



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:27 PM UTC

PDB ID : 1NQG / pdb_00001nqg
Title : OUTER MEMBRANE COBALAMIN TRANSPORTER (BTUB) FROM E. COLI, WITH BOUND CALCIUM
Authors : Chimento, D.P.; Mohanty, A.K.; Kadner, R.J.; Wiener, M.C.
Deposited on : 2003-01-21
Resolution : 3.31 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

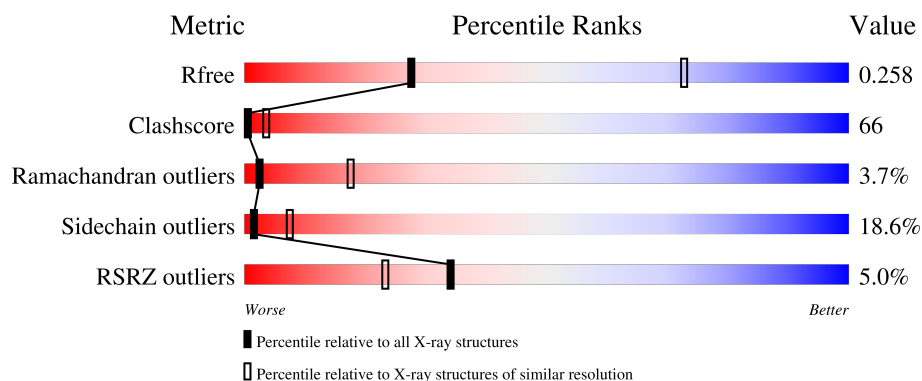
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (3.34-3.30)

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	5% 32% 41% 20% • •

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	C8E	A	800	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4685 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.

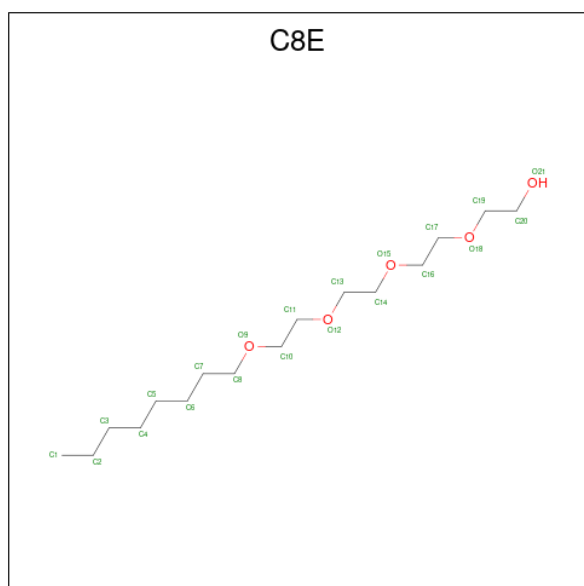
- Molecule 1 is a protein called vitamin b12 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	576	Total	C	N	O	S	0	0	0
			4555	2863	781	909	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 (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (CCD ID: C8E) (formula: C₁₆H₃₄O₅).



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

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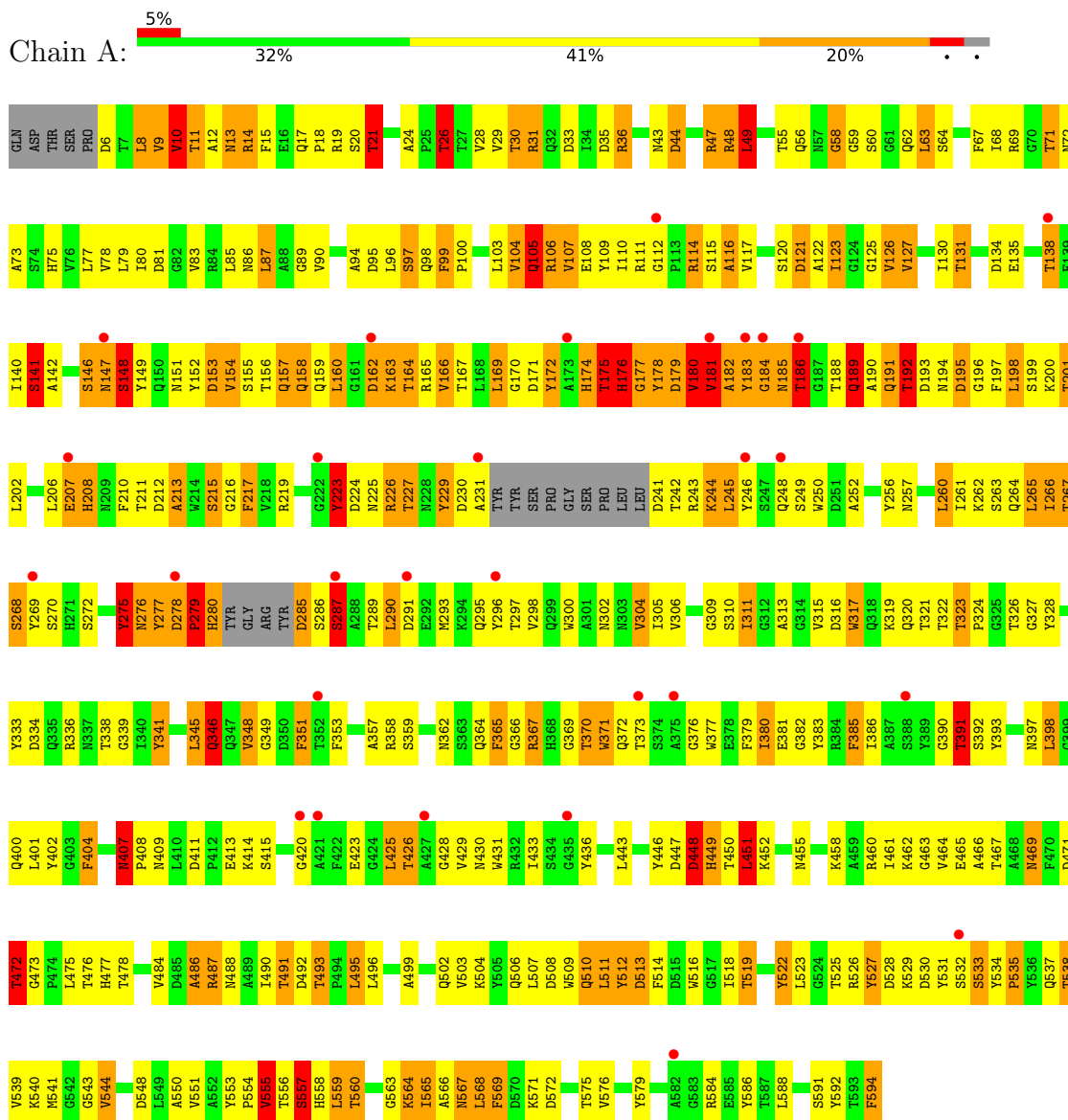
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			21	16	5		

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	81.63Å 81.63Å 225.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.31 20.00 – 3.31	Depositor EDS
% Data completeness (in resolution range)	95.1 (20.00-3.31) 94.5 (20.00-3.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.68 (at 3.31Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.234 , 0.259 0.230 , 0.258	Depositor DCC
R_{free} test set	643 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	69.2	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 67.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	4685	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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

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	1.77	74/4666 (1.6%)	1.74	105/6352 (1.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	ILE	CA-CB	-11.15	1.44	1.55
1	A	311	ILE	CA-CB	-9.10	1.42	1.55
1	A	83	VAL	CA-CB	-8.73	1.44	1.54
1	A	306	VAL	CA-CB	-8.65	1.42	1.53
1	A	10	VAL	CA-CB	-8.18	1.43	1.54
1	A	380	ILE	CA-CB	-8.13	1.43	1.54
1	A	377	TRP	C-O	-8.01	1.15	1.24
1	A	26	THR	C-O	-7.62	1.14	1.23
1	A	478	THR	CA-CB	-7.51	1.42	1.52
1	A	305	ILE	CA-CB	-7.39	1.44	1.53
1	A	265	LEU	CA-C	-7.23	1.44	1.52
1	A	464	VAL	CA-CB	-7.16	1.45	1.54
1	A	461	ILE	CA-CB	-7.05	1.45	1.54
1	A	365	PHE	CA-C	-7.04	1.43	1.52
1	A	29	VAL	CA-C	-6.99	1.44	1.52
1	A	154	VAL	CA-CB	-6.94	1.45	1.54
1	A	484	VAL	CA-CB	-6.90	1.45	1.53
1	A	462	LYS	CA-C	-6.88	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	VAL	CA-CB	-6.86	1.44	1.54
1	A	310	SER	CA-C	-6.85	1.44	1.52
1	A	80	ILE	CA-CB	-6.78	1.46	1.54
1	A	401	LEU	CA-C	-6.70	1.45	1.52
1	A	512	TYR	N-CA	-6.67	1.39	1.47
1	A	104	VAL	C-O	-6.66	1.17	1.24
1	A	407	ASN	CA-C	-6.53	1.44	1.52
1	A	313	ALA	CA-CB	-6.49	1.43	1.53
1	A	380	ILE	CA-C	-6.46	1.44	1.52
1	A	117	VAL	N-CA	-6.42	1.39	1.46
1	A	266	ILE	CA-CB	-6.36	1.44	1.55
1	A	49	LEU	C-O	-6.28	1.17	1.23
1	A	109	TYR	C-O	-6.22	1.17	1.23
1	A	522	TYR	CA-CB	-6.20	1.44	1.53
1	A	466	ALA	CA-CB	-6.18	1.43	1.53
1	A	486	ALA	CA-CB	-6.16	1.45	1.53
1	A	157	GLN	CA-C	-6.05	1.45	1.52
1	A	512	TYR	CA-CB	-6.02	1.46	1.53
1	A	29	VAL	CA-CB	-6.00	1.47	1.54
1	A	401	LEU	N-CA	-5.99	1.38	1.46
1	A	140	ILE	CA-C	-5.88	1.45	1.52
1	A	298	VAL	CA-CB	-5.88	1.47	1.54
1	A	346	GLN	N-CA	-5.87	1.38	1.46
1	A	36	ARG	CA-C	-5.82	1.45	1.52
1	A	503	VAL	CA-CB	-5.77	1.47	1.54
1	A	367	ARG	CA-C	-5.77	1.45	1.52
1	A	28	VAL	CA-C	-5.76	1.45	1.52
1	A	78	VAL	CA-CB	-5.74	1.47	1.54
1	A	366	GLY	CA-C	-5.74	1.46	1.52
1	A	575	THR	CA-C	-5.69	1.45	1.52
1	A	164	THR	CA-CB	-5.65	1.43	1.53
1	A	341	TYR	CA-CB	-5.63	1.43	1.54
1	A	467	THR	CA-C	-5.60	1.45	1.52
1	A	99	PHE	C-N	-5.57	1.28	1.33
1	A	430	ASN	CA-CB	-5.57	1.45	1.53
1	A	215	SER	CA-C	-5.51	1.45	1.52
1	A	26	THR	CA-C	-5.51	1.45	1.52
1	A	460	ARG	NE-CZ	5.38	1.39	1.33
1	A	527	TYR	C-O	-5.38	1.17	1.23
1	A	29	VAL	N-CA	-5.33	1.40	1.46
1	A	35	ASP	CA-C	-5.31	1.45	1.52
1	A	567	ASN	CA-C	-5.29	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	341	TYR	CA-C	-5.29	1.46	1.52
1	A	158	GLN	CA-C	-5.26	1.46	1.52
1	A	201	THR	CA-C	-5.24	1.46	1.52
1	A	555	VAL	CA-CB	-5.24	1.48	1.54
1	A	9	VAL	CA-C	-5.20	1.46	1.52
1	A	44	ASP	CA-C	-5.20	1.46	1.52
1	A	351	PHE	CA-C	-5.17	1.46	1.52
1	A	73	ALA	CA-CB	-5.12	1.44	1.53
1	A	223	TYR	CA-C	-5.11	1.46	1.52
1	A	518	ILE	CA-CB	-5.10	1.48	1.54
1	A	63	LEU	CA-C	-5.07	1.46	1.52
1	A	71	THR	CA-CB	-5.05	1.45	1.53
1	A	9	VAL	CA-CB	-5.05	1.47	1.54
1	A	30	THR	CA-CB	-5.05	1.45	1.53

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	306	VAL	CB-CA-C	-10.43	99.51	111.09
1	A	386	ILE	N-CA-C	10.14	122.55	107.75
1	A	472	THR	CB-CA-C	-9.32	96.64	110.24
1	A	575	THR	N-CA-C	-8.68	102.70	113.38
1	A	327	GLY	N-CA-C	-8.62	102.56	115.32
1	A	511	LEU	CA-C-N	-8.52	109.86	121.71
1	A	511	LEU	C-N-CA	-8.52	109.86	121.71
1	A	272	SER	N-CA-C	8.30	123.15	109.95
1	A	448	ASP	N-CA-C	-8.14	102.37	111.82
1	A	544	VAL	N-CA-C	7.64	117.85	108.53
1	A	513	ASP	N-CA-C	-7.29	102.79	114.09
1	A	123	ILE	CB-CA-C	-7.27	105.53	111.71
1	A	386	ILE	N-CA-CB	-7.08	102.44	111.64
1	A	323	THR	CB-CA-C	-7.06	98.52	109.11
1	A	463	GLY	N-CA-C	7.03	121.36	111.10
1	A	31	ARG	N-CA-C	-6.81	104.44	112.89
1	A	495	LEU	N-CA-C	-6.73	99.98	110.42
1	A	415	SER	N-CA-C	6.67	120.28	109.40
1	A	305	ILE	N-CA-C	6.65	117.62	108.84
1	A	512	TYR	N-CA-C	-6.60	97.75	110.56
1	A	484	VAL	N-CA-CB	-6.53	104.25	112.15
1	A	563	GLY	N-CA-C	-6.47	98.54	110.97
1	A	130	ILE	N-CA-C	6.46	117.60	108.36
1	A	275	TYR	CA-C-N	-6.44	112.82	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	275	TYR	C-N-CA	-6.44	112.82	122.74
1	A	316	ASP	N-CA-CB	-6.42	100.88	110.90
1	A	110	ILE	N-CA-CB	-6.40	103.12	111.82
1	A	385	PHE	N-CA-C	6.39	119.13	108.96
1	A	484	VAL	N-CA-C	6.38	116.87	106.72
1	A	518	ILE	N-CA-CB	-6.38	102.57	111.25
1	A	304	VAL	N-CA-C	6.28	117.82	108.46
1	A	21	THR	OG1-CB-CG2	-6.22	96.86	109.30
1	A	371	TRP	N-CA-C	6.21	118.57	108.76
1	A	565	ILE	N-CA-C	-6.20	98.70	107.75
1	A	423	GLU	N-CA-C	-6.18	98.56	109.06
1	A	428	GLY	N-CA-C	-6.17	106.58	115.27
1	A	391	THR	N-CA-CB	-6.14	100.15	110.83
1	A	94	ALA	N-CA-C	6.07	119.15	110.10
1	A	317	TRP	N-CA-C	6.04	119.31	109.59
1	A	311	ILE	N-CA-C	-5.98	99.87	108.42
1	A	557	SER	N-CA-C	-5.94	98.14	110.80
1	A	276	ASN	N-CA-C	5.94	118.80	108.76
1	A	166	VAL	CB-CA-C	-5.91	101.40	110.50
1	A	366	GLY	O-C-N	5.88	126.90	123.08
1	A	588	LEU	N-CA-C	-5.87	98.84	108.76
1	A	83	VAL	N-CA-C	5.79	116.28	108.17
1	A	512	TYR	CB-CA-C	5.78	122.34	112.00
1	A	569	PHE	CA-C-N	-5.77	110.51	121.54
1	A	569	PHE	C-N-CA	-5.77	110.51	121.54
1	A	126	VAL	CB-CA-C	-5.71	102.03	110.82
1	A	30	THR	N-CA-C	5.69	118.14	109.95
1	A	89	GLY	N-CA-C	5.68	119.55	112.73
1	A	487	ARG	NE-CZ-NH1	-5.68	115.82	121.50
1	A	346	GLN	CA-C-N	-5.65	115.21	123.00
1	A	346	GLN	C-N-CA	-5.65	115.21	123.00
1	A	106	ARG	NE-CZ-NH1	-5.64	115.86	121.50
1	A	30	THR	CB-CA-C	-5.64	100.72	111.48
1	A	386	ILE	CB-CA-C	-5.63	102.77	110.77
1	A	85	LEU	CB-CA-C	-5.62	102.89	109.80
1	A	28	VAL	CA-C-N	-5.60	115.81	123.14
1	A	28	VAL	C-N-CA	-5.60	115.81	123.14
1	A	58	GLY	CA-C-N	-5.60	115.36	122.19
1	A	58	GLY	C-N-CA	-5.60	115.36	122.19
1	A	217	PHE	N-CA-C	5.59	117.57	109.07
1	A	43	ASN	N-CA-C	-5.59	105.29	111.71
1	A	380	ILE	CA-C-N	-5.58	113.03	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	ILE	C-N-CA	-5.58	113.03	120.90
1	A	177	GLY	N-CA-C	5.58	126.40	113.18
1	A	429	VAL	N-CA-C	5.55	115.85	107.75
1	A	126	VAL	CA-C-N	-5.54	115.12	122.98
1	A	126	VAL	C-N-CA	-5.54	115.12	122.98
1	A	430	ASN	N-CA-C	5.52	117.74	108.96
1	A	105	GLN	N-CA-C	-5.49	107.13	113.88
1	A	268	SER	N-CA-C	5.49	117.43	108.76
1	A	420	GLY	O-C-N	-5.47	118.34	123.48
1	A	392	SER	N-CA-C	5.42	116.22	108.74
1	A	550	ALA	N-CA-C	5.39	117.59	109.23
1	A	85	LEU	N-CA-C	5.39	118.61	110.64
1	A	12	ALA	N-CA-C	5.37	117.13	111.28
1	A	48	ARG	N-CA-C	5.36	119.54	112.89
1	A	20	SER	N-CA-C	-5.36	105.37	112.34
1	A	544	VAL	N-CA-CB	-5.36	106.16	112.32
1	A	116	ALA	CA-C-N	-5.33	117.17	122.77
1	A	116	ALA	C-N-CA	-5.33	117.17	122.77
1	A	345	LEU	CB-CG-CD1	-5.33	94.72	110.70
1	A	10	VAL	CB-CA-C	-5.30	102.60	111.29
1	A	148	SER	CB-CA-C	-5.28	102.76	111.36
1	A	127	VAL	CA-C-N	-5.27	115.37	123.07
1	A	127	VAL	C-N-CA	-5.27	115.37	123.07
1	A	315	VAL	CB-CA-C	-5.26	102.78	110.62
1	A	131	THR	O-C-N	5.26	128.61	122.24
1	A	429	VAL	CB-CA-C	-5.25	103.32	110.77
1	A	141	SER	N-CA-CB	-5.21	103.44	111.46
1	A	491	THR	OG1-CB-CG2	-5.17	98.96	109.30
1	A	208	HIS	N-CA-C	5.16	116.83	108.26
1	A	449	HIS	N-CA-C	-5.16	105.66	111.28
1	A	107	VAL	CB-CA-C	-5.16	101.79	110.71
1	A	122	ALA	CA-C-N	-5.16	117.92	122.97
1	A	122	ALA	C-N-CA	-5.16	117.92	122.97
1	A	535	PRO	N-CD-CG	-5.14	97.63	103.80
1	A	297	THR	N-CA-C	5.13	117.44	108.76
1	A	180	VAL	CB-CA-C	-5.12	102.88	111.29
1	A	175	THR	CB-CA-C	-5.08	103.97	111.70
1	A	499	ALA	N-CA-C	5.07	117.57	109.96
1	A	328	TYR	N-CA-C	-5.05	104.45	111.52

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	275	TYR	Peptide
1	A	279	PRO	Peptide
1	A	472	THR	Mainchain

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	4555	0	4272	586	0
2	A	4	0	0	0	0
3	A	126	0	204	37	0
All	All	4685	0	4476	603	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 66.

All (603) 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:278:ASP:CG	1:A:279:PRO:HA	1.27	1.52
1:A:181:VAL:CG1	1:A:182:ALA:H	1.29	1.44
1:A:244:LYS:HE3	1:A:246:TYR:CZ	1.59	1.38
1:A:358:ARG:O	3:A:800:C8E:H72	1.33	1.29
1:A:510:GLN:HE21	1:A:510:GLN:N	1.36	1.23
1:A:190:ALA:O	1:A:191:GLN:HG2	1.37	1.22
1:A:142:ALA:HB1	1:A:151:ASN:O	1.36	1.22
1:A:527:TYR:CZ	1:A:540:LYS:HD2	1.74	1.21
1:A:278:ASP:CG	1:A:279:PRO:CA	2.12	1.21
1:A:510:GLN:N	1:A:510:GLN:NE2	1.89	1.21
1:A:555:VAL:HG12	1:A:556:THR:HG23	1.24	1.20
1:A:181:VAL:HG12	1:A:182:ALA:N	1.30	1.19
1:A:226:ARG:NH1	1:A:244:LYS:NZ	1.91	1.17
1:A:226:ARG:NH1	1:A:244:LYS:CE	2.08	1.16
1:A:398:LEU:CD2	1:A:398:LEU:H	1.59	1.16
1:A:226:ARG:NH1	1:A:244:LYS:HZ3	1.42	1.15
1:A:162:ASP:C	1:A:163:LYS:HG2	1.68	1.14
1:A:278:ASP:HB2	1:A:279:PRO:C	1.71	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:TRP:C	1:A:510:GLN:HE21	1.56	1.13
1:A:309:GLY:HA3	1:A:346:GLN:NE2	1.63	1.13
1:A:169:LEU:HD13	1:A:170:GLY:N	1.62	1.12
1:A:286:SER:O	1:A:287:SER:HB2	1.44	1.12
1:A:277:TYR:HB2	1:A:278:ASP:HB3	1.32	1.11
1:A:527:TYR:OH	1:A:540:LYS:HD2	1.50	1.11
1:A:290:LEU:HD12	1:A:290:LEU:C	1.70	1.10
1:A:509:TRP:C	1:A:510:GLN:NE2	2.09	1.10
1:A:181:VAL:CG1	1:A:182:ALA:N	1.94	1.10
1:A:278:ASP:OD1	1:A:279:PRO:HA	1.50	1.09
1:A:180:VAL:HG23	1:A:180:VAL:O	1.51	1.09
1:A:277:TYR:HB2	1:A:278:ASP:CB	1.82	1.09
1:A:278:ASP:CB	1:A:279:PRO:HA	1.83	1.08
1:A:491:THR:HG23	1:A:493:THR:HG23	1.09	1.07
1:A:77:LEU:HD21	1:A:79:LEU:HD21	1.31	1.07
1:A:244:LYS:CE	1:A:246:TYR:CZ	2.37	1.07
1:A:277:TYR:HB2	1:A:278:ASP:CA	1.84	1.07
1:A:398:LEU:H	1:A:398:LEU:HD23	1.09	1.06
1:A:451:LEU:N	1:A:451:LEU:HD22	1.63	1.06
1:A:190:ALA:O	1:A:191:GLN:CG	2.03	1.05
1:A:189:GLN:HA	1:A:189:GLN:OE1	1.57	1.05
1:A:506:GLN:NE2	1:A:519:THR:HB	1.72	1.04
1:A:226:ARG:HH12	1:A:244:LYS:HE2	1.18	1.04
1:A:169:LEU:CD1	1:A:169:LEU:C	2.28	1.02
1:A:226:ARG:HH11	1:A:244:LYS:NZ	1.50	1.02
1:A:446:TYR:OH	1:A:451:LEU:HD13	1.60	1.01
1:A:189:GLN:OE1	1:A:189:GLN:CA	2.09	1.00
1:A:278:ASP:CB	1:A:279:PRO:CA	2.35	1.00
1:A:172:TYR:HD2	1:A:172:TYR:O	1.43	0.99
1:A:555:VAL:HG12	1:A:556:THR:CG2	1.92	0.99
1:A:397:ASN:H	1:A:400:GLN:HE21	1.08	0.99
1:A:162:ASP:O	1:A:163:LYS:CG	2.10	0.99
1:A:160:LEU:HD22	1:A:166:VAL:HG21	1.42	0.98
1:A:172:TYR:O	1:A:172:TYR:CD2	2.17	0.98
1:A:527:TYR:CE1	1:A:540:LYS:HG3	1.97	0.98
1:A:397:ASN:H	1:A:400:GLN:NE2	1.62	0.97
1:A:244:LYS:HE3	1:A:246:TYR:CE1	1.99	0.97
1:A:169:LEU:HD13	1:A:169:LEU:C	1.87	0.97
1:A:165:ARG:HG3	1:A:207:GLU:OE1	1.63	0.97
1:A:278:ASP:HB2	1:A:279:PRO:O	1.62	0.97
1:A:527:TYR:OH	1:A:540:LYS:HE3	1.63	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:THR:HA	1:A:231:ALA:HB2	1.47	0.97
1:A:527:TYR:OH	1:A:540:LYS:CD	2.13	0.95
1:A:226:ARG:NH1	1:A:244:LYS:HE2	1.76	0.95
1:A:534:TYR:CG	1:A:535:PRO:HA	2.00	0.95
1:A:142:ALA:HB2	1:A:152:TYR:HA	1.47	0.94
1:A:379:PHE:O	1:A:380:ILE:HG13	1.67	0.94
1:A:527:TYR:OH	1:A:540:LYS:CE	2.16	0.94
1:A:160:LEU:HD22	1:A:166:VAL:CG2	1.96	0.94
1:A:77:LEU:CD2	1:A:79:LEU:HD21	1.98	0.93
1:A:290:LEU:HD12	1:A:291:ASP:N	1.83	0.93
1:A:398:LEU:CD2	1:A:398:LEU:N	2.27	0.93
1:A:526:ARG:CG	1:A:541:MET:HE2	1.98	0.93
1:A:120:SER:HB2	1:A:393:TYR:CE1	2.03	0.93
1:A:184:GLY:H	1:A:532:SER:CB	1.75	0.92
1:A:323:THR:HG22	1:A:324:PRO:O	1.68	0.92
1:A:451:LEU:HD22	1:A:451:LEU:H	1.30	0.92
1:A:526:ARG:CD	1:A:541:MET:HE2	1.99	0.92
1:A:446:TYR:OH	1:A:451:LEU:CD1	2.16	0.91
1:A:174:HIS:C	1:A:174:HIS:CD2	2.48	0.91
1:A:451:LEU:N	1:A:451:LEU:CD2	2.32	0.91
1:A:491:THR:CG2	1:A:493:THR:HG23	2.00	0.91
1:A:114:ARG:HA	1:A:372:GLN:HE22	1.33	0.91
1:A:10:VAL:HG12	1:A:11:THR:N	1.82	0.91
1:A:510:GLN:HE21	1:A:510:GLN:CA	1.83	0.90
1:A:190:ALA:O	1:A:191:GLN:NE2	2.04	0.89
1:A:197:PHE:CD2	1:A:227:THR:CG2	2.56	0.89
1:A:184:GLY:H	1:A:532:SER:HB3	1.37	0.89
1:A:358:ARG:O	3:A:800:C8E:C7	2.20	0.88
1:A:404:PHE:HD2	1:A:404:PHE:O	1.56	0.88
1:A:425:LEU:C	1:A:425:LEU:CD2	2.47	0.88
1:A:142:ALA:CB	1:A:151:ASN:O	2.19	0.88
1:A:411:ASP:H	1:A:455:ASN:HD21	1.17	0.88
1:A:226:ARG:HH11	1:A:244:LYS:HZ3	0.91	0.87
1:A:165:ARG:O	1:A:207:GLU:OE1	1.93	0.87
1:A:244:LYS:CE	1:A:246:TYR:OH	2.22	0.87
1:A:278:ASP:HB2	1:A:279:PRO:CA	2.00	0.86
1:A:290:LEU:C	1:A:290:LEU:CD1	2.47	0.86
1:A:278:ASP:O	1:A:280:HIS:CD2	2.28	0.86
1:A:472:THR:O	1:A:472:THR:OG1	1.88	0.86
1:A:197:PHE:HD2	1:A:227:THR:CG2	1.89	0.85
1:A:425:LEU:C	1:A:425:LEU:HD23	2.01	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:TYR:CE2	1:A:290:LEU:HD22	2.10	0.85
1:A:244:LYS:HE3	1:A:246:TYR:OH	1.76	0.85
1:A:172:TYR:CD2	1:A:172:TYR:C	2.54	0.84
1:A:319:LYS:HE3	1:A:336:ARG:NH2	1.92	0.84
1:A:426:THR:CG2	1:A:431:TRP:HE1	1.90	0.84
1:A:279:PRO:C	1:A:280:HIS:O	2.20	0.83
1:A:8:LEU:O	1:A:8:LEU:CD1	2.26	0.83
1:A:263:SER:OG	1:A:302:ASN:ND2	2.11	0.83
1:A:90:VAL:HG22	1:A:293:MET:HE3	1.60	0.83
1:A:162:ASP:O	1:A:163:LYS:HG2	1.70	0.82
1:A:286:SER:O	1:A:287:SER:CB	2.27	0.82
1:A:189:GLN:OE1	1:A:189:GLN:N	2.13	0.82
1:A:488:ASN:N	1:A:495:LEU:HD21	1.94	0.82
1:A:362:ASN:ND2	1:A:364:GLN:H	1.75	0.81
1:A:293:MET:HE2	1:A:322:THR:HG22	1.61	0.81
1:A:317:TRP:HD1	1:A:338:THR:OG1	1.62	0.81
1:A:278:ASP:C	1:A:280:HIS:HD2	1.87	0.81
1:A:190:ALA:C	1:A:191:GLN:HG2	2.05	0.81
1:A:277:TYR:CB	1:A:278:ASP:HB3	2.09	0.81
1:A:192:THR:O	1:A:192:THR:HG22	1.80	0.80
1:A:81:ASP:OD2	1:A:131:THR:OG1	1.99	0.80
1:A:277:TYR:HB2	1:A:278:ASP:HA	1.63	0.80
1:A:279:PRO:O	1:A:280:HIS:O	1.99	0.80
1:A:280:HIS:CE1	1:A:285:ASP:OD2	2.34	0.80
1:A:24:ALA:O	1:A:26:THR:HG22	1.81	0.80
1:A:169:LEU:C	1:A:169:LEU:HD12	2.05	0.80
1:A:527:TYR:CZ	1:A:540:LYS:CD	2.61	0.80
1:A:506:GLN:HE22	1:A:519:THR:HB	1.40	0.80
1:A:180:VAL:O	1:A:180:VAL:CG2	2.25	0.80
1:A:358:ARG:C	3:A:800:C8E:H72	2.05	0.80
1:A:226:ARG:HD2	1:A:244:LYS:HG3	1.62	0.80
1:A:13:ASN:O	1:A:14:ARG:HB2	1.81	0.79
1:A:526:ARG:HD3	1:A:541:MET:HE2	1.62	0.79
1:A:369:GLY:HA3	3:A:800:C8E:H82	1.64	0.78
1:A:56:GLN:HG3	1:A:64:SER:HB3	1.66	0.78
1:A:407:ASN:C	1:A:407:ASN:HD22	1.89	0.78
1:A:197:PHE:CD2	1:A:227:THR:HG22	2.18	0.78
1:A:197:PHE:HD2	1:A:227:THR:CB	1.95	0.78
1:A:226:ARG:HH11	1:A:244:LYS:CE	1.83	0.78
1:A:280:HIS:HE1	1:A:285:ASP:OD2	1.65	0.78
1:A:398:LEU:N	1:A:398:LEU:HD22	1.98	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:TRP:CE3	1:A:551:VAL:CG1	2.66	0.77
1:A:13:ASN:HD22	1:A:13:ASN:C	1.92	0.77
1:A:527:TYR:CE1	1:A:540:LYS:CG	2.67	0.77
1:A:81:ASP:OD2	1:A:219:ARG:NH1	2.18	0.77
1:A:191:GLN:HB3	1:A:230:ASP:OD2	1.84	0.77
1:A:527:TYR:HE1	1:A:540:LYS:HG3	1.46	0.76
1:A:162:ASP:O	1:A:163:LYS:HG3	1.85	0.76
1:A:95:ASP:OD1	1:A:97:SER:HB3	1.86	0.76
1:A:186:THR:CA	1:A:231:ALA:HB2	2.16	0.76
1:A:446:TYR:CZ	1:A:451:LEU:HA	2.21	0.75
1:A:148:SER:O	1:A:148:SER:OG	2.05	0.75
1:A:245:LEU:CD2	1:A:246:TYR:N	2.49	0.75
1:A:179:ASP:HA	1:A:195:ASP:OD2	1.87	0.75
1:A:175:THR:O	1:A:176:HIS:C	2.27	0.75
1:A:160:LEU:CD2	1:A:166:VAL:HG21	2.17	0.75
1:A:186:THR:N	1:A:231:ALA:HB1	2.03	0.74
1:A:534:TYR:CD1	1:A:535:PRO:CA	2.70	0.74
1:A:309:GLY:CA	1:A:346:GLN:NE2	2.45	0.74
1:A:186:THR:H	1:A:231:ALA:HB1	1.51	0.74
1:A:506:GLN:HE22	1:A:519:THR:CB	1.99	0.74
1:A:527:TYR:N	1:A:527:TYR:CD1	2.54	0.74
1:A:142:ALA:CB	1:A:152:TYR:HA	2.17	0.73
1:A:174:HIS:CD2	1:A:174:HIS:O	2.41	0.73
1:A:190:ALA:O	1:A:191:GLN:CD	2.31	0.73
1:A:426:THR:HG23	1:A:431:TRP:HE1	1.52	0.73
1:A:90:VAL:HA	1:A:293:MET:HE1	1.70	0.73
1:A:450:THR:O	1:A:451:LEU:C	2.32	0.73
1:A:556:THR:OG1	1:A:557:SER:N	2.13	0.73
1:A:186:THR:N	1:A:231:ALA:CB	2.52	0.72
1:A:277:TYR:N	1:A:277:TYR:CD2	2.55	0.72
1:A:527:TYR:CE1	1:A:540:LYS:HD2	2.21	0.72
1:A:8:LEU:O	1:A:8:LEU:HD12	1.90	0.72
1:A:186:THR:HA	1:A:231:ALA:CB	2.18	0.71
1:A:8:LEU:O	1:A:8:LEU:HD13	1.90	0.71
1:A:13:ASN:ND2	1:A:15:PHE:H	1.87	0.71
1:A:245:LEU:HD23	1:A:246:TYR:N	2.06	0.71
1:A:526:ARG:HD3	1:A:541:MET:CE	2.19	0.71
1:A:487:ARG:NH1	1:A:492:ASP:O	2.23	0.71
1:A:153:ASP:HB2	1:A:171:ASP:OD1	1.89	0.71
1:A:165:ARG:HG3	1:A:207:GLU:CD	2.15	0.71
1:A:126:VAL:CG1	1:A:127:VAL:N	2.53	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:TRP:CE2	3:A:805:C8E:H62	2.26	0.70
1:A:381:GLU:HG3	1:A:382:GLY:N	2.06	0.70
1:A:527:TYR:HH	1:A:540:LYS:HD2	1.56	0.70
1:A:277:TYR:H	1:A:277:TYR:HD2	1.33	0.70
1:A:357:ALA:HB1	3:A:800:C8E:H52	1.73	0.70
1:A:114:ARG:HA	1:A:372:GLN:NE2	2.06	0.70
1:A:135:GLU:H	1:A:157:GLN:HE22	1.39	0.70
1:A:244:LYS:HE2	1:A:246:TYR:OH	1.90	0.70
1:A:373:THR:HG21	3:A:803:C8E:H131	1.74	0.70
1:A:357:ALA:HB2	3:A:805:C8E:H13	1.74	0.70
1:A:526:ARG:CD	1:A:541:MET:CE	2.69	0.70
1:A:278:ASP:HB2	1:A:280:HIS:O	1.92	0.69
1:A:404:PHE:HD2	1:A:404:PHE:C	2.00	0.69
1:A:149:TYR:HA	1:A:175:THR:HB	1.74	0.69
3:A:802:C8E:H13	3:A:802:C8E:H52	1.72	0.69
1:A:201:THR:HG22	1:A:202:LEU:N	2.06	0.69
1:A:277:TYR:CB	1:A:278:ASP:CA	2.69	0.69
1:A:511:LEU:HD21	1:A:512:TYR:CE2	2.27	0.69
1:A:527:TYR:CE1	1:A:540:LYS:CD	2.76	0.69
1:A:104:VAL:C	1:A:105:GLN:HE21	2.01	0.69
1:A:185:ASN:O	1:A:186:THR:HB	1.93	0.69
1:A:197:PHE:CD2	1:A:227:THR:HB	2.27	0.69
1:A:197:PHE:HD2	1:A:227:THR:HB	1.58	0.69
1:A:165:ARG:C	1:A:207:GLU:OE1	2.35	0.69
1:A:277:TYR:N	1:A:277:TYR:HD2	1.91	0.69
1:A:534:TYR:CD1	1:A:535:PRO:HA	2.28	0.69
3:A:802:C8E:H11	3:A:802:C8E:H171	1.75	0.69
1:A:511:LEU:HG	1:A:512:TYR:N	2.06	0.68
1:A:153:ASP:C	1:A:153:ASP:OD1	2.36	0.68
1:A:491:THR:HG23	1:A:493:THR:CG2	2.05	0.67
1:A:527:TYR:N	1:A:527:TYR:HD1	1.90	0.67
1:A:407:ASN:ND2	1:A:409:ASN:H	1.91	0.67
1:A:77:LEU:CG	1:A:79:LEU:HD21	2.24	0.67
1:A:506:GLN:HE21	1:A:519:THR:HB	1.59	0.67
1:A:291:ASP:HA	1:A:326:THR:HG23	1.76	0.67
1:A:534:TYR:CG	1:A:535:PRO:CA	2.75	0.67
1:A:47:ARG:NH2	1:A:548:ASP:OD2	2.27	0.67
1:A:370:THR:N	3:A:800:C8E:H81	2.10	0.67
1:A:516:TRP:CE3	1:A:551:VAL:HG13	2.29	0.67
1:A:275:TYR:CE2	1:A:290:LEU:CD2	2.77	0.67
1:A:526:ARG:C	1:A:527:TYR:HD1	2.03	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:PHE:C	1:A:404:PHE:CD2	2.72	0.67
1:A:185:ASN:O	1:A:186:THR:CB	2.43	0.66
1:A:188:THR:C	1:A:189:GLN:OE1	2.38	0.66
1:A:197:PHE:CD2	1:A:227:THR:CB	2.78	0.66
1:A:278:ASP:C	1:A:280:HIS:CD2	2.72	0.66
1:A:293:MET:HE2	1:A:322:THR:CG2	2.25	0.66
1:A:44:ASP:OD2	1:A:47:ARG:NH1	2.28	0.66
1:A:224:ASP:C	1:A:224:ASP:OD1	2.37	0.66
1:A:183:TYR:O	1:A:185:ASN:OD1	2.12	0.66
1:A:371:TRP:CD2	3:A:805:C8E:H51	2.31	0.66
1:A:184:GLY:N	1:A:532:SER:CB	2.51	0.66
1:A:446:TYR:OH	1:A:451:LEU:HA	1.94	0.66
1:A:229:TYR:CZ	1:A:241:ASP:HB3	2.31	0.66
1:A:506:GLN:HE22	1:A:519:THR:CG2	2.10	0.65
1:A:229:TYR:O	1:A:230:ASP:OD1	2.14	0.65
1:A:13:ASN:C	1:A:13:ASN:ND2	2.52	0.65
1:A:181:VAL:HG13	1:A:182:ALA:N	2.09	0.65
1:A:291:ASP:CA	1:A:326:THR:HG23	2.27	0.65
1:A:191:GLN:O	1:A:193:ASP:N	2.28	0.65
1:A:529:LYS:NZ	1:A:538:THR:HG23	2.11	0.65
1:A:112:GLY:O	1:A:125:GLY:HA2	1.97	0.65
1:A:8:LEU:HD12	1:A:8:LEU:H	1.62	0.64
1:A:176:HIS:HA	1:A:196:GLY:CA	2.28	0.64
1:A:177:GLY:C	1:A:194:ASN:HB3	2.23	0.64
1:A:291:ASP:CB	1:A:326:THR:HG23	2.27	0.64
1:A:397:ASN:OD1	1:A:400:GLN:HG3	1.97	0.64
1:A:186:THR:CA	1:A:231:ALA:CB	2.75	0.64
1:A:245:LEU:CD2	1:A:245:LEU:C	2.70	0.64
1:A:397:ASN:N	1:A:400:GLN:HE21	1.90	0.64
1:A:370:THR:OG1	1:A:391:THR:HG22	1.97	0.64
1:A:317:TRP:CD1	1:A:338:THR:OG1	2.49	0.64
1:A:506:GLN:NE2	1:A:519:THR:CB	2.53	0.64
1:A:55:THR:HB	1:A:576:VAL:CG2	2.27	0.64
1:A:245:LEU:HD22	1:A:246:TYR:N	2.12	0.64
1:A:309:GLY:HA3	1:A:346:GLN:HE22	1.62	0.64
1:A:458:LYS:HD2	1:A:490:ILE:HD11	1.78	0.64
1:A:227:THR:O	1:A:227:THR:OG1	2.16	0.63
1:A:146:SER:OG	1:A:586:TYR:HB2	1.98	0.63
1:A:516:TRP:CZ3	1:A:551:VAL:CG1	2.82	0.63
1:A:169:LEU:HD12	1:A:169:LEU:O	1.96	0.63
1:A:250:TRP:N	1:A:269:TYR:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LEU:HD23	1:A:246:TYR:H	1.63	0.63
1:A:398:LEU:HD23	1:A:398:LEU:N	1.94	0.63
1:A:534:TYR:HA	1:A:535:PRO:C	2.24	0.63
1:A:197:PHE:CE2	1:A:227:THR:CG2	2.82	0.62
1:A:534:TYR:CD1	1:A:535:PRO:HG3	2.34	0.62
1:A:362:ASN:CG	1:A:365:PHE:CE2	2.77	0.62
1:A:162:ASP:C	1:A:163:LYS:CG	2.43	0.62
1:A:226:ARG:CD	1:A:244:LYS:HZ3	2.12	0.62
1:A:162:ASP:HB2	1:A:163:LYS:HZ3	1.65	0.62
1:A:169:LEU:HD13	1:A:170:GLY:CA	2.28	0.62
1:A:425:LEU:HD23	1:A:426:THR:N	2.14	0.62
1:A:226:ARG:CZ	1:A:244:LYS:HZ3	2.10	0.62
1:A:323:THR:HG23	1:A:324:PRO:HD2	1.82	0.62
1:A:36:ARG:NH1	1:A:508:ASP:OD1	2.33	0.61
1:A:309:GLY:HA3	1:A:346:GLN:HE21	1.59	0.61
1:A:592:TYR:HE1	1:A:594:PHE:CG	2.18	0.61
1:A:425:LEU:C	1:A:425:LEU:HD22	2.25	0.61
1:A:362:ASN:CB	1:A:365:PHE:CE2	2.83	0.61
1:A:477:HIS:CE1	1:A:507:LEU:HD11	2.36	0.61
1:A:341:TYR:CD1	1:A:341:TYR:C	2.79	0.61
1:A:379:PHE:C	1:A:380:ILE:HG13	2.25	0.61
1:A:555:VAL:CG1	1:A:556:THR:CG2	2.74	0.61
1:A:31:ARG:O	1:A:31:ARG:HD3	2.01	0.61
1:A:567:ASN:O	1:A:584:ARG:HB2	2.01	0.61
1:A:278:ASP:O	1:A:280:HIS:HD2	1.75	0.60
1:A:224:ASP:OD1	1:A:226:ARG:HD3	2.01	0.60
1:A:533:SER:O	1:A:535:PRO:O	2.20	0.60
1:A:115:SER:O	1:A:358:ARG:HD3	2.02	0.60
1:A:534:TYR:CE1	1:A:535:PRO:HG3	2.37	0.60
1:A:126:VAL:HG12	1:A:127:VAL:N	2.14	0.59
1:A:180:VAL:O	1:A:181:VAL:C	2.45	0.59
1:A:290:LEU:CD1	1:A:291:ASP:N	2.59	0.59
3:A:802:C8E:H161	3:A:802:C8E:H12	1.85	0.59
1:A:179:ASP:OD1	1:A:192:THR:HA	2.03	0.59
1:A:212:ASP:O	1:A:213:ALA:HB2	2.02	0.59
3:A:802:C8E:H11	3:A:802:C8E:C17	2.32	0.59
1:A:241:ASP:OD1	1:A:277:TYR:O	2.21	0.58
1:A:90:VAL:CG2	1:A:293:MET:HE3	2.32	0.58
1:A:407:ASN:HD22	1:A:408:PRO:N	2.00	0.58
1:A:528:ASP:CG	1:A:529:LYS:H	2.11	0.58
1:A:407:ASN:C	1:A:407:ASN:ND2	2.53	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:TYR:CD2	1:A:535:PRO:HA	2.37	0.58
1:A:488:ASN:HB3	1:A:491:THR:HG22	1.85	0.58
1:A:30:THR:O	1:A:33:ASP:HB2	2.04	0.58
1:A:181:VAL:HG12	1:A:182:ALA:H	0.45	0.58
1:A:212:ASP:O	1:A:212:ASP:OD2	2.22	0.58
1:A:77:LEU:HD11	1:A:79:LEU:CD2	2.34	0.58
1:A:472:THR:O	1:A:475:LEU:HB2	2.04	0.58
1:A:529:LYS:HZ3	1:A:538:THR:HG23	1.69	0.58
1:A:201:THR:CG2	1:A:202:LEU:N	2.66	0.57
1:A:446:TYR:OH	1:A:451:LEU:HD12	2.00	0.57
1:A:371:TRP:CZ2	3:A:805:C8E:H62	2.39	0.57
1:A:19:ARG:NH2	1:A:26:THR:O	2.37	0.57
1:A:197:PHE:HD2	1:A:227:THR:HG22	1.56	0.57
1:A:198:LEU:HD13	1:A:198:LEU:C	2.30	0.57
1:A:277:TYR:CB	1:A:278:ASP:HA	2.32	0.57
1:A:77:LEU:CG	1:A:79:LEU:CD2	2.82	0.57
1:A:592:TYR:CD1	1:A:592:TYR:C	2.83	0.57
1:A:160:LEU:CD2	1:A:166:VAL:CG2	2.79	0.57
1:A:296:TYR:HB2	1:A:319:LYS:HB3	1.87	0.57
1:A:176:HIS:HA	1:A:196:GLY:HA2	1.86	0.57
1:A:226:ARG:HH11	1:A:244:LYS:CD	2.18	0.57
1:A:380:ILE:O	1:A:381:GLU:C	2.44	0.57
3:A:803:C8E:C10	3:A:803:C8E:H172	2.34	0.57
1:A:116:ALA:HB2	1:A:370:THR:HG23	1.86	0.57
1:A:146:SER:HG	1:A:586:TYR:HB2	1.70	0.57
1:A:362:ASN:HD22	1:A:364:GLN:H	1.50	0.57
1:A:175:THR:O	1:A:176:HIS:O	2.23	0.57
1:A:197:PHE:CE2	1:A:227:THR:HG22	2.39	0.56
1:A:357:ALA:CB	3:A:800:C8E:H52	2.34	0.56
1:A:502:GLN:HG2	1:A:523:LEU:HD23	1.86	0.56
1:A:516:TRP:CZ3	1:A:551:VAL:HG11	2.40	0.56
1:A:534:TYR:CE1	1:A:535:PRO:HB3	2.40	0.56
1:A:556:THR:HG1	1:A:558:HIS:H	1.51	0.56
1:A:594:PHE:CD1	1:A:594:PHE:N	2.73	0.56
1:A:257:ASN:CG	1:A:257:ASN:O	2.47	0.56
1:A:166:VAL:HG12	1:A:167:THR:N	2.21	0.56
1:A:135:GLU:H	1:A:157:GLN:NE2	2.04	0.55
1:A:323:THR:HG22	1:A:324:PRO:N	2.22	0.55
1:A:162:ASP:HB2	1:A:163:LYS:NZ	2.20	0.55
1:A:174:HIS:C	1:A:174:HIS:HD2	2.08	0.55
1:A:142:ALA:HB2	1:A:152:TYR:CA	2.30	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASN:O	1:A:186:THR:HG22	2.07	0.55
1:A:249:SER:HA	1:A:270:SER:HA	1.87	0.55
1:A:383:TYR:OH	1:A:426:THR:HB	2.06	0.55
1:A:371:TRP:CG	3:A:805:C8E:H51	2.42	0.55
1:A:487:ARG:C	1:A:495:LEU:HD21	2.30	0.55
1:A:184:GLY:N	1:A:532:SER:HB3	2.13	0.55
1:A:69:ARG:HD3	1:A:436:TYR:CE1	2.42	0.55
1:A:369:GLY:CA	3:A:800:C8E:H82	2.35	0.55
1:A:357:ALA:CB	3:A:805:C8E:H13	2.37	0.55
1:A:526:ARG:HG3	1:A:541:MET:HE2	1.86	0.55
1:A:309:GLY:CA	1:A:346:GLN:HE22	2.15	0.55
1:A:164:THR:OG1	1:A:208:HIS:HD2	1.90	0.54
1:A:383:TYR:CE2	3:A:801:C8E:H42	2.41	0.54
1:A:175:THR:O	1:A:175:THR:OG1	2.14	0.54
1:A:528:ASP:O	1:A:538:THR:HA	2.07	0.54
1:A:290:LEU:HD12	1:A:291:ASP:CA	2.37	0.54
1:A:146:SER:OG	1:A:586:TYR:N	2.35	0.54
1:A:6:ASP:HB2	1:A:106:ARG:HH22	1.72	0.54
1:A:120:SER:HB2	1:A:393:TYR:CZ	2.40	0.54
1:A:555:VAL:CG1	1:A:556:THR:HG23	2.16	0.54
1:A:68:ILE:HD13	1:A:68:ILE:N	2.23	0.53
1:A:531:TYR:C	1:A:533:SER:N	2.64	0.53
1:A:496:LEU:HD12	1:A:496:LEU:N	2.22	0.53
1:A:17:GLN:OE1	1:A:21:THR:HG22	2.07	0.53
1:A:164:THR:OG1	1:A:208:HIS:CD2	2.61	0.53
1:A:567:ASN:C	1:A:567:ASN:HD22	2.16	0.53
1:A:594:PHE:N	1:A:594:PHE:HD1	2.07	0.53
1:A:160:LEU:HD22	1:A:166:VAL:HG23	1.86	0.53
1:A:264:GLN:O	1:A:300:TRP:HD1	1.92	0.53
1:A:488:ASN:N	1:A:495:LEU:CD2	2.69	0.53
1:A:528:ASP:OD1	1:A:529:LYS:N	2.35	0.53
1:A:176:HIS:HA	1:A:196:GLY:HA3	1.91	0.53
1:A:197:PHE:CE2	1:A:227:THR:HG21	2.44	0.53
1:A:397:ASN:OD1	1:A:397:ASN:C	2.52	0.53
1:A:138:THR:HB	1:A:156:THR:HB	1.89	0.53
1:A:169:LEU:HD13	1:A:170:GLY:C	2.34	0.53
1:A:197:PHE:HA	1:A:227:THR:HA	1.91	0.53
1:A:379:PHE:CE1	1:A:380:ILE:HD12	2.44	0.53
1:A:502:GLN:OE1	1:A:523:LEU:CD2	2.57	0.53
1:A:151:ASN:CG	1:A:152:TYR:N	2.67	0.52
1:A:567:ASN:HD21	1:A:571:LYS:H	1.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:HIS:CG	1:A:123:ILE:HD12	2.44	0.52
1:A:179:ASP:O	1:A:180:VAL:C	2.50	0.52
1:A:266:ILE:CG2	1:A:267:THR:N	2.70	0.52
1:A:120:SER:OG	1:A:121:ASP:OD1	2.20	0.52
1:A:134:ASP:C	1:A:134:ASP:OD1	2.51	0.52
1:A:278:ASP:OD2	1:A:278:ASP:N	2.41	0.52
1:A:77:LEU:HD11	1:A:79:LEU:HD23	1.90	0.52
1:A:178:TYR:O	1:A:179:ASP:CB	2.57	0.52
1:A:379:PHE:O	1:A:380:ILE:CG1	2.51	0.52
1:A:556:THR:OG1	1:A:558:HIS:N	2.33	0.52
1:A:18:PRO:O	1:A:21:THR:HB	2.09	0.52
1:A:69:ARG:NH1	1:A:436:TYR:CD1	2.78	0.51
1:A:212:ASP:O	1:A:213:ALA:CB	2.59	0.51
1:A:13:ASN:O	1:A:14:ARG:CB	2.53	0.51
1:A:111:ARG:NH2	1:A:465:GLU:OE2	2.43	0.51
1:A:153:ASP:OD1	1:A:154:VAL:N	2.44	0.51
1:A:198:LEU:HD13	1:A:199:SER:N	2.25	0.51
1:A:426:THR:HG23	1:A:431:TRP:NE1	2.22	0.51
1:A:165:ARG:CG	1:A:207:GLU:OE1	2.49	0.51
1:A:81:ASP:CG	1:A:219:ARG:HH12	2.19	0.51
1:A:19:ARG:C	1:A:21:THR:N	2.68	0.51
1:A:55:THR:HB	1:A:576:VAL:HG22	1.92	0.51
1:A:135:GLU:N	1:A:157:GLN:HE22	2.07	0.51
1:A:278:ASP:CG	1:A:279:PRO:N	2.65	0.51
1:A:509:TRP:C	1:A:510:GLN:HE22	2.13	0.51
1:A:185:ASN:O	1:A:186:THR:CG2	2.59	0.50
1:A:534:TYR:CD1	1:A:535:PRO:CG	2.94	0.50
1:A:473:GLY:C	1:A:475:LEU:H	2.19	0.50
1:A:477:HIS:CE1	1:A:507:LEU:CD1	2.94	0.50
1:A:277:TYR:CG	1:A:278:ASP:HB3	2.46	0.50
1:A:146:SER:O	1:A:147:ASN:CG	2.54	0.50
1:A:245:LEU:C	1:A:245:LEU:HD22	2.36	0.50
1:A:198:LEU:C	1:A:198:LEU:CD1	2.85	0.50
1:A:568:LEU:HD23	1:A:569:PHE:CE1	2.47	0.50
1:A:172:TYR:OH	1:A:174:HIS:ND1	2.27	0.50
1:A:522:TYR:CD1	1:A:544:VAL:O	2.65	0.50
1:A:77:LEU:HG	1:A:79:LEU:CD2	2.41	0.50
1:A:450:THR:C	1:A:452:LYS:N	2.69	0.50
1:A:333:TYR:CE1	1:A:402:TYR:CD1	3.00	0.49
1:A:514:PHE:CE2	1:A:553:TYR:CE1	3.00	0.49
1:A:592:TYR:CE1	1:A:594:PHE:HB3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ARG:HG2	1:A:48:ARG:N	2.10	0.49
1:A:289:THR:O	1:A:289:THR:OG1	2.29	0.49
1:A:534:TYR:CD1	1:A:535:PRO:N	2.81	0.49
1:A:116:ALA:HA	1:A:370:THR:CG2	2.43	0.49
1:A:309:GLY:N	1:A:346:GLN:HE22	2.10	0.49
1:A:385:PHE:C	1:A:385:PHE:CD2	2.88	0.49
1:A:398:LEU:O	1:A:402:TYR:N	2.29	0.49
1:A:81:ASP:CG	1:A:219:ARG:NH1	2.70	0.49
1:A:179:ASP:O	1:A:180:VAL:HG22	2.13	0.49
1:A:197:PHE:CD2	1:A:227:THR:HG21	2.47	0.49
1:A:13:ASN:HD22	1:A:14:ARG:N	2.11	0.49
1:A:86:ASN:CG	1:A:87:LEU:N	2.70	0.49
1:A:185:ASN:OD1	1:A:185:ASN:N	2.32	0.49
1:A:226:ARG:HD2	1:A:244:LYS:HZ3	1.76	0.49
1:A:511:LEU:C	1:A:511:LEU:HD12	2.37	0.49
1:A:534:TYR:CE1	1:A:535:PRO:CB	2.96	0.49
1:A:450:THR:OG1	1:A:452:LYS:HB2	2.13	0.49
1:A:516:TRP:CH2	1:A:551:VAL:HG11	2.48	0.49
1:A:98:GLN:OE1	1:A:227:THR:HG21	2.13	0.48
1:A:162:ASP:CB	1:A:163:LYS:NZ	2.76	0.48
1:A:516:TRP:CZ3	1:A:551:VAL:HG13	2.48	0.48
1:A:397:ASN:O	1:A:398:LEU:C	2.57	0.48
1:A:362:ASN:HD22	1:A:365:PHE:H	1.61	0.48
1:A:529:LYS:HZ3	1:A:538:THR:CG2	2.25	0.48
1:A:96:LEU:O	1:A:97:SER:C	2.56	0.48
1:A:208:HIS:C	1:A:208:HIS:ND1	2.71	0.48
1:A:192:THR:O	1:A:192:THR:CG2	2.51	0.48
3:A:804:C8E:H112	3:A:804:C8E:H81	1.14	0.48
1:A:141:SER:O	1:A:142:ALA:HB2	2.14	0.48
1:A:351:PHE:CD1	1:A:351:PHE:N	2.82	0.48
1:A:62:GLN:O	1:A:63:LEU:C	2.54	0.48
1:A:210:PHE:C	1:A:211:THR:HG23	2.39	0.48
1:A:534:TYR:CD1	1:A:535:PRO:CB	2.97	0.48
1:A:179:ASP:C	1:A:180:VAL:HG13	2.37	0.48
1:A:8:LEU:HD12	1:A:8:LEU:N	2.24	0.48
1:A:185:ASN:ND2	1:A:579:TYR:OH	2.47	0.48
1:A:486:ALA:O	1:A:495:LEU:HG	2.14	0.47
1:A:510:GLN:NE2	1:A:510:GLN:CA	2.50	0.47
1:A:275:TYR:CD2	1:A:290:LEU:HB2	2.50	0.47
1:A:381:GLU:HG3	1:A:382:GLY:H	1.79	0.47
1:A:511:LEU:HG	1:A:512:TYR:CG	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:VAL:HG12	1:A:182:ALA:CA	2.33	0.47
1:A:323:THR:CG2	1:A:324:PRO:N	2.74	0.47
1:A:469:ASN:N	1:A:469:ASN:ND2	2.61	0.47
1:A:530:ASP:OD1	1:A:530:ASP:C	2.56	0.47
1:A:244:LYS:NZ	1:A:246:TYR:CE2	2.83	0.47
1:A:404:PHE:O	1:A:404:PHE:CD2	2.48	0.47
1:A:543:GLY:C	1:A:544:VAL:HG13	2.40	0.47
1:A:226:ARG:NH1	1:A:244:LYS:CD	2.72	0.47
1:A:516:TRP:CD2	1:A:551:VAL:CG1	2.97	0.47
1:A:229:TYR:N	1:A:229:TYR:CD2	2.82	0.47
1:A:217:PHE:O	1:A:252:ALA:HA	2.15	0.46
1:A:371:TRP:CE2	3:A:805:C8E:C6	2.97	0.46
1:A:87:LEU:HD11	1:A:223:TYR:OH	2.15	0.46
1:A:291:ASP:HB3	1:A:326:THR:HG23	1.96	0.46
3:A:803:C8E:H172	3:A:803:C8E:H112	1.97	0.46
1:A:208:HIS:O	1:A:216:GLY:N	2.46	0.46
1:A:260:LEU:HA	1:A:260:LEU:HD12	1.50	0.46
1:A:397:ASN:CG	1:A:400:GLN:NE2	2.74	0.46
1:A:157:GLN:OE1	1:A:165:ARG:NH1	2.48	0.46
1:A:195:ASP:OD2	1:A:195:ASP:N	2.48	0.46
1:A:226:ARG:HH11	1:A:244:LYS:HG3	1.80	0.46
1:A:250:TRP:O	1:A:268:SER:OG	2.34	0.46
1:A:169:LEU:CD1	1:A:170:GLY:N	2.46	0.46
1:A:511:LEU:CD2	1:A:512:TYR:CE2	2.98	0.46
1:A:105:GLN:HA	1:A:105:GLN:NE2	2.29	0.46
1:A:278:ASP:CB	1:A:280:HIS:O	2.63	0.46
1:A:321:THR:HA	1:A:333:TYR:O	2.16	0.45
1:A:446:TYR:HH	1:A:451:LEU:HD12	1.80	0.45
1:A:450:THR:O	1:A:452:LYS:N	2.49	0.45
1:A:179:ASP:O	1:A:181:VAL:N	2.49	0.45
1:A:86:ASN:CG	1:A:87:LEU:H	2.25	0.45
1:A:447:ASP:CG	1:A:449:HIS:HB2	2.40	0.45
1:A:413:GLU:HG2	1:A:443:LEU:HA	1.97	0.45
1:A:425:LEU:HD22	1:A:425:LEU:O	2.17	0.45
1:A:99:PHE:HA	1:A:100:PRO:HD3	1.64	0.45
1:A:248:GLN:O	1:A:270:SER:HA	2.17	0.45
1:A:261:ILE:HA	1:A:304:VAL:HG12	1.97	0.45
1:A:290:LEU:HD12	1:A:291:ASP:C	2.42	0.45
1:A:450:THR:C	1:A:451:LEU:CD2	2.88	0.45
1:A:525:THR:OG1	1:A:541:MET:O	2.35	0.45
3:A:802:C8E:H31	3:A:802:C8E:H61	1.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:ASN:O	1:A:569:PHE:O	2.35	0.45
3:A:803:C8E:H172	3:A:803:C8E:C11	2.45	0.45
1:A:81:ASP:CB	1:A:219:ARG:HH12	2.30	0.45
1:A:126:VAL:HG13	1:A:127:VAL:N	2.31	0.45
1:A:166:VAL:HG22	1:A:206:LEU:HD11	1.99	0.45
1:A:516:TRP:CD2	1:A:551:VAL:HG12	2.51	0.45
1:A:295:GLN:HG3	1:A:320:GLN:HG3	1.99	0.45
1:A:67:PHE:C	1:A:68:ILE:HD13	2.42	0.45
1:A:105:GLN:NE2	1:A:105:GLN:CA	2.79	0.45
3:A:800:C8E:H101	3:A:800:C8E:H131	1.74	0.45
1:A:296:TYR:N	1:A:319:LYS:O	2.36	0.44
1:A:290:LEU:CD1	1:A:291:ASP:C	2.90	0.44
1:A:362:ASN:HB3	1:A:365:PHE:CE2	2.52	0.44
1:A:592:TYR:HD1	1:A:592:TYR:O	2.01	0.44
1:A:245:LEU:HD23	1:A:245:LEU:HA	1.78	0.44
1:A:317:TRP:CD1	1:A:338:THR:HG1	2.36	0.44
1:A:446:TYR:CE2	1:A:451:LEU:HA	2.53	0.44
1:A:471:ASP:OD1	1:A:476:THR:HG23	2.18	0.44
3:A:803:C8E:H101	3:A:803:C8E:H72	1.09	0.44
1:A:206:LEU:HA	1:A:206:LEU:HD12	1.78	0.44
1:A:323:THR:O	1:A:324:PRO:C	2.60	0.44
1:A:334:ASP:OD1	1:A:334:ASP:C	2.59	0.44
1:A:502:GLN:OE1	1:A:523:LEU:HD21	2.18	0.44
1:A:592:TYR:CD1	1:A:592:TYR:O	2.70	0.44
1:A:181:VAL:O	1:A:182:ALA:HB2	2.17	0.44
1:A:446:TYR:HH	1:A:451:LEU:CD1	2.24	0.44
1:A:160:LEU:HA	1:A:160:LEU:HD12	1.13	0.43
3:A:802:C8E:H13	3:A:802:C8E:C5	2.45	0.43
1:A:36:ARG:NH2	1:A:508:ASP:OD1	2.50	0.43
1:A:213:ALA:O	1:A:256:TYR:HA	2.17	0.43
1:A:116:ALA:HA	1:A:370:THR:HG22	2.00	0.43
1:A:446:TYR:CE1	1:A:448:ASP:HA	2.54	0.43
1:A:448:ASP:O	1:A:449:HIS:C	2.60	0.43
1:A:138:THR:HA	1:A:155:SER:O	2.19	0.43
1:A:48:ARG:HH12	1:A:519:THR:HG21	1.83	0.43
1:A:98:GLN:NE2	1:A:225:ASN:CB	2.82	0.43
1:A:193:ASP:O	1:A:195:ASP:OD2	2.35	0.43
1:A:559:LEU:HD23	1:A:560:THR:N	2.34	0.43
1:A:98:GLN:HE22	1:A:225:ASN:CB	2.31	0.42
1:A:275:TYR:CZ	1:A:290:LEU:HD22	2.52	0.42
1:A:120:SER:C	1:A:121:ASP:OD1	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LEU:CD1	1:A:79:LEU:HD23	2.49	0.42
1:A:369:GLY:HA3	3:A:800:C8E:C8	2.43	0.42
1:A:59:GLY:O	1:A:62:GLN:HG2	2.20	0.42
1:A:71:THR:O	1:A:72:ASN:C	2.61	0.42
1:A:559:LEU:CD2	1:A:560:THR:N	2.83	0.42
1:A:142:ALA:HA	1:A:151:ASN:OD1	2.19	0.42
1:A:379:PHE:CD1	1:A:380:ILE:HD12	2.55	0.42
1:A:531:TYR:O	1:A:532:SER:C	2.63	0.42
1:A:191:GLN:CB	1:A:230:ASP:OD2	2.64	0.42
1:A:226:ARG:HH11	1:A:244:LYS:CG	2.32	0.42
1:A:323:THR:HB	1:A:326:THR:OG1	2.19	0.42
1:A:175:THR:C	1:A:176:HIS:O	2.63	0.42
1:A:334:ASP:OD2	1:A:336:ARG:NH2	2.33	0.42
3:A:804:C8E:H172	3:A:804:C8E:H201	1.49	0.42
1:A:293:MET:HE3	1:A:293:MET:HB2	1.79	0.41
1:A:371:TRP:O	1:A:391:THR:HB	2.20	0.41
1:A:473:GLY:C	1:A:475:LEU:N	2.78	0.41
1:A:509:TRP:CA	1:A:510:GLN:NE2	2.81	0.41
1:A:566:ALA:O	1:A:584:ARG:HA	2.21	0.41
1:A:370:THR:N	3:A:800:C8E:C8	2.82	0.41
1:A:77:LEU:CD1	1:A:79:LEU:CD2	2.98	0.41
1:A:278:ASP:CB	1:A:279:PRO:C	2.58	0.41
1:A:348:VAL:O	1:A:349:GLY:C	2.61	0.41
1:A:496:LEU:N	1:A:496:LEU:CD1	2.84	0.41
1:A:523:LEU:HD23	1:A:523:LEU:HA	1.80	0.41
3:A:804:C8E:H41	3:A:804:C8E:H71	1.89	0.41
1:A:353:PHE:HB3	3:A:803:C8E:H191	2.02	0.41
1:A:553:TYR:HA	1:A:554:PRO:HD3	1.67	0.41
1:A:564:LYS:HG3	1:A:565:ILE:N	2.36	0.41
1:A:56:GLN:C	1:A:58:GLY:H	2.28	0.41
1:A:104:VAL:C	1:A:105:GLN:NE2	2.74	0.41
1:A:166:VAL:HG22	1:A:206:LEU:CD1	2.51	0.41
1:A:263:SER:CB	1:A:302:ASN:ND2	2.83	0.41
1:A:372:GLN:HA	1:A:390:GLY:HA2	2.03	0.41
1:A:407:ASN:HA	1:A:408:PRO:HD3	1.82	0.41
1:A:509:TRP:C	1:A:509:TRP:CD1	2.99	0.41
3:A:802:C8E:C17	3:A:802:C8E:C1	2.98	0.41
3:A:804:C8E:H171	3:A:804:C8E:H141	1.50	0.41
1:A:162:ASP:HB3	1:A:163:LYS:HZ2	1.87	0.40
1:A:351:PHE:HA	1:A:376:GLY:O	2.22	0.40
1:A:358:ARG:HB3	1:A:370:THR:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:800:C8E:H81	3:A:800:C8E:H112	1.86	0.40
1:A:49:LEU:O	1:A:504:LYS:NZ	2.54	0.40
1:A:107:VAL:HG12	1:A:108:GLU:N	2.36	0.40
1:A:210:PHE:C	1:A:211:THR:CG2	2.94	0.40
1:A:339:GLY:HA2	1:A:359:SER:O	2.21	0.40
1:A:162:ASP:OD1	1:A:162:ASP:N	2.54	0.40
1:A:86:ASN:O	1:A:87:LEU:C	2.64	0.40
1:A:87:LEU:HD23	1:A:87:LEU:HA	1.64	0.40
1:A:159:GLN:O	1:A:160:LEU:HD13	2.22	0.40
1:A:9:VAL:HG13	1:A:19:ARG:HG2	2.03	0.40
1:A:77:LEU:HD21	1:A:79:LEU:CD2	2.24	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	570/594 (96%)	499 (88%)	50 (9%)	21 (4%)	2 17

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	181	VAL
1	A	182	ALA
1	A	191	GLN
1	A	192	THR
1	A	278	ASP
1	A	287	SER
1	A	11	THR
1	A	147	ASN
1	A	176	HIS
1	A	184	GLY

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Mol	Chain	Res	Type
1	A	186	THR
1	A	213	ALA
1	A	146	SER
1	A	178	TYR
1	A	179	ASP
1	A	14	ARG
1	A	87	LEU
1	A	183	TYR
1	A	189	GLN
1	A	451	LEU
1	A	279	PRO

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	479/495 (97%)	390 (81%)	89 (19%)	1 7

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	10	VAL
1	A	13	ASN
1	A	21	THR
1	A	26	THR
1	A	47	ARG
1	A	49	LEU
1	A	60	SER
1	A	97	SER
1	A	103	LEU
1	A	105	GLN
1	A	114	ARG
1	A	121	ASP
1	A	138	THR
1	A	141	SER

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Mol	Chain	Res	Type
1	A	148	SER
1	A	153	ASP
1	A	158	GLN
1	A	160	LEU
1	A	162	ASP
1	A	163	LYS
1	A	169	LEU
1	A	172	TYR
1	A	174	HIS
1	A	175	THR
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	192	THR
1	A	195	ASP
1	A	198	LEU
1	A	200	LYS
1	A	207	GLU
1	A	215	SER
1	A	223	TYR
1	A	226	ARG
1	A	227	THR
1	A	229	TYR
1	A	242	THR
1	A	243	ARG
1	A	244	LYS
1	A	245	LEU
1	A	260	LEU
1	A	262	LYS
1	A	265	LEU
1	A	267	THR
1	A	276	ASN
1	A	277	TYR
1	A	280	HIS
1	A	285	ASP
1	A	287	SER
1	A	290	LEU
1	A	311	ILE
1	A	345	LEU

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Mol	Chain	Res	Type
1	A	346	GLN
1	A	348	VAL
1	A	367	ARG
1	A	370	THR
1	A	391	THR
1	A	398	LEU
1	A	404	PHE
1	A	407	ASN
1	A	414	LYS
1	A	425	LEU
1	A	426	THR
1	A	433	ILE
1	A	448	ASP
1	A	451	LEU
1	A	469	ASN
1	A	493	THR
1	A	510	GLN
1	A	513	ASP
1	A	519	THR
1	A	533	SER
1	A	537	GLN
1	A	538	THR
1	A	539	VAL
1	A	555	VAL
1	A	557	SER
1	A	559	LEU
1	A	560	THR
1	A	564	LYS
1	A	568	LEU
1	A	572	ASP
1	A	591	SER
1	A	594	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	32	GLN
1	A	105	GLN
1	A	147	ASN
1	A	157	GLN
1	A	208	HIS

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Mol	Chain	Res	Type
1	A	209	ASN
1	A	280	HIS
1	A	295	GLN
1	A	302	ASN
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	469	ASN
1	A	506	GLN
1	A	510	GLN
1	A	521	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	$\# Z > 2$
3	C8E	A	804	-	20,20,20	0.46	0	19,19,19	0.65	0
3	C8E	A	803	-	20,20,20	0.45	0	19,19,19	0.99	1 (5%)
3	C8E	A	802	-	20,20,20	0.43	0	19,19,19	1.34	1 (5%)
3	C8E	A	801	-	20,20,20	0.49	0	19,19,19	0.59	0
3	C8E	A	805	-	20,20,20	0.57	0	19,19,19	0.96	0
3	C8E	A	800	-	20,20,20	0.53	0	19,19,19	1.50	4 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	C8E	A	804	-	-	11/18/18/18	-
3	C8E	A	803	-	-	10/18/18/18	-
3	C8E	A	802	-	-	11/18/18/18	-
3	C8E	A	801	-	-	13/18/18/18	-
3	C8E	A	805	-	-	11/18/18/18	-
3	C8E	A	800	-	-	12/18/18/18	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	800	C8E	O12-C13-C14	-3.03	96.53	110.35
3	A	800	C8E	O15-C14-C13	-3.01	96.65	110.35
3	A	802	C8E	C19-O18-C17	-2.68	101.54	113.26
3	A	800	C8E	O21-C20-C19	-2.45	97.42	111.82
3	A	803	C8E	O18-C19-C20	-2.22	100.31	110.11
3	A	800	C8E	C19-O18-C17	-2.20	103.62	113.26

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	C8E	C14-C13-O12-C11

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Mol	Chain	Res	Type	Atoms
3	A	804	C8E	C11-C10-O9-C8
3	A	801	C8E	C11-C10-O9-C8
3	A	803	C8E	C17-C16-O15-C14
3	A	803	C8E	C14-C13-O12-C11
3	A	804	C8E	C20-C19-O18-C17
3	A	801	C8E	C13-C14-O15-C16
3	A	805	C8E	C11-C10-O9-C8
3	A	804	C8E	C17-C16-O15-C14
3	A	803	C8E	C7-C8-O9-C10
3	A	805	C8E	O9-C10-C11-O12
3	A	804	C8E	O15-C16-C17-O18
3	A	804	C8E	O18-C19-C20-O21
3	A	804	C8E	O9-C10-C11-O12
3	A	801	C8E	C6-C7-C8-O9
3	A	805	C8E	C17-C16-O15-C14
3	A	803	C8E	C4-C5-C6-C7
3	A	801	C8E	O18-C19-C20-O21
3	A	805	C8E	O15-C16-C17-O18
3	A	801	C8E	O12-C13-C14-O15
3	A	803	C8E	O18-C19-C20-O21
3	A	800	C8E	C4-C5-C6-C7
3	A	800	C8E	C3-C4-C5-C6
3	A	805	C8E	C10-C11-O12-C13
3	A	800	C8E	O15-C16-C17-O18
3	A	802	C8E	C5-C6-C7-C8
3	A	800	C8E	O12-C13-C14-O15
3	A	801	C8E	O9-C10-C11-O12
3	A	802	C8E	O9-C10-C11-O12
3	A	801	C8E	C4-C5-C6-C7
3	A	800	C8E	O18-C19-C20-O21
3	A	804	C8E	C3-C4-C5-C6
3	A	804	C8E	C2-C3-C4-C5
3	A	804	C8E	C1-C2-C3-C4
3	A	802	C8E	C6-C7-C8-O9
3	A	802	C8E	C10-C11-O12-C13
3	A	801	C8E	C16-C17-O18-C19
3	A	800	C8E	C13-C14-O15-C16
3	A	804	C8E	C14-C13-O12-C11
3	A	802	C8E	O15-C16-C17-O18
3	A	802	C8E	C2-C3-C4-C5
3	A	801	C8E	C20-C19-O18-C17
3	A	805	C8E	O12-C13-C14-O15

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Mol	Chain	Res	Type	Atoms
3	A	801	C8E	C17-C16-O15-C14
3	A	805	C8E	C7-C8-O9-C10
3	A	802	C8E	C3-C4-C5-C6
3	A	802	C8E	C1-C2-C3-C4
3	A	802	C8E	C17-C16-O15-C14
3	A	800	C8E	C14-C13-O12-C11
3	A	803	C8E	C20-C19-O18-C17
3	A	803	C8E	C11-C10-O9-C8
3	A	801	C8E	C14-C13-O12-C11
3	A	803	C8E	O12-C13-C14-O15
3	A	805	C8E	C13-C14-O15-C16
3	A	805	C8E	C2-C3-C4-C5
3	A	800	C8E	C10-C11-O12-C13
3	A	805	C8E	C5-C6-C7-C8
3	A	803	C8E	C5-C6-C7-C8
3	A	805	C8E	C14-C13-O12-C11
3	A	804	C8E	C10-C11-O12-C13
3	A	800	C8E	C1-C2-C3-C4
3	A	800	C8E	O9-C10-C11-O12
3	A	802	C8E	C7-C8-O9-C10
3	A	801	C8E	C10-C11-O12-C13
3	A	801	C8E	O15-C16-C17-O18
3	A	800	C8E	C11-C10-O9-C8
3	A	803	C8E	O9-C10-C11-O12
3	A	800	C8E	C6-C7-C8-O9

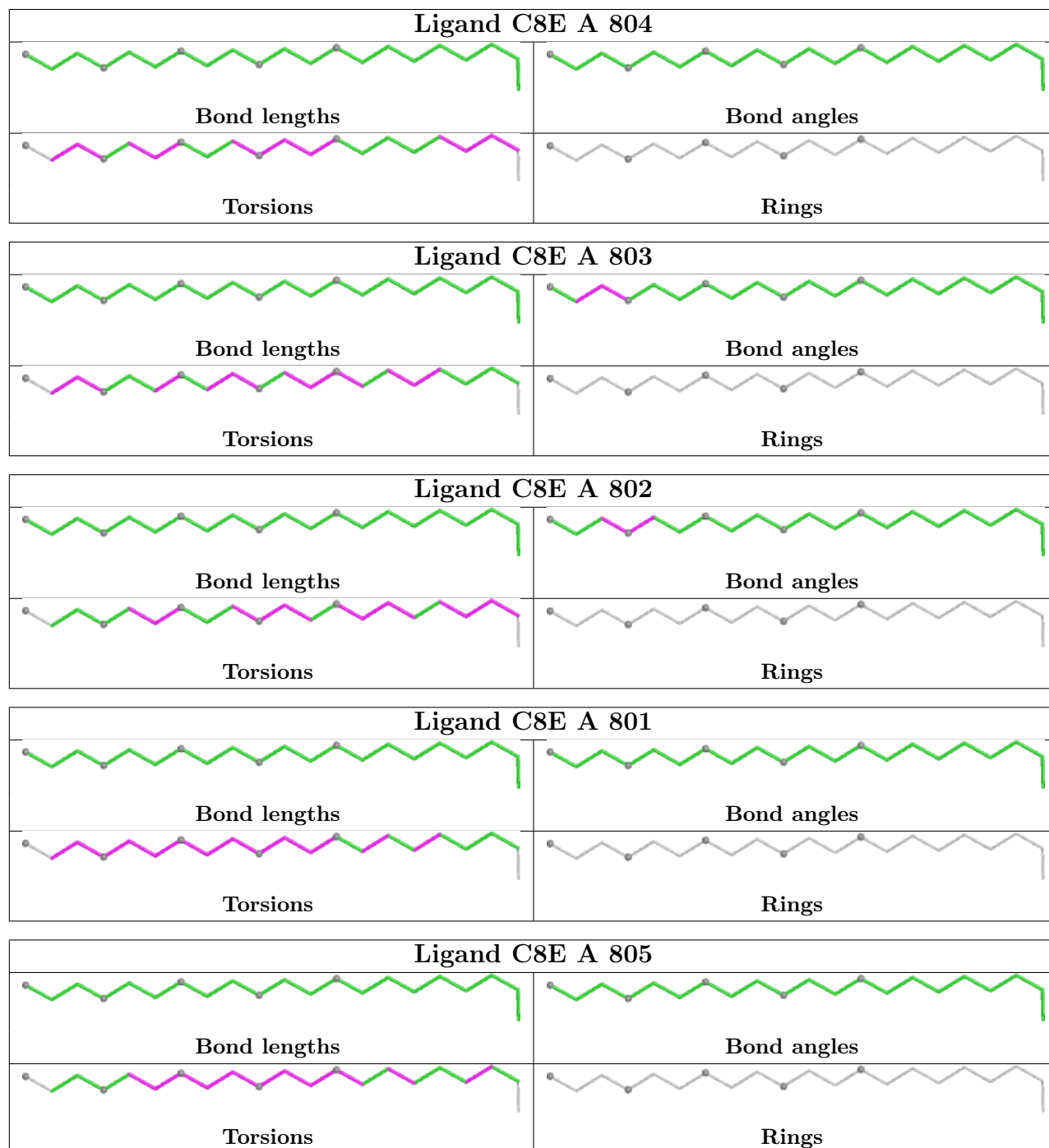
There are no ring outliers.

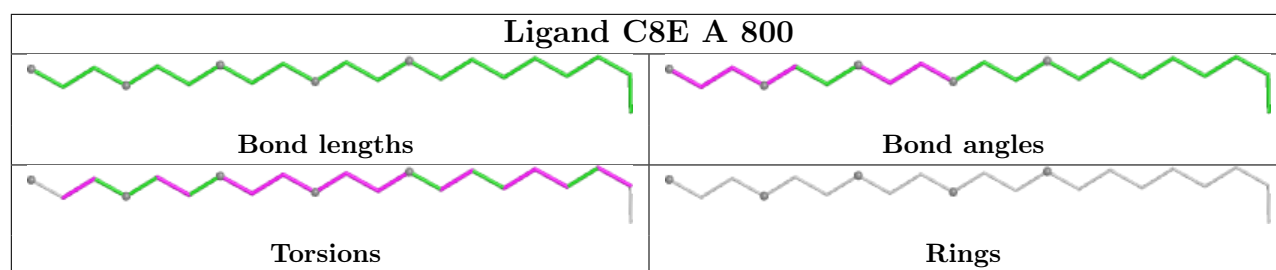
6 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	804	C8E	4	0
3	A	803	C8E	6	0
3	A	802	C8E	7	0
3	A	801	C8E	1	0
3	A	805	C8E	7	0
3	A	800	C8E	12	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	576/594 (96%)	0.42	29 (5%) 34 23	17, 30, 45, 61	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	532	SER	5.1
1	A	278	ASP	5.0
1	A	184	GLY	4.4
1	A	246	TYR	3.5
1	A	173	ALA	3.3
1	A	373	THR	3.1
1	A	287	SER	2.7
1	A	231	ALA	2.7
1	A	248	GLN	2.6
1	A	186	THR	2.5
1	A	582	ALA	2.5
1	A	352	THR	2.5
1	A	181	VAL	2.4
1	A	435	GLY	2.3
1	A	296	TYR	2.3
1	A	375	ALA	2.3
1	A	112	GLY	2.3
1	A	207	GLU	2.3
1	A	269	TYR	2.2
1	A	388	SER	2.2
1	A	138	THR	2.2
1	A	183	TYR	2.2
1	A	147	ASN	2.1
1	A	291	ASP	2.1
1	A	427	ALA	2.1
1	A	162	ASP	2.0
1	A	420	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	421	ALA	2.0
1	A	222	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

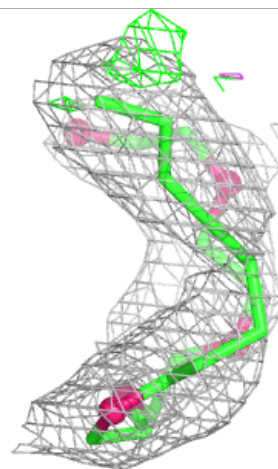
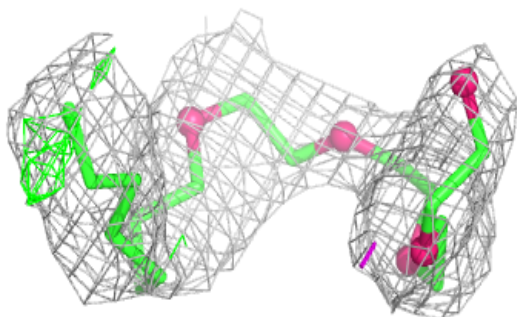
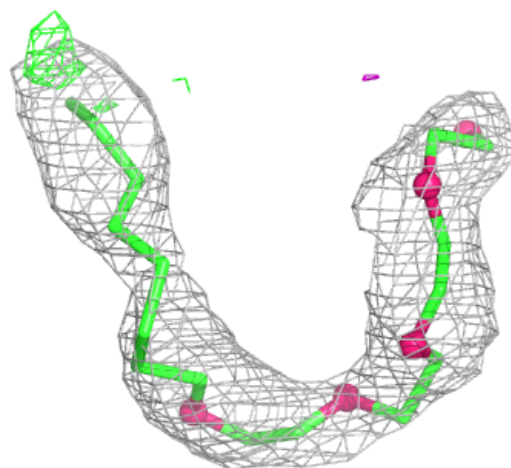
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	C8E	A	804	21/21	0.69	0.20	48,69,82,88	0
3	C8E	A	803	21/21	0.76	0.17	55,79,97,103	0
3	C8E	A	805	21/21	0.78	0.16	48,86,117,120	0
3	C8E	A	801	21/21	0.79	0.20	45,76,99,107	0
2	CA	A	597	1/1	0.85	0.13	99,99,99,99	0
2	CA	A	598	1/1	0.85	0.10	111,111,111,111	0
3	C8E	A	802	21/21	0.87	0.16	39,58,75,77	0
3	C8E	A	800	21/21	0.88	0.14	51,66,75,83	0
2	CA	A	596	1/1	0.93	0.06	94,94,94,94	0
2	CA	A	595	1/1	0.97	0.04	78,78,78,78	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.

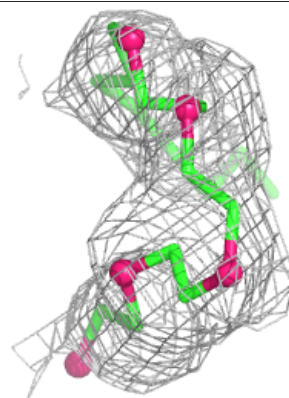
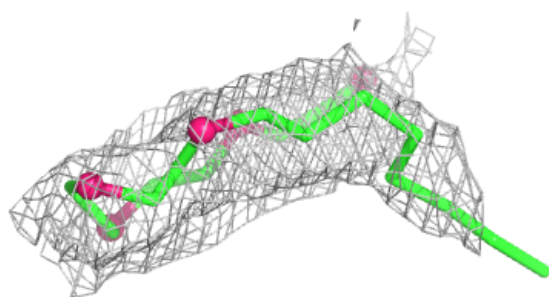
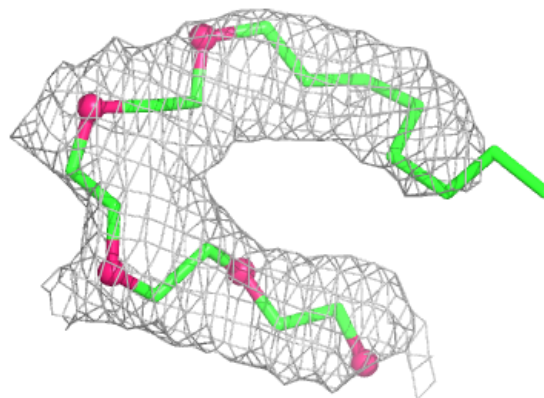
Electron density around C8E A 804:

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

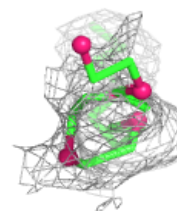
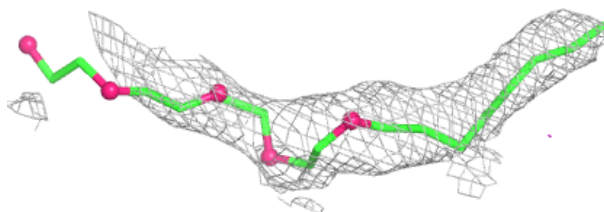


Electron density around C8E A 803:

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

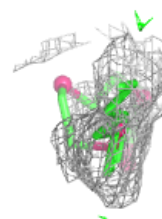
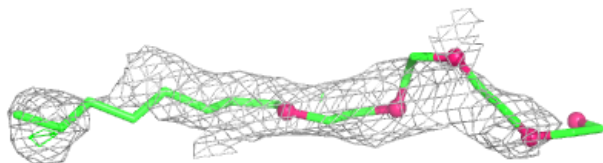
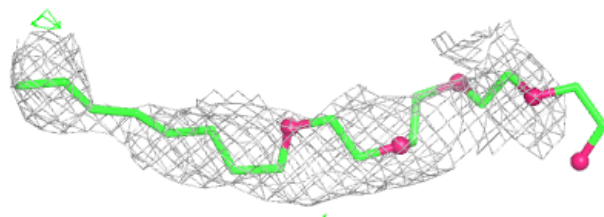
**Electron density around C8E A 805:**

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



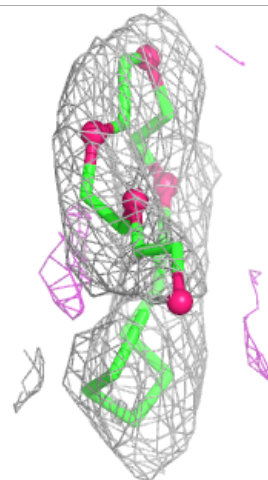
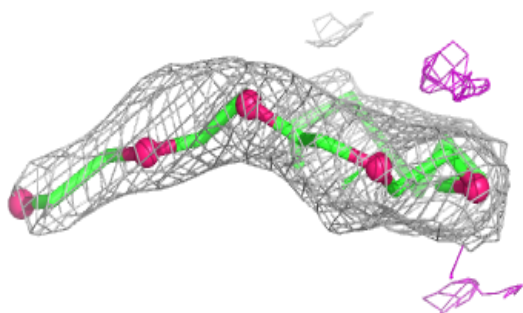
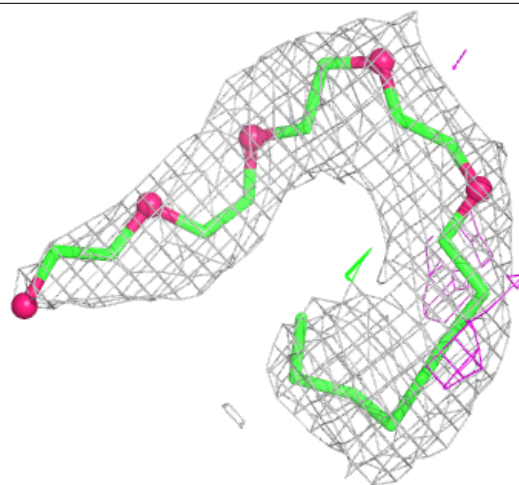
Electron density around C8E A 801:

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



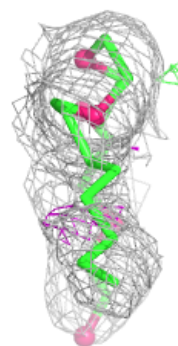
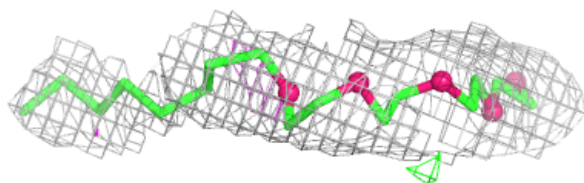
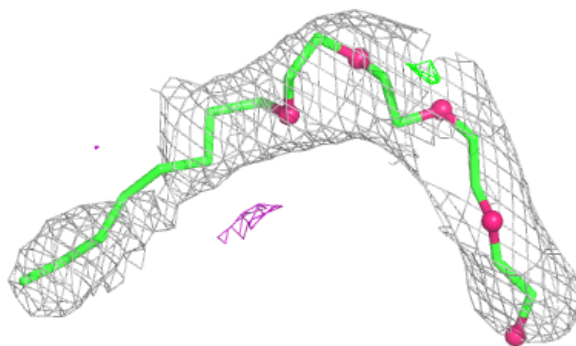
Electron density around C8E A 802:

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



Electron density around 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.