



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 12:09 AM EDT

PDB ID : 1NQH / pdb_00001nqh
Title : OUTER MEMBRANE COBALAMIN TRANSPORTER (BTUB) FROM E. COLI, WITH BOUND CALCIUM AND CYANOCOBALAMIN (VITAMIN B12) SUBSTRATE
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Deposited on : 2003-01-21
Resolution : 3.10 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

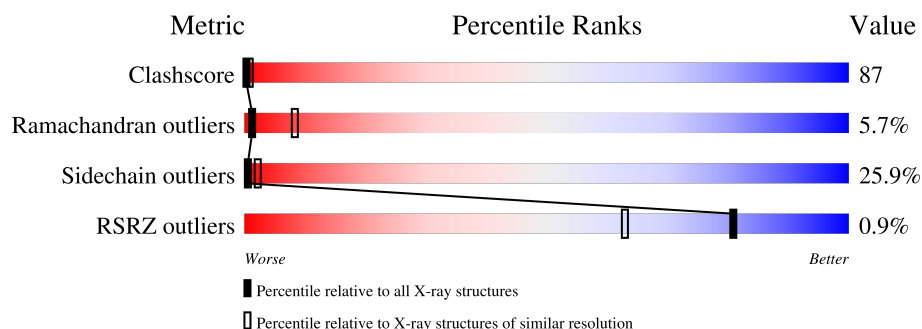
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	594	

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	CNC	A	701	X	-	X	-
4	C8E	A	802	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	C8E	A	803	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4853 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.

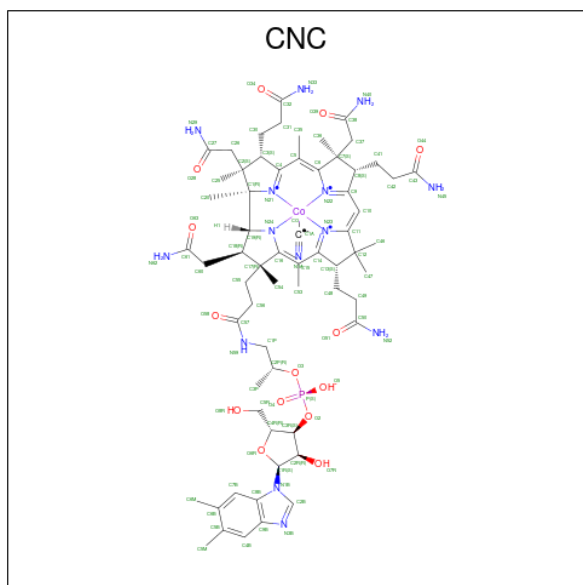
- Molecule 1 is a protein called VITAMIN B12 RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	584	Total	C	N	O	S	0	0	0
			4630	2915	792	921	2			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Ca	0	0
			4	4		

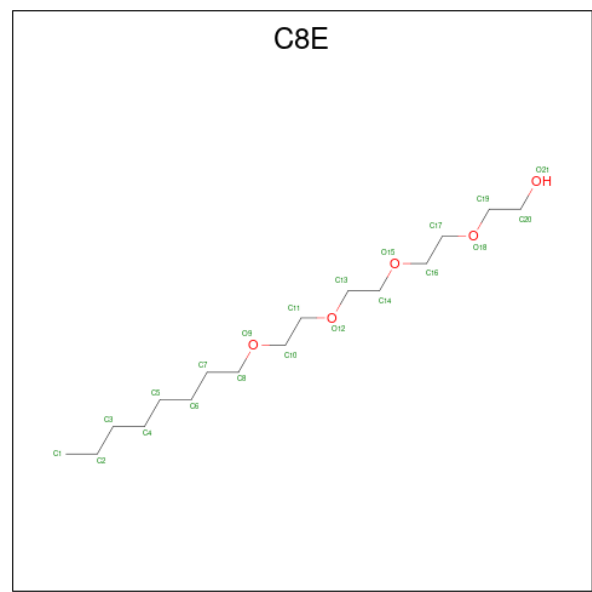
- Molecule 3 is CYANOCOBALAMIN (CCD ID: CNC) (formula: C₆₃H₈₉CoN₁₄O₁₄P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Co	N	O	P	0	0
			93	63	1	14	14	1		

- Molecule 4 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (CCD ID: C8E)

(formula: C₁₆H₃₄O₅).

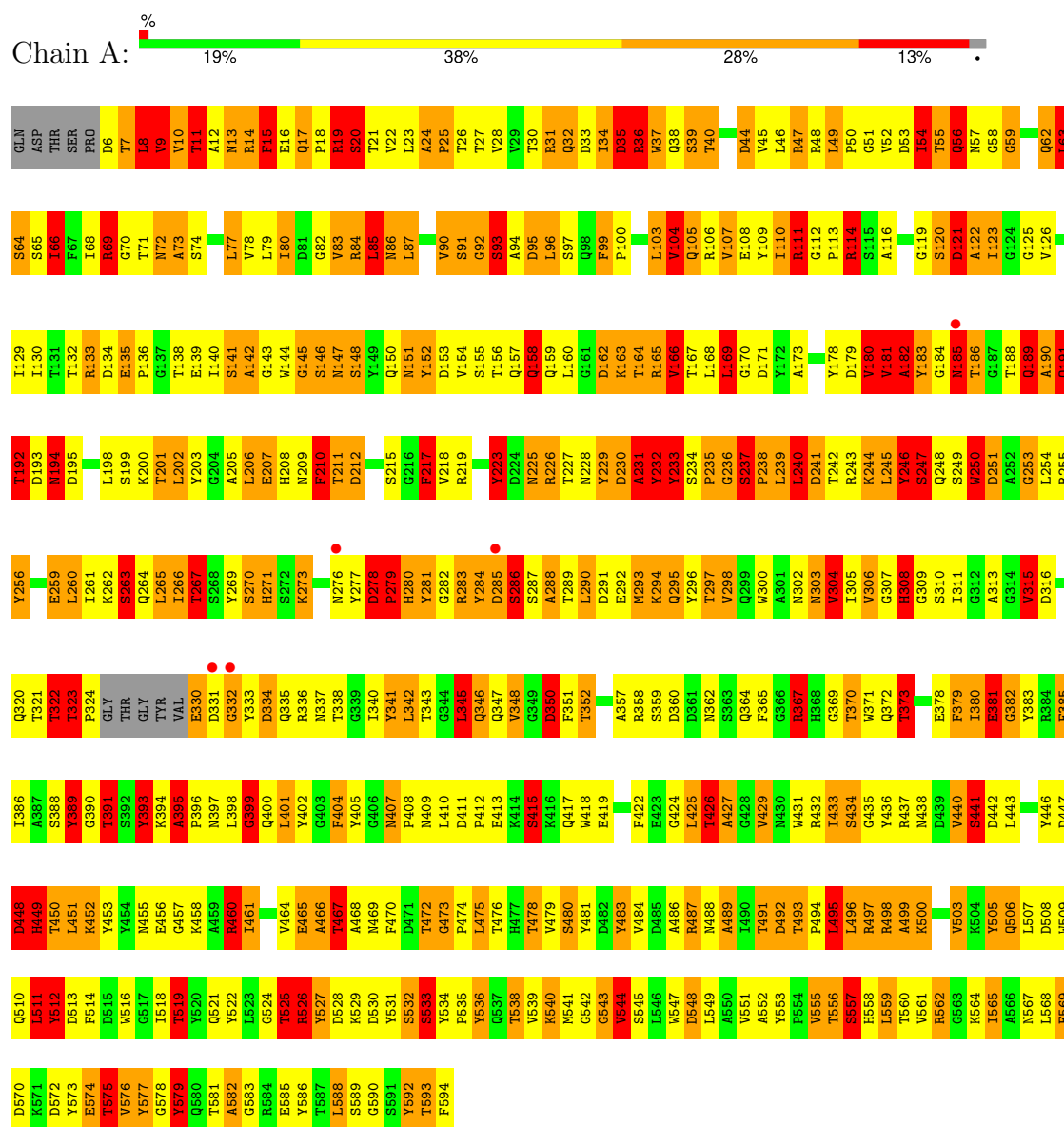


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			21	16	5		
4	A	1	Total	C	O	0	0
			21	16	5		
4	A	1	Total	C	O	0	0
			21	16	5		
4	A	1	Total	C	O	0	0
			21	16	5		
4	A	1	Total	C	O	0	0
			21	16	5		
4	A	1	Total	C	O	0	0
			21	16	5		

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: VITAMIN B12 RECEPTOR



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	81.69Å 81.69Å 225.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.10 20.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-3.10) 99.5 (20.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.44 (at 3.11Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.224 , 0.265 0.230 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	62.9	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4853	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, C8E, CNC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.90	102/4747 (2.1%)	1.89	136/6465 (2.1%)

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	A	3	100

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	ILE	CA-CB	-12.22	1.39	1.54
1	A	230	ASP	CA-C	12.15	1.69	1.52
1	A	54	ILE	CA-CB	-10.53	1.39	1.55
1	A	306	VAL	CA-CB	-9.96	1.41	1.54
1	A	293	MET	SD-CE	9.17	2.02	1.79
1	A	544	VAL	CA-CB	-8.34	1.43	1.54
1	A	338	THR	CA-CB	-8.14	1.39	1.53
1	A	388	SER	CA-C	-8.01	1.42	1.52
1	A	467	THR	CA-C	-7.89	1.42	1.52
1	A	104	VAL	CA-C	-7.63	1.43	1.52
1	A	110	ILE	CA-CB	-7.57	1.44	1.54
1	A	28	VAL	C-O	-7.38	1.16	1.24
1	A	380	ILE	CA-CB	-7.33	1.44	1.55
1	A	147	ASN	CA-C	-7.23	1.45	1.53
1	A	129	ILE	CA-CB	-7.15	1.45	1.54
1	A	427	ALA	CA-CB	-7.08	1.41	1.53
1	A	180	VAL	CA-CB	-7.00	1.45	1.54
1	A	111	ARG	CZ-NH1	-6.90	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	298	VAL	CA-CB	-6.89	1.45	1.54
1	A	386	ILE	CA-CB	-6.69	1.46	1.54
1	A	464	VAL	C-O	-6.68	1.17	1.24
1	A	401	LEU	CA-C	-6.66	1.46	1.53
1	A	218	VAL	CA-CB	-6.66	1.45	1.54
1	A	34	ILE	CA-CB	-6.62	1.45	1.54
1	A	270	SER	CA-C	-6.59	1.44	1.52
1	A	303	ASN	CA-C	-6.53	1.44	1.52
1	A	496	LEU	C-O	-6.52	1.15	1.23
1	A	129	ILE	CA-C	-6.51	1.44	1.52
1	A	391	THR	CA-CB	-6.50	1.43	1.53
1	A	104	VAL	C-O	-6.49	1.17	1.24
1	A	518	ILE	CA-CB	-6.48	1.46	1.54
1	A	111	ARG	NE-CZ	-6.43	1.25	1.33
1	A	343	THR	CA-CB	-6.43	1.41	1.53
1	A	25	PRO	CA-C	-6.42	1.45	1.52
1	A	84	ARG	C-O	-6.41	1.16	1.23
1	A	472	THR	CA-CB	-6.40	1.45	1.53
1	A	278	ASP	C-O	-6.38	1.16	1.24
1	A	395	ALA	CA-C	-6.37	1.45	1.53
1	A	489	ALA	CA-CB	-6.29	1.43	1.53
1	A	267	THR	CA-CB	-6.28	1.43	1.53
1	A	217	PHE	CA-C	-6.26	1.44	1.52
1	A	233	TYR	CA-C	-6.22	1.44	1.52
1	A	129	ILE	N-CA	-6.13	1.38	1.46
1	A	40	THR	CA-CB	-6.03	1.44	1.53
1	A	499	ALA	CA-CB	-6.02	1.45	1.53
1	A	499	ALA	C-O	-6.02	1.16	1.24
1	A	107	VAL	CA-CB	-5.99	1.46	1.54
1	A	468	ALA	CA-CB	-5.99	1.43	1.53
1	A	379	PHE	C-O	-5.93	1.16	1.24
1	A	83	VAL	C-O	-5.93	1.17	1.24
1	A	338	THR	CA-C	-5.89	1.45	1.52
1	A	123	ILE	CA-CB	-5.87	1.48	1.55
1	A	304	VAL	CA-CB	-5.86	1.46	1.55
1	A	24	ALA	CA-CB	-5.83	1.44	1.53
1	A	136	PRO	CA-C	-5.81	1.45	1.52
1	A	250	TRP	CA-C	-5.80	1.45	1.52
1	A	484	VAL	CA-CB	-5.72	1.46	1.53
1	A	40	THR	C-O	-5.71	1.16	1.24
1	A	388	SER	C-O	-5.66	1.17	1.23
1	A	461	ILE	CA-CB	-5.66	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	323	THR	CA-CB	-5.64	1.45	1.53
1	A	52	VAL	CA-CB	-5.63	1.47	1.54
1	A	308	HIS	CA-C	-5.59	1.45	1.52
1	A	495	LEU	CA-C	-5.58	1.45	1.53
1	A	505	TYR	CA-C	-5.56	1.45	1.52
1	A	565	ILE	CA-CB	-5.56	1.47	1.53
1	A	71	THR	CA-CB	-5.52	1.44	1.53
1	A	426	THR	CA-C	-5.49	1.46	1.52
1	A	503	VAL	C-O	-5.49	1.17	1.24
1	A	434	SER	CA-CB	-5.46	1.44	1.53
1	A	35	ASP	CA-C	-5.45	1.45	1.52
1	A	347	GLN	C-O	-5.45	1.17	1.24
1	A	466	ALA	CA-CB	-5.44	1.43	1.53
1	A	296	TYR	CA-C	-5.40	1.46	1.52
1	A	106	ARG	CA-C	-5.40	1.45	1.52
1	A	514	PHE	N-CA	-5.40	1.39	1.46
1	A	478	THR	CA-CB	-5.39	1.45	1.53
1	A	66	ILE	CA-C	-5.36	1.46	1.52
1	A	310	SER	CA-C	-5.35	1.46	1.52
1	A	472	THR	N-CA	-5.32	1.41	1.46
1	A	389	TYR	C-O	-5.30	1.17	1.23
1	A	111	ARG	CZ-NH2	-5.28	1.26	1.33
1	A	104	VAL	CA-CB	-5.25	1.48	1.54
1	A	381	GLU	CA-C	-5.23	1.45	1.52
1	A	521	GLN	C-O	-5.22	1.17	1.23
1	A	418	TRP	C-O	-5.22	1.17	1.23
1	A	346	GLN	CA-C	-5.21	1.46	1.52
1	A	593	THR	CA-CB	-5.20	1.43	1.53
1	A	582	ALA	CA-CB	-5.18	1.44	1.53
1	A	271	HIS	CA-C	-5.16	1.46	1.52
1	A	147	ASN	CA-CB	-5.14	1.49	1.53
1	A	429	VAL	CA-CB	-5.14	1.48	1.54
1	A	297	THR	CA-CB	-5.13	1.45	1.53
1	A	511	LEU	CA-C	-5.10	1.46	1.52
1	A	315	VAL	CA-CB	-5.08	1.46	1.55
1	A	182	ALA	CA-CB	-5.07	1.45	1.53
1	A	83	VAL	CA-CB	-5.05	1.48	1.54
1	A	166	VAL	CA-CB	-5.04	1.46	1.54
1	A	35	ASP	C-O	-5.04	1.18	1.24
1	A	72	ASN	C-O	-5.02	1.17	1.23
1	A	229	TYR	CA-C	5.01	1.58	1.53
1	A	246	TYR	CA-C	-5.00	1.46	1.52

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	569	PHE	CA-C-N	-12.67	102.89	123.04
1	A	569	PHE	C-N-CA	-12.67	102.89	123.04
1	A	399	GLY	N-CA-C	-10.28	100.05	112.49
1	A	123	ILE	N-CA-C	9.37	120.57	111.67
1	A	10	VAL	CB-CA-C	-8.88	96.73	111.29
1	A	230	ASP	N-CA-C	8.83	129.62	110.80
1	A	145	GLY	N-CA-C	8.82	124.75	111.42
1	A	495	LEU	CA-C-O	-8.76	112.08	121.98
1	A	96	LEU	N-CA-C	-8.68	103.23	113.21
1	A	293	MET	N-CA-C	8.66	123.19	109.50
1	A	278	ASP	N-CA-C	-8.47	97.53	110.32
1	A	104	VAL	CB-CA-C	-8.24	100.99	110.96
1	A	232	TYR	N-CA-C	-8.12	93.49	110.80
1	A	472	THR	N-CA-C	-8.05	99.34	111.34
1	A	83	VAL	N-CA-C	7.96	119.58	108.12
1	A	279	PRO	N-CD-CG	-7.77	94.48	103.80
1	A	180	VAL	CB-CA-C	-7.57	102.39	112.46
1	A	74	SER	N-CA-C	-7.55	103.18	113.30
1	A	230	ASP	O-C-N	-7.39	112.76	122.59
1	A	235	PRO	CA-C-O	-7.34	112.33	120.92
1	A	37	TRP	N-CA-C	-7.32	104.33	113.18
1	A	448	ASP	N-CA-C	-7.25	102.17	111.02
1	A	298	VAL	N-CA-C	7.16	117.80	108.35
1	A	575	THR	N-CA-C	-7.16	104.41	113.72
1	A	512	TYR	O-C-N	-7.08	114.74	122.38
1	A	66	ILE	CB-CA-C	-6.95	100.35	110.63
1	A	238	PRO	N-CA-C	6.95	121.26	111.33
1	A	9	VAL	CB-CA-C	-6.91	99.96	111.29
1	A	306	VAL	CB-CA-C	-6.83	98.63	110.65
1	A	382	GLY	N-CA-C	-6.75	105.19	114.64
1	A	158	GLN	CB-CA-C	-6.70	98.15	110.62
1	A	39	SER	N-CA-C	6.68	119.70	110.35
1	A	381	GLU	N-CA-C	-6.65	99.98	109.96
1	A	315	VAL	CB-CA-C	-6.65	100.06	110.69
1	A	231	ALA	N-CA-C	6.62	124.89	110.80
1	A	495	LEU	N-CA-C	-6.42	99.78	109.60
1	A	64	SER	N-CA-C	6.40	118.50	108.96
1	A	236	GLY	N-CA-C	6.37	128.29	113.18
1	A	66	ILE	CA-C-O	-6.33	113.74	120.39
1	A	369	GLY	O-C-N	-6.31	118.18	123.73
1	A	218	VAL	N-CA-C	6.29	117.83	108.46
1	A	235	PRO	CA-C-N	-6.27	109.12	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	PRO	C-N-CA	-6.27	109.12	121.41
1	A	469	ASN	N-CA-C	6.26	118.93	109.23
1	A	579	TYR	CA-C-N	-6.25	112.48	121.42
1	A	579	TYR	C-N-CA	-6.25	112.48	121.42
1	A	143	GLY	CA-C-O	-6.23	115.07	121.61
1	A	133	ARG	N-CA-C	6.22	119.79	110.14
1	A	59	GLY	N-CA-C	-6.19	103.64	112.55
1	A	511	LEU	CA-CB-CG	-6.05	95.13	116.30
1	A	308	HIS	N-CA-C	-6.04	97.93	110.80
1	A	476	THR	N-CA-C	6.04	119.31	109.59
1	A	514	PHE	N-CA-C	-6.04	100.02	109.25
1	A	545	SER	N-CA-C	6.02	118.22	108.41
1	A	369	GLY	N-CA-C	6.01	120.08	111.12
1	A	169	LEU	CA-C-N	6.00	126.32	122.18
1	A	169	LEU	C-N-CA	6.00	126.32	122.18
1	A	235	PRO	N-CA-C	-6.00	101.08	110.50
1	A	491	THR	OG1-CB-CG2	-6.00	97.29	109.30
1	A	498	ARG	NE-CZ-NH1	-6.00	115.50	121.50
1	A	164	THR	N-CA-C	6.00	119.26	109.06
1	A	346	GLN	N-CA-C	5.90	117.75	108.96
1	A	582	ALA	CA-C-N	-5.89	113.52	122.06
1	A	582	ALA	C-N-CA	-5.89	113.52	122.06
1	A	460	ARG	NE-CZ-NH1	-5.88	115.61	121.50
1	A	332	GLY	O-C-N	-5.85	118.47	122.62
1	A	498	ARG	NE-CZ-NH2	5.85	124.46	119.20
1	A	525	THR	N-CA-C	-5.85	102.65	110.55
1	A	126	VAL	CA-C-N	-5.84	115.30	123.13
1	A	126	VAL	C-N-CA	-5.84	115.30	123.13
1	A	119	GLY	N-CA-C	5.83	120.86	110.95
1	A	122	ALA	CA-C-N	-5.83	115.69	122.63
1	A	122	ALA	C-N-CA	-5.83	115.69	122.63
1	A	69	ARG	NE-CZ-NH2	5.80	124.42	119.20
1	A	472	THR	CA-C-O	5.79	125.77	119.40
1	A	263	SER	N-CA-C	5.79	118.91	109.24
1	A	27	THR	N-CA-C	-5.76	99.94	108.99
1	A	8	LEU	CA-C-N	-5.73	111.66	121.97
1	A	8	LEU	C-N-CA	-5.73	111.66	121.97
1	A	562	ARG	N-CA-C	5.71	117.91	109.69
1	A	512	TYR	CB-CA-C	5.68	122.17	112.00
1	A	579	TYR	O-C-N	-5.67	116.87	123.27
1	A	512	TYR	CA-C-N	-5.58	112.04	121.18
1	A	512	TYR	C-N-CA	-5.58	112.04	121.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	557	SER	N-CA-C	-5.57	98.94	110.80
1	A	544	VAL	N-CA-C	5.57	120.91	109.34
1	A	484	VAL	N-CA-CB	-5.56	104.89	111.90
1	A	467	THR	CA-C-O	-5.56	115.12	121.40
1	A	130	ILE	N-CA-C	5.55	115.88	108.11
1	A	480	SER	N-CA-C	5.54	118.10	109.52
1	A	111	ARG	N-CA-C	-5.53	102.34	110.52
1	A	526	ARG	N-CA-C	5.52	116.36	108.74
1	A	261	ILE	N-CA-C	-5.50	100.41	108.11
1	A	484	VAL	N-CA-C	5.47	115.98	107.28
1	A	415	SER	N-CA-C	5.46	118.39	109.59
1	A	36	ARG	CG-CD-NE	5.46	124.01	112.00
1	A	336	ARG	N-CA-C	5.46	118.36	109.24
1	A	347	GLN	CA-C-N	-5.46	115.58	123.11
1	A	347	GLN	C-N-CA	-5.46	115.58	123.11
1	A	487	ARG	N-CA-C	5.43	118.56	110.14
1	A	294	LYS	N-CA-C	5.43	117.52	108.02
1	A	441	SER	O-C-N	5.39	128.79	123.46
1	A	15	PHE	CA-C-O	-5.36	114.92	121.78
1	A	20	SER	CA-C-N	-5.33	114.16	122.73
1	A	20	SER	C-N-CA	-5.33	114.16	122.73
1	A	511	LEU	CA-C-N	-5.32	114.31	121.71
1	A	511	LEU	C-N-CA	-5.32	114.31	121.71
1	A	229	TYR	CA-C-O	-5.31	114.41	121.47
1	A	237	SER	CA-C-N	5.30	126.05	120.11
1	A	237	SER	C-N-CA	5.30	126.05	120.11
1	A	304	VAL	N-CA-C	5.30	116.65	108.44
1	A	350	ASP	CB-CA-C	-5.28	102.23	110.94
1	A	73	ALA	N-CA-C	-5.26	106.84	113.20
1	A	71	THR	N-CA-C	5.26	117.31	110.53
1	A	521	GLN	O-C-N	-5.24	117.41	123.33
1	A	576	VAL	N-CA-C	5.23	116.23	107.18
1	A	342	LEU	N-CA-C	5.22	117.91	109.40
1	A	194	ASN	N-CA-C	-5.20	102.58	110.28
1	A	25	PRO	N-CD-CG	-5.17	95.44	103.20
1	A	578	GLY	N-CA-C	5.17	120.84	114.69
1	A	54	ILE	CB-CA-C	-5.16	102.88	110.82
1	A	120	SER	O-C-N	5.14	129.08	123.01
1	A	509	TRP	N-CA-C	5.13	116.64	108.79
1	A	233	TYR	CB-CA-C	-5.13	100.22	110.42
1	A	210	PHE	N-CA-C	-5.12	106.98	113.18
1	A	52	VAL	N-CA-CB	-5.10	104.87	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	532	SER	N-CA-C	-5.10	106.75	112.87
1	A	549	LEU	CA-C-N	-5.07	114.53	122.73
1	A	549	LEU	C-N-CA	-5.07	114.53	122.73
1	A	393	TYR	N-CA-C	5.06	115.98	108.60
1	A	525	THR	OG1-CB-CG2	-5.04	99.22	109.30
1	A	590	GLY	N-CA-C	5.02	119.39	110.80
1	A	367	ARG	CG-CD-NE	5.02	123.05	112.00
1	A	536	TYR	CA-C-O	-5.01	114.88	120.54
1	A	456	GLU	N-CA-C	5.01	121.06	114.75
1	A	19	ARG	N-CA-C	5.01	116.43	111.07

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	231	ALA	CA
1	A	279	PRO	CA
1	A	283	ARG	CA

All (100) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	VAL	Mainchain
1	A	11	THR	Mainchain
1	A	111	ARG	Sidechain
1	A	114	ARG	Sidechain
1	A	12	ALA	Mainchain
1	A	133	ARG	Sidechain
1	A	15	PHE	Sidechain,Mainchain
1	A	152	TYR	Mainchain
1	A	158	GLN	Sidechain,Mainchain
1	A	165	ARG	Mainchain
1	A	169	LEU	Mainchain
1	A	173	ALA	Mainchain
1	A	183	TYR	Sidechain
1	A	19	ARG	Mainchain
1	A	191	GLN	Mainchain
1	A	192	THR	Mainchain
1	A	195	ASP	Mainchain
1	A	199	SER	Mainchain
1	A	201	THR	Mainchain
1	A	203	TYR	Sidechain
1	A	211	THR	Mainchain

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Mol	Chain	Res	Type	Group
1	A	217	PHE	Sidechain,Peptide,Mainchain
1	A	223	TYR	Mainchain
1	A	225	ASN	Mainchain
1	A	231	ALA	Mainchain
1	A	232	TYR	Mainchain
1	A	233	TYR	Peptide
1	A	235	PRO	Mainchain
1	A	238	PRO	Mainchain
1	A	240	LEU	Peptide,Mainchain
1	A	246	TYR	Sidechain
1	A	247	SER	Mainchain
1	A	250	TRP	Mainchain
1	A	251	ASP	Mainchain
1	A	253	GLY	Peptide
1	A	254	LEU	Mainchain
1	A	266	ILE	Mainchain
1	A	281	TYR	Mainchain
1	A	285	ASP	Mainchain
1	A	289	THR	Mainchain
1	A	308	HIS	Mainchain
1	A	315	VAL	Mainchain
1	A	322	THR	Mainchain
1	A	341	TYR	Mainchain
1	A	345	LEU	Mainchain
1	A	35	ASP	Mainchain
1	A	350	ASP	Mainchain
1	A	367	ARG	Sidechain
1	A	373	THR	Mainchain
1	A	385	PHE	Sidechain
1	A	389	TYR	Sidechain
1	A	391	THR	Mainchain
1	A	393	TYR	Sidechain
1	A	395	ALA	Mainchain
1	A	399	GLY	Mainchain
1	A	415	SER	Mainchain
1	A	426	THR	Mainchain
1	A	44	ASP	Mainchain
1	A	448	ASP	Peptide
1	A	465	GLU	Mainchain
1	A	467	THR	Mainchain
1	A	473	GLY	Peptide
1	A	478	THR	Mainchain

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Mol	Chain	Res	Type	Group
1	A	492	ASP	Mainchain
1	A	495	LEU	Mainchain
1	A	497	ARG	Sidechain
1	A	503	VAL	Mainchain
1	A	505	TYR	Mainchain
1	A	511	LEU	Mainchain
1	A	512	TYR	Peptide,Mainchain
1	A	519	THR	Mainchain
1	A	525	THR	Mainchain
1	A	526	ARG	Mainchain
1	A	527	TYR	Sidechain
1	A	533	SER	Mainchain
1	A	536	TYR	Mainchain
1	A	538	THR	Mainchain
1	A	543	GLY	Peptide
1	A	544	VAL	Mainchain
1	A	556	THR	Peptide,Mainchain
1	A	559	LEU	Mainchain
1	A	56	GLN	Mainchain
1	A	57	ASN	Mainchain
1	A	574	GLU	Sidechain
1	A	577	TYR	Sidechain
1	A	586	TYR	Mainchain
1	A	588	LEU	Mainchain
1	A	592	TYR	Mainchain
1	A	63	LEU	Mainchain
1	A	65	SER	Mainchain
1	A	66	ILE	Mainchain
1	A	77	LEU	Mainchain
1	A	99	PHE	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4630	0	4342	773	0
2	A	4	0	0	0	0
3	A	93	0	82	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	126	0	204	33	0
All	All	4853	0	4628	821	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 87.

All (821) 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:447:ASP:HB2	1:A:449:HIS:CG	1.36	1.55
1:A:285:ASP:HB3	1:A:286:SER:CA	1.29	1.52
1:A:527:TYR:CE1	1:A:540:LYS:HG3	1.47	1.49
1:A:293:MET:SD	1:A:293:MET:CE	2.02	1.45
1:A:279:PRO:CD	1:A:280:HIS:H	1.32	1.42
3:A:701:CNC:H302	3:A:701:CNC:C35	1.27	1.39
1:A:236:GLY:HA3	1:A:237:SER:CB	1.35	1.38
1:A:142:ALA:CB	1:A:151:ASN:O	1.72	1.37
1:A:236:GLY:CA	1:A:237:SER:HB2	1.44	1.34
1:A:447:ASP:CA	1:A:449:HIS:ND1	1.93	1.31
1:A:497:ARG:NH1	1:A:576:VAL:HG13	1.44	1.29
1:A:244:LYS:HE3	1:A:246:TYR:OH	1.33	1.27
1:A:447:ASP:CG	1:A:449:HIS:HB2	1.57	1.27
1:A:285:ASP:CB	1:A:286:SER:HA	1.57	1.27
1:A:18:PRO:O	1:A:21:THR:HG22	1.23	1.26
1:A:281:TYR:CD2	1:A:285:ASP:OD1	1.86	1.26
3:A:701:CNC:H353	3:A:701:CNC:C30	1.57	1.26
1:A:13:ASN:HD22	1:A:13:ASN:C	1.42	1.24
1:A:497:ARG:HH12	1:A:576:VAL:CG1	1.51	1.23
1:A:527:TYR:HE1	1:A:540:LYS:CG	1.51	1.21
1:A:404:PHE:HD2	1:A:404:PHE:O	1.19	1.21
1:A:6:ASP:OD2	1:A:20:SER:HB3	1.39	1.21
1:A:497:ARG:NH1	1:A:576:VAL:CG1	2.04	1.20
1:A:180:VAL:O	1:A:180:VAL:CG2	1.89	1.20
1:A:447:ASP:CB	1:A:449:HIS:CG	2.25	1.20
1:A:18:PRO:HD2	1:A:21:THR:HG21	1.23	1.19
1:A:244:LYS:NZ	1:A:246:TYR:CE1	2.11	1.19
1:A:279:PRO:HD3	1:A:280:HIS:N	1.36	1.18
1:A:286:SER:OG	1:A:288:ALA:HB3	1.44	1.17
1:A:293:MET:HE2	1:A:322:THR:HG22	1.19	1.17
1:A:330:GLU:N	1:A:333:TYR:HH	1.42	1.16
3:A:701:CNC:C35	3:A:701:CNC:C30	2.10	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:LYS:CE	1:A:246:TYR:CZ	2.28	1.15
1:A:448:ASP:N	1:A:449:HIS:ND1	1.95	1.15
1:A:404:PHE:O	1:A:404:PHE:CD2	2.01	1.12
1:A:244:LYS:HE3	1:A:246:TYR:CZ	1.84	1.11
1:A:437:ARG:HH21	1:A:460:ARG:CD	1.64	1.11
1:A:95:ASP:OD1	1:A:95:ASP:O	1.67	1.10
1:A:191:GLN:NE2	1:A:230:ASP:OD2	1.83	1.10
1:A:283:ARG:HA	1:A:284:TYR:HB2	1.14	1.10
3:A:701:CNC:C53	3:A:701:CNC:H482	1.80	1.10
1:A:447:ASP:C	1:A:449:HIS:ND1	2.10	1.10
1:A:286:SER:HA	1:A:287:SER:HB3	1.33	1.09
1:A:451:LEU:N	1:A:451:LEU:CD1	2.14	1.08
1:A:8:LEU:HD23	1:A:8:LEU:H	1.04	1.08
1:A:167:THR:O	1:A:168:LEU:HD23	1.52	1.08
1:A:142:ALA:HB2	1:A:152:TYR:HA	1.31	1.07
1:A:447:ASP:HA	1:A:449:HIS:ND1	1.61	1.07
1:A:397:ASN:ND2	1:A:400:GLN:HG3	1.67	1.07
1:A:87:LEU:HD13	1:A:92:GLY:O	1.53	1.07
1:A:437:ARG:HH21	1:A:460:ARG:HD3	1.02	1.07
1:A:447:ASP:HB2	1:A:449:HIS:ND1	1.68	1.07
1:A:285:ASP:N	1:A:286:SER:HB2	1.67	1.07
1:A:447:ASP:CB	1:A:449:HIS:ND1	2.16	1.07
1:A:511:LEU:HD23	1:A:512:TYR:CD2	1.89	1.06
1:A:397:ASN:ND2	1:A:400:GLN:CD	2.13	1.06
1:A:556:THR:OG1	1:A:557:SER:N	1.77	1.06
1:A:497:ARG:HH12	1:A:576:VAL:HG11	1.16	1.06
1:A:397:ASN:CG	1:A:400:GLN:HG3	1.81	1.05
1:A:283:ARG:HA	1:A:284:TYR:CB	1.83	1.05
1:A:191:GLN:O	1:A:193:ASP:HB3	1.54	1.05
1:A:397:ASN:ND2	1:A:400:GLN:CG	2.19	1.05
1:A:244:LYS:CE	1:A:246:TYR:OH	2.04	1.05
1:A:180:VAL:O	1:A:180:VAL:HG23	1.40	1.04
1:A:285:ASP:CB	1:A:286:SER:CB	2.35	1.04
1:A:85:LEU:O	1:A:86:ASN:CB	2.05	1.04
1:A:451:LEU:N	1:A:451:LEU:HD13	1.72	1.04
1:A:285:ASP:CB	1:A:286:SER:HB2	1.87	1.04
1:A:447:ASP:HA	1:A:449:HIS:CE1	1.92	1.03
1:A:285:ASP:N	1:A:286:SER:CB	2.20	1.03
1:A:85:LEU:O	1:A:86:ASN:HB2	1.23	1.03
1:A:511:LEU:HD23	1:A:512:TYR:CE2	1.93	1.03
1:A:281:TYR:CE2	1:A:285:ASP:OD1	2.13	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:GLY:HA3	1:A:346:GLN:NE2	1.74	1.02
3:A:701:CNC:H482	3:A:701:CNC:H533	1.42	1.01
1:A:142:ALA:HB1	1:A:151:ASN:O	0.85	1.01
1:A:543:GLY:C	1:A:544:VAL:HG13	1.81	1.01
1:A:573:TYR:O	1:A:581:THR:HG23	1.59	1.00
1:A:159:GLN:C	1:A:160:LEU:HD12	1.87	1.00
1:A:324:PRO:HD3	1:A:333:TYR:HE2	1.23	1.00
1:A:184:GLY:O	1:A:185:ASN:CG	2.03	1.00
1:A:7:THR:O	1:A:9:VAL:N	1.95	0.99
1:A:111:ARG:HG2	1:A:111:ARG:HH11	1.23	0.99
1:A:447:ASP:HB2	1:A:449:HIS:CB	1.91	0.99
1:A:530:ASP:OD1	1:A:532:SER:HB3	1.62	0.99
1:A:8:LEU:HD23	1:A:8:LEU:N	1.68	0.99
1:A:8:LEU:O	1:A:17:GLN:O	1.79	0.98
1:A:8:LEU:O	1:A:9:VAL:O	1.80	0.98
1:A:192:THR:O	1:A:192:THR:HG22	1.61	0.97
1:A:527:TYR:CE1	1:A:540:LYS:CG	2.35	0.97
3:A:701:CNC:C30	3:A:701:CNC:H352	1.95	0.97
3:A:701:CNC:H302	3:A:701:CNC:H352	1.46	0.97
1:A:324:PRO:HD3	1:A:333:TYR:CE2	2.00	0.97
1:A:226:ARG:NH1	1:A:244:LYS:HE2	1.79	0.96
1:A:191:GLN:O	1:A:193:ASP:CB	2.13	0.96
1:A:121:ASP:O	1:A:123:ILE:N	1.96	0.96
1:A:281:TYR:HD2	1:A:285:ASP:OD1	1.32	0.96
1:A:437:ARG:NH2	1:A:460:ARG:HD3	1.81	0.96
1:A:290:LEU:HD12	1:A:291:ASP:N	1.81	0.96
1:A:285:ASP:CA	1:A:286:SER:CB	2.44	0.96
1:A:13:ASN:C	1:A:13:ASN:ND2	2.16	0.95
1:A:323:THR:HG23	1:A:324:PRO:HD2	1.48	0.95
1:A:448:ASP:O	1:A:451:LEU:CD1	2.15	0.95
1:A:543:GLY:C	1:A:544:VAL:CG1	2.39	0.94
1:A:66:ILE:HD11	1:A:96:LEU:HD12	1.49	0.94
1:A:324:PRO:CD	1:A:333:TYR:HE2	1.82	0.93
1:A:279:PRO:O	1:A:280:HIS:CG	2.22	0.93
1:A:447:ASP:CB	1:A:449:HIS:HB2	1.99	0.93
1:A:191:GLN:O	1:A:193:ASP:N	2.02	0.93
1:A:10:VAL:HG23	1:A:10:VAL:O	1.66	0.93
1:A:135:GLU:H	1:A:157:GLN:HE22	1.14	0.93
1:A:9:VAL:O	1:A:9:VAL:HG12	1.69	0.92
1:A:283:ARG:HG2	1:A:284:TYR:CD2	2.04	0.92
1:A:167:THR:C	1:A:168:LEU:HD23	1.93	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:GLY:CA	1:A:346:GLN:NE2	2.33	0.92
1:A:285:ASP:HB3	1:A:286:SER:CB	1.99	0.92
1:A:594:PHE:CG	1:A:594:PHE:O	2.22	0.92
1:A:184:GLY:O	1:A:185:ASN:ND2	2.03	0.91
1:A:447:ASP:CB	1:A:449:HIS:CB	2.48	0.91
1:A:450:THR:C	1:A:451:LEU:HD13	1.95	0.91
1:A:263:SER:OG	1:A:302:ASN:ND2	2.03	0.91
1:A:402:TYR:CE2	1:A:408:PRO:HB3	2.06	0.91
1:A:111:ARG:HG2	1:A:111:ARG:NH1	1.82	0.90
1:A:304:VAL:HG23	1:A:305:ILE:N	1.85	0.90
1:A:447:ASP:CG	1:A:449:HIS:CB	2.43	0.90
1:A:239:LEU:O	1:A:240:LEU:HG	1.69	0.90
1:A:18:PRO:O	1:A:21:THR:CG2	2.16	0.90
1:A:330:GLU:C	1:A:333:TYR:HE1	1.80	0.89
1:A:50:PRO:HB2	1:A:111:ARG:HE	1.36	0.89
1:A:13:ASN:ND2	1:A:15:PHE:H	1.70	0.89
1:A:497:ARG:HH11	1:A:576:VAL:HG13	1.37	0.89
1:A:593:THR:O	1:A:594:PHE:HB3	1.73	0.89
1:A:192:THR:O	1:A:192:THR:CG2	2.21	0.88
1:A:407:ASN:C	1:A:407:ASN:HD22	1.82	0.88
1:A:104:VAL:C	1:A:105:GLN:HE21	1.81	0.88
1:A:285:ASP:HB3	1:A:287:SER:HB3	1.56	0.88
1:A:448:ASP:O	1:A:451:LEU:HD11	1.74	0.88
1:A:47:ARG:HG2	1:A:48:ARG:N	1.88	0.88
3:A:701:CNC:C53	3:A:701:CNC:C48	2.49	0.88
1:A:244:LYS:CE	1:A:246:TYR:CE1	2.57	0.87
1:A:397:ASN:H	1:A:400:GLN:HE21	1.20	0.87
1:A:345:LEU:O	1:A:346:GLN:HG2	1.74	0.87
1:A:285:ASP:H	1:A:286:SER:HB3	1.38	0.87
1:A:86:ASN:HD21	1:A:295:GLN:HB3	1.40	0.87
1:A:473:GLY:H	1:A:475:LEU:HB2	1.39	0.87
1:A:69:ARG:HB3	1:A:436:TYR:OH	1.74	0.86
3:A:701:CNC:H533	3:A:701:CNC:C48	2.05	0.86
1:A:72:ASN:ND2	1:A:73:ALA:H	1.73	0.86
3:A:701:CNC:H471	3:A:701:CNC:H492	1.54	0.86
1:A:543:GLY:O	1:A:544:VAL:HG12	1.74	0.86
1:A:90:VAL:HG23	1:A:90:VAL:O	1.74	0.85
1:A:240:LEU:HD22	1:A:277:TYR:HA	1.58	0.85
1:A:397:ASN:HD21	1:A:400:GLN:CG	1.87	0.85
1:A:447:ASP:HB2	1:A:449:HIS:CD2	2.11	0.85
1:A:293:MET:CE	1:A:322:THR:HG22	2.06	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:LEU:HD11	1:A:352:THR:CG2	2.08	0.84
3:A:701:CNC:H482	3:A:701:CNC:H532	1.58	0.84
1:A:191:GLN:O	1:A:192:THR:C	2.19	0.84
1:A:266:ILE:CG2	1:A:267:THR:N	2.41	0.83
1:A:516:TRP:CZ3	1:A:551:VAL:CG1	2.61	0.83
1:A:286:SER:OG	1:A:288:ALA:CB	2.25	0.83
1:A:111:ARG:NH2	1:A:465:GLU:OE2	2.09	0.83
1:A:135:GLU:H	1:A:157:GLN:NE2	1.77	0.83
1:A:244:LYS:NZ	1:A:246:TYR:CZ	2.46	0.83
1:A:285:ASP:H	1:A:286:SER:CB	1.91	0.83
1:A:8:LEU:N	1:A:8:LEU:CD2	2.39	0.82
1:A:18:PRO:HD2	1:A:21:THR:CG2	2.06	0.82
1:A:285:ASP:HB2	1:A:286:SER:HB2	1.61	0.82
1:A:293:MET:HE3	1:A:293:MET:HB2	1.61	0.82
1:A:169:LEU:HD12	1:A:169:LEU:C	2.04	0.82
1:A:334:ASP:OD1	1:A:334:ASP:C	2.21	0.82
1:A:284:TYR:CD1	1:A:284:TYR:N	2.40	0.82
1:A:285:ASP:CA	1:A:286:SER:HB2	2.05	0.82
1:A:134:ASP:C	1:A:134:ASP:OD1	2.22	0.82
1:A:293:MET:CE	1:A:293:MET:HB2	2.10	0.82
3:A:701:CNC:H471	3:A:701:CNC:C49	2.08	0.82
1:A:286:SER:HA	1:A:287:SER:CB	2.10	0.81
1:A:165:ARG:NH2	1:A:207:GLU:CD	2.38	0.81
1:A:279:PRO:CD	1:A:280:HIS:N	1.98	0.81
1:A:90:VAL:N	3:A:701:CNC:N45	2.28	0.81
1:A:244:LYS:HE3	1:A:246:TYR:CE1	2.16	0.81
1:A:543:GLY:O	1:A:544:VAL:CG1	2.27	0.81
1:A:426:THR:HG23	1:A:431:TRP:HE1	1.45	0.81
1:A:7:THR:O	1:A:8:LEU:C	2.17	0.81
1:A:534:TYR:HA	1:A:535:PRO:C	2.06	0.80
1:A:506:GLN:NE2	1:A:519:THR:HB	1.95	0.80
1:A:285:ASP:CB	1:A:286:SER:CA	2.11	0.80
1:A:180:VAL:O	1:A:180:VAL:HG22	1.82	0.80
1:A:511:LEU:CD2	1:A:512:TYR:CE2	2.64	0.80
1:A:311:ILE:CD1	4:A:803:C8E:H12	2.12	0.80
1:A:311:ILE:HD11	4:A:803:C8E:H12	1.64	0.79
1:A:404:PHE:CD2	1:A:404:PHE:C	2.59	0.79
1:A:448:ASP:OD1	1:A:449:HIS:N	2.13	0.79
1:A:266:ILE:HG22	1:A:267:THR:N	1.96	0.79
1:A:279:PRO:HD3	1:A:280:HIS:H	0.64	0.79
1:A:293:MET:HG3	1:A:294:LYS:N	1.98	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:GLU:C	1:A:333:TYR:CE1	2.60	0.79
1:A:56:GLN:C	1:A:58:GLY:H	1.88	0.79
1:A:411:ASP:H	1:A:455:ASN:HD21	1.30	0.79
1:A:185:ASN:O	1:A:231:ALA:C	2.25	0.78
1:A:309:GLY:N	1:A:346:GLN:NE2	2.32	0.78
1:A:573:TYR:O	1:A:581:THR:CG2	2.30	0.78
1:A:138:THR:HG22	1:A:156:THR:OG1	1.83	0.78
1:A:330:GLU:N	1:A:333:TYR:OH	2.16	0.78
1:A:159:GLN:O	1:A:160:LEU:HD12	1.82	0.78
1:A:367:ARG:HH21	4:A:800:C8E:H192	1.48	0.78
3:A:701:CNC:H533	3:A:701:CNC:H521	1.47	0.78
1:A:488:ASN:CG	1:A:491:THR:HG22	2.08	0.77
1:A:23:LEU:HD11	1:A:352:THR:HG22	1.66	0.77
1:A:160:LEU:HD12	1:A:160:LEU:N	1.98	0.77
1:A:142:ALA:HB1	1:A:151:ASN:C	1.98	0.77
1:A:323:THR:HG23	1:A:324:PRO:CD	2.13	0.77
1:A:190:ALA:C	1:A:191:GLN:HG2	2.07	0.77
1:A:279:PRO:CG	1:A:280:HIS:N	2.46	0.77
1:A:13:ASN:HD22	1:A:14:ARG:N	1.83	0.77
1:A:188:THR:O	1:A:189:GLN:HB2	1.84	0.77
1:A:184:GLY:C	1:A:185:ASN:CG	2.51	0.76
1:A:244:LYS:HE3	1:A:246:TYR:HH	1.51	0.76
1:A:279:PRO:CD	1:A:282:GLY:H	1.98	0.76
1:A:293:MET:HE2	1:A:322:THR:CG2	2.08	0.76
1:A:398:LEU:HD23	1:A:398:LEU:N	1.95	0.76
1:A:162:ASP:O	1:A:164:THR:N	2.19	0.76
1:A:210:PHE:CD1	1:A:210:PHE:N	2.54	0.76
1:A:287:SER:O	1:A:288:ALA:HB2	1.84	0.76
1:A:397:ASN:H	1:A:400:GLN:NE2	1.83	0.76
1:A:281:TYR:CD2	1:A:281:TYR:O	2.39	0.76
1:A:309:GLY:HA3	1:A:346:GLN:HE21	1.48	0.76
1:A:362:ASN:ND2	1:A:365:PHE:CD2	2.54	0.76
3:A:701:CNC:C3	3:A:701:CNC:O28	2.33	0.75
3:A:701:CNC:H601	3:A:701:CNC:H252	1.68	0.75
1:A:290:LEU:HD12	1:A:290:LEU:C	2.07	0.75
4:A:802:C8E:H13	4:A:802:C8E:H52	1.69	0.75
1:A:451:LEU:N	1:A:451:LEU:HD12	2.01	0.75
1:A:66:ILE:HD11	1:A:96:LEU:CD1	2.16	0.75
1:A:105:GLN:HA	1:A:105:GLN:NE2	2.00	0.75
1:A:181:VAL:O	1:A:182:ALA:HB3	1.86	0.75
1:A:279:PRO:CG	1:A:280:HIS:H	2.00	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:VAL:HG12	1:A:16:GLU:HA	1.69	0.74
1:A:18:PRO:C	1:A:21:THR:HG22	2.12	0.74
1:A:142:ALA:CB	1:A:152:TYR:HA	2.16	0.74
1:A:513:ASP:HB2	1:A:553:TYR:CE1	2.23	0.74
1:A:486:ALA:O	1:A:495:LEU:HG	1.87	0.74
1:A:491:THR:HG23	1:A:493:THR:HG23	1.68	0.74
1:A:283:ARG:CA	1:A:284:TYR:HB2	2.08	0.74
1:A:114:ARG:HA	1:A:372:GLN:HE22	1.53	0.73
1:A:31:ARG:O	1:A:32:GLN:C	2.30	0.73
1:A:95:ASP:OD1	1:A:95:ASP:C	2.32	0.73
1:A:55:THR:HA	1:A:575:THR:OG1	1.89	0.73
1:A:169:LEU:C	1:A:169:LEU:CD1	2.62	0.73
1:A:324:PRO:HB3	1:A:333:TYR:OH	1.88	0.73
1:A:528:ASP:CG	1:A:529:LYS:H	1.96	0.73
1:A:92:GLY:O	1:A:93:SER:C	2.31	0.72
1:A:99:PHE:C	1:A:99:PHE:CD2	2.65	0.72
1:A:293:MET:CG	1:A:294:LYS:N	2.52	0.72
1:A:245:LEU:HD22	1:A:246:TYR:N	2.04	0.72
1:A:393:TYR:CD1	1:A:393:TYR:C	2.66	0.72
1:A:426:THR:CG2	1:A:431:TRP:HE1	2.02	0.72
1:A:451:LEU:CD1	1:A:451:LEU:H	2.03	0.72
1:A:450:THR:CA	1:A:451:LEU:HD13	2.20	0.71
1:A:68:ILE:O	1:A:69:ARG:C	2.33	0.71
1:A:579:TYR:CD1	1:A:579:TYR:N	2.56	0.71
1:A:13:ASN:O	1:A:14:ARG:HB2	1.89	0.71
1:A:285:ASP:CB	1:A:287:SER:HB3	2.20	0.71
1:A:116:ALA:HB1	1:A:357:ALA:HA	1.73	0.71
1:A:240:LEU:N	1:A:278:ASP:HB3	2.05	0.71
1:A:467:THR:HG22	1:A:480:SER:HB3	1.71	0.71
1:A:479:VAL:HG13	1:A:479:VAL:O	1.91	0.71
1:A:231:ALA:O	1:A:232:TYR:HB2	1.88	0.70
1:A:309:GLY:HA3	1:A:346:GLN:CD	2.15	0.70
1:A:556:THR:OG1	1:A:558:HIS:N	2.24	0.70
1:A:397:ASN:OD1	1:A:400:GLN:HG3	1.92	0.70
1:A:13:ASN:ND2	1:A:13:ASN:O	2.24	0.70
1:A:188:THR:O	1:A:189:GLN:CB	2.38	0.70
1:A:244:LYS:NZ	1:A:246:TYR:CD1	2.53	0.70
1:A:210:PHE:HD1	1:A:210:PHE:H	1.36	0.70
1:A:91:SER:O	1:A:93:SER:N	2.25	0.70
1:A:160:LEU:HD13	1:A:166:VAL:HG23	1.73	0.69
1:A:407:ASN:O	1:A:410:LEU:HG	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LEU:N	1:A:160:LEU:CD1	2.53	0.69
1:A:72:ASN:CG	1:A:73:ALA:H	2.00	0.69
1:A:245:LEU:CD2	1:A:246:TYR:N	2.55	0.69
1:A:15:PHE:CD1	1:A:303:ASN:HB2	2.28	0.69
1:A:156:THR:O	1:A:156:THR:HG23	1.92	0.69
1:A:279:PRO:HD2	1:A:282:GLY:CA	2.23	0.69
1:A:448:ASP:OD1	1:A:449:HIS:CG	2.46	0.69
1:A:516:TRP:CE3	1:A:551:VAL:HG12	2.27	0.69
1:A:448:ASP:O	1:A:449:HIS:C	2.36	0.69
1:A:217:PHE:CE2	1:A:253:GLY:HA3	2.29	0.68
1:A:286:SER:HG	1:A:288:ALA:HB3	1.56	0.68
1:A:443:LEU:HB2	1:A:457:GLY:O	1.94	0.68
1:A:565:ILE:HG21	1:A:568:LEU:CD1	2.22	0.68
1:A:321:THR:HA	1:A:333:TYR:O	1.93	0.68
1:A:273:LYS:HG2	1:A:292:GLU:HG3	1.75	0.68
1:A:19:ARG:NH2	1:A:26:THR:O	2.27	0.68
1:A:479:VAL:O	1:A:479:VAL:CG1	2.40	0.68
1:A:105:GLN:NE2	1:A:105:GLN:CA	2.57	0.68
1:A:157:GLN:C	1:A:158:GLN:HG2	2.16	0.68
1:A:90:VAL:O	1:A:90:VAL:CG2	2.42	0.68
1:A:198:LEU:HD11	1:A:200:LYS:HE2	1.76	0.68
1:A:178:TYR:C	1:A:194:ASN:HA	2.20	0.67
1:A:279:PRO:HD2	1:A:282:GLY:H	1.59	0.67
1:A:309:GLY:CA	1:A:345:LEU:O	2.43	0.67
1:A:111:ARG:NH1	1:A:111:ARG:CG	2.47	0.67
1:A:373:THR:HG21	4:A:803:C8E:H131	1.76	0.67
1:A:24:ALA:O	1:A:26:THR:HG23	1.93	0.67
1:A:240:LEU:CD2	1:A:277:TYR:HA	2.24	0.67
1:A:8:LEU:H	1:A:8:LEU:CD2	1.93	0.67
1:A:407:ASN:C	1:A:407:ASN:ND2	2.41	0.67
1:A:446:TYR:HB2	1:A:453:TYR:CE1	2.30	0.66
1:A:13:ASN:HD21	1:A:15:PHE:HB2	1.61	0.66
1:A:285:ASP:N	1:A:286:SER:HB3	2.00	0.66
1:A:402:TYR:HE2	1:A:408:PRO:HB3	1.57	0.66
1:A:135:GLU:N	1:A:157:GLN:HE22	1.90	0.66
1:A:284:TYR:N	1:A:284:TYR:HD1	1.90	0.66
1:A:205:ALA:O	1:A:206:LEU:HD12	1.95	0.66
1:A:306:VAL:O	1:A:346:GLN:NE2	2.29	0.66
1:A:287:SER:O	1:A:288:ALA:CB	2.44	0.66
1:A:529:LYS:NZ	1:A:538:THR:CG2	2.59	0.66
1:A:210:PHE:C	1:A:211:THR:CG2	2.69	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:TYR:HE1	1:A:294:LYS:HG2	1.61	0.66
1:A:337:ASN:ND2	1:A:362:ASN:HB2	2.11	0.66
1:A:293:MET:CE	1:A:293:MET:CB	2.74	0.65
3:A:701:CNC:C49	3:A:701:CNC:C47	2.74	0.65
1:A:157:GLN:HA	1:A:166:VAL:O	1.96	0.65
1:A:63:LEU:H	3:A:701:CNC:H332	1.41	0.65
1:A:160:LEU:HD13	1:A:166:VAL:CG2	2.26	0.65
1:A:337:ASN:HD21	1:A:362:ASN:HB2	1.62	0.65
3:A:701:CNC:C4B	3:A:701:CNC:H412	2.27	0.65
1:A:397:ASN:HD21	1:A:400:GLN:HG3	1.50	0.65
1:A:448:ASP:H	1:A:449:HIS:CE1	2.14	0.65
1:A:277:TYR:CE1	1:A:279:PRO:HG2	2.31	0.65
1:A:293:MET:CE	1:A:293:MET:CG	2.75	0.65
1:A:565:ILE:HG21	1:A:568:LEU:HD12	1.78	0.65
1:A:13:ASN:HD21	1:A:15:PHE:H	1.45	0.64
1:A:62:GLN:O	1:A:63:LEU:C	2.37	0.64
4:A:803:C8E:C10	4:A:803:C8E:H172	2.28	0.64
3:A:701:CNC:H302	3:A:701:CNC:H353	0.64	0.64
1:A:279:PRO:HD2	1:A:282:GLY:N	2.12	0.64
1:A:367:ARG:NH2	4:A:800:C8E:H192	2.13	0.64
1:A:594:PHE:O	1:A:594:PHE:CD2	2.51	0.64
1:A:63:LEU:HD22	1:A:64:SER:N	2.13	0.63
1:A:59:GLY:O	1:A:62:GLN:HG2	1.98	0.63
1:A:279:PRO:HD3	1:A:282:GLY:H	1.62	0.63
1:A:411:ASP:N	1:A:455:ASN:HD21	1.96	0.63
1:A:14:ARG:HD2	1:A:264:GLN:NE2	2.13	0.63
1:A:243:ARG:HG2	1:A:244:LYS:N	2.14	0.63
1:A:63:LEU:HD22	1:A:95:ASP:HB2	1.81	0.63
1:A:109:TYR:CZ	1:A:111:ARG:HD3	2.33	0.63
1:A:244:LYS:HE2	1:A:246:TYR:CZ	2.30	0.63
1:A:279:PRO:HD2	1:A:282:GLY:HA3	1.80	0.63
1:A:506:GLN:CD	1:A:519:THR:HB	2.24	0.63
1:A:63:LEU:CD2	1:A:95:ASP:HB2	2.28	0.63
1:A:90:VAL:N	3:A:701:CNC:H452	1.97	0.63
1:A:529:LYS:HZ1	1:A:538:THR:CG2	2.10	0.63
1:A:63:LEU:HD23	1:A:95:ASP:OD2	1.98	0.63
1:A:266:ILE:CG2	1:A:267:THR:H	2.10	0.63
1:A:451:LEU:HD12	1:A:451:LEU:H	1.62	0.63
1:A:105:GLN:HE21	1:A:105:GLN:N	1.96	0.62
1:A:240:LEU:HD23	1:A:278:ASP:H	1.64	0.62
1:A:309:GLY:HA3	1:A:345:LEU:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:LYS:NZ	1:A:538:THR:HG23	2.14	0.62
1:A:379:PHE:CD1	1:A:380:ILE:HG13	2.34	0.62
1:A:153:ASP:C	1:A:153:ASP:OD1	2.42	0.62
1:A:191:GLN:O	1:A:193:ASP:CA	2.47	0.62
1:A:472:THR:OG1	1:A:473:GLY:N	2.32	0.62
1:A:526:ARG:HD3	1:A:541:MET:HE3	1.80	0.62
1:A:531:TYR:C	1:A:533:SER:H	2.07	0.62
1:A:358:ARG:NH2	1:A:360:ASP:OD2	2.29	0.62
3:A:701:CNC:H551	3:A:701:CNC:C61	2.30	0.62
1:A:256:TYR:C	1:A:256:TYR:CD2	2.78	0.61
1:A:13:ASN:O	1:A:14:ARG:CB	2.47	0.61
1:A:397:ASN:C	1:A:401:LEU:HD12	2.25	0.61
1:A:56:GLN:HG3	1:A:64:SER:HB3	1.83	0.61
3:A:701:CNC:H4B	3:A:701:CNC:C6	2.29	0.61
1:A:341:TYR:HB2	1:A:357:ALA:O	2.00	0.61
1:A:156:THR:O	1:A:156:THR:CG2	2.49	0.61
1:A:138:THR:HG22	1:A:156:THR:HG1	1.63	0.61
1:A:266:ILE:HG23	1:A:267:THR:H	1.65	0.61
1:A:407:ASN:HD21	1:A:409:ASN:HB2	1.65	0.61
1:A:72:ASN:CG	1:A:73:ALA:N	2.58	0.60
1:A:364:GLN:NE2	1:A:410:LEU:O	2.35	0.60
1:A:15:PHE:CE1	1:A:303:ASN:HB2	2.37	0.60
1:A:525:THR:HG23	1:A:525:THR:O	2.00	0.60
1:A:179:ASP:OD1	1:A:191:GLN:NE2	2.33	0.60
1:A:446:TYR:HB2	1:A:453:TYR:CD1	2.36	0.60
1:A:543:GLY:CA	1:A:544:VAL:HG13	2.31	0.60
1:A:19:ARG:C	1:A:21:THR:N	2.58	0.60
1:A:135:GLU:OE1	1:A:135:GLU:HA	2.01	0.60
1:A:393:TYR:HD1	1:A:394:LYS:N	2.00	0.60
1:A:426:THR:HG23	1:A:431:TRP:NE1	2.16	0.60
1:A:94:ALA:O	1:A:95:ASP:CB	2.45	0.59
1:A:163:LYS:O	1:A:208:HIS:HA	2.02	0.59
1:A:239:LEU:O	1:A:240:LEU:CG	2.48	0.59
1:A:405:TYR:CG	1:A:446:TYR:HE2	2.20	0.59
1:A:283:ARG:HA	1:A:284:TYR:CG	2.37	0.59
1:A:94:ALA:O	1:A:95:ASP:HB3	2.02	0.59
1:A:140:ILE:HG22	1:A:141:SER:N	2.16	0.59
1:A:516:TRP:CZ3	1:A:551:VAL:HG12	2.37	0.59
1:A:105:GLN:HE21	1:A:105:GLN:CA	2.15	0.59
1:A:209:ASN:N	1:A:209:ASN:ND2	2.50	0.59
1:A:285:ASP:HB3	1:A:286:SER:HA	0.60	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:THR:CG2	1:A:108:GLU:OE1	2.50	0.59
1:A:86:ASN:ND2	1:A:295:GLN:HB3	2.12	0.59
1:A:311:ILE:HD11	4:A:803:C8E:C1	2.32	0.59
1:A:491:THR:HG23	1:A:493:THR:CG2	2.32	0.59
1:A:18:PRO:O	1:A:21:THR:N	2.27	0.59
1:A:393:TYR:CD1	1:A:394:LYS:N	2.70	0.59
1:A:14:ARG:NH1	1:A:82:GLY:O	2.36	0.58
1:A:334:ASP:OD1	1:A:335:GLN:N	2.35	0.58
1:A:8:LEU:O	1:A:9:VAL:C	2.37	0.58
1:A:240:LEU:H	1:A:278:ASP:HB3	1.67	0.58
1:A:555:VAL:O	1:A:555:VAL:HG13	2.03	0.58
1:A:234:SER:HB2	1:A:237:SER:CB	2.33	0.58
1:A:271:HIS:HA	1:A:293:MET:O	2.04	0.58
1:A:13:ASN:HD22	1:A:15:PHE:H	1.49	0.58
1:A:162:ASP:C	1:A:164:THR:H	2.11	0.58
1:A:446:TYR:HA	1:A:453:TYR:HA	1.85	0.58
1:A:572:ASP:O	1:A:573:TYR:HB3	2.03	0.57
4:A:802:C8E:H11	4:A:802:C8E:H172	1.86	0.57
4:A:803:C8E:H172	4:A:803:C8E:C11	2.35	0.57
1:A:191:GLN:C	1:A:193:ASP:N	2.58	0.57
1:A:17:GLN:HG3	1:A:21:THR:CG2	2.35	0.57
1:A:229:TYR:CZ	1:A:240:LEU:O	2.57	0.57
1:A:72:ASN:ND2	1:A:73:ALA:N	2.48	0.57
1:A:181:VAL:O	1:A:191:GLN:OE1	2.23	0.57
4:A:803:C8E:H172	4:A:803:C8E:H112	1.85	0.57
1:A:142:ALA:HB2	1:A:152:TYR:CA	2.21	0.57
1:A:240:LEU:H	1:A:278:ASP:CB	2.18	0.57
1:A:44:ASP:O	1:A:47:ARG:HD3	2.05	0.57
1:A:240:LEU:HD23	1:A:278:ASP:N	2.17	0.57
1:A:422:PHE:CG	4:A:801:C8E:H11	2.39	0.57
1:A:6:ASP:OD2	1:A:20:SER:CB	2.33	0.56
1:A:191:GLN:CD	1:A:230:ASP:OD2	2.47	0.56
1:A:63:LEU:HD22	1:A:64:SER:H	1.70	0.56
1:A:168:LEU:HD23	1:A:168:LEU:N	2.16	0.56
1:A:234:SER:HB2	1:A:237:SER:HB3	1.87	0.56
1:A:255:ARG:NH1	1:A:264:GLN:OE1	2.39	0.56
1:A:362:ASN:ND2	1:A:365:PHE:H	2.03	0.56
1:A:491:THR:CG2	1:A:493:THR:HG23	2.35	0.56
1:A:56:GLN:C	1:A:58:GLY:N	2.58	0.56
1:A:95:ASP:C	1:A:97:SER:H	2.13	0.56
1:A:499:ALA:O	1:A:500:LYS:C	2.48	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ARG:HB3	1:A:436:TYR:CZ	2.41	0.56
1:A:488:ASN:OD1	1:A:491:THR:HG22	2.06	0.56
1:A:529:LYS:HZ1	1:A:538:THR:HG23	1.69	0.56
1:A:534:TYR:CD1	1:A:535:PRO:N	2.74	0.56
1:A:496:LEU:O	1:A:497:ARG:HB2	2.04	0.56
1:A:533:SER:O	1:A:533:SER:OG	2.17	0.56
1:A:23:LEU:HD11	1:A:352:THR:HG21	1.86	0.56
1:A:552:ALA:HB2	1:A:562:ARG:HD3	1.88	0.56
1:A:24:ALA:O	1:A:26:THR:CG2	2.53	0.55
1:A:244:LYS:HE2	1:A:246:TYR:OH	2.02	0.55
1:A:470:PHE:N	1:A:470:PHE:CD2	2.74	0.55
1:A:267:THR:O	1:A:267:THR:HG22	2.05	0.55
1:A:397:ASN:HD22	1:A:400:GLN:CD	2.12	0.55
1:A:112:GLY:O	1:A:125:GLY:HA2	2.06	0.55
1:A:239:LEU:O	1:A:240:LEU:CB	2.54	0.55
1:A:281:TYR:O	1:A:281:TYR:CG	2.59	0.55
1:A:579:TYR:N	1:A:579:TYR:HD1	2.04	0.55
1:A:209:ASN:ND2	1:A:209:ASN:H	2.04	0.55
1:A:567:ASN:C	1:A:567:ASN:HD22	2.15	0.55
1:A:25:PRO:HG3	1:A:432:ARG:NH2	2.21	0.55
1:A:37:TRP:O	1:A:38:GLN:HB2	2.06	0.55
1:A:87:LEU:HD23	1:A:87:LEU:H	1.72	0.55
1:A:527:TYR:CE1	1:A:540:LYS:CB	2.90	0.55
1:A:188:THR:OG1	1:A:233:TYR:O	2.25	0.55
1:A:163:LYS:HB2	1:A:209:ASN:O	2.07	0.55
1:A:569:PHE:CD1	1:A:569:PHE:N	2.74	0.55
1:A:63:LEU:CD2	1:A:95:ASP:CB	2.85	0.55
1:A:265:LEU:HD23	1:A:300:TRP:HB2	1.89	0.55
1:A:332:GLY:O	1:A:333:TYR:CG	2.59	0.55
1:A:379:PHE:O	1:A:380:ILE:HG12	2.07	0.55
3:A:701:CNC:H562	3:A:701:CNC:N62	2.21	0.55
1:A:82:GLY:C	1:A:83:VAL:HG23	2.33	0.54
1:A:315:VAL:HG12	1:A:316:ASP:H	1.71	0.54
1:A:433:ILE:HG12	1:A:434:SER:H	1.72	0.54
1:A:146:SER:O	1:A:147:ASN:CG	2.50	0.54
1:A:297:THR:C	1:A:298:VAL:HG23	2.31	0.54
1:A:313:ALA:HB2	1:A:342:LEU:HD12	1.89	0.54
1:A:283:ARG:C	1:A:284:TYR:CD1	2.85	0.54
1:A:185:ASN:ND2	1:A:579:TYR:OH	2.40	0.54
1:A:210:PHE:O	1:A:211:THR:HG22	2.06	0.54
1:A:309:GLY:CA	1:A:346:GLN:HE21	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:TYR:HB3	1:A:451:LEU:O	2.07	0.54
1:A:31:ARG:O	1:A:34:ILE:N	2.41	0.54
1:A:77:LEU:HD21	1:A:79:LEU:HD21	1.89	0.54
1:A:323:THR:CG2	1:A:324:PRO:N	2.67	0.54
1:A:113:PRO:HD3	1:A:417:GLN:OE1	2.08	0.54
1:A:487:ARG:NH1	1:A:494:PRO:HD3	2.22	0.54
1:A:488:ASN:CG	1:A:491:THR:CG2	2.80	0.54
1:A:121:ASP:C	1:A:123:ILE:N	2.64	0.54
1:A:304:VAL:O	1:A:304:VAL:HG22	2.06	0.54
1:A:516:TRP:CE3	1:A:551:VAL:CG1	2.90	0.54
1:A:179:ASP:OD2	1:A:193:ASP:N	2.28	0.53
1:A:283:ARG:C	1:A:284:TYR:CG	2.85	0.53
1:A:30:THR:O	1:A:33:ASP:HB2	2.09	0.53
1:A:362:ASN:HD22	1:A:365:PHE:H	1.55	0.53
1:A:183:TYR:O	1:A:183:TYR:CD2	2.61	0.53
1:A:231:ALA:O	1:A:232:TYR:CB	2.52	0.53
1:A:91:SER:O	1:A:92:GLY:C	2.51	0.53
1:A:140:ILE:C	1:A:141:SER:OG	2.49	0.53
1:A:210:PHE:C	1:A:211:THR:HG23	2.34	0.53
1:A:165:ARG:HH21	1:A:207:GLU:CD	2.16	0.53
1:A:417:GLN:HG2	1:A:438:ASN:HB2	1.89	0.53
1:A:488:ASN:HB3	1:A:491:THR:CG2	2.38	0.53
1:A:25:PRO:HG3	1:A:432:ARG:HH21	1.73	0.53
1:A:208:HIS:C	1:A:208:HIS:ND1	2.66	0.53
1:A:232:TYR:CD2	1:A:233:TYR:N	2.75	0.53
1:A:531:TYR:C	1:A:533:SER:N	2.65	0.53
1:A:167:THR:HB	1:A:205:ALA:HB3	1.91	0.53
1:A:315:VAL:HG12	1:A:316:ASP:N	2.23	0.53
1:A:437:ARG:NH2	1:A:460:ARG:CD	2.50	0.53
1:A:55:THR:CA	1:A:575:THR:OG1	2.57	0.52
1:A:370:THR:H	4:A:800:C8E:H81	1.74	0.52
1:A:239:LEU:C	1:A:240:LEU:HG	2.35	0.52
1:A:331:ASP:N	1:A:333:TYR:HE1	2.07	0.52
1:A:419:GLU:HA	1:A:435:GLY:O	2.09	0.52
1:A:448:ASP:OD1	1:A:449:HIS:ND1	2.42	0.52
1:A:593:THR:HG22	1:A:594:PHE:N	2.24	0.52
1:A:201:THR:O	1:A:202:LEU:HD12	2.09	0.52
1:A:236:GLY:CA	1:A:237:SER:CB	2.29	0.52
1:A:86:ASN:HD21	1:A:295:GLN:CB	2.18	0.52
1:A:383:TYR:CE2	4:A:801:C8E:H42	2.44	0.52
1:A:229:TYR:CD1	3:A:701:CNC:H311	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ASP:H	1:A:455:ASN:ND2	2.05	0.52
1:A:31:ARG:NH1	1:A:35:ASP:OD1	2.42	0.52
1:A:269:TYR:CE1	1:A:294:LYS:HG2	2.44	0.52
1:A:283:ARG:HG2	1:A:284:TYR:CG	2.43	0.52
1:A:472:THR:OG1	1:A:475:LEU:HB2	2.10	0.52
1:A:8:LEU:O	1:A:9:VAL:CB	2.51	0.52
1:A:180:VAL:C	1:A:181:VAL:HG23	2.35	0.52
1:A:528:ASP:CG	1:A:529:LYS:N	2.65	0.52
1:A:560:THR:HG22	1:A:561:VAL:N	2.25	0.52
1:A:234:SER:HB2	1:A:237:SER:OG	2.09	0.52
1:A:534:TYR:CD1	1:A:534:TYR:C	2.88	0.52
1:A:54:ILE:HG22	1:A:55:THR:N	2.24	0.52
1:A:160:LEU:CD1	1:A:166:VAL:CG2	2.88	0.52
1:A:179:ASP:HA	1:A:193:ASP:O	2.09	0.52
1:A:226:ARG:CZ	1:A:244:LYS:HD2	2.40	0.52
1:A:530:ASP:OD1	1:A:532:SER:CB	2.49	0.52
1:A:437:ARG:HH21	1:A:460:ARG:CG	2.20	0.52
1:A:279:PRO:O	1:A:280:HIS:ND1	2.43	0.51
1:A:391:THR:HG22	1:A:391:THR:O	2.09	0.51
1:A:69:ARG:HD3	1:A:436:TYR:CZ	2.44	0.51
1:A:217:PHE:CE2	1:A:253:GLY:CA	2.93	0.51
4:A:802:C8E:H161	4:A:802:C8E:H12	1.91	0.51
1:A:529:LYS:NZ	1:A:538:THR:HG22	2.25	0.51
1:A:286:SER:OG	1:A:287:SER:C	2.53	0.51
1:A:488:ASN:CB	1:A:491:THR:HG22	2.41	0.51
1:A:245:LEU:CD2	1:A:245:LEU:C	2.82	0.51
1:A:304:VAL:CG2	1:A:305:ILE:N	2.50	0.51
1:A:488:ASN:O	1:A:492:ASP:N	2.42	0.51
1:A:497:ARG:HH11	1:A:576:VAL:HG22	1.76	0.51
1:A:516:TRP:CZ3	1:A:551:VAL:HG13	2.45	0.51
1:A:17:GLN:HG3	1:A:21:THR:HG23	1.93	0.51
1:A:182:ALA:O	1:A:183:TYR:HB3	2.10	0.51
1:A:185:ASN:CG	1:A:579:TYR:OH	2.54	0.51
1:A:139:GLU:N	1:A:155:SER:O	2.39	0.51
1:A:385:PHE:C	1:A:385:PHE:CD2	2.88	0.51
1:A:574:GLU:HA	1:A:581:THR:CG2	2.41	0.51
1:A:77:LEU:HG	1:A:77:LEU:O	2.11	0.50
1:A:226:ARG:HH11	1:A:244:LYS:HE2	1.70	0.50
1:A:473:GLY:C	1:A:475:LEU:H	2.19	0.50
1:A:565:ILE:HG21	1:A:568:LEU:HD13	1.92	0.50
1:A:245:LEU:HD23	1:A:246:TYR:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ASN:HD22	1:A:408:PRO:N	2.09	0.50
1:A:447:ASP:OD2	1:A:450:THR:HG23	2.12	0.50
1:A:160:LEU:CD2	1:A:166:VAL:HG21	2.41	0.50
1:A:277:TYR:CD1	1:A:279:PRO:HG2	2.46	0.50
1:A:436:TYR:O	1:A:436:TYR:CD2	2.64	0.50
1:A:245:LEU:HD22	1:A:245:LEU:C	2.36	0.50
1:A:531:TYR:O	1:A:533:SER:N	2.45	0.50
1:A:491:THR:HG23	1:A:493:THR:H	1.77	0.50
1:A:398:LEU:HA	1:A:401:LEU:HB2	1.94	0.50
1:A:407:ASN:ND2	1:A:409:ASN:H	2.09	0.50
1:A:104:VAL:O	1:A:104:VAL:HG12	2.09	0.49
1:A:324:PRO:CD	1:A:333:TYR:CE2	2.72	0.49
4:A:801:C8E:H141	4:A:801:C8E:H102	1.94	0.49
1:A:22:VAL:HG11	1:A:26:THR:HG21	1.94	0.49
1:A:11:THR:HG23	1:A:108:GLU:OE1	2.13	0.49
1:A:46:LEU:O	1:A:49:LEU:HG	2.12	0.49
1:A:245:LEU:HD23	1:A:246:TYR:H	1.77	0.49
1:A:593:THR:CG2	1:A:594:PHE:N	2.76	0.49
1:A:134:ASP:OD1	1:A:135:GLU:N	2.44	0.49
1:A:285:ASP:OD2	1:A:287:SER:HB3	2.12	0.49
3:A:701:CNC:H492	3:A:701:CNC:C47	2.33	0.49
1:A:307:GLY:HA3	1:A:346:GLN:HE22	1.77	0.49
1:A:425:LEU:HD23	1:A:429:VAL:O	2.13	0.49
1:A:583:GLY:O	1:A:585:GLU:HG3	2.13	0.49
1:A:240:LEU:HD22	1:A:277:TYR:CA	2.35	0.49
1:A:397:ASN:OD1	1:A:399:GLY:N	2.46	0.49
1:A:32:GLN:O	1:A:33:ASP:C	2.56	0.49
1:A:107:VAL:HG12	1:A:108:GLU:N	2.28	0.49
1:A:217:PHE:N	1:A:217:PHE:CD2	2.78	0.49
1:A:488:ASN:HB3	1:A:491:THR:HG22	1.95	0.49
1:A:78:VAL:HG11	1:A:96:LEU:HD21	1.94	0.48
1:A:95:ASP:C	1:A:97:SER:N	2.70	0.48
1:A:286:SER:CA	1:A:287:SER:HB3	2.23	0.48
1:A:340:ILE:O	1:A:340:ILE:HG23	2.12	0.48
1:A:436:TYR:CD2	1:A:436:TYR:C	2.90	0.48
1:A:14:ARG:HD2	1:A:264:GLN:HE22	1.75	0.48
1:A:348:VAL:O	1:A:351:PHE:HB2	2.13	0.48
3:A:701:CNC:H533	3:A:701:CNC:N52	2.24	0.48
1:A:83:VAL:O	1:A:84:ARG:C	2.53	0.48
1:A:528:ASP:O	1:A:538:THR:HA	2.13	0.48
1:A:367:ARG:HH21	4:A:800:C8E:C19	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:TRP:CE2	4:A:805:C8E:H62	2.48	0.48
1:A:147:ASN:O	1:A:148:SER:C	2.55	0.48
1:A:248:GLN:NE2	1:A:250:TRP:HE1	2.12	0.48
4:A:803:C8E:H172	4:A:803:C8E:H142	1.61	0.48
1:A:249:SER:C	1:A:250:TRP:CD1	2.92	0.48
1:A:259:GLU:O	1:A:260:LEU:HD12	2.13	0.48
1:A:265:LEU:CD2	1:A:300:TRP:HB2	2.43	0.48
1:A:265:LEU:HD23	1:A:300:TRP:CB	2.42	0.48
1:A:497:ARG:HE	3:A:701:CNC:H1P1	1.78	0.48
1:A:525:THR:O	1:A:525:THR:CG2	2.62	0.48
1:A:50:PRO:HB2	1:A:111:ARG:NE	2.18	0.48
1:A:69:ARG:CB	1:A:436:TYR:OH	2.56	0.48
1:A:411:ASP:HB3	1:A:412:PRO:CD	2.44	0.48
1:A:24:ALA:HB1	1:A:25:PRO:CD	2.43	0.48
1:A:286:SER:CB	1:A:288:ALA:HB3	2.40	0.48
1:A:522:TYR:CZ	1:A:524:GLY:HA2	2.48	0.48
1:A:153:ASP:OD1	1:A:154:VAL:N	2.47	0.47
1:A:309:GLY:HA3	1:A:346:GLN:CG	2.43	0.47
1:A:555:VAL:HG12	1:A:556:THR:N	2.28	0.47
1:A:277:TYR:HE1	1:A:279:PRO:HG2	1.74	0.47
1:A:309:GLY:HA3	1:A:346:GLN:HG2	1.96	0.47
1:A:283:ARG:CA	1:A:284:TYR:CB	2.66	0.47
1:A:433:ILE:HG12	1:A:434:SER:N	2.29	0.47
1:A:160:LEU:CD1	1:A:166:VAL:HG21	2.45	0.47
1:A:483:TYR:CD2	1:A:483:TYR:C	2.93	0.47
4:A:800:C8E:H81	4:A:800:C8E:H112	1.44	0.47
4:A:802:C8E:H11	4:A:802:C8E:C17	2.44	0.47
1:A:160:LEU:HD22	1:A:166:VAL:HG21	1.96	0.47
1:A:209:ASN:H	1:A:209:ASN:HD22	1.62	0.47
4:A:802:C8E:H141	4:A:802:C8E:H112	1.56	0.47
1:A:233:TYR:CE2	1:A:239:LEU:HD22	2.50	0.47
1:A:380:ILE:O	1:A:381:GLU:C	2.58	0.47
1:A:405:TYR:CD2	1:A:446:TYR:HE2	2.33	0.47
1:A:56:GLN:H	1:A:575:THR:HG1	1.63	0.47
1:A:217:PHE:O	1:A:217:PHE:CG	2.68	0.47
1:A:576:VAL:O	1:A:577:TYR:C	2.58	0.47
3:A:701:CNC:H412	3:A:701:CNC:C5B	2.44	0.47
1:A:337:ASN:ND2	1:A:362:ASN:CB	2.78	0.47
1:A:497:ARG:NH2	3:A:701:CNC:N62	2.61	0.47
1:A:526:ARG:C	1:A:527:TYR:HD1	2.23	0.47
1:A:45:VAL:O	1:A:46:LEU:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ARG:CZ	1:A:207:GLU:OE1	2.63	0.46
1:A:527:TYR:HE1	1:A:540:LYS:HG3	0.56	0.46
1:A:567:ASN:C	1:A:567:ASN:ND2	2.72	0.46
1:A:341:TYR:CB	1:A:357:ALA:O	2.63	0.46
1:A:146:SER:O	1:A:147:ASN:ND2	2.48	0.46
1:A:443:LEU:HB2	1:A:457:GLY:C	2.39	0.46
4:A:804:C8E:H201	4:A:804:C8E:H172	1.43	0.46
1:A:69:ARG:HD3	1:A:436:TYR:CE1	2.51	0.46
1:A:295:GLN:HE21	1:A:320:GLN:CG	2.29	0.46
1:A:405:TYR:HD2	1:A:451:LEU:HB3	1.80	0.46
1:A:405:TYR:O	1:A:452:LYS:HA	2.15	0.46
1:A:281:TYR:CD2	1:A:281:TYR:C	2.94	0.46
1:A:285:ASP:CG	1:A:287:SER:HB3	2.40	0.46
1:A:290:LEU:HD12	1:A:291:ASP:H	1.72	0.46
1:A:401:LEU:HB3	1:A:402:TYR:CD1	2.49	0.46
1:A:330:GLU:O	1:A:333:TYR:CE1	2.67	0.46
1:A:51:GLY:O	1:A:68:ILE:HA	2.16	0.46
1:A:286:SER:CA	1:A:287:SER:CB	2.83	0.46
1:A:140:ILE:CG2	1:A:141:SER:N	2.79	0.46
1:A:36:ARG:HH11	1:A:36:ARG:CG	2.29	0.45
1:A:256:TYR:CD2	1:A:256:TYR:O	2.70	0.45
1:A:506:GLN:HG3	1:A:507:LEU:N	2.32	0.45
1:A:251:ASP:HA	1:A:267:THR:O	2.16	0.45
1:A:410:LEU:HD23	1:A:410:LEU:HA	1.71	0.45
1:A:495:LEU:C	1:A:496:LEU:HD12	2.42	0.45
1:A:10:VAL:HG12	1:A:16:GLU:CA	2.45	0.45
1:A:100:PRO:HB2	1:A:103:LEU:HD22	1.99	0.45
1:A:189:GLN:O	1:A:190:ALA:HB2	2.16	0.45
1:A:159:GLN:C	1:A:160:LEU:CD1	2.73	0.45
1:A:99:PHE:C	1:A:99:PHE:HD2	2.22	0.45
1:A:308:HIS:N	1:A:346:GLN:HE22	2.14	0.45
1:A:209:ASN:HB3	1:A:211:THR:O	2.17	0.45
1:A:405:TYR:HB3	1:A:451:LEU:C	2.41	0.45
4:A:804:C8E:H112	4:A:804:C8E:H81	1.44	0.45
1:A:283:ARG:CA	1:A:284:TYR:CG	2.99	0.45
1:A:446:TYR:C	1:A:446:TYR:CD1	2.94	0.45
1:A:525:THR:HB	1:A:542:GLY:O	2.17	0.45
4:A:800:C8E:H131	4:A:800:C8E:H101	1.36	0.45
1:A:82:GLY:C	1:A:83:VAL:CG2	2.90	0.45
1:A:95:ASP:OD2	1:A:97:SER:OG	2.35	0.45
1:A:446:TYR:CE2	1:A:451:LEU:HA	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ASP:OD2	1:A:449:HIS:HB2	2.09	0.45
1:A:8:LEU:O	1:A:9:VAL:HB	2.16	0.45
1:A:185:ASN:O	1:A:232:TYR:N	2.49	0.44
1:A:323:THR:CG2	1:A:324:PRO:CD	2.91	0.44
1:A:472:THR:O	1:A:473:GLY:O	2.34	0.44
1:A:483:TYR:CD2	1:A:483:TYR:O	2.70	0.44
1:A:331:ASP:O	1:A:333:TYR:HD1	2.00	0.44
1:A:447:ASP:CB	1:A:449:HIS:CE1	2.97	0.44
1:A:511:LEU:HD23	1:A:512:TYR:CG	2.48	0.44
1:A:208:HIS:C	1:A:208:HIS:HD1	2.26	0.44
1:A:229:TYR:CG	3:A:701:CNC:H311	2.52	0.44
1:A:260:LEU:HA	1:A:305:ILE:HD12	1.99	0.44
1:A:528:ASP:OD1	1:A:529:LYS:N	2.46	0.44
3:A:701:CNC:C61	3:A:701:CNC:C55	2.96	0.44
1:A:226:ARG:CZ	1:A:244:LYS:HE2	2.45	0.44
1:A:350:ASP:HB3	1:A:378:GLU:O	2.17	0.44
1:A:450:THR:O	1:A:450:THR:OG1	2.24	0.44
1:A:169:LEU:CD1	1:A:170:GLY:N	2.81	0.44
1:A:170:GLY:HA2	1:A:201:THR:O	2.18	0.44
1:A:179:ASP:N	1:A:194:ASN:HA	2.32	0.44
1:A:293:MET:HE3	1:A:293:MET:CB	2.37	0.44
1:A:440:VAL:HG12	1:A:441:SER:H	1.83	0.44
1:A:37:TRP:C	1:A:39:SER:H	2.26	0.44
1:A:49:LEU:N	1:A:49:LEU:HD23	2.31	0.44
1:A:59:GLY:N	1:A:62:GLN:HG3	2.32	0.44
1:A:494:PRO:C	1:A:495:LEU:O	2.57	0.44
1:A:19:ARG:C	1:A:21:THR:H	2.23	0.44
1:A:165:ARG:NH2	1:A:207:GLU:OE2	2.50	0.44
1:A:331:ASP:O	1:A:333:TYR:CD1	2.70	0.44
1:A:426:THR:O	1:A:427:ALA:C	2.61	0.44
1:A:483:TYR:O	1:A:483:TYR:HD2	2.00	0.44
4:A:802:C8E:H13	4:A:802:C8E:C5	2.45	0.44
1:A:260:LEU:HD12	1:A:260:LEU:HA	1.69	0.44
1:A:276:ASN:O	1:A:277:TYR:HB3	2.17	0.44
1:A:495:LEU:N	1:A:495:LEU:HD23	2.33	0.44
1:A:511:LEU:HD12	1:A:511:LEU:HA	1.86	0.44
1:A:25:PRO:C	1:A:111:ARG:HH12	2.25	0.43
1:A:255:ARG:HG2	1:A:264:GLN:HB3	2.00	0.43
1:A:588:LEU:HA	1:A:588:LEU:HD22	1.48	0.43
1:A:146:SER:HB2	1:A:585:GLU:HB3	2.00	0.43
1:A:417:GLN:HA	1:A:437:ARG:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:ILE:HG13	1:A:466:ALA:HB2	2.00	0.43
1:A:26:THR:HG22	1:A:110:ILE:HG23	2.01	0.43
1:A:171:ASP:OD2	1:A:171:ASP:C	2.60	0.43
1:A:231:ALA:H	3:A:701:CNC:H292	1.66	0.43
1:A:440:VAL:HG12	1:A:441:SER:N	2.33	0.43
1:A:443:LEU:CB	1:A:457:GLY:O	2.65	0.43
4:A:802:C8E:H172	4:A:802:C8E:C1	2.47	0.43
1:A:31:ARG:O	1:A:33:ASP:N	2.50	0.43
1:A:264:GLN:OE1	1:A:266:ILE:HD11	2.18	0.43
1:A:321:THR:HA	1:A:334:ASP:HA	2.00	0.43
1:A:560:THR:CG2	1:A:561:VAL:N	2.81	0.43
1:A:36:ARG:NH2	1:A:508:ASP:OD1	2.39	0.43
1:A:68:ILE:C	1:A:70:GLY:N	2.74	0.43
1:A:239:LEU:HB3	1:A:240:LEU:H	1.72	0.43
1:A:279:PRO:O	1:A:280:HIS:CB	2.62	0.43
1:A:407:ASN:HD22	1:A:408:PRO:CD	2.32	0.43
1:A:68:ILE:O	1:A:70:GLY:N	2.51	0.43
1:A:265:LEU:HD23	1:A:300:TRP:CG	2.53	0.43
1:A:321:THR:O	1:A:321:THR:OG1	2.33	0.43
1:A:413:GLU:HG2	1:A:442:ASP:O	2.18	0.43
1:A:422:PHE:CD2	4:A:801:C8E:H11	2.54	0.43
1:A:443:LEU:HD12	1:A:457:GLY:C	2.43	0.43
1:A:212:ASP:OD2	1:A:212:ASP:N	2.42	0.43
1:A:293:MET:HG3	1:A:294:LYS:H	1.77	0.43
1:A:150:GLN:HG2	1:A:151:ASN:N	2.33	0.42
1:A:458:LYS:HB2	1:A:489:ALA:HB3	2.00	0.42
3:A:701:CNC:H4B	3:A:701:CNC:C5	2.49	0.42
1:A:389:TYR:CG	1:A:390:GLY:N	2.84	0.42
1:A:488:ASN:N	1:A:495:LEU:HD21	2.34	0.42
1:A:497:ARG:NH1	1:A:576:VAL:CG2	2.82	0.42
3:A:701:CNC:H601	3:A:701:CNC:C25	2.46	0.42
1:A:8:LEU:HA	1:A:17:GLN:O	2.20	0.42
1:A:365:PHE:CD1	1:A:365:PHE:C	2.97	0.42
1:A:80:ILE:HD12	1:A:99:PHE:CE1	2.54	0.42
1:A:169:LEU:HD13	1:A:170:GLY:N	2.34	0.42
1:A:239:LEU:O	1:A:240:LEU:HB2	2.18	0.42
1:A:534:TYR:CG	1:A:535:PRO:HA	2.55	0.42
1:A:56:GLN:HB3	1:A:58:GLY:O	2.19	0.42
1:A:186:THR:O	1:A:233:TYR:CB	2.68	0.42
1:A:433:ILE:HD12	4:A:802:C8E:C1	2.49	0.42
1:A:123:ILE:O	1:A:417:GLN:NE2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ASP:C	1:A:163:LYS:HG2	2.44	0.42
3:A:701:CNC:C14	3:A:701:CNC:H2B	2.50	0.42
1:A:182:ALA:O	1:A:183:TYR:CB	2.61	0.42
1:A:228:ASN:OD1	1:A:242:THR:HG23	2.19	0.42
1:A:481:TYR:OH	1:A:483:TYR:HB2	2.20	0.42
1:A:547:TRP:C	1:A:548:ASP:OD1	2.62	0.42
1:A:68:ILE:HD12	1:A:68:ILE:HG23	1.84	0.41
4:A:801:C8E:H102	4:A:801:C8E:C14	2.50	0.41
1:A:417:GLN:HG2	1:A:438:ASN:CB	2.49	0.41
1:A:529:LYS:HZ3	1:A:538:THR:CG2	2.30	0.41
1:A:164:THR:HA	1:A:207:GLU:O	2.21	0.41
1:A:217:PHE:CE1	1:A:219:ARG:NH2	2.88	0.41
1:A:425:LEU:HD23	1:A:425:LEU:HA	1.73	0.41
4:A:803:C8E:H101	4:A:803:C8E:H72	1.22	0.41
1:A:53:ASP:C	1:A:54:ILE:HG12	2.28	0.41
1:A:180:VAL:HG23	1:A:579:TYR:HA	2.01	0.41
1:A:206:LEU:HD12	1:A:206:LEU:HA	1.56	0.41
1:A:331:ASP:OD1	1:A:331:ASP:C	2.63	0.41
1:A:592:TYR:HE1	1:A:594:PHE:HB3	1.86	0.41
4:A:802:C8E:H12	4:A:802:C8E:C16	2.51	0.41
1:A:63:LEU:HD23	1:A:63:LEU:HA	1.80	0.41
1:A:120:SER:C	1:A:121:ASP:CG	2.89	0.41
1:A:223:TYR:CZ	1:A:247:SER:OG	2.69	0.41
1:A:307:GLY:CA	1:A:346:GLN:HE22	2.32	0.41
1:A:382:GLY:O	1:A:424:GLY:HA2	2.21	0.41
1:A:395:ALA:HA	1:A:396:PRO:HD3	1.91	0.41
1:A:188:THR:O	1:A:189:GLN:CG	2.69	0.41
1:A:116:ALA:HA	1:A:370:THR:HG22	2.02	0.41
1:A:332:GLY:O	1:A:333:TYR:CD2	2.74	0.41
1:A:225:ASN:N	1:A:225:ASN:HD22	2.18	0.41
1:A:570:ASP:C	1:A:570:ASP:OD1	2.60	0.41
1:A:162:ASP:O	1:A:163:LYS:C	2.64	0.40
1:A:186:THR:O	1:A:233:TYR:HB2	2.21	0.40
1:A:189:GLN:HE21	1:A:189:GLN:HB3	1.57	0.40
1:A:297:THR:C	1:A:298:VAL:CG2	2.94	0.40
1:A:323:THR:CG2	1:A:324:PRO:HD2	2.34	0.40
1:A:447:ASP:OD2	1:A:449:HIS:CB	2.67	0.40
1:A:145:GLY:O	1:A:147:ASN:N	2.54	0.40
1:A:165:ARG:NH2	1:A:207:GLU:OE1	2.52	0.40
1:A:309:GLY:N	1:A:346:GLN:HE22	2.14	0.40
1:A:55:THR:HG22	1:A:575:THR:CB	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:GLY:O	1:A:62:GLN:CG	2.67	0.40
1:A:63:LEU:HD21	3:A:701:CNC:HM61	2.03	0.40
1:A:178:TYR:CZ	1:A:582:ALA:HA	2.57	0.40
1:A:179:ASP:OD2	1:A:192:THR:N	2.54	0.40
1:A:415:SER:OG	1:A:438:ASN:OD1	2.34	0.40
1:A:511:LEU:CD2	1:A:512:TYR:CD2	2.81	0.40
4:A:804:C8E:H171	4:A:804:C8E:H141	1.56	0.40
1:A:283:ARG:CG	1:A:284:TYR:CD2	2.92	0.40
1:A:405:TYR:CG	1:A:446:TYR:CE2	3.05	0.40
1:A:565:ILE:O	1:A:565:ILE:HG22	2.17	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	580/594 (98%)	480 (83%)	67 (12%)	33 (6%)	1 8

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	9	VAL
1	A	20	SER
1	A	86	ASN
1	A	92	GLY
1	A	122	ALA
1	A	135	GLU
1	A	146	SER
1	A	189	GLN
1	A	231	ALA
1	A	232	TYR

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Mol	Chain	Res	Type
1	A	240	LEU
1	A	241	ASP
1	A	279	PRO
1	A	283	ARG
1	A	288	ALA
1	A	449	HIS
1	A	85	LEU
1	A	163	LYS
1	A	190	ALA
1	A	273	LYS
1	A	280	HIS
1	A	93	SER
1	A	121	ASP
1	A	181	VAL
1	A	182	ALA
1	A	192	THR
1	A	69	ARG
1	A	142	ALA
1	A	185	ASN
1	A	286	SER
1	A	533	SER
1	A	237	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	487/495 (98%)	361 (74%)	126 (26%)	0 2

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	8	LEU
1	A	9	VAL
1	A	11	THR

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Mol	Chain	Res	Type
1	A	13	ASN
1	A	14	ARG
1	A	17	GLN
1	A	31	ARG
1	A	32	GLN
1	A	36	ARG
1	A	40	THR
1	A	47	ARG
1	A	49	LEU
1	A	54	ILE
1	A	55	THR
1	A	56	GLN
1	A	62	GLN
1	A	63	LEU
1	A	80	ILE
1	A	85	LEU
1	A	87	LEU
1	A	90	VAL
1	A	91	SER
1	A	93	SER
1	A	95	ASP
1	A	103	LEU
1	A	105	GLN
1	A	111	ARG
1	A	114	ARG
1	A	121	ASP
1	A	132	THR
1	A	141	SER
1	A	144	TRP
1	A	148	SER
1	A	151	ASN
1	A	158	GLN
1	A	162	ASP
1	A	166	VAL
1	A	169	LEU
1	A	180	VAL
1	A	181	VAL
1	A	185	ASN
1	A	186	THR
1	A	189	GLN
1	A	191	GLN
1	A	192	THR

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Mol	Chain	Res	Type
1	A	194	ASN
1	A	202	LEU
1	A	206	LEU
1	A	207	GLU
1	A	210	PHE
1	A	212	ASP
1	A	215	SER
1	A	217	PHE
1	A	223	TYR
1	A	226	ARG
1	A	227	THR
1	A	237	SER
1	A	239	LEU
1	A	241	ASP
1	A	244	LYS
1	A	245	LEU
1	A	247	SER
1	A	256	TYR
1	A	259	GLU
1	A	260	LEU
1	A	262	LYS
1	A	263	SER
1	A	265	LEU
1	A	267	THR
1	A	270	SER
1	A	278	ASP
1	A	284	TYR
1	A	286	SER
1	A	290	LEU
1	A	295	GLN
1	A	304	VAL
1	A	322	THR
1	A	323	THR
1	A	330	GLU
1	A	334	ASP
1	A	345	LEU
1	A	348	VAL
1	A	352	THR
1	A	359	SER
1	A	370	THR
1	A	373	THR
1	A	381	GLU

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Mol	Chain	Res	Type
1	A	391	THR
1	A	393	TYR
1	A	404	PHE
1	A	407	ASN
1	A	425	LEU
1	A	426	THR
1	A	433	ILE
1	A	440	VAL
1	A	441	SER
1	A	449	HIS
1	A	450	THR
1	A	451	LEU
1	A	452	LYS
1	A	460	ARG
1	A	461	ILE
1	A	467	THR
1	A	474	PRO
1	A	475	LEU
1	A	483	TYR
1	A	493	THR
1	A	498	ARG
1	A	500	LYS
1	A	506	GLN
1	A	510	GLN
1	A	519	THR
1	A	525	THR
1	A	526	ARG
1	A	533	SER
1	A	539	VAL
1	A	540	LYS
1	A	548	ASP
1	A	555	VAL
1	A	557	SER
1	A	559	LEU
1	A	564	LYS
1	A	575	THR
1	A	579	TYR
1	A	589	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	32	GLN
1	A	56	GLN
1	A	57	ASN
1	A	72	ASN
1	A	75	HIS
1	A	86	ASN
1	A	98	GLN
1	A	105	GLN
1	A	147	ASN
1	A	157	GLN
1	A	185	ASN
1	A	189	GLN
1	A	209	ASN
1	A	225	ASN
1	A	248	GLN
1	A	257	ASN
1	A	295	GLN
1	A	302	ASN
1	A	318	GLN
1	A	320	GLN
1	A	335	GLN
1	A	337	ASN
1	A	346	GLN
1	A	347	GLN
1	A	362	ASN
1	A	372	GLN
1	A	400	GLN
1	A	407	ASN
1	A	455	ASN
1	A	506	GLN
1	A	567	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	C8E	A	804	-	20,20,20	0.45	0	19,19,19	0.97	2 (10%)
4	C8E	A	800	-	20,20,20	0.52	0	19,19,19	0.97	0
4	C8E	A	801	-	20,20,20	0.41	0	19,19,19	1.03	1 (5%)
4	C8E	A	805	-	20,20,20	0.69	0	19,19,19	0.75	0
3	CNC	A	701	-	93,103,103	1.38	14 (15%)	149,171,171	2.97	70 (46%)
4	C8E	A	803	-	20,20,20	0.56	0	19,19,19	1.11	0
4	C8E	A	802	-	20,20,20	0.39	0	19,19,19	1.18	1 (5%)

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
4	C8E	A	804	-	-	10/18/18/18	-
4	C8E	A	800	-	-	10/18/18/18	-
4	C8E	A	801	-	-	10/18/18/18	-
4	C8E	A	805	-	-	10/18/18/18	-
3	CNC	A	701	-	1/1/36/38	15/56/235/235	0/3/11/11
4	C8E	A	803	-	-	9/18/18/18	-
4	C8E	A	802	-	-	13/18/18/18	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	CNC	C12-C13	-4.52	1.42	1.55
3	A	701	CNC	C18-C19	-4.41	1.45	1.54
3	A	701	CNC	C1-N21	-4.19	1.43	1.50
3	A	701	CNC	C61-N62	-3.06	1.22	1.32
3	A	701	CNC	C1-C19	-2.66	1.47	1.54
3	A	701	CNC	C2R-C3R	-2.64	1.47	1.53
3	A	701	CNC	O63-C61	2.50	1.31	1.23
3	A	701	CNC	C2-C3	-2.47	1.50	1.57
3	A	701	CNC	C48-C13	-2.45	1.48	1.54
3	A	701	CNC	C2B-N3B	2.42	1.36	1.31
3	A	701	CNC	O44-C43	2.29	1.31	1.23
3	A	701	CNC	P-O3	-2.27	1.52	1.59
3	A	701	CNC	C3R-C4R	-2.19	1.47	1.52
3	A	701	CNC	C17-C18	-2.14	1.50	1.54

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	CNC	C15-C16-N24	-10.33	112.00	122.38
3	A	701	CNC	C17-C16-C15	8.22	139.06	126.70
3	A	701	CNC	O6R-C1R-N1B	7.39	122.27	108.09
3	A	701	CNC	C12-C11-C10	-7.05	117.20	123.54
3	A	701	CNC	C35-C5-C4	-6.79	103.04	116.79
3	A	701	CNC	O6R-C4R-C5R	6.72	123.42	109.22
3	A	701	CNC	C41-C8-C9	6.69	122.86	111.19
3	A	701	CNC	C54-C17-C18	-6.66	103.43	112.99
3	A	701	CNC	C3-C4-N21	6.24	119.73	111.98
3	A	701	CNC	C1-C19-C18	-6.03	112.70	121.75
3	A	701	CNC	C31-C30-C3	5.97	131.57	114.65
3	A	701	CNC	C17-C18-C19	-5.55	95.95	102.70
3	A	701	CNC	C54-C17-C55	5.21	117.93	109.27
3	A	701	CNC	C55-C17-C16	5.02	127.10	116.17
3	A	701	CNC	C7-C6-N22	-4.91	98.98	107.94
3	A	701	CNC	C25-C2-C1	4.88	121.05	113.75
3	A	701	CNC	C48-C49-C50	-4.76	96.36	112.55
3	A	701	CNC	C30-C3-C2	4.58	129.09	119.00
3	A	701	CNC	C35-C5-C6	4.57	129.78	122.41
3	A	701	CNC	C41-C8-C7	4.53	126.66	114.19
3	A	701	CNC	C9B-N3B-C2B	-4.22	99.23	104.40
3	A	701	CNC	C3R-C2R-C1R	4.02	108.74	99.89
3	A	701	CNC	C7B-C8B-C9B	3.95	127.21	122.47
3	A	701	CNC	C18-C19-N24	3.88	108.10	101.92
3	A	701	CNC	C3-C4-C5	-3.76	117.52	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	CNC	C20-C1-C19	-3.66	102.96	110.23
3	A	701	CNC	C13-C14-C15	-3.59	117.81	123.82
3	A	701	CNC	C16-C15-C14	3.59	126.16	121.29
3	A	701	CNC	C55-C17-C18	-3.52	104.40	111.12
3	A	701	CNC	O39-C38-C37	-3.42	111.38	121.98
3	A	701	CNC	C5-C4-N21	-3.38	118.76	124.19
3	A	701	CNC	O63-C61-C60	-3.35	113.86	120.87
3	A	701	CNC	O28-C27-N29	-3.31	113.69	122.53
3	A	701	CNC	C30-C3-C4	3.30	117.41	109.66
3	A	701	CNC	C7B-C8B-N1B	-3.27	124.93	131.39
3	A	701	CNC	C2-C1-N21	3.20	106.23	101.78
3	A	701	CNC	C4B-C5B-C6B	3.19	124.38	119.69
3	A	701	CNC	C19-N24-C16	-3.15	106.92	111.96
3	A	701	CNC	O7R-C2R-C1R	3.12	120.85	110.10
3	A	701	CNC	C5M-C5B-C6B	-3.11	114.42	120.76
3	A	701	CNC	C7-C6-C5	3.10	132.93	128.07
3	A	701	CNC	C12-C11-N23	-3.01	108.28	111.49
3	A	701	CNC	C26-C2-C3	-2.96	102.26	107.42
3	A	701	CNC	C37-C7-C6	-2.88	98.20	107.11
3	A	701	CNC	C8B-N1B-C2B	-2.86	103.66	106.26
3	A	701	CNC	O58-C57-C56	-2.86	116.83	122.02
3	A	701	CNC	O2-C3R-C4R	2.79	119.87	110.03
3	A	701	CNC	N1B-C2B-N3B	2.70	117.77	113.94
3	A	701	CNC	C3P-C2P-C1P	2.70	116.63	111.42
3	A	701	CNC	C8-C9-C10	2.68	129.04	123.33
3	A	701	CNC	C6-C5-C4	2.68	126.32	121.55
3	A	701	CNC	P-O3-C2P	-2.66	112.02	121.10
4	A	802	C8E	C19-O18-C17	-2.63	101.76	113.26
3	A	701	CNC	C9-C10-C11	-2.62	121.99	125.84
3	A	701	CNC	C2R-C1R-N1B	2.60	119.77	113.30
3	A	701	CNC	C13-C12-C11	2.57	104.31	100.86
3	A	701	CNC	C5R-C4R-C3R	2.56	122.89	114.84
3	A	701	CNC	C8B-C7B-C6B	-2.55	114.09	119.22
3	A	701	CNC	C9B-C4B-C5B	-2.53	116.15	120.83
4	A	804	C8E	O12-C13-C14	-2.50	98.96	110.35
3	A	701	CNC	C10-C9-N22	-2.50	122.89	125.74
3	A	701	CNC	O7R-C2R-C3R	2.45	118.04	111.19
3	A	701	CNC	C2-C3-C4	-2.39	98.96	101.64
3	A	701	CNC	C9B-C8B-N1B	2.38	106.36	105.30
4	A	801	C8E	O12-C13-C14	-2.37	99.57	110.35
3	A	701	CNC	O6R-C4R-C3R	2.28	109.73	104.92
3	A	701	CNC	O39-C38-N40	2.28	128.61	122.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	CNC	C36-C7-C37	2.25	114.56	110.74
3	A	701	CNC	C25-C2-C26	2.24	114.19	109.74
3	A	701	CNC	C8-C7-C6	-2.21	97.17	100.92
3	A	701	CNC	C4B-C9B-C8B	-2.20	118.14	120.16
4	A	804	C8E	O18-C17-C16	-2.12	100.68	110.35
3	A	701	CNC	O3-C2P-C1P	-2.07	102.84	106.94
3	A	701	CNC	O63-C61-N62	2.05	128.01	122.53

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	701	CNC	N24

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	802	C8E	C14-C13-O12-C11
4	A	803	C8E	C17-C16-O15-C14
4	A	804	C8E	C11-C10-O9-C8
4	A	805	C8E	C17-C16-O15-C14
4	A	801	C8E	C11-C10-O9-C8
4	A	803	C8E	C14-C13-O12-C11
4	A	804	C8E	C20-C19-O18-C17
4	A	801	C8E	C13-C14-O15-C16
3	A	701	CNC	C3R-C4R-C5R-O8R
4	A	803	C8E	C7-C8-O9-C10
4	A	805	C8E	C11-C10-O9-C8
4	A	804	C8E	O15-C16-C17-O18
4	A	800	C8E	C10-C11-O12-C13
4	A	803	C8E	O12-C13-C14-O15
3	A	701	CNC	O6R-C4R-C5R-O8R
4	A	805	C8E	O9-C10-C11-O12
4	A	805	C8E	C10-C11-O12-C13
4	A	804	C8E	C17-C16-O15-C14
4	A	800	C8E	O15-C16-C17-O18
4	A	801	C8E	O18-C19-C20-O21
4	A	802	C8E	C6-C7-C8-O9
3	A	701	CNC	C42-C41-C8-C9
4	A	801	C8E	O9-C10-C11-O12
4	A	804	C8E	O9-C10-C11-O12
3	A	701	CNC	C12-C13-C48-C49
4	A	803	C8E	C16-C17-O18-C19

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Mol	Chain	Res	Type	Atoms
4	A	800	C8E	O18-C19-C20-O21
4	A	804	C8E	O18-C19-C20-O21
3	A	701	CNC	C38-C37-C7-C8
4	A	805	C8E	C4-C5-C6-C7
4	A	801	C8E	O12-C13-C14-O15
4	A	801	C8E	C6-C7-C8-O9
4	A	803	C8E	C4-C5-C6-C7
4	A	805	C8E	O15-C16-C17-O18
4	A	802	C8E	C5-C6-C7-C8
3	A	701	CNC	N59-C1P-C2P-C3P
4	A	804	C8E	C3-C4-C5-C6
4	A	800	C8E	C4-C5-C6-C7
4	A	800	C8E	C11-C10-O9-C8
4	A	800	C8E	C3-C4-C5-C6
4	A	802	C8E	C1-C2-C3-C4
4	A	800	C8E	O12-C13-C14-O15
4	A	804	C8E	C1-C2-C3-C4
4	A	800	C8E	C13-C14-O15-C16
4	A	800	C8E	C14-C13-O12-C11
4	A	802	C8E	C17-C16-O15-C14
4	A	801	C8E	C14-C13-O12-C11
4	A	805	C8E	C20-C19-O18-C17
4	A	801	C8E	C17-C16-O15-C14
4	A	803	C8E	C10-C11-O12-C13
4	A	801	C8E	C20-C19-O18-C17
4	A	802	C8E	C20-C19-O18-C17
4	A	802	C8E	O18-C19-C20-O21
3	A	701	CNC	C18-C60-C61-O63
4	A	802	C8E	C16-C17-O18-C19
4	A	802	C8E	O9-C10-C11-O12
4	A	805	C8E	C7-C8-O9-C10
4	A	805	C8E	C14-C13-O12-C11
4	A	804	C8E	C10-C11-O12-C13
3	A	701	CNC	C18-C60-C61-N62
4	A	805	C8E	C3-C4-C5-C6
4	A	801	C8E	C16-C17-O18-C19
3	A	701	CNC	O58-C57-N59-C1P
3	A	701	CNC	C1-C2-C26-C27
4	A	803	C8E	C5-C6-C7-C8
3	A	701	CNC	C2R-C1R-N1B-C8B
4	A	802	C8E	C10-C11-O12-C13
4	A	804	C8E	C2-C3-C4-C5

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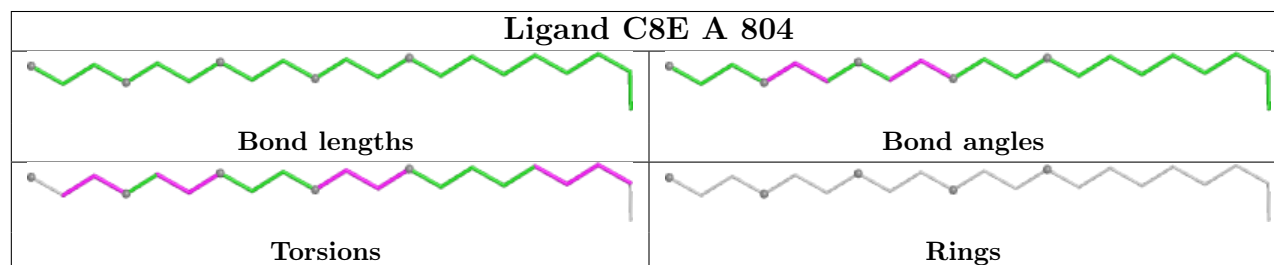
Mol	Chain	Res	Type	Atoms
4	A	803	C8E	O15-C16-C17-O18
3	A	701	CNC	C38-C37-C7-C36
3	A	701	CNC	C48-C49-C50-N52
4	A	800	C8E	C7-C8-O9-C10
3	A	701	CNC	C13-C48-C49-C50
4	A	802	C8E	C7-C8-O9-C10
3	A	701	CNC	C7-C37-C38-N40
4	A	802	C8E	C11-C10-O9-C8
4	A	802	C8E	O12-C13-C14-O15

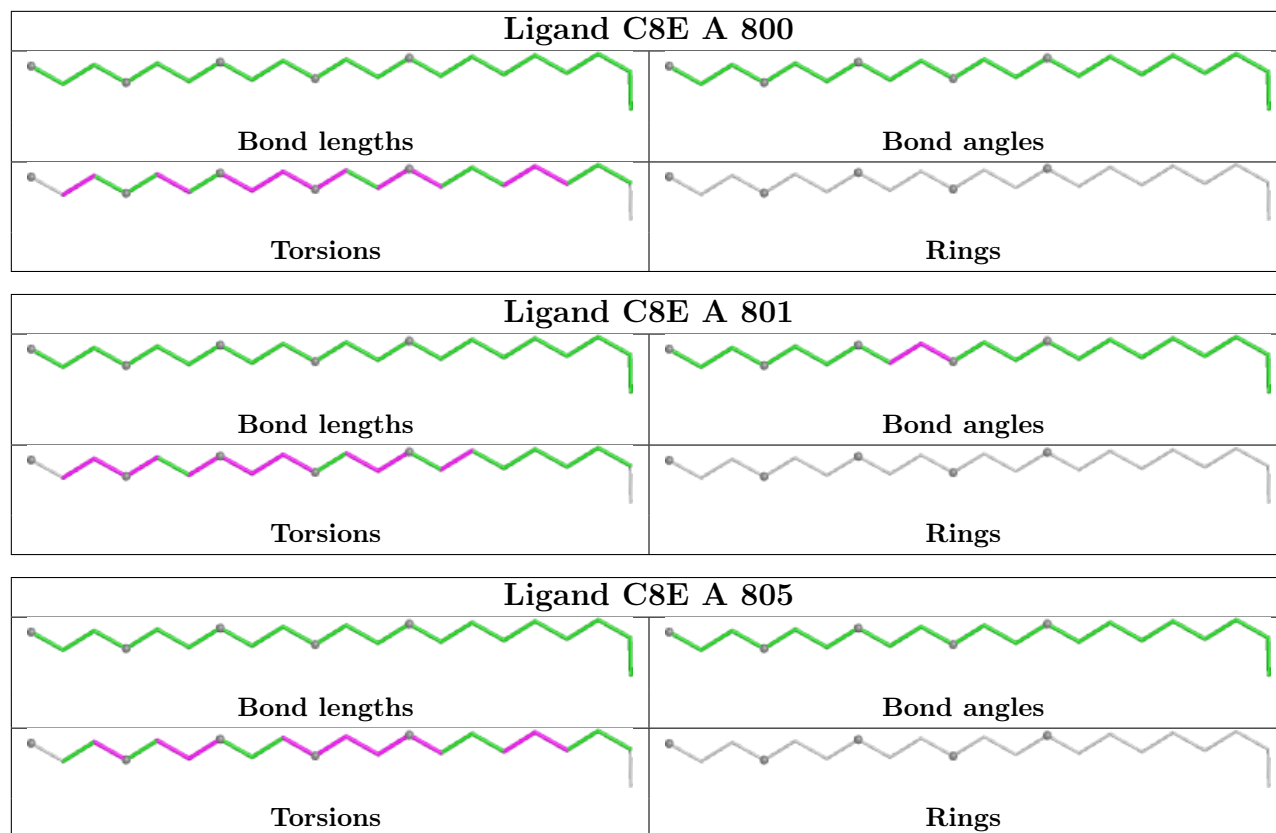
There are no ring outliers.

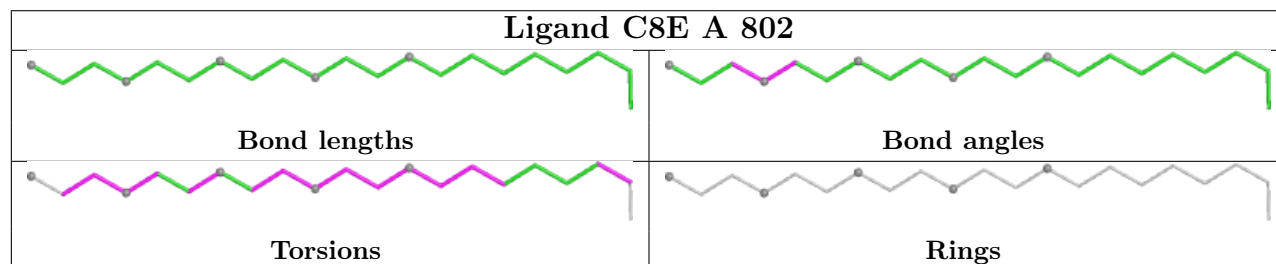
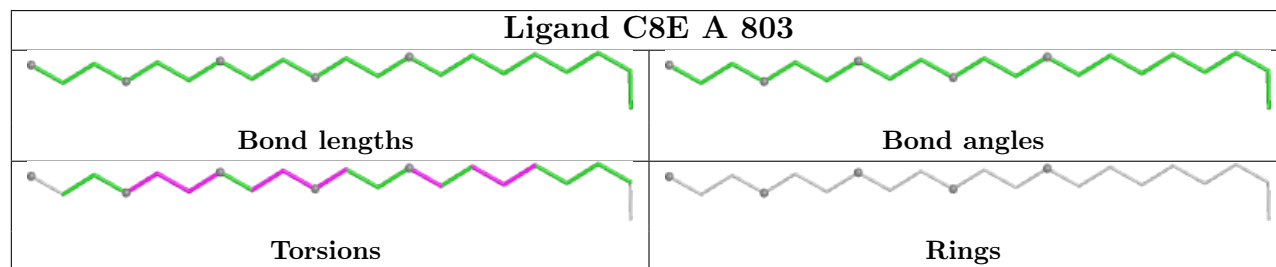
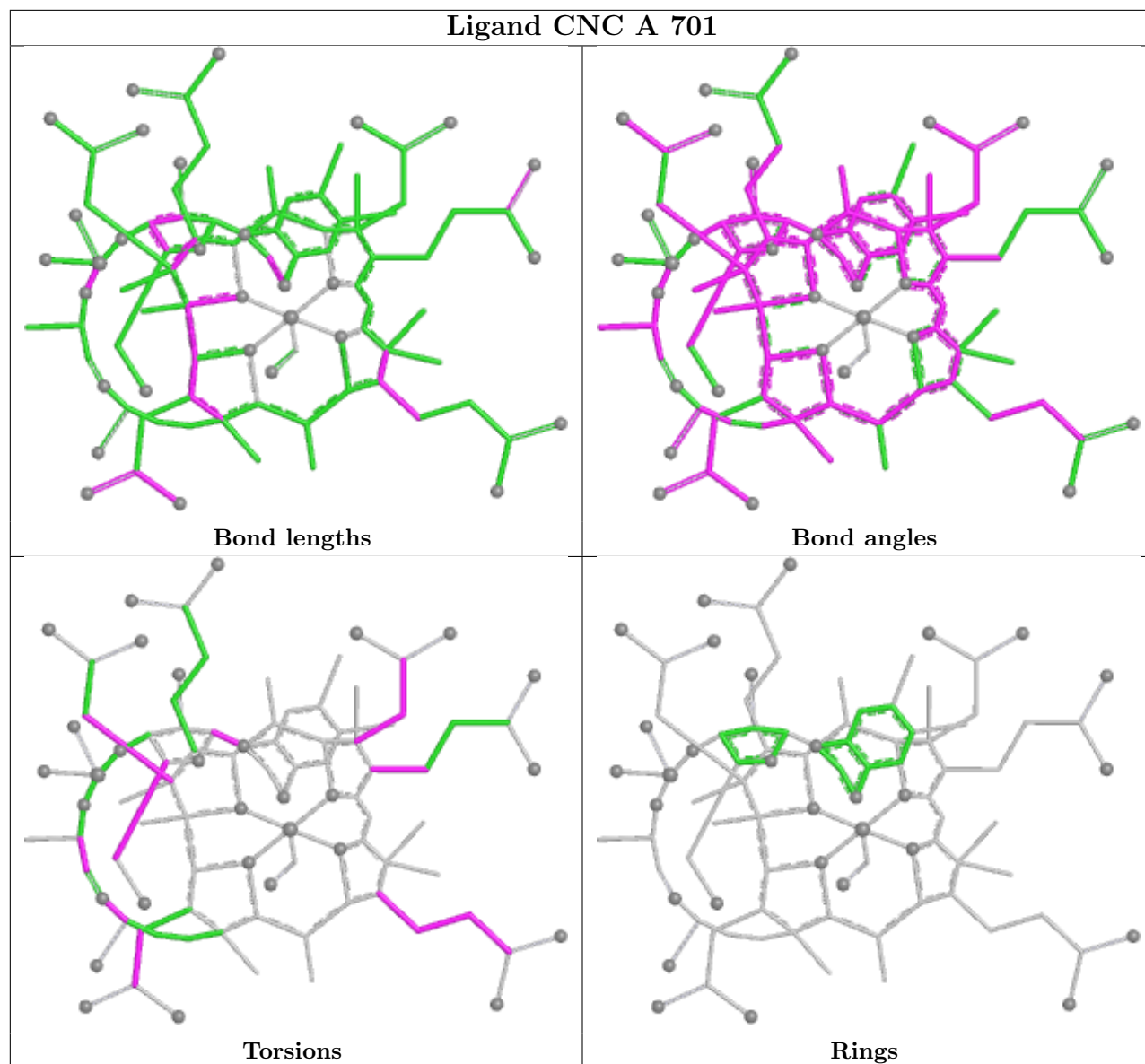
7 monomers are involved in 70 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	804	C8E	3	0
4	A	800	C8E	6	0
4	A	801	C8E	5	0
4	A	805	C8E	1	0
3	A	701	CNC	37	0
4	A	803	C8E	9	0
4	A	802	C8E	9	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

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	584/594 (98%)	0.07	5 (0%) 81 63	13, 22, 32, 49	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	331	ASP	4.6
1	A	332	GLY	3.8
1	A	185	ASN	3.7
1	A	285	ASP	2.6
1	A	276	ASN	2.3

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	CA	A	598	1/1	0.60	0.10	76,76,76,76	0
4	C8E	A	804	21/21	0.79	0.18	41,50,61,66	0

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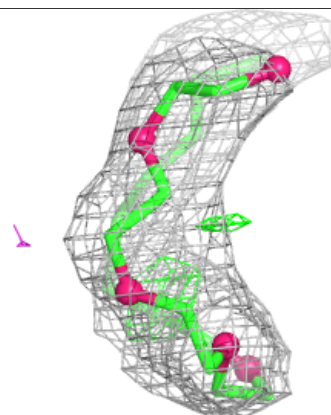
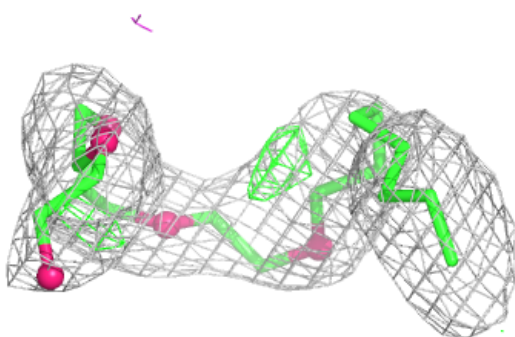
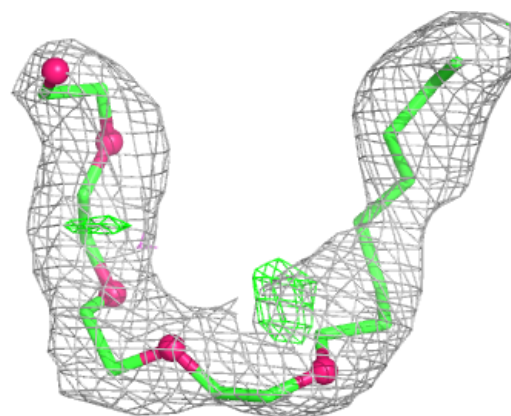
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	C8E	A	805	21/21	0.82	0.16	43,65,82,86	0
4	C8E	A	803	21/21	0.85	0.15	45,64,70,74	0
2	CA	A	597	1/1	0.86	0.11	76,76,76,76	0
4	C8E	A	801	21/21	0.87	0.16	40,56,69,72	0
4	C8E	A	800	21/21	0.90	0.12	38,44,50,52	0
4	C8E	A	802	21/21	0.91	0.14	40,48,54,63	0
3	CNC	A	701	93/93	0.93	0.12	29,51,69,81	0
2	CA	A	596	1/1	0.97	0.04	57,57,57,57	0
2	CA	A	595	1/1	0.98	0.08	54,54,54,54	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.

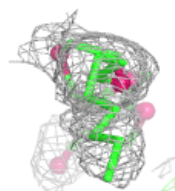
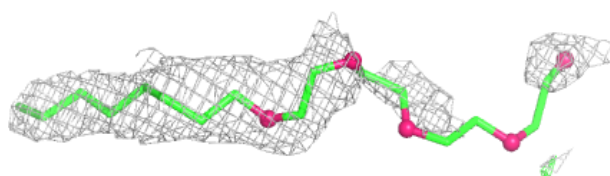
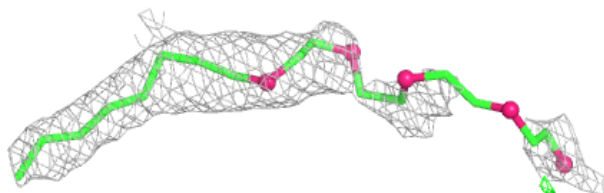
Electron density around C8E A 804:

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

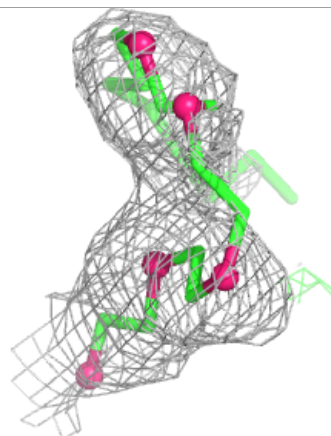
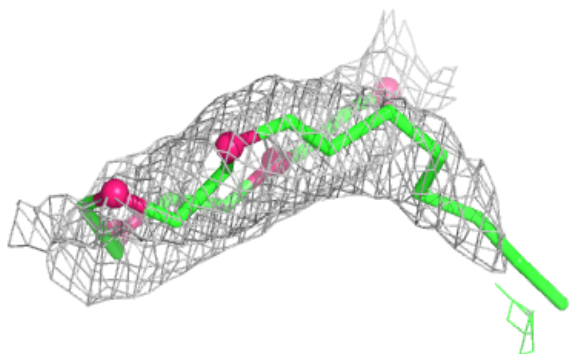
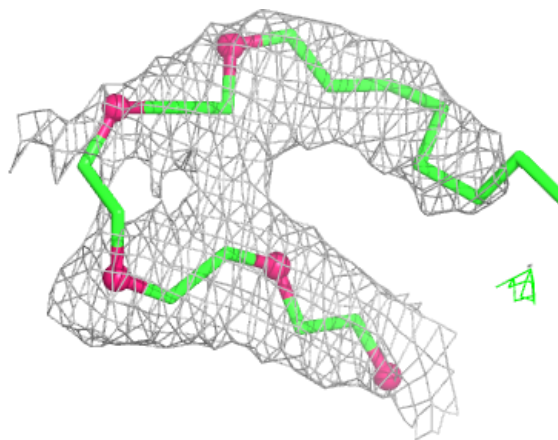


Electron density around C8E A 805:

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

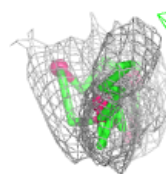
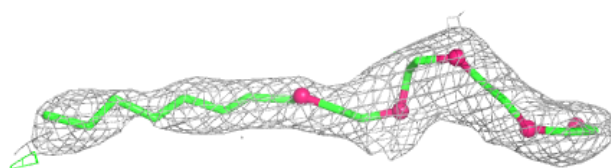
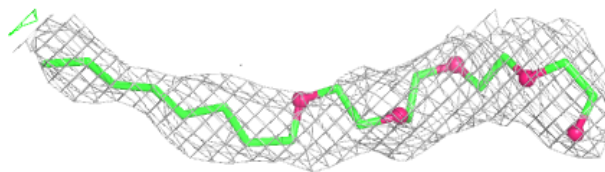
**Electron density around C8E A 803:**

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

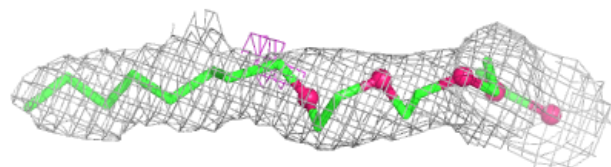
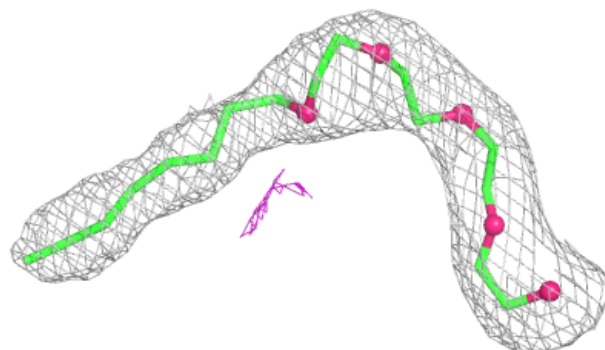


Electron density around C8E A 801:

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

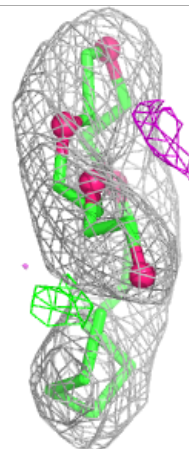
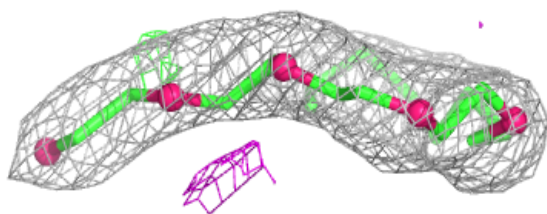
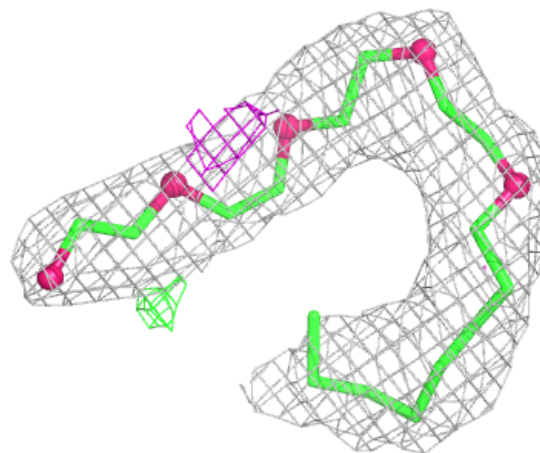
**Electron density around C8E A 800:**

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



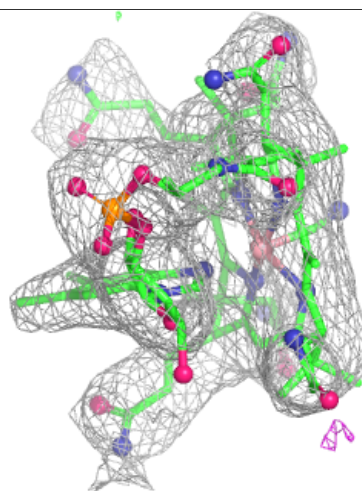
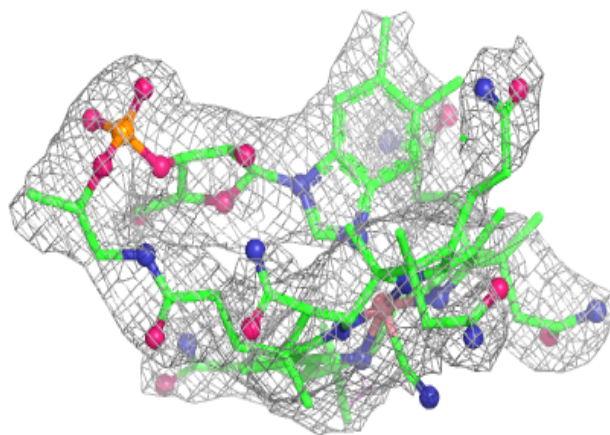
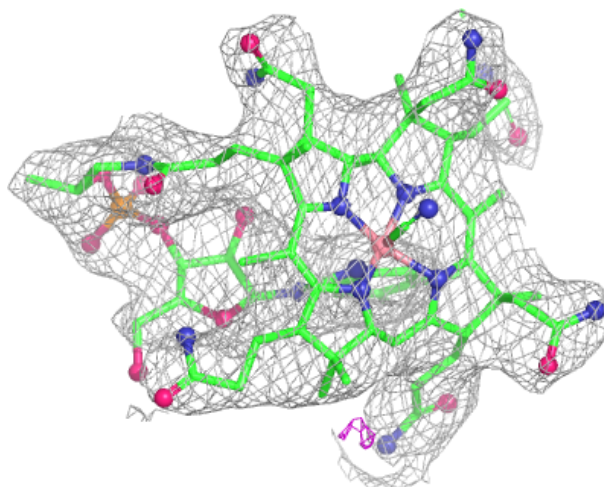
Electron density around C8E A 802:

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



Electron density around CNC A 701:

$2mF_o-DF_c$ (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.