-7.69	102.86	111.71
1	A	261	TYR	N-CA-C	7.53	120.96	111.69
1	B	309	GLN	N-CA-C	7.45	121.98	110.20
1	B	101	PHE	CA-C-N	-7.10	111.02	122.30
1	B	101	PHE	C-N-CA	-7.10	111.02	122.30
1	B	192	GLY	N-CA-C	7.08	121.83	112.77
1	B	99	SER	N-CA-C	-7.03	95.83	110.80
1	A	366	CYS	N-CA-C	-7.01	103.27	112.24
1	B	98	LYS	N-CA-C	6.86	125.41	110.80
1	A	114	LYS	N-CA-C	-6.84	103.75	111.14
1	B	99	SER	CA-C-N	-6.80	108.55	121.54
1	B	99	SER	C-N-CA	-6.80	108.55	121.54
1	A	309	GLN	N-CA-C	6.65	120.71	110.20
1	B	114	LYS	N-CA-C	-6.60	104.02	111.14
1	A	352	ASP	CA-C-N	-6.54	113.64	120.38
1	A	352	ASP	C-N-CA	-6.54	113.64	120.38
1	B	560	ILE	N-CA-C	6.46	118.34	108.71
1	A	560	ILE	N-CA-C	6.34	117.72	108.53
1	B	337	ARG	N-CA-C	-6.31	105.40	113.23
1	A	213	ASN	CA-C-N	6.29	126.24	119.76
1	A	213	ASN	C-N-CA	6.29	126.24	119.76
1	B	175	LEU	N-CA-C	6.28	121.08	113.17
1	A	240	TYR	N-CA-C	-6.09	104.55	111.07
1	A	175	LEU	N-CA-C	6.08	120.90	112.45
1	A	387	ASP	N-CA-C	-6.04	100.78	109.48
1	A	378	GLY	N-CA-C	-6.01	107.78	115.42
1	A	51	LYS	N-CA-C	-5.98	105.82	113.23
1	A	403	THR	N-CA-C	5.95	119.86	110.58
1	B	387	ASP	N-CA-C	-5.95	100.91	109.48
1	B	214	PRO	N-CA-C	5.92	120.38	111.14
1	A	67	VAL	N-CA-C	-5.92	104.56	110.30
1	A	352	ASP	N-CA-C	-5.90	102.72	110.39
1	B	51	LYS	N-CA-C	-5.81	106.35	113.50
1	B	403	THR	N-CA-C	5.81	119.65	110.58
1	A	343	MET	N-CA-C	-5.75	104.70	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	TYR	N-CA-C	-5.67	105.02	111.14
1	B	534	LEU	N-CA-C	-5.64	101.69	110.42
1	B	144	VAL	N-CA-C	5.59	115.83	107.51
1	A	144	VAL	N-CA-C	5.58	115.82	107.51
1	A	214	PRO	N-CA-C	5.57	119.83	111.14
1	A	280	ARG	N-CA-C	5.45	118.08	109.96
1	B	100	LYS	CA-C-O	5.33	128.14	120.51
1	B	67	VAL	N-CA-C	-5.32	105.31	110.42
1	B	423	MET	N-CA-C	5.30	117.97	111.82
1	B	352	ASP	N-CA-C	-5.29	102.33	110.32
1	A	92	THR	CA-C-N	5.28	125.82	120.38
1	A	92	THR	C-N-CA	5.28	125.82	120.38
1	A	148	GLN	CA-C-N	5.25	125.70	120.14
1	A	148	GLN	C-N-CA	5.25	125.70	120.14
1	A	550	TRP	N-CA-C	5.24	116.99	111.28
1	B	378	GLY	N-CA-C	-5.18	108.75	115.59
1	B	343	MET	N-CA-C	-5.16	105.34	110.97
1	A	245	LEU	N-CA-C	5.16	117.71	109.81
1	B	352	ASP	CA-C-N	-5.16	115.07	120.38
1	B	352	ASP	C-N-CA	-5.16	115.07	120.38
1	B	62	ASP	N-CA-C	-5.16	106.09	112.38
1	A	355	GLN	N-CA-C	5.15	116.16	109.72
1	B	454	ILE	N-CA-C	5.14	115.53	108.12
1	A	122	VAL	N-CA-C	-5.13	98.67	109.34
1	B	280	ARG	N-CA-C	5.13	117.60	109.96
1	B	349	PRO	CA-C-N	5.09	126.21	119.84
1	B	349	PRO	C-N-CA	5.09	126.21	119.84
1	B	148	GLN	CA-C-N	5.06	125.50	120.14
1	B	148	GLN	C-N-CA	5.06	125.50	120.14
1	B	181	THR	N-CA-C	5.02	120.94	114.56
1	A	327	ALA	N-CA-C	-5.00	106.60	113.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	100	LYS	Mainchain

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	4065	0	4071	213	0
1	B	4078	0	4084	207	0
2	A	25	0	13	0	0
2	B	25	0	13	0	0
All	All	8193	0	8181	418	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 26.

All (418) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:MET:HE1	1:A:297:LEU:HB2	1.36	1.07
1:A:261:TYR:HE1	1:A:284:VAL:HG11	1.17	1.06
1:B:230:GLU:HB3	1:B:262:ILE:HD11	1.39	1.03
1:A:254:LYS:HE3	1:B:254:LYS:HE3	1.42	0.97
1:B:377:SER:HB2	1:B:379:LYS:HG3	1.45	0.96
1:A:230:GLU:HB3	1:A:262:ILE:HD11	1.48	0.94
1:B:175:LEU:HD11	1:B:261:TYR:HE2	1.32	0.92
1:A:221:THR:HG1	1:A:224:PHE:HD1	0.93	0.91
1:A:261:TYR:CE1	1:A:284:VAL:HG11	2.09	0.87
1:B:44:SER:HB2	1:B:47:LEU:HD12	1.57	0.86
1:A:377:SER:HB2	1:A:379:LYS:HG3	1.59	0.85
1:A:309:GLN:O	1:A:324:CYS:HB2	1.80	0.82
1:A:191:TYR:O	1:A:194:GLN:HG2	1.79	0.82
1:B:170:CYS:HA	1:B:173:MET:HE3	1.62	0.81
1:A:163:PRO:HB2	1:A:167:VAL:HB	1.64	0.79
1:B:191:TYR:O	1:B:194:GLN:HG2	1.82	0.79
1:B:74:LYS:O	1:B:77:THR:HB	1.83	0.79
1:B:163:PRO:HB2	1:B:167:VAL:HB	1.64	0.79
1:B:71:MET:CE	1:B:297:LEU:HB2	2.13	0.78
1:A:76:SER:HA	1:A:242:CYS:O	1.83	0.78
1:A:79:LYS:HA	1:A:244:ASP:HB3	1.65	0.78
1:A:44:SER:HB2	1:A:47:LEU:HD12	1.66	0.77
1:A:74:LYS:O	1:A:77:THR:HB	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:ARG:O	1:A:398:GLU:HG3	1.84	0.77
1:B:175:LEU:HD13	1:B:286:THR:CG2	2.14	0.77
1:B:230:GLU:HB3	1:B:262:ILE:CD1	2.14	0.76
1:B:221:THR:HG1	1:B:224:PHE:HD1	1.30	0.76
1:B:309:GLN:O	1:B:324:CYS:HB2	1.86	0.76
1:A:171:GLU:OE1	1:A:284:VAL:HG12	1.84	0.76
1:B:303:CYS:SG	1:B:308:LEU:HD11	2.26	0.75
1:A:230:GLU:HB3	1:A:262:ILE:CD1	2.16	0.75
1:B:79:LYS:HA	1:B:244:ASP:HB3	1.68	0.75
1:A:303:CYS:SG	1:A:308:LEU:HD11	2.28	0.74
1:A:126:LEU:HA	1:A:259:ARG:NH1	2.02	0.74
1:B:245:LEU:HB2	1:B:250:ARG:HE	1.53	0.74
1:B:63:HIS:O	1:B:67:VAL:HG23	1.87	0.74
1:A:141:LYS:HG3	1:A:160:ILE:CG1	2.18	0.73
1:B:82:LEU:HD13	1:B:249:ALA:HB2	1.70	0.73
1:A:232:ASP:O	1:A:236:GLU:HG3	1.89	0.73
1:B:175:LEU:HD13	1:B:286:THR:HG23	1.68	0.73
1:A:175:LEU:HD13	1:A:286:THR:CG2	2.18	0.72
1:A:175:LEU:HD11	1:A:261:TYR:HE2	1.55	0.72
1:B:230:GLU:CB	1:B:262:ILE:HD11	2.17	0.72
1:A:261:TYR:HE1	1:A:284:VAL:CG1	1.99	0.71
1:B:80:ALA:HB3	1:B:245:LEU:CD2	2.20	0.71
1:B:122:VAL:O	1:B:126:LEU:HB2	1.89	0.71
1:B:71:MET:HE2	1:B:297:LEU:HD12	1.72	0.70
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.73	0.70
1:A:230:GLU:CB	1:A:262:ILE:HD11	2.19	0.70
1:A:201:VAL:HG22	1:A:384:LEU:HG	1.73	0.70
1:B:141:LYS:HG3	1:B:160:ILE:CG1	2.21	0.69
1:A:182:LEU:HB3	1:A:183:PRO:HD3	1.74	0.69
1:B:448:TYR:CE2	1:B:551:PHE:HD1	2.11	0.69
1:A:80:ALA:HB3	1:A:245:LEU:CD2	2.23	0.69
1:B:182:LEU:HB3	1:B:183:PRO:HD3	1.74	0.69
1:B:126:LEU:HA	1:B:259:ARG:NH1	2.07	0.69
1:B:175:LEU:CD1	1:B:261:TYR:HE2	2.06	0.69
1:B:76:SER:HA	1:B:242:CYS:O	1.93	0.68
1:A:175:LEU:HD13	1:A:286:THR:HG23	1.73	0.68
1:B:94:PRO:HG3	1:B:109:ARG:HH11	1.58	0.67
1:B:149:PRO:O	1:B:150:GLU:HB2	1.93	0.67
1:B:232:ASP:O	1:B:236:GLU:HG3	1.94	0.67
1:B:237:GLU:HG3	1:B:257:THR:HG21	1.76	0.67
1:A:485:VAL:O	1:A:489:LEU:HG	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LYS:CG	1:A:160:ILE:HD11	2.25	0.66
1:B:148:GLN:O	1:B:151:LYS:HA	1.95	0.66
1:A:122:VAL:O	1:A:126:LEU:HB2	1.96	0.66
1:B:67:VAL:HG21	1:B:301:ALA:HB2	1.76	0.66
1:B:175:LEU:HD11	1:B:261:TYR:CE2	2.23	0.66
1:A:264:GLY:HA2	1:A:276:TYR:CZ	2.31	0.66
1:B:365:SER:O	1:B:366:CYS:HB2	1.96	0.66
1:B:388:PRO:O	1:B:392:LEU:HG	1.95	0.66
1:A:128:GLU:OE2	1:B:69:LYS:HE2	1.96	0.65
1:A:141:LYS:HG2	1:A:160:ILE:HD11	1.76	0.65
1:A:245:LEU:HB2	1:A:250:ARG:HE	1.61	0.65
1:A:171:GLU:OE1	1:A:284:VAL:CG1	2.44	0.65
1:B:99:SER:C	1:B:101:PHE:N	2.49	0.65
1:B:236:GLU:OE2	1:B:280:ARG:NH2	2.30	0.65
1:B:67:VAL:O	1:B:71:MET:HG2	1.97	0.64
1:B:445:CYS:HB3	1:B:454:ILE:HD12	1.78	0.64
1:B:68:LEU:CD1	1:B:72:LYS:HE3	2.26	0.64
1:B:68:LEU:HD11	1:B:72:LYS:HE3	1.79	0.64
1:B:126:LEU:HD21	1:B:256:LEU:HG	1.80	0.64
1:B:394:ARG:O	1:B:398:GLU:HG3	1.98	0.63
1:B:94:PRO:HG3	1:B:109:ARG:NH1	2.12	0.63
1:A:63:HIS:O	1:A:67:VAL:HG23	1.98	0.63
1:B:48:ARG:HG2	1:B:159:LEU:HG	1.81	0.62
1:A:71:MET:HE1	1:A:297:LEU:CB	2.23	0.62
1:B:263:GLY:HA2	1:B:277:ARG:NH1	2.14	0.62
1:A:237:GLU:HG3	1:A:257:THR:HG21	1.82	0.62
1:B:296:TYR:O	1:B:300:SER:HB2	2.00	0.62
1:A:48:ARG:HG2	1:A:159:LEU:HG	1.80	0.62
1:A:68:LEU:HG	1:A:72:LYS:HE3	1.82	0.61
1:A:197:PRO:O	1:A:201:VAL:HG23	2.00	0.61
1:A:263:GLY:HA3	1:A:277:ARG:O	1.99	0.61
1:A:408:TRP:HB2	1:A:429:PHE:CE2	2.36	0.60
1:B:141:LYS:CG	1:B:160:ILE:HD11	2.31	0.60
1:A:388:PRO:O	1:A:392:LEU:HG	2.01	0.60
1:B:99:SER:O	1:B:100:LYS:C	2.44	0.60
1:B:141:LYS:HG2	1:B:160:ILE:HD11	1.83	0.59
1:B:149:PRO:C	1:B:151:LYS:H	2.08	0.59
1:B:419:LEU:HD23	1:B:477:TYR:CG	2.37	0.59
1:A:235:VAL:O	1:A:238:SER:HB3	2.03	0.59
1:A:448:TYR:CE2	1:A:551:PHE:HD1	2.20	0.59
1:A:224:PHE:CG	1:A:318:ASP:HB3	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:GLY:HA3	1:B:277:ARG:O	2.03	0.58
1:A:68:LEU:CG	1:A:72:LYS:HE3	2.32	0.58
1:A:68:LEU:HD11	1:A:72:LYS:HE3	1.83	0.58
1:B:201:VAL:HG22	1:B:384:LEU:HG	1.84	0.58
1:A:31:LEU:HA	1:A:494:VAL:HG12	1.85	0.58
1:A:175:LEU:O	1:A:178:VAL:N	2.26	0.58
1:B:71:MET:HE2	1:B:297:LEU:HB2	1.86	0.58
1:B:309:GLN:HG2	1:B:325:GLU:HB2	1.85	0.58
1:A:68:LEU:CD1	1:A:72:LYS:HE3	2.34	0.58
1:A:72:LYS:HB3	1:A:242:CYS:SG	2.44	0.58
1:A:126:LEU:HD21	1:A:256:LEU:HG	1.85	0.58
1:A:219:TYR:CZ	1:A:350:PRO:HB3	2.38	0.58
1:B:408:TRP:HB2	1:B:429:PHE:CE2	2.39	0.58
1:A:105:ALA:O	1:A:109:ARG:HG3	2.03	0.58
1:A:56:ARG:NH1	1:A:279:CYS:HB3	2.19	0.57
1:A:175:LEU:HD11	1:A:261:TYR:CE2	2.38	0.57
1:A:257:THR:HA	1:A:261:TYR:HB2	1.86	0.57
1:A:264:GLY:HA2	1:A:276:TYR:CE1	2.39	0.57
1:A:246:ALA:O	1:A:249:ALA:HB3	2.05	0.57
1:A:78:VAL:HG21	1:A:185:VAL:HG21	1.86	0.57
1:B:237:GLU:HA	1:B:240:TYR:CD2	2.40	0.57
1:A:211:LYS:HB2	1:A:214:PRO:HB3	1.87	0.57
1:A:230:GLU:HB3	1:A:262:ILE:CG1	2.35	0.57
1:B:141:LYS:HE3	1:B:158:ARG:HB2	1.87	0.57
1:B:246:ALA:O	1:B:249:ALA:HB3	2.04	0.57
1:B:261:TYR:HE1	1:B:284:VAL:HG11	1.69	0.57
1:A:445:CYS:HB3	1:A:454:ILE:HD12	1.87	0.57
1:A:78:VAL:CG2	1:A:185:VAL:HG21	2.35	0.56
1:B:78:VAL:HG21	1:B:185:VAL:HG21	1.87	0.56
1:B:191:TYR:CD1	1:B:292:THR:HG21	2.39	0.56
1:B:264:GLY:HA2	1:B:276:TYR:CZ	2.41	0.56
1:A:192:GLY:HA3	1:A:316:ASN:OD1	2.05	0.56
1:B:175:LEU:HD13	1:B:286:THR:HG21	1.88	0.56
1:B:134:ILE:HG13	1:B:259:ARG:HB3	1.87	0.56
1:A:58:GLN:HG2	1:A:346:TYR:O	2.06	0.56
1:A:83:LEU:HB2	1:A:173:MET:HA	1.88	0.56
1:A:221:THR:OG1	1:A:224:PHE:HD1	1.75	0.56
1:A:263:GLY:HA2	1:A:277:ARG:NH1	2.21	0.56
1:A:56:ARG:HH12	1:A:279:CYS:HB3	1.70	0.56
1:B:415:TYR:O	1:B:418:THR:HG23	2.06	0.56
1:B:175:LEU:CD1	1:B:261:TYR:CE2	2.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:VAL:HG21	1:A:165:LEU:HD21	1.88	0.55
1:A:134:ILE:HG13	1:A:259:ARG:HB3	1.89	0.55
1:B:398:GLU:OE1	1:B:408:TRP:HD1	1.89	0.55
1:A:433:LEU:HB3	1:A:439:LEU:HD23	1.88	0.55
1:A:489:LEU:HD22	1:A:494:VAL:CG2	2.37	0.55
1:B:191:TYR:HD1	1:B:292:THR:HG21	1.70	0.54
1:B:221:THR:OG1	1:B:224:PHE:HD1	1.88	0.54
1:B:224:PHE:CG	1:B:318:ASP:HB3	2.42	0.54
1:B:245:LEU:HD12	1:B:250:ARG:HG2	1.89	0.54
1:A:365:SER:O	1:A:366:CYS:HB2	2.07	0.54
1:B:71:MET:HE1	1:B:297:LEU:HB2	1.89	0.54
1:A:144:VAL:HG21	1:A:397:TRP:CD2	2.43	0.54
1:A:237:GLU:HA	1:A:240:TYR:CD2	2.42	0.54
1:B:40:THR:O	1:B:142:ASN:HA	2.06	0.54
1:B:108:VAL:HG21	1:B:165:LEU:HD21	1.89	0.54
1:A:40:THR:O	1:A:142:ASN:HA	2.06	0.54
1:A:67:VAL:HG12	1:A:71:MET:HE3	1.90	0.54
1:B:48:ARG:HA	1:B:51:LYS:HD3	1.90	0.54
1:B:80:ALA:HB3	1:B:245:LEU:HD23	1.90	0.54
1:A:419:LEU:HD23	1:A:477:TYR:CG	2.42	0.53
1:B:423:MET:HG2	1:B:528:TRP:CZ3	2.44	0.53
1:B:377:SER:C	1:B:379:LYS:H	2.17	0.53
1:A:165:LEU:O	1:A:169:VAL:HG23	2.09	0.53
1:A:32:ARG:HB2	1:A:493:GLY:O	2.09	0.53
1:A:200:ARG:HD3	1:A:384:LEU:CD1	2.39	0.53
1:A:284:VAL:O	1:A:287:THR:HG22	2.08	0.52
1:B:58:GLN:HG2	1:B:346:TYR:O	2.09	0.52
1:B:48:ARG:CG	1:B:159:LEU:HG	2.40	0.52
1:B:144:VAL:HG21	1:B:397:TRP:CD2	2.45	0.52
1:A:241:GLN:HE22	1:A:250:ARG:HA	1.73	0.52
1:B:469:LEU:HD11	1:B:538:PRO:HA	1.91	0.52
1:A:241:GLN:HE22	1:A:250:ARG:CA	2.23	0.52
1:B:219:TYR:CZ	1:B:350:PRO:HB3	2.45	0.52
1:B:44:SER:CB	1:B:47:LEU:HD12	2.34	0.52
1:B:72:LYS:HB3	1:B:242:CYS:SG	2.49	0.52
1:B:83:LEU:O	1:B:173:MET:HG2	2.10	0.52
1:A:423:MET:HG2	1:A:528:TRP:CZ3	2.45	0.51
1:A:499:VAL:HG12	1:A:503:ARG:NE	2.26	0.51
1:B:268:ASN:HD21	1:B:272:GLN:HB2	1.75	0.51
1:A:219:TYR:HE2	1:A:221:THR:HG22	1.73	0.51
1:A:303:CYS:SG	1:A:308:LEU:HD21	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:HIS:O	1:A:476:SER:HB2	2.09	0.51
1:A:56:ARG:NH1	1:A:226:SER:O	2.44	0.51
1:A:236:GLU:OE2	1:A:280:ARG:NH2	2.39	0.51
1:B:85:VAL:HG11	1:B:116:VAL:HG13	1.93	0.51
1:B:141:LYS:HG3	1:B:160:ILE:HG12	1.91	0.51
1:B:170:CYS:HA	1:B:173:MET:CE	2.38	0.51
1:B:224:PHE:HE2	1:B:291:ASN:HA	1.76	0.51
1:A:224:PHE:CB	1:A:318:ASP:HB3	2.41	0.51
1:A:141:LYS:HG3	1:A:160:ILE:HG12	1.92	0.51
1:B:39:ALA:HB2	1:B:144:VAL:HG22	1.93	0.51
1:B:105:ALA:O	1:B:109:ARG:HG3	2.11	0.50
1:B:149:PRO:C	1:B:151:LYS:N	2.67	0.50
1:A:255:SER:O	1:A:259:ARG:HG3	2.11	0.50
1:B:478:SER:O	1:B:482:ILE:HG13	2.11	0.50
1:B:237:GLU:OE1	1:B:241:GLN:HG3	2.11	0.50
1:A:366:CYS:C	1:A:368:SER:H	2.20	0.50
1:A:377:SER:C	1:A:379:LYS:H	2.19	0.50
1:B:211:LYS:HB2	1:B:214:PRO:HB3	1.94	0.50
1:A:406:ASN:H	1:A:406:ASN:HD22	1.60	0.50
1:A:48:ARG:CG	1:A:159:LEU:HG	2.41	0.50
1:B:75:ALA:C	1:B:77:THR:H	2.20	0.50
1:B:200:ARG:HD3	1:B:384:LEU:CD1	2.42	0.49
1:A:44:SER:CB	1:A:47:LEU:HD12	2.41	0.49
1:B:68:LEU:HA	1:B:71:MET:HG3	1.93	0.49
1:B:78:VAL:CG2	1:B:185:VAL:HG21	2.42	0.49
1:A:56:ARG:HD3	1:A:226:SER:O	2.11	0.49
1:B:475:HIS:O	1:B:476:SER:HB2	2.11	0.49
1:A:246:ALA:HB3	1:A:249:ALA:HB2	1.94	0.49
1:B:408:TRP:CB	1:B:429:PHE:CE2	2.95	0.49
1:A:191:TYR:HD1	1:A:292:THR:HG21	1.78	0.49
1:A:224:PHE:O	1:A:228:VAL:HG23	2.12	0.49
1:A:82:LEU:CD1	1:A:249:ALA:HB2	2.43	0.49
1:B:125:ASP:C	1:B:125:ASP:OD1	2.56	0.49
1:B:419:LEU:C	1:B:419:LEU:HD12	2.38	0.49
1:A:31:LEU:HD21	1:A:34:HIS:HA	1.93	0.49
1:A:126:LEU:HA	1:A:259:ARG:HH12	1.74	0.49
1:A:451:CYS:HB3	1:A:561:TYR:HD1	1.78	0.49
1:B:422:ARG:NH2	1:B:528:TRP:HB3	2.28	0.49
1:B:264:GLY:HA2	1:B:276:TYR:CE1	2.47	0.49
1:A:39:ALA:HB2	1:A:144:VAL:HG22	1.95	0.48
1:A:237:GLU:HA	1:A:240:TYR:HD2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:THR:HB	1:B:391:PRO:HD3	1.95	0.48
1:A:224:PHE:HE2	1:A:291:ASN:HA	1.78	0.48
1:A:200:ARG:HD3	1:A:384:LEU:HD11	1.95	0.48
1:B:144:VAL:HB	1:B:394:ARG:HG2	1.94	0.48
1:B:237:GLU:OE1	1:B:241:GLN:CG	2.62	0.48
1:A:141:LYS:HG3	1:A:160:ILE:HD11	1.94	0.48
1:A:47:LEU:HB2	1:A:156:PRO:HB3	1.95	0.48
1:A:408:TRP:CB	1:A:429:PHE:CE2	2.96	0.48
1:B:182:LEU:HD21	1:B:293:LEU:HD21	1.95	0.48
1:A:233:ILE:O	1:A:236:GLU:HB2	2.14	0.48
1:A:48:ARG:HA	1:A:51:LYS:HD3	1.95	0.48
1:A:246:ALA:O	1:A:249:ALA:N	2.46	0.48
1:A:455:GLU:O	1:A:458:ASP:HB2	2.13	0.48
1:B:66:ASP:HB3	1:B:304:ARG:HH12	1.78	0.48
1:B:125:ASP:OD1	1:B:259:ARG:NH2	2.43	0.48
1:B:175:LEU:O	1:B:178:VAL:HG12	2.13	0.48
1:A:383:TYR:HE2	1:A:385:THR:HB	1.79	0.48
1:A:398:GLU:OE1	1:A:408:TRP:HD1	1.97	0.48
1:B:230:GLU:HB3	1:B:262:ILE:CG1	2.42	0.48
1:B:419:LEU:HD11	1:B:485:VAL:HG11	1.96	0.48
1:A:80:ALA:HB3	1:A:245:LEU:HD23	1.95	0.48
1:A:303:CYS:SG	1:A:308:LEU:CD1	3.01	0.48
1:A:415:TYR:O	1:A:418:THR:HG23	2.13	0.48
1:A:56:ARG:HE	1:A:229:THR:HG22	1.78	0.47
1:A:296:TYR:O	1:A:300:SER:HB2	2.13	0.47
1:A:36:MET:HE1	1:A:491:LYS:O	2.14	0.47
1:A:191:TYR:CD1	1:A:292:THR:HG21	2.49	0.47
1:B:284:VAL:HG23	1:B:287:THR:HB	1.94	0.47
1:A:243:CYS:O	1:A:245:LEU:HG	2.14	0.47
1:B:366:CYS:C	1:B:368:SER:H	2.21	0.47
1:B:187:MET:HE1	1:B:292:THR:HG22	1.97	0.47
1:A:85:VAL:HG11	1:A:116:VAL:HG13	1.97	0.47
1:B:47:LEU:HB2	1:B:156:PRO:HB3	1.97	0.47
1:B:56:ARG:HH11	1:B:56:ARG:HG3	1.80	0.47
1:B:339:PHE:O	1:B:343:MET:HG2	2.15	0.47
1:B:126:LEU:HA	1:B:259:ARG:HH11	1.80	0.47
1:B:141:LYS:HG3	1:B:160:ILE:HD11	1.97	0.47
1:B:284:VAL:O	1:B:287:THR:HG22	2.15	0.47
1:A:124:LYS:O	1:A:128:GLU:HG3	2.15	0.46
1:A:398:GLU:OE2	1:A:406:ASN:HA	2.15	0.46
1:A:419:LEU:C	1:A:419:LEU:HD12	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:THR:HA	1:B:261:TYR:HB2	1.96	0.46
1:A:383:TYR:CE2	1:A:385:THR:HB	2.51	0.46
1:B:163:PRO:HB2	1:B:167:VAL:CB	2.40	0.46
1:B:233:ILE:O	1:B:236:GLU:HB2	2.15	0.46
1:B:398:GLU:OE2	1:B:406:ASN:HA	2.16	0.46
1:A:422:ARG:NH2	1:A:528:TRP:HB3	2.30	0.46
1:B:176:TYR:HA	1:B:285:LEU:HD21	1.96	0.46
1:A:97:ALA:O	1:A:168:ARG:NH2	2.48	0.46
1:A:125:ASP:C	1:A:125:ASP:OD1	2.59	0.46
1:A:141:LYS:HG3	1:A:160:ILE:CD1	2.45	0.46
1:B:64:TYR:C	1:B:64:TYR:CD2	2.94	0.46
1:A:31:LEU:HD22	1:A:37:VAL:HG21	1.98	0.46
1:A:164:ASP:O	1:A:165:LEU:C	2.57	0.46
1:B:192:GLY:HA3	1:B:316:ASN:OD1	2.15	0.46
1:A:94:PRO:HG3	1:A:109:ARG:NH1	2.31	0.46
1:A:506:SER:O	1:A:510:ARG:HG3	2.16	0.46
1:A:78:VAL:HB	1:A:243:CYS:SG	2.56	0.45
1:B:303:CYS:SG	1:B:308:LEU:CD1	3.02	0.45
1:A:94:PRO:HG3	1:A:109:ARG:HH11	1.81	0.45
1:B:84:SER:OG	1:B:87:GLU:HG3	2.16	0.45
1:B:237:GLU:CG	1:B:257:THR:HG21	2.45	0.45
1:A:56:ARG:HD3	1:A:227:THR:HA	1.97	0.45
1:A:377:SER:CB	1:A:379:LYS:HG3	2.36	0.45
1:A:489:LEU:HD22	1:A:494:VAL:HG21	1.97	0.45
1:A:499:VAL:CG1	1:A:503:ARG:HE	2.29	0.45
1:B:456:PRO:C	1:B:458:ASP:H	2.23	0.45
1:A:110:ASN:O	1:A:111:LEU:HB2	2.15	0.45
1:B:39:ALA:HA	1:B:143:GLU:O	2.16	0.45
1:A:245:LEU:HD12	1:A:250:ARG:HG2	1.99	0.45
1:A:263:GLY:HA2	1:A:277:ARG:CZ	2.47	0.45
1:B:165:LEU:O	1:B:169:VAL:HG23	2.17	0.45
1:A:126:LEU:HA	1:A:259:ARG:HH11	1.78	0.45
1:B:78:VAL:HB	1:B:243:CYS:SG	2.57	0.45
1:B:108:VAL:CG2	1:B:165:LEU:HD21	2.46	0.45
1:B:469:LEU:HD11	1:B:538:PRO:CA	2.46	0.45
1:A:292:THR:HG23	1:A:315:VAL:HG12	1.97	0.45
1:A:56:ARG:NH2	1:A:278:ARG:O	2.49	0.45
1:A:70:GLU:O	1:A:73:ALA:HB3	2.17	0.44
1:A:141:LYS:HE3	1:A:158:ARG:HB2	1.99	0.44
1:A:423:MET:HA	1:A:528:TRP:CZ2	2.52	0.44
1:B:175:LEU:O	1:B:179:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ALA:O	1:B:249:ALA:N	2.48	0.44
1:A:75:ALA:C	1:A:77:THR:H	2.26	0.44
1:A:176:TYR:HA	1:A:285:LEU:HD21	1.99	0.44
1:B:465:ARG:NH1	1:B:543:SER:HA	2.32	0.44
1:A:92:THR:HA	1:A:93:PRO:HD3	1.80	0.44
1:A:303:CYS:SG	1:A:308:LEU:CG	3.05	0.44
1:A:36:MET:O	1:A:146:CYS:HA	2.17	0.44
1:A:175:LEU:HD13	1:A:286:THR:HG21	1.94	0.44
1:A:182:LEU:O	1:A:185:VAL:N	2.47	0.44
1:A:421:ALA:O	1:A:426:MET:HG3	2.18	0.44
1:A:457:LEU:HB3	1:A:517:ARG:HB3	2.00	0.44
1:B:56:ARG:HD2	1:B:229:THR:HG22	2.00	0.44
1:A:224:PHE:CB	1:A:318:ASP:CB	2.96	0.44
1:B:155:LYS:HA	1:B:156:PRO:HD3	1.82	0.44
1:B:163:PRO:HB3	1:B:167:VAL:HG21	1.99	0.44
1:B:179:VAL:HG12	1:B:289:CYS:CB	2.47	0.44
1:B:383:TYR:CE2	1:B:385:THR:HB	2.53	0.44
1:B:55:ASP:OD1	1:B:56:ARG:N	2.51	0.44
1:B:224:PHE:CB	1:B:318:ASP:HB3	2.48	0.44
1:A:163:PRO:CB	1:A:167:VAL:HB	2.42	0.44
1:B:179:VAL:HG12	1:B:289:CYS:HB2	2.00	0.44
1:B:261:TYR:HE1	1:B:284:VAL:CG1	2.31	0.44
1:A:388:PRO:C	1:A:391:PRO:HD2	2.42	0.43
1:B:255:SER:O	1:B:259:ARG:HG3	2.18	0.43
1:A:182:LEU:HB3	1:A:183:PRO:CD	2.47	0.43
1:B:45:ALA:O	1:B:49:GLN:HG3	2.18	0.43
1:B:366:CYS:C	1:B:368:SER:N	2.76	0.43
1:A:469:LEU:HD11	1:A:538:PRO:HA	2.00	0.43
1:B:406:ASN:HD22	1:B:406:ASN:H	1.66	0.43
1:A:518:ALA:O	1:A:521:CYS:HB2	2.19	0.43
1:B:183:PRO:HB3	1:B:187:MET:CE	2.48	0.43
1:B:433:LEU:HB3	1:B:439:LEU:HD23	1.99	0.43
1:A:71:MET:HE2	1:A:296:TYR:CD2	2.53	0.43
1:A:408:TRP:HB2	1:A:429:PHE:CD2	2.54	0.43
1:B:61:ASP:C	1:B:63:HIS:N	2.73	0.43
1:B:63:HIS:O	1:B:64:TYR:C	2.62	0.43
1:B:542:ALA:O	1:B:543:SER:HB2	2.18	0.43
1:A:31:LEU:CD2	1:A:34:HIS:HA	2.49	0.43
1:A:439:LEU:HB3	1:A:457:LEU:HD21	2.01	0.43
1:B:173:MET:HE3	1:B:173:MET:HB2	1.88	0.43
1:A:56:ARG:HH21	1:A:229:THR:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:SER:O	1:A:482:ILE:HG13	2.18	0.43
1:B:282:SER:O	1:B:287:THR:HG21	2.19	0.43
1:A:182:LEU:O	1:A:183:PRO:C	2.62	0.43
1:A:469:LEU:HD23	1:A:469:LEU:HA	1.88	0.43
1:B:141:LYS:HG3	1:B:160:ILE:CD1	2.48	0.43
1:B:224:PHE:CB	1:B:318:ASP:CB	2.97	0.43
1:B:408:TRP:HB2	1:B:429:PHE:CD2	2.53	0.43
1:A:267:THR:HG22	1:A:268:ASN:O	2.19	0.42
1:A:79:LYS:HG2	1:A:244:ASP:CG	2.44	0.42
1:A:236:GLU:O	1:A:237:GLU:C	2.62	0.42
1:B:126:LEU:HA	1:B:259:ARG:HH12	1.82	0.42
1:B:359:ASP:HB3	1:B:362:LEU:HD22	2.00	0.42
1:B:499:VAL:HG12	1:B:503:ARG:NE	2.34	0.42
1:B:555:TYR:O	1:B:556:SER:C	2.62	0.42
1:B:32:ARG:O	1:B:34:HIS:N	2.48	0.42
1:A:164:ASP:O	1:A:167:VAL:N	2.53	0.42
1:A:308:LEU:HD11	1:A:311:CYS:SG	2.59	0.42
1:A:155:LYS:HA	1:A:156:PRO:HD3	1.83	0.42
1:B:66:ASP:HB3	1:B:304:ARG:NH1	2.34	0.42
1:B:134:ILE:HG22	1:B:135:ASP:N	2.35	0.42
1:B:56:ARG:HE	1:B:229:THR:HG22	1.85	0.42
1:B:495:PRO:HA	1:B:496:PRO:HD3	1.90	0.42
1:A:39:ALA:HA	1:A:143:GLU:O	2.20	0.42
1:A:183:PRO:HB3	1:A:187:MET:CE	2.50	0.42
1:B:190:SER:HA	1:B:313:MET:O	2.19	0.42
1:B:315:VAL:HG22	1:B:320:LEU:CD1	2.50	0.42
1:A:390:THR:HB	1:A:391:PRO:HD3	2.02	0.42
1:B:182:LEU:O	1:B:183:PRO:C	2.63	0.42
1:A:237:GLU:OE1	1:A:241:GLN:CG	2.68	0.41
1:B:197:PRO:O	1:B:201:VAL:HG23	2.20	0.41
1:B:313:MET:HG2	1:B:322:VAL:HG22	2.02	0.41
1:B:377:SER:C	1:B:379:LYS:N	2.78	0.41
1:A:148:GLN:HG3	1:A:153:GLY:O	2.20	0.41
1:B:196:SER:HA	1:B:551:PHE:CD1	2.55	0.41
1:A:93:PRO:HA	1:A:94:PRO:HD3	1.90	0.41
1:A:68:LEU:HD12	1:A:68:LEU:HA	1.82	0.41
1:A:224:PHE:CZ	1:A:295:CYS:HB2	2.56	0.41
1:A:45:ALA:O	1:A:49:GLN:HG3	2.21	0.41
1:B:178:VAL:CG1	1:B:179:VAL:N	2.82	0.41
1:B:237:GLU:HG2	1:B:257:THR:OG1	2.20	0.41
1:A:366:CYS:C	1:A:368:SER:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:ILE:HG23	1:A:540:PRO:HD2	2.01	0.41
1:B:172:LYS:HE2	1:B:559:ASP:O	2.20	0.41
1:A:104:GLY:O	1:A:108:VAL:HG23	2.21	0.41
1:A:146:CYS:SG	1:A:492:LEU:HD21	2.60	0.41
1:B:221:THR:OG1	1:B:224:PHE:CD1	2.69	0.41
1:A:63:HIS:O	1:A:64:TYR:C	2.63	0.41
1:A:357:GLU:OE2	1:A:362:LEU:HD23	2.21	0.41
1:B:33:HIS:C	1:B:35:ASN:H	2.29	0.41
1:B:36:MET:O	1:B:146:CYS:HA	2.21	0.41
1:B:374:HIS:CE1	1:B:380:ARG:HG3	2.56	0.41
1:A:82:LEU:HA	1:A:82:LEU:HD12	1.86	0.41
1:A:172:LYS:HA	1:A:176:TYR:HB2	2.02	0.41
1:B:237:GLU:HA	1:B:240:TYR:HD2	1.84	0.41
1:B:451:CYS:HB3	1:B:561:TYR:HD1	1.85	0.41
1:B:455:GLU:O	1:B:458:ASP:HB2	2.21	0.41
1:B:56:ARG:HG3	1:B:56:ARG:NH1	2.35	0.40
1:A:139:MET:HE1	1:A:269:SER:HB3	2.03	0.40
1:A:508:ARG:O	1:A:512:LEU:HG	2.21	0.40
1:B:277:ARG:CZ	1:B:281:ALA:HB2	2.52	0.40
1:B:148:GLN:HG3	1:B:153:GLY:O	2.22	0.40
1:B:311:CYS:HA	1:B:324:CYS:HB3	2.03	0.40
1:B:455:GLU:O	1:B:456:PRO:C	2.64	0.40
1:A:375:ASP:OD1	1:A:377:SER:N	2.47	0.40
1:B:228:VAL:HG21	1:B:280:ARG:HB2	2.01	0.40
1:A:521:CYS:O	1:A:525:LEU:HB2	2.22	0.40
1:B:110:ASN:O	1:B:111:LEU:HB2	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	509/578 (88%)	466 (92%)	41 (8%)	2 (0%)	30	59
1	B	515/578 (89%)	464 (90%)	46 (9%)	5 (1%)	12	39
All	All	1024/1156 (89%)	930 (91%)	87 (8%)	7 (1%)	18	48

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	98	LYS
1	A	165	LEU
1	B	34	HIS
1	B	33	HIS
1	A	271	GLY
1	B	457	LEU
1	B	271	GLY

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	443/492 (90%)	416 (94%)	27 (6%)	17	46
1	B	444/492 (90%)	415 (94%)	29 (6%)	15	44
All	All	887/984 (90%)	831 (94%)	56 (6%)	16	45

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	57	LEU
1	A	76	SER
1	A	77	THR
1	A	82	LEU
1	A	92	THR
1	A	112	SER
1	A	125	ASP
1	A	126	LEU

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Mol	Chain	Res	Type
1	A	138	ILE
1	A	185	VAL
1	A	233	ILE
1	A	235	VAL
1	A	242	CYS
1	A	247	PRO
1	A	262	ILE
1	A	303	CYS
1	A	316	ASN
1	A	350	PRO
1	A	362	LEU
1	A	406	ASN
1	A	425	LEU
1	A	431	SER
1	A	433	LEU
1	A	451	CYS
1	A	456	PRO
1	A	556	SER
1	B	52	VAL
1	B	77	THR
1	B	82	LEU
1	B	85	VAL
1	B	92	THR
1	B	112	SER
1	B	125	ASP
1	B	126	LEU
1	B	138	ILE
1	B	173	MET
1	B	178	VAL
1	B	185	VAL
1	B	233	ILE
1	B	235	VAL
1	B	242	CYS
1	B	247	PRO
1	B	262	ILE
1	B	284	VAL
1	B	300	SER
1	B	303	CYS
1	B	316	ASN
1	B	350	PRO
1	B	362	LEU
1	B	425	LEU

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Mol	Chain	Res	Type
1	B	431	SER
1	B	451	CYS
1	B	456	PRO
1	B	520	THR
1	B	556	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	ASN
1	A	241	GLN
1	B	95	HIS
1	B	120	HIS
1	B	194	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	452	A	579	-	26,26,26	2.31	12 (46%)	36,36,36	1.22	4 (11%)
2	452	B	579	-	26,26,26	2.43	12 (46%)	36,36,36	1.22	3 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	452	A	579	-	-	0/17/17/17	0/2/2/2
2	452	B	579	-	-	0/17/17/17	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	579	452	C7-C8	4.72	1.47	1.39
2	B	579	452	C3-C8	4.18	1.47	1.41
2	A	579	452	C7-C8	4.14	1.46	1.39
2	A	579	452	C4-C5	4.09	1.44	1.37
2	B	579	452	C4-C3	3.98	1.46	1.39
2	A	579	452	C16-C11	3.71	1.46	1.41
2	A	579	452	C4-C3	3.66	1.45	1.39
2	B	579	452	C4-C5	3.66	1.44	1.37
2	A	579	452	C12-C11	3.42	1.45	1.39
2	B	579	452	C16-C11	3.32	1.46	1.41
2	B	579	452	C6-C5	3.27	1.43	1.38
2	A	579	452	C6-C5	3.17	1.43	1.38
2	B	579	452	C12-C11	2.99	1.44	1.39
2	A	579	452	C15-C16	2.97	1.44	1.39
2	B	579	452	C15-C16	2.81	1.44	1.39
2	B	579	452	C8-N1	2.76	1.44	1.37
2	A	579	452	C3-C8	2.72	1.45	1.41
2	B	579	452	C3-C2	2.70	1.54	1.48
2	B	579	452	C9-N1	2.57	1.49	1.45
2	B	579	452	C7-C6	2.38	1.42	1.38
2	A	579	452	C10-N2	2.30	1.40	1.35
2	A	579	452	C8-N1	2.28	1.43	1.37
2	A	579	452	C3-C2	2.21	1.53	1.48
2	A	579	452	C11-N2	2.03	1.45	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	579	452	C9-N1-C8	3.19	128.66	123.94
2	A	579	452	C9-N1-C8	2.92	128.26	123.94
2	B	579	452	O2-C10-N2	2.24	127.66	123.64
2	A	579	452	C8-C7-C6	2.18	123.50	120.05
2	B	579	452	C8-C7-C6	2.13	123.42	120.05
2	A	579	452	C11-C16-C17	2.02	123.98	121.72
2	A	579	452	O2-C10-N2	2.00	127.23	123.64

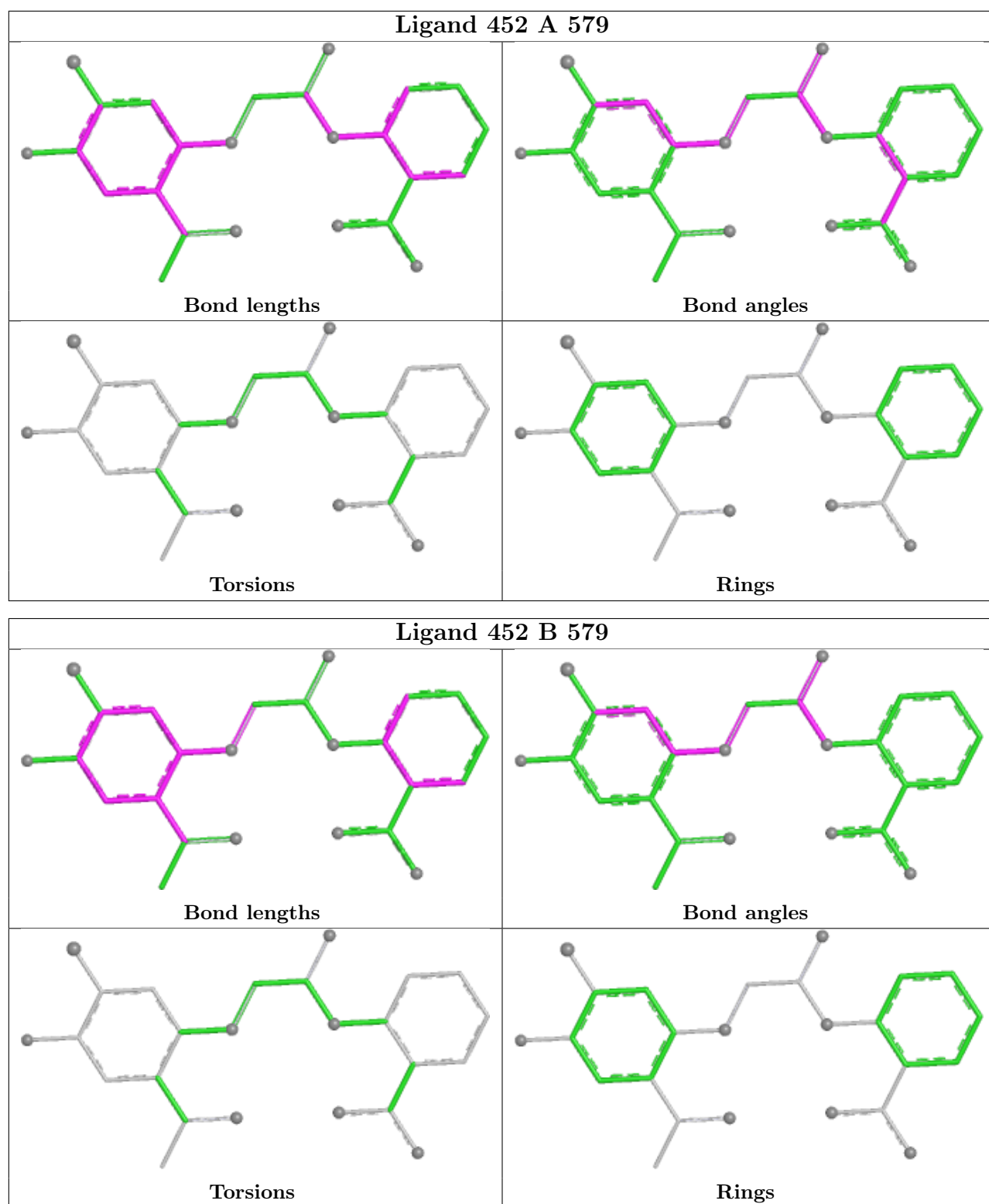
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	521/578 (90%)	-1.25	0 100 100	18, 43, 77, 119	0
1	B	523/578 (90%)	-1.24	0 100 100	19, 43, 79, 115	0
All	All	1044/1156 (90%)	-1.24	0 100 100	18, 43, 78, 119	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

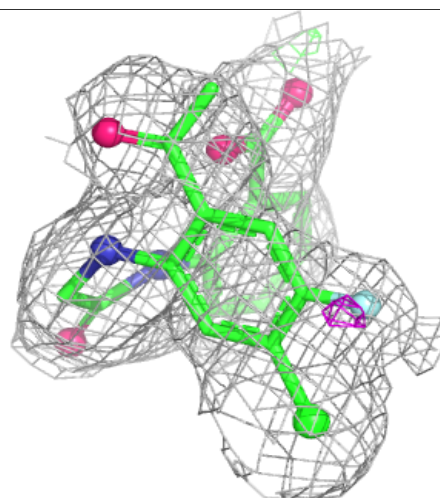
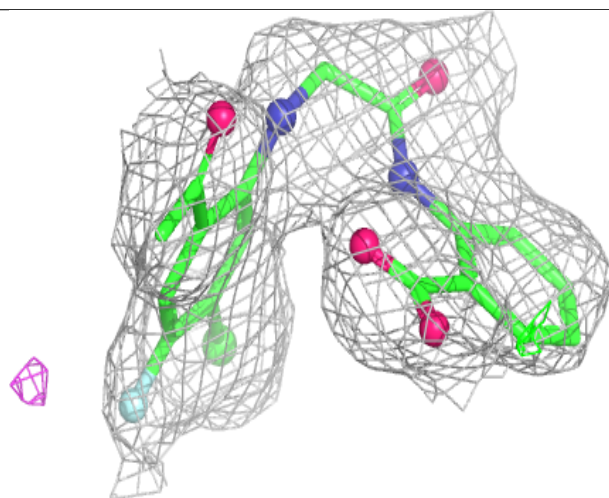
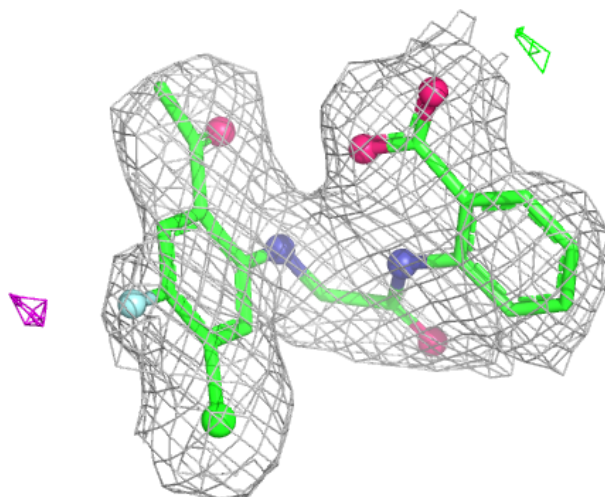
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	452	A	579	25/25	0.99	0.03	22,32,37,42	0
2	452	B	579	25/25	0.99	0.03	22,31,37,39	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.

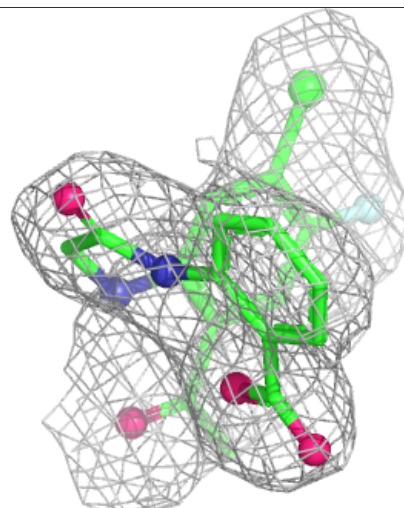
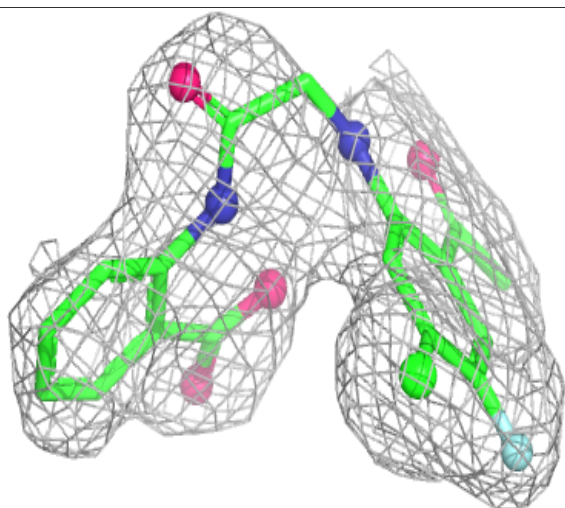
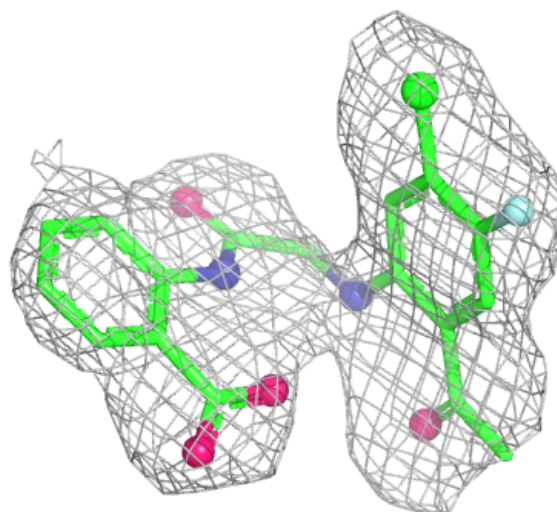
Electron density around 452 A 579:

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



Electron density around 452 B 579:

$2mF_o-DF_c$ (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.