



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:53 PM UTC

PDB ID : 1W2X / pdb_00001w2x
Title : Crystal structure of the carboxyltransferase domain of acetyl- coenzyme A
carboxylase in complex with CP-640186
Authors : Zhang, H.; Tweel, B.; Li, J.; Tong, L.
Deposited on : 2004-07-09
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

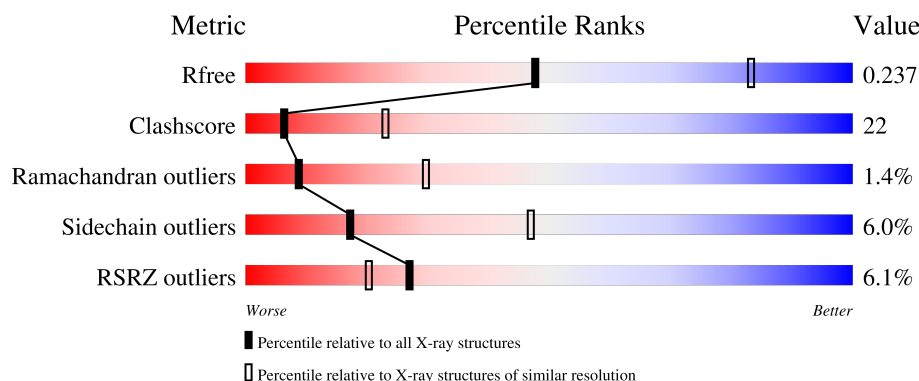
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	758	5% 55% 32% • 10%
1	B	758	7% 50% 35% • 11%
1	C	758	5% 50% 33% 5% 12%

2 Entry composition [i](#)

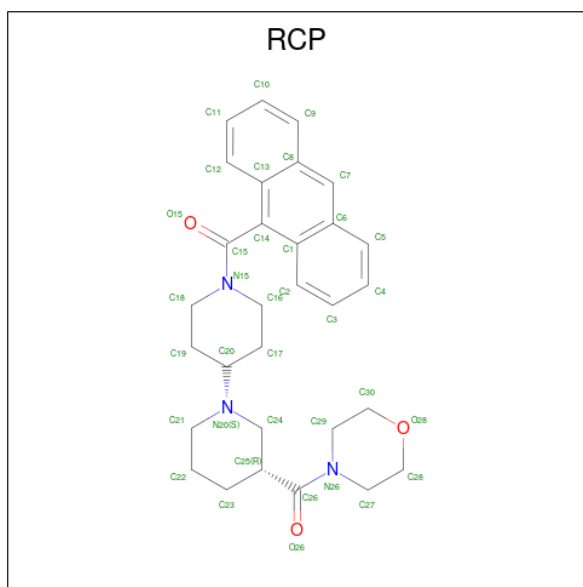
There are 3 unique types of molecules in this entry. The entry contains 16588 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACETYL-COA CARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	682	Total	C	N	O	S	0	0	1
			5425	3459	931	1016	19			
1	B	676	Total	C	N	O	S	0	0	1
			5377	3427	924	1007	19			
1	C	666	Total	C	N	O	S	0	0	1
			5299	3374	913	993	19			

- Molecule 2 is (3R)-1'-(9-ANTHRYLCARBONYL)-3-(MORPHOLIN-4-YLCARBONYL)-1,4'-BIPIPERIDINE (CCD ID: RCP) (formula: C₃₀H₃₅N₃O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			36	30	3	3		
2	B	1	Total	C	N	O	0	0
			36	30	3	3		
2	C	1	Total	C	N	O	0	0
			36	30	3	3		

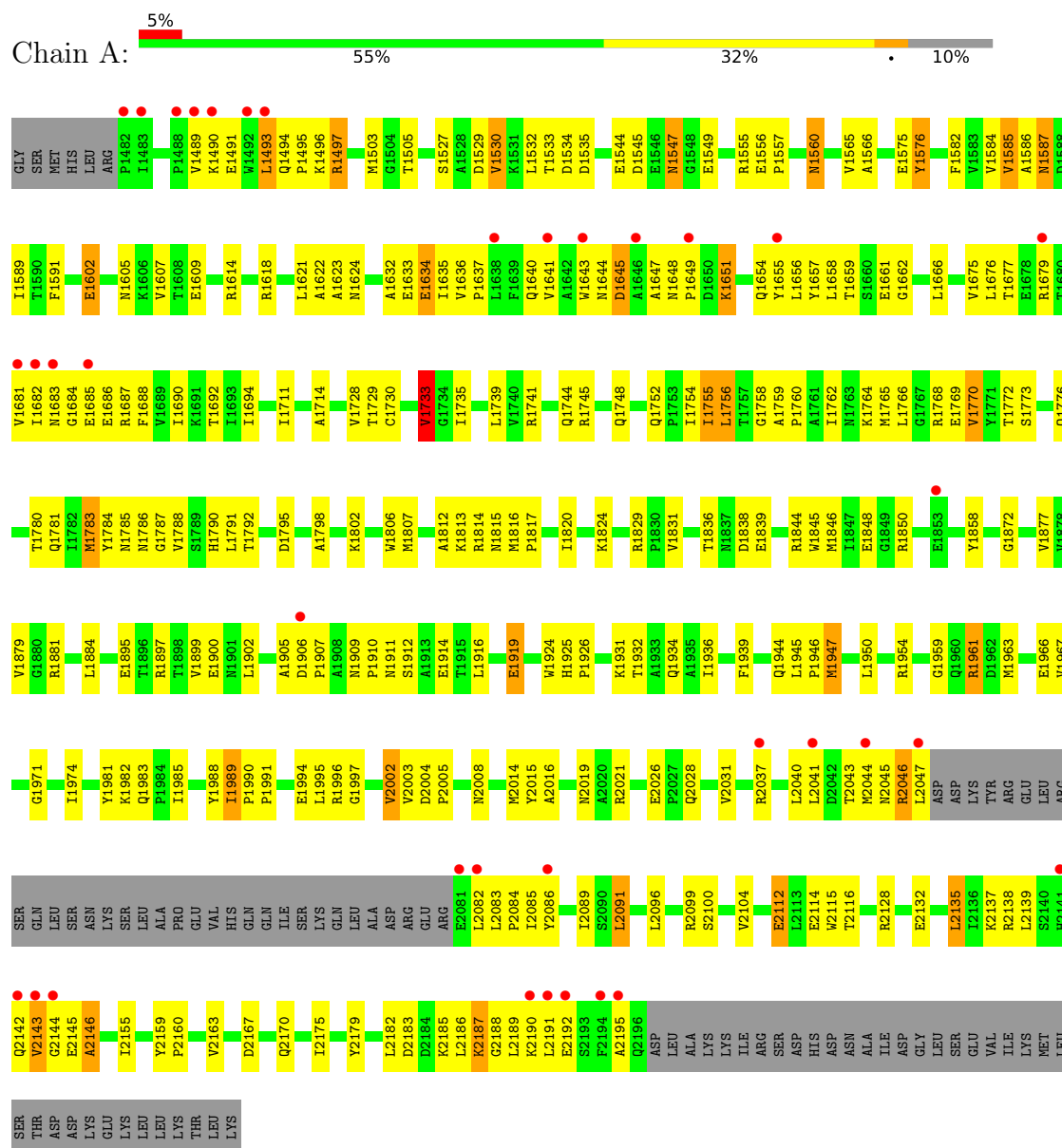
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	147	Total 147	O 147	0	0
3	B	128	Total 128	O 128	0	0
3	C	104	Total 104	O 104	0	0

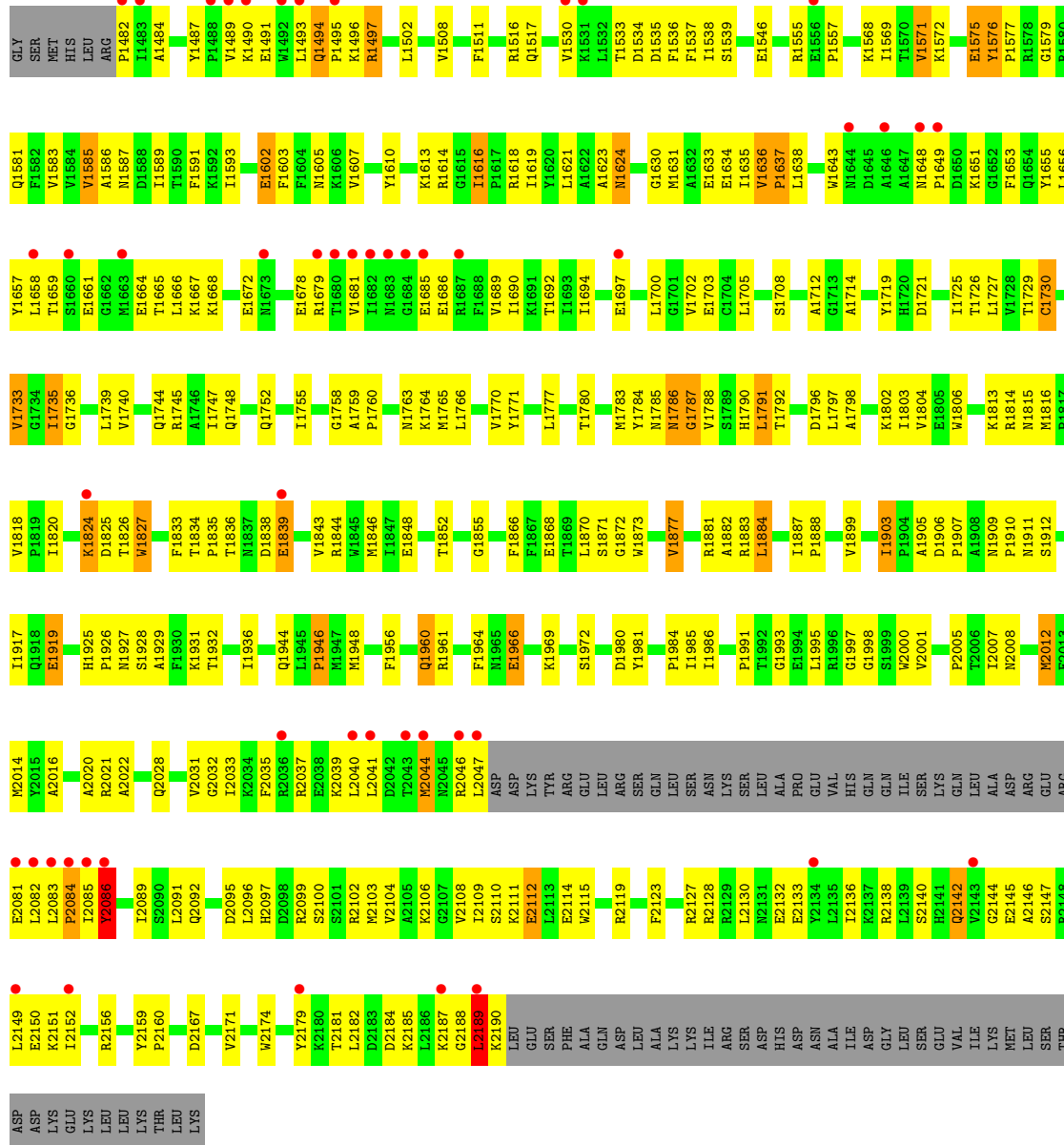
3 Residue-property plots

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.

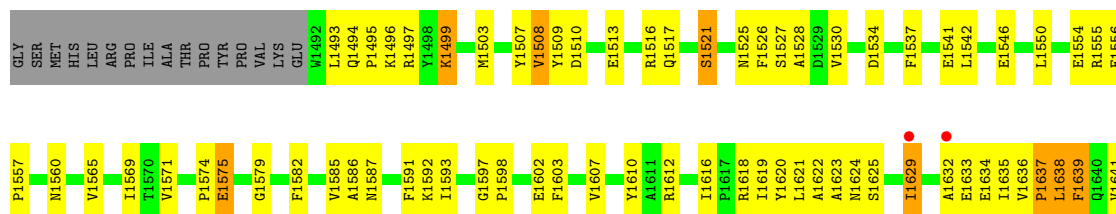
• Molecule 1: ACETYL-COA CARBOXYLASE

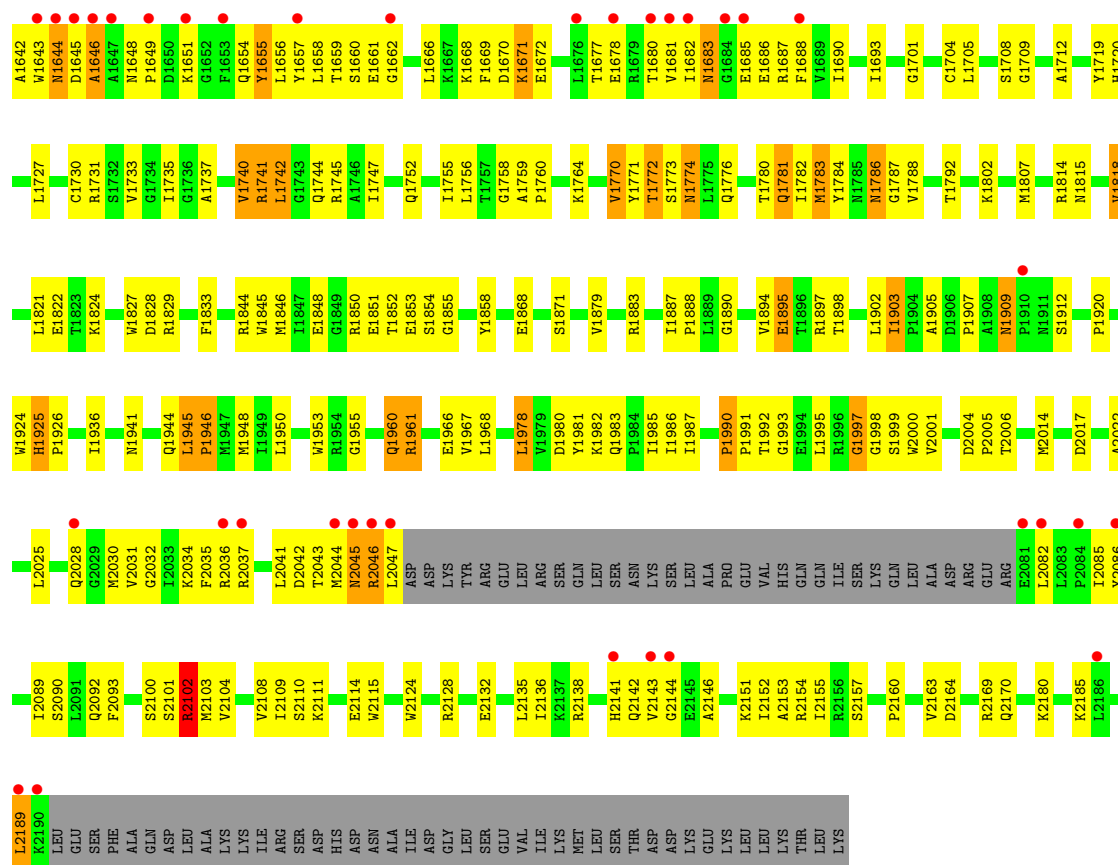


• Molecule 1: ACETYL-COA CARBOXYLASE



• Molecule 1: ACETYL-COA CARBOXYLASE





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	246.59Å 124.60Å 145.60Å 90.00° 93.85° 90.00°	Depositor
Resolution (Å)	29.66 – 2.80 29.66 – 2.80	Depositor EDS
% Data completeness (in resolution range)	85.7 (29.66-2.80) 89.8 (29.66-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.76Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.197 , 0.234 0.199 , 0.237	Depositor DCC
R_{free} test set	10186 reflections (9.92%)	wwPDB-VP
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16588	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: RCP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.46	1/5547 (0.0%)	0.95	22/7516 (0.3%)
1	B	0.46	2/5498 (0.0%)	0.96	24/7451 (0.3%)
1	C	0.45	1/5416 (0.0%)	0.92	19/7337 (0.3%)
All	All	0.46	4/16461 (0.0%)	0.94	65/22304 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2012	MET	SD-CE	-5.64	1.65	1.79
1	B	2189	LEU	C-N	-5.55	1.25	1.33
1	A	2195	ALA	C-N	-5.39	1.25	1.33
1	C	2189	LEU	C-N	-5.39	1.25	1.33

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1989	ILE	CA-C-N	7.87	128.49	120.38
1	A	1989	ILE	C-N-CA	7.87	128.49	120.38
1	C	1787	GLY	N-CA-C	-7.79	104.33	114.85
1	B	1494	GLN	CA-C-N	7.77	127.43	119.82
1	B	1494	GLN	C-N-CA	7.77	127.43	119.82
1	B	1787	GLY	N-CA-C	-7.68	103.95	115.00
1	A	1576	TYR	CA-C-N	7.46	127.82	119.32
1	A	1576	TYR	C-N-CA	7.46	127.82	119.32
1	B	1827	TRP	N-CA-C	6.79	119.69	111.82
1	B	2112	GLU	N-CA-C	-6.54	99.64	110.17
1	A	1787	GLY	N-CA-C	-6.53	105.74	114.95
1	A	1587	ASN	N-CA-C	-6.45	102.02	110.53
1	C	1946	PRO	N-CA-C	-6.41	101.58	111.13
1	A	1919	GLU	CA-C-N	6.33	126.35	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1919	GLU	C-N-CA	6.33	126.35	119.90
1	B	1636	VAL	CB-CA-C	-6.32	107.65	114.35
1	C	1909	ASN	CA-C-N	6.22	125.71	119.24
1	C	1909	ASN	C-N-CA	6.22	125.71	119.24
1	B	2086	TYR	N-CA-C	-6.05	105.89	113.28
1	A	1966	GLU	N-CA-C	6.03	119.72	111.39
1	A	1755	ILE	N-CA-C	6.02	118.89	108.95
1	A	1733	VAL	N-CA-C	6.00	118.10	108.85
1	B	1535	ASP	N-CA-C	-5.99	105.95	113.20
1	B	1730	CYS	N-CA-C	-5.87	100.64	108.74
1	B	1733	VAL	N-CA-C	5.81	116.84	108.48
1	B	1946	PRO	N-CA-C	-5.74	102.84	111.57
1	C	2157	SER	N-CA-C	-5.74	106.23	113.18
1	B	1712	ALA	N-CA-C	-5.72	104.96	111.14
1	A	2112	GLU	N-CA-C	-5.66	100.02	109.24
1	A	1946	PRO	N-CA-C	-5.65	101.31	110.40
1	B	2044	MET	N-CA-C	-5.61	106.28	113.01
1	B	1624	ASN	N-CA-C	5.58	115.91	108.38
1	A	1788	VAL	N-CA-C	-5.54	105.12	110.72
1	C	1783	MET	N-CA-C	5.54	118.25	111.82
1	C	1712	ALA	N-CA-C	-5.52	105.18	111.14
1	B	1903	ILE	N-CA-C	5.50	113.31	107.76
1	A	2046	ARG	N-CA-C	-5.44	106.37	114.64
1	C	2102	ARG	N-CA-C	-5.44	105.25	111.07
1	C	1890	GLY	N-CA-C	-5.37	104.85	112.37
1	A	1770	VAL	N-CA-C	5.37	116.03	110.82
1	B	1919	GLU	CA-C-N	5.36	125.28	119.76
1	B	1919	GLU	C-N-CA	5.36	125.28	119.76
1	B	1576	TYR	CA-C-N	5.35	125.42	119.32
1	B	1576	TYR	C-N-CA	5.35	125.42	119.32
1	A	1493	LEU	N-CA-C	-5.35	105.85	112.38
1	A	1945	LEU	N-CA-C	5.35	117.53	110.36
1	C	1616	ILE	CA-C-N	5.32	125.31	119.89
1	C	1616	ILE	C-N-CA	5.32	125.31	119.89
1	A	1783	MET	N-CA-C	5.32	117.99	111.82
1	B	1493	LEU	N-CA-C	-5.30	105.91	112.38
1	C	1990	PRO	N-CA-C	5.29	117.15	110.70
1	C	1945	LEU	N-CA-C	5.25	117.40	110.36
1	B	1929	ALA	N-CA-C	-5.25	105.64	111.36
1	A	1622	ALA	N-CA-C	5.25	117.30	108.96
1	B	1572	LYS	N-CA-C	-5.21	100.74	109.24
1	C	1966	GLU	N-CA-C	5.19	118.60	111.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2004	ASP	CA-C-N	5.19	124.99	119.28
1	A	2004	ASP	C-N-CA	5.19	124.99	119.28
1	C	1925	HIS	N-CA-C	-5.17	102.51	110.58
1	C	1818	VAL	CA-C-N	5.14	126.27	119.84
1	C	1818	VAL	C-N-CA	5.14	126.27	119.84
1	B	2012	MET	N-CA-C	5.13	118.43	110.17
1	B	1966	GLU	N-CA-C	5.06	118.72	112.24
1	C	1770	VAL	N-CA-C	5.03	116.48	111.00
1	C	1521	SER	N-CA-C	-5.03	105.80	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5425	0	5365	220	0
1	B	5377	0	5316	249	0
1	C	5299	0	5234	267	0
2	A	36	0	35	4	0
2	B	36	0	35	3	0
2	C	36	0	35	3	0
3	A	147	0	0	4	0
3	B	128	0	0	7	0
3	C	104	0	0	1	0
All	All	16588	0	16020	712	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 22.

All (712) 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:1813:LYS:HG2	1:A:1816:MET:HE2	1.33	1.05
1:B:1730:CYS:HA	1:B:1752:GLN:HE21	1.21	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1936:ILE:HG12	1:A:1947:MET:HE1	1.39	1.02
1:C:1772:THR:H	1:C:1776:GLN:NE2	1.59	1.01
1:C:1773:SER:H	1:C:1776:GLN:HE21	1.09	1.00
1:B:2007:ILE:HB	1:B:2012:MET:HE1	1.43	0.99
1:B:1815:ASN:H	1:B:1944:GLN:HE22	0.98	0.98
1:A:1773:SER:H	1:A:1776:GLN:HE21	1.13	0.96
1:A:1772:THR:H	1:A:1776:GLN:HE22	0.95	0.92
1:C:1637:PRO:HG2	1:C:1638:LEU:HD23	1.49	0.92
1:B:2181:THR:HG22	1:B:2185:LYS:HE2	1.51	0.91
1:B:2031:VAL:HG21	1:B:2091:LEU:HD23	1.54	0.91
1:C:1772:THR:H	1:C:1776:GLN:HE22	0.90	0.89
1:A:1772:THR:N	1:A:1776:GLN:HE22	1.71	0.87
1:B:2005:PRO:HD3	1:B:2014:MET:HE3	1.54	0.87
1:B:1764:LYS:HD2	2:B:3000:RCP:H5	1.57	0.86
1:B:1511:PHE:HZ	1:B:1729:THR:HG21	1.42	0.85
1:A:1772:THR:H	1:A:1776:GLN:NE2	1.76	0.84
1:B:1638:LEU:HD23	1:B:1638:LEU:H	1.42	0.84
1:C:1648:ASN:HB2	1:C:1651:LYS:HD3	1.58	0.84
1:A:1813:LYS:HG2	1:A:1816:MET:CE	2.08	0.84
1:A:1733:VAL:HG13	1:A:1755:ILE:HG13	1.61	0.83
1:B:1877:VAL:HG13	1:B:1931:LYS:HD3	1.60	0.82
1:B:1836:THR:HB	1:B:1839:GLU:HB3	1.62	0.80
1:C:1772:THR:N	1:C:1776:GLN:HE22	1.75	0.80
1:A:1633:GLU:O	1:A:1636:VAL:HG12	1.81	0.80
1:A:1939:PHE:HD1	1:A:1947:MET:HE3	1.47	0.80
1:B:2147:SER:HB3	1:B:2150:GLU:HG3	1.62	0.80
1:B:1494:GLN:HB3	1:B:1497:ARG:HH21	1.46	0.78
1:B:1692:THR:HG21	1:C:2101:SER:HB2	1.64	0.78
1:C:1493:LEU:HB2	1:C:1497:ARG:NH1	1.99	0.78
1:C:1646:ALA:HB3	1:C:1651:LYS:HG2	1.63	0.78
1:C:2031:VAL:HG23	1:C:2035:PHE:HB3	1.65	0.78
1:B:1494:GLN:NE2	1:B:1496:LYS:HG3	1.99	0.78
1:C:2160:PRO:HD2	1:C:2163:VAL:HG21	1.65	0.77
1:B:2044:MET:SD	1:B:2082:LEU:HD21	2.24	0.77
1:C:1773:SER:N	1:C:1776:GLN:HE21	1.81	0.77
1:B:1836:THR:HG22	1:B:1838:ASP:H	1.50	0.76
1:A:1773:SER:H	1:A:1776:GLN:NE2	1.83	0.76
1:B:2140:SER:O	1:B:2144:GLY:HA3	1.87	0.75
1:B:1827:TRP:HA	1:B:2119:ARG:NH1	2.01	0.75
1:A:1533:THR:HB	1:A:1535:ASP:OD1	1.86	0.74
1:B:1511:PHE:CZ	1:B:1729:THR:HG21	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1773:SER:H	1:C:1776:GLN:NE2	1.84	0.74
1:A:1657:TYR:CE2	1:A:1687:ARG:HD2	2.23	0.74
1:A:2135:LEU:HB3	1:A:2155:ILE:HD13	1.69	0.74
1:B:1827:TRP:HA	1:B:2119:ARG:HH12	1.53	0.74
1:C:1625:SER:HB3	1:C:1731:ARG:NH2	2.02	0.74
1:C:1638:LEU:HD23	1:C:1638:LEU:H	1.52	0.74
1:B:1763:ASN:ND2	1:B:1770:VAL:H	1.86	0.74
1:C:1759:ALA:H	1:C:1774:ASN:ND2	1.86	0.73
1:B:2008:ASN:HB3	1:B:2012:MET:HE2	1.69	0.73
1:B:1667:LYS:HG2	1:B:1672:GLU:HB3	1.70	0.73
1:A:2183:ASP:HB2	1:B:1482:PRO:HG3	1.71	0.73
1:A:1846:MET:HE1	1:A:1990:PRO:HB3	1.71	0.72
1:C:1786:ASN:HB3	1:C:1788:VAL:HG23	1.71	0.72
1:A:1813:LYS:CG	1:A:1816:MET:HE2	2.18	0.72
1:C:2138:ARG:HH11	1:C:2138:ARG:HB3	1.55	0.71
1:A:1587:ASN:HD22	1:A:1623:ALA:H	1.37	0.71
1:A:1991:PRO:HG3	1:A:2115:TRP:HB2	1.72	0.71
1:A:1741:ARG:HH22	1:A:1934:GLN:NE2	1.88	0.71
1:C:1764:LYS:HD2	2:C:3000:RCP:H5	1.71	0.71
1:C:1783:MET:HA	1:C:1786:ASN:HB2	1.72	0.71
1:C:1772:THR:N	1:C:1776:GLN:NE2	2.35	0.70
1:B:2008:ASN:H	1:B:2012:MET:HE3	1.56	0.70
1:B:1631:MET:HE2	1:C:2034:LYS:HB3	1.72	0.70
1:C:1815:ASN:ND2	1:C:1944:GLN:HE22	1.89	0.70
1:B:2108:VAL:HG23	1:B:2109:ILE:HG23	1.74	0.70
1:C:1759:ALA:H	1:C:1774:ASN:HD21	1.38	0.69
1:C:1909:ASN:HD22	1:C:1912:SER:HB2	1.57	0.69
1:C:1641:VAL:HG12	1:C:1642:ALA:H	1.57	0.69
1:C:2036:ARG:HB3	1:C:2036:ARG:NH1	2.07	0.69
1:A:1899:VAL:HB	1:A:1919:GLU:HB2	1.74	0.69
1:B:2100:SER:O	1:B:2104:VAL:HG23	1.93	0.69
1:C:1550:LEU:HD21	1:C:1607:VAL:HG22	1.74	0.69
1:C:1903:ILE:N	1:C:1903:ILE:HD12	2.08	0.69
1:C:1998:GLY:O	1:C:2001:VAL:HG12	1.92	0.69
1:B:1852:THR:HG22	1:B:1855:GLY:O	1.93	0.68
1:C:1991:PRO:HG2	1:C:2115:TRP:HB2	1.75	0.68
1:A:1585:VAL:HG13	1:A:1607:VAL:HG11	1.75	0.68
1:B:1658:LEU:HD13	1:B:1690:ILE:HD11	1.76	0.68
1:B:1638:LEU:HD11	1:B:1666:LEU:CD1	2.24	0.68
1:B:1763:ASN:HD21	1:B:1771:TYR:H	1.42	0.67
1:B:1998:GLY:O	1:B:2001:VAL:HG12	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1936:ILE:HD13	1:C:1978:LEU:HD13	1.76	0.67
1:B:1815:ASN:H	1:B:1944:GLN:NE2	1.82	0.67
1:B:2189:LEU:HD23	1:B:2189:LEU:H	1.59	0.67
1:C:2138:ARG:HB3	1:C:2138:ARG:NH1	2.10	0.67
1:B:2082:LEU:HD23	1:B:2082:LEU:H	1.58	0.67
1:C:1782:ILE:HG22	1:C:1783:MET:HE2	1.76	0.67
1:A:1895:GLU:OE1	1:A:1897:ARG:HD3	1.94	0.67
1:C:1815:ASN:HD22	1:C:1944:GLN:HE22	1.42	0.67
1:C:2045:ASN:C	1:C:2045:ASN:HD22	2.03	0.67
1:B:1815:ASN:N	1:B:1944:GLN:HE22	1.82	0.67
1:C:2160:PRO:HB2	1:C:2163:VAL:HG23	1.75	0.67
1:B:2008:ASN:CB	1:B:2012:MET:HE2	2.25	0.66
1:C:1658:LEU:HG	1:C:1690:ILE:HD11	1.76	0.66
1:A:1677:THR:HG22	1:A:1690:ILE:HA	1.77	0.66
1:A:2041:LEU:HA	1:A:2044:MET:HG2	1.75	0.66
1:A:2190:LYS:C	1:A:2192:GLU:H	2.02	0.66
1:A:2037:ARG:O	1:A:2041:LEU:HG	1.96	0.66
1:A:1836:THR:HG22	1:A:1838:ASP:H	1.60	0.66
1:A:1836:THR:HB	1:A:1839:GLU:HB2	1.79	0.65
1:C:2164:ASP:H	1:C:2170:GLN:NE2	1.93	0.65
1:B:1735:ILE:HD13	1:B:1739:LEU:HG	1.79	0.65
1:C:2036:ARG:HB3	1:C:2036:ARG:HH11	1.61	0.65
1:A:1547:ASN:HB2	1:A:1549:GLU:HG2	1.78	0.65
1:C:2100:SER:O	1:C:2104:VAL:HG23	1.97	0.65
1:A:2160:PRO:HD2	1:A:2163:VAL:HG21	1.78	0.64
1:A:1632:ALA:HB1	1:A:1634:GLU:OE2	1.97	0.64
1:B:2047:LEU:HD21	1:C:1649:PRO:HG3	1.78	0.64
1:A:2040:LEU:HD21	1:A:2086:TYR:HB3	1.79	0.64
1:B:1735:ILE:HD13	1:B:1735:ILE:O	1.96	0.64
1:A:1905:ALA:O	1:A:1907:PRO:HD3	1.98	0.64
1:A:1909:ASN:ND2	1:A:1911:ASN:H	1.96	0.64
1:C:1772:THR:HG23	1:C:1776:GLN:NE2	2.12	0.64
1:A:1812:ALA:HB3	1:A:1816:MET:CE	2.28	0.64
1:A:2044:MET:SD	1:A:2082:LEU:HD11	2.38	0.64
1:C:1909:ASN:ND2	1:C:1912:SER:HB2	2.13	0.64
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.47	0.63
1:B:2008:ASN:N	1:B:2012:MET:CE	2.62	0.63
1:B:1745:ARG:NH2	3:B:4057:HOH:O	2.31	0.63
1:C:1772:THR:HG23	1:C:1776:GLN:HE22	1.64	0.62
1:C:1585:VAL:HG22	1:C:1607:VAL:HG11	1.81	0.62
1:C:1936:ILE:HD13	1:C:1978:LEU:CD1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2096:LEU:HD23	1:A:2099:ARG:NH1	2.15	0.62
1:C:1781:GLN:H	1:C:1781:GLN:HE21	1.47	0.62
1:C:1660:SER:HB2	1:C:1686:GLU:HB2	1.82	0.62
1:C:1747:ILE:HD13	1:C:1802:LYS:HB2	1.82	0.62
1:B:1909:ASN:HB3	1:B:1912:SER:HB2	1.82	0.61
1:A:2046:ARG:O	1:A:2047:LEU:HG	1.99	0.61
1:C:1745:ARG:NH2	3:C:4033:HOH:O	2.33	0.61
1:C:1782:ILE:CG2	1:C:1783:MET:HE2	2.31	0.61
1:C:1554:GLU:O	1:C:1554:GLU:HG3	1.99	0.61
1:A:1939:PHE:CD1	1:A:1947:MET:HE3	2.33	0.61
1:B:2037:ARG:HD2	1:B:2083:LEU:HD21	1.83	0.61
1:C:1991:PRO:CG	1:C:2115:TRP:HB2	2.30	0.61
1:B:1681:VAL:HA	1:B:1685:GLU:O	2.01	0.61
1:B:1909:ASN:HD21	1:B:1911:ASN:ND2	1.99	0.61
1:A:2085:ILE:O	1:A:2089:ILE:HG13	2.01	0.61
1:C:1546:GLU:CD	1:C:1546:GLU:H	2.09	0.61
1:A:2186:LEU:C	1:A:2188:GLY:H	2.07	0.60
1:B:1729:THR:HG22	1:B:1796:ASP:OD1	2.00	0.60
1:A:1824:LYS:HE2	1:A:1824:LYS:H	1.65	0.60
1:B:1637:PRO:HG2	1:B:1638:LEU:HD23	1.82	0.60
1:A:1730:CYS:HA	1:A:1752:GLN:NE2	2.16	0.60
1:C:1960:GLN:HG3	1:C:1961:ARG:N	2.12	0.60
1:A:1582:PHE:CD2	1:A:1807:MET:HE1	2.36	0.60
1:B:2000:TRP:CD1	1:C:1705:LEU:HB3	2.36	0.60
1:A:2128:ARG:HE	1:A:2132:GLU:CD	2.08	0.60
1:A:1686:GLU:O	1:A:1686:GLU:HG3	2.01	0.59
1:A:1991:PRO:O	1:A:2019:ASN:O	2.19	0.59
1:B:2110:SER:O	1:B:2111:LYS:HG3	2.01	0.59
1:C:1509:TYR:HE2	1:C:1541:GLU:OE1	1.85	0.59
1:B:1824:LYS:HG3	1:B:1825:ASP:H	1.67	0.59
1:A:2143:VAL:HG13	1:A:2144:GLY:H	1.66	0.59
1:C:1493:LEU:HB2	1:C:1497:ARG:HH12	1.66	0.59
1:C:1755:ILE:HD12	1:C:1758:GLY:HA2	1.84	0.59
1:A:1490:LYS:HD2	1:A:1497:ARG:NH2	2.17	0.59
1:A:1605:ASN:O	1:A:1609:GLU:HG3	2.03	0.59
1:C:1670:ASP:C	1:C:1672:GLU:H	2.11	0.59
1:A:1656:LEU:HB2	1:A:1690:ILE:HD11	1.85	0.58
1:A:1959:GLY:O	1:A:1963:MET:HB2	2.02	0.58
1:A:1560:ASN:H	1:A:1560:ASN:HD22	1.51	0.58
1:B:1491:GLU:O	1:B:1495:PRO:HA	2.02	0.58
1:B:2086:TYR:HA	1:B:2089:ILE:HD12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1555:ARG:NH2	1:C:1560:ASN:HA	2.17	0.58
1:B:2147:SER:HB3	1:B:2150:GLU:CG	2.33	0.58
1:C:1655:TYR:OH	1:C:1687:ARG:HD3	2.04	0.58
1:C:1655:TYR:C	1:C:1656:LEU:HD12	2.29	0.58
1:C:2041:LEU:HA	1:C:2044:MET:CG	2.33	0.58
1:B:1755:ILE:HD12	1:B:1758:GLY:HA2	1.85	0.58
1:C:1991:PRO:HG3	1:C:2017:ASP:CG	2.29	0.58
1:C:2082:LEU:O	1:C:2085:ILE:HG22	2.05	0.57
1:C:1660:SER:HB2	1:C:1686:GLU:CB	2.34	0.57
1:C:1677:THR:HG22	1:C:1690:ILE:HD13	1.85	0.57
1:C:1824:LYS:H	1:C:1824:LYS:HE2	1.69	0.57
1:A:2041:LEU:O	1:A:2044:MET:N	2.37	0.57
1:A:2138:ARG:HB3	1:A:2186:LEU:HD13	1.86	0.57
1:B:1694:ILE:HA	1:C:2102:ARG:HD3	1.86	0.57
1:A:1676:LEU:HD13	1:A:1694:ILE:HD13	1.86	0.57
1:A:1932:THR:O	1:A:1936:ILE:HG13	2.04	0.57
1:B:1585:VAL:HG13	1:B:1607:VAL:HG11	1.86	0.57
1:C:1655:TYR:O	1:C:1656:LEU:HD12	2.05	0.57
1:B:1708:SER:CB	1:B:1735:ILE:HG13	2.35	0.57
1:C:2041:LEU:HA	1:C:2044:MET:HG2	1.85	0.57
1:A:2003:VAL:HG12	1:A:2003:VAL:O	2.03	0.57
1:B:1785:ASN:HA	1:B:1872:GLY:O	2.05	0.57
1:C:1607:VAL:O	1:C:1610:TYR:HB3	2.04	0.57
1:C:1587:ASN:HD22	1:C:1623:ALA:H	1.53	0.57
1:B:1634:GLU:O	1:B:1638:LEU:HD21	2.05	0.56
1:C:2164:ASP:H	1:C:2170:GLN:HE22	1.52	0.56
1:A:1758:GLY:O	1:A:1762:ILE:HG13	2.05	0.56
1:A:2008:ASN:C	1:A:2008:ASN:HD22	2.10	0.56
1:C:1612:ARG:O	1:C:1814:ARG:NH2	2.38	0.56
1:A:2100:SER:O	1:A:2104:VAL:HG23	2.05	0.56
1:B:1624:ASN:ND2	1:B:1733:VAL:H	2.04	0.56
1:B:1984:PRO:HD3	1:B:2133:GLU:HG3	1.87	0.56
1:B:2028:GLN:H	1:B:2028:GLN:CD	2.14	0.56
1:A:1654:GLN:O	1:A:1655:TYR:HB3	2.06	0.56
1:B:1490:LYS:HG3	1:B:1497:ARG:NH1	2.21	0.56
1:A:1493:LEU:C	1:A:1494:GLN:HG3	2.31	0.56
1:A:2183:ASP:CB	1:B:1482:PRO:HG3	2.36	0.56
1:B:1616:ILE:HD11	3:B:4022:HOH:O	2.06	0.56
1:B:2085:ILE:O	1:B:2089:ILE:HG13	2.05	0.56
1:C:1883:ARG:HA	1:C:1887:ILE:O	2.05	0.56
1:A:2179:TYR:HD1	1:B:1489:VAL:HA	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1587:ASN:ND2	1:C:1624:ASN:HD22	2.03	0.56
1:B:1991:PRO:HG2	1:B:2115:TRP:HB2	1.88	0.55
1:C:1586:ALA:HB2	1:C:1621:LEU:HB2	1.88	0.55
1:A:1829:ARG:CZ	1:A:1858:TYR:HB3	2.36	0.55
1:A:1902:LEU:HD11	1:A:1914:GLU:CG	2.36	0.55
1:B:2081:GLU:HB3	1:B:2083:LEU:HD13	1.88	0.55
1:C:1555:ARG:HH22	1:C:1560:ASN:HA	1.71	0.55
1:C:1846:MET:HE1	1:C:1990:PRO:HB2	1.87	0.55
1:B:1494:GLN:HE21	1:B:1496:LYS:HG3	1.69	0.55
1:C:2028:GLN:O	1:C:2031:VAL:HG12	2.07	0.55
1:A:2185:LYS:O	1:A:2189:LEU:HD13	2.07	0.55
1:B:1530:VAL:O	1:B:1530:VAL:HG13	2.06	0.55
1:A:1645:ASP:OD2	1:A:1647:ALA:HB3	2.06	0.55
1:A:1909:ASN:HB3	1:A:1912:SER:HB3	1.87	0.55
1:C:1641:VAL:HG12	1:C:1642:ALA:N	2.22	0.55
1:B:1991:PRO:CG	1:B:2115:TRP:HB2	2.37	0.55
1:B:2008:ASN:N	1:B:2012:MET:HE3	2.21	0.55
1:A:1902:LEU:HD11	1:A:1914:GLU:HG2	1.88	0.55
1:B:1637:PRO:HG2	1:B:1638:LEU:CD2	2.36	0.55
1:B:2188:GLY:O	1:B:2190:LYS:N	2.40	0.55
1:C:2180:LYS:NZ	1:C:2180:LYS:HB3	2.22	0.55
1:A:1527:SER:O	1:A:1530:VAL:HG22	2.07	0.54
1:B:2021:ARG:NH2	1:B:2099:ARG:NE	2.55	0.54
1:B:1786:ASN:HB3	1:B:1788:VAL:HG23	1.89	0.54
1:B:2097:HIS:CE1	1:C:1632:ALA:H	2.26	0.54
1:B:1719:TYR:CE2	1:B:1744:GLN:HG3	2.42	0.54
1:C:1629:ILE:HD12	1:C:1629:ILE:H	1.72	0.54
1:A:1936:ILE:HG12	1:A:1947:MET:CE	2.27	0.54
1:B:1636:VAL:N	1:B:1637:PRO:HD2	2.22	0.54
1:C:2045:ASN:C	1:C:2045:ASN:ND2	2.64	0.54
1:B:1624:ASN:HD21	1:B:1733:VAL:H	1.55	0.54
1:B:1765:MET:HE1	2:B:3000:RCP:H302	1.90	0.54
1:B:2008:ASN:H	1:B:2012:MET:CE	2.20	0.54
1:C:1681:VAL:HG13	1:C:1685:GLU:O	2.07	0.54
1:C:1733:VAL:HA	1:C:1755:ILE:O	2.08	0.54
1:A:1503:MET:HG2	1:A:1589:ILE:HG12	1.89	0.54
1:A:1982:LYS:HB2	1:A:1983:GLN:OE1	2.08	0.54
1:C:1719:TYR:CE2	1:C:1744:GLN:HG3	2.42	0.54
1:A:1812:ALA:HB3	1:A:1816:MET:HE1	1.90	0.54
1:B:2146:ALA:O	1:B:2151:LYS:HE3	2.07	0.54
1:C:2146:ALA:O	1:C:2151:LYS:HE3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1636:VAL:N	1:A:1637:PRO:HD2	2.22	0.54
1:A:1768:ARG:HG2	1:A:1769:GLU:N	2.23	0.54
1:B:1575:GLU:H	1:B:1575:GLU:CD	2.16	0.54
1:B:1730:CYS:HA	1:B:1752:GLN:NE2	2.06	0.54
1:C:1682:ILE:HG21	1:C:1687:ARG:NH1	2.22	0.54
1:A:1764:LYS:HG2	2:A:3000:RCP:H7	1.89	0.53
1:C:1648:ASN:CB	1:C:1651:LYS:HD3	2.36	0.53
1:B:1546:GLU:H	1:B:1546:GLU:CD	2.16	0.53
1:B:2097:HIS:HE1	1:C:1632:ALA:H	1.57	0.53
1:A:1489:VAL:O	1:A:1493:LEU:HG	2.09	0.53
1:A:1682:ILE:O	1:A:1683:ASN:C	2.49	0.53
1:B:1616:ILE:HD12	1:B:1813:LYS:HB3	1.91	0.53
1:B:1946:PRO:HG3	1:B:2130:LEU:HD21	1.90	0.53
1:C:1682:ILE:HG21	1:C:1687:ARG:HH11	1.74	0.53
1:C:2041:LEU:O	1:C:2044:MET:HB2	2.08	0.53
1:A:2183:ASP:OD1	1:A:2187:LYS:HE3	2.09	0.53
1:A:2189:LEU:O	1:A:2192:GLU:HB2	2.09	0.53
1:A:2028:GLN:O	1:A:2031:VAL:HG22	2.09	0.53
1:C:1720:HIS:HA	1:C:1941:ASN:HD22	1.74	0.53
1:A:1635:ILE:HG22	1:A:1635:ILE:O	2.10	0.52
1:A:1636:VAL:N	1:A:1637:PRO:CD	2.72	0.52
1:B:1866:PHE:CE1	1:B:1868:GLU:HB2	2.44	0.52
1:C:1770:VAL:HG13	1:C:1771:TYR:CD1	2.44	0.52
1:A:2143:VAL:HB	1:A:2192:GLU:OE2	2.09	0.52
1:C:1633:GLU:HA	1:C:1636:VAL:HG23	1.91	0.52
1:C:2185:LYS:O	1:C:2189:LEU:HD13	2.09	0.52
1:B:1927:ASN:OD1	1:B:1928:SER:N	2.43	0.52
1:A:2041:LEU:HA	1:A:2044:MET:CG	2.40	0.52
1:C:2085:ILE:HG23	1:C:2086:TYR:HD1	1.74	0.52
1:B:1932:THR:O	1:B:1936:ILE:HG13	2.09	0.52
1:C:1730:CYS:HA	1:C:1752:GLN:OE1	2.09	0.52
3:B:4128:HOH:O	1:C:1925:HIS:HE1	1.92	0.52
1:C:2004:ASP:OD2	1:C:2006:THR:HG23	2.10	0.52
1:A:1544:GLU:OE1	1:A:1602:GLU:OE2	2.28	0.52
1:A:1995:LEU:CD2	1:A:2014:MET:HE1	2.40	0.52
1:B:1820:ILE:HD12	1:B:1887:ILE:HG12	1.92	0.52
1:C:1575:GLU:CD	1:C:1575:GLU:H	2.18	0.52
1:B:1877:VAL:CG1	1:B:1931:LYS:HD3	2.36	0.52
1:C:1645:ASP:O	1:C:1646:ALA:HB2	2.10	0.52
1:B:1748:GLN:HE22	1:B:1783:MET:HB2	1.75	0.51
1:A:1657:TYR:O	1:A:1658:LEU:HD23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1633:GLU:HA	1:B:1636:VAL:HG23	1.92	0.51
1:B:1678:GLU:O	1:B:1689:VAL:HG12	2.09	0.51
1:B:1694:ILE:N	1:B:1694:ILE:HD12	2.25	0.51
1:C:1556:GLU:HG3	1:C:1557:PRO:HD2	1.92	0.51
1:A:2160:PRO:HD2	1:A:2163:VAL:CG2	2.41	0.51
1:A:1906:ASP:H	1:A:1912:SER:HB2	1.75	0.51
1:C:1643:TRP:C	1:C:1645:ASP:H	2.19	0.51
1:C:1995:LEU:CD2	1:C:2014:MET:HE1	2.40	0.51
1:C:2100:SER:HA	1:C:2103:MET:HE3	1.93	0.51
1:A:1648:ASN:O	1:A:1651:LYS:HB2	2.11	0.51
1:C:1494:GLN:N	1:C:1495:PRO:HD2	2.26	0.51
1:C:1585:VAL:CG2	1:C:1607:VAL:HG11	2.40	0.51
1:C:1991:PRO:C	1:C:1992:THR:HG23	2.36	0.51
1:A:1994:GLU:HA	1:A:2021:ARG:O	2.10	0.51
1:B:2102:ARG:NH1	1:B:2106:LYS:HG3	2.25	0.51
1:A:2114:GLU:HB3	3:A:4135:HOH:O	2.09	0.51
1:B:1745:ARG:HG2	1:B:1806:TRP:CZ2	2.46	0.51
1:B:2182:LEU:HA	1:B:2185:LYS:HD3	1.92	0.51
1:C:1657:TYR:CG	1:C:1687:ARG:HG3	2.46	0.51
1:C:1661:GLU:HG3	1:C:1662:GLY:N	2.26	0.51
1:B:1537:PHE:CD1	1:B:1537:PHE:C	2.89	0.50
1:C:2136:ILE:HD11	1:C:2152:ILE:CG2	2.41	0.50
1:B:2022:ALA:HB3	1:B:2103:MET:HE2	1.92	0.50
1:C:1730:CYS:O	1:C:1731:ARG:C	2.54	0.50
1:C:1987:ILE:CG2	1:C:2014:MET:HE3	2.41	0.50
1:B:1638:LEU:H	1:B:1638:LEU:CD2	2.19	0.50
1:C:1903:ILE:N	1:C:1903:ILE:CD1	2.73	0.50
1:B:1581:GLN:O	1:B:1616:ILE:HG13	2.12	0.50
1:B:2037:ARG:HA	1:B:2040:LEU:HB3	1.93	0.50
1:C:1507:TYR:HB3	1:C:1510:ASP:OD2	2.12	0.50
1:C:1591:PHE:C	1:C:1591:PHE:CD2	2.89	0.50
1:A:1995:LEU:HD23	1:A:2014:MET:HE1	1.94	0.50
1:B:2016:ALA:O	1:B:2112:GLU:HA	2.12	0.50
1:B:1605:ASN:ND2	1:B:1714:ALA:HB2	2.26	0.50
1:B:1697:GLU:O	1:B:1700:LEU:HD13	2.11	0.50
1:C:1759:ALA:HB3	1:C:1760:PRO:HD3	1.92	0.50
1:C:2044:MET:HA	1:C:2086:TYR:CE2	2.46	0.50
1:C:2138:ARG:HA	1:C:2141:HIS:CD2	2.46	0.50
1:B:1780:THR:O	1:B:1784:TYR:HB3	2.12	0.50
1:B:2167:ASP:O	1:B:2171:VAL:HG23	2.12	0.50
1:B:1490:LYS:HG3	1:B:1497:ARG:CZ	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1814:ARG:O	1:B:1815:ASN:HB2	2.12	0.50
1:B:1909:ASN:HD22	1:B:1910:PRO:CD	2.25	0.50
1:C:1646:ALA:C	1:C:1648:ASN:H	2.19	0.50
1:C:1643:TRP:O	1:C:1645:ASP:N	2.44	0.50
1:C:1780:THR:O	1:C:1784:TYR:HB3	2.11	0.50
1:A:1605:ASN:ND2	1:A:1714:ALA:HB2	2.26	0.49
1:B:1638:LEU:HD11	1:B:1666:LEU:HD13	1.93	0.49
1:C:1646:ALA:CB	1:C:1651:LYS:HG2	2.38	0.49
1:B:1909:ASN:HD22	1:B:1910:PRO:HD2	1.78	0.49
1:A:1755:ILE:HD12	1:A:1758:GLY:HA2	1.93	0.49
1:C:1981:TYR:CB	1:C:1985:ILE:HD11	2.42	0.49
1:A:1936:ILE:CG1	1:A:1947:MET:HE1	2.27	0.49
1:A:1576:TYR:CZ	1:A:1812:ALA:HB2	2.48	0.49
1:A:1614:ARG:HG3	1:A:1614:ARG:HH11	1.77	0.49
1:A:2186:LEU:C	1:A:2188:GLY:N	2.71	0.49
1:B:1835:PRO:HG2	1:B:1846:MET:SD	2.51	0.49
1:C:1852:THR:HG22	1:C:1853:GLU:N	2.27	0.49
1:A:2143:VAL:HG22	1:A:2144:GLY:N	2.28	0.49
1:B:2100:SER:HA	1:B:2103:MET:HE3	1.94	0.49
1:C:1493:LEU:HD12	1:C:1497:ARG:HH12	1.76	0.49
1:C:1586:ALA:CB	1:C:1621:LEU:HB2	2.42	0.49
1:C:1829:ARG:NH1	1:C:1858:TYR:HB3	2.28	0.49
1:B:1736:GLY:O	1:B:1740:VAL:HG23	2.13	0.49
1:C:1582:PHE:CD2	1:C:1807:MET:HE1	2.48	0.49
1:C:1955:GLY:HA2	1:C:1999:SER:OG	2.13	0.49
1:A:1681:VAL:HG23	1:A:1681:VAL:O	2.13	0.49
1:B:1907:PRO:HD2	1:C:1960:GLN:HG2	1.95	0.49
1:C:1991:PRO:C	1:C:1993:GLY:H	2.20	0.48
1:A:1643:TRP:CZ3	1:A:1649:PRO:HB3	2.47	0.48
1:A:1814:ARG:O	1:A:1815:ASN:HB2	2.13	0.48
1:B:1643:TRP:CD1	1:B:1643:TRP:H	2.29	0.48
1:B:2156:ARG:HD3	1:B:2159:TYR:CE1	2.48	0.48
1:C:1636:VAL:O	1:C:1639:PHE:HD2	1.95	0.48
1:C:1818:VAL:HG11	1:C:1946:PRO:HD3	1.95	0.48
1:B:1679:ARG:O	1:B:1679:ARG:HG3	2.12	0.48
1:B:2044:MET:HA	1:B:2086:TYR:CE2	2.48	0.48
1:B:1766:LEU:HD13	1:B:1770:VAL:HG21	1.94	0.48
1:C:1987:ILE:HG21	1:C:2014:MET:HE3	1.95	0.48
1:B:1538:ILE:HG22	1:B:1539:SER:N	2.29	0.48
1:B:1665:THR:O	1:B:1668:LYS:HB3	2.13	0.48
1:A:1759:ALA:HB3	1:A:1760:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1961:ARG:HH11	1:A:1961:ARG:HB3	1.78	0.48
1:A:2043:THR:C	1:A:2045:ASN:N	2.72	0.48
1:A:1768:ARG:HE	1:A:1770:VAL:HG22	1.79	0.48
1:A:2135:LEU:HD21	1:A:2182:LEU:HD13	1.96	0.48
1:C:1657:TYR:CD2	1:C:1687:ARG:HG3	2.49	0.48
1:A:1692:THR:HG22	1:A:1694:ILE:HD12	1.95	0.47
1:B:2096:LEU:HB3	1:C:1693:ILE:HG13	1.96	0.47
1:A:1560:ASN:H	1:A:1560:ASN:ND2	2.08	0.47
1:A:1735:ILE:O	1:A:1739:LEU:HG	2.14	0.47
1:A:1824:LYS:H	1:A:1824:LYS:CE	2.27	0.47
1:B:1884:LEU:HD22	1:B:2123:PHE:HB2	1.97	0.47
1:B:2007:ILE:CB	1:B:2012:MET:HE1	2.31	0.47
1:C:1527:SER:O	1:C:1530:VAL:HG13	2.13	0.47
1:A:1728:VAL:HG21	1:A:1754:ILE:HD11	1.96	0.47
1:B:1824:LYS:HG3	1:B:1825:ASP:N	2.28	0.47
1:C:1496:LYS:O	1:C:1497:ARG:C	2.57	0.47
1:C:1619:ILE:HD12	1:C:1619:ILE:N	2.28	0.47
1:C:1670:ASP:O	1:C:1672:GLU:N	2.45	0.47
1:A:2016:ALA:O	1:A:2112:GLU:HA	2.15	0.47
1:B:2020:ALA:O	1:B:2021:ARG:HD2	2.14	0.47
1:A:2044:MET:CE	1:A:2082:LEU:HD11	2.44	0.47
1:B:2000:TRP:CD1	1:B:2000:TRP:C	2.93	0.47
1:A:1640:GLN:HA	1:A:1640:GLN:NE2	2.30	0.47
1:A:1772:THR:N	1:A:1776:GLN:NE2	2.47	0.47
1:A:1783:MET:HA	1:A:1786:ASN:HB2	1.95	0.47
1:A:2002:VAL:HG13	1:A:2003:VAL:HG23	1.97	0.47
1:B:1657:TYR:O	1:B:1658:LEU:HD12	2.14	0.47
1:B:1969:LYS:HG2	1:C:1741:ARG:CZ	2.45	0.47
1:B:2082:LEU:H	1:B:2082:LEU:CD2	2.27	0.47
1:A:2003:VAL:O	1:A:2003:VAL:CG1	2.63	0.47
1:C:1845:TRP:CE2	1:C:1850:ARG:HD3	2.49	0.47
1:A:1547:ASN:N	1:A:1547:ASN:ND2	2.63	0.47
1:C:1513:GLU:O	1:C:1517:GLN:HG3	2.15	0.47
1:C:1591:PHE:C	1:C:1591:PHE:HD2	2.23	0.47
1:B:1587:ASN:HB2	1:B:1623:ALA:O	2.14	0.46
1:B:2136:ILE:HD11	1:B:2152:ILE:HG12	1.96	0.46
1:B:1619:ILE:N	1:B:1619:ILE:HD12	2.31	0.46
1:B:1727:LEU:HB2	1:B:1803:ILE:HD11	1.96	0.46
1:C:1669:PHE:C	1:C:1671:LYS:H	2.22	0.46
1:C:1852:THR:HG22	1:C:1854:SER:H	1.79	0.46
1:C:1909:ASN:O	1:C:1912:SER:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1633:GLU:C	1:B:1635:ILE:H	2.23	0.46
1:B:1679:ARG:HH21	1:B:1681:VAL:HG23	1.81	0.46
1:B:1833:PHE:C	1:B:1833:PHE:CD2	2.93	0.46
1:B:2046:ARG:NH1	1:C:1639:PHE:O	2.49	0.46
1:C:1635:ILE:HG22	1:C:1635:ILE:O	2.15	0.46
1:C:1981:TYR:CG	1:C:1985:ILE:HD11	2.50	0.46
1:A:1497:ARG:HH11	1:A:1497:ARG:HB2	1.80	0.46
1:B:1786:ASN:HD22	1:B:1786:ASN:HA	1.47	0.46
1:B:2040:LEU:HD11	1:B:2086:TYR:O	2.15	0.46
1:C:1510:ASP:O	1:C:1513:GLU:HB3	2.16	0.46
1:C:2128:ARG:HE	1:C:2132:GLU:CD	2.23	0.46
1:A:1925:HIS:O	1:A:1926:PRO:C	2.57	0.46
1:B:1665:THR:HA	1:B:1668:LYS:HE3	1.97	0.46
1:C:1682:ILE:HG23	1:C:1682:ILE:O	2.16	0.46
1:C:1868:GLU:HG2	1:C:1871:SER:HB3	1.97	0.46
1:A:1711:ILE:HD12	1:A:1739:LEU:HD11	1.96	0.46
1:A:2005:PRO:HG3	1:A:2014:MET:HB2	1.97	0.46
1:C:1569:ILE:HG22	1:C:1571:VAL:HG23	1.98	0.46
1:C:2042:ASP:O	1:C:2045:ASN:ND2	2.49	0.46
1:A:1762:ILE:O	1:A:1766:LEU:HD13	2.15	0.46
1:B:1610:TYR:CE1	1:B:1614:ARG:CZ	2.99	0.46
1:B:1826:THR:O	1:B:2119:ARG:NH1	2.41	0.46
1:B:1906:ASP:N	1:B:1912:SER:OG	2.46	0.46
2:B:3000:RCP:O15	1:C:2025:LEU:HB3	2.16	0.46
1:C:1634:GLU:O	1:C:1638:LEU:HD21	2.15	0.46
1:C:2136:ILE:HD11	1:C:2152:ILE:HG22	1.98	0.46
1:A:2041:LEU:C	1:A:2043:THR:N	2.70	0.46
1:B:1881:ARG:HH11	1:B:1881:ARG:HG2	1.81	0.46
1:C:1497:ARG:HA	1:C:1507:TYR:HB2	1.98	0.46
1:C:1995:LEU:HD23	1:C:2014:MET:HE1	1.97	0.46
1:A:1845:TRP:CE2	1:A:1850:ARG:HD3	2.51	0.46
1:B:1633:GLU:O	1:B:1636:VAL:HG23	2.15	0.46
1:C:1587:ASN:HB2	1:C:1623:ALA:O	2.15	0.46
1:C:1669:PHE:O	1:C:1670:ASP:HB2	2.16	0.46
1:C:2160:PRO:HD2	1:C:2163:VAL:CG2	2.41	0.46
1:A:1785:ASN:HA	1:A:1872:GLY:O	2.16	0.45
1:B:1658:LEU:CD1	1:B:1690:ILE:HD11	2.44	0.45
1:B:1966:GLU:HB3	1:B:1969:LYS:HD2	1.99	0.45
1:B:2102:ARG:HD3	3:B:4116:HOH:O	2.16	0.45
1:C:1643:TRP:C	1:C:1645:ASP:N	2.74	0.45
1:A:1605:ASN:HD22	1:A:1714:ALA:HB2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1701:GLY:O	1:C:1704:CYS:HB2	2.16	0.45
1:C:1783:MET:CA	1:C:1786:ASN:HB2	2.43	0.45
1:A:1575:GLU:CD	1:A:1575:GLU:H	2.25	0.45
1:A:1988:TYR:HA	1:A:2015:TYR:O	2.16	0.45
1:A:1656:LEU:CB	1:A:1690:ILE:HD11	2.45	0.45
1:A:1662:GLY:O	1:A:1666:LEU:HD23	2.16	0.45
1:A:1676:LEU:HD13	1:A:1694:ILE:CD1	2.46	0.45
1:A:1820:ILE:HD13	1:B:1487:TYR:CZ	2.52	0.45
1:B:1571:VAL:O	1:B:1579:GLY:HA2	2.17	0.45
1:B:1883:ARG:HA	1:B:1887:ILE:O	2.17	0.45
1:B:2138:ARG:O	1:B:2142:GLN:HG2	2.16	0.45
1:B:2156:ARG:HG3	1:B:2156:ARG:HH11	1.81	0.45
1:C:1654:GLN:O	1:C:1655:TYR:HB3	2.15	0.45
1:C:1708:SER:HB3	1:C:1735:ILE:HD13	1.98	0.45
1:C:2092:GLN:NE2	1:C:2092:GLN:HA	2.31	0.45
1:C:2143:VAL:O	1:C:2143:VAL:HG23	2.17	0.45
1:C:1727:LEU:HD12	1:C:1747:ILE:O	2.16	0.45
1:C:1741:ARG:O	1:C:1741:ARG:HD3	2.16	0.45
1:A:1838:ASP:O	1:A:1839:GLU:HG3	2.16	0.45
1:C:1620:TYR:CE1	1:C:1622:ALA:HB2	2.51	0.45
1:C:1682:ILE:O	1:C:1683:ASN:C	2.59	0.45
1:A:1659:THR:C	1:A:1661:GLU:N	2.72	0.45
1:B:1664:GLU:O	1:B:1668:LYS:HB2	2.17	0.45
1:B:1848:GLU:HB2	3:B:4081:HOH:O	2.17	0.45
1:B:1903:ILE:HD11	1:B:1917:ILE:HD12	1.98	0.45
1:C:2037:ARG:O	1:C:2041:LEU:HG	2.16	0.45
1:C:2135:LEU:HB3	1:C:2155:ILE:HD13	1.99	0.45
1:A:1555:ARG:HH22	1:A:1560:ASN:HA	1.82	0.45
1:C:1850:ARG:CG	1:C:1851:GLU:N	2.80	0.45
1:A:1676:LEU:HB2	1:A:1692:THR:HB	1.99	0.45
1:A:1745:ARG:HG2	1:A:1806:TRP:CZ2	2.52	0.45
1:A:1926:PRO:HD3	1:A:1967:VAL:HB	1.99	0.45
1:A:2128:ARG:HD3	1:A:2128:ARG:C	2.42	0.45
1:B:1747:ILE:HD12	1:B:1803:ILE:HG13	1.98	0.45
1:B:2184:ASP:O	1:B:2187:LYS:HB3	2.16	0.45
1:C:1526:PHE:CD1	1:C:1574:PRO:HB3	2.52	0.45
1:C:1644:ASN:HD21	1:C:1687:ARG:HH12	1.65	0.45
1:B:1956:PHE:HB2	1:C:1756:LEU:HD13	1.99	0.44
1:B:2096:LEU:HD13	1:C:1690:ILE:CG2	2.47	0.44
1:B:2149:LEU:HD13	1:B:2149:LEU:C	2.43	0.44
1:C:1493:LEU:HB2	1:C:1497:ARG:HH11	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1844:ARG:HH11	1:C:1844:ARG:HG3	1.82	0.44
1:C:1894:VAL:HG22	1:C:1953:TRP:CZ2	2.52	0.44
1:B:2021:ARG:NH2	1:B:2095:ASP:OD1	2.48	0.44
1:A:1493:LEU:O	1:A:1494:GLN:HG3	2.17	0.44
1:A:1815:ASN:ND2	1:A:1944:GLN:HE22	2.14	0.44
1:A:2159:TYR:OH	1:A:2175:ILE:HD11	2.17	0.44
1:B:1637:PRO:HG2	1:B:1638:LEU:H	1.82	0.44
1:B:2083:LEU:N	1:B:2084:PRO:CD	2.81	0.44
1:C:1685:GLU:HB3	1:C:1686:GLU:H	1.58	0.44
1:C:1833:PHE:CZ	1:C:1845:TRP:HE3	2.36	0.44
1:A:1529:ASP:O	1:A:1530:VAL:C	2.60	0.44
1:A:2008:ASN:C	1:A:2008:ASN:ND2	2.75	0.44
1:B:1763:ASN:HD21	1:B:1770:VAL:H	1.63	0.44
1:B:2147:SER:CB	1:B:2150:GLU:HG3	2.42	0.44
1:A:1812:ALA:HB3	1:A:1816:MET:HE3	1.99	0.44
1:B:1703:GLU:OE2	1:C:2102:ARG:NH2	2.51	0.44
1:B:2083:LEU:C	1:B:2085:ILE:H	2.26	0.44
1:A:1748:GLN:HE22	1:A:1783:MET:HB2	1.82	0.44
2:A:3000:RCP:H25	2:A:3000:RCP:H291	1.81	0.44
1:B:1630:GLY:O	1:C:2030:MET:HE1	2.18	0.44
1:B:2033:ILE:HD11	2:C:3000:RCP:H3	1.99	0.44
1:C:1603:PHE:O	1:C:1607:VAL:HG23	2.16	0.44
1:C:1786:ASN:HD22	1:C:1786:ASN:HA	1.55	0.44
1:C:2135:LEU:CB	1:C:2155:ILE:HD13	2.48	0.44
1:A:1981:TYR:CB	1:A:1985:ILE:HD11	2.48	0.44
1:B:1798:ALA:O	1:B:1802:LYS:HG3	2.18	0.44
1:A:1623:ALA:HB2	1:A:1729:THR:HG23	2.00	0.44
1:A:1817:PRO:HD3	1:B:1484:ALA:HB1	1.99	0.44
1:B:1616:ILE:HD12	1:B:1616:ILE:HA	1.83	0.44
1:B:2085:ILE:O	1:B:2085:ILE:HG22	2.17	0.44
1:C:1625:SER:HB3	1:C:1731:ARG:CZ	2.47	0.44
1:C:1783:MET:C	1:C:1786:ASN:HB2	2.43	0.44
1:A:1624:ASN:ND2	1:A:1733:VAL:H	2.15	0.44
1:A:1741:ARG:HH22	1:A:1934:GLN:HE22	1.63	0.44
1:B:1787:GLY:HA3	1:B:1873:TRP:CE3	2.53	0.44
1:C:1493:LEU:HD11	1:C:1557:PRO:HB2	2.00	0.44
1:C:1814:ARG:O	1:C:1815:ASN:HB2	2.18	0.44
1:C:1905:ALA:O	1:C:1907:PRO:HD3	2.18	0.44
1:C:1982:LYS:HB2	1:C:1983:GLN:OE1	2.18	0.44
1:B:1619:ILE:HG13	1:B:1725:ILE:CG2	2.48	0.43
1:B:1643:TRP:CZ3	1:B:1649:PRO:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1591:PHE:CE2	1:C:1592:LYS:HG3	2.53	0.43
1:A:1844:ARG:HG3	1:A:1844:ARG:HH11	1.82	0.43
1:B:1960:GLN:HG3	1:C:1776:GLN:O	2.18	0.43
1:B:1981:TYR:CB	1:B:1985:ILE:HD11	2.49	0.43
1:B:2102:ARG:O	1:B:2106:LYS:HG2	2.18	0.43
1:A:1954:ARG:HD2	1:A:2026:GLU:OE1	2.18	0.43
1:A:1981:TYR:CG	1:A:1985:ILE:HD11	2.52	0.43
1:B:1591:PHE:C	1:B:1591:PHE:CD2	2.96	0.43
1:C:1895:GLU:OE2	1:C:1897:ARG:NH2	2.51	0.43
1:C:2189:LEU:HD12	1:C:2189:LEU:N	2.34	0.43
1:A:1545:ASP:OD2	1:A:1545:ASP:C	2.62	0.43
1:A:2031:VAL:HG11	1:A:2091:LEU:HD12	2.00	0.43
1:A:2186:LEU:O	1:A:2188:GLY:N	2.52	0.43
2:A:3000:RCP:H281	3:A:4045:HOH:O	2.17	0.43
1:B:1576:TYR:N	1:B:1577:PRO:HD3	2.34	0.43
1:A:1790:HIS:HD2	3:A:4078:HOH:O	2.01	0.43
1:B:1870:LEU:HD22	1:B:1873:TRP:HE3	1.83	0.43
1:C:1659:THR:C	1:C:1661:GLU:N	2.75	0.43
1:C:2154:ARG:HG3	1:C:2154:ARG:HH11	1.83	0.43
1:A:1494:GLN:HB3	1:A:1496:LYS:HE3	2.00	0.43
1:A:1829:ARG:HG3	1:A:1829:ARG:HH11	1.84	0.43
1:B:2035:PHE:CD1	1:B:2039:LYS:HE3	2.54	0.43
1:C:1678:GLU:HA	1:C:1678:GLU:OE2	2.19	0.43
1:C:1844:ARG:O	1:C:1848:GLU:HG2	2.18	0.43
1:A:1682:ILE:HG22	1:A:1685:GLU:O	2.19	0.43
1:A:1745:ARG:NH2	3:A:4035:HOH:O	2.42	0.43
1:C:1509:TYR:HE1	1:C:1560:ASN:ND2	2.16	0.43
1:C:1571:VAL:O	1:C:1579:GLY:HA2	2.19	0.43
1:C:1737:ALA:O	1:C:1740:VAL:HG22	2.19	0.43
1:C:1747:ILE:HD13	1:C:1802:LYS:CB	2.48	0.43
1:A:1566:ALA:HA	1:A:1584:VAL:O	2.18	0.43
1:A:1624:ASN:HD21	1:A:1733:VAL:H	1.67	0.43
1:B:1589:ILE:O	1:B:1593:ILE:HA	2.18	0.43
1:B:1964:PHE:O	1:C:1786:ASN:ND2	2.47	0.43
1:C:1597:GLY:O	1:C:1598:PRO:C	2.61	0.43
1:C:2004:ASP:HA	1:C:2005:PRO:HD3	1.91	0.43
1:A:1591:PHE:C	1:A:1591:PHE:CD2	2.97	0.43
1:A:1651:LYS:HE3	1:A:1651:LYS:O	2.19	0.43
1:A:1877:VAL:CG2	1:A:1931:LYS:HD3	2.49	0.43
1:A:1954:ARG:O	1:A:1996:ARG:HB2	2.19	0.43
1:B:1868:GLU:HG2	1:B:1871:SER:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1660:SER:HB2	1:C:1686:GLU:HG3	2.00	0.43
1:A:1494:GLN:NE2	1:A:1557:PRO:HB2	2.33	0.42
1:A:1971:GLY:O	1:A:1974:ILE:HB	2.19	0.42
1:B:1702:VAL:CG2	1:C:2108:VAL:HG21	2.49	0.42
1:B:1790:HIS:O	1:B:1791:LEU:HD13	2.18	0.42
1:C:2000:TRP:CD1	1:C:2000:TRP:C	2.96	0.42
1:C:2045:ASN:ND2	1:C:2045:ASN:O	2.51	0.42
1:A:1644:ASN:ND2	1:A:1651:LYS:O	2.53	0.42
1:A:1780:THR:O	1:A:1784:TYR:HB3	2.19	0.42
1:A:2043:THR:C	1:A:2045:ASN:H	2.27	0.42
1:B:2083:LEU:O	1:B:2085:ILE:N	2.52	0.42
1:C:1521:SER:O	1:C:1525:ASN:ND2	2.52	0.42
1:C:1537:PHE:C	1:C:1537:PHE:CD1	2.96	0.42
1:C:1677:THR:HB	1:C:1688:PHE:HB3	2.01	0.42
1:C:1682:ILE:CG2	1:C:1687:ARG:HD2	2.50	0.42
1:C:1948:MET:HA	1:C:1986:ILE:O	2.18	0.42
1:B:1833:PHE:HE2	1:B:1835:PRO:HG3	1.85	0.42
1:C:2090:SER:O	1:C:2093:PHE:HB3	2.18	0.42
1:C:2110:SER:O	1:C:2111:LYS:HB2	2.18	0.42
1:A:1677:THR:CG2	1:A:1690:ILE:HG22	2.48	0.42
1:A:1815:ASN:HD22	1:A:1944:GLN:HE22	1.68	0.42
1:B:1991:PRO:C	1:B:1993:GLY:H	2.27	0.42
1:C:1894:VAL:HG22	1:C:1953:TRP:CE2	2.54	0.42
1:C:1926:PRO:HG3	1:C:1967:VAL:HB	2.00	0.42
1:A:1733:VAL:HA	1:A:1755:ILE:O	2.19	0.42
1:B:1636:VAL:N	1:B:1637:PRO:CD	2.82	0.42
1:B:1972:SER:HB3	1:C:1742:LEU:HD13	2.01	0.42
1:C:1759:ALA:N	1:C:1760:PRO:CD	2.82	0.42
1:C:1995:LEU:HD12	1:C:1995:LEU:HA	1.91	0.42
1:A:1675:VAL:HG21	1:A:1690:ILE:HG22	2.02	0.42
1:A:2139:LEU:O	1:A:2143:VAL:HG12	2.20	0.42
1:C:2124:TRP:CZ3	1:C:2169:ARG:HG3	2.54	0.42
1:B:1494:GLN:NE2	1:B:1496:LYS:CG	2.77	0.42
1:B:1651:LYS:HB2	3:B:4038:HOH:O	2.19	0.42
1:B:2128:ARG:HE	1:B:2132:GLU:CD	2.27	0.42
1:B:2156:ARG:HD3	1:B:2159:TYR:HE1	1.84	0.42
1:A:1679:ARG:NE	1:A:1686:GLU:OE1	2.50	0.42
1:B:1844:ARG:O	1:B:1848:GLU:HG2	2.19	0.42
1:B:1882:ALA:O	1:B:1888:PRO:HA	2.19	0.42
1:B:2149:LEU:HD13	1:B:2149:LEU:O	2.20	0.42
1:C:2043:THR:HG22	1:C:2043:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2152:ILE:HG13	1:C:2153:ALA:N	2.35	0.42
1:A:1677:THR:HG22	1:A:1690:ILE:HG22	2.01	0.42
1:A:2040:LEU:O	1:A:2043:THR:HB	2.19	0.42
1:B:1497:ARG:HE	1:B:1497:ARG:HB2	1.53	0.42
1:C:1821:LEU:HD23	1:C:1821:LEU:O	2.20	0.42
1:C:1850:ARG:HG2	1:C:1851:GLU:N	2.34	0.42
1:A:2083:LEU:N	1:A:2084:PRO:CD	2.83	0.42
1:C:1516:ARG:HA	1:C:1537:PHE:CD2	2.55	0.42
1:A:1895:GLU:OE2	1:A:1897:ARG:NH1	2.53	0.41
1:B:1708:SER:HB3	1:B:1735:ILE:HG13	2.01	0.41
1:B:1759:ALA:HB3	1:B:1760:PRO:HD3	2.02	0.41
1:B:2114:GLU:HB3	3:B:4118:HOH:O	2.20	0.41
1:C:1681:VAL:HG13	1:C:1685:GLU:C	2.45	0.41
1:A:1881:ARG:CZ	1:A:1939:PHE:HE2	2.32	0.41
1:A:2170:GLN:HG3	1:B:1517:GLN:NE2	2.35	0.41
1:B:1818:VAL:HB	1:B:1888:PRO:HG2	2.02	0.41
2:C:3000:RCP:H172	2:C:3000:RCP:H211	1.86	0.41
1:A:1623:ALA:HB2	1:A:1729:THR:CG2	2.50	0.41
1:A:1795:ASP:O	1:A:1798:ALA:HB3	2.21	0.41
1:B:1569:ILE:HG22	1:B:1571:VAL:HG22	2.01	0.41
1:B:1605:ASN:HD22	1:B:1714:ALA:HB2	1.84	0.41
1:A:1657:TYR:CD2	1:A:1687:ARG:HB3	2.56	0.41
1:A:1900:GLU:OE2	1:A:1916:LEU:HD21	2.19	0.41
1:B:1586:ALA:HB2	1:B:1621:LEU:HB2	2.01	0.41
1:B:1763:ASN:ND2	1:B:1770:VAL:N	2.63	0.41
1:B:1995:LEU:HD23	1:B:2000:TRP:CE3	2.56	0.41
1:B:2147:SER:HB3	1:B:2150:GLU:CD	2.46	0.41
1:C:1818:VAL:HB	1:C:1888:PRO:HG2	2.02	0.41
1:C:1852:THR:HB	1:C:1855:GLY:O	2.21	0.41
1:A:1790:HIS:O	1:A:1791:LEU:HD23	2.21	0.41
1:A:1909:ASN:HD22	1:A:1910:PRO:CD	2.34	0.41
1:A:1989:ILE:HA	1:A:1990:PRO:HD3	1.79	0.41
1:A:2086:TYR:HA	1:A:2089:ILE:HD12	2.01	0.41
1:B:1681:VAL:HG22	1:B:1686:GLU:HA	2.01	0.41
1:C:1527:SER:O	1:C:1528:ALA:C	2.63	0.41
1:A:1556:GLU:HA	1:A:1557:PRO:HD3	1.93	0.41
2:A:3000:RCP:H242	2:A:3000:RCP:H191	1.86	0.41
1:B:1653:PHE:CD1	1:B:1653:PHE:N	2.88	0.41
1:C:1991:PRO:HG2	1:C:2115:TRP:CB	2.47	0.41
1:A:1844:ARG:O	1:A:1848:GLU:HG2	2.20	0.41
1:B:1494:GLN:CB	1:B:1497:ARG:HH21	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1694:ILE:HA	1:C:2102:ARG:CD	2.50	0.41
1:B:1881:ARG:HG2	1:B:1881:ARG:NH1	2.36	0.41
1:B:2021:ARG:NH2	1:B:2099:ARG:HE	2.18	0.41
1:C:1592:LYS:O	1:C:1593:ILE:HG12	2.20	0.41
1:C:1648:ASN:O	1:C:1651:LYS:HB2	2.20	0.41
1:A:1505:THR:HB	1:A:1730:CYS:HB2	2.01	0.41
1:A:2145:GLU:O	1:A:2146:ALA:HB2	2.21	0.41
1:C:2041:LEU:HA	1:C:2044:MET:HG3	2.03	0.41
1:A:1565:VAL:HG12	1:A:1566:ALA:N	2.36	0.41
1:A:1752:GLN:NE2	1:A:1752:GLN:HA	2.35	0.41
1:A:1756:LEU:HD12	1:A:1756:LEU:HA	1.90	0.41
1:A:2137:LYS:O	1:A:2138:ARG:C	2.64	0.41
1:A:2167:ASP:HB3	1:A:2170:GLN:HB3	2.02	0.41
1:B:1816:MET:HE2	1:B:1816:MET:HB3	1.84	0.41
1:B:1905:ALA:O	1:B:1907:PRO:HD3	2.21	0.41
1:B:1998:GLY:O	1:B:2001:VAL:CG1	2.67	0.41
1:C:1682:ILE:HG22	1:C:1687:ARG:HD2	2.03	0.41
1:A:1784:TYR:CD1	1:A:1792:THR:HG23	2.56	0.41
1:A:1909:ASN:ND2	1:A:1909:ASN:C	2.78	0.41
1:B:1631:MET:HE3	1:B:1631:MET:HB2	2.00	0.41
1:B:1721:ASP:OD2	1:B:1814:ARG:NH1	2.54	0.41
1:C:1666:LEU:C	1:C:1668:LYS:N	2.79	0.41
1:A:1831:VAL:HB	1:A:2116:THR:HA	2.02	0.40
1:A:2190:LYS:O	1:A:2192:GLU:N	2.54	0.40
1:B:1602:GLU:HG3	1:B:1603:PHE:N	2.36	0.40
1:B:1655:TYR:O	1:B:1656:LEU:HD23	2.22	0.40
1:B:1820:ILE:CD1	1:B:1887:ILE:HA	2.51	0.40
1:B:2160:PRO:HD3	1:B:2174:TRP:CZ2	2.56	0.40
1:C:1637:PRO:HG2	1:C:1638:LEU:H	1.86	0.40
1:A:1491:GLU:O	1:A:1495:PRO:HA	2.22	0.40
1:A:1679:ARG:HB2	1:A:1688:PHE:CE2	2.56	0.40
1:A:2044:MET:HA	1:A:2086:TYR:CE2	2.56	0.40
1:B:1834:THR:HA	1:B:1835:PRO:HD3	1.86	0.40
1:B:1925:HIS:O	1:B:1926:PRO:C	2.63	0.40
1:B:2185:LYS:H	1:B:2185:LYS:HD2	1.85	0.40
1:C:1827:TRP:CG	1:C:1828:ASP:N	2.89	0.40
1:C:1920:PRO:HD2	1:C:1925:HIS:CE1	2.56	0.40
1:A:1772:THR:HB	1:A:1776:GLN:NE2	2.36	0.40
1:B:1659:THR:C	1:B:1661:GLU:N	2.78	0.40
1:B:1899:VAL:HB	1:B:1919:GLU:HB2	2.02	0.40
1:B:1948:MET:HA	1:B:1986:ILE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1591:PHE:CD2	1:C:1592:LYS:HG3	2.57	0.40
1:C:1680:THR:O	1:C:1687:ARG:HB3	2.21	0.40
1:C:2022:ALA:HB3	1:C:2103:MET:HE2	2.03	0.40
1:C:2043:THR:O	1:C:2046:ARG:HB2	2.22	0.40
1:C:2108:VAL:HG23	1:C:2109:ILE:HG23	2.03	0.40
1:A:1586:ALA:HB2	1:A:1621:LEU:HB2	2.02	0.40
1:B:2083:LEU:C	1:B:2085:ILE:N	2.80	0.40
1:C:2031:VAL:HG13	1:C:2032:GLY:N	2.35	0.40
1:C:2085:ILE:O	1:C:2089:ILE:HG13	2.21	0.40
1:B:1705:LEU:HD21	1:C:1997:GLY:HA2	2.04	0.40
1:B:2001:VAL:HG23	1:C:1709:GLY:HA2	2.04	0.40
1:C:1499:LYS:O	1:C:1503:MET:HG2	2.22	0.40
1:C:1741:ARG:HD3	1:C:1741:ARG:C	2.46	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	678/758 (89%)	618 (91%)	52 (8%)	8 (1%)	10	34
1	B	672/758 (89%)	611 (91%)	51 (8%)	10 (2%)	8	28
1	C	662/758 (87%)	588 (89%)	64 (10%)	10 (2%)	8	28
All	All	2012/2274 (88%)	1817 (90%)	167 (8%)	28 (1%)	9	30

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2145	GLU
1	B	2189	LEU
1	C	1644	ASN
1	A	1684	GLY

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Mol	Chain	Res	Type
1	A	1997	GLY
1	A	2146	ALA
1	B	1997	GLY
1	B	2142	GLN
1	C	1508	VAL
1	C	1534	ASP
1	C	1671	LYS
1	C	1997	GLY
1	A	2187	LYS
1	B	1839	GLU
1	C	1646	ALA
1	C	1655	TYR
1	C	1683	ASN
1	C	2144	GLY
1	A	1530	VAL
1	A	1645	ASP
1	A	2191	LEU
1	B	1533	THR
1	A	1744	GLN
1	B	2084	PRO
1	B	1637	PRO
1	B	2032	GLY
1	C	1637	PRO
1	B	1557	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	577/648 (89%)	550 (95%)	27 (5%)	23	57
1	B	572/648 (88%)	535 (94%)	37 (6%)	15	43
1	C	563/648 (87%)	525 (93%)	38 (7%)	15	42
All	All	1712/1944 (88%)	1610 (94%)	102 (6%)	17	47

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1497	ARG
1	A	1532	LEU
1	A	1534	ASP
1	A	1547	ASN
1	A	1560	ASN
1	A	1585	VAL
1	A	1602	GLU
1	A	1618	ARG
1	A	1634	GLU
1	A	1641	VAL
1	A	1651	LYS
1	A	1733	VAL
1	A	1756	LEU
1	A	1765	MET
1	A	1781	GLN
1	A	1802	LYS
1	A	1879	VAL
1	A	1884	LEU
1	A	1924	TRP
1	A	1947	MET
1	A	1950	LEU
1	A	1961	ARG
1	A	2002	VAL
1	A	2091	LEU
1	A	2135	LEU
1	A	2142	GLN
1	A	2143	VAL
1	B	1497	ARG
1	B	1502	LEU
1	B	1508	VAL
1	B	1516	ARG
1	B	1534	ASP
1	B	1536	PHE
1	B	1555	ARG
1	B	1568	LYS
1	B	1571	VAL
1	B	1575	GLU
1	B	1583	VAL
1	B	1585	VAL
1	B	1602	GLU
1	B	1613	LYS
1	B	1616	ILE
1	B	1618	ARG

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Mol	Chain	Res	Type
1	B	1648	ASN
1	B	1726	THR
1	B	1735	ILE
1	B	1777	LEU
1	B	1786	ASN
1	B	1791	LEU
1	B	1792	THR
1	B	1797	LEU
1	B	1804	VAL
1	B	1824	LYS
1	B	1843	VAL
1	B	1877	VAL
1	B	1884	LEU
1	B	1960	GLN
1	B	1961	ARG
1	B	1980	ASP
1	B	2041	LEU
1	B	2086	TYR
1	B	2092	GLN
1	B	2127	ARG
1	B	2179	TYR
1	C	1499	LYS
1	C	1508	VAL
1	C	1542	LEU
1	C	1565	VAL
1	C	1575	GLU
1	C	1602	GLU
1	C	1618	ARG
1	C	1629	ILE
1	C	1638	LEU
1	C	1639	PHE
1	C	1740	VAL
1	C	1741	ARG
1	C	1742	LEU
1	C	1772	THR
1	C	1774	ASN
1	C	1781	GLN
1	C	1786	ASN
1	C	1792	THR
1	C	1822	GLU
1	C	1879	VAL
1	C	1895	GLU

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Mol	Chain	Res	Type
1	C	1898	THR
1	C	1902	LEU
1	C	1903	ILE
1	C	1924	TRP
1	C	1945	LEU
1	C	1950	LEU
1	C	1960	GLN
1	C	1961	ARG
1	C	1968	LEU
1	C	1978	LEU
1	C	1980	ASP
1	C	2045	ASN
1	C	2046	ARG
1	C	2047	LEU
1	C	2102	ARG
1	C	2114	GLU
1	C	2142	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1494	GLN
1	A	1522	GLN
1	A	1525	ASN
1	A	1547	ASN
1	A	1560	ASN
1	A	1587	ASN
1	A	1605	ASN
1	A	1624	ASN
1	A	1640	GLN
1	A	1644	ASN
1	A	1748	GLN
1	A	1752	GLN
1	A	1776	GLN
1	A	1790	HIS
1	A	1815	ASN
1	A	1909	ASN
1	A	1922	GLN
1	A	1925	HIS
1	A	1934	GLN
1	A	2008	ASN
1	A	2088	GLN

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Mol	Chain	Res	Type
1	A	2092	GLN
1	A	2131	ASN
1	B	1494	GLN
1	B	1517	GLN
1	B	1525	ASN
1	B	1587	ASN
1	B	1605	ASN
1	B	1624	ASN
1	B	1644	ASN
1	B	1654	GLN
1	B	1683	ASN
1	B	1748	GLN
1	B	1752	GLN
1	B	1763	ASN
1	B	1786	ASN
1	B	1815	ASN
1	B	1837	ASN
1	B	1909	ASN
1	B	1911	ASN
1	B	1934	GLN
1	B	1937	ASN
1	B	1941	ASN
1	B	1944	GLN
1	B	2028	GLN
1	B	2045	ASN
1	B	2092	GLN
1	B	2097	HIS
1	B	2131	ASN
1	C	1517	GLN
1	C	1522	GLN
1	C	1525	ASN
1	C	1560	ASN
1	C	1581	GLN
1	C	1587	ASN
1	C	1640	GLN
1	C	1644	ASN
1	C	1654	GLN
1	C	1683	ASN
1	C	1748	GLN
1	C	1774	ASN
1	C	1776	GLN
1	C	1781	GLN

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Mol	Chain	Res	Type
1	C	1786	ASN
1	C	1815	ASN
1	C	1909	ASN
1	C	1911	ASN
1	C	1918	GLN
1	C	1925	HIS
1	C	1934	GLN
1	C	1941	ASN
1	C	1960	GLN
1	C	2011	GLN
1	C	2045	ASN
1	C	2092	GLN
1	C	2142	GLN
1	C	2170	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	RCP	C	3000	-	41,41,41	0.97	1 (2%)	58,58,58	1.27	7 (12%)
2	RCP	A	3000	-	41,41,41	0.98	1 (2%)	58,58,58	1.25	7 (12%)
2	RCP	B	3000	-	41,41,41	0.97	1 (2%)	58,58,58	1.24	7 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	RCP	C	3000	-	-	4/20/48/48	0/6/6/6
2	RCP	A	3000	-	-	0/20/48/48	0/6/6/6
2	RCP	B	3000	-	-	4/20/48/48	0/6/6/6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3000	RCP	C14-C15	2.99	1.53	1.50
2	B	3000	RCP	C14-C15	2.92	1.53	1.50
2	A	3000	RCP	C14-C15	2.90	1.53	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3000	RCP	C27-N26-C29	4.04	120.92	112.68
2	B	3000	RCP	C27-N26-C29	3.74	120.31	112.68
2	A	3000	RCP	C16-N15-C18	3.48	119.78	112.68
2	A	3000	RCP	C27-N26-C29	3.47	119.76	112.68
2	B	3000	RCP	C16-N15-C18	3.37	119.56	112.68
2	C	3000	RCP	C16-N15-C18	3.30	119.41	112.68
2	C	3000	RCP	C14-C15-N15	3.07	121.15	117.76
2	A	3000	RCP	C14-C15-N15	3.03	121.11	117.76
2	B	3000	RCP	C14-C15-N15	2.74	120.79	117.76
2	A	3000	RCP	C25-C26-N26	2.69	121.34	118.80
2	C	3000	RCP	C25-C26-N26	2.42	121.08	118.80
2	B	3000	RCP	O26-C26-N26	-2.24	118.94	121.61
2	B	3000	RCP	C25-C26-N26	2.22	120.89	118.80
2	C	3000	RCP	O26-C26-N26	-2.20	118.99	121.61
2	A	3000	RCP	O26-C26-N26	-2.19	119.00	121.61
2	C	3000	RCP	C12-C13-C14	-2.05	120.71	122.82
2	C	3000	RCP	O15-C15-N15	-2.05	119.12	122.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3000	RCP	O15-C15-N15	-2.05	119.12	122.35
2	B	3000	RCP	C12-C13-C14	-2.03	120.73	122.82
2	B	3000	RCP	C2-C1-C14	-2.03	120.74	122.82
2	A	3000	RCP	C2-C1-C14	-2.00	120.76	122.82

There are no chirality outliers.

All (8) torsion outliers are listed below:

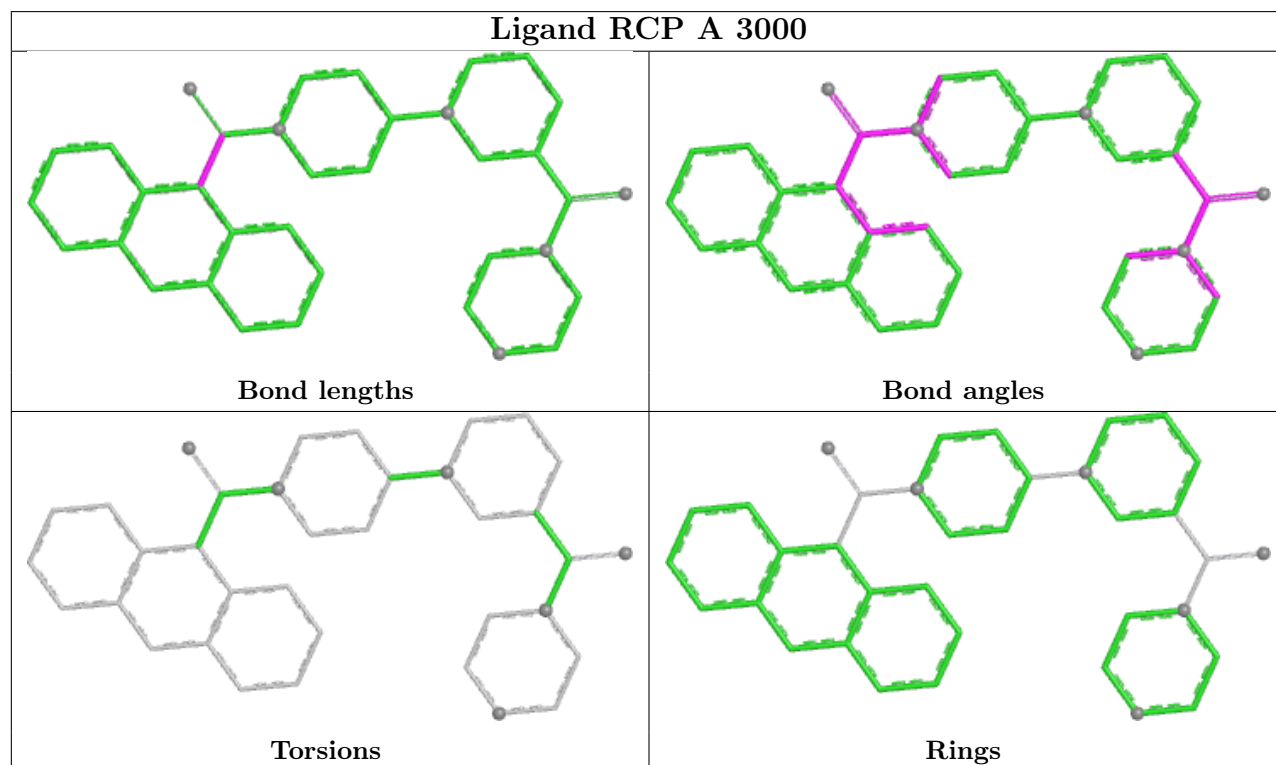
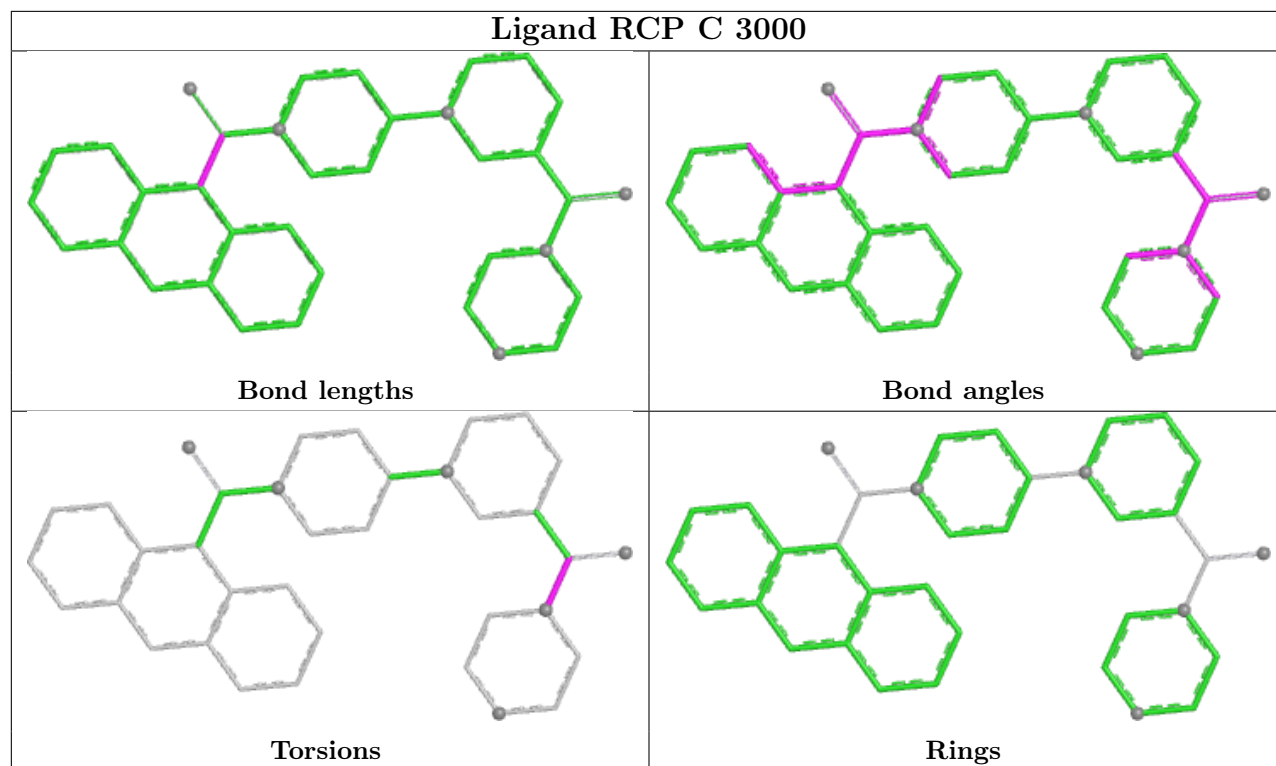
Mol	Chain	Res	Type	Atoms
2	B	3000	RCP	O26-C26-N26-C29
2	B	3000	RCP	C25-C26-N26-C29
2	C	3000	RCP	O26-C26-N26-C29
2	C	3000	RCP	C25-C26-N26-C29
2	B	3000	RCP	O26-C26-N26-C27
2	C	3000	RCP	O26-C26-N26-C27
2	B	3000	RCP	C25-C26-N26-C27
2	C	3000	RCP	C25-C26-N26-C27

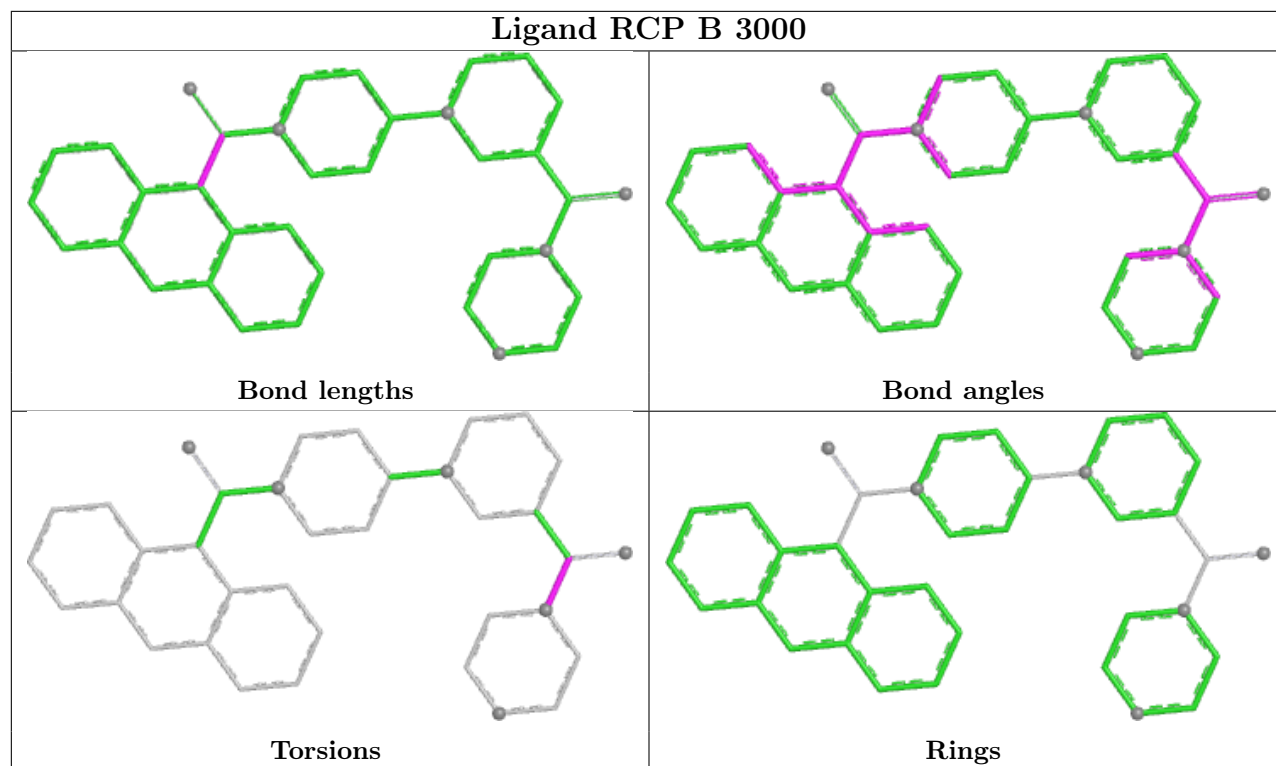
There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3000	RCP	3	0
2	A	3000	RCP	4	0
2	B	3000	RCP	3	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	682/758 (89%)	0.06	36 (5%)	32	24	22, 47, 98, 99	0
1	B	676/758 (89%)	0.11	50 (7%)	20	15	24, 49, 98, 99	0
1	C	666/758 (87%)	0.06	38 (5%)	29	22	22, 49, 99, 99	0
All	All	2024/2274 (89%)	0.07	124 (6%)	27	20	22, 48, 99, 99	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2082	LEU	6.5
1	C	2047	LEU	6.4
1	A	2047	LEU	5.4
1	B	2047	LEU	5.4
1	A	1493	LEU	5.3
1	A	1489	VAL	5.0
1	B	1680	THR	4.9
1	B	1488	PRO	4.8
1	A	2082	LEU	4.6
1	B	1683	ASN	4.6
1	B	1646	ALA	4.6
1	A	1492	TRP	4.4
1	A	2194	PHE	4.3
1	A	1482	PRO	4.2
1	C	1646	ALA	4.2
1	A	1488	PRO	4.1
1	B	2189	LEU	4.0
1	C	1644	ASN	4.0
1	A	2191	LEU	4.0
1	B	1483	ILE	3.8
1	C	1681	VAL	3.8
1	C	2037	ARG	3.8
1	B	1682	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	2149	LEU	3.6
1	A	1483	ILE	3.6
1	C	2081	GLU	3.5
1	B	1492	TRP	3.5
1	A	2143	VAL	3.5
1	B	1490	LYS	3.5
1	B	1685	GLU	3.5
1	A	1655	TYR	3.5
1	C	2143	VAL	3.4
1	C	1649	PRO	3.4
1	B	1493	LEU	3.4
1	B	2083	LEU	3.3
1	A	1649	PRO	3.2
1	B	2043	THR	3.2
1	B	2041	LEU	3.2
1	B	1489	VAL	3.1
1	C	2190	LYS	3.1
1	B	1660	SER	3.1
1	C	1685	GLU	3.1
1	C	2082	LEU	3.0
1	A	2144	GLY	2.9
1	B	1482	PRO	2.9
1	A	1490	LYS	2.9
1	B	2085	ILE	2.8
1	C	1684	GLY	2.8
1	A	1643	TRP	2.8
1	B	2086	TYR	2.8
1	A	2195	ALA	2.8
1	C	2044	MET	2.8
1	A	1646	ALA	2.8
1	A	2041	LEU	2.7
1	B	2187	LYS	2.7
1	B	2081	GLU	2.7
1	C	1629	ILE	2.7
1	C	1682	ILE	2.7
1	B	2179	TYR	2.7
1	B	1679	ARG	2.7
1	B	1556	GLU	2.7
1	C	2086	TYR	2.7
1	C	1645	ASP	2.6
1	C	1688	PHE	2.6
1	A	2081	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	2044	MET	2.6
1	A	2141	HIS	2.6
1	A	1681	VAL	2.6
1	C	2028	GLN	2.6
1	B	1649	PRO	2.5
1	A	1683	ASN	2.5
1	B	1531	LYS	2.5
1	B	1824	LYS	2.5
1	C	1647	ALA	2.5
1	A	2037	ARG	2.5
1	C	1678	GLU	2.5
1	C	2045	ASN	2.5
1	B	2152	ILE	2.4
1	B	1648	ASN	2.4
1	C	1643	TRP	2.4
1	B	1673	ASN	2.4
1	B	1839	GLU	2.4
1	C	1910	PRO	2.4
1	B	2143	VAL	2.4
1	B	1687	ARG	2.4
1	A	1641	VAL	2.3
1	A	1638	LEU	2.3
1	A	2086	TYR	2.3
1	C	1657	TYR	2.3
1	A	1682	ILE	2.3
1	A	1679	ARG	2.3
1	C	2036	ARG	2.3
1	A	2142	GLN	2.3
1	A	2190	LYS	2.3
1	C	2046	ARG	2.2
1	B	2134	TYR	2.2
1	B	1684	GLY	2.2
1	C	1632	ALA	2.2
1	B	1644	ASN	2.2
1	B	1495	PRO	2.2
1	C	1651	LYS	2.2
1	C	1676	LEU	2.2
1	A	1906	ASP	2.2
1	B	2084	PRO	2.2
1	B	1663	MET	2.2
1	C	1680	THR	2.2
1	C	1653	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	2186	LEU	2.2
1	B	1697	GLU	2.2
1	C	1662	GLY	2.1
1	C	2189	LEU	2.1
1	A	1685	GLU	2.1
1	C	2144	GLY	2.1
1	C	2141	HIS	2.1
1	B	1681	VAL	2.1
1	C	2084	PRO	2.1
1	B	1530	VAL	2.1
1	B	2040	LEU	2.1
1	B	2036	ARG	2.1
1	B	2046	ARG	2.1
1	B	1658	LEU	2.0
1	A	1853	GLU	2.0
1	A	2192	GLU	2.0
1	A	2044	MET	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.

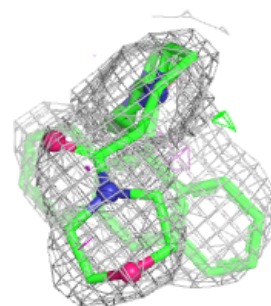
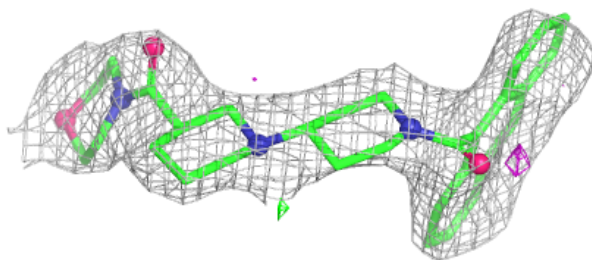
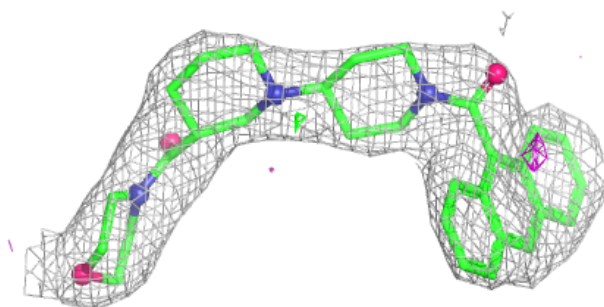
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	RCP	C	3000	36/36	0.92	0.15	73,87,94,95	0
2	RCP	B	3000	36/36	0.94	0.11	58,63,71,71	0
2	RCP	A	3000	36/36	0.95	0.10	60,68,69,70	0

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.

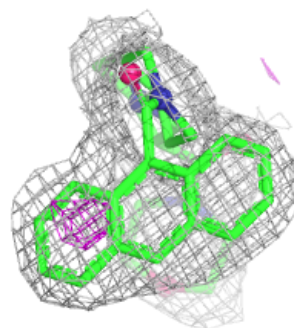
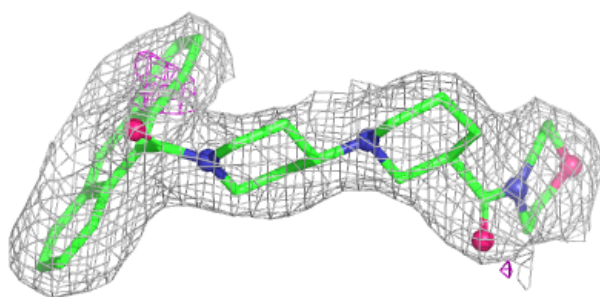
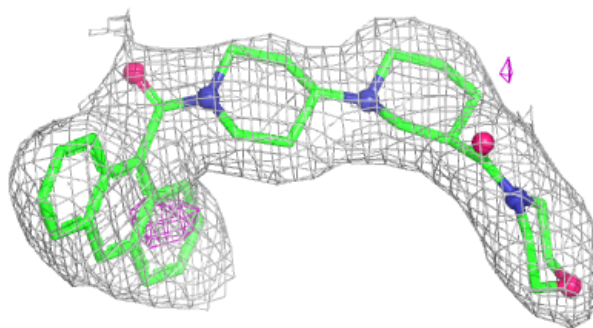
Electron density around RCP C 3000:

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

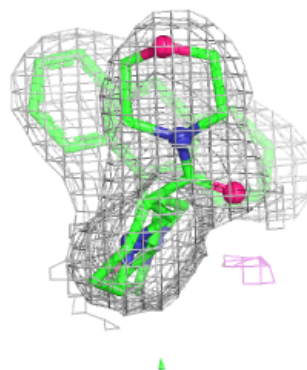
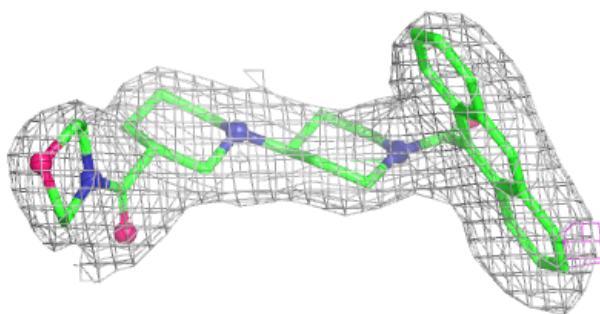
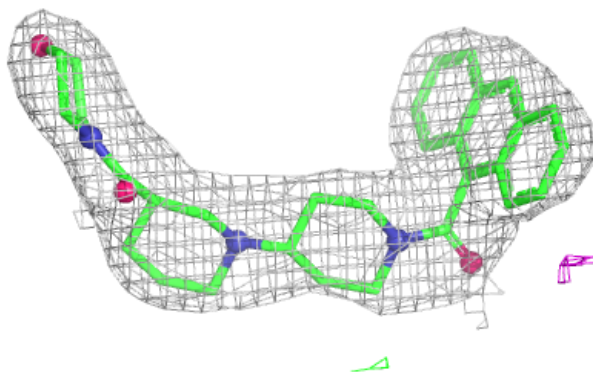


Electron density around RCP B 3000:

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

**Electron density around RCP A 3000:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.