



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:29 AM UTC

PDB ID : 1GSZ / pdb_00001gsz
Title : Crystal Structure of a Squalene Cyclase in Complex with the Potential Anti-cholesteremic Drug Ro48-8071
Authors : Lenhart, A.; Weihofen, W.A.; Pleschke, A.E.W.; Schulz, G.E.
Deposited on : 2002-01-09
Resolution : 2.80 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

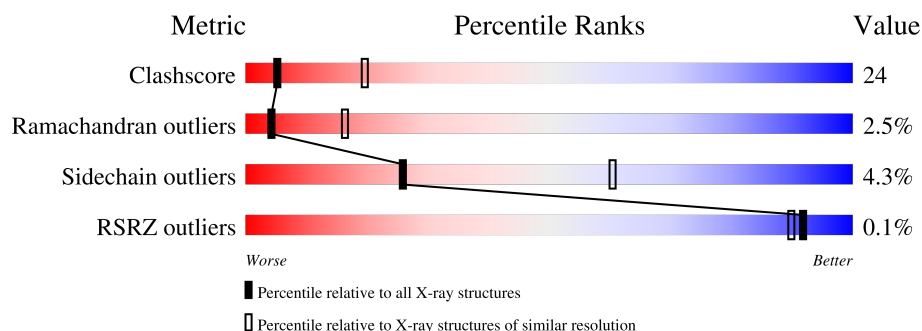
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

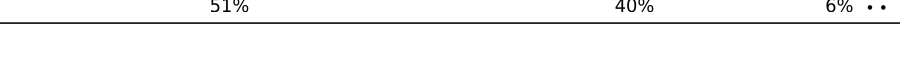
The reported resolution of this entry is 2.80 Å.

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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	631	
1	B	631	
1	C	631	

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	R71	A	1630[B]	-	X	-	-

2 Entry composition [i](#)

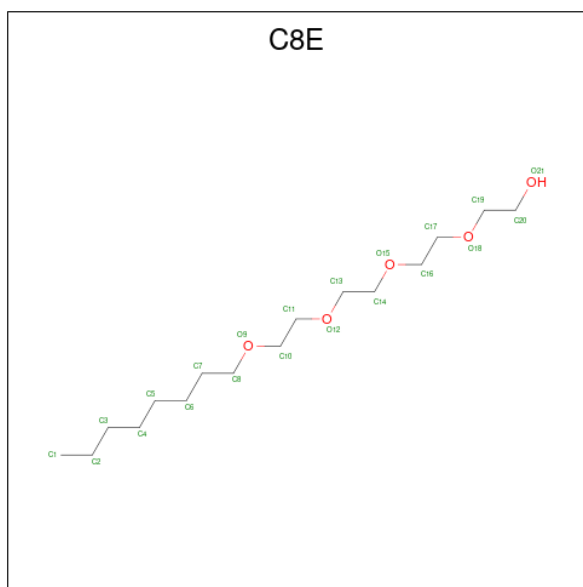
There are 4 unique types of molecules in this entry. The entry contains 15378 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SQUALENE-HOPENE CYCLASE.

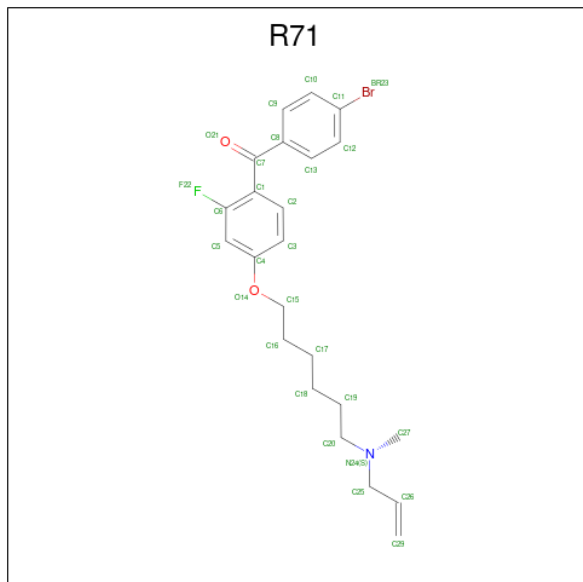
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	620	Total	C	N	O	S	0	0	1
			4964	3188	859	897	20			
1	B	620	Total	C	N	O	S	0	0	1
			4964	3188	859	897	20			
1	C	620	Total	C	N	O	S	0	0	1
			4964	3188	859	897	20			

- Molecule 2 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (CCD ID: C8E) (formula: C₁₆H₃₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			21	16	5		
2	B	1	Total	C	O	0	0
			21	16	5		
2	C	1	Total	C	O	0	0
			21	16	5		

- Molecule 3 is [4-({6-[ALLYL(METHYL)AMINO]HEXYL}OXY)-2-FLUOROPHENYL](4-BROMOPHENYL)METHANONE (CCD ID: R71) (formula: $C_{23}H_{27}BrFNO_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	Br	C	F	N	O	0	1
			56	2	46	2	2	4		
3	B	1	Total	Br	C	F	N	O	0	1
			56	2	46	2	2	4		
3	C	1	Total	Br	C	F	N	O	0	1
			56	2	46	2	2	4		

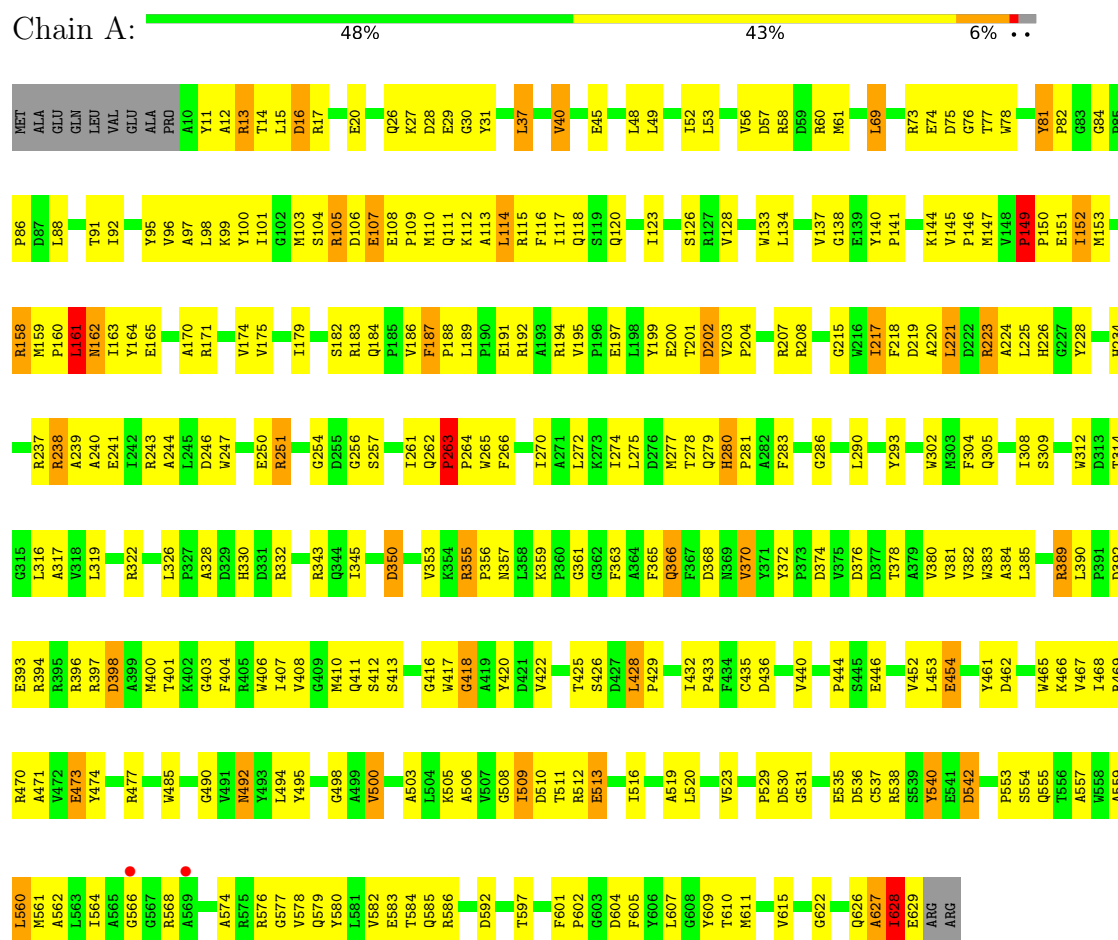
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	80	Total	O	0	0
			80	80		
4	B	94	Total	O	0	0
			94	94		
4	C	81	Total	O	0	0
			81	81		

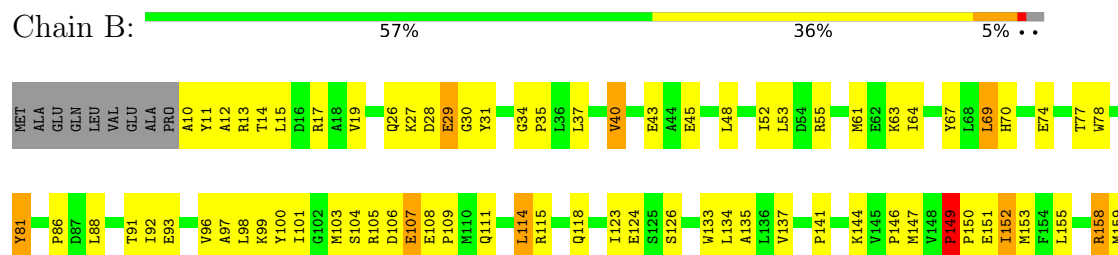
3 Residue-property plots

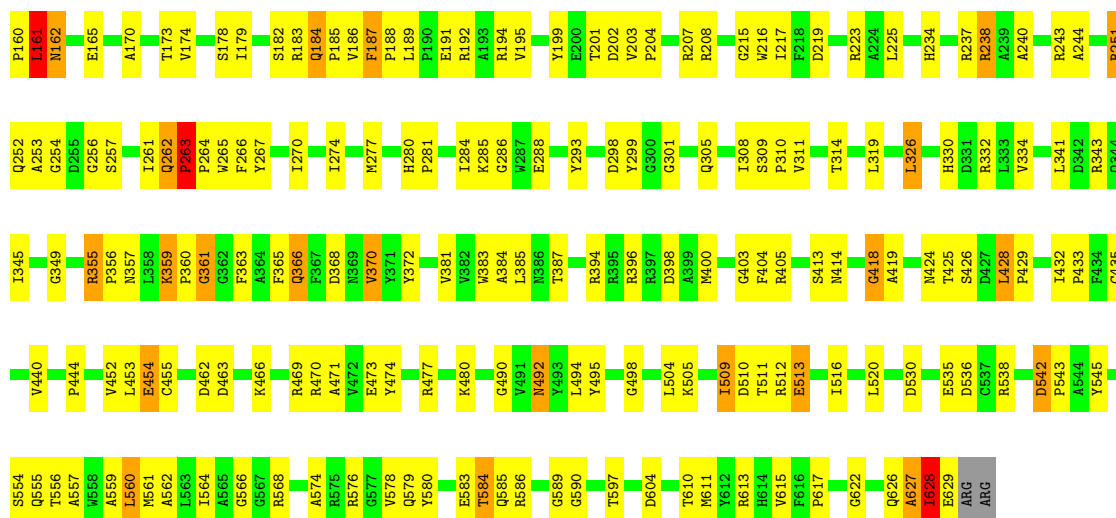
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: SQUALENE-HOPENE CYCLASE



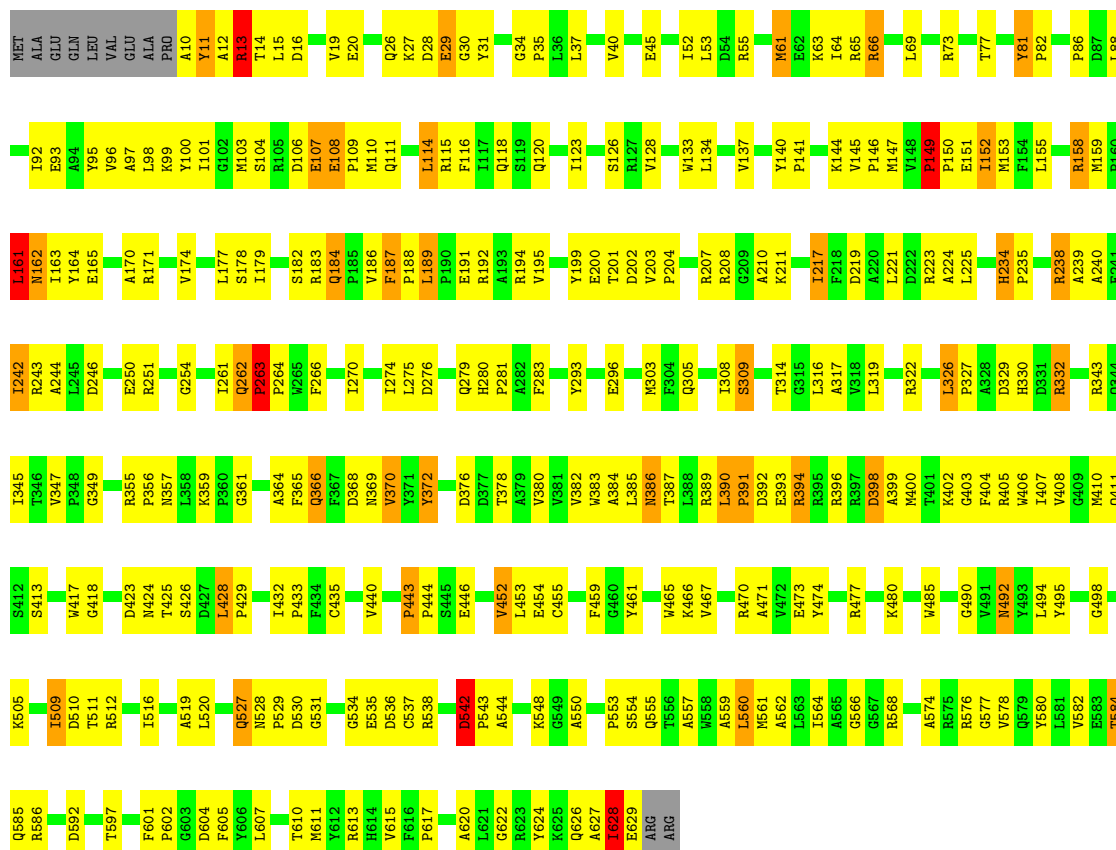
• Molecule 1: SQUALENE-HOPENE CYCLASE





● Molecule 1: SQUALENE-HOPENE CYCLASE

Chain C: 51% 40% 6% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.90Å 140.90Å 244.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.80 25.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	78.0 (25.00-2.80) 77.8 (25.00-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.80Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.203 , 0.259 0.195 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 61.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15378	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.80 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9651e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: C8E, R71

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	1/5117 (0.0%)	1.09	39/6967 (0.6%)
1	B	0.63	1/5117 (0.0%)	1.11	37/6967 (0.5%)
1	C	0.62	1/5117 (0.0%)	1.11	42/6967 (0.6%)
All	All	0.62	3/15351 (0.0%)	1.10	118/20901 (0.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	628	ILE	C-N	-5.40	1.25	1.33
1	C	628	ILE	C-N	-5.27	1.25	1.33
1	B	628	ILE	C-N	-5.25	1.25	1.33

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	PRO	N-CA-C	8.66	121.27	110.70
1	B	149	PRO	N-CA-C	7.98	120.43	110.70
1	B	615	VAL	N-CA-C	7.62	117.70	110.53
1	B	355	ARG	CA-C-N	7.57	127.28	119.56
1	B	355	ARG	C-N-CA	7.57	127.28	119.56
1	C	149	PRO	N-CA-C	7.54	119.91	110.70
1	B	263	PRO	N-CA-C	7.52	119.88	110.70
1	B	359	LYS	CA-C-N	7.51	127.56	119.90
1	B	359	LYS	C-N-CA	7.51	127.56	119.90
1	A	187	PHE	CA-C-N	7.35	127.39	119.90
1	A	187	PHE	C-N-CA	7.35	127.39	119.90
1	B	413	SER	N-CA-C	7.17	119.71	111.11
1	C	615	VAL	N-CA-C	7.04	117.15	110.53
1	C	217	ILE	CB-CA-C	-7.02	102.83	112.02
1	A	435	CYS	N-CA-C	7.01	120.54	109.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	542	ASP	CA-C-N	6.98	128.56	119.84
1	A	542	ASP	C-N-CA	6.98	128.56	119.84
1	A	615	VAL	N-CA-C	6.93	117.05	110.53
1	C	542	ASP	CA-C-N	6.93	128.50	119.84
1	C	542	ASP	C-N-CA	6.93	128.50	119.84
1	B	542	ASP	CA-C-N	6.90	128.47	119.84
1	B	542	ASP	C-N-CA	6.90	128.47	119.84
1	C	263	PRO	N-CA-C	6.84	119.05	110.70
1	B	370	VAL	N-CA-C	6.74	119.51	111.09
1	B	162	ASN	N-CA-C	-6.71	101.68	110.53
1	A	418	GLY	N-CA-C	-6.68	103.05	112.60
1	A	263	PRO	N-CA-C	6.67	118.84	110.70
1	B	604	ASP	N-CA-C	6.63	122.26	114.04
1	C	13	ARG	N-CA-C	-6.55	104.22	111.36
1	B	394	ARG	N-CA-C	-6.54	103.77	111.03
1	A	223	ARG	N-CA-C	-6.53	104.20	111.71
1	B	435	CYS	N-CA-C	6.49	119.71	109.39
1	B	187	PHE	CA-C-N	6.44	126.47	119.90
1	B	187	PHE	C-N-CA	6.44	126.47	119.90
1	C	161	LEU	N-CA-C	6.41	121.05	113.23
1	A	215	GLY	N-CA-C	-6.34	99.43	110.71
1	C	604	ASP	N-CA-C	6.29	121.84	114.04
1	C	390	LEU	CA-C-N	6.29	127.70	119.84
1	C	390	LEU	C-N-CA	6.29	127.70	119.84
1	C	480	LYS	CA-C-N	6.22	126.41	119.32
1	C	480	LYS	C-N-CA	6.22	126.41	119.32
1	A	161	LEU	N-CA-C	6.21	120.81	113.23
1	B	14	THR	N-CA-C	-6.18	103.86	111.40
1	C	359	LYS	CA-C-N	6.18	126.51	119.83
1	C	359	LYS	C-N-CA	6.18	126.51	119.83
1	A	370	VAL	N-CA-C	6.18	118.81	111.09
1	C	187	PHE	CA-C-N	6.17	126.19	119.90
1	C	187	PHE	C-N-CA	6.17	126.19	119.90
1	C	370	VAL	N-CA-C	6.13	118.75	111.09
1	C	262	GLN	N-CA-C	6.05	120.97	112.75
1	C	372	TYR	N-CA-C	6.01	119.41	109.79
1	A	359	LYS	CA-C-N	6.00	126.02	119.90
1	A	359	LYS	C-N-CA	6.00	126.02	119.90
1	B	165	GLU	N-CA-C	-5.88	106.15	113.38
1	A	84	GLY	CA-C-N	5.83	123.86	119.66
1	A	84	GLY	C-N-CA	5.83	123.86	119.66
1	A	355	ARG	CA-C-N	5.83	125.69	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	355	ARG	C-N-CA	5.83	125.69	119.28
1	C	435	CYS	N-CA-C	5.80	118.61	109.39
1	A	350	ASP	N-CA-C	-5.74	105.77	112.89
1	A	280	HIS	CA-C-N	5.73	127.01	119.84
1	A	280	HIS	C-N-CA	5.73	127.01	119.84
1	C	347	VAL	N-CA-C	5.72	113.88	109.19
1	B	251	ARG	N-CA-C	5.68	120.48	113.50
1	A	398	ASP	N-CA-C	5.66	117.26	111.14
1	C	66	ARG	N-CA-C	-5.65	104.33	111.11
1	B	372	TYR	N-CA-C	5.64	117.71	109.30
1	C	184	GLN	CA-C-N	5.63	125.83	120.31
1	C	184	GLN	C-N-CA	5.63	125.83	120.31
1	C	418	GLY	N-CA-C	-5.62	104.56	112.60
1	A	162	ASN	N-CA-C	-5.61	102.59	110.50
1	C	326	LEU	N-CA-C	5.61	116.05	109.60
1	B	326	LEU	CA-C-N	5.57	125.50	119.76
1	B	326	LEU	C-N-CA	5.57	125.50	119.76
1	B	462	ASP	N-CA-C	5.56	115.45	108.45
1	B	424	ASN	N-CA-C	-5.55	101.29	109.62
1	C	108	GLU	CA-C-N	5.54	125.63	119.32
1	C	108	GLU	C-N-CA	5.54	125.63	119.32
1	A	473	GLU	N-CA-C	-5.51	105.35	111.36
1	B	179	ILE	CB-CA-C	-5.51	104.62	112.22
1	B	262	GLN	N-CA-C	5.50	120.23	112.75
1	C	61	MET	N-CA-C	-5.49	105.38	111.36
1	C	165	GLU	N-CA-C	-5.45	106.68	113.38
1	A	372	TYR	N-CA-C	5.44	117.41	109.30
1	B	480	LYS	CA-C-N	5.44	125.52	119.32
1	B	480	LYS	C-N-CA	5.44	125.52	119.32
1	A	165	GLU	N-CA-C	-5.43	106.70	113.38
1	B	161	LEU	N-CA-C	5.43	121.10	113.56
1	A	604	ASP	N-CA-C	5.38	120.70	114.04
1	C	452	VAL	N-CA-C	-5.37	105.37	110.42
1	C	162	ASN	N-CA-C	-5.37	102.93	110.50
1	C	424	ASN	N-CA-C	-5.35	101.60	109.62
1	C	40	VAL	N-CA-C	5.34	120.45	109.34
1	B	418	GLY	N-CA-C	-5.33	103.16	112.55
1	B	234	HIS	CA-C-N	5.31	125.61	119.93
1	B	234	HIS	C-N-CA	5.31	125.61	119.93
1	B	556	THR	N-CA-C	-5.31	105.41	111.14
1	B	40	VAL	N-CA-C	5.31	120.38	109.34
1	A	540	TYR	N-CA-C	-5.27	106.98	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	ILE	CB-CA-C	-5.26	104.96	112.22
1	A	40	VAL	N-CA-C	5.24	120.24	109.34
1	B	184	GLN	CA-C-N	5.23	125.43	120.31
1	B	184	GLN	C-N-CA	5.23	125.43	120.31
1	A	390	LEU	CA-C-N	5.18	126.32	119.84
1	A	390	LEU	C-N-CA	5.18	126.32	119.84
1	C	443	PRO	CA-C-N	5.18	125.09	119.76
1	C	443	PRO	C-N-CA	5.18	125.09	119.76
1	A	240	ALA	N-CA-C	-5.13	105.68	111.28
1	C	189	LEU	N-CA-C	-5.13	103.21	110.29
1	A	202	ASP	N-CA-C	-5.13	107.15	113.41
1	C	11	TYR	N-CA-C	5.09	117.73	111.82
1	C	620	ALA	N-CA-C	-5.08	105.66	111.14
1	A	13	ARG	N-CA-C	-5.06	105.84	111.36
1	A	413	SER	N-CA-C	5.06	116.79	111.28
1	C	234	HIS	CA-C-N	5.05	125.33	119.93
1	C	234	HIS	C-N-CA	5.05	125.33	119.93
1	A	461	TYR	N-CA-C	5.05	116.91	108.23
1	A	385	LEU	N-CA-C	-5.03	105.88	111.36

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	4964	0	4787	253	0
1	B	4964	0	4787	222	0
1	C	4964	0	4787	252	0
2	A	21	0	34	0	0
2	B	21	0	34	2	0
2	C	21	0	34	1	0
3	A	56	0	54	0	0
3	B	56	0	54	1	0
3	C	56	0	54	1	0
4	A	80	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	94	0	0	10	0
4	C	81	0	0	5	0
All	All	15378	0	14625	726	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 24.

All (726) 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:580:TYR:O	1:B:584:THR:HG23	1.48	1.13
1:A:238:ARG:HH11	1:A:238:ARG:HB2	1.16	1.10
1:A:254:GLY:HA3	1:A:368:ASP:OD2	1.60	1.00
1:C:238:ARG:HH11	1:C:238:ARG:HB2	1.32	0.95
1:B:207:ARG:HG3	4:B:2015:HOH:O	1.67	0.94
1:B:238:ARG:HH11	1:B:238:ARG:HB2	1.35	0.92
1:B:254:GLY:HA3	1:B:368:ASP:OD2	1.68	0.90
1:C:238:ARG:HH11	1:C:238:ARG:CB	1.84	0.90
1:C:254:GLY:HA3	1:C:368:ASP:OD2	1.70	0.90
1:B:520:LEU:HD21	1:B:566:GLY:HA3	1.56	0.88
1:A:520:LEU:HD21	1:A:566:GLY:HA3	1.54	0.88
1:A:561:MET:HB2	4:A:2073:HOH:O	1.74	0.88
1:A:221:LEU:O	1:A:224:ALA:HB3	1.75	0.86
1:C:520:LEU:HD21	1:C:566:GLY:HA3	1.57	0.86
1:C:123:ILE:HD11	1:C:134:LEU:HD13	1.57	0.86
1:C:394:ARG:HA	1:C:394:ARG:HH11	1.41	0.84
1:C:627:ALA:C	1:C:628:ILE:HD12	2.00	0.84
1:A:492:ASN:HB3	1:A:535:GLU:OE2	1.77	0.84
1:A:123:ILE:HD11	1:A:134:LEU:HD13	1.59	0.83
1:B:466:LYS:O	1:B:470:ARG:HG3	1.78	0.83
1:C:394:ARG:HA	1:C:394:ARG:NH1	1.93	0.83
1:B:123:ILE:HD11	1:B:134:LEU:HD13	1.61	0.82
1:A:86:PRO:HB2	1:A:116:PHE:CE2	2.13	0.82
1:A:578:VAL:O	1:A:582:VAL:HG23	1.78	0.82
1:B:627:ALA:C	1:B:628:ILE:HD12	2.05	0.82
1:B:345:ILE:HD12	1:B:370:VAL:HA	1.62	0.81
1:A:345:ILE:HD12	1:A:370:VAL:HA	1.61	0.81
1:A:221:LEU:O	1:A:221:LEU:HD12	1.81	0.80
1:C:170:ALA:O	1:C:174:VAL:HG23	1.81	0.80
1:A:149:PRO:O	1:A:152:ILE:HG22	1.82	0.80
1:A:473:GLU:O	1:A:477:ARG:HG3	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ARG:O	1:A:400:MET:HG3	1.83	0.78
1:B:217:ILE:HD12	1:B:217:ILE:H	1.49	0.78
1:B:219:ASP:O	1:B:223:ARG:HG3	1.83	0.78
1:B:114:LEU:O	1:B:118:GLN:HG3	1.84	0.77
1:B:396:ARG:HG2	1:B:400:MET:HE2	1.65	0.77
1:C:466:LYS:O	1:C:470:ARG:HG3	1.83	0.77
1:C:345:ILE:HD12	1:C:370:VAL:HA	1.65	0.76
1:A:239:ALA:O	1:A:243:ARG:HG2	1.85	0.76
1:C:73:ARG:HD3	1:C:77:THR:O	1.85	0.76
1:A:238:ARG:HB2	1:A:238:ARG:NH1	1.99	0.76
1:A:627:ALA:C	1:A:628:ILE:HD12	2.11	0.76
1:B:15:LEU:O	1:B:19:VAL:HG23	1.85	0.75
1:B:419:ALA:HB1	4:B:2061:HOH:O	1.87	0.75
1:B:576:ARG:HG3	1:B:576:ARG:HH11	1.51	0.75
1:A:238:ARG:HH11	1:A:238:ARG:CB	1.99	0.75
1:B:473:GLU:O	1:B:477:ARG:HG3	1.87	0.75
1:A:576:ARG:HH11	1:A:576:ARG:HG3	1.50	0.74
1:C:208:ARG:HH11	1:C:208:ARG:HB3	1.52	0.74
1:A:406:TRP:O	1:A:410:MET:HG2	1.88	0.73
1:C:473:GLU:O	1:C:477:ARG:HG3	1.88	0.73
1:A:61:MET:HB3	1:A:101:ILE:HG23	1.69	0.73
1:C:246:ASP:O	1:C:250:GLU:HG3	1.88	0.73
1:A:170:ALA:O	1:A:174:VAL:HG23	1.87	0.73
1:C:576:ARG:HG3	1:C:576:ARG:HH11	1.52	0.73
1:B:622:GLY:O	1:B:626:GLN:HG2	1.89	0.72
1:B:326:LEU:HD22	1:B:330:HIS:CD2	2.24	0.72
1:B:238:ARG:HH11	1:B:238:ARG:CB	2.02	0.72
1:B:383:TRP:CH2	1:B:454:GLU:HG2	2.25	0.72
1:C:622:GLY:O	1:C:626:GLN:HG2	1.89	0.72
1:A:203:VAL:HG13	1:A:204:PRO:HD2	1.72	0.72
1:C:219:ASP:O	1:C:223:ARG:HG3	1.90	0.71
1:A:40:VAL:HG13	4:A:2008:HOH:O	1.88	0.71
1:A:561:MET:HE3	4:A:2073:HOH:O	1.88	0.71
1:B:326:LEU:HD22	1:B:330:HIS:HD2	1.55	0.71
1:C:149:PRO:O	1:C:152:ILE:HG22	1.90	0.71
1:B:203:VAL:HG13	1:B:204:PRO:HD2	1.73	0.71
1:C:141:PRO:HG2	1:C:144:LYS:HG3	1.72	0.71
1:B:208:ARG:HH11	1:B:208:ARG:HB3	1.54	0.70
1:C:45:GLU:HG2	1:C:133:TRP:CE2	2.26	0.70
1:A:14:THR:OG1	1:A:582:VAL:HG13	1.91	0.70
1:A:628:ILE:HG22	1:A:629:GLU:N	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:585:GLN:NE2	1:B:589:GLY:HA2	2.07	0.70
1:A:560:LEU:O	1:A:564:ILE:HG13	1.91	0.69
1:B:170:ALA:O	1:B:174:VAL:HG23	1.92	0.69
1:C:11:TYR:O	1:C:14:THR:HB	1.92	0.69
1:A:45:GLU:HG2	1:A:133:TRP:CE2	2.28	0.69
1:A:123:ILE:CD1	1:A:134:LEU:HD13	2.23	0.69
1:A:208:ARG:HH11	1:A:208:ARG:HB3	1.57	0.69
1:A:270:ILE:O	1:A:274:ILE:HG12	1.93	0.68
1:B:414:ASN:HD21	1:B:444:PRO:HG2	1.58	0.68
1:C:329:ASP:HB3	1:C:389:ARG:HB2	1.76	0.68
1:A:246:ASP:O	1:A:250:GLU:HG3	1.94	0.68
1:B:106:ASP:O	1:B:111:GLN:HG2	1.94	0.67
1:C:628:ILE:HG22	1:C:629:GLU:N	2.08	0.67
1:A:622:GLY:O	1:A:626:GLN:HG2	1.94	0.67
1:B:123:ILE:CD1	1:B:134:LEU:HD13	2.25	0.67
1:C:13:ARG:HG2	1:C:13:ARG:HH11	1.60	0.67
1:A:383:TRP:CH2	1:A:454:GLU:HG2	2.29	0.67
1:C:544:ALA:O	1:C:548:LYS:HD3	1.93	0.67
1:A:141:PRO:HG2	1:A:144:LYS:HG3	1.76	0.67
1:B:10:ALA:N	4:B:2001:HOH:O	2.27	0.67
1:C:492:ASN:HB3	1:C:535:GLU:OE2	1.94	0.67
1:A:322:ARG:NH2	1:A:328:ALA:HB2	2.10	0.66
1:C:203:VAL:HG13	1:C:204:PRO:HD2	1.76	0.66
1:B:149:PRO:O	1:B:152:ILE:HG22	1.95	0.66
1:C:14:THR:OG1	1:C:582:VAL:HG13	1.95	0.66
1:C:61:MET:HB3	1:C:101:ILE:HG23	1.76	0.66
1:B:97:ALA:O	1:B:101:ILE:HG13	1.96	0.66
1:C:627:ALA:O	1:C:628:ILE:HD12	1.96	0.66
1:C:326:LEU:HD22	1:C:330:HIS:HD2	1.60	0.66
1:A:106:ASP:O	1:A:111:GLN:HG2	1.96	0.65
1:A:114:LEU:O	1:A:118:GLN:HG3	1.95	0.65
1:A:150:PRO:HG3	1:A:182:SER:HB2	1.77	0.65
1:A:326:LEU:HD22	1:A:330:HIS:CD2	2.30	0.65
1:A:466:LYS:O	1:A:470:ARG:HG3	1.97	0.65
1:C:403:GLY:O	1:C:407:ILE:HG12	1.95	0.65
1:C:452:VAL:O	1:C:455:CYS:HB3	1.97	0.65
1:A:471:ALA:O	1:A:474:TYR:HB3	1.97	0.65
1:A:12:ALA:O	1:A:16:ASP:HB2	1.96	0.65
1:C:557:ALA:O	1:C:561:MET:HG3	1.98	0.64
1:A:108:GLU:HB2	1:A:109:PRO:HD3	1.79	0.64
1:B:330:HIS:O	1:B:334:VAL:HG23	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:LEU:HD22	1:C:330:HIS:CD2	2.33	0.63
1:B:99:LYS:HD3	1:B:195:VAL:HG12	1.78	0.63
1:B:150:PRO:HG3	1:B:182:SER:HB2	1.81	0.63
1:C:11:TYR:CD1	1:C:12:ALA:N	2.66	0.63
1:A:326:LEU:HD22	1:A:330:HIS:HD2	1.62	0.63
1:C:404:PHE:O	1:C:408:VAL:HG23	1.99	0.63
1:B:498:GLY:HA2	1:B:562:ALA:HB2	1.79	0.63
1:C:97:ALA:O	1:C:101:ILE:HG13	1.99	0.63
1:C:221:LEU:O	1:C:224:ALA:HB3	1.98	0.63
1:C:150:PRO:HG3	1:C:182:SER:HB2	1.81	0.63
1:C:280:HIS:ND1	1:C:281:PRO:HD2	2.13	0.63
1:C:610:THR:HG22	1:C:611:MET:HE2	1.80	0.63
1:C:123:ILE:CD1	1:C:134:LEU:HD13	2.29	0.62
1:C:11:TYR:HD1	1:C:12:ALA:N	1.96	0.62
1:A:113:ALA:O	1:A:117:ILE:HG12	2.00	0.62
1:A:498:GLY:HA2	1:A:562:ALA:HB2	1.80	0.62
1:B:45:GLU:HG2	1:B:133:TRP:CE2	2.34	0.62
1:A:494:LEU:HD22	1:A:559:ALA:HB2	1.80	0.62
1:C:494:LEU:HD22	1:C:559:ALA:HB2	1.80	0.62
1:A:11:TYR:CD1	1:A:12:ALA:N	2.68	0.62
1:C:99:LYS:HD3	1:C:195:VAL:HG12	1.81	0.62
1:B:492:ASN:HB3	1:B:535:GLU:OE2	2.00	0.62
1:A:554:SER:OG	1:A:597:THR:HG21	2.00	0.61
1:B:13:ARG:HH12	1:B:17:ARG:NH2	1.98	0.61
1:A:557:ALA:O	1:A:561:MET:HG3	2.01	0.61
1:A:261:ILE:HG13	1:A:264:PRO:HD2	1.82	0.61
1:C:417:TRP:O	1:C:444:PRO:HA	2.00	0.61
1:A:92:ILE:O	1:A:96:VAL:HG23	2.01	0.61
1:B:251:ARG:O	1:B:252:GLN:C	2.44	0.61
1:C:309:SER:HB3	1:C:365:PHE:CZ	2.35	0.61
1:C:411:GLN:HB2	1:C:417:TRP:CZ2	2.36	0.61
1:C:498:GLY:HA2	1:C:562:ALA:HB2	1.83	0.60
1:C:560:LEU:O	1:C:564:ILE:HG13	2.00	0.60
1:B:141:PRO:HG2	1:B:144:LYS:HG3	1.81	0.60
1:C:396:ARG:HG2	1:C:400:MET:HE2	1.82	0.60
1:C:261:ILE:HG13	1:C:264:PRO:HD2	1.83	0.60
1:A:536:ASP:OD2	1:A:538:ARG:HG3	2.01	0.60
1:C:319:LEU:HD21	1:C:384:ALA:HA	1.83	0.60
1:C:392:ASP:O	1:C:394:ARG:N	2.34	0.60
1:C:69:LEU:HD11	1:C:103:MET:CE	2.32	0.60
1:B:158:ARG:O	1:B:158:ARG:HG2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:628:ILE:HG22	1:B:629:GLU:N	2.17	0.60
1:A:440:VAL:HG12	1:A:440:VAL:O	2.01	0.59
1:C:141:PRO:CG	1:C:144:LYS:HG3	2.32	0.59
1:A:404:PHE:O	1:A:408:VAL:HG23	2.01	0.59
1:C:115:ARG:HB3	1:C:115:ARG:HH11	1.68	0.59
1:C:95:TYR:CE1	1:C:110:MET:HE3	2.37	0.59
1:A:11:TYR:HD1	1:A:12:ALA:N	2.01	0.59
1:A:88:LEU:O	1:A:92:ILE:HG13	2.03	0.59
1:B:61:MET:HB3	1:B:101:ILE:HG23	1.83	0.59
1:C:10:ALA:N	4:C:2001:HOH:O	2.35	0.59
1:C:158:ARG:O	1:C:158:ARG:HG2	2.03	0.58
1:C:114:LEU:HD22	1:C:118:GLN:HG3	1.86	0.58
1:C:239:ALA:O	1:C:243:ARG:HG2	2.02	0.58
1:B:536:ASP:OD2	1:B:538:ARG:HG3	2.03	0.58
1:B:31:TYR:HB2	1:B:314:THR:OG1	2.03	0.58
1:B:520:LEU:HD12	1:B:520:LEU:H	1.69	0.58
1:B:277:MET:HE2	1:B:280:HIS:CD2	2.39	0.58
1:C:238:ARG:HB2	1:C:238:ARG:NH1	2.11	0.58
1:A:237:ARG:O	1:A:241:GLU:HG3	2.04	0.58
1:A:263:PRO:HB2	1:A:264:PRO:CD	2.34	0.58
1:C:92:ILE:O	1:C:96:VAL:HG23	2.04	0.57
1:B:153:MET:HE2	1:B:244:ALA:HA	1.86	0.57
1:B:560:LEU:O	1:B:564:ILE:HG13	2.04	0.57
1:B:516:ILE:O	1:B:520:LEU:HD12	2.04	0.57
1:A:31:TYR:HB2	1:A:314:THR:OG1	2.05	0.57
1:A:95:TYR:CE1	1:A:110:MET:HE3	2.39	0.57
1:A:13:ARG:HG2	1:A:13:ARG:HH11	1.69	0.57
1:A:99:LYS:HD3	1:A:195:VAL:HG12	1.84	0.57
1:A:141:PRO:CG	1:A:144:LYS:HG3	2.34	0.57
1:A:579:GLN:O	1:A:583:GLU:HG3	2.04	0.57
1:C:63:LYS:NZ	1:C:296:GLU:OE1	2.37	0.57
1:A:410:MET:HE3	1:A:422:VAL:HG22	1.87	0.56
1:B:208:ARG:HB3	1:B:208:ARG:NH1	2.20	0.56
1:C:471:ALA:O	1:C:474:TYR:HB3	2.05	0.56
1:A:98:LEU:HB3	1:A:103:MET:HG3	1.86	0.56
1:C:243:ARG:HG3	1:C:243:ARG:HH11	1.69	0.56
1:C:536:ASP:OD2	1:C:538:ARG:HG3	2.06	0.56
1:B:404:PHE:C	1:B:404:PHE:HD1	2.12	0.56
1:A:56:VAL:HG13	1:A:61:MET:HE3	1.86	0.56
1:C:208:ARG:HB3	1:C:208:ARG:NH1	2.19	0.56
1:A:159:MET:HE2	1:A:160:PRO:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:LEU:HB3	1:B:103:MET:HG3	1.88	0.56
1:C:31:TYR:HB2	1:C:314:THR:OG1	2.05	0.56
1:A:256:GLY:O	1:A:286:GLY:HA2	2.06	0.56
1:B:404:PHE:C	1:B:404:PHE:CD1	2.83	0.56
1:C:509:ILE:HG22	1:C:510:ASP:N	2.21	0.56
1:B:29:GLU:CD	1:B:29:GLU:H	2.14	0.56
1:B:557:ALA:O	1:B:561:MET:HG3	2.05	0.56
1:A:520:LEU:H	1:A:520:LEU:HD12	1.71	0.55
1:A:626:GLN:C	1:A:628:ILE:H	2.15	0.55
1:B:309:SER:HB3	1:B:365:PHE:CZ	2.41	0.55
1:A:97:ALA:O	1:A:101:ILE:HG13	2.06	0.55
1:B:440:VAL:HG12	1:B:440:VAL:O	2.07	0.55
1:C:98:LEU:HB3	1:C:103:MET:HG3	1.88	0.55
1:C:263:PRO:HB2	1:C:264:PRO:CD	2.36	0.55
1:C:531:GLY:O	1:C:577:GLY:HA2	2.06	0.55
1:A:91:THR:HG22	1:A:117:ILE:HD11	1.86	0.55
1:A:462:ASP:O	1:A:468:ILE:HG13	2.06	0.55
1:B:432:ILE:HG22	1:B:433:PRO:HD2	1.88	0.55
1:B:574:ALA:O	1:B:578:VAL:HG23	2.06	0.55
1:A:580:TYR:CD1	1:A:580:TYR:C	2.84	0.55
1:C:332:ARG:HH11	1:C:332:ARG:HG2	1.70	0.55
1:A:627:ALA:O	1:A:628:ILE:HD12	2.05	0.55
1:C:238:ARG:HH11	1:C:238:ARG:CG	2.19	0.55
1:A:383:TRP:CZ3	1:A:454:GLU:HG2	2.41	0.55
1:A:576:ARG:HG3	1:A:576:ARG:NH1	2.21	0.55
1:C:364:ALA:HA	4:C:2049:HOH:O	2.07	0.55
1:B:383:TRP:O	1:B:387:THR:HG23	2.07	0.54
1:B:579:GLN:O	1:B:583:GLU:HG3	2.08	0.54
1:B:191:GLU:HA	1:B:194:ARG:HG2	1.89	0.54
1:C:440:VAL:HG12	1:C:440:VAL:O	2.07	0.54
1:A:308:ILE:HA	4:A:2003:HOH:O	2.07	0.54
1:C:345:ILE:HD12	1:C:370:VAL:HG12	1.88	0.54
1:A:411:GLN:HB2	1:A:417:TRP:CZ2	2.42	0.54
1:B:627:ALA:O	1:B:628:ILE:HD12	2.07	0.54
1:C:26:GLN:OE1	1:C:332:ARG:HG3	2.08	0.54
1:B:108:GLU:HB3	1:B:109:PRO:HD3	1.90	0.54
1:B:576:ARG:HG3	1:B:576:ARG:NH1	2.22	0.54
1:C:413:SER:HG	1:C:423:ASP:CG	2.16	0.54
1:A:49:LEU:HD11	1:A:53:LEU:HD11	1.90	0.53
1:A:158:ARG:O	1:A:158:ARG:HG2	2.08	0.53
1:B:580:TYR:CD1	1:B:580:TYR:C	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:626:GLN:C	1:C:628:ILE:H	2.16	0.53
1:B:48:LEU:O	1:B:52:ILE:HG12	2.08	0.53
1:B:257:SER:HB2	1:B:265:TRP:CE3	2.43	0.53
1:C:106:ASP:O	1:C:111:GLN:HG2	2.08	0.53
1:C:554:SER:OG	1:C:597:THR:HG21	2.08	0.53
1:A:191:GLU:HA	1:A:194:ARG:HG2	1.89	0.53
1:B:137:VAL:HB	1:B:189:LEU:HG	1.90	0.53
1:C:357:ASN:N	1:C:357:ASN:HD22	2.06	0.53
1:A:208:ARG:HB3	1:A:208:ARG:NH1	2.22	0.53
1:C:263:PRO:HG2	3:C:1630[B]:R71:H9	1.88	0.53
1:C:580:TYR:CD1	1:C:580:TYR:C	2.86	0.53
1:A:191:GLU:HA	1:A:194:ARG:CG	2.37	0.53
1:A:516:ILE:O	1:A:520:LEU:HD12	2.08	0.53
1:B:554:SER:OG	1:B:597:THR:HG21	2.08	0.53
1:A:531:GLY:O	1:A:577:GLY:HA2	2.08	0.53
1:C:208:ARG:NH1	1:C:208:ARG:CB	2.72	0.53
1:C:516:ILE:O	1:C:520:LEU:HD12	2.08	0.53
1:B:141:PRO:CG	1:B:144:LYS:HG3	2.39	0.53
1:C:585:GLN:CG	1:C:586:ARG:N	2.71	0.53
1:A:263:PRO:HD2	1:A:264:PRO:HD2	1.91	0.52
1:A:278:THR:HG22	1:A:283:PHE:CZ	2.44	0.52
1:A:428:LEU:N	1:A:429:PRO:HD2	2.24	0.52
1:A:492:ASN:HB3	1:A:535:GLU:CD	2.33	0.52
1:A:137:VAL:HB	1:A:189:LEU:HG	1.91	0.52
1:B:494:LEU:HD22	1:B:559:ALA:HB2	1.90	0.52
1:A:115:ARG:HG3	1:A:115:ARG:HH11	1.74	0.52
1:A:150:PRO:CG	1:A:182:SER:HB2	2.39	0.52
1:B:106:ASP:O	1:B:111:GLN:CG	2.56	0.52
1:B:626:GLN:C	1:B:628:ILE:H	2.18	0.52
1:C:529:PRO:C	1:C:531:GLY:H	2.17	0.52
1:B:92:ILE:O	1:B:96:VAL:HG23	2.09	0.52
1:C:520:LEU:HD12	1:C:520:LEU:H	1.75	0.52
1:A:393:GLU:O	1:A:397:ARG:HB2	2.10	0.52
1:B:238:ARG:HH11	1:B:238:ARG:CG	2.22	0.52
1:C:319:LEU:CD2	1:C:384:ALA:HA	2.40	0.52
1:C:407:ILE:O	1:C:410:MET:HB2	2.09	0.52
1:A:81:TYR:N	1:A:81:TYR:CD1	2.77	0.52
1:C:153:MET:HE2	1:C:244:ALA:HA	1.91	0.52
1:C:329:ASP:O	1:C:330:HIS:C	2.53	0.51
1:C:574:ALA:O	1:C:578:VAL:HG23	2.10	0.51
1:C:580:TYR:O	1:C:584:THR:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:GLU:O	1:B:111:GLN:HB2	2.11	0.51
1:B:509:ILE:HG22	1:B:510:ASP:N	2.26	0.51
1:B:610:THR:HG22	1:B:611:MET:HE2	1.92	0.51
1:A:263:PRO:HB2	1:A:264:PRO:HD3	1.92	0.51
1:B:332:ARG:HG2	1:B:332:ARG:HH11	1.75	0.51
1:C:100:TYR:O	1:C:192:ARG:NH2	2.43	0.51
1:A:221:LEU:HD12	1:A:221:LEU:C	2.35	0.51
1:A:490:GLY:HA3	1:A:495:TYR:CD2	2.45	0.51
1:B:185:PRO:HG3	1:B:274:ILE:CD1	2.40	0.51
1:B:208:ARG:NH1	1:B:208:ARG:CB	2.74	0.51
1:A:29:GLU:CD	1:A:29:GLU:H	2.19	0.51
1:A:509:ILE:HG22	1:A:510:ASP:N	2.25	0.51
1:B:263:PRO:HG2	3:B:1630[B]:R71:H9	1.91	0.51
1:C:16:ASP:O	1:C:20:GLU:HG2	2.11	0.51
1:A:153:MET:HE2	1:A:244:ALA:HA	1.91	0.51
1:A:605:PHE:CE2	1:A:607:LEU:HD21	2.45	0.51
1:B:357:ASN:N	1:B:357:ASN:HD22	2.09	0.51
1:C:183:ARG:O	1:C:184:GLN:C	2.53	0.51
1:C:275:LEU:O	1:C:276:ASP:C	2.54	0.51
1:B:345:ILE:HD11	4:B:2049:HOH:O	2.10	0.51
1:A:100:TYR:O	1:A:192:ARG:NH2	2.44	0.50
1:B:13:ARG:NH2	1:C:528:ASN:HA	2.26	0.50
1:B:88:LEU:O	1:B:92:ILE:HG13	2.11	0.50
1:B:261:ILE:HG13	1:B:264:PRO:HD2	1.93	0.50
1:C:115:ARG:HB3	1:C:115:ARG:NH1	2.26	0.50
1:C:137:VAL:HB	1:C:189:LEU:HG	1.91	0.50
1:A:279:GLN:HB2	4:A:2036:HOH:O	2.10	0.50
1:B:252:GLN:HB3	4:B:2028:HOH:O	2.10	0.50
1:B:263:PRO:HB2	1:B:264:PRO:CD	2.42	0.50
1:A:319:LEU:HD21	1:A:384:ALA:HA	1.92	0.50
1:C:29:GLU:CD	1:C:29:GLU:H	2.20	0.50
1:C:280:HIS:CE1	1:C:281:PRO:HD2	2.45	0.50
1:A:345:ILE:HG21	1:A:370:VAL:O	2.12	0.50
1:B:191:GLU:HA	1:B:194:ARG:CG	2.41	0.50
1:B:452:VAL:O	1:B:455:CYS:HB3	2.12	0.50
1:A:76:GLY:HA3	1:A:112:LYS:HB3	1.93	0.50
1:B:28:ASP:O	1:B:30:GLY:N	2.45	0.50
1:C:81:TYR:CD1	1:C:81:TYR:N	2.80	0.50
1:A:383:TRP:CD1	1:A:383:TRP:C	2.89	0.50
1:A:485:TRP:CG	1:A:500:VAL:HG21	2.47	0.50
1:A:123:ILE:HG21	1:A:199:TYR:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:ARG:CB	1:B:115:ARG:HH11	2.25	0.49
1:B:363:PHE:CE2	1:B:381:VAL:HG11	2.47	0.49
1:C:243:ARG:HG3	1:C:243:ARG:NH1	2.27	0.49
1:A:81:TYR:HB2	1:A:82:PRO:HD2	1.93	0.49
1:A:516:ILE:O	1:A:519:ALA:HB3	2.11	0.49
1:B:202:ASP:OD1	1:B:202:ASP:N	2.43	0.49
1:C:52:ILE:HD12	1:C:187:PHE:CD2	2.47	0.49
1:A:151:GLU:C	1:A:153:MET:N	2.67	0.49
1:A:332:ARG:HG2	1:A:332:ARG:HH11	1.78	0.49
1:B:345:ILE:HD12	1:B:370:VAL:HG12	1.95	0.49
1:A:137:VAL:HA	1:A:187:PHE:O	2.13	0.49
1:A:505:LYS:NZ	1:A:511:THR:HG21	2.27	0.49
1:B:137:VAL:HA	1:B:187:PHE:O	2.13	0.49
1:B:343:ARG:HH11	1:B:343:ARG:HG2	1.78	0.49
1:A:219:ASP:O	1:A:223:ARG:HG3	2.13	0.49
1:C:365:PHE:HB3	1:C:366:GLN:OE1	2.13	0.49
1:C:534:GLY:HA3	1:C:550:ALA:O	2.12	0.49
1:B:11:TYR:CD1	1:B:12:ALA:N	2.81	0.48
1:B:115:ARG:HH11	1:B:115:ARG:HB3	1.78	0.48
1:C:432:ILE:HG22	1:C:433:PRO:HD2	1.94	0.48
1:A:11:TYR:O	1:A:14:THR:HB	2.14	0.48
1:A:503:ALA:O	1:A:506:ALA:N	2.47	0.48
1:A:610:THR:HG22	1:A:611:MET:HE2	1.95	0.48
1:B:253:ALA:HA	4:B:2053:HOH:O	2.13	0.48
1:C:461:TYR:HD1	1:C:461:TYR:H	1.58	0.48
1:A:152:ILE:O	1:A:152:ILE:HG12	2.12	0.48
1:A:138:GLY:HA2	4:A:2021:HOH:O	2.12	0.48
1:B:207:ARG:HH11	1:B:207:ARG:HB3	1.79	0.48
1:B:293:TYR:O	1:B:305:GLN:HG3	2.14	0.48
1:C:191:GLU:HA	1:C:194:ARG:HG2	1.94	0.48
1:C:207:ARG:HH11	1:C:207:ARG:HB3	1.78	0.48
1:A:92:ILE:HD12	1:A:126:SER:HB3	1.95	0.48
1:A:505:LYS:HZ3	1:A:511:THR:HG21	1.78	0.48
1:C:202:ASP:OD1	1:C:202:ASP:N	2.45	0.48
1:C:428:LEU:N	1:C:429:PRO:HD2	2.27	0.48
1:A:86:PRO:HB2	1:A:116:PHE:CZ	2.49	0.48
1:C:151:GLU:C	1:C:153:MET:N	2.69	0.48
1:C:69:LEU:HD11	1:C:103:MET:HE2	1.96	0.48
1:A:52:ILE:HD12	1:A:187:PHE:CD2	2.49	0.48
1:A:396:ARG:NH1	1:A:400:MET:CE	2.77	0.48
1:A:417:TRP:CZ3	1:A:452:VAL:HG11	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:PRO:O	1:A:432:ILE:HG12	2.14	0.48
1:B:504:LEU:HD13	1:B:516:ILE:HD11	1.95	0.48
1:A:208:ARG:NH1	1:A:208:ARG:CB	2.76	0.47
1:C:406:TRP:CZ2	1:C:410:MET:HE2	2.49	0.47
1:A:293:TYR:O	1:A:305:GLN:HG3	2.14	0.47
1:A:343:ARG:NH1	1:A:343:ARG:HG2	2.29	0.47
1:B:383:TRP:CD1	1:B:383:TRP:C	2.92	0.47
1:C:28:ASP:C	1:C:30:GLY:N	2.71	0.47
1:C:108:GLU:HB3	1:C:109:PRO:HD3	1.96	0.47
1:B:52:ILE:HD12	1:B:187:PHE:CD2	2.49	0.47
1:B:100:TYR:O	1:B:192:ARG:NH2	2.47	0.47
1:C:576:ARG:HG3	1:C:576:ARG:NH1	2.24	0.47
1:A:280:HIS:CG	1:A:281:PRO:HD2	2.49	0.47
1:B:11:TYR:CD1	1:B:11:TYR:C	2.93	0.47
1:B:215:GLY:C	1:B:217:ILE:H	2.22	0.47
1:B:356:PRO:C	1:B:357:ASN:HD22	2.23	0.47
1:C:53:LEU:O	1:C:55:ARG:HG3	2.14	0.47
1:A:440:VAL:O	1:A:440:VAL:CG1	2.62	0.47
1:B:217:ILE:H	1:B:217:ILE:CD1	2.23	0.47
1:C:263:PRO:HB2	1:C:264:PRO:HD3	1.97	0.47
1:C:535:GLU:HA	1:C:548:LYS:O	2.14	0.47
1:A:110:MET:O	1:A:114:LEU:HB2	2.15	0.47
1:B:28:ASP:C	1:B:30:GLY:N	2.70	0.47
1:B:201:THR:HG22	1:B:203:VAL:N	2.30	0.47
1:A:207:ARG:HB3	1:A:207:ARG:HH11	1.79	0.47
1:A:319:LEU:CD2	1:A:384:ALA:HA	2.43	0.47
1:B:359:LYS:HA	1:B:360:PRO:HD3	1.77	0.47
1:C:385:LEU:C	1:C:387:THR:H	2.23	0.47
1:C:386:ASN:HA	1:C:396:ARG:HH12	1.80	0.47
1:A:161:LEU:HD11	1:A:432:ILE:HD11	1.97	0.47
1:A:316:LEU:O	1:A:317:ALA:C	2.58	0.47
1:A:535:GLU:HB3	1:A:555:GLN:NE2	2.30	0.47
1:B:319:LEU:HD21	1:B:384:ALA:HA	1.97	0.47
1:C:376:ASP:O	1:C:380:VAL:HG23	2.15	0.47
1:C:510:ASP:OD2	1:C:512:ARG:NH1	2.48	0.47
1:B:159:MET:HE2	1:B:159:MET:HB3	1.84	0.47
1:B:343:ARG:HG2	1:B:343:ARG:NH1	2.30	0.47
1:C:14:THR:HG23	1:C:585:GLN:OE1	2.15	0.47
1:A:48:LEU:O	1:A:52:ILE:HG12	2.14	0.47
1:A:396:ARG:NH1	1:A:400:MET:HE1	2.30	0.47
1:A:574:ALA:O	1:A:578:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:LEU:O	1:B:70:HIS:C	2.56	0.47
1:B:77:THR:OG1	1:B:86:PRO:HB3	2.15	0.47
1:C:392:ASP:C	1:C:394:ARG:H	2.22	0.47
1:A:147:MET:HG2	1:A:225:LEU:HB3	1.96	0.46
1:A:159:MET:HE2	1:A:159:MET:HB3	1.81	0.46
1:A:201:THR:HG22	1:A:203:VAL:N	2.30	0.46
1:A:392:ASP:C	1:A:394:ARG:N	2.72	0.46
1:A:432:ILE:HG22	1:A:433:PRO:HD2	1.96	0.46
1:A:465:TRP:CE2	1:A:467:VAL:HG21	2.50	0.46
1:C:147:MET:HG2	1:C:225:LEU:HB3	1.96	0.46
1:B:217:ILE:HD12	1:B:217:ILE:N	2.25	0.46
1:C:114:LEU:HD22	1:C:118:GLN:CG	2.45	0.46
1:C:398:ASP:O	1:C:399:ALA:C	2.59	0.46
1:C:585:GLN:HG3	1:C:586:ARG:H	1.80	0.46
1:B:366:GLN:O	4:B:2048:HOH:O	2.21	0.46
1:A:446:GLU:OE1	1:A:446:GLU:N	2.28	0.46
1:B:81:TYR:N	1:B:81:TYR:CD1	2.83	0.46
1:B:440:VAL:O	1:B:440:VAL:CG1	2.64	0.46
1:C:45:GLU:OE2	1:C:93:GLU:OE1	2.32	0.46
1:B:284:ILE:O	1:B:288:GLU:HG2	2.16	0.46
1:C:440:VAL:O	1:C:440:VAL:CG1	2.63	0.46
1:B:92:ILE:HD12	1:B:126:SER:HB3	1.97	0.46
1:B:186:VAL:O	1:B:188:PRO:HD3	2.15	0.46
1:C:392:ASP:C	1:C:394:ARG:N	2.74	0.46
1:B:215:GLY:C	1:B:217:ILE:N	2.72	0.46
1:C:262:GLN:HG2	1:C:266:PHE:CE1	2.50	0.46
1:C:378:THR:HG22	1:C:407:ILE:HD11	1.97	0.46
1:C:553:PRO:HG2	1:C:592:ASP:O	2.15	0.46
1:A:389:ARG:HE	1:A:389:ARG:HB3	1.62	0.46
1:B:147:MET:HG2	1:B:225:LEU:HB3	1.98	0.46
1:B:299:TYR:CD1	1:B:299:TYR:C	2.93	0.46
1:A:115:ARG:HG3	1:A:115:ARG:NH1	2.31	0.46
1:A:418:GLY:HA2	1:A:444:PRO:HA	1.98	0.46
1:B:135:ALA:O	4:B:2016:HOH:O	2.20	0.46
1:C:64:ILE:O	1:C:64:ILE:CG2	2.63	0.46
1:C:123:ILE:HG21	1:C:199:TYR:CE1	2.51	0.46
1:C:385:LEU:O	1:C:387:THR:N	2.49	0.46
1:C:490:GLY:HA3	1:C:495:TYR:CD2	2.50	0.46
1:A:27:LYS:HE3	4:A:2002:HOH:O	2.17	0.46
1:B:262:GLN:HG2	1:B:266:PHE:CE1	2.51	0.46
1:C:238:ARG:O	1:C:242:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:ARG:HH11	1:C:394:ARG:CA	2.21	0.46
1:C:413:SER:OG	1:C:423:ASP:OD1	2.31	0.46
1:A:378:THR:O	1:A:382:VAL:HG23	2.16	0.45
1:B:69:LEU:HD11	1:B:103:MET:CE	2.46	0.45
1:B:383:TRP:CZ3	1:B:454:GLU:HG2	2.50	0.45
1:B:510:ASP:OD2	1:B:512:ARG:NH1	2.49	0.45
1:A:392:ASP:C	1:A:394:ARG:H	2.25	0.45
1:C:542:ASP:HA	1:C:543:PRO:HD2	1.72	0.45
1:A:510:ASP:OD2	1:A:512:ARG:NH1	2.50	0.45
1:A:529:PRO:C	1:A:531:GLY:H	2.24	0.45
1:B:173:THR:HG23	1:B:267:TYR:CD2	2.52	0.45
1:B:326:LEU:HD13	1:B:330:HIS:CD2	2.51	0.45
1:C:66:ARG:HG2	1:C:66:ARG:HH11	1.81	0.45
1:C:369:ASN:HD21	1:C:372:TYR:HB2	1.81	0.45
1:C:446:GLU:HB2	4:C:2059:HOH:O	2.16	0.45
1:A:146:PRO:HB3	1:A:433:PRO:HB2	1.99	0.45
1:A:202:ASP:OD1	1:A:202:ASP:N	2.46	0.45
1:B:63:LYS:O	1:B:301:GLY:HA2	2.16	0.45
1:B:471:ALA:O	1:B:474:TYR:HB3	2.17	0.45
1:C:326:LEU:HD13	1:C:330:HIS:CD2	2.51	0.45
1:C:383:TRP:CD1	1:C:383:TRP:C	2.94	0.45
1:C:425:THR:O	1:C:426:SER:C	2.57	0.45
1:A:228:TYR:O	1:A:228:TYR:CD1	2.69	0.45
1:A:353:VAL:HG12	1:A:353:VAL:O	2.17	0.45
1:B:243:ARG:HG3	1:B:243:ARG:HH11	1.81	0.45
1:C:92:ILE:HD12	1:C:126:SER:HB3	1.98	0.45
1:C:613:ARG:O	1:C:617:PRO:HG2	2.16	0.45
1:A:160:PRO:O	1:A:161:LEU:HB2	2.17	0.45
1:A:343:ARG:HG2	1:A:343:ARG:HH11	1.81	0.45
1:B:26:GLN:HG2	1:B:27:LYS:O	2.17	0.45
1:B:237:ARG:HD3	4:B:2026:HOH:O	2.16	0.45
1:B:453:LEU:HD11	1:B:471:ALA:CB	2.46	0.45
1:A:105:ARG:HE	1:A:105:ARG:HB2	1.56	0.45
1:B:256:GLY:HA3	1:B:285:LYS:HG3	1.99	0.45
1:C:238:ARG:NH1	1:C:238:ARG:CG	2.79	0.45
1:A:37:LEU:O	1:A:607:LEU:HA	2.17	0.45
1:A:357:ASN:N	1:A:357:ASN:HD22	2.14	0.45
1:A:330:HIS:CE1	1:A:332:ARG:HB2	2.51	0.45
1:B:146:PRO:HB3	1:B:433:PRO:HB2	1.99	0.45
1:B:160:PRO:O	1:B:161:LEU:HB2	2.16	0.45
1:C:586:ARG:HD3	1:C:592:ASP:OD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ILE:HG21	1:B:199:TYR:CE1	2.52	0.44
1:C:159:MET:HE2	1:C:159:MET:HB3	1.81	0.44
1:C:505:LYS:O	1:C:505:LYS:HD3	2.17	0.44
1:B:155:LEU:HB2	1:B:162:ASN:HA	1.98	0.44
1:C:179:ILE:O	1:C:182:SER:HB3	2.17	0.44
1:C:509:ILE:CG2	1:C:510:ASP:N	2.80	0.44
1:A:118:GLN:C	1:A:120:GLN:H	2.25	0.44
1:A:417:TRP:CH2	1:A:452:VAL:HG11	2.52	0.44
1:C:535:GLU:HB3	1:C:555:GLN:NE2	2.33	0.44
1:A:512:ARG:O	1:A:512:ARG:HG2	2.17	0.44
1:B:151:GLU:C	1:B:153:MET:N	2.74	0.44
1:C:145:VAL:O	1:C:146:PRO:C	2.59	0.44
1:B:183:ARG:O	1:B:184:GLN:C	2.60	0.44
1:C:383:TRP:CH2	1:C:454:GLU:HG2	2.52	0.44
1:A:17:ARG:HA	1:A:20:GLU:HG2	1.99	0.44
1:A:149:PRO:HA	1:A:150:PRO:HD3	1.90	0.44
1:B:159:MET:HE2	1:B:160:PRO:HD2	1.99	0.44
1:B:201:THR:CG2	1:B:202:ASP:N	2.81	0.44
1:B:256:GLY:CA	1:B:285:LYS:HG3	2.48	0.44
1:C:605:PHE:CE2	1:C:607:LEU:HD21	2.53	0.44
1:A:583:GLU:O	1:A:585:GLN:N	2.51	0.44
1:B:99:LYS:HD3	1:B:195:VAL:CG1	2.45	0.44
1:B:355:ARG:N	1:B:356:PRO:HD3	2.32	0.44
1:C:86:PRO:HB2	1:C:116:PHE:CZ	2.52	0.44
1:A:151:GLU:C	1:A:153:MET:H	2.24	0.44
1:A:505:LYS:O	1:A:505:LYS:HD3	2.18	0.44
1:B:365:PHE:HB3	1:B:366:GLN:OE1	2.17	0.44
1:B:535:GLU:HB3	1:B:555:GLN:NE2	2.33	0.44
1:C:69:LEU:HD11	1:C:103:MET:HE1	1.99	0.44
1:A:309:SER:HB3	1:A:365:PHE:CZ	2.53	0.44
1:B:256:GLY:O	1:B:286:GLY:HA2	2.18	0.44
1:B:361:GLY:O	1:B:403:GLY:HA2	2.18	0.44
1:C:28:ASP:O	1:C:30:GLY:N	2.51	0.44
1:C:88:LEU:O	1:C:92:ILE:HG13	2.18	0.44
1:C:326:LEU:HA	1:C:327:PRO:HD3	1.88	0.44
1:A:416:GLY:O	1:A:444:PRO:HB3	2.17	0.43
1:B:345:ILE:HG21	1:B:370:VAL:O	2.17	0.43
1:C:406:TRP:O	1:C:407:ILE:C	2.61	0.43
1:A:355:ARG:N	1:A:356:PRO:HD3	2.33	0.43
1:B:104:SER:C	1:B:106:ASP:H	2.26	0.43
1:C:137:VAL:HA	1:C:187:PHE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:LEU:HD11	1:B:103:MET:HE2	1.99	0.43
1:B:349:GLY:O	2:B:1629:C8E:H132	2.18	0.43
1:B:505:LYS:NZ	1:B:511:THR:HG21	2.33	0.43
1:C:15:LEU:O	1:C:19:VAL:HG23	2.18	0.43
1:C:283:PHE:CD1	1:C:283:PHE:C	2.95	0.43
1:C:511:THR:HG23	4:C:2068:HOH:O	2.17	0.43
1:A:163:ILE:O	1:A:171:ARG:HG3	2.18	0.43
1:B:207:ARG:NH1	1:B:207:ARG:CB	2.81	0.43
1:B:404:PHE:HD1	1:B:404:PHE:O	2.02	0.43
1:C:191:GLU:HA	1:C:194:ARG:CG	2.48	0.43
1:C:201:THR:HG22	1:C:203:VAL:N	2.34	0.43
1:A:26:GLN:HG2	1:A:27:LYS:O	2.18	0.43
1:A:403:GLY:O	1:A:404:PHE:C	2.61	0.43
1:B:43:GLU:HG2	1:B:67:TYR:CD2	2.53	0.43
1:C:378:THR:O	1:C:382:VAL:HG23	2.18	0.43
1:C:474:TYR:HA	1:C:477:ARG:NH1	2.33	0.43
1:A:145:VAL:O	1:A:226:HIS:CE1	2.71	0.43
1:A:186:VAL:O	1:A:188:PRO:HD3	2.19	0.43
1:A:538:ARG:C	1:A:540:TYR:H	2.26	0.43
1:A:601:PHE:O	1:A:602:PRO:C	2.58	0.43
1:A:78:TRP:CE3	1:A:91:THR:HG23	2.53	0.43
1:B:396:ARG:NH1	1:B:400:MET:CE	2.82	0.43
1:C:192:ARG:HG2	1:C:192:ARG:HH11	1.84	0.43
1:C:349:GLY:O	2:C:1629:C8E:H132	2.19	0.43
1:A:57:ASP:O	1:A:58:ARG:C	2.61	0.43
1:A:128:VAL:HG23	1:A:436:ASP:CG	2.44	0.43
1:A:251:ARG:NH1	1:A:350:ASP:OD1	2.51	0.43
1:A:262:GLN:HG2	1:A:266:PHE:CE1	2.54	0.43
1:A:374:ASP:HB3	1:A:420:TYR:CE1	2.53	0.43
1:A:609:TYR:HA	4:A:2004:HOH:O	2.18	0.43
1:A:490:GLY:HA3	1:A:495:TYR:CE2	2.54	0.43
1:B:203:VAL:CG1	1:B:204:PRO:HD2	2.44	0.43
1:B:270:ILE:O	1:B:274:ILE:HG12	2.19	0.43
1:B:509:ILE:CG2	1:B:510:ASP:N	2.82	0.43
1:C:114:LEU:O	1:C:118:GLN:HG3	2.18	0.43
1:C:322:ARG:NH1	1:C:326:LEU:O	2.51	0.43
1:B:43:GLU:HG2	1:B:67:TYR:CE2	2.54	0.43
1:B:310:PRO:HG2	1:B:311:VAL:H	1.84	0.43
1:B:332:ARG:HG2	1:B:332:ARG:NH1	2.34	0.43
1:B:586:ARG:HH21	1:B:590:GLY:HA3	1.83	0.43
1:C:115:ARG:NH1	1:C:115:ARG:CB	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:GLN:C	1:A:120:GLN:N	2.77	0.42
1:A:508:GLY:O	1:A:509:ILE:C	2.61	0.42
1:B:428:LEU:N	1:B:429:PRO:HD2	2.34	0.42
1:B:469:ARG:HH11	1:B:469:ARG:HB3	1.84	0.42
1:B:505:LYS:HD3	1:B:505:LYS:O	2.18	0.42
1:C:118:GLN:C	1:C:120:GLN:H	2.27	0.42
1:C:210:ALA:O	1:C:211:LYS:C	2.61	0.42
1:C:316:LEU:O	1:C:317:ALA:C	2.61	0.42
1:A:494:LEU:CD2	1:A:559:ALA:HB2	2.48	0.42
1:A:512:ARG:NH1	1:A:512:ARG:HB3	2.34	0.42
1:B:107:GLU:O	1:B:108:GLU:C	2.62	0.42
1:C:140:TYR:CG	1:C:141:PRO:HD2	2.54	0.42
1:C:390:LEU:HA	1:C:391:PRO:HD3	1.91	0.42
1:C:527:GLN:O	1:C:528:ASN:C	2.62	0.42
1:A:261:ILE:HG13	1:A:264:PRO:CD	2.49	0.42
1:A:312:TRP:CZ3	1:A:380:VAL:HG21	2.54	0.42
1:A:490:GLY:CA	1:A:495:TYR:CD2	3.03	0.42
1:A:553:PRO:HG2	1:A:592:ASP:O	2.19	0.42
1:B:53:LEU:O	1:B:55:ARG:HG3	2.19	0.42
1:B:474:TYR:HA	1:B:477:ARG:NH1	2.34	0.42
1:C:106:ASP:O	1:C:107:GLU:C	2.61	0.42
1:C:343:ARG:NH1	1:C:343:ARG:HG2	2.34	0.42
1:C:345:ILE:HG21	1:C:370:VAL:O	2.19	0.42
1:C:385:LEU:C	1:C:387:THR:N	2.77	0.42
1:C:601:PHE:O	1:C:602:PRO:C	2.62	0.42
1:A:365:PHE:HB3	1:A:366:GLN:OE1	2.19	0.42
1:A:453:LEU:HD11	1:A:471:ALA:CB	2.49	0.42
1:B:425:THR:O	1:B:426:SER:C	2.60	0.42
1:C:26:GLN:HG2	1:C:27:LYS:O	2.20	0.42
1:A:58:ARG:HA	1:A:58:ARG:HD3	1.82	0.42
1:A:140:TYR:CG	1:A:141:PRO:HD2	2.54	0.42
1:B:215:GLY:O	1:B:217:ILE:N	2.53	0.42
1:B:280:HIS:O	1:B:281:PRO:C	2.62	0.42
1:B:396:ARG:NH1	1:B:400:MET:HE1	2.34	0.42
1:C:13:ARG:HH11	1:C:13:ARG:CG	2.29	0.42
1:C:386:ASN:HA	1:C:400:MET:SD	2.59	0.42
1:A:13:ARG:HG2	1:A:13:ARG:NH1	2.34	0.42
1:A:60:ARG:NH1	1:A:302:TRP:CZ2	2.87	0.42
1:C:207:ARG:NH1	1:C:207:ARG:CB	2.83	0.42
1:C:240:ALA:O	1:C:243:ARG:HB2	2.19	0.42
1:C:392:ASP:OD1	1:C:394:ARG:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:TYR:CD2	1:A:537:CYS:HB2	2.55	0.42
1:A:376:ASP:O	1:A:380:VAL:HG23	2.19	0.42
1:B:34:GLY:HA2	1:B:35:PRO:HD3	1.92	0.42
1:B:243:ARG:HG3	1:B:243:ARG:NH1	2.34	0.42
1:C:64:ILE:O	1:C:64:ILE:HG22	2.19	0.42
1:C:453:LEU:HD11	1:C:471:ALA:CB	2.49	0.42
1:C:465:TRP:CE2	1:C:467:VAL:HB	2.55	0.42
1:C:585:GLN:CG	1:C:586:ARG:H	2.33	0.42
1:B:150:PRO:CG	1:B:182:SER:HB2	2.48	0.42
1:B:238:ARG:CG	1:B:238:ARG:NH1	2.81	0.42
1:B:308:ILE:HA	4:B:2038:HOH:O	2.20	0.42
1:B:383:TRP:O	1:B:383:TRP:CD1	2.73	0.42
1:B:613:ARG:O	1:B:617:PRO:HG2	2.19	0.42
1:C:512:ARG:O	1:C:512:ARG:HG2	2.19	0.42
1:A:106:ASP:O	1:A:107:GLU:O	2.37	0.42
1:B:104:SER:O	1:B:106:ASP:N	2.53	0.42
1:B:512:ARG:O	1:B:513:GLU:O	2.38	0.42
1:C:128:VAL:HG13	1:C:146:PRO:HD2	2.01	0.42
1:C:192:ARG:HG2	1:C:192:ARG:NH1	2.35	0.42
1:C:386:ASN:OD1	1:C:459:PHE:CE1	2.73	0.42
1:C:461:TYR:CD1	1:C:461:TYR:N	2.86	0.42
1:A:118:GLN:HB3	1:A:201:THR:OG1	2.19	0.42
1:A:228:TYR:O	1:A:234:HIS:CD2	2.73	0.42
1:A:275:LEU:O	1:A:277:MET:HG3	2.20	0.42
1:A:586:ARG:HD3	1:A:592:ASP:CG	2.45	0.42
1:C:177:LEU:HD23	1:C:177:LEU:HA	1.87	0.42
1:C:308:ILE:HG13	1:C:366:GLN:HB3	2.01	0.42
1:A:290:LEU:HD22	1:A:304:PHE:CE2	2.55	0.41
1:B:13:ARG:HH22	1:C:528:ASN:HA	1.84	0.41
1:B:469:ARG:NH1	1:B:469:ARG:CB	2.83	0.41
1:C:201:THR:CG2	1:C:202:ASP:N	2.83	0.41
1:C:293:TYR:O	1:C:305:GLN:HG3	2.20	0.41
1:A:108:GLU:CB	1:A:109:PRO:HD3	2.49	0.41
1:B:52:ILE:HG23	1:B:187:PHE:CD2	2.55	0.41
1:B:150:PRO:C	1:B:240:ALA:HB1	2.46	0.41
1:B:512:ARG:O	1:B:512:ARG:HG2	2.20	0.41
2:B:1629:C8E:O21	2:B:1629:C8E:H52	2.19	0.41
1:C:413:SER:OG	1:C:423:ASP:CG	2.63	0.41
1:C:529:PRO:C	1:C:531:GLY:N	2.78	0.41
1:A:106:ASP:O	1:A:107:GLU:C	2.63	0.41
1:B:43:GLU:OE1	1:B:67:TYR:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:TYR:HB2	1:C:82:PRO:HD2	2.02	0.41
1:A:28:ASP:O	1:A:30:GLY:N	2.54	0.41
1:A:203:VAL:CG1	1:A:204:PRO:HD2	2.45	0.41
1:A:257:SER:HB2	1:A:265:TRP:CE3	2.55	0.41
1:C:161:LEU:HD11	1:C:432:ILE:HD11	2.02	0.41
1:C:355:ARG:N	1:C:356:PRO:HD3	2.36	0.41
1:C:356:PRO:C	1:C:357:ASN:HD22	2.29	0.41
1:A:512:ARG:HB3	1:A:512:ARG:HH11	1.86	0.41
1:C:155:LEU:HB2	1:C:162:ASN:HA	2.01	0.41
1:C:398:ASP:OD2	1:C:402:LYS:HE3	2.20	0.41
1:C:492:ASN:HB3	1:C:535:GLU:CD	2.44	0.41
1:C:505:LYS:NZ	1:C:511:THR:HG21	2.34	0.41
1:C:516:ILE:O	1:C:519:ALA:HB3	2.20	0.41
1:B:543:PRO:C	1:B:545:TYR:H	2.28	0.41
1:A:228:TYR:OH	1:A:234:HIS:HB3	2.21	0.41
1:A:272:LEU:HD13	1:A:283:PHE:HB2	2.03	0.41
1:B:341:LEU:HD23	1:B:341:LEU:HA	1.81	0.41
1:B:512:ARG:NH1	1:B:512:ARG:HB3	2.36	0.41
1:C:34:GLY:HA2	1:C:35:PRO:HD3	1.96	0.41
1:C:177:LEU:O	1:C:178:SER:C	2.63	0.41
1:C:234:HIS:HA	1:C:235:PRO:HD2	1.88	0.41
1:C:270:ILE:O	1:C:274:ILE:HG12	2.21	0.41
1:C:343:ARG:HG2	1:C:343:ARG:HH11	1.86	0.41
1:A:28:ASP:C	1:A:30:GLY:N	2.77	0.41
1:A:73:ARG:HD3	1:A:77:THR:O	2.21	0.41
1:A:75:ASP:OD1	1:A:77:THR:OG1	2.36	0.41
1:A:217:ILE:O	1:A:220:ALA:HB3	2.21	0.41
1:A:228:TYR:CE1	1:A:234:HIS:CD2	3.09	0.41
1:A:586:ARG:HD3	1:A:592:ASP:OD2	2.20	0.41
1:B:45:GLU:OE2	1:B:93:GLU:OE1	2.38	0.41
1:B:201:THR:CG2	1:B:203:VAL:HB	2.51	0.41
1:B:405:ARG:HG2	1:B:405:ARG:HH11	1.85	0.41
1:C:162:ASN:OD1	1:C:164:TYR:HB2	2.20	0.41
1:C:343:ARG:NE	1:C:343:ARG:HA	2.36	0.41
1:C:366:GLN:OE1	1:C:366:GLN:N	2.51	0.41
1:C:443:PRO:HA	1:C:444:PRO:HD3	1.87	0.41
1:C:624:TYR:C	1:C:626:GLN:H	2.28	0.41
1:A:356:PRO:C	1:A:357:ASN:HD22	2.29	0.41
1:B:124:GLU:OE2	1:B:144:LYS:NZ	2.39	0.41
1:B:178:SER:O	1:B:182:SER:HB2	2.21	0.41
1:B:192:ARG:HG2	1:B:192:ARG:HH11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:PRO:HB2	1:B:264:PRO:HD3	2.03	0.41
1:B:469:ARG:HB3	1:B:469:ARG:NH1	2.35	0.41
1:C:65:ARG:O	1:C:66:ARG:C	2.60	0.41
1:C:485:TRP:HA	4:C:2063:HOH:O	2.20	0.41
1:A:69:LEU:HD12	1:A:69:LEU:HA	1.95	0.40
1:A:104:SER:O	1:A:106:ASP:N	2.54	0.40
1:B:78:TRP:CE3	1:B:91:THR:HG23	2.56	0.40
1:B:185:PRO:HG3	1:B:274:ILE:HD11	2.02	0.40
1:C:303:MET:O	1:C:303:MET:HG3	2.19	0.40
1:C:357:ASN:N	1:C:357:ASN:ND2	2.69	0.40
1:A:52:ILE:HG23	1:A:187:PHE:CD2	2.57	0.40
1:A:77:THR:HG22	1:A:116:PHE:CD2	2.56	0.40
1:A:162:ASN:OD1	1:A:164:TYR:HB2	2.22	0.40
1:A:183:ARG:O	1:A:184:GLN:C	2.64	0.40
1:A:319:LEU:HG	1:A:384:ALA:HB2	2.03	0.40
1:A:326:LEU:HD13	1:A:330:HIS:CD2	2.56	0.40
1:A:509:ILE:CG2	1:A:510:ASP:N	2.84	0.40
1:B:26:GLN:OE1	1:B:332:ARG:HG3	2.21	0.40
1:C:108:GLU:N	1:C:109:PRO:CD	2.85	0.40
1:C:163:ILE:O	1:C:171:ARG:HG3	2.21	0.40
1:A:207:ARG:NH1	1:A:207:ARG:CB	2.84	0.40
1:A:403:GLY:O	1:A:407:ILE:HG13	2.21	0.40
1:B:418:GLY:HA2	1:B:444:PRO:HA	2.02	0.40
1:C:243:ARG:HA	1:C:243:ARG:HD2	1.89	0.40
1:A:159:MET:CE	1:A:160:PRO:HD2	2.50	0.40
1:A:425:THR:O	1:A:426:SER:C	2.61	0.40
1:A:469:ARG:NH1	1:A:469:ARG:HB3	2.36	0.40
1:B:298:ASP:OD1	1:B:299:TYR:N	2.53	0.40
1:B:385:LEU:C	1:B:387:THR:H	2.29	0.40
1:B:585:GLN:HG2	1:B:586:ARG:N	2.36	0.40
1:C:178:SER:O	1:C:182:SER:HB2	2.21	0.40
1:A:175:VAL:HG21	1:A:247:TRP:CE3	2.57	0.40
1:A:218:PHE:HA	1:A:221:LEU:HB3	2.03	0.40
1:A:363:PHE:CE2	1:A:381:VAL:HG11	2.56	0.40
1:A:512:ARG:O	1:A:513:GLU:C	2.64	0.40
1:B:243:ARG:HA	1:B:243:ARG:HD2	1.86	0.40
1:B:490:GLY:HA3	1:B:495:TYR:CD2	2.56	0.40
1:C:81:TYR:CD2	1:C:537:CYS:HB2	2.57	0.40
1:C:186:VAL:O	1:C:188:PRO:HD3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	618/631 (98%)	545 (88%)	57 (9%)	16 (3%)	4	15
1	B	618/631 (98%)	559 (90%)	44 (7%)	15 (2%)	4	17
1	C	618/631 (98%)	542 (88%)	61 (10%)	15 (2%)	4	17
All	All	1854/1893 (98%)	1646 (89%)	162 (9%)	46 (2%)	4	16

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	GLU
1	A	509	ILE
1	C	393	GLU
1	A	200	GLU
1	C	107	GLU
1	C	386	ASN
1	C	509	ILE
1	A	530	ASP
1	A	568	ARG
1	A	584	THR
1	B	29	GLU
1	B	105	ARG
1	B	107	GLU
1	C	527	GLN
1	C	568	ARG
1	A	197	GLU
1	A	627	ALA
1	B	216	TRP
1	B	361	GLY
1	B	463	ASP
1	B	530	ASP
1	B	568	ARG
1	C	492	ASN
1	C	530	ASP

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Mol	Chain	Res	Type
1	A	361	GLY
1	A	492	ASN
1	C	29	GLU
1	C	200	GLU
1	C	361	GLY
1	C	584	THR
1	A	105	ARG
1	B	492	ASN
1	B	509	ILE
1	B	627	ALA
1	A	628	ILE
1	C	628	ILE
1	A	263	PRO
1	A	500	VAL
1	A	513	GLU
1	B	40	VAL
1	B	513	GLU
1	C	263	PRO
1	A	523	VAL
1	B	263	PRO
1	B	628	ILE
1	C	309	SER

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	503/513 (98%)	479 (95%)	24 (5%)	23	56
1	B	503/513 (98%)	485 (96%)	18 (4%)	31	66
1	C	503/513 (98%)	480 (95%)	23 (5%)	24	58
All	All	1509/1539 (98%)	1444 (96%)	65 (4%)	26	60

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	16	ASP
1	A	37	LEU
1	A	69	LEU
1	A	74	GLU
1	A	81	TYR
1	A	114	LEU
1	A	149	PRO
1	A	152	ILE
1	A	158	ARG
1	A	161	LEU
1	A	217	ILE
1	A	221	LEU
1	A	238	ARG
1	A	251	ARG
1	A	366	GLN
1	A	389	ARG
1	A	398	ASP
1	A	401	THR
1	A	412	SER
1	A	428	LEU
1	A	454	GLU
1	A	542	ASP
1	A	560	LEU
1	B	37	LEU
1	B	64	ILE
1	B	69	LEU
1	B	74	GLU
1	B	81	TYR
1	B	114	LEU
1	B	149	PRO
1	B	152	ILE
1	B	158	ARG
1	B	161	LEU
1	B	238	ARG
1	B	366	GLN
1	B	398	ASP
1	B	428	LEU
1	B	454	GLU
1	B	542	ASP
1	B	560	LEU
1	B	584	THR
1	C	13	ARG

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Mol	Chain	Res	Type
1	C	37	LEU
1	C	81	TYR
1	C	104	SER
1	C	114	LEU
1	C	149	PRO
1	C	152	ILE
1	C	158	ARG
1	C	161	LEU
1	C	217	ILE
1	C	238	ARG
1	C	242	ILE
1	C	251	ARG
1	C	279	GLN
1	C	332	ARG
1	C	366	GLN
1	C	391	PRO
1	C	394	ARG
1	C	398	ASP
1	C	405	ARG
1	C	428	LEU
1	C	542	ASP
1	C	560	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	226	HIS
1	A	234	HIS
1	A	357	ASN
1	A	614	HIS
1	B	51	HIS
1	B	226	HIS
1	B	279	GLN
1	B	357	ASN
1	B	369	ASN
1	B	386	ASN
1	B	414	ASN
1	B	555	GLN
1	B	614	HIS
1	C	118	GLN
1	C	279	GLN

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Mol	Chain	Res	Type
1	C	357	ASN
1	C	369	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	C8E	C	1629	-	20,20,20	0.78	0	19,19,19	1.72	6 (31%)
3	R71	A	1630[B]	-	29,29,29	2.29	15 (51%)	36,37,37	1.32	3 (8%)
3	R71	A	1630[A]	-	29,29,29	2.15	10 (34%)	36,37,37	1.19	3 (8%)
3	R71	C	1630[A]	-	29,29,29	2.12	9 (31%)	36,37,37	1.24	3 (8%)
3	R71	B	1630[B]	-	29,29,29	2.25	14 (48%)	36,37,37	1.22	3 (8%)
3	R71	C	1630[B]	-	29,29,29	2.19	14 (48%)	36,37,37	1.10	3 (8%)
2	C8E	A	1629	-	20,20,20	0.88	0	19,19,19	1.80	6 (31%)
3	R71	B	1630[A]	-	29,29,29	2.18	11 (37%)	36,37,37	1.10	2 (5%)
2	C8E	B	1629	-	20,20,20	0.76	0	19,19,19	1.75	6 (31%)

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	C8E	C	1629	-	-	13/18/18/18	-
3	R71	A	1630[B]	-	-	18/21/21/21	0/2/2/2
3	R71	A	1630[A]	-	-	8/21/21/21	0/2/2/2
3	R71	C	1630[A]	-	-	6/21/21/21	0/2/2/2
3	R71	B	1630[B]	-	-	17/21/21/21	0/2/2/2
3	R71	C	1630[B]	-	-	14/21/21/21	0/2/2/2
2	C8E	A	1629	-	-	13/18/18/18	-
3	R71	B	1630[A]	-	-	13/21/21/21	0/2/2/2
2	C8E	B	1629	-	-	12/18/18/18	-

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1630[A]	R71	O21-C7	6.46	1.34	1.22
3	C	1630[A]	R71	O21-C7	6.44	1.34	1.22
3	A	1630[B]	R71	O21-C7	6.30	1.34	1.22
3	C	1630[B]	R71	O21-C7	6.24	1.34	1.22
3	B	1630[B]	R71	O21-C7	6.23	1.34	1.22
3	A	1630[A]	R71	O21-C7	6.20	1.33	1.22
3	A	1630[A]	R71	C1-C6	4.66	1.45	1.38
3	B	1630[A]	R71	C1-C6	4.14	1.44	1.38
3	B	1630[B]	R71	C1-C6	4.05	1.44	1.38
3	A	1630[B]	R71	C1-C6	4.03	1.44	1.38
3	C	1630[A]	R71	C1-C6	3.96	1.44	1.38
3	C	1630[B]	R71	C1-C6	3.79	1.43	1.38
3	C	1630[A]	R71	C5-C6	3.49	1.43	1.37
3	B	1630[A]	R71	C5-C6	3.43	1.43	1.37
3	B	1630[B]	R71	C5-C6	3.28	1.43	1.37
3	C	1630[B]	R71	C5-C6	3.16	1.43	1.37
3	A	1630[B]	R71	C8-C7	3.04	1.54	1.49
3	A	1630[B]	R71	C5-C6	2.98	1.42	1.37
3	A	1630[A]	R71	C9-C8	2.97	1.43	1.39
3	A	1630[B]	R71	C12-C13	2.95	1.43	1.38
3	B	1630[A]	R71	C10-C11	2.93	1.44	1.38
3	B	1630[A]	R71	C9-C10	2.83	1.43	1.38
3	A	1630[B]	R71	C9-C10	2.77	1.43	1.38
3	A	1630[B]	R71	C1-C7	2.74	1.55	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1630[B]	R71	C2-C1	2.71	1.44	1.39
3	A	1630[A]	R71	C9-C10	2.70	1.43	1.38
3	A	1630[A]	R71	C10-C11	2.68	1.43	1.38
3	B	1630[B]	R71	C8-C7	2.67	1.53	1.49
3	A	1630[A]	R71	C8-C7	2.66	1.53	1.49
3	B	1630[A]	R71	C2-C3	2.65	1.43	1.38
3	C	1630[B]	R71	C12-C13	2.64	1.43	1.38
3	A	1630[B]	R71	C9-C8	2.63	1.43	1.39
3	B	1630[B]	R71	C9-C10	2.62	1.43	1.38
3	B	1630[A]	R71	C3-C4	2.62	1.43	1.38
3	B	1630[B]	R71	C1-C7	2.61	1.55	1.49
3	B	1630[B]	R71	C2-C3	2.61	1.43	1.38
3	C	1630[A]	R71	C3-C4	2.60	1.43	1.38
3	A	1630[B]	R71	C10-C11	2.59	1.43	1.38
3	B	1630[B]	R71	C9-C8	2.57	1.43	1.39
3	C	1630[B]	R71	C9-C8	2.55	1.43	1.39
3	A	1630[A]	R71	C5-C6	2.55	1.42	1.37
3	A	1630[B]	R71	C2-C1	2.54	1.43	1.39
3	A	1630[B]	R71	C12-C11	2.53	1.43	1.38
3	C	1630[B]	R71	C2-C3	2.51	1.42	1.38
3	B	1630[B]	R71	C10-C11	2.45	1.43	1.38
3	A	1630[B]	R71	C13-C8	2.45	1.43	1.39
3	C	1630[B]	R71	C1-C7	2.42	1.54	1.49
3	B	1630[B]	R71	C12-C13	2.37	1.42	1.38
3	B	1630[A]	R71	C13-C8	2.37	1.43	1.39
3	C	1630[B]	R71	C2-C1	2.37	1.43	1.39
3	C	1630[B]	R71	C12-C11	2.35	1.42	1.38
3	C	1630[A]	R71	C10-C11	2.35	1.42	1.38
3	C	1630[A]	R71	C2-C3	2.34	1.42	1.38
3	B	1630[B]	R71	C13-C8	2.33	1.42	1.39
3	C	1630[B]	R71	C5-C4	2.31	1.42	1.39
3	C	1630[B]	R71	C8-C7	2.30	1.53	1.49
3	C	1630[B]	R71	C3-C4	2.29	1.43	1.38
3	C	1630[A]	R71	C9-C8	2.27	1.42	1.39
3	B	1630[A]	R71	C8-C7	2.26	1.53	1.49
3	A	1630[B]	R71	C2-C3	2.23	1.42	1.38
3	A	1630[A]	R71	C13-C8	2.18	1.42	1.39
3	C	1630[B]	R71	BR23-C11	-2.17	1.86	1.90
3	B	1630[A]	R71	C1-C7	2.11	1.54	1.49
3	A	1630[B]	R71	C3-C4	2.11	1.42	1.38
3	B	1630[B]	R71	C5-C4	2.11	1.42	1.39
3	A	1630[A]	R71	C12-C13	2.11	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1630[A]	R71	C2-C1	2.09	1.43	1.39
3	C	1630[A]	R71	C9-C10	2.07	1.42	1.38
3	A	1630[B]	R71	C5-C4	2.06	1.42	1.39
3	B	1630[B]	R71	C12-C11	2.05	1.42	1.38
3	A	1630[A]	R71	C5-C4	2.05	1.42	1.39
3	B	1630[A]	R71	C9-C8	2.05	1.42	1.39
3	C	1630[B]	R71	C9-C10	2.03	1.42	1.38

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1630[B]	R71	C1-C7-C8	4.80	127.24	119.56
2	A	1629	C8E	O15-C14-C13	4.56	131.12	110.35
2	B	1629	C8E	O15-C14-C13	4.41	130.44	110.35
3	B	1630[B]	R71	C1-C7-C8	4.39	126.59	119.56
2	C	1629	C8E	O15-C14-C13	4.34	130.15	110.35
3	C	1630[A]	R71	C1-C7-C8	4.27	126.39	119.56
3	A	1630[A]	R71	C1-C7-C8	3.86	125.72	119.56
3	C	1630[B]	R71	C1-C7-C8	3.62	125.36	119.56
3	B	1630[A]	R71	C1-C7-C8	3.40	125.00	119.56
3	A	1630[A]	R71	C5-C6-C1	-3.03	120.13	123.48
3	B	1630[A]	R71	C5-C6-C1	-2.88	120.30	123.48
2	A	1629	C8E	O15-C16-C17	2.87	123.43	110.35
3	C	1630[B]	R71	C5-C6-C1	-2.81	120.38	123.48
3	A	1630[B]	R71	C5-C6-C1	-2.79	120.40	123.48
3	C	1630[A]	R71	C5-C6-C1	-2.78	120.41	123.48
2	B	1629	C8E	C19-O18-C17	-2.76	101.20	113.26
2	A	1629	C8E	O18-C19-C20	2.75	122.24	110.11
2	B	1629	C8E	O15-C16-C17	2.75	122.87	110.35
2	B	1629	C8E	O18-C19-C20	2.72	122.11	110.11
2	C	1629	C8E	O15-C16-C17	2.71	122.72	110.35
3	B	1630[B]	R71	C5-C6-C1	-2.71	120.48	123.48
2	C	1629	C8E	C19-O18-C17	-2.70	101.43	113.26
3	A	1630[B]	R71	O21-C7-C8	-2.68	115.85	120.15
2	A	1629	C8E	C19-O18-C17	-2.61	101.83	113.26
3	B	1630[B]	R71	O21-C7-C8	-2.50	116.14	120.15
3	C	1630[A]	R71	O21-C7-C8	-2.50	116.14	120.15
2	C	1629	C8E	O18-C19-C20	2.47	120.99	110.11
2	A	1629	C8E	C7-C6-C5	-2.34	102.54	114.37
2	C	1629	C8E	C7-C6-C5	-2.27	102.89	114.37
2	B	1629	C8E	C7-C6-C5	-2.17	103.38	114.37
2	B	1629	C8E	C16-O15-C14	-2.14	103.90	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1629	C8E	C16-O15-C14	-2.11	104.03	113.26
3	A	1630[A]	R71	O21-C7-C8	-2.09	116.80	120.15
2	A	1629	C8E	C16-O15-C14	-2.06	104.25	113.26
3	C	1630[B]	R71	O21-C7-C8	-2.02	116.91	120.15

There are no chirality outliers.

All (114) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1630[A]	R71	C26-C25-N24-C20
3	B	1630[B]	R71	C26-C25-N24-C20
3	A	1630[A]	R71	N24-C25-C26-C29
3	A	1630[B]	R71	N24-C25-C26-C29
3	B	1630[B]	R71	C5-C4-O14-C15
3	B	1630[B]	R71	C3-C4-O14-C15
3	A	1630[A]	R71	C3-C4-O14-C15
3	A	1630[A]	R71	C5-C4-O14-C15
3	B	1630[A]	R71	N24-C25-C26-C29
3	B	1630[A]	R71	C18-C19-C20-N24
3	B	1630[B]	R71	C18-C19-C20-N24
3	C	1630[B]	R71	C18-C19-C20-N24
3	C	1630[B]	R71	C3-C4-O14-C15
3	A	1630[B]	R71	C5-C4-O14-C15
3	A	1630[B]	R71	C3-C4-O14-C15
3	C	1630[A]	R71	C18-C19-C20-N24
3	B	1630[B]	R71	N24-C25-C26-C29
3	C	1630[B]	R71	C5-C4-O14-C15
2	A	1629	C8E	O15-C16-C17-O18
2	B	1629	C8E	O15-C16-C17-O18
3	B	1630[A]	R71	C5-C4-O14-C15
3	B	1630[A]	R71	C3-C4-O14-C15
2	C	1629	C8E	C6-C7-C8-O9
3	A	1630[B]	R71	C6-C1-C7-C8
2	A	1629	C8E	O18-C19-C20-O21
2	B	1629	C8E	O18-C19-C20-O21
2	A	1629	C8E	C6-C7-C8-O9
3	C	1630[A]	R71	C5-C4-O14-C15
2	C	1629	C8E	O15-C16-C17-O18
3	C	1630[A]	R71	C19-C20-N24-C27
3	C	1630[A]	R71	C3-C4-O14-C15
3	A	1630[B]	R71	O21-C7-C8-C13
3	A	1630[A]	R71	C18-C19-C20-N24

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Mol	Chain	Res	Type	Atoms
2	C	1629	C8E	O18-C19-C20-O21
3	A	1630[B]	R71	O21-C7-C8-C9
3	A	1630[B]	R71	O14-C15-C16-C17
3	A	1630[B]	R71	C1-C7-C8-C9
2	A	1629	C8E	C4-C5-C6-C7
2	B	1629	C8E	C2-C3-C4-C5
3	A	1630[B]	R71	C6-C1-C7-O21
3	A	1630[B]	R71	C2-C1-C7-O21
3	A	1630[B]	R71	C1-C7-C8-C13
3	B	1630[B]	R71	O14-C15-C16-C17
3	B	1630[B]	R71	C6-C1-C7-C8
2	B	1629	C8E	C4-C5-C6-C7
3	A	1630[B]	R71	C2-C1-C7-C8
2	C	1629	C8E	C4-C5-C6-C7
3	C	1630[B]	R71	O14-C15-C16-C17
2	C	1629	C8E	C2-C3-C4-C5
3	A	1630[A]	R71	C19-C20-N24-C27
3	A	1630[B]	R71	C19-C20-N24-C27
3	C	1630[B]	R71	C19-C20-N24-C27
3	B	1630[A]	R71	O21-C7-C8-C13
2	A	1629	C8E	C2-C3-C4-C5
3	A	1630[A]	R71	C19-C20-N24-C25
3	A	1630[B]	R71	C19-C20-N24-C25
3	C	1630[A]	R71	C19-C20-N24-C25
3	C	1630[B]	R71	C19-C20-N24-C25
3	B	1630[B]	R71	C2-C1-C7-O21
3	B	1630[B]	R71	C2-C1-C7-C8
3	B	1630[B]	R71	C6-C1-C7-O21
3	C	1630[B]	R71	C6-C1-C7-C8
2	C	1629	C8E	C3-C4-C5-C6
3	B	1630[A]	R71	O21-C7-C8-C9
3	A	1630[A]	R71	C15-C16-C17-C18
3	B	1630[A]	R71	C1-C7-C8-C13
3	B	1630[A]	R71	O14-C15-C16-C17
2	C	1629	C8E	C1-C2-C3-C4
2	A	1629	C8E	C1-C2-C3-C4
3	B	1630[B]	R71	O21-C7-C8-C13
3	A	1630[B]	R71	C15-C16-C17-C18
2	B	1629	C8E	C1-C2-C3-C4
2	A	1629	C8E	C3-C4-C5-C6
3	C	1630[A]	R71	O14-C15-C16-C17
3	B	1630[A]	R71	C1-C7-C8-C9

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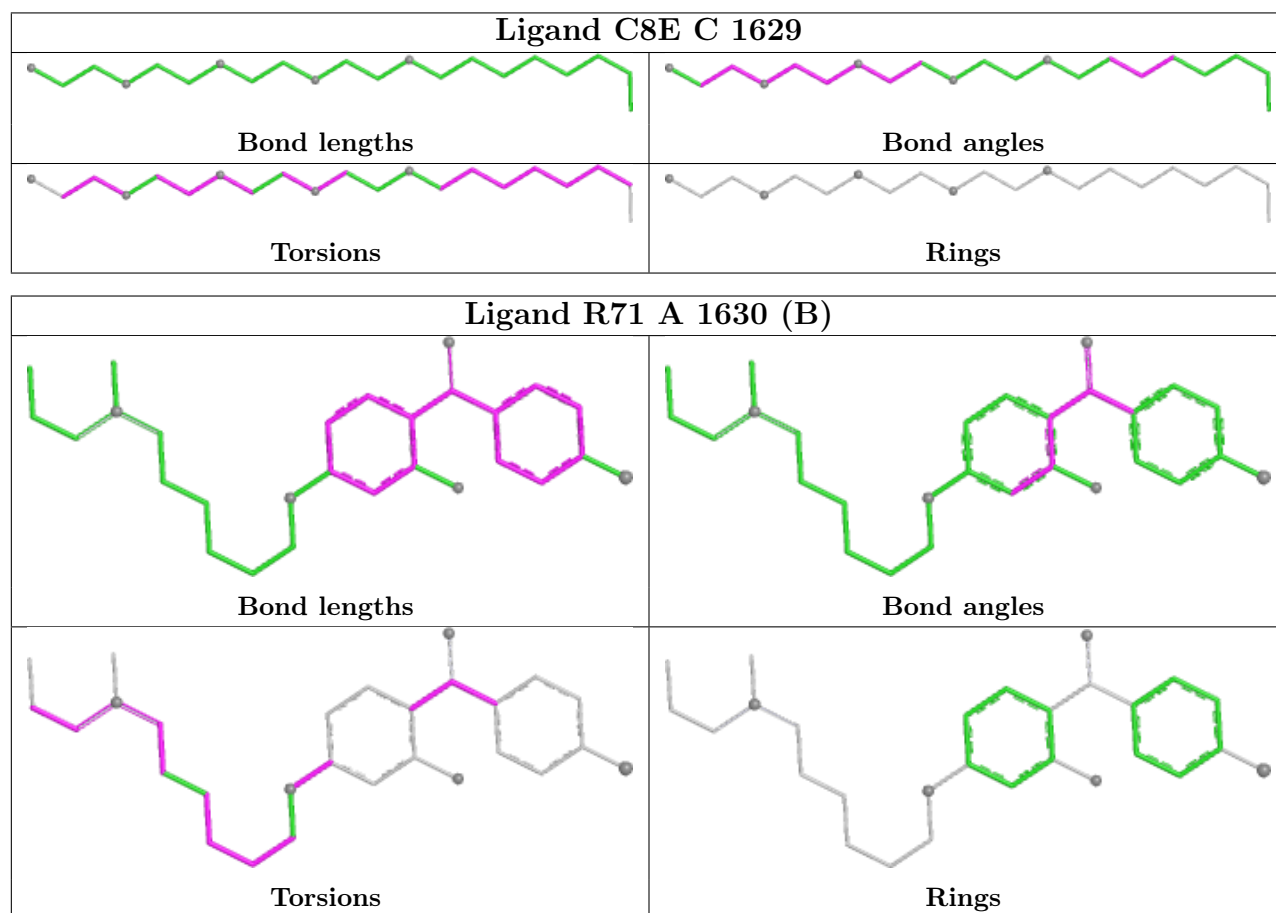
Mol	Chain	Res	Type	Atoms
3	B	1630[B]	R71	C1-C7-C8-C13
3	A	1630[B]	R71	C18-C19-C20-N24
2	A	1629	C8E	C13-C14-O15-C16
3	B	1630[A]	R71	C15-C16-C17-C18
2	C	1629	C8E	C14-C13-O12-C11
3	C	1630[B]	R71	C2-C1-C7-C8
2	B	1629	C8E	C13-C14-O15-C16
3	B	1630[B]	R71	O21-C7-C8-C9
2	B	1629	C8E	C20-C19-O18-C17
3	A	1630[B]	R71	C16-C17-C18-C19
2	C	1629	C8E	C10-C11-O12-C13
2	A	1629	C8E	C14-C13-O12-C11
2	A	1629	C8E	C10-C11-O12-C13
2	B	1629	C8E	C14-C13-O12-C11
2	B	1629	C8E	O12-C13-C14-O15
2	C	1629	C8E	C13-C14-O15-C16
3	C	1630[B]	R71	C1-C7-C8-C13
3	C	1630[B]	R71	O21-C7-C8-C13
3	B	1630[B]	R71	C1-C7-C8-C9
2	B	1629	C8E	C7-C8-O9-C10
3	C	1630[B]	R71	C2-C1-C7-O21
3	C	1630[B]	R71	C6-C1-C7-O21
3	B	1630[B]	R71	C15-C16-C17-C18
2	B	1629	C8E	C17-C16-O15-C14
2	A	1629	C8E	C17-C16-O15-C14
2	B	1629	C8E	C10-C11-O12-C13
2	C	1629	C8E	C20-C19-O18-C17
2	C	1629	C8E	C5-C6-C7-C8
2	C	1629	C8E	C17-C16-O15-C14
3	B	1630[A]	R71	C26-C25-N24-C27
3	B	1630[B]	R71	C26-C25-N24-C27
3	B	1630[B]	R71	C16-C17-C18-C19
3	B	1630[A]	R71	C16-C17-C18-C19
3	C	1630[B]	R71	O21-C7-C8-C9
3	C	1630[B]	R71	C1-C7-C8-C9
2	A	1629	C8E	O12-C13-C14-O15
3	A	1630[B]	R71	C26-C25-N24-C20
2	A	1629	C8E	C20-C19-O18-C17
3	A	1630[A]	R71	C16-C17-C18-C19

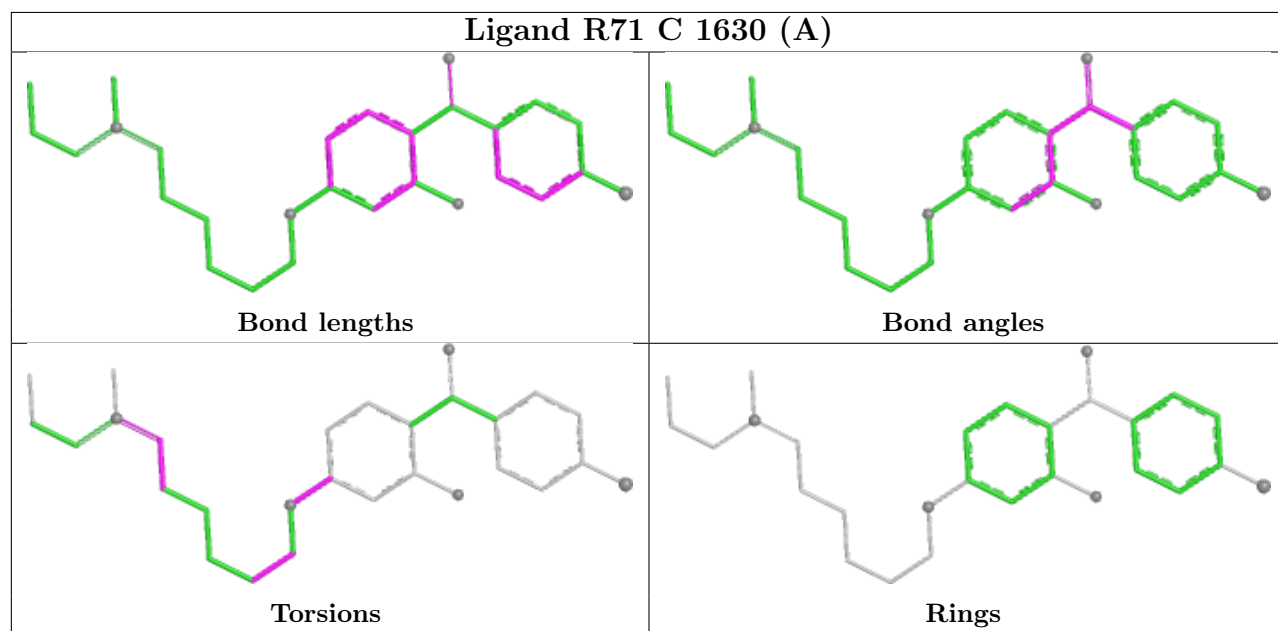
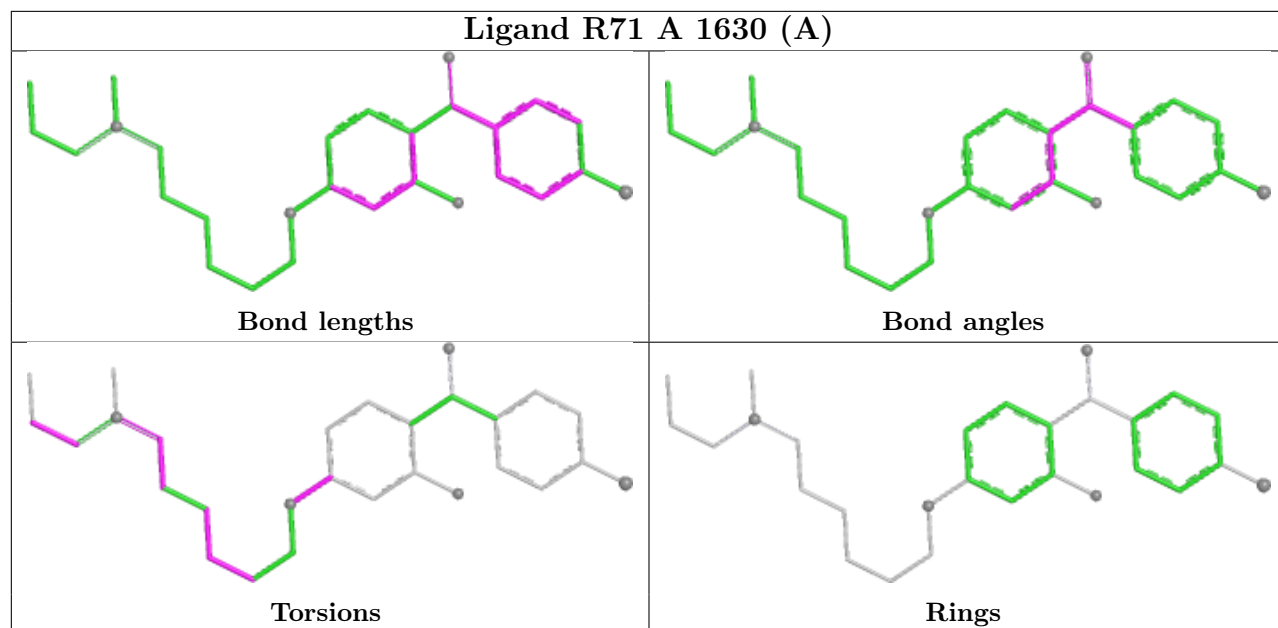
There are no ring outliers.

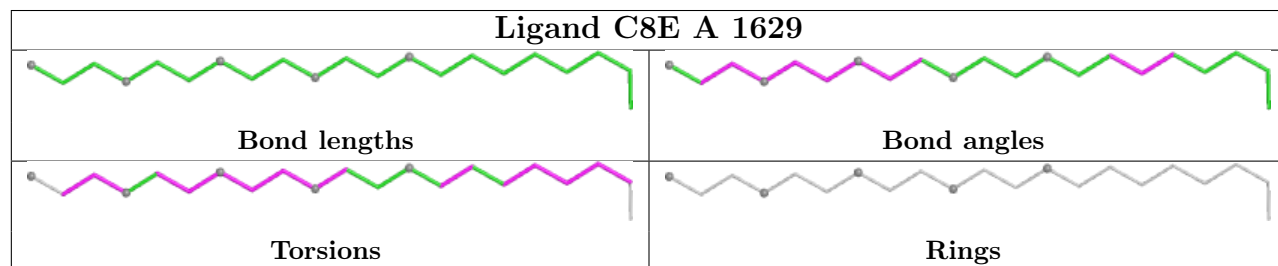
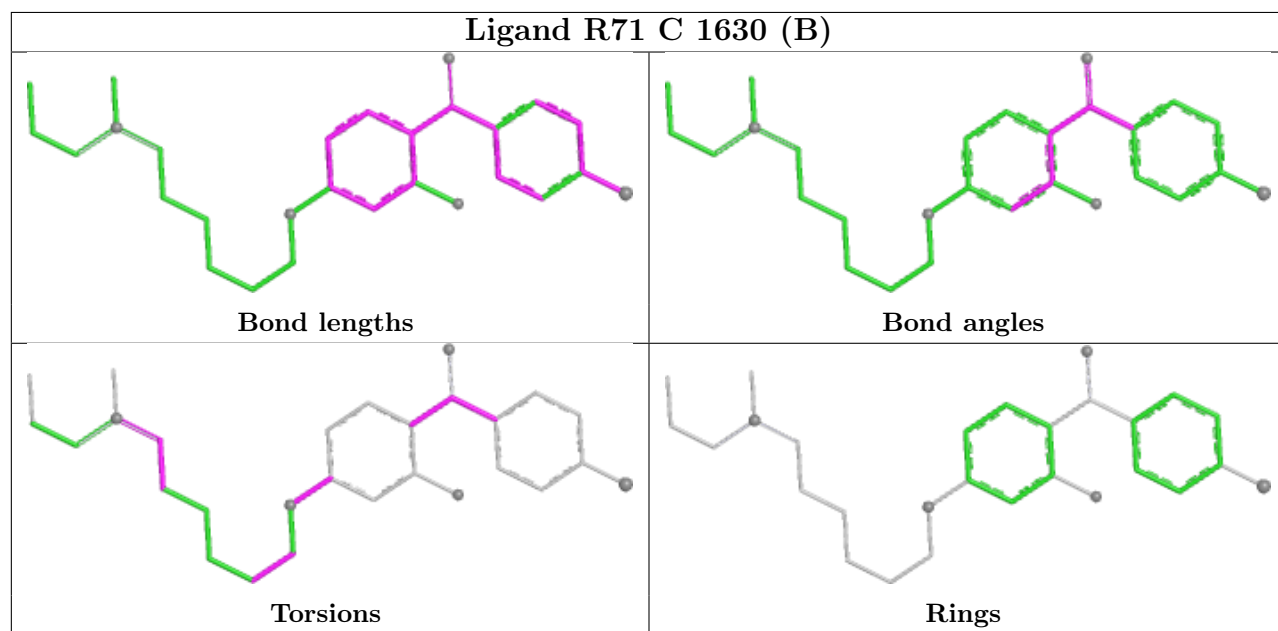
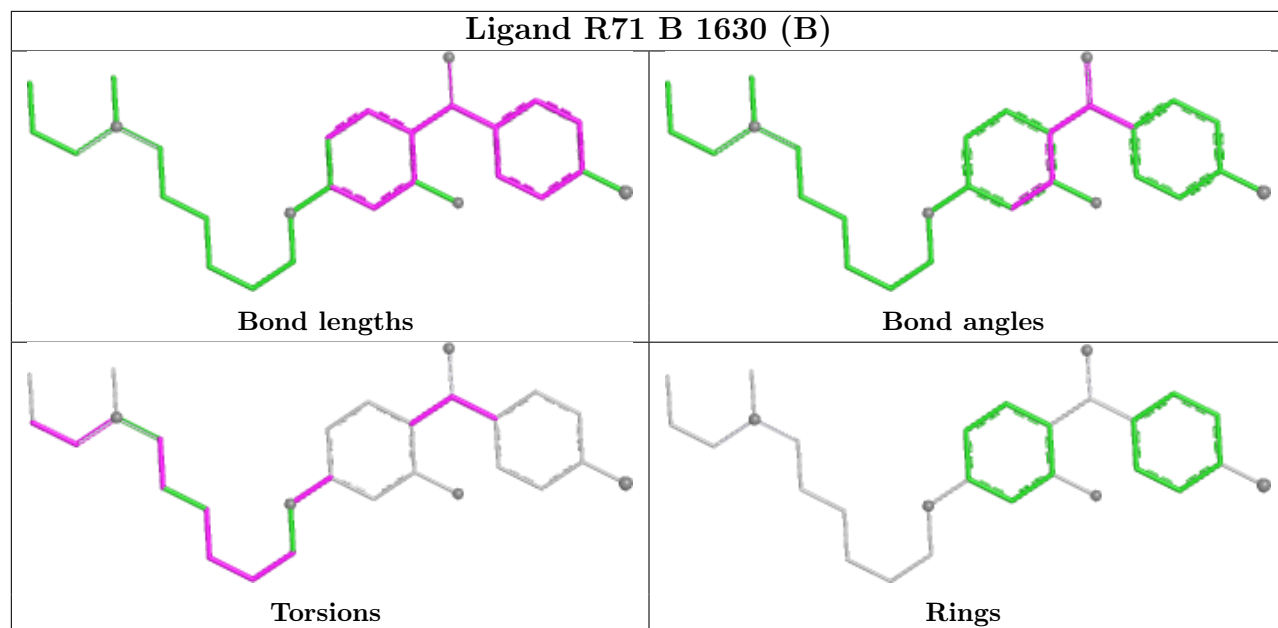
4 monomers are involved in 5 short contacts:

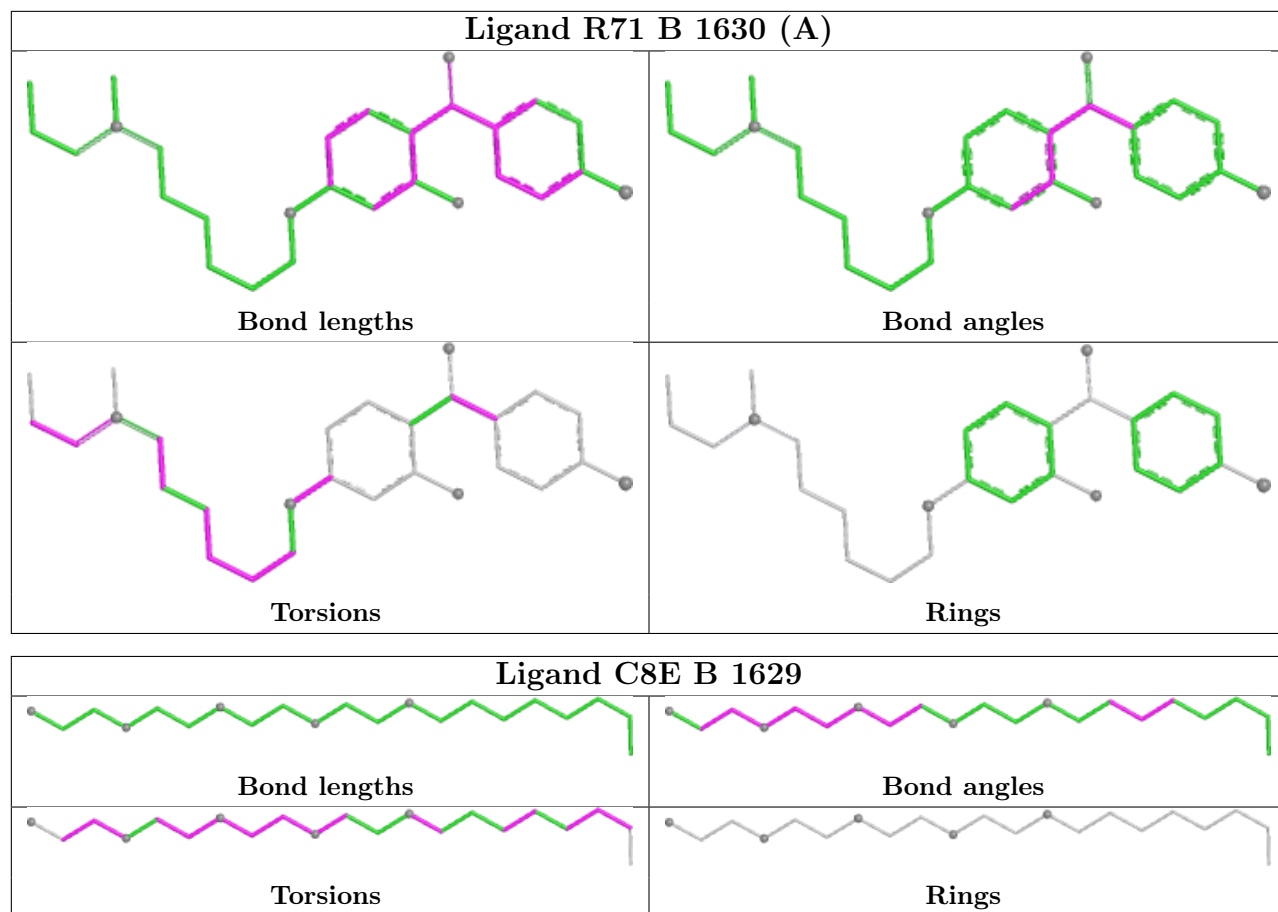
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1629	C8E	1	0
3	B	1630[B]	R71	1	0
3	C	1630[B]	R71	1	0
2	B	1629	C8E	2	0

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.









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	620/631 (98%)	-0.50	2 (0%) 90 86	8, 46, 90, 99	0
1	B	620/631 (98%)	-0.81	0 100 100	4, 31, 76, 99	0
1	C	620/631 (98%)	-0.71	0 100 100	4, 37, 84, 99	0
All	All	1860/1893 (98%)	-0.67	2 (0%) 92 90	4, 37, 85, 99	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	569	ALA	2.2
1	A	566	GLY	2.2

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	C8E	B	1629	21/21	0.86	0.19	68,81,89,89	0

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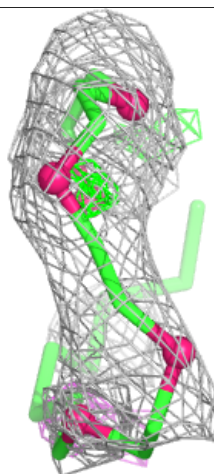
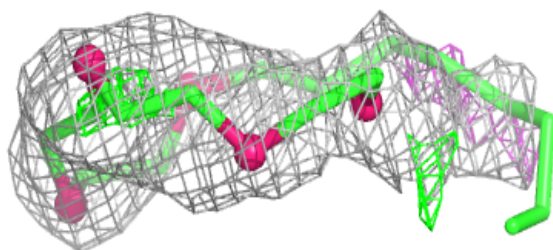
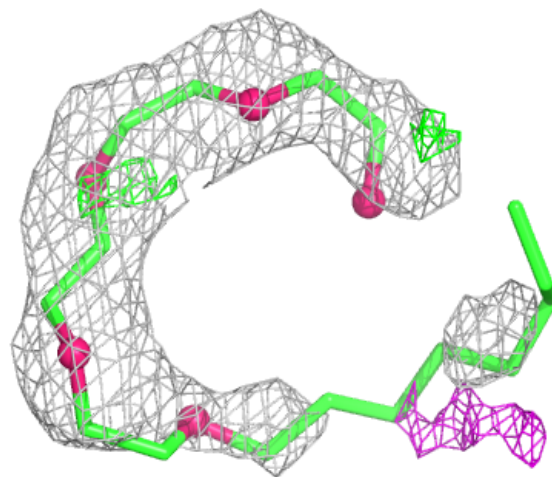
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	C8E	C	1629	21/21	0.88	0.20	71,84,92,92	0
2	C8E	A	1629	21/21	0.89	0.18	75,89,96,96	0
3	R71	A	1630[A]	28/28	0.97	0.08	19,41,55,55	28
3	R71	A	1630[B]	28/28	0.97	0.08	19,41,50,50	28
3	R71	B	1630[A]	28/28	0.98	0.07	12,41,49,49	28
3	R71	B	1630[B]	28/28	0.98	0.07	22,33,41,41	28
3	R71	C	1630[A]	28/28	0.99	0.07	23,34,41,41	28
3	R71	C	1630[B]	28/28	0.99	0.07	39,42,55,55	28

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.

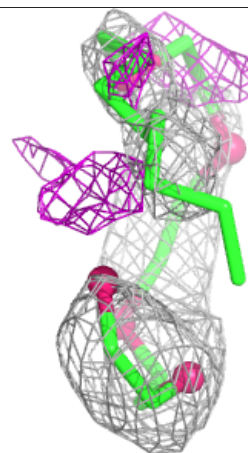
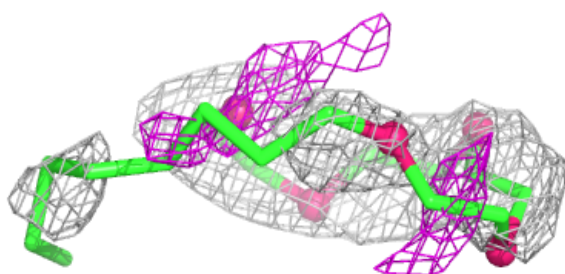
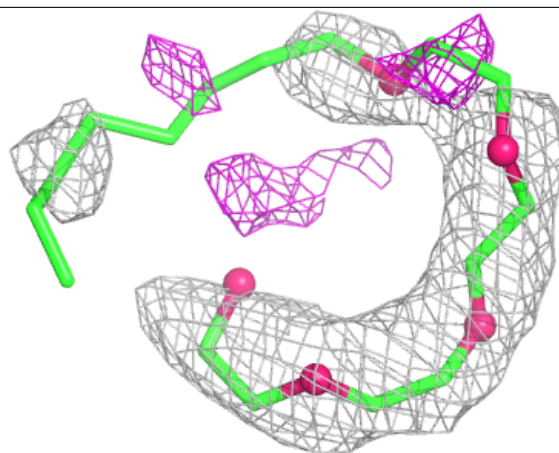
Electron density around C8E B 1629:

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



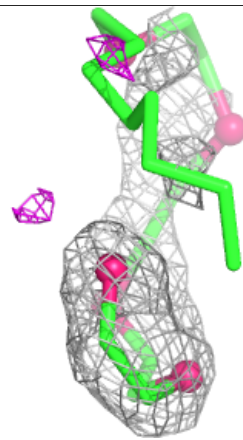
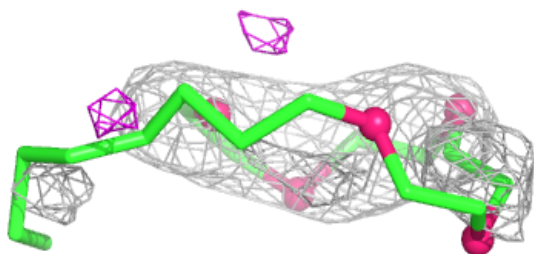
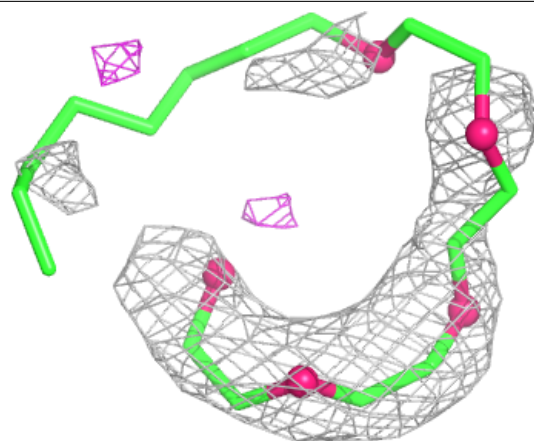
Electron density around C8E C 1629:

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

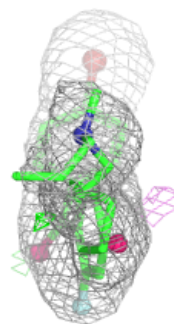
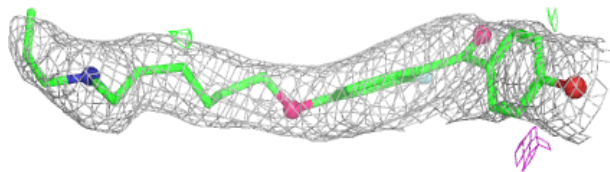
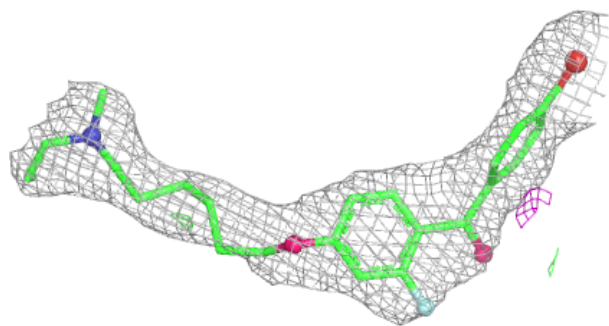


Electron density around C8E A 1629:

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

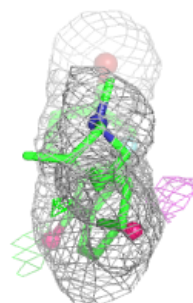
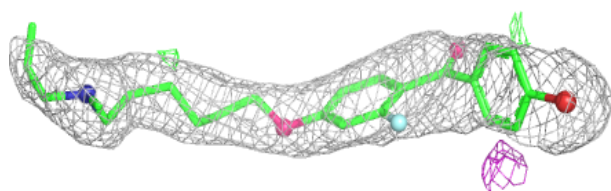
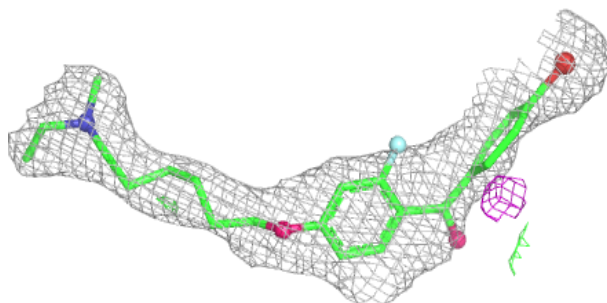
**Electron density around R71 A 1630 (A):**

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

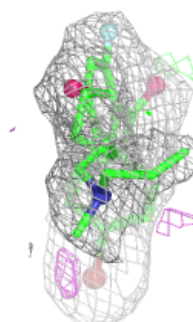
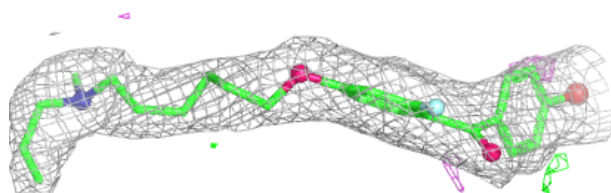
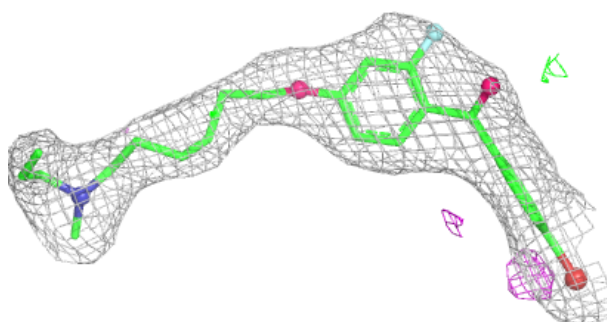


Electron density around R71 A 1630 (B):

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

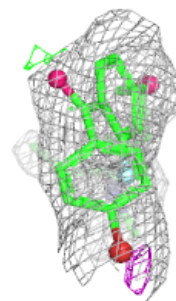
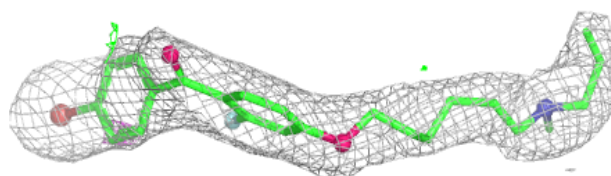
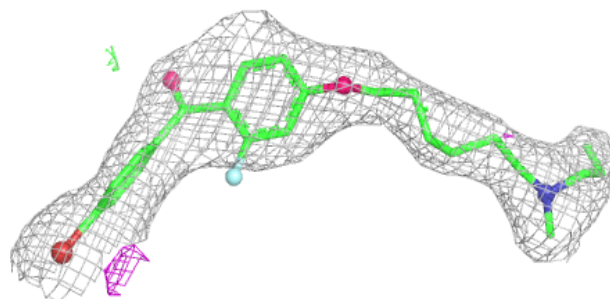
**Electron density around R71 B 1630 (A):**

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

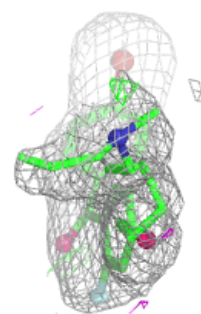
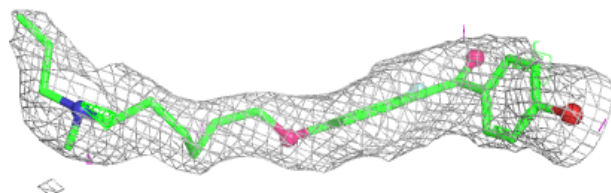
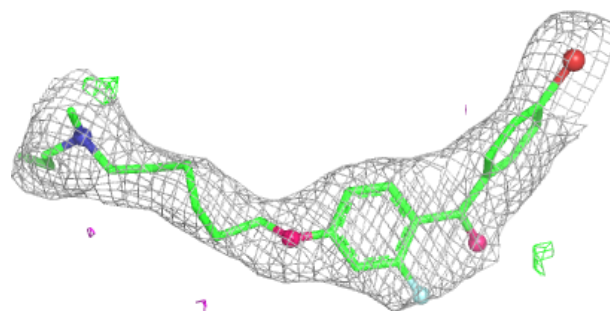


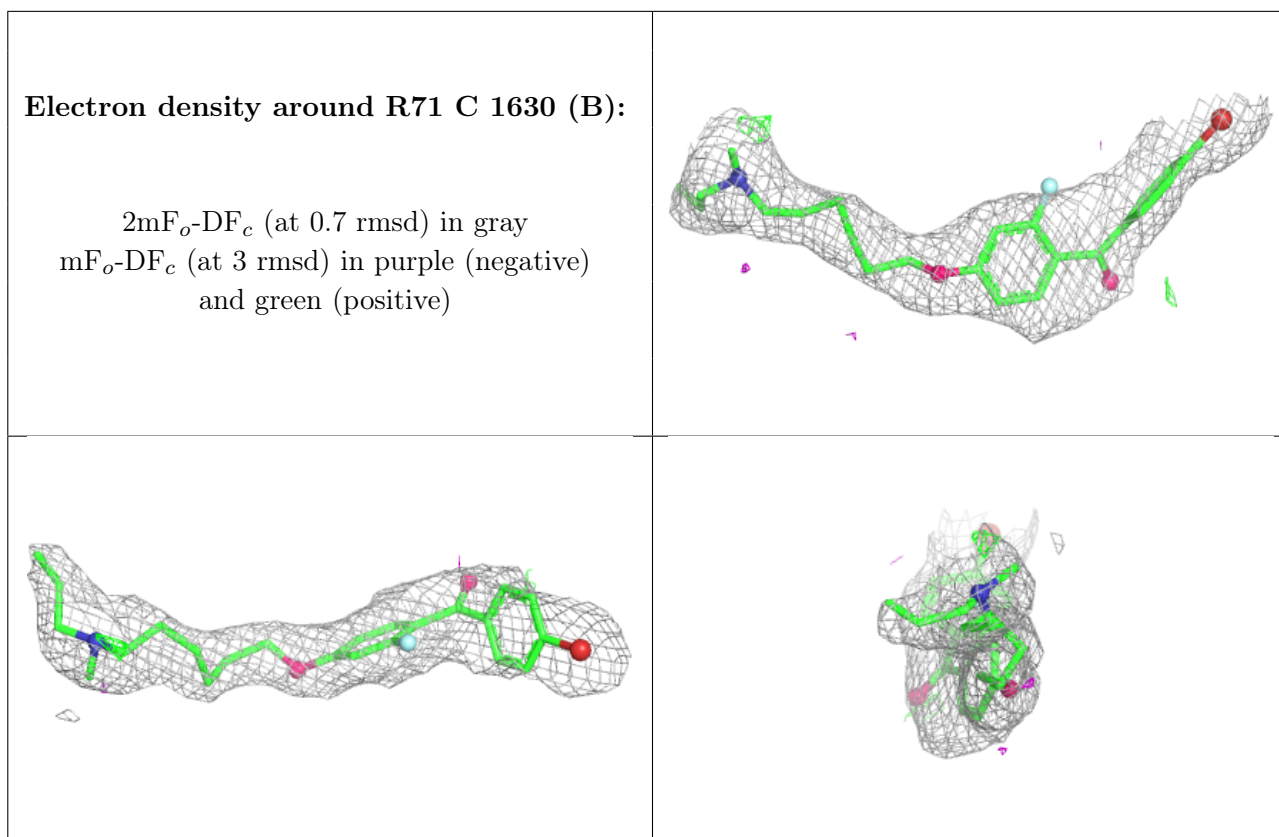
Electron density around R71 B 1630 (B):

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

**Electron density around R71 C 1630 (A):**

$2mF_o-DF_c$ (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.