Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2023 – 12:19 AM EDT

PDB ID	:	1NQH
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 (i) 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 (i)) were used in the production of this report:

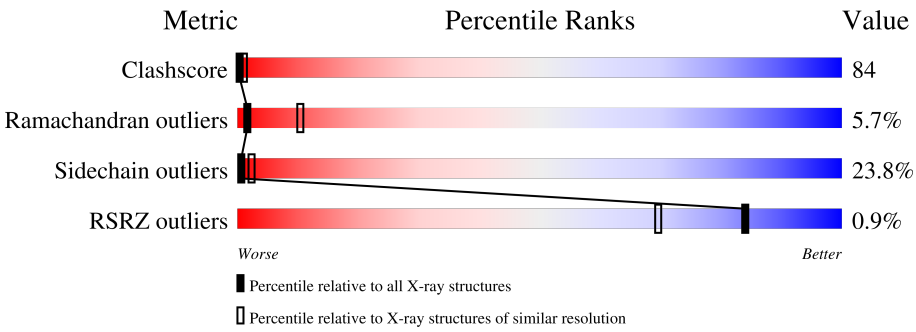
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (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 <=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	% 24% 39% 22% 13% •

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	-
4	C8E	A	805	-	-	-	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.

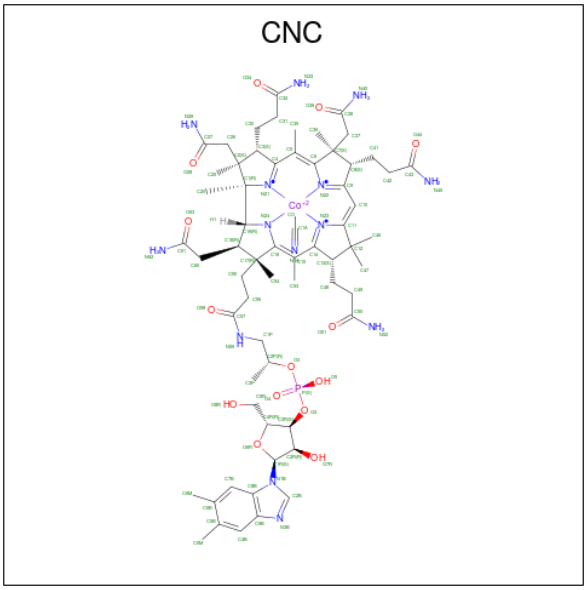
- Molecule 1 is a protein called VITAMIN B12 RECEPTOR.

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

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

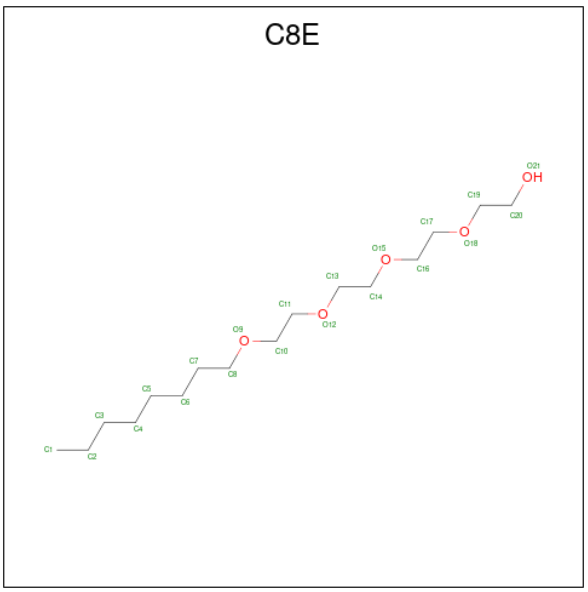
- Molecule 3 is CYANOCOBALAMIN (three-letter code: CNC) (formula: $C_{63}H_{89}CoN_{14}O_{14}P$).



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

- Molecule 4 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code:

C8E) (formula: $C_{16}H_{34}O_5$).



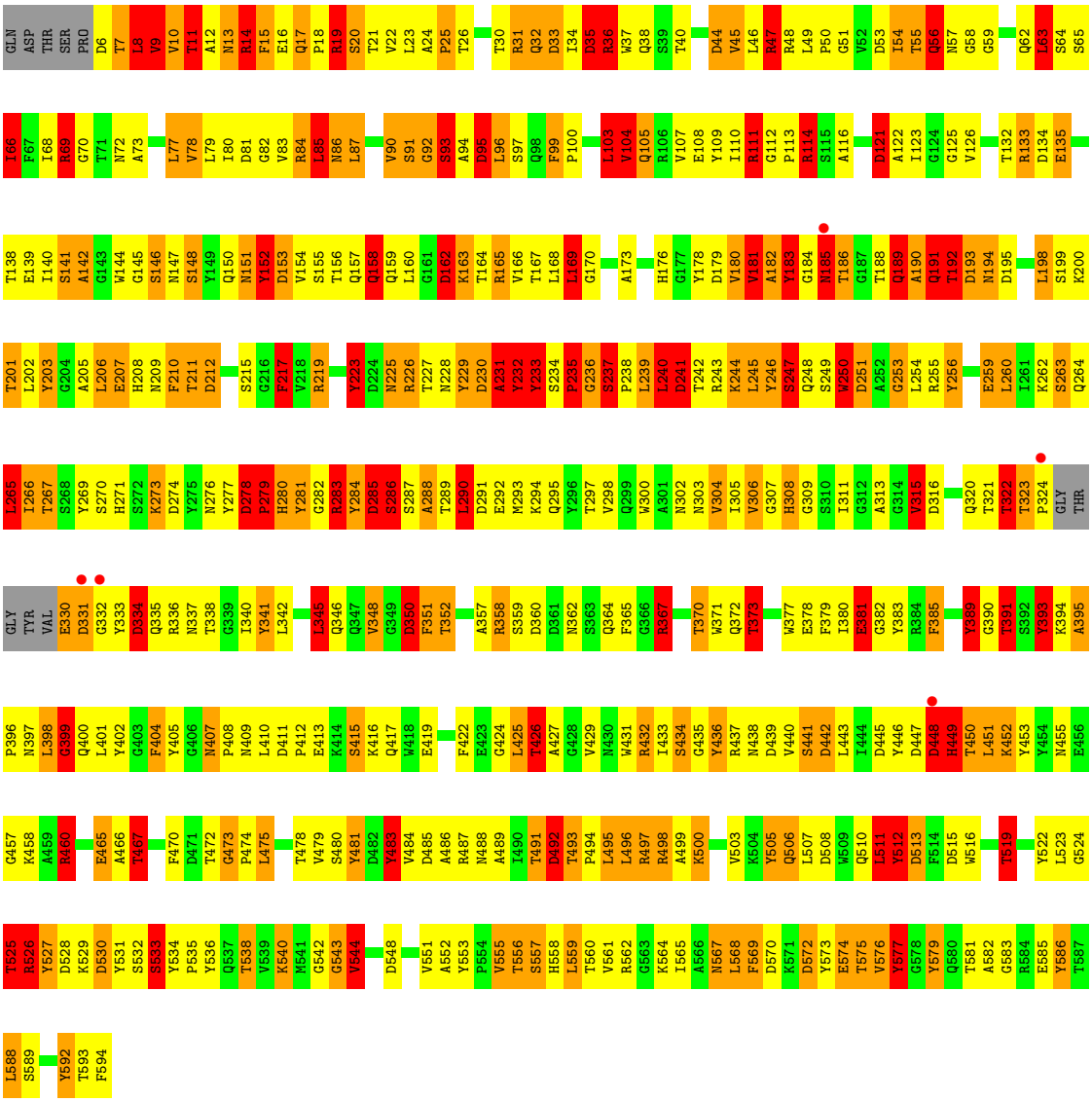
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	21	16	5	0	0
			Total	C	O		
4	A	1	21	16	5	0	0
			Total	C	O		
4	A	1	21	16	5	0	0
			Total	C	O		
4	A	1	21	16	5	0	0
			Total	C	O		
4	A	1	21	16	5	0	0
			Total	C	O		
4	A	1	21	16	5	0	0

3 Residue-property plots (i)

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

Chain A:



4 Data and refinement statistics (i)

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 29.97 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-3.10) 99.8 (29.97-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [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)	0.29 , 52.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o,F_c correlation	0.89	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CNC, C8E, CA

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	1.53	38/4747 (0.8%)	1.61	86/6465 (1.3%)

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 (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	377	TRP	CB-CG	-8.50	1.34	1.50
1	A	381	GLU	CD-OE1	8.12	1.34	1.25
1	A	78	VAL	CB-CG1	-7.66	1.36	1.52
1	A	111	ARG	CZ-NH1	-7.66	1.23	1.33
1	A	152	TYR	CD1-CE1	7.38	1.50	1.39
1	A	152	TYR	CD2-CE2	7.29	1.50	1.39
1	A	126	VAL	CB-CG2	-7.11	1.38	1.52
1	A	223	TYR	CE1-CZ	-6.96	1.29	1.38
1	A	54	ILE	CA-CB	-6.87	1.39	1.54
1	A	66	ILE	CA-CB	-6.70	1.39	1.54
1	A	544	VAL	CB-CG2	-6.69	1.38	1.52
1	A	484	VAL	CB-CG2	-6.59	1.39	1.52
1	A	434	SER	CB-OG	-6.58	1.33	1.42
1	A	577	TYR	CD1-CE1	-6.47	1.29	1.39
1	A	306	VAL	CA-CB	-6.47	1.41	1.54
1	A	9	VAL	CB-CG2	-6.45	1.39	1.52
1	A	481	TYR	CD2-CE2	-6.44	1.29	1.39
1	A	436	TYR	CE1-CZ	-6.42	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	VAL	CB-CG1	-6.37	1.39	1.52
1	A	250	TRP	CB-CG	-6.31	1.38	1.50
1	A	230	ASP	CA-C	6.19	1.69	1.52
1	A	306	VAL	CB-CG2	-6.18	1.39	1.52
1	A	577	TYR	CD2-CE2	-6.07	1.30	1.39
1	A	576	VAL	CB-CG1	-6.05	1.40	1.52
1	A	152	TYR	CE2-CZ	5.87	1.46	1.38
1	A	483	TYR	CG-CD2	-5.86	1.31	1.39
1	A	544	VAL	CA-CB	-5.54	1.43	1.54
1	A	19	ARG	CB-CG	-5.48	1.37	1.52
1	A	111	ARG	NE-CZ	-5.45	1.25	1.33
1	A	434	SER	CA-CB	-5.40	1.44	1.52
1	A	351	PHE	CB-CG	-5.36	1.42	1.51
1	A	10	VAL	CB-CG2	-5.33	1.41	1.52
1	A	586	TYR	CE2-CZ	-5.23	1.31	1.38
1	A	389	TYR	CD2-CE2	-5.23	1.31	1.39
1	A	427	ALA	CA-CB	-5.21	1.41	1.52
1	A	338	THR	CA-CB	-5.21	1.39	1.53
1	A	133	ARG	CG-CD	5.14	1.64	1.51
1	A	203	TYR	CE1-CZ	-5.05	1.31	1.38

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	358	ARG	NE-CZ-NH1	10.79	125.69	120.30
1	A	442	ASP	CB-CG-OD2	10.37	127.63	118.30
1	A	492	ASP	CB-CG-OD2	10.36	127.62	118.30
1	A	241	ASP	CB-CG-OD2	10.25	127.52	118.30
1	A	334	ASP	CB-CG-OD2	9.70	127.03	118.30
1	A	498	ARG	NE-CZ-NH1	-9.61	115.50	120.30
1	A	460	ARG	NE-CZ-NH1	-9.37	115.61	120.30
1	A	193	ASP	CB-CG-OD2	8.88	126.30	118.30
1	A	511	LEU	CA-CB-CG	-8.77	95.13	115.30
1	A	162	ASP	CB-CG-OD2	8.74	126.17	118.30
1	A	439	ASP	CB-CG-OD2	8.73	126.16	118.30
1	A	498	ARG	NE-CZ-NH2	8.33	124.46	120.30
1	A	274	ASP	CB-CG-OD2	8.26	125.73	118.30
1	A	69	ARG	NE-CZ-NH2	8.24	124.42	120.30
1	A	358	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	A	81	ASP	CB-CG-OD2	7.99	125.49	118.30
1	A	47	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	A	230	ASP	CB-CG-OD1	7.85	125.37	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	95	ASP	CB-CG-OD2	7.80	125.32	118.30
1	A	10	VAL	CB-CA-C	-7.72	96.73	111.40
1	A	569	PHE	C-N-CA	-7.52	102.89	121.70
1	A	570	ASP	CB-CG-OD1	-7.46	111.59	118.30
1	A	530	ASP	CB-CG-OD2	7.33	124.90	118.30
1	A	448	ASP	CB-CG-OD2	7.21	124.79	118.30
1	A	103	LEU	CB-CG-CD2	-7.02	99.06	111.00
1	A	570	ASP	CB-CG-OD2	7.02	124.62	118.30
1	A	278	ASP	CB-CG-OD2	7.00	124.60	118.30
1	A	513	ASP	CB-CG-OD2	6.92	124.53	118.30
1	A	230	ASP	N-CA-C	6.89	129.62	111.00
1	A	445	ASP	CB-CG-OD2	6.79	124.41	118.30
1	A	241	ASP	CB-CG-OD1	-6.78	112.19	118.30
1	A	285	ASP	CB-CG-OD2	6.77	124.39	118.30
1	A	53	ASP	CB-CG-OD2	6.76	124.38	118.30
1	A	95	ASP	CB-CG-OD1	-6.73	112.24	118.30
1	A	306	VAL	CB-CA-C	-6.72	98.63	111.40
1	A	198	LEU	CA-CB-CG	6.61	130.51	115.30
1	A	232	TYR	N-CA-C	-6.48	93.49	111.00
1	A	111	ARG	NE-CZ-NH1	-6.48	117.06	120.30
1	A	398	LEU	CA-CB-CG	-6.37	100.65	115.30
1	A	235	PRO	C-N-CA	-6.28	109.12	122.30
1	A	183	TYR	CB-CG-CD1	-6.21	117.27	121.00
1	A	230	ASP	O-C-N	-6.21	112.76	122.70
1	A	432	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	A	350	ASP	CB-CG-OD1	-6.17	112.75	118.30
1	A	158	GLN	CB-CA-C	-6.12	98.15	110.40
1	A	496	LEU	CB-CG-CD1	-6.12	100.59	111.00
1	A	206	LEU	CA-CB-CG	-6.11	101.24	115.30
1	A	33	ASP	CB-CG-OD1	6.09	123.78	118.30
1	A	236	GLY	N-CA-C	6.08	128.29	113.10
1	A	9	VAL	CB-CA-C	-6.02	99.96	111.40
1	A	568	LEU	CA-CB-CG	-5.99	101.53	115.30
1	A	315	VAL	CB-CA-C	-5.97	100.06	111.40
1	A	512	TYR	CB-CA-C	5.89	122.17	110.40
1	A	47	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	14	ARG	NE-CZ-NH2	5.87	123.24	120.30
1	A	153	ASP	CB-CG-OD2	5.86	123.57	118.30
1	A	331	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	36	ARG	CG-CD-NE	5.81	124.01	111.80
1	A	279	PRO	N-CD-CG	-5.81	94.48	103.20
1	A	219	ARG	NE-CZ-NH1	-5.70	117.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	283	ARG	NE-CZ-NH1	-5.69	117.45	120.30
1	A	260	LEU	CB-CG-CD1	-5.65	101.39	111.00
1	A	66	ILE	CB-CA-C	-5.63	100.35	111.60
1	A	523	LEU	CB-CG-CD2	-5.58	101.52	111.00
1	A	491	THR	OG1-CB-CG2	-5.53	97.29	110.00
1	A	230	ASP	OD1-CG-OD2	-5.50	112.84	123.30
1	A	104	VAL	CB-CA-C	-5.48	100.99	111.40
1	A	515	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	416	LYS	CD-CE-NZ	-5.41	99.25	111.70
1	A	367	ARG	CG-CD-NE	5.36	123.05	111.80
1	A	485	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	505	TYR	CB-CA-C	-5.28	99.84	110.40
1	A	114	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	A	399	GLY	N-CA-C	-5.22	100.05	113.10
1	A	265	LEU	CA-CB-CG	5.21	127.29	115.30
1	A	35	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	25	PRO	N-CD-CG	-5.17	95.44	103.20
1	A	84	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	A	231	ALA	N-CA-C	5.14	124.89	111.00
1	A	229	TYR	CB-CA-C	5.11	120.61	110.40
1	A	233	TYR	CB-CA-C	-5.09	100.22	110.40
1	A	96	LEU	CA-CB-CG	-5.09	103.60	115.30
1	A	572	ASP	CB-CG-OD1	-5.03	113.77	118.30
1	A	290	LEU	CB-CG-CD1	-5.02	102.47	111.00
1	A	439	ASP	OD1-CG-OD2	-5.01	113.78	123.30
1	A	206	LEU	CB-CG-CD1	-5.00	102.49	111.00

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

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Mol	Chain	Res	Type	Group
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
1	A	217	PHE	Peptide,Sidechain,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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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 (i)

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	749	0
2	A	4	0	0	0	0
3	A	93	0	82	37	0
4	A	126	0	204	33	0
All	All	4853	0	4628	797	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 84.

All (797) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:701:CNC:H353	3:A:701:CNC:C30	1.57	1.26
1:A:497:ARG:HH12	1:A:576:VAL:CG1	1.51	1.23
1:A:447:ASP:CG	1:A:449:HIS:HB2	1.57	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:13:ASN:HD22	1:A:13:ASN:C	1.42	1.19
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: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
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: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: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:283:ARG:HA	1:A:284:TYR:CB	1.83	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:447:ASP:C	1:A:449:HIS:ND1	2.10	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
1:A:309:GLY:HA3	1:A:346:GLN:NE2	1.74	1.02
1:A:397:ASN:ND2	1:A:400:GLN:CD	2.13	1.01
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:397:ASN:CG	1:A:400:GLN:HG3	1.81	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:324:PRO:HD3	1:A:333:TYR:HE2	1.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:THR:HG23	1:A:324:PRO:HD2	1.48	0.95
1:A:159:GLN:C	1:A:160:LEU:HD12	1.87	0.95
1:A:184:GLY:O	1:A:185:ASN:CG	2.03	0.95
1:A:448:ASP:O	1:A:451:LEU:CD1	2.15	0.95
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:293:MET:HE2	1:A:322:THR:HG22	1.48	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: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:13:ASN:C	1:A:13:ASN:ND2	2.16	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: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:543:GLY:C	1:A:544:VAL:CG1	2.39	0.90
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: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:167:THR:C	1:A:168:LEU:HD23	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ASN:HD21	1:A:295:GLN:HB3	1.40	0.87
1:A:447:ASP:CG	1:A:449:HIS:CB	2.43	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
1:A:450:THR:C	1:A:451:LEU:HD13	1.95	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:330:GLU:C	1:A:333:TYR:HE1	1.80	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
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:266:ILE:CG2	1:A:267:THR:N	2.41	0.83
1:A:407:ASN:C	1:A:407:ASN:HD22	1.82	0.83
1:A:516:TRP:CZ3	1:A:551:VAL:CG1	2.61	0.83
1:A:104:VAL:C	1:A:105:GLN:HE21	1.81	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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:448:ASP:OD1	1:A:449:HIS:N	2.13	0.79
1:A:191:GLN:O	1:A:192:THR:C	2.19	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
1:A:411:ASP:H	1:A:455:ASN:HD21	1.30	0.79
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:169:LEU:HD12	1:A:169:LEU:C	2.04	0.78
1:A:334:ASP:OD1	1:A:334:ASP:C	2.21	0.78
1:A:165:ARG:NH2	1:A:207:GLU:CD	2.38	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:134:ASP:C	1:A:134:ASP:OD1	2.22	0.77
1:A:323:THR:HG23	1:A:324:PRO:CD	2.13	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:105:GLN:HA	1:A:105:GLN:NE2	2.00	0.76
1:A:279:PRO:CD	1:A:282:GLY:H	1.98	0.76
1:A:398:LEU:HD23	1:A:398:LEU:N	1.95	0.76
1:A:7:THR:O	1:A:8:LEU:C	2.17	0.76
1:A:56:GLN:C	1:A:58:GLY:H	1.88	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:534:TYR:HA	1:A:535:PRO:C	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:701:CNC:H601	3:A:701:CNC:H252	1.68	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: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
1:A:404:PHE:CD2	1:A:404:PHE:C	2.59	0.74
1:A:10:VAL:HG12	1:A:16:GLU:HA	1.69	0.74
1:A:330:GLU:C	1:A:333:TYR:CE1	2.60	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:185:ASN:O	1:A:231:ALA:C	2.25	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:407:ASN:C	1:A:407:ASN:ND2	2.41	0.73
1:A:488:ASN:CG	1:A:491:THR:HG22	2.08	0.73
1:A:55:THR:HA	1:A:575:THR:OG1	1.89	0.73
1:A:324:PRO:HB3	1:A:333:TYR:OH	1.88	0.73
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: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: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:304:VAL:CG2	1:A:305:ILE:N	2.50	0.71
1:A:190:ALA:C	1:A:191:GLN:HG2	2.07	0.71
1:A:479:VAL:HG13	1:A:479:VAL:O	1.91	0.71
1:A:290:LEU:HD12	1:A:290:LEU:C	2.07	0.71
1:A:231:ALA:O	1:A:232:TYR:HB2	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:160:LEU:N	1:A:160:LEU:CD1	2.53	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:479:VAL:O	1:A:479:VAL:CG1	2.40	0.69
1:A:31:ARG:O	1:A:32:GLN:C	2.30	0.68
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:95:ASP:OD1	1:A:95:ASP:C	2.32	0.68
1:A:321:THR:HA	1:A:333:TYR:O	1.93	0.68
1:A:169:LEU:C	1:A:169:LEU:CD1	2.62	0.68
1:A:273:LYS:HG2	1:A:292:GLU:HG3	1.75	0.68
1:A:528:ASP:CG	1:A:529:LYS:H	1.96	0.68
1:A:19:ARG:NH2	1:A:26:THR:O	2.27	0.68
1:A:99:PHE:C	1:A:99:PHE:CD2	2.65	0.68
1:A:92:GLY:O	1:A:93:SER:C	2.31	0.68
1:A:105:GLN:NE2	1:A:105:GLN:CA	2.57	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:393:TYR:CD1	1:A:393:TYR:C	2.66	0.68
1:A:184:GLY:C	1:A:185:ASN:CG	2.51	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:68:ILE:O	1:A:69:ARG:C	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:309:GLY:HA3	1:A:346:GLN:CD	2.15	0.66
1:A:283:ARG:CA	1:A:284:TYR:CB	2.66	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: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:293:MET:HE2	1:A:293:MET:HB2	1.75	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:72:ASN:CG	1:A:73:ALA:H	2.00	0.64
1:A:13:ASN:HD21	1:A:15:PHE:H	1.45	0.64
1:A:18:PRO:C	1:A:21:THR:HG22	2.12	0.64
1:A:448:ASP:O	1:A:449:HIS:C	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:529:LYS:NZ	1:A:538:THR:HG23	2.14	0.62
1:A:178:TYR:C	1:A:194:ASN:HA	2.20	0.62
1:A:379:PHE:CD1	1:A:380:ILE:HG13	2.34	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: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:13:ASN:O	1:A:14:ARG:CB	2.47	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:210:PHE:C	1:A:211:THR:CG2	2.69	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:157:GLN:C	1:A:158:GLN:HG2	2.16	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:135:GLU:OE1	1:A:135:GLU:HA	2.01	0.60
1:A:140:ILE:HG22	1:A:141:SER:N	2.16	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:62:GLN:O	1:A:63:LEU:C	2.37	0.59
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:240:LEU:H	1:A:278:ASP:HB3	1.67	0.58
1:A:506:GLN:CD	1:A:519:THR:HB	2.24	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: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
1:A:153:ASP:C	1:A:153:ASP:OD1	2.42	0.57
4:A:802:C8E:H11	4:A:802:C8E:H172	1.86	0.57
1:A:323:THR:CG2	1:A:324:PRO:N	2.67	0.57
4:A:803:C8E:H172	4:A:803:C8E:C11	2.35	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:256:TYR:C	1:A:256:TYR:CD2	2.78	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:397:ASN:C	1:A:401:LEU:HD12	2.25	0.57
1:A:422:PHE:CG	4:A:801:C8E:H11	2.39	0.57
1:A:72:ASN:CG	1:A:73:ALA:N	2.58	0.57
1:A:6:ASP:OD2	1:A:20:SER:CB	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:GLN:C	1:A:58:GLY:N	2.58	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:531:TYR:C	1:A:533:SER:H	2.07	0.56
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:293:MET:HE2	1:A:322:THR:CG2	2.29	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:HG22	1:A:267:THR:O	2.05	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:19:ARG:C	1:A:21:THR:N	2.58	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:286:SER:CA	1:A:287:SER:CB	2.83	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:315:VAL:HG12	1:A:316:ASP:H	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:ILE:HG12	1:A:434:SER:H	1.72	0.54
1:A:313:ALA:HB2	1:A:342:LEU:HD12	1.89	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
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: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:8:LEU:O	1:A:9:VAL:C	2.37	0.54
1:A:304:VAL:HG22	1:A:304:VAL:O	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: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:162:ASP:C	1:A:164:THR:H	2.11	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: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:232:TYR:CD2	1:A:233:TYR:N	2.75	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:191:GLN:C	1:A:193:ASP:N	2.58	0.52
1:A:370:THR:H	4:A:800:C8E:H81	1.74	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:63:LEU:HD21	3:A:701:CNC:HM63	1.92	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:191:GLN:CD	1:A:230:ASP:OD2	2.47	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: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:95:ASP:C	1:A:97:SER:H	2.13	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:499:ALA:O	1:A:500:LYS:C	2.48	0.51
1:A:529:LYS:NZ	1:A:538:THR:HG22	2.25	0.51
1:A:488:ASN:CB	1:A:491:THR:HG22	2.41	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:139:GLU:N	1:A:155:SER:O	2.39	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:297:THR:C	1:A:298:VAL:HG23	2.31	0.50
1:A:565:ILE:HG21	1:A:568:LEU:HD13	1.92	0.50
1:A:567:ASN:C	1:A:567:ASN:HD22	2.15	0.50
1:A:245:LEU:HD23	1:A:246:TYR:N	2.26	0.50
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:531:TYR:O	1:A:533:SER:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:THR:HG23	1:A:493:THR:H	1.77	0.50
1:A:82:GLY:C	1:A:83:VAL:HG23	2.33	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:283:ARG:C	1:A:284:TYR:CD1	2.85	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:146:SER:O	1:A:147:ASN:CG	2.50	0.49
1:A:245:LEU:HD23	1:A:246:TYR:H	1.77	0.49
1:A:283:ARG:C	1:A:284:TYR:CG	2.85	0.49
1:A:56:GLN:H	1:A:575:THR:HG1	1.61	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:140:ILE:C	1:A:141:SER:OG	2.49	0.49
1:A:285:ASP:OD2	1:A:287:SER:HB3	2.12	0.49
1:A:488:ASN:CG	1:A:491:THR:CG2	2.80	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:528:ASP:CG	1:A:529:LYS:N	2.65	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: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: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:14:ARG:HD2	1:A:264:GLN:HE22	1.75	0.48
1:A:309:GLY:HA3	1:A:346:GLN:CG	2.43	0.48
1:A:348:VAL:O	1:A:351:PHE:HB2	2.13	0.48
1:A:531:TYR:C	1:A:533:SER:N	2.65	0.48
3:A:701:CNC:H533	3:A:701:CNC:N52	2.24	0.48
1:A:165:ARG:HH21	1:A:207:GLU:CD	2.16	0.48
1:A:528:ASP:O	1:A:538:THR:HA	2.13	0.48
1:A:91:SER:O	1:A:92:GLY:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:PHE:C	1:A:211:THR:HG23	2.34	0.48
1:A:367:ARG:HH21	4:A:800:C8E:C19	2.21	0.48
1:A:371:TRP:CE2	4:A:805:C8E:H62	2.48	0.48
1:A:248:GLN:NE2	1:A:250:TRP:HE1	2.12	0.48
1:A:208:HIS:C	1:A:208:HIS:ND1	2.66	0.48
4:A:803:C8E:H172	4:A:803:C8E:H142	1.61	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:293:MET:CE	1:A:322:THR:CG2	2.87	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: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:286:SER:OG	1:A:287:SER:C	2.53	0.47
1:A:330:GLU:O	1:A:333:TYR:CE1	2.67	0.47
1:A:534:TYR:CD1	1:A:534:TYR:C	2.88	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:405:TYR:CD2	1:A:446:TYR:HE2	2.33	0.47
1:A:217:PHE:O	1:A:217:PHE:CG	2.68	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:165:ARG:CZ	1:A:207:GLU:OE1	2.63	0.46
1:A:180:VAL:C	1:A:181:VAL:HG23	2.35	0.46
1:A:527:TYR:HE1	1:A:540:LYS:HG3	0.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:389:TYR:CG	1:A:390:GLY:N	2.84	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:185:ASN:CG	1:A:579:TYR:OH	2.54	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:385:PHE:C	1:A:385:PHE:CD2	2.88	0.46
1:A:473:GLY:C	1:A:475:LEU:H	2.19	0.46
1:A:51:GLY:O	1:A:68:ILE:HA	2.16	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:245:LEU:HD22	1:A:245:LEU:C	2.36	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:10:VAL:HG12	1:A:16:GLU:CA	2.45	0.45
1:A:83:VAL:O	1:A:84:ARG:C	2.53	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:323:THR:HG23	1:A:324:PRO:N	2.30	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
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: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:95:ASP:OD2	1:A:97:SER:OG	2.35	0.45
1:A:185:ASN:O	1:A:232:TYR:N	2.49	0.45
1:A:446:TYR:CE2	1:A:451:LEU:HA	2.52	0.45
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:245:LEU:CD2	1:A:245:LEU:C	2.82	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:95:ASP:C	1:A:97:SER:N	2.70	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:32:GLN:O	1:A:33:ASP:C	2.56	0.44
1:A:45:VAL:O	1:A:46:LEU:C	2.54	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:440:VAL:HG12	1:A:441:SER:H	1.83	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:436:TYR:CD2	1:A:436:TYR:C	2.90	0.44
1:A:68:ILE:O	1:A:70:GLY:N	2.51	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: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: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:147:ASN:O	1:A:148:SER:C	2.55	0.43
1:A:417:GLN:HA	1:A:437:ARG:O	2.17	0.43
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:150:GLN:HG2	1:A:151:ASN:N	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ARG:O	1:A:33:ASP:N	2.50	0.43
1:A:249:SER:C	1:A:250:TRP:CD1	2.92	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: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:265:LEU:HD23	1:A:300:TRP:CG	2.53	0.43
1:A:293:MET:HE1	1:A:322:THR:HG22	1.92	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: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: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:483:TYR:CD2	1:A:483:TYR:C	2.93	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: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:526:ARG:CG	1:A:527:TYR:N	2.82	0.42
1:A:534:TYR:CG	1:A:535:PRO:HA	2.55	0.42
1:A:223:TYR:CZ	1:A:247:SER:OG	2.69	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:380:ILE:O	1:A:381:GLU:C	2.58	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
1:A:239:LEU:C	1:A:240:LEU:HG	2.35	0.42
1:A:526:ARG:C	1:A:527:TYR:HD1	2.23	0.42
1:A:576:VAL:O	1:A:577:TYR:C	2.58	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:567:ASN:C	1:A:567:ASN:ND2	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:LEU:HB2	1:A:457:GLY:C	2.39	0.42
1:A:481:TYR:OH	1:A:483:TYR:HB2	2.20	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:281:TYR:CD2	1:A:281:TYR:C	2.94	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:285:ASP:CG	1:A:287:SER:HB3	2.40	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: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:495:LEU:C	1:A:496:LEU:HD12	2.42	0.41
1:A:225:ASN:N	1:A:225:ASN:HD22	2.18	0.41
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: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
1:A:59:GLY:O	1:A:62:GLN:CG	2.67	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:405:TYR:HB3	1:A:451:LEU:C	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:TYR:CG	1:A:446:TYR:CE2	3.05	0.40
1:A:446:TYR:CD1	1:A:446:TYR:C	2.94	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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	580/594 (98%)	480 (83%)	67 (12%)	33 (6%)	1 10

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
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

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Mol	Chain	Res	Type
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	487/495 (98%)	371 (76%)	116 (24%)	0 2

All (116) residues with a non-rotameric sidechain are listed below:

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

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Mol	Chain	Res	Type
1	A	55	THR
1	A	56	GLN
1	A	63	LEU
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	169	LEU
1	A	176	HIS
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
1	A	194	ASN
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	235	PRO
1	A	237	SER
1	A	239	LEU

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Mol	Chain	Res	Type
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	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	304	VAL
1	A	322	THR
1	A	323	THR
1	A	330	GLU
1	A	334	ASP
1	A	336	ARG
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
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	441	SER
1	A	449	HIS
1	A	450	THR
1	A	451	LEU
1	A	452	LYS
1	A	460	ARG
1	A	467	THR
1	A	474	PRO

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Mol	Chain	Res	Type
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	540	LYS
1	A	548	ASP
1	A	555	VAL
1	A	557	SER
1	A	559	LEU
1	A	564	LYS
1	A	567	ASN
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 (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	32	GLN
1	A	56	GLN
1	A	72	ASN
1	A	86	ASN
1	A	98	GLN
1	A	105	GLN
1	A	147	ASN
1	A	157	GLN
1	A	158	GLN
1	A	185	ASN
1	A	189	GLN
1	A	209	ASN
1	A	225	ASN
1	A	248	GLN
1	A	295	GLN
1	A	302	ASN

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Mol	Chain	Res	Type
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 (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 monosaccharides 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	800	-	20,20,20	0.50	0	19,19,19	0.98	0
4	C8E	A	802	-	20,20,20	0.37	0	19,19,19	1.19	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	CNC	A	701	-	90,103,103	1.33	13 (14%)	139,171,171	2.95	61 (43%)
4	C8E	A	804	-	20,20,20	0.43	0	19,19,19	0.98	2 (10%)
4	C8E	A	803	-	20,20,20	0.54	0	19,19,19	1.11	0
4	C8E	A	805	-	20,20,20	0.68	0	19,19,19	0.75	0
4	C8E	A	801	-	20,20,20	0.40	0	19,19,19	1.03	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	800	-	-	10/18/18/18	-
4	C8E	A	802	-	-	13/18/18/18	-
3	CNC	A	701	-	1/1/36/38	15/52/235/235	0/3/11/11
4	C8E	A	804	-	-	10/18/18/18	-
4	C8E	A	803	-	-	9/18/18/18	-
4	C8E	A	805	-	-	10/18/18/18	-
4	C8E	A	801	-	-	11/18/18/18	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	CNC	C12-C13	-4.44	1.42	1.55
3	A	701	CNC	C18-C19	-4.28	1.45	1.54
3	A	701	CNC	P-O3	-3.11	1.52	1.60
3	A	701	CNC	C61-N62	-3.04	1.22	1.32
3	A	701	CNC	C1-C19	-2.62	1.47	1.54
3	A	701	CNC	C2R-C3R	-2.57	1.47	1.52
3	A	701	CNC	O63-C61	2.57	1.31	1.24
3	A	701	CNC	C48-C13	-2.42	1.48	1.54
3	A	701	CNC	C2-C3	-2.37	1.50	1.57
3	A	701	CNC	O44-C43	2.36	1.31	1.24
3	A	701	CNC	C3R-C4R	-2.09	1.47	1.52
3	A	701	CNC	C17-C18	-2.08	1.50	1.54
3	A	701	CNC	P-O2	-2.05	1.55	1.60

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	701	CNC	C15-C16-N24	-10.22	112.00	122.38
3	A	701	CNC	C17-C16-C15	8.11	139.06	126.73
3	A	701	CNC	C12-C11-C10	-6.94	117.20	123.54
3	A	701	CNC	C35-C5-C4	-6.74	103.04	116.79
3	A	701	CNC	C7B-C8B-C9B	6.74	127.21	120.54
3	A	701	CNC	C41-C8-C9	6.62	122.86	111.19
3	A	701	CNC	O6R-C4R-C5R	6.57	123.42	109.21
3	A	701	CNC	C54-C17-C18	-6.47	103.43	112.98
3	A	701	CNC	C3-C4-N21	6.20	119.73	111.97
3	A	701	CNC	C1-C19-C18	-6.16	112.70	121.81
3	A	701	CNC	C31-C30-C3	5.84	131.57	114.73
3	A	701	CNC	C17-C18-C19	-5.57	95.95	102.66
3	A	701	CNC	C54-C17-C55	5.26	117.93	109.25
3	A	701	CNC	C55-C17-C16	5.05	127.10	116.24
3	A	701	CNC	C7-C6-N22	-4.90	98.98	107.94
3	A	701	CNC	C25-C2-C1	4.82	121.05	113.78
3	A	701	CNC	C48-C49-C50	-4.78	96.36	112.59
3	A	701	CNC	C30-C3-C2	4.73	129.09	119.09
3	A	701	CNC	C35-C5-C6	4.62	129.78	122.43
3	A	701	CNC	C41-C8-C7	4.55	126.66	114.14
3	A	701	CNC	C3R-C2R-C1R	4.00	108.74	99.89
3	A	701	CNC	C18-C19-N24	3.92	108.10	101.88
3	A	701	CNC	C3-C4-C5	-3.73	117.52	123.81
3	A	701	CNC	C20-C1-C19	-3.62	102.96	110.23
3	A	701	CNC	C5B-C4B-C9B	-3.58	116.15	121.22
3	A	701	CNC	C13-C14-C15	-3.56	117.81	123.81
3	A	701	CNC	C16-C15-C14	3.54	126.16	121.30
3	A	701	CNC	C55-C17-C18	-3.49	104.40	111.15
3	A	701	CNC	O39-C38-C37	-3.35	111.38	121.99
3	A	701	CNC	C5-C4-N21	-3.34	118.76	124.19
3	A	701	CNC	C30-C3-C4	3.34	117.41	109.63
3	A	701	CNC	O63-C61-C60	-3.33	113.86	120.87
3	A	701	CNC	O28-C27-N29	-3.23	113.69	122.50
3	A	701	CNC	C2-C1-N21	3.20	106.23	101.77
3	A	701	CNC	C19-N24-C16	-3.12	106.92	111.96
3	A	701	CNC	C7-C6-C5	3.09	132.93	128.07
3	A	701	CNC	C5M-C5B-C6B	-3.08	114.42	120.74
3	A	701	CNC	C12-C11-N23	-2.95	108.28	111.48
3	A	701	CNC	C26-C2-C3	-2.91	102.26	107.41
3	A	701	CNC	C4B-C9B-C8B	-2.89	118.14	121.10
3	A	701	CNC	C37-C7-C6	-2.84	98.20	107.12
3	A	701	CNC	O58-C57-C56	-2.83	116.83	122.02
3	A	701	CNC	O2-C3R-C4R	2.71	119.87	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	701	CNC	O7R-C2R-C1R	2.71	120.85	110.85
3	A	701	CNC	C3P-C2P-C1P	2.70	116.63	111.39
3	A	701	CNC	C6-C5-C4	2.67	126.32	121.54
4	A	802	C8E	C19-O18-C17	-2.66	101.76	113.29
3	A	701	CNC	C4B-C5B-C6B	2.65	124.38	119.91
3	A	701	CNC	C8-C9-C10	2.65	129.04	123.32
3	A	701	CNC	C9-C10-C11	-2.64	121.99	125.88
4	A	804	C8E	O12-C13-C14	-2.54	98.96	110.39
3	A	701	CNC	C5R-C4R-C3R	2.53	122.89	114.85
3	A	701	CNC	C13-C12-C11	2.50	104.31	100.90
3	A	701	CNC	C10-C9-N22	-2.48	122.89	125.73
3	A	701	CNC	O7R-C2R-C3R	2.42	118.04	111.17
4	A	801	C8E	O12-C13-C14	-2.40	99.57	110.39
3	A	701	CNC	C2-C3-C4	-2.35	98.96	101.63
3	A	701	CNC	C36-C7-C37	2.28	114.56	110.80
3	A	701	CNC	O6R-C4R-C3R	2.27	109.73	104.87
3	A	701	CNC	O39-C38-N40	2.24	128.61	122.50
3	A	701	CNC	C25-C2-C26	2.21	114.19	109.71
3	A	701	CNC	C8-C7-C6	-2.19	97.17	100.92
4	A	804	C8E	O18-C17-C16	-2.15	100.68	110.39
3	A	701	CNC	O3-C2P-C1P	-2.04	102.84	106.92
3	A	701	CNC	O63-C61-N62	2.02	128.01	122.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	701	CNC	N24

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	802	C8E	C14-C13-O12-C11
4	A	801	C8E	C11-C10-O9-C8
4	A	803	C8E	C14-C13-O12-C11
4	A	804	C8E	C11-C10-O9-C8
4	A	805	C8E	C17-C16-O15-C14
4	A	803	C8E	C17-C16-O15-C14
4	A	804	C8E	C20-C19-O18-C17
4	A	803	C8E	C7-C8-O9-C10
4	A	801	C8E	C13-C14-O15-C16
3	A	701	CNC	C3R-C4R-C5R-O8R
4	A	805	C8E	C11-C10-O9-C8

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Mol	Chain	Res	Type	Atoms
4	A	800	C8E	C10-C11-O12-C13
4	A	804	C8E	O15-C16-C17-O18
4	A	803	C8E	O12-C13-C14-O15
4	A	805	C8E	C10-C11-O12-C13
4	A	805	C8E	O9-C10-C11-O12
4	A	804	C8E	C17-C16-O15-C14
3	A	701	CNC	O6R-C4R-C5R-O8R
4	A	800	C8E	O15-C16-C17-O18
3	A	701	CNC	C42-C41-C8-C9
4	A	802	C8E	C6-C7-C8-O9
4	A	801	C8E	O18-C19-C20-O21
4	A	801	C8E	O9-C10-C11-O12
4	A	803	C8E	C16-C17-O18-C19
4	A	804	C8E	O9-C10-C11-O12
4	A	804	C8E	O18-C19-C20-O21
3	A	701	CNC	C12-C13-C48-C49
3	A	701	CNC	C38-C37-C7-C8
4	A	800	C8E	O18-C19-C20-O21
4	A	805	C8E	C4-C5-C6-C7
4	A	801	C8E	O12-C13-C14-O15
4	A	803	C8E	C4-C5-C6-C7
4	A	801	C8E	C6-C7-C8-O9
4	A	805	C8E	O15-C16-C17-O18
4	A	804	C8E	C3-C4-C5-C6
4	A	802	C8E	C5-C6-C7-C8
3	A	701	CNC	C18-C60-C61-O63
4	A	800	C8E	C4-C5-C6-C7
4	A	800	C8E	C11-C10-O9-C8
3	A	701	CNC	N59-C1P-C2P-C3P
4	A	800	C8E	C3-C4-C5-C6
4	A	802	C8E	C1-C2-C3-C4
4	A	804	C8E	C1-C2-C3-C4
3	A	701	CNC	C18-C60-C61-N62
4	A	800	C8E	O12-C13-C14-O15
4	A	805	C8E	C20-C19-O18-C17
4	A	800	C8E	C14-C13-O12-C11
4	A	800	C8E	C13-C14-O15-C16
4	A	801	C8E	C14-C13-O12-C11
4	A	801	C8E	C17-C16-O15-C14
4	A	802	C8E	C17-C16-O15-C14
4	A	801	C8E	C20-C19-O18-C17
4	A	802	C8E	C20-C19-O18-C17

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Mol	Chain	Res	Type	Atoms
4	A	802	C8E	O9-C10-C11-O12
4	A	803	C8E	C10-C11-O12-C13
4	A	802	C8E	C16-C17-O18-C19
4	A	805	C8E	C7-C8-O9-C10
4	A	802	C8E	O18-C19-C20-O21
4	A	805	C8E	C14-C13-O12-C11
4	A	804	C8E	C10-C11-O12-C13
4	A	805	C8E	C3-C4-C5-C6
3	A	701	CNC	O58-C57-N59-C1P
4	A	801	C8E	C16-C17-O18-C19
4	A	803	C8E	C5-C6-C7-C8
4	A	803	C8E	O15-C16-C17-O18
3	A	701	CNC	C1-C2-C26-C27
3	A	701	CNC	C48-C49-C50-N52
4	A	804	C8E	C2-C3-C4-C5
4	A	800	C8E	C7-C8-O9-C10
4	A	802	C8E	C10-C11-O12-C13
3	A	701	CNC	C38-C37-C7-C36
3	A	701	CNC	C13-C48-C49-C50
4	A	802	C8E	C11-C10-O9-C8
3	A	701	CNC	C7-C37-C38-N40
4	A	802	C8E	O12-C13-C14-O15
4	A	802	C8E	C7-C8-O9-C10
3	A	701	CNC	C48-C49-C50-O51
4	A	801	C8E	O15-C16-C17-O18

There are no ring outliers.

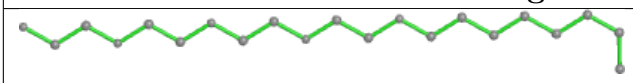
7 monomers are involved in 70 short contacts:

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

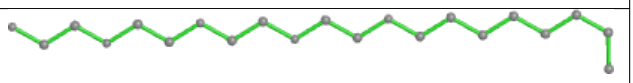
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

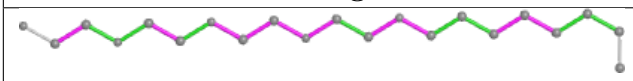
Ligand C8E A 800



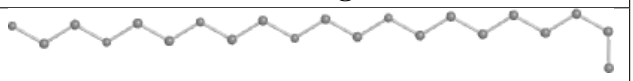
Bond lengths



Bond angles

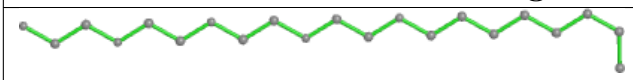


Torsions

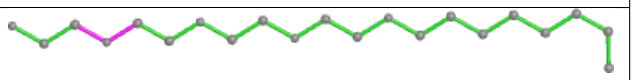


Rings

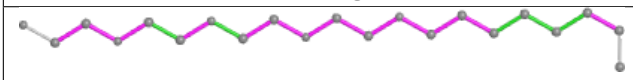
Ligand C8E A 802



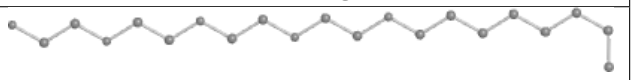
Bond lengths



Bond angles

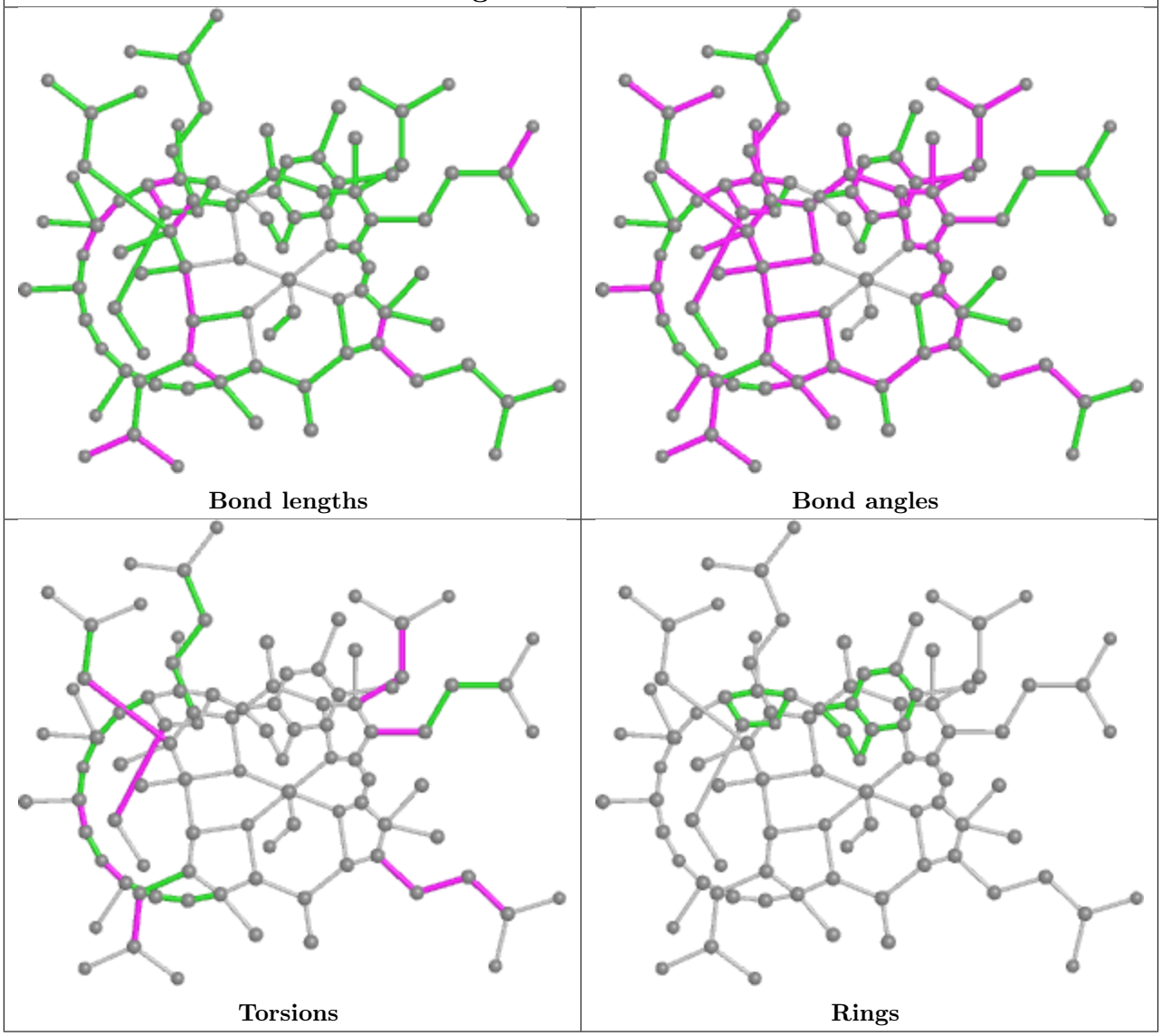


Torsions

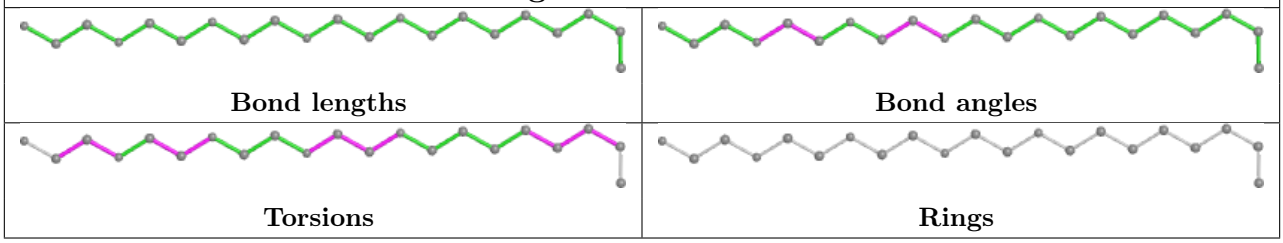


Rings

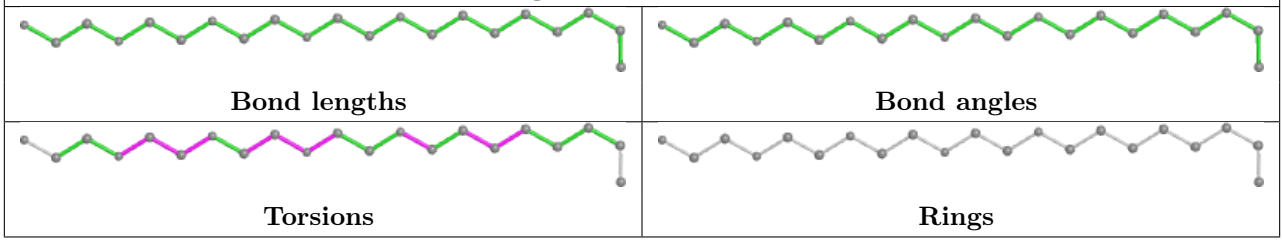
Ligand CNC A 701

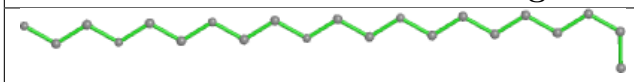
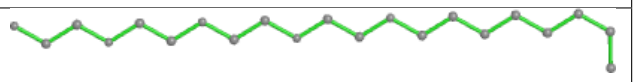
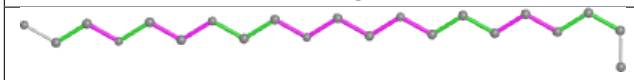
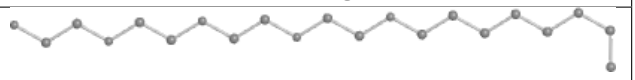


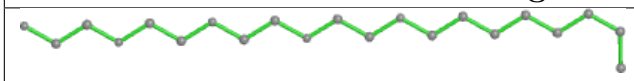
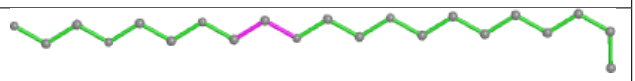
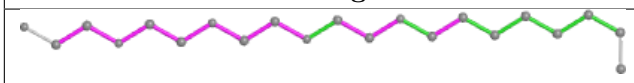
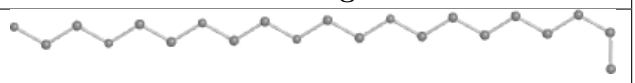
Ligand C8E A 804



Ligand C8E A 803



Ligand C8E A 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand C8E A 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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%)	-0.48	5 (0%) 84 69	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	2.3
1	A	324	PRO	2.2
1	A	448	ASP	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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	597	1/1	0.72	0.14	76,76,76,76	0
4	C8E	A	805	21/21	0.76	0.47	43,65,82,86	0

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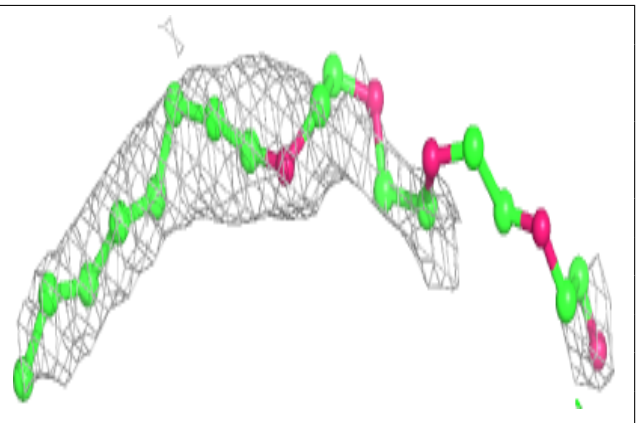
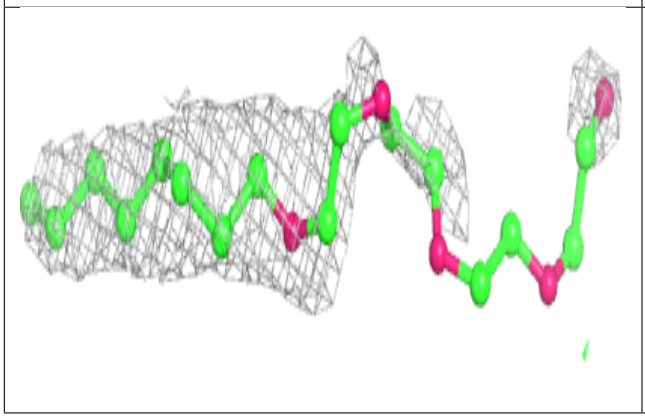
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	A	598	1/1	0.79	0.12	76,76,76,76	0
4	C8E	A	803	21/21	0.86	0.30	45,64,70,74	0
4	C8E	A	804	21/21	0.87	0.25	41,50,61,66	0
4	C8E	A	801	21/21	0.89	0.32	40,56,69,72	0
4	C8E	A	800	21/21	0.94	0.17	38,44,50,52	0
3	CNC	A	701	93/93	0.94	0.17	29,51,69,81	0
4	C8E	A	802	21/21	0.94	0.22	40,48,54,63	0
2	CA	A	595	1/1	0.97	0.06	54,54,54,54	0
2	CA	A	596	1/1	0.98	0.07	57,57,57,57	0

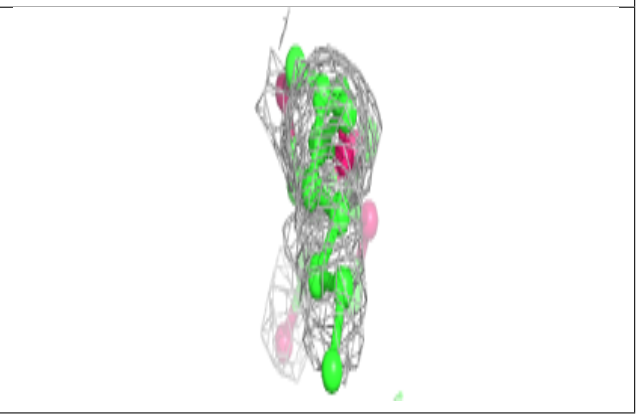
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around C8E A 805:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

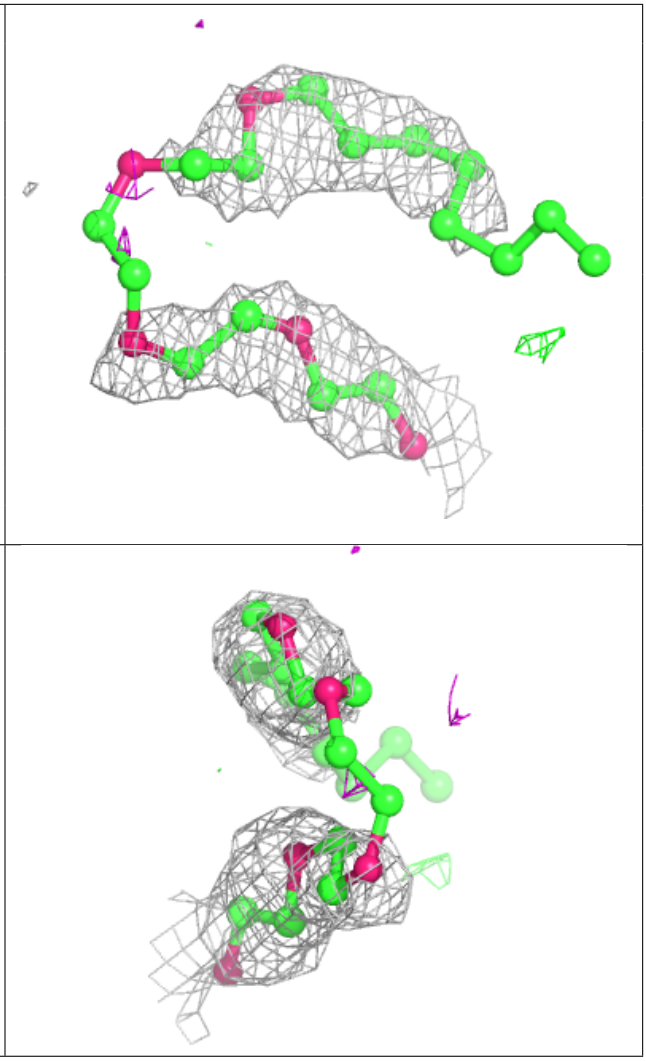






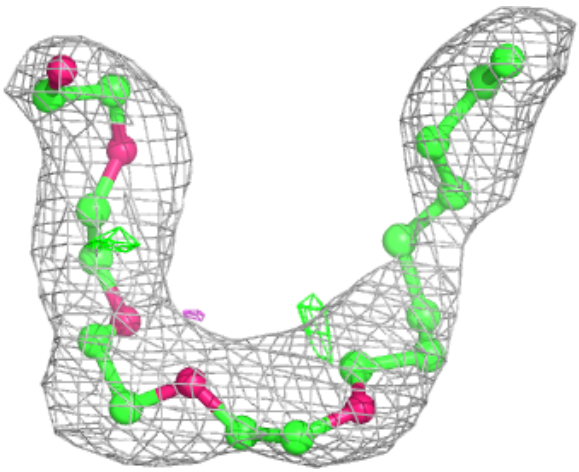
Electron density around C8E A 803:

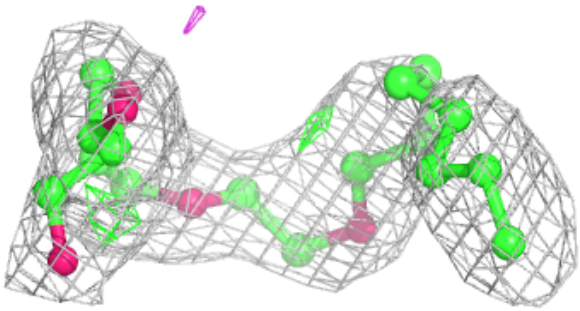
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

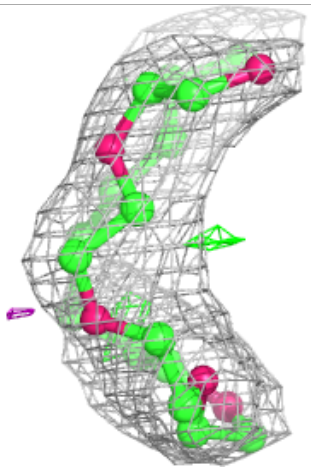


Electron density around C8E A 804:

$2mF_o$-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 801:

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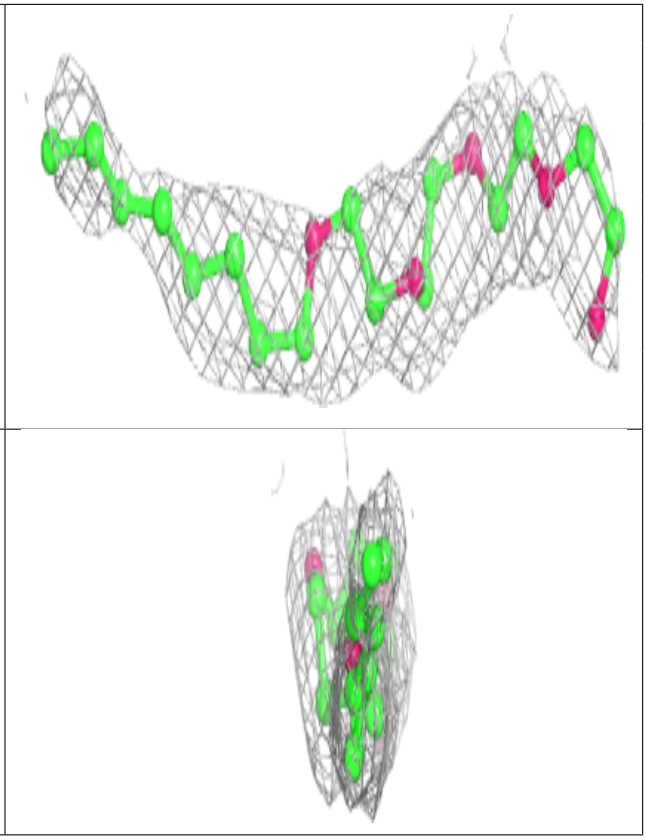
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around C8E A 800:

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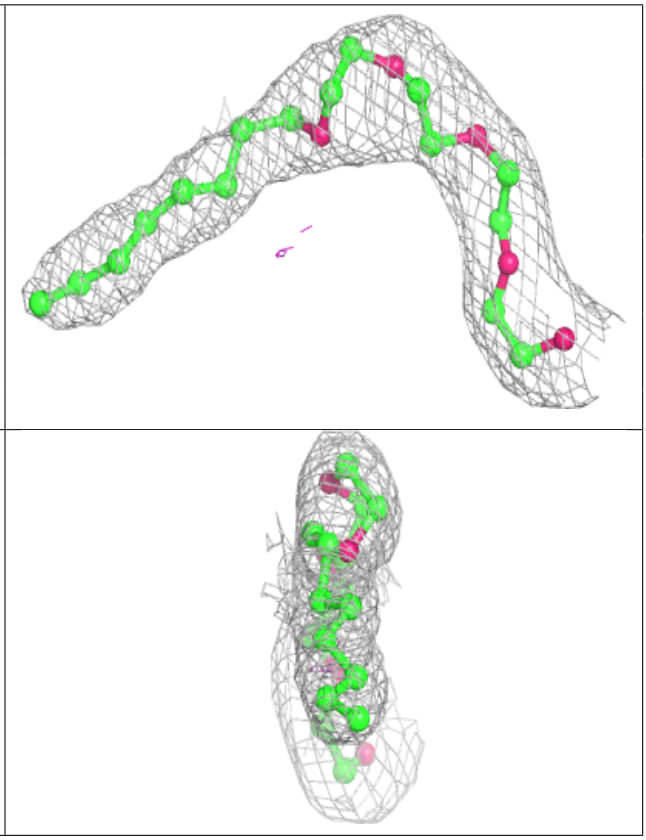
and green (positive)



Electron density around CNC A 701:

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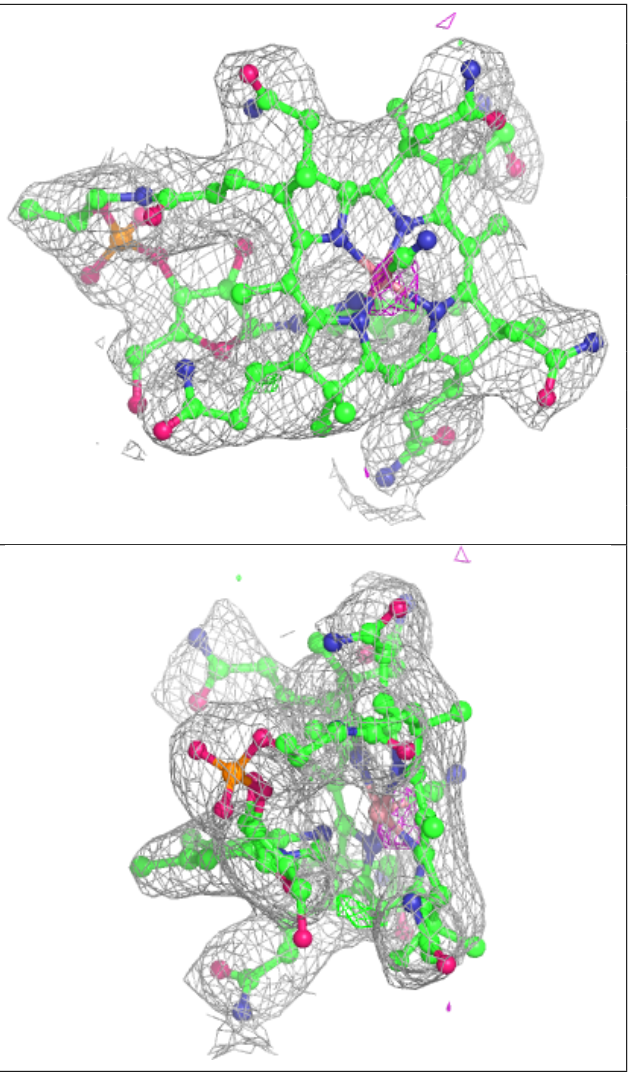
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around C8E A 802:

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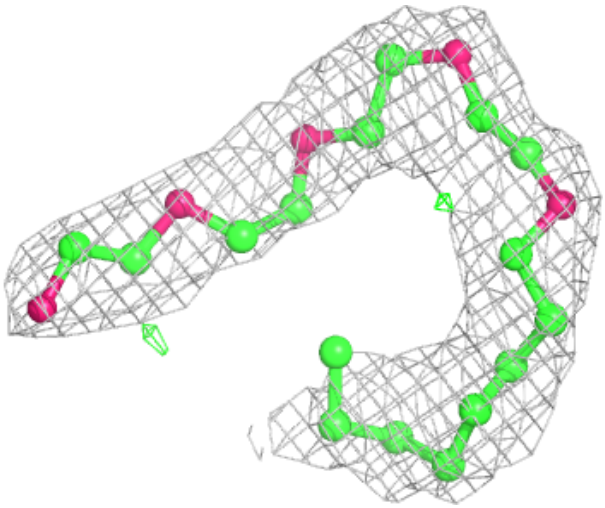
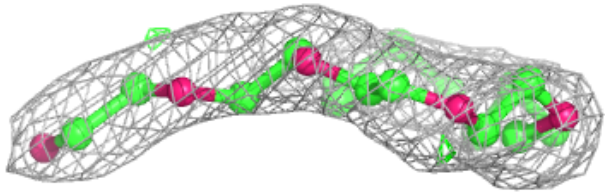
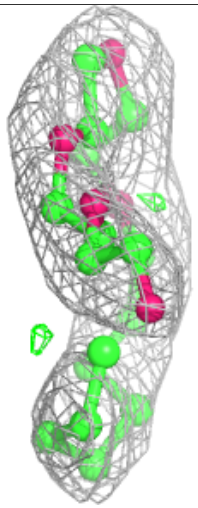
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.