



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:05 AM UTC

PDB ID : 1UYS / pdb_00001uys
Title : Acetyl-CoA carboxylase carboxyltransferase domain in complex with inhibitor haloxyfop
Authors : Zhang, H.; Tweel, B.; Tong, L.
Deposited on : 2004-03-02
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

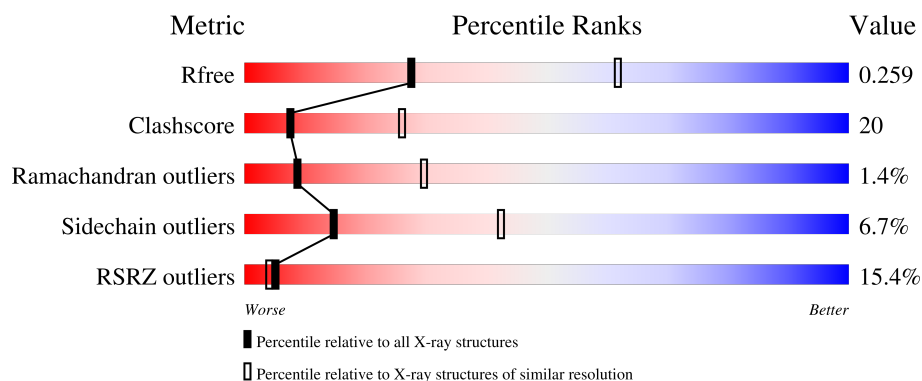
1 Overall quality at a glance

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	737	12% 56% 32% • 9%
1	B	737	15% 53% 34% • 9%
1	C	737	14% 52% 33% • • 10%

2 Entry composition [i](#)

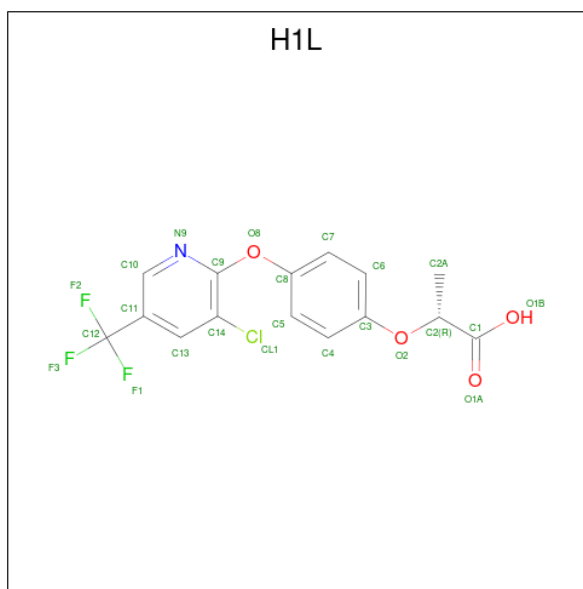
There are 3 unique types of molecules in this entry. The entry contains 16130 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	670	Total	C	N	O	S	Se	0	0	1
			5326	3396	914	998	2	16			
1	B	670	Total	C	N	O	S	Se	0	0	1
			5326	3396	914	998	2	16			
1	C	660	Total	C	N	O	S	Se	0	0	1
			5248	3343	903	984	2	16			

- Molecule 2 is (2R)-2-(4-{[3-chloro-5-(trifluoromethyl)pyridin-2-yl]oxy}phenoxy)propanoic acid (CCD ID: H1L) (formula: C₁₅H₁₁ClF₃NO₄).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0	0
			24	15	1	3	1	4		
2	B	1	Total	C	Cl	F	N	O	0	0
			24	15	1	3	1	4		
2	C	1	Total	C	Cl	F	N	O	0	0
			24	15	1	3	1	4		

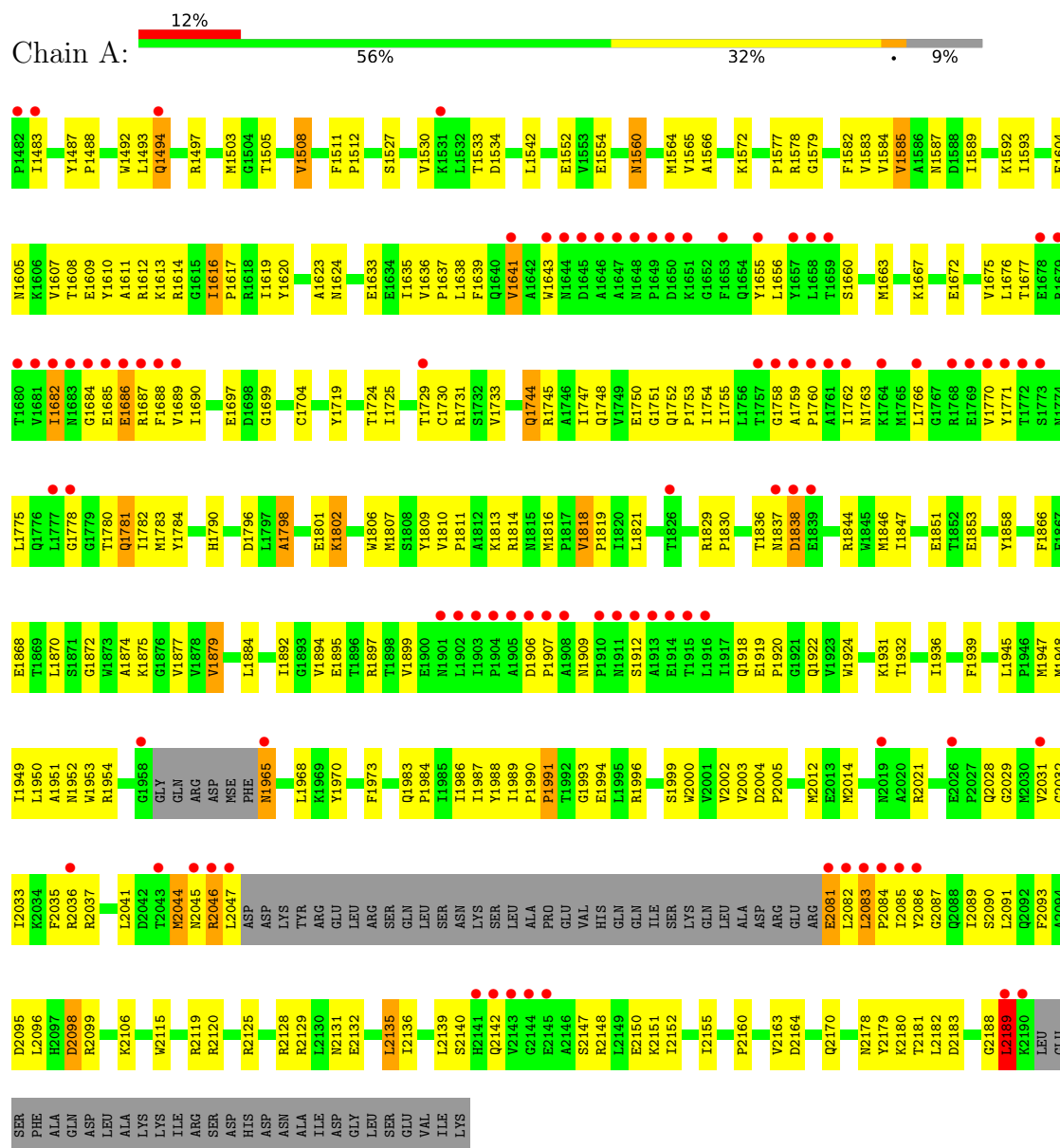
- Molecule 3 is water.

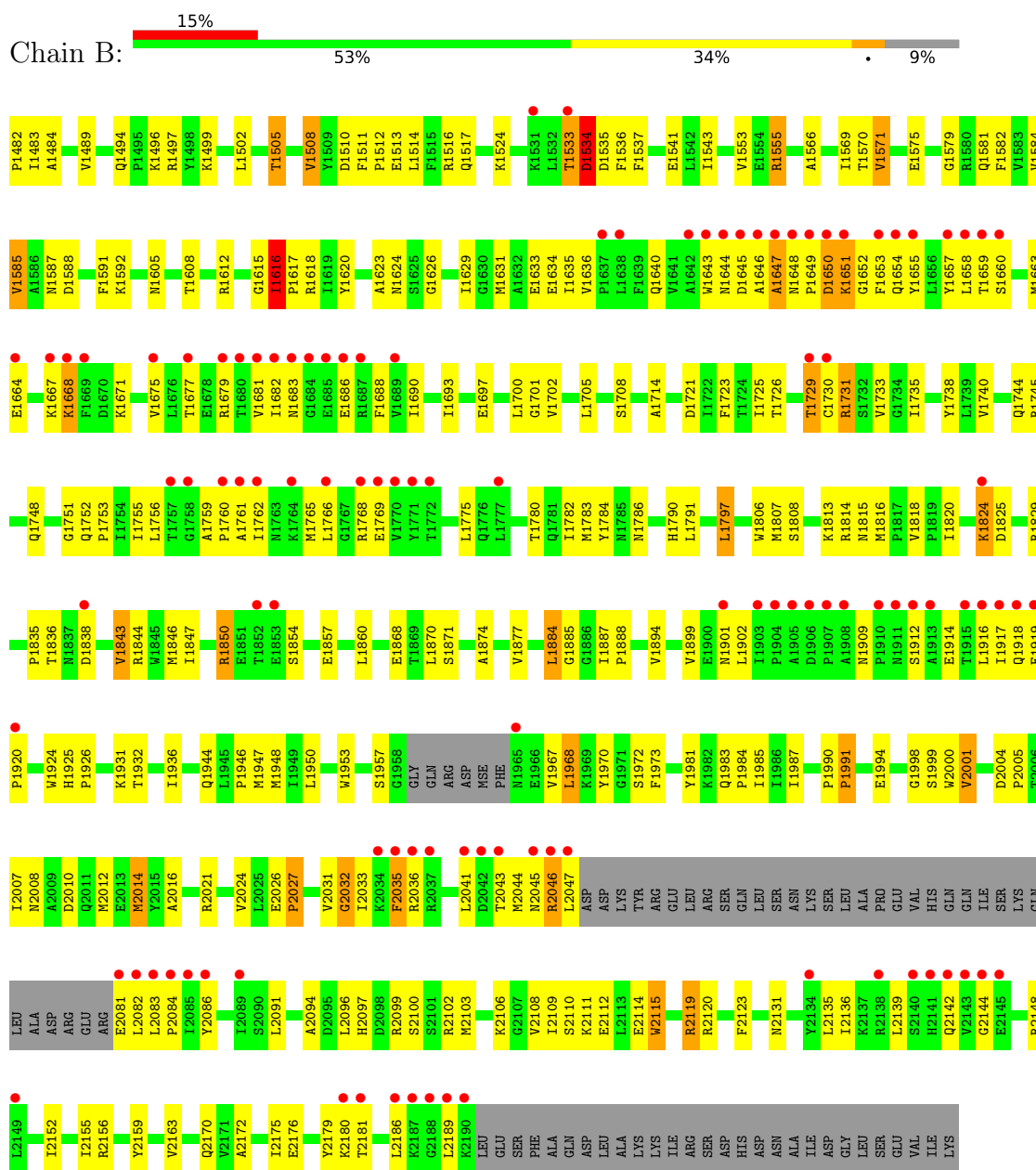
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	69	Total 69	O 69	0	0
3	B	50	Total 50	O 50	0	0
3	C	39	Total 39	O 39	0	0

3 Residue-property plots

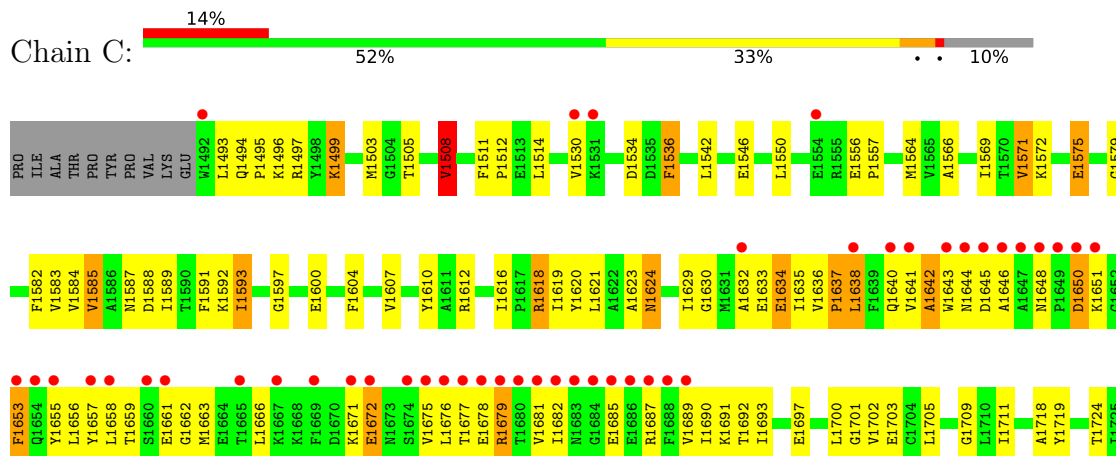
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

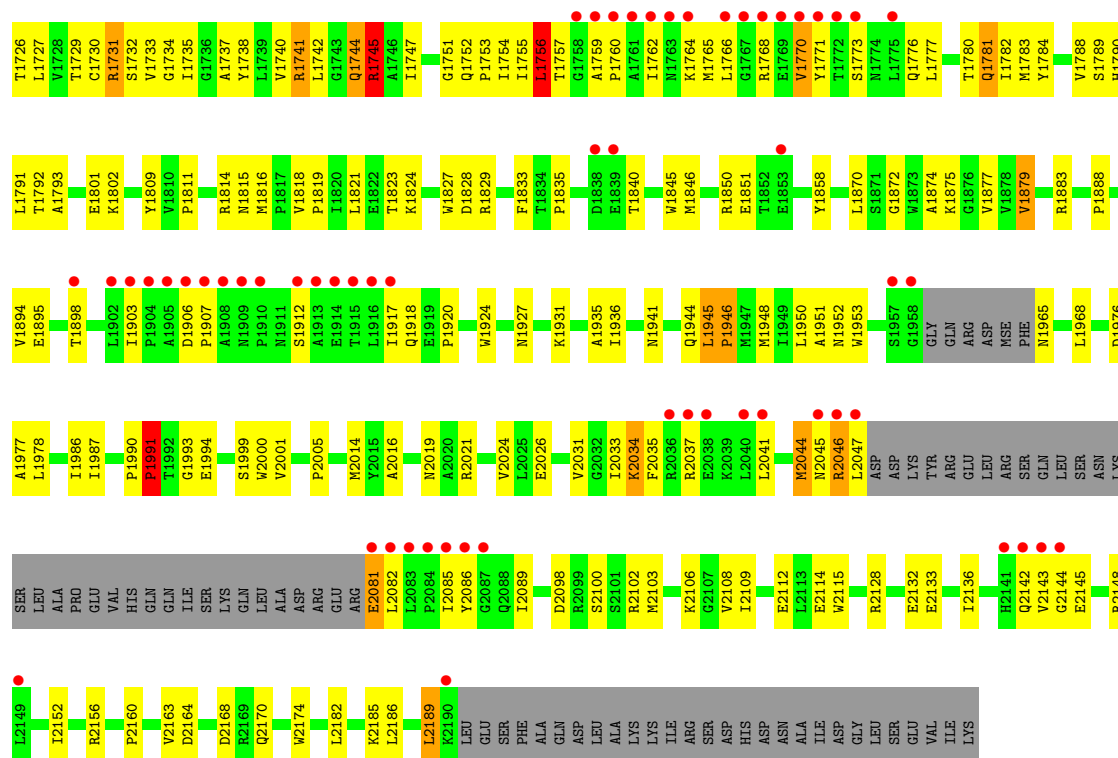
• Molecule 1: ACETYL-COA CARBOXYLASE





• Molecule 1: ACETYL-COA CARBOXYLASE





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	246.21Å 125.58Å 146.88Å 90.00° 94.08° 90.00°	Depositor
Resolution (Å)	27.42 – 2.80 27.42 – 2.80	Depositor EDS
% Data completeness (in resolution range)	87.6 (27.42-2.80) 94.3 (27.42-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.252 0.225 , 0.259	Depositor DCC
R_{free} test set	10734 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.8	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	0.90	EDS
Total number of atoms	16130	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: H1L

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	0.63	1/5429 (0.0%)	0.93	8/7332 (0.1%)
1	B	0.55	1/5429 (0.0%)	0.88	4/7332 (0.1%)
1	C	0.56	1/5347 (0.0%)	0.89	11/7218 (0.2%)
All	All	0.58	3/16205 (0.0%)	0.90	23/21882 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2189	LEU	C-N	-5.89	1.25	1.33
1	B	2189	LEU	C-N	-5.61	1.25	1.33
1	C	2189	LEU	C-N	-5.58	1.25	1.33

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1818	VAL	CA-C-N	9.07	131.18	119.84
1	A	1818	VAL	C-N-CA	9.07	131.18	119.84
1	A	1821	LEU	N-CA-C	7.79	120.18	107.32
1	C	1745	ARG	NE-CZ-NH2	7.53	125.98	119.20
1	C	1745	ARG	NE-CZ-NH1	-7.49	114.02	121.50
1	A	2012	MSE	N-CA-C	6.55	120.50	109.76
1	C	1745	ARG	CD-NE-CZ	-6.39	115.46	124.40
1	C	1976	ASP	N-CA-C	-6.31	104.48	111.36
1	C	1624	ASN	N-CA-C	5.67	115.77	108.34
1	C	2026	GLU	CA-C-N	5.67	126.93	119.84
1	C	2026	GLU	C-N-CA	5.67	126.93	119.84
1	B	1946	PRO	N-CA-C	-5.59	102.79	111.13
1	C	1756	LEU	N-CA-C	-5.38	106.40	113.12
1	C	1946	PRO	N-CA-C	-5.25	103.87	111.22
1	A	1798	ALA	N-CA-C	-5.22	105.67	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2168	ASP	N-CA-C	5.19	116.62	110.97
1	A	1989	ILE	CA-C-N	5.16	125.70	120.38
1	A	1989	ILE	C-N-CA	5.16	125.70	120.38
1	A	1796	ASP	N-CA-C	5.15	116.58	111.07
1	B	1616	ILE	CA-C-N	5.15	125.08	119.78
1	B	1616	ILE	C-N-CA	5.15	125.08	119.78
1	C	1782	ILE	CB-CA-C	-5.13	107.35	111.71
1	B	2001	VAL	N-CA-C	5.05	116.38	110.62

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	5326	0	5269	207	1
1	B	5326	0	5269	223	0
1	C	5248	0	5187	237	0
2	A	24	0	10	0	0
2	B	24	0	10	4	0
2	C	24	0	10	6	0
3	A	69	0	0	4	0
3	B	50	0	0	3	0
3	C	39	0	0	4	0
All	All	16130	0	15755	641	1

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 20.

All (641) 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:C:1618:ARG:HG2	1:C:1618:ARG:HH11	1.25	1.01
1:C:1637:PRO:HG2	1:C:1638:LEU:HD23	1.40	1.00
1:C:1823:THR:HG22	1:C:1824:LYS:H	1.33	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2045:ASN:HB2	1:A:2046:ARG:CZ	1.99	0.92
1:A:1582:PHE:HA	1:A:1616:ILE:HG23	1.54	0.90
1:C:1754:ILE:HD12	1:C:1783:MSE:HG2	1.54	0.88
1:A:2135:LEU:HB3	1:A:2155:ILE:HD13	1.57	0.87
1:A:1624:ASN:ND2	1:A:1733:VAL:H	1.74	0.86
1:A:2045:ASN:HB2	1:A:2046:ARG:NH2	1.90	0.86
1:B:1899:VAL:HB	1:B:1919:GLU:HB2	1.58	0.85
1:B:2031:VAL:HG21	1:B:2091:LEU:HD23	1.59	0.85
1:A:1874:ALA:HB3	1:A:1931:LYS:HD2	1.60	0.84
1:B:1508:VAL:HG21	1:B:1588:ASP:HA	1.61	0.82
1:C:2045:ASN:HB2	1:C:2046:ARG:NH2	1.95	0.81
1:B:1708:SER:HB3	1:B:1735:ILE:HD13	1.63	0.81
1:C:1493:LEU:HB2	1:C:1497:ARG:NH1	1.96	0.80
1:A:1948:MSE:HE2	1:A:1950:LEU:CD1	2.11	0.79
1:A:1624:ASN:HD21	1:A:1733:VAL:H	1.32	0.78
1:A:2183:ASP:HB2	1:B:1482:PRO:HG3	1.67	0.77
1:C:1754:ILE:HB	1:C:1783:MSE:HE3	1.65	0.77
1:B:1756:LEU:HD21	1:C:1968:LEU:HD13	1.66	0.77
1:C:1737:ALA:O	1:C:1740:VAL:HG22	1.85	0.77
1:C:2081:GLU:HG2	1:C:2082:LEU:H	1.49	0.76
1:B:1677:THR:HG22	1:B:1690:ILE:HA	1.68	0.76
1:A:1965:ASN:HD22	1:A:1965:ASN:N	1.84	0.76
1:A:2031:VAL:HG23	1:A:2035:PHE:HB3	1.68	0.75
1:C:1618:ARG:HG2	1:C:1618:ARG:NH1	1.93	0.75
1:C:1672:GLU:CD	1:C:1672:GLU:H	1.95	0.74
1:A:2140:SER:OG	1:A:2151:LYS:HE2	1.88	0.74
1:B:1730:CYS:HA	1:B:1752:GLN:HG3	1.67	0.74
1:B:1702:VAL:HA	1:B:1705:LEU:HD12	1.68	0.74
1:A:1899:VAL:HB	1:A:1919:GLU:HB2	1.71	0.73
1:B:1733:VAL:HG12	1:B:1755:ILE:HB	1.71	0.73
1:C:1592:LYS:C	1:C:1593:ILE:HG13	2.12	0.73
1:A:1750:GLU:HA	1:A:1780:THR:HG21	1.71	0.73
1:A:1948:MSE:HE2	1:A:1950:LEU:HD13	1.69	0.73
1:A:1939:PHE:CD1	1:A:1947:MSE:HE3	2.24	0.73
1:C:2047:LEU:HD13	1:C:2082:LEU:HD11	1.70	0.73
1:B:1836:THR:HG22	1:B:1838:ASP:H	1.52	0.72
1:B:2135:LEU:HB3	1:B:2155:ILE:HD13	1.70	0.72
1:C:2031:VAL:HG23	1:C:2035:PHE:HB3	1.72	0.72
1:B:1679:ARG:HH21	1:B:1681:VAL:HG21	1.54	0.71
1:C:1658:LEU:HG	1:C:1690:ILE:HD11	1.71	0.71
1:C:1676:LEU:HD12	1:C:1692:THR:HB	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1906:ASP:HB3	1:A:1912:SER:OG	1.90	0.71
1:B:1681:VAL:HA	1:B:1686:GLU:HA	1.73	0.70
1:C:1638:LEU:HD23	1:C:1638:LEU:H	1.56	0.70
1:C:1991:PRO:HG3	1:C:2115:TRP:HB2	1.72	0.70
1:B:1640:GLN:HG3	1:B:1659:THR:HG23	1.73	0.70
1:C:1759:ALA:HB3	1:C:1760:PRO:HD3	1.74	0.70
1:C:2148:ARG:CZ	1:C:2152:ILE:HD11	2.22	0.70
1:B:1968:LEU:HA	2:C:3000:H1L:CL1	2.29	0.70
1:A:1682:ILE:HD13	1:A:1682:ILE:H	1.56	0.69
1:B:1623:ALA:HB2	1:B:1729:THR:HG23	1.74	0.69
2:B:3000:H1L:CL1	1:C:1968:LEU:HA	2.30	0.69
1:C:2045:ASN:HB2	1:C:2046:ARG:CZ	2.22	0.69
1:B:1762:ILE:HG22	1:B:1766:LEU:HD12	1.75	0.69
1:B:2024:VAL:HG23	1:C:1701:GLY:HA2	1.75	0.68
1:B:1644:ASN:HB3	1:B:1654:GLN:HE21	1.58	0.68
1:C:1747:ILE:HD13	1:C:1802:LYS:HB2	1.75	0.68
1:A:1560:ASN:H	1:A:1560:ASN:HD22	1.40	0.67
1:A:1936:ILE:HG12	1:A:1947:MSE:HE1	1.76	0.67
1:A:1766:LEU:CD2	1:A:1770:VAL:HG11	2.25	0.67
1:A:1948:MSE:HE3	1:A:1988:TYR:HB3	1.75	0.67
1:A:2086:TYR:HA	1:A:2089:ILE:HD12	1.78	0.66
1:C:1651:LYS:H	1:C:1651:LYS:HD2	1.60	0.66
1:A:1656:LEU:HB2	1:A:1690:ILE:HD11	1.77	0.66
1:A:1560:ASN:H	1:A:1560:ASN:ND2	1.94	0.66
1:B:1582:PHE:HA	1:B:1616:ILE:HG23	1.77	0.66
1:A:1846:MSE:HE1	1:A:1991:PRO:HD2	1.76	0.66
1:B:1790:HIS:HA	1:B:1870:LEU:HD23	1.77	0.66
1:A:1936:ILE:HA	1:A:1947:MSE:HE1	1.78	0.66
1:B:1663:MSE:O	1:B:1667:LYS:HG3	1.95	0.66
1:B:1494:GLN:HE21	1:B:1496:LYS:H	1.44	0.66
1:A:1766:LEU:HD22	1:A:1770:VAL:HG11	1.78	0.66
1:A:1572:LYS:HA	1:A:1579:GLY:HA2	1.78	0.66
1:B:2108:VAL:HG23	1:B:2109:ILE:HG23	1.77	0.66
1:B:2082:LEU:HD23	1:B:2082:LEU:H	1.60	0.65
1:A:1587:ASN:HD22	1:A:1623:ALA:H	1.44	0.65
1:A:1939:PHE:HD1	1:A:1947:MSE:HE3	1.60	0.65
1:B:1843:VAL:HG21	1:B:1894:VAL:O	1.97	0.65
1:C:1493:LEU:HD12	1:C:1497:ARG:HH12	1.62	0.65
1:B:2045:ASN:HB2	1:B:2046:ARG:CZ	2.27	0.65
1:A:1614:ARG:HG3	1:A:1614:ARG:HH11	1.63	0.64
1:A:1682:ILE:HG12	1:A:1684:GLY:H	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1846:MSE:HE1	1:C:1990:PRO:HB3	1.79	0.64
1:A:2037:ARG:NH1	1:A:2037:ARG:HB2	2.12	0.64
1:B:1643:TRP:HA	1:B:1653:PHE:HA	1.79	0.64
1:B:1730:CYS:CA	1:B:1752:GLN:HG3	2.26	0.64
1:A:1623:ALA:HB2	1:A:1729:THR:CG2	2.27	0.63
1:C:1877:VAL:HG23	1:C:1931:LYS:HE2	1.79	0.63
1:C:1636:VAL:N	1:C:1637:PRO:HD2	2.13	0.63
1:B:1617:PRO:HB3	1:B:1723:PHE:HB3	1.80	0.63
1:C:1726:THR:HG21	1:C:1740:VAL:HG12	1.81	0.63
1:B:1970:TYR:O	1:B:1973:PHE:HB2	1.99	0.62
1:B:1998:GLY:HA2	1:B:2001:VAL:HG12	1.79	0.62
1:C:2148:ARG:NH1	1:C:2152:ILE:HD11	2.14	0.62
1:C:1637:PRO:HG2	1:C:1638:LEU:H	1.65	0.62
1:B:1902:LEU:HD12	1:B:1916:LEU:HD13	1.82	0.62
1:C:1783:MSE:HG3	1:C:1788:VAL:HB	1.81	0.62
1:A:1605:ASN:O	1:A:1609:GLU:HG2	2.00	0.62
1:A:1748:GLN:HE22	1:A:1783:MSE:HB2	1.65	0.62
1:B:1868:GLU:HG2	1:B:1871:SER:HB3	1.81	0.62
1:C:1793:ALA:HA	3:C:4012:HOH:O	1.99	0.62
1:B:2094:ALA:HA	1:B:2097:HIS:HD2	1.64	0.61
1:A:1530:VAL:HG23	1:A:1530:VAL:O	2.01	0.61
1:B:1483:ILE:HD12	1:B:1484:ALA:H	1.65	0.61
1:C:1818:VAL:HG12	1:C:1945:LEU:HD12	1.82	0.61
1:A:1948:MSE:HE2	1:A:1950:LEU:HD11	1.81	0.61
1:B:1645:ASP:OD2	1:B:1651:LYS:HB2	2.00	0.61
1:B:2001:VAL:HG11	2:C:3000:H1L:C6	2.30	0.61
1:A:2028:GLN:HE21	1:A:2091:LEU:HD21	1.65	0.61
1:B:1884:LEU:HD13	1:B:2123:PHE:HA	1.82	0.61
1:A:2180:LYS:HA	1:B:1482:PRO:HD3	1.82	0.61
1:C:2182:LEU:O	1:C:2186:LEU:HD23	2.00	0.61
1:B:1814:ARG:HA	1:B:1944:GLN:HE22	1.65	0.61
1:B:1829:ARG:HG3	1:B:1829:ARG:HH11	1.66	0.61
1:A:1578:ARG:HD2	1:A:1578:ARG:N	2.16	0.60
1:A:1730:CYS:HA	1:A:1752:GLN:NE2	2.16	0.60
1:C:1682:ILE:HG21	1:C:1687:ARG:HD2	1.82	0.60
1:A:2095:ASP:O	1:A:2099:ARG:NH1	2.34	0.60
1:B:1730:CYS:O	1:B:1731:ARG:C	2.45	0.60
1:C:2108:VAL:HG23	1:C:2109:ILE:HG23	1.84	0.60
1:C:1508:VAL:HG21	1:C:1588:ASP:HA	1.84	0.60
1:A:1759:ALA:HB3	1:A:1760:PRO:HD3	1.83	0.60
1:C:1874:ALA:HB3	1:C:1931:LYS:HD3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1818:VAL:HG11	1:C:1946:PRO:HD3	1.83	0.59
1:C:1757:THR:HB	1:C:1762:ILE:HD11	1.83	0.59
1:A:2180:LYS:HG2	1:B:1482:PRO:HD3	1.84	0.59
1:B:1745:ARG:HG2	1:B:1806:TRP:CZ2	2.38	0.58
1:A:2044:MSE:SE	1:A:2082:LEU:HD11	2.53	0.58
1:B:2036:ARG:HH11	1:B:2036:ARG:HG2	1.68	0.58
1:A:1682:ILE:HD12	1:A:1687:ARG:HG3	1.86	0.58
1:A:1811:PRO:HG3	1:A:1818:VAL:HA	1.85	0.58
1:C:1898:THR:HG22	1:C:1920:PRO:HA	1.84	0.58
1:A:1623:ALA:HB2	1:A:1729:THR:HG23	1.84	0.58
1:A:1724:THR:H	1:A:1745:ARG:HH21	1.50	0.58
1:A:2028:GLN:NE2	1:A:2091:LEU:HD21	2.19	0.58
1:B:1790:HIS:HD2	3:B:4039:HOH:O	1.85	0.58
1:A:2164:ASP:H	1:A:2170:GLN:HE22	1.49	0.58
1:B:1733:VAL:HA	1:B:1755:ILE:O	2.04	0.58
1:A:1809:TYR:O	1:A:1945:LEU:HD21	2.04	0.58
1:C:1737:ALA:HB3	1:C:1756:LEU:HD12	1.86	0.58
1:A:1996:ARG:HG3	1:A:1996:ARG:HH11	1.69	0.57
1:C:1823:THR:HB	3:C:4016:HOH:O	2.04	0.57
1:B:1679:ARG:HH21	1:B:1681:VAL:CG2	2.17	0.57
1:B:2031:VAL:HG13	1:B:2035:PHE:HB3	1.85	0.57
1:C:1823:THR:HG22	1:C:1824:LYS:N	2.12	0.57
1:B:2142:GLN:HG3	1:B:2186:LEU:HB3	1.87	0.57
1:C:1572:LYS:HA	1:C:1579:GLY:HA2	1.87	0.57
1:B:1608:THR:O	1:B:1612:ARG:HG2	2.04	0.57
1:B:2096:LEU:HB3	1:C:1693:ILE:HG13	1.87	0.57
1:A:1894:VAL:HG11	1:A:1952:ASN:O	2.05	0.57
1:A:2136:ILE:HD11	1:A:2152:ILE:HD13	1.87	0.57
1:A:1846:MSE:HE2	1:A:2115:TRP:CH2	2.40	0.57
1:C:2160:PRO:HD2	1:C:2163:VAL:HG21	1.85	0.57
1:A:1582:PHE:HA	1:A:1616:ILE:CG2	2.33	0.57
1:B:2136:ILE:HD11	1:B:2152:ILE:HG12	1.87	0.56
1:A:1922:GLN:HB3	1:A:1954:ARG:HG3	1.87	0.56
1:B:1874:ALA:HB3	1:B:1931:LYS:HD3	1.86	0.56
1:B:1582:PHE:CB	1:B:1617:PRO:HG2	2.35	0.56
1:B:1818:VAL:HB	1:B:1888:PRO:HG2	1.88	0.56
1:B:1846:MSE:HE1	1:B:1990:PRO:HB2	1.87	0.56
1:A:1624:ASN:HD21	1:A:1733:VAL:N	2.00	0.56
1:B:1748:GLN:HE22	1:B:1783:MSE:HB2	1.70	0.56
1:B:1874:ALA:HB3	1:B:1931:LYS:CD	2.36	0.56
1:B:1782:ILE:HG22	1:B:1783:MSE:HE2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2081:GLU:CD	1:C:2081:GLU:N	2.64	0.56
1:C:1623:ALA:HB2	1:C:1729:THR:HG23	1.87	0.56
1:C:1677:THR:HG22	1:C:1690:ILE:HD13	1.88	0.56
1:C:1612:ARG:HD3	1:C:1718:ALA:HA	1.88	0.56
1:C:1633:GLU:C	1:C:1635:ILE:H	2.14	0.56
1:A:2147:SER:HB3	1:A:2150:GLU:HG3	1.88	0.56
1:A:1592:LYS:O	1:A:1593:ILE:HG12	2.06	0.55
1:A:1747:ILE:HD13	1:A:1802:LYS:HB3	1.89	0.55
1:C:2086:TYR:HA	1:C:2089:ILE:HD12	1.89	0.55
1:B:1605:ASN:ND2	1:B:1714:ALA:HB2	2.22	0.55
1:B:1768:ARG:HG2	1:B:1768:ARG:HH11	1.71	0.55
1:B:1991:PRO:HG3	1:B:2115:TRP:HB2	1.87	0.55
1:C:1815:ASN:HD22	1:C:1944:GLN:HE22	1.54	0.55
1:B:2001:VAL:HG11	2:C:3000:H1L:H6	1.89	0.55
1:B:2156:ARG:HD3	1:B:2159:TYR:HE1	1.72	0.55
1:C:1724:THR:O	1:C:1745:ARG:HG2	2.06	0.55
1:B:1582:PHE:HB3	1:B:1617:PRO:HG2	1.89	0.55
1:A:1948:MSE:HE3	1:A:1988:TYR:CB	2.37	0.55
1:B:1824:LYS:HE2	1:B:1825:ASP:N	2.22	0.55
1:B:1987:ILE:HG22	1:B:2014:MSE:HE3	1.89	0.55
1:A:1585:VAL:HG13	1:A:1607:VAL:HG11	1.89	0.55
1:C:1505:THR:HB	1:C:1730:CYS:HB2	1.90	0.54
1:A:1508:VAL:HG23	3:A:4018:HOH:O	2.05	0.54
1:A:2106:LYS:HA	1:A:2106:LYS:HE2	1.89	0.54
1:B:2102:ARG:O	1:B:2106:LYS:HG2	2.06	0.54
1:C:1681:VAL:HG13	1:C:1685:GLU:O	2.08	0.54
1:B:2031:VAL:C	1:B:2033:ILE:H	2.16	0.54
1:A:1790:HIS:HA	1:A:1870:LEU:HD23	1.88	0.54
1:A:1948:MSE:CE	1:A:1988:TYR:HD1	2.20	0.54
1:A:1970:TYR:O	1:A:1973:PHE:HB2	2.07	0.54
1:B:1968:LEU:HD22	1:C:1741:ARG:HG3	1.90	0.54
1:A:1758:GLY:O	1:A:1762:ILE:HG13	2.07	0.54
1:C:2041:LEU:HD23	1:C:2044:MSE:HE3	1.89	0.54
1:A:2029:GLY:O	1:A:2033:ILE:HG12	2.07	0.54
1:B:1651:LYS:HE3	1:B:1651:LYS:HA	1.90	0.54
1:C:1874:ALA:HA	1:C:1927:ASN:HD22	1.73	0.54
1:B:1860:LEU:O	1:B:2119:ARG:HG3	2.07	0.54
1:B:1947:MSE:HE2	1:B:1985:ILE:HG12	1.90	0.54
1:B:2047:LEU:HD22	1:B:2082:LEU:HD22	1.90	0.54
1:C:1618:ARG:NH1	1:C:1620:TYR:HB2	2.22	0.54
1:C:1630:GLY:HA3	1:C:1700:LEU:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1987:ILE:CG2	1:B:2014:MSE:HE3	2.38	0.54
1:B:2081:GLU:HB3	1:B:2083:LEU:HD13	1.88	0.54
1:A:1895:GLU:OE1	1:A:1897:ARG:HD3	2.09	0.53
1:C:1587:ASN:HD22	1:C:1623:ALA:H	1.56	0.53
1:A:1633:GLU:O	1:A:1636:VAL:HG12	2.07	0.53
1:A:1730:CYS:HA	1:A:1752:GLN:HE21	1.71	0.53
1:B:1820:ILE:HD12	1:B:1887:ILE:HG12	1.90	0.53
1:B:1566:ALA:HA	1:B:1584:VAL:O	2.08	0.53
1:B:1629:ILE:HG22	1:C:2024:VAL:HG11	1.90	0.53
1:B:1972:SER:HB3	1:C:1742:LEU:HD12	1.90	0.53
1:C:1765:MSE:HE2	1:C:1766:LEU:HG	1.91	0.53
1:A:2002:VAL:HG13	1:A:2003:VAL:HG13	1.89	0.53
1:A:2085:ILE:HG23	1:A:2086:TYR:N	2.24	0.53
1:B:1681:VAL:HG22	1:B:1686:GLU:HB2	1.90	0.53
1:C:2016:ALA:O	1:C:2112:GLU:HA	2.07	0.53
1:C:1645:ASP:OD2	1:C:1651:LYS:HB2	2.08	0.53
1:C:1655:TYR:C	1:C:1656:LEU:HD12	2.33	0.53
1:C:1755:ILE:HD12	1:C:1755:ILE:N	2.23	0.53
1:A:2032:GLY:O	1:A:2033:ILE:HD13	2.09	0.53
1:B:1721:ASP:OD2	1:B:1814:ARG:NH1	2.41	0.53
1:B:1909:ASN:HB3	1:B:1912:SER:OG	2.09	0.53
1:C:1918:GLN:O	1:C:1920:PRO:HD3	2.08	0.53
1:A:1667:LYS:HG3	1:A:1672:GLU:OE2	2.09	0.53
1:C:1991:PRO:O	1:C:2019:ASN:O	2.27	0.53
1:A:1733:VAL:HA	1:A:1755:ILE:O	2.09	0.53
1:A:1635:ILE:O	1:A:1639:PHE:HB3	2.08	0.52
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.58	0.52
1:B:1655:TYR:HE1	1:B:1657:TYR:HB3	1.74	0.52
1:A:1780:THR:O	1:A:1784:TYR:HB3	2.09	0.52
1:C:1569:ILE:HG22	1:C:1571:VAL:HG22	1.92	0.52
1:C:1894:VAL:HG11	1:C:1952:ASN:O	2.08	0.52
1:C:1702:VAL:HA	1:C:1705:LEU:HD12	1.90	0.52
1:C:1823:THR:CG2	1:C:1824:LYS:H	2.14	0.52
1:B:1932:THR:O	1:B:1936:ILE:HG13	2.09	0.52
1:C:1642:ALA:HB2	1:C:1657:TYR:CE1	2.45	0.52
1:A:2000:TRP:CD1	1:A:2000:TRP:C	2.86	0.52
1:C:1638:LEU:O	1:C:1658:LEU:HD21	2.10	0.52
1:C:1643:TRP:C	1:C:1645:ASP:H	2.16	0.52
1:A:1807:MSE:O	1:A:1810:VAL:HG22	2.09	0.52
1:C:1781:GLN:H	1:C:1781:GLN:NE2	2.06	0.52
1:A:2119:ARG:HB3	3:A:4041:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1902:LEU:HD21	1:B:1914:GLU:CG	2.39	0.52
1:B:2001:VAL:HG23	1:C:1709:GLY:N	2.25	0.52
1:A:1614:ARG:HG3	1:A:1614:ARG:NH1	2.24	0.51
1:B:1664:GLU:O	1:B:1668:LYS:HG3	2.10	0.51
1:A:1836:THR:HG22	1:A:1838:ASP:H	1.75	0.51
1:A:2164:ASP:H	1:A:2170:GLN:NE2	2.09	0.51
1:B:1605:ASN:HD22	1:B:1714:ALA:HB2	1.74	0.51
1:C:2100:SER:HA	1:C:2103:MSE:HE3	1.93	0.51
1:A:1829:ARG:CZ	1:A:1858:TYR:HB3	2.40	0.51
1:C:1546:GLU:CD	1:C:1546:GLU:H	2.18	0.51
1:B:1824:LYS:HZ3	1:B:1825:ASP:H	1.59	0.51
1:A:1948:MSE:HE1	1:A:1988:TYR:HD1	1.75	0.51
1:B:1738:TYR:CG	2:B:3000:H1L:H7	2.46	0.51
1:B:1860:LEU:HD21	1:B:1948:MSE:HE1	1.92	0.51
1:A:1751:GLY:O	1:A:1775:LEU:HD21	2.11	0.51
1:B:2008:ASN:HB3	1:B:2012:MSE:HG3	1.91	0.51
1:B:2156:ARG:HD3	1:B:2159:TYR:CE1	2.46	0.51
1:B:1660:SER:O	1:B:1664:GLU:HG2	2.11	0.50
1:B:1494:GLN:NE2	1:B:1496:LYS:HG2	2.26	0.50
1:C:1809:TYR:O	1:C:1945:LEU:HD11	2.10	0.50
1:C:1883:ARG:HG3	1:C:1883:ARG:HH11	1.75	0.50
1:A:1608:THR:O	1:A:1612:ARG:HG3	2.12	0.50
1:A:1918:GLN:O	1:A:1920:PRO:HD3	2.11	0.50
1:A:2005:PRO:HG3	1:A:2014:MSE:HB2	1.93	0.50
1:B:1605:ASN:HD22	1:B:1714:ALA:CB	2.24	0.50
1:C:1814:ARG:O	1:C:1815:ASN:HB2	2.12	0.50
1:C:2160:PRO:HB2	1:C:2163:VAL:HG23	1.92	0.50
1:A:2179:TYR:HD1	1:B:1489:VAL:HA	1.75	0.50
1:B:1649:PRO:O	1:B:1651:LYS:N	2.44	0.50
1:B:1705:LEU:HB3	1:C:2000:TRP:CD1	2.45	0.50
1:B:1981:TYR:CG	1:B:1985:ILE:HD11	2.47	0.50
1:C:1818:VAL:HB	1:C:1888:PRO:HG2	1.93	0.50
1:C:1835:PRO:HG2	1:C:1991:PRO:HB2	1.93	0.50
1:A:1936:ILE:HA	1:A:1947:MSE:CE	2.42	0.50
1:B:1647:ALA:C	1:B:1649:PRO:HD3	2.37	0.50
1:B:1733:VAL:CG1	1:B:1755:ILE:HB	2.39	0.50
1:B:1753:PRO:HB2	1:B:1755:ILE:HD11	1.93	0.50
1:C:1987:ILE:HB	1:C:2014:MSE:HG3	1.93	0.50
1:C:1719:TYR:CE2	1:C:1744:GLN:HG3	2.46	0.50
1:A:2093:PHE:HA	1:A:2096:LEU:HD12	1.94	0.50
1:B:1634:GLU:HG3	1:B:1671:LYS:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1697:GLU:O	1:B:1700:LEU:HD13	2.12	0.50
1:C:1493:LEU:HB2	1:C:1497:ARG:HH11	1.73	0.50
1:C:1621:LEU:HD22	1:C:1727:LEU:HD23	1.94	0.50
1:C:1659:THR:OG1	1:C:1661:GLU:HG3	2.12	0.50
1:C:1730:CYS:O	1:C:1731:ARG:C	2.55	0.50
1:C:1737:ALA:CB	1:C:1756:LEU:HD12	2.42	0.50
1:C:1780:THR:O	1:C:1784:TYR:HB3	2.12	0.50
1:C:1582:PHE:CD1	1:C:1619:ILE:HD13	2.47	0.50
1:C:1629:ILE:HG13	1:C:1629:ILE:O	2.09	0.50
1:A:1719:TYR:CE2	1:A:1744:GLN:HG3	2.47	0.49
1:A:2037:ARG:HB2	1:A:2037:ARG:CZ	2.42	0.49
1:B:1570:THR:HG23	1:B:1581:GLN:HG2	1.93	0.49
1:B:1918:GLN:O	1:B:1920:PRO:HD3	2.12	0.49
1:A:1564:MSE:HE3	1:A:1604:PHE:HB2	1.93	0.49
1:A:1636:VAL:N	1:A:1637:PRO:HD2	2.27	0.49
1:B:2045:ASN:HB2	1:B:2046:ARG:NH2	2.27	0.49
1:C:2021:ARG:HA	1:C:2098:ASP:O	2.12	0.49
1:A:1636:VAL:CG1	1:A:1637:PRO:HD3	2.42	0.49
1:B:1534:ASP:C	1:B:1536:PHE:H	2.20	0.49
1:C:1493:LEU:HD12	1:C:1497:ARG:NH1	2.28	0.49
1:C:1697:GLU:HB3	1:C:1700:LEU:HD11	1.94	0.49
1:B:1569:ILE:HG22	1:B:1571:VAL:HG22	1.93	0.49
1:B:1998:GLY:O	1:B:2001:VAL:HG12	2.12	0.49
1:B:2100:SER:HA	1:B:2103:MSE:HE3	1.94	0.49
1:A:1619:ILE:HD12	1:A:1619:ILE:N	2.27	0.49
1:B:1983:GLN:HB3	1:B:1984:PRO:HD2	1.94	0.49
1:B:1541:GLU:CD	1:B:1555:ARG:HH11	2.21	0.49
1:B:1652:GLY:HA2	1:C:2085:ILE:HD11	1.94	0.49
1:B:2001:VAL:HG23	1:C:1709:GLY:CA	2.42	0.49
1:B:2099:ARG:HB2	1:C:1692:THR:HG23	1.95	0.49
1:A:1636:VAL:N	1:A:1637:PRO:CD	2.76	0.49
1:A:2041:LEU:O	1:A:2044:MSE:HB2	2.13	0.49
1:C:1811:PRO:HA	1:C:1819:PRO:HD3	1.95	0.49
1:A:2170:GLN:HG3	1:B:1517:GLN:NE2	2.28	0.49
1:B:1533:THR:OG1	1:B:1534:ASP:N	2.46	0.49
1:A:2135:LEU:HB3	1:A:2155:ILE:CD1	2.37	0.49
1:A:1572:LYS:HG2	1:A:1577:PRO:O	2.13	0.48
1:A:1660:SER:HB2	1:A:1686:GLU:OE2	2.12	0.48
1:B:1686:GLU:HG3	1:B:1686:GLU:O	2.12	0.48
1:B:1780:THR:O	1:B:1784:TYR:HB3	2.13	0.48
1:B:2103:MSE:HG2	1:C:1702:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1641:VAL:HG12	1:C:1653:PHE:HB3	1.94	0.48
1:A:1487:TYR:HB3	1:A:1488:PRO:HD2	1.95	0.48
1:A:2044:MSE:HG3	1:A:2086:TYR:CE2	2.48	0.48
1:B:1631:MSE:HE2	1:C:2034:LYS:HB3	1.96	0.48
1:B:2004:ASP:CG	1:B:2005:PRO:HD2	2.38	0.48
1:B:2120:ARG:HG3	3:B:4035:HOH:O	2.11	0.48
1:C:1592:LYS:O	1:C:1593:ILE:HG13	2.12	0.48
1:C:2128:ARG:HE	1:C:2132:GLU:CD	2.22	0.48
1:C:1550:LEU:HD11	1:C:1607:VAL:HA	1.95	0.48
1:C:1651:LYS:HD2	1:C:1651:LYS:N	2.26	0.48
1:A:1948:MSE:HA	1:A:1986:ILE:O	2.14	0.48
1:C:1951:ALA:O	1:C:1990:PRO:HD2	2.12	0.48
1:C:2133:GLU:HA	1:C:2136:ILE:HD12	1.93	0.48
1:C:2142:GLN:O	1:C:2144:GLY:N	2.46	0.48
1:A:1754:ILE:HD12	1:A:1783:MSE:HG3	1.95	0.48
1:A:1994:GLU:HA	1:A:2021:ARG:O	2.13	0.48
1:A:2005:PRO:CG	1:A:2014:MSE:HB2	2.43	0.48
1:B:2036:ARG:HG2	1:B:2036:ARG:NH1	2.28	0.48
1:A:1987:ILE:HB	1:A:2014:MSE:HG3	1.96	0.48
1:B:1829:ARG:HG3	1:B:1829:ARG:NH1	2.27	0.48
1:C:2164:ASP:H	1:C:2170:GLN:HE22	1.60	0.48
1:C:1646:ALA:C	1:C:1648:ASN:H	2.22	0.48
1:C:1879:VAL:CG1	1:C:1931:LYS:HE3	2.43	0.48
1:B:1649:PRO:C	1:B:1651:LYS:H	2.21	0.48
1:B:1755:ILE:N	1:B:1755:ILE:HD12	2.28	0.48
1:B:1780:THR:C	1:B:1782:ILE:H	2.22	0.48
1:C:2081:GLU:N	1:C:2081:GLU:OE1	2.47	0.48
1:A:1503:MSE:HB3	1:A:1505:THR:HG22	1.95	0.48
1:B:2044:MSE:HA	1:B:2086:TYR:CE2	2.49	0.48
1:C:1650:ASP:HB2	1:C:1651:LYS:HD2	1.96	0.48
1:C:2185:LYS:O	1:C:2189:LEU:HD13	2.13	0.48
1:A:1798:ALA:O	1:A:1802:LYS:HD3	2.13	0.48
1:B:1994:GLU:HA	1:B:2021:ARG:O	2.13	0.48
1:C:1499:LYS:O	1:C:1503:MSE:HG2	2.14	0.48
1:C:1948:MSE:HA	1:C:1986:ILE:O	2.13	0.47
1:C:1784:TYR:HA	1:C:1789:SER:HB2	1.95	0.47
1:C:2044:MSE:HG2	1:C:2086:TYR:CE2	2.49	0.47
1:A:1682:ILE:HD13	1:A:1682:ILE:N	2.25	0.47
1:A:1932:THR:O	1:A:1936:ILE:HG13	2.14	0.47
1:B:2131:ASN:HB3	1:B:2175:ILE:HG21	1.96	0.47
1:A:1830:PRO:HG3	1:A:2120:ARG:HH12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2001:VAL:O	1:B:2007:ILE:HD11	2.14	0.47
1:A:2085:ILE:O	1:A:2089:ILE:HG13	2.14	0.47
1:A:2128:ARG:HD3	1:A:2128:ARG:C	2.39	0.47
1:A:2178:ASN:HB3	1:A:2181:THR:HB	1.96	0.47
2:B:3000:H1L:H2A1	1:C:2001:VAL:CG2	2.45	0.47
1:B:1537:PHE:HD2	1:B:1571:VAL:HG13	1.80	0.47
1:B:1868:GLU:CG	1:B:1871:SER:HB3	2.45	0.47
1:B:1925:HIS:CE1	1:B:1957:SER:HB3	2.49	0.47
1:C:1566:ALA:HA	1:C:1584:VAL:O	2.15	0.47
1:C:1738:TYR:CG	2:C:3000:H1L:H7	2.49	0.47
1:B:1682:ILE:HG22	1:B:1683:ASN:H	1.80	0.47
1:B:1846:MSE:HE1	1:B:1990:PRO:CB	2.44	0.47
1:C:1636:VAL:N	1:C:1637:PRO:CD	2.77	0.47
1:C:1681:VAL:HG22	1:C:1685:GLU:O	2.14	0.47
1:C:2152:ILE:O	1:C:2156:ARG:HG3	2.15	0.47
1:A:1844:ARG:HA	1:A:1847:ILE:HD12	1.96	0.47
1:B:1635:ILE:O	1:B:1635:ILE:HG22	2.14	0.47
1:B:2001:VAL:HG23	1:C:1709:GLY:HA2	1.95	0.47
1:C:1623:ALA:HB2	1:C:1729:THR:CG2	2.44	0.47
1:A:1582:PHE:CD1	1:A:1619:ILE:HD13	2.50	0.47
1:A:1875:LYS:HB2	1:A:1899:VAL:CG1	2.45	0.47
1:A:2135:LEU:HD21	1:A:2182:LEU:HD13	1.97	0.47
1:A:2179:TYR:HB2	1:B:1489:VAL:HG13	1.97	0.47
1:B:1786:ASN:OD1	1:C:1965:ASN:HB3	2.15	0.47
1:C:1790:HIS:HA	1:C:1870:LEU:HD23	1.97	0.47
1:B:1681:VAL:O	1:B:1682:ILE:HD13	2.14	0.46
1:B:1759:ALA:HA	1:B:1762:ILE:HD12	1.97	0.46
1:B:1991:PRO:CG	1:B:2115:TRP:HB2	2.45	0.46
1:C:2160:PRO:HD3	1:C:2174:TRP:CE2	2.49	0.46
1:A:1894:VAL:HG11	1:A:1922:GLN:HA	1.97	0.46
1:A:2095:ASP:C	1:A:2099:ARG:NH1	2.73	0.46
1:B:2114:GLU:O	1:B:2115:TRP:C	2.57	0.46
1:C:2164:ASP:H	1:C:2170:GLN:NE2	2.13	0.46
1:A:1542:LEU:CD2	1:A:1552:GLU:HG2	2.46	0.46
1:B:1663:MSE:HG3	1:B:1688:PHE:CD2	2.49	0.46
1:C:1906:ASP:HB2	1:C:1912:SER:HB3	1.97	0.46
1:B:2163:VAL:HG13	1:B:2170:GLN:HG2	1.98	0.46
1:C:1827:TRP:CD2	1:C:1828:ASP:N	2.83	0.46
1:B:1835:PRO:HG2	1:B:1846:MSE:SE	2.65	0.46
1:C:1872:GLY:HA2	1:C:1875:LYS:HE3	1.97	0.46
1:B:1658:LEU:O	1:B:1688:PHE:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2148:ARG:O	1:C:2152:ILE:HG13	2.15	0.46
1:B:1624:ASN:ND2	1:B:1733:VAL:H	2.13	0.46
1:B:1768:ARG:HG2	1:B:1768:ARG:NH1	2.31	0.46
1:A:1675:VAL:HG22	1:A:1676:LEU:N	2.31	0.46
1:A:1965:ASN:N	1:A:1965:ASN:ND2	2.56	0.46
1:A:1583:VAL:HG21	1:A:1611:ALA:HB2	1.98	0.45
1:A:1990:PRO:HG2	1:A:1993:GLY:HA3	1.98	0.45
1:B:1571:VAL:O	1:B:1579:GLY:HA2	2.16	0.45
1:B:1591:PHE:O	1:B:1592:LYS:C	2.57	0.45
1:B:2000:TRP:CD1	1:C:1705:LEU:HB3	2.51	0.45
1:A:1760:PRO:HA	1:A:1763:ASN:HD22	1.81	0.45
1:A:2160:PRO:HD2	1:A:2163:VAL:HG21	1.97	0.45
2:B:3000:H1L:CL1	1:C:1968:LEU:HD12	2.53	0.45
1:C:1733:VAL:HA	1:C:1755:ILE:O	2.16	0.45
1:A:1494:GLN:HG3	1:A:1497:ARG:NH1	2.31	0.45
1:A:1801:GLU:HG2	3:A:4006:HOH:O	2.16	0.45
1:A:1813:LYS:HA	3:A:4033:HOH:O	2.15	0.45
1:A:2021:ARG:HA	1:A:2098:ASP:O	2.16	0.45
1:B:1514:LEU:HD22	1:B:1797:LEU:HG	1.99	0.45
1:B:1616:ILE:HG13	1:B:1617:PRO:HD2	1.97	0.45
1:B:1759:ALA:N	1:B:1760:PRO:CD	2.79	0.45
1:B:2024:VAL:HG11	1:C:1629:ILE:HG22	1.98	0.45
1:C:1550:LEU:HD12	1:C:1610:TYR:HB2	1.98	0.45
1:A:1770:VAL:HG13	1:A:1771:TYR:CD1	2.51	0.45
1:A:1745:ARG:HG2	1:A:1806:TRP:CZ2	2.51	0.45
1:A:1872:GLY:HA2	1:A:1875:LYS:HE2	1.98	0.45
1:A:2188:GLY:O	1:A:2189:LEU:HD12	2.17	0.45
1:B:1885:GLY:HA3	1:B:2123:PHE:CE1	2.52	0.45
1:C:1642:ALA:HB2	1:C:1657:TYR:CD1	2.51	0.45
1:C:2102:ARG:O	1:C:2106:LYS:HG2	2.16	0.45
1:B:1682:ILE:HG22	1:B:1683:ASN:N	2.31	0.45
1:B:2046:ARG:HD2	1:B:2046:ARG:N	2.32	0.45
1:B:2110:SER:O	1:B:2111:LYS:HB3	2.17	0.45
1:C:1766:LEU:HD13	1:C:1770:VAL:HG11	1.99	0.45
1:C:1883:ARG:HG3	1:C:1883:ARG:NH1	2.32	0.45
1:B:1761:ALA:O	1:B:1765:MSE:HG3	2.16	0.45
1:B:1797:LEU:HB2	3:B:4029:HOH:O	2.17	0.45
1:B:2094:ALA:HA	1:B:2097:HIS:CD2	2.49	0.45
1:C:1591:PHE:CD2	1:C:1592:LYS:HG3	2.52	0.45
1:C:2082:LEU:O	1:C:2086:TYR:HB2	2.16	0.45
1:A:1527:SER:O	1:A:1530:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1494:GLN:NE2	1:B:1496:LYS:H	2.12	0.45
1:B:1615:GLY:HA2	1:B:1814:ARG:NH1	2.32	0.45
1:B:1675:VAL:HG12	1:B:1693:ILE:HA	1.98	0.45
1:C:1875:LYS:O	1:C:1895:GLU:HG3	2.17	0.45
1:B:2179:TYR:HB2	1:B:2180:LYS:NZ	2.31	0.45
1:C:1682:ILE:CG2	1:C:1687:ARG:HD2	2.46	0.45
1:A:1682:ILE:C	1:A:1684:GLY:N	2.73	0.45
1:C:1564:MSE:HE3	1:C:1604:PHE:HB2	1.98	0.45
1:A:1633:GLU:C	1:A:1635:ILE:H	2.25	0.44
1:A:1750:GLU:HA	1:A:1780:THR:CG2	2.45	0.44
1:A:2081:GLU:OE1	1:A:2081:GLU:N	2.50	0.44
1:B:1633:GLU:HA	1:B:1636:VAL:HG23	1.99	0.44
1:C:1663:MSE:HE3	1:C:1666:LEU:HD12	1.99	0.44
1:A:1578:ARG:HD2	1:A:1578:ARG:H	1.83	0.44
1:C:1879:VAL:HG12	1:C:1931:LYS:HE3	1.99	0.44
1:C:1990:PRO:HG2	1:C:1993:GLY:HA3	1.98	0.44
1:C:2031:VAL:CG2	1:C:2035:PHE:HB3	2.45	0.44
1:A:1492:TRP:CE3	1:A:1493:LEU:HD23	2.53	0.44
1:B:1730:CYS:HA	1:B:1752:GLN:HE21	1.82	0.44
1:B:1901:ASN:ND2	1:B:1917:ILE:HD12	2.33	0.44
1:C:1655:TYR:O	1:C:1656:LEU:HD12	2.18	0.44
1:A:1635:ILE:C	1:A:1637:PRO:HD2	2.43	0.44
1:A:1875:LYS:HB2	1:A:1899:VAL:HG11	1.99	0.44
1:B:1731:ARG:HA	1:B:1753:PRO:O	2.18	0.44
1:B:1953:TRP:HB2	1:B:1999:SER:HB3	2.00	0.44
1:B:2083:LEU:N	1:B:2084:PRO:CD	2.81	0.44
1:A:1503:MSE:HG2	1:A:1589:ILE:HG12	1.98	0.44
1:A:2125:ARG:O	1:A:2129:ARG:HG3	2.17	0.44
1:B:1582:PHE:CD2	1:B:1807:MSE:HE1	2.52	0.44
1:C:1493:LEU:HB2	1:C:1497:ARG:HH12	1.78	0.44
1:C:1730:CYS:SG	1:C:1731:ARG:N	2.90	0.44
1:C:1903:ILE:HD13	1:C:1917:ILE:HG12	1.99	0.44
1:A:1656:LEU:CB	1:A:1690:ILE:HD11	2.47	0.44
1:A:1892:ILE:CD1	1:A:1947:MSE:HE2	2.48	0.44
1:C:1655:TYR:OH	1:C:1687:ARG:NH1	2.51	0.44
1:C:1675:VAL:HG12	1:C:1693:ILE:HG23	1.99	0.44
1:C:1729:THR:O	1:C:1752:GLN:HG3	2.18	0.44
1:C:1745:ARG:HH11	1:C:1745:ARG:HD2	1.31	0.44
1:B:1824:LYS:HE2	1:B:1825:ASP:H	1.83	0.44
1:C:1619:ILE:HD12	1:C:1619:ILE:N	2.33	0.44
1:C:1703:GLU:OE1	1:C:1703:GLU:N	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1690:ILE:HG13	1:A:1690:ILE:O	2.17	0.43
1:A:1991:PRO:C	1:A:1993:GLY:H	2.25	0.43
1:C:1583:VAL:HG13	1:C:1616:ILE:HD11	1.98	0.43
1:A:2132:GLU:O	1:A:2136:ILE:HG13	2.18	0.43
1:B:1505:THR:HB	1:B:1730:CYS:HB2	2.00	0.43
1:A:1778:GLY:HA2	1:A:1783:MSE:HE3	2.00	0.43
1:C:2000:TRP:CD1	1:C:2000:TRP:C	2.96	0.43
1:A:1641:VAL:HG13	1:A:1643:TRP:NE1	2.34	0.43
1:A:1663:MSE:HG3	1:A:1688:PHE:CD1	2.54	0.43
1:A:1699:GLY:HA2	1:A:1704:CYS:SG	2.59	0.43
1:B:2172:ALA:O	1:B:2176:GLU:HG3	2.18	0.43
1:C:1494:GLN:HB3	1:C:1495:PRO:CD	2.48	0.43
1:C:1879:VAL:HG12	1:C:1931:LYS:CE	2.49	0.43
1:A:1655:TYR:CE1	1:A:1689:VAL:HG22	2.54	0.43
1:A:1983:GLN:HB3	1:A:1984:PRO:HD2	2.00	0.43
1:B:1646:ALA:C	1:B:1648:ASN:H	2.26	0.43
1:C:1640:GLN:HB2	1:C:1657:TYR:CE1	2.54	0.43
1:C:1936:ILE:CG2	1:C:1977:ALA:HB1	2.48	0.43
1:B:1643:TRP:CZ3	1:B:1649:PRO:HB3	2.53	0.43
1:B:1759:ALA:HB3	1:B:1760:PRO:HD3	2.00	0.43
1:C:1575:GLU:CD	1:C:1575:GLU:H	2.25	0.43
1:C:1607:VAL:O	1:C:1610:TYR:HB3	2.19	0.43
1:C:1738:TYR:HB2	2:C:3000:H1L:C7	2.49	0.43
1:A:1892:ILE:HD11	1:A:1947:MSE:HE2	2.00	0.43
1:B:1815:ASN:H	1:B:1944:GLN:HE22	1.65	0.43
1:C:1644:ASN:N	1:C:1644:ASN:HD22	2.16	0.43
1:A:1677:THR:HA	1:A:1689:VAL:O	2.19	0.43
1:A:1682:ILE:C	1:A:1684:GLY:H	2.27	0.43
1:B:1844:ARG:HA	1:B:1847:ILE:HD12	2.01	0.43
1:A:1584:VAL:HA	1:A:1619:ILE:O	2.19	0.42
1:A:1879:VAL:HG13	1:A:1931:LYS:HE2	2.00	0.42
1:C:1811:PRO:HB2	1:C:1816:MSE:HB2	2.01	0.42
1:C:1827:TRP:CG	1:C:1828:ASP:N	2.87	0.42
1:A:1846:MSE:CE	1:A:1991:PRO:HD2	2.45	0.42
1:A:2180:LYS:HG2	1:B:1482:PRO:CD	2.48	0.42
1:B:2010:ASP:CG	1:B:2148:ARG:HD3	2.44	0.42
1:C:1534:ASP:C	1:C:1536:PHE:H	2.27	0.42
1:C:1677:THR:HA	1:C:1689:VAL:O	2.20	0.42
1:A:2180:LYS:CA	1:B:1482:PRO:HD3	2.49	0.42
1:B:1643:TRP:CD1	1:B:1643:TRP:H	2.35	0.42
1:B:1751:GLY:C	1:B:1775:LEU:HD21	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2044:MSE:C	1:A:2045:ASN:HD22	2.27	0.42
1:C:1597:GLY:H	1:C:1600:GLU:HB2	1.84	0.42
1:C:2128:ARG:HD3	1:C:2128:ARG:C	2.44	0.42
1:A:1619:ILE:HG13	1:A:1725:ILE:CG2	2.49	0.42
1:A:1844:ARG:HG3	1:A:1844:ARG:HH11	1.83	0.42
1:B:1582:PHE:HB2	1:B:1617:PRO:HG2	2.01	0.42
1:B:1726:THR:HG21	1:B:1740:VAL:HG22	2.02	0.42
1:B:1926:PRO:HG3	1:B:1967:VAL:HG23	2.00	0.42
1:C:1634:GLU:HG3	1:C:1671:LYS:HD3	2.01	0.42
1:C:2037:ARG:O	1:C:2041:LEU:HG	2.19	0.42
1:A:1996:ARG:O	1:A:1999:SER:HB2	2.19	0.42
1:B:2102:ARG:NH1	1:B:2106:LYS:HG3	2.35	0.42
1:C:1756:LEU:HD21	2:C:3000:H1L:CL1	2.57	0.42
1:C:1773:SER:HB3	1:C:1776:GLN:HG3	2.02	0.42
1:C:1833:PHE:CZ	1:C:1845:TRP:HE3	2.38	0.42
1:A:1907:PRO:C	1:A:1909:ASN:H	2.28	0.42
1:A:1953:TRP:HB2	1:A:1999:SER:HB3	2.02	0.42
1:A:2087:GLY:O	1:A:2090:SER:HB2	2.18	0.42
1:B:1543:ILE:HD11	1:B:1553:VAL:HG11	2.01	0.42
1:B:1585:VAL:O	1:B:1620:TYR:HA	2.19	0.42
1:C:1790:HIS:HD2	3:C:4018:HOH:O	2.02	0.42
1:A:1866:PHE:CE1	1:A:1868:GLU:HB2	2.54	0.42
1:A:1877:VAL:CG2	1:A:1931:LYS:HD3	2.50	0.42
1:B:1701:GLY:HA2	1:C:2024:VAL:HG23	2.01	0.42
1:C:1792:THR:CG2	1:C:1793:ALA:N	2.83	0.42
1:A:1753:PRO:HA	1:A:1778:GLY:O	2.20	0.42
1:B:1624:ASN:HD22	1:B:1626:GLY:H	1.68	0.42
1:B:1729:THR:C	1:B:1752:GLN:HG2	2.44	0.42
1:B:2010:ASP:OD2	1:B:2148:ARG:HD3	2.20	0.42
1:B:2156:ARG:HG3	1:B:2156:ARG:HH11	1.84	0.42
1:C:1751:GLY:O	1:C:1753:PRO:HD3	2.19	0.42
1:C:1829:ARG:CZ	1:C:1858:TYR:HB3	2.49	0.42
1:A:1565:VAL:HG12	1:A:1566:ALA:N	2.34	0.42
1:B:1818:VAL:HB	1:B:1888:PRO:CG	2.48	0.42
1:B:1850:ARG:NH1	1:B:1857:GLU:OE2	2.52	0.42
1:C:1711:ILE:HD11	1:C:1735:ILE:HG12	2.02	0.42
1:C:1790:HIS:O	1:C:1791:LEU:HD23	2.20	0.42
1:A:1505:THR:HB	1:A:1730:CYS:HB2	2.02	0.41
1:A:1585:VAL:O	1:A:1620:TYR:HA	2.20	0.41
1:A:2083:LEU:N	1:A:2084:PRO:CD	2.82	0.41
1:B:1494:GLN:NE2	1:B:1496:LYS:CG	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1537:PHE:CD2	1:B:1571:VAL:HG13	2.55	0.41
1:A:1807:MSE:HA	1:A:1810:VAL:HG22	2.02	0.41
1:B:2027:PRO:O	1:B:2031:VAL:HG23	2.19	0.41
1:C:1753:PRO:CG	1:C:1755:ILE:HD11	2.50	0.41
1:A:1616:ILE:HA	1:A:1617:PRO:HD3	1.91	0.41
1:B:2016:ALA:O	1:B:2112:GLU:HA	2.19	0.41
1:C:1585:VAL:O	1:C:1620:TYR:HA	2.20	0.41
1:C:1678:GLU:OE2	1:C:1691:LYS:HD2	2.20	0.41
1:A:1780:THR:C	1:A:1782:ILE:H	2.28	0.41
1:A:1655:TYR:CD1	1:A:1689:VAL:HG13	2.55	0.41
1:A:1781:GLN:O	1:A:1782:ILE:HD13	2.20	0.41
1:B:1543:ILE:HD13	1:B:1553:VAL:HG21	2.02	0.41
1:C:1587:ASN:ND2	1:C:1623:ALA:H	2.18	0.41
1:C:1759:ALA:HB2	1:C:1777:LEU:HD12	2.02	0.41
1:C:1850:ARG:HG2	1:C:1851:GLU:N	2.35	0.41
1:C:2033:ILE:HG22	1:C:2034:LYS:HD2	2.02	0.41
1:A:1542:LEU:HD21	1:A:1552:GLU:HG2	2.02	0.41
1:B:1648:ASN:ND2	1:B:1650:ASP:OD2	2.53	0.41
1:B:1780:THR:C	1:B:1782:ILE:N	2.78	0.41
1:C:1530:VAL:O	1:C:1530:VAL:HG23	2.21	0.41
1:C:1589:ILE:HD12	1:C:1589:ILE:HA	1.95	0.41
1:C:2081:GLU:CG	1:C:2082:LEU:H	2.23	0.41
1:C:1493:LEU:O	1:C:1494:GLN:C	2.63	0.41
1:C:1587:ASN:ND2	1:C:1624:ASN:HD22	2.18	0.41
1:A:1592:LYS:C	1:A:1593:ILE:HG12	2.46	0.41
1:C:1733:VAL:HG12	1:C:1734:GLY:N	2.35	0.41
1:C:1770:VAL:HG13	1:C:1771:TYR:H	1.85	0.41
1:A:1607:VAL:O	1:A:1610:TYR:HB3	2.21	0.41
1:B:1524:LYS:HA	1:B:1524:LYS:HE2	2.03	0.41
1:C:1633:GLU:C	1:C:1635:ILE:N	2.79	0.41
1:C:1661:GLU:HG3	1:C:1662:GLY:N	2.35	0.41
1:C:1679:ARG:HB2	1:C:1679:ARG:HH11	1.85	0.41
1:C:1753:PRO:HG2	1:C:1755:ILE:HD11	2.02	0.41
1:C:2005:PRO:HG3	1:C:2014:MSE:HB2	2.03	0.41
1:A:1951:ALA:O	1:A:1990:PRO:HD2	2.21	0.41
1:C:1569:ILE:CG2	1:C:1571:VAL:HG22	2.51	0.41
1:C:1719:TYR:O	1:C:1941:ASN:HB3	2.21	0.41
1:C:1764:LYS:N	1:C:1764:LYS:HD2	2.36	0.41
1:C:1818:VAL:CG1	1:C:1945:LEU:HD12	2.50	0.41
1:A:1813:LYS:O	1:A:1816:MSE:HB2	2.21	0.40
1:B:1497:ARG:HD3	1:B:1510:ASP:OD1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1511:PHE:O	1:B:1512:PRO:C	2.64	0.40
1:C:1766:LEU:C	1:C:1768:ARG:H	2.29	0.40
1:A:1636:VAL:HG12	1:A:1637:PRO:HD3	2.03	0.40
1:A:2131:ASN:ND2	1:A:2179:TYR:OH	2.54	0.40
1:B:2032:GLY:C	1:B:2033:ILE:HG13	2.45	0.40
1:B:2139:LEU:HD22	1:B:2155:ILE:HG13	2.03	0.40
1:C:1575:GLU:OE1	1:C:1821:LEU:HD22	2.21	0.40
1:C:1792:THR:HG22	1:C:1793:ALA:N	2.36	0.40
1:C:2148:ARG:HG2	1:C:2148:ARG:HH11	1.85	0.40
1:A:2004:ASP:HA	1:A:2005:PRO:HD3	1.98	0.40
1:C:1511:PHE:O	1:C:1512:PRO:C	2.62	0.40
1:C:1556:GLU:HA	1:C:1557:PRO:HD3	1.92	0.40
1:C:1754:ILE:HB	1:C:1783:MSE:CE	2.45	0.40
1:C:1935:ALA:HA	3:C:4024:HOH:O	2.22	0.40
1:B:1537:PHE:CD1	1:B:1537:PHE:C	3.00	0.40
1:C:1505:THR:CB	1:C:1730:CYS:HB2	2.51	0.40
1:C:1666:LEU:HB3	1:C:1671:LYS:O	2.21	0.40
1:C:1953:TRP:HB2	1:C:1999:SER:HB3	2.04	0.40
1:A:1511:PHE:N	1:A:1512:PRO:CD	2.84	0.40
1:A:1762:ILE:O	1:A:1766:LEU:HD13	2.22	0.40
1:A:1949:ILE:HD12	1:A:1987:ILE:CD1	2.52	0.40
1:B:1575:GLU:OE1	1:B:1808:SER:HB2	2.22	0.40
1:C:1994:GLU:HA	1:C:2021:ARG:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1970:TYR:OH	1:A:1970:TYR:OH[2_555]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	664/737 (90%)	602 (91%)	57 (9%)	5 (1%)	16	44
1	B	664/737 (90%)	597 (90%)	57 (9%)	10 (2%)	8	28
1	C	654/737 (89%)	576 (88%)	66 (10%)	12 (2%)	6	23
All	All	1982/2211 (90%)	1775 (90%)	180 (9%)	27 (1%)	9	30

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1991	PRO
1	B	1534	ASP
1	B	1650	ASP
1	B	1731	ARG
1	C	1632	ALA
1	C	2143	VAL
1	A	2036	ARG
1	B	1744	GLN
1	C	1642	ALA
1	C	1744	GLN
1	C	1907	PRO
1	A	1731	ARG
1	A	1744	GLN
1	B	1533	THR
1	C	1634	GLU
1	C	1637	PRO
1	C	1731	ARG
1	A	1819	PRO
1	B	1991	PRO
1	B	2115	TRP
1	C	1508	VAL
1	C	1653	PHE
1	B	1647	ALA
1	B	2144	GLY
1	C	1650	ASP
1	B	2032	GLY
1	C	1991	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	567/611 (93%)	528 (93%)	39 (7%)	14	41
1	B	567/611 (93%)	527 (93%)	40 (7%)	13	39
1	C	558/611 (91%)	524 (94%)	34 (6%)	17	46
All	All	1692/1833 (92%)	1579 (93%)	113 (7%)	15	42

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1483	ILE
1	A	1494	GLN
1	A	1508	VAL
1	A	1533	THR
1	A	1534	ASP
1	A	1554	GLU
1	A	1560	ASN
1	A	1585	VAL
1	A	1613	LYS
1	A	1616	ILE
1	A	1638	LEU
1	A	1641	VAL
1	A	1682	ILE
1	A	1685	GLU
1	A	1686	GLU
1	A	1697	GLU
1	A	1781	GLN
1	A	1802	LYS
1	A	1814	ARG
1	A	1837	ASN
1	A	1838	ASP
1	A	1851	GLU
1	A	1853	GLU
1	A	1879	VAL
1	A	1884	LEU
1	A	1924	TRP
1	A	1965	ASN
1	A	1968	LEU
1	A	2044	MSE
1	A	2046	ARG
1	A	2047	LEU

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Mol	Chain	Res	Type
1	A	2081	GLU
1	A	2083	LEU
1	A	2098	ASP
1	A	2135	LEU
1	A	2139	LEU
1	A	2142	GLN
1	A	2148	ARG
1	A	2189	LEU
1	B	1499	LYS
1	B	1502	LEU
1	B	1505	THR
1	B	1508	VAL
1	B	1513	GLU
1	B	1516	ARG
1	B	1534	ASP
1	B	1535	ASP
1	B	1555	ARG
1	B	1571	VAL
1	B	1585	VAL
1	B	1616	ILE
1	B	1618	ARG
1	B	1651	LYS
1	B	1668	LYS
1	B	1725	ILE
1	B	1729	THR
1	B	1769	GLU
1	B	1791	LEU
1	B	1797	LEU
1	B	1813	LYS
1	B	1816	MSE
1	B	1824	LYS
1	B	1843	VAL
1	B	1850	ARG
1	B	1854	SER
1	B	1877	VAL
1	B	1884	LEU
1	B	1924	TRP
1	B	1950	LEU
1	B	1968	LEU
1	B	2014	MSE
1	B	2026	GLU
1	B	2027	PRO

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Mol	Chain	Res	Type
1	B	2035	PHE
1	B	2041	LEU
1	B	2043	THR
1	B	2046	ARG
1	B	2119	ARG
1	B	2181	THR
1	C	1496	LYS
1	C	1499	LYS
1	C	1508	VAL
1	C	1514	LEU
1	C	1536	PHE
1	C	1542	LEU
1	C	1571	VAL
1	C	1575	GLU
1	C	1585	VAL
1	C	1593	ILE
1	C	1618	ARG
1	C	1638	LEU
1	C	1672	GLU
1	C	1679	ARG
1	C	1732	SER
1	C	1741	ARG
1	C	1745	ARG
1	C	1756	LEU
1	C	1770	VAL
1	C	1781	GLN
1	C	1801	GLU
1	C	1840	THR
1	C	1879	VAL
1	C	1924	TRP
1	C	1945	LEU
1	C	1950	LEU
1	C	1978	LEU
1	C	1991	PRO
1	C	2034	LYS
1	C	2044	MSE
1	C	2046	ARG
1	C	2081	GLU
1	C	2114	GLU
1	C	2145	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1517	GLN
1	A	1547	ASN
1	A	1560	ASN
1	A	1587	ASN
1	A	1624	ASN
1	A	1748	GLN
1	A	1752	GLN
1	A	1774	ASN
1	A	1815	ASN
1	A	1937	ASN
1	A	2008	ASN
1	A	2028	GLN
1	A	2045	ASN
1	A	2088	GLN
1	A	2092	GLN
1	A	2131	ASN
1	A	2170	GLN
1	A	2178	ASN
1	B	1494	GLN
1	B	1517	GLN
1	B	1525	ASN
1	B	1547	ASN
1	B	1581	GLN
1	B	1587	ASN
1	B	1599	GLN
1	B	1605	ASN
1	B	1624	ASN
1	B	1654	GLN
1	B	1720	HIS
1	B	1748	GLN
1	B	1752	GLN
1	B	1763	ASN
1	B	1774	ASN
1	B	1790	HIS
1	B	1815	ASN
1	B	1901	ASN
1	B	1909	ASN
1	B	1922	GLN
1	B	1941	ASN
1	B	1944	GLN
1	B	2019	ASN
1	B	2045	ASN
1	B	2097	HIS

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Mol	Chain	Res	Type
1	B	2178	ASN
1	C	1522	GLN
1	C	1560	ASN
1	C	1587	ASN
1	C	1605	ASN
1	C	1640	GLN
1	C	1644	ASN
1	C	1654	GLN
1	C	1683	ASN
1	C	1744	GLN
1	C	1748	GLN
1	C	1763	ASN
1	C	1781	GLN
1	C	1786	ASN
1	C	1790	HIS
1	C	1815	ASN
1	C	1922	GLN
1	C	1925	HIS
1	C	1927	ASN
1	C	1941	ASN
1	C	2011	GLN
1	C	2092	GLN
1	C	2170	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	H1L	C	3000	-	25,25,25	0.97	0	36,36,36	1.58	7 (19%)
2	H1L	A	3000	-	25,25,25	1.09	2 (8%)	36,36,36	1.49	8 (22%)
2	H1L	B	3000	-	25,25,25	1.31	4 (16%)	36,36,36	1.59	10 (27%)

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	H1L	C	3000	-	-	6/18/18/18	0/2/2/2
2	H1L	A	3000	-	-	4/18/18/18	0/2/2/2
2	H1L	B	3000	-	-	4/18/18/18	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3000	H1L	C7-C6	2.75	1.43	1.38
2	B	3000	H1L	C12-C11	2.39	1.54	1.49
2	B	3000	H1L	C5-C8	2.34	1.43	1.38
2	A	3000	H1L	O2-C3	-2.12	1.34	1.38
2	B	3000	H1L	C4-C3	2.03	1.42	1.38
2	A	3000	H1L	O1B-C1	-2.02	1.24	1.30

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3000	H1L	C14-C9-N9	-4.31	118.93	122.69
2	A	3000	H1L	C11-C10-N9	-3.89	119.73	123.38
2	B	3000	H1L	C11-C10-N9	-3.43	120.16	123.38
2	C	3000	H1L	C11-C10-N9	-3.29	120.29	123.38
2	C	3000	H1L	O8-C9-N9	3.06	123.56	119.47
2	B	3000	H1L	C13-C11-C10	2.93	121.07	118.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3000	H1L	C8-O8-C9	-2.83	112.14	118.27
2	B	3000	H1L	F3-C12-C11	-2.82	106.86	112.90
2	B	3000	H1L	O2-C2-C1	-2.75	107.86	111.34
2	C	3000	H1L	C10-N9-C9	2.67	122.96	116.51
2	A	3000	H1L	C3-O2-C2	-2.55	114.25	118.40
2	A	3000	H1L	O2-C2-C1	-2.54	108.13	111.34
2	C	3000	H1L	C8-O8-C9	-2.36	113.16	118.27
2	A	3000	H1L	C10-N9-C9	2.31	122.08	116.51
2	A	3000	H1L	C13-C11-C10	2.31	120.58	118.78
2	C	3000	H1L	C3-O2-C2	-2.30	114.64	118.40
2	B	3000	H1L	O8-C9-N9	2.23	122.45	119.47
2	A	3000	H1L	F2-C12-C11	-2.21	108.16	112.90
2	B	3000	H1L	O1B-C1-O1A	-2.20	119.08	124.08
2	C	3000	H1L	O1B-C1-O1A	-2.20	119.09	124.08
2	A	3000	H1L	C13-C14-CL1	2.11	121.90	118.45
2	B	3000	H1L	C14-C13-C11	-2.10	117.05	119.59
2	A	3000	H1L	C8-O8-C9	-2.05	113.83	118.27
2	B	3000	H1L	C10-N9-C9	2.03	121.39	116.51
2	B	3000	H1L	C3-O2-C2	-2.02	115.11	118.40

There are no chirality outliers.

All (14) torsion outliers are listed below:

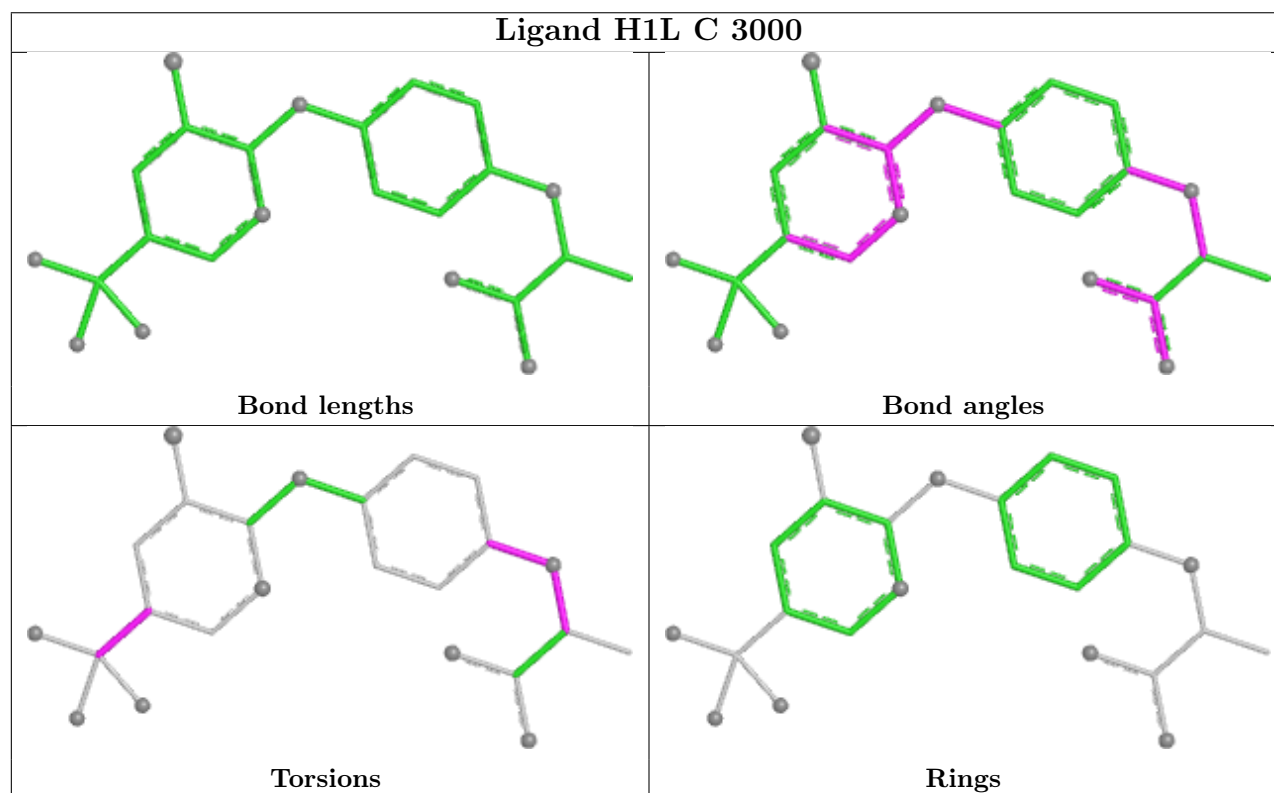
Mol	Chain	Res	Type	Atoms
2	B	3000	H1L	O1A-C1-C2-O2
2	A	3000	H1L	C1-C2-O2-C3
2	B	3000	H1L	C1-C2-O2-C3
2	C	3000	H1L	C1-C2-O2-C3
2	C	3000	H1L	C2A-C2-O2-C3
2	B	3000	H1L	O1B-C1-C2-O2
2	A	3000	H1L	C2A-C2-O2-C3
2	B	3000	H1L	C2A-C2-O2-C3
2	A	3000	H1L	C4-C3-O2-C2
2	C	3000	H1L	C4-C3-O2-C2
2	A	3000	H1L	C6-C3-O2-C2
2	C	3000	H1L	C10-C11-C12-F2
2	C	3000	H1L	C10-C11-C12-F1
2	C	3000	H1L	C10-C11-C12-F3

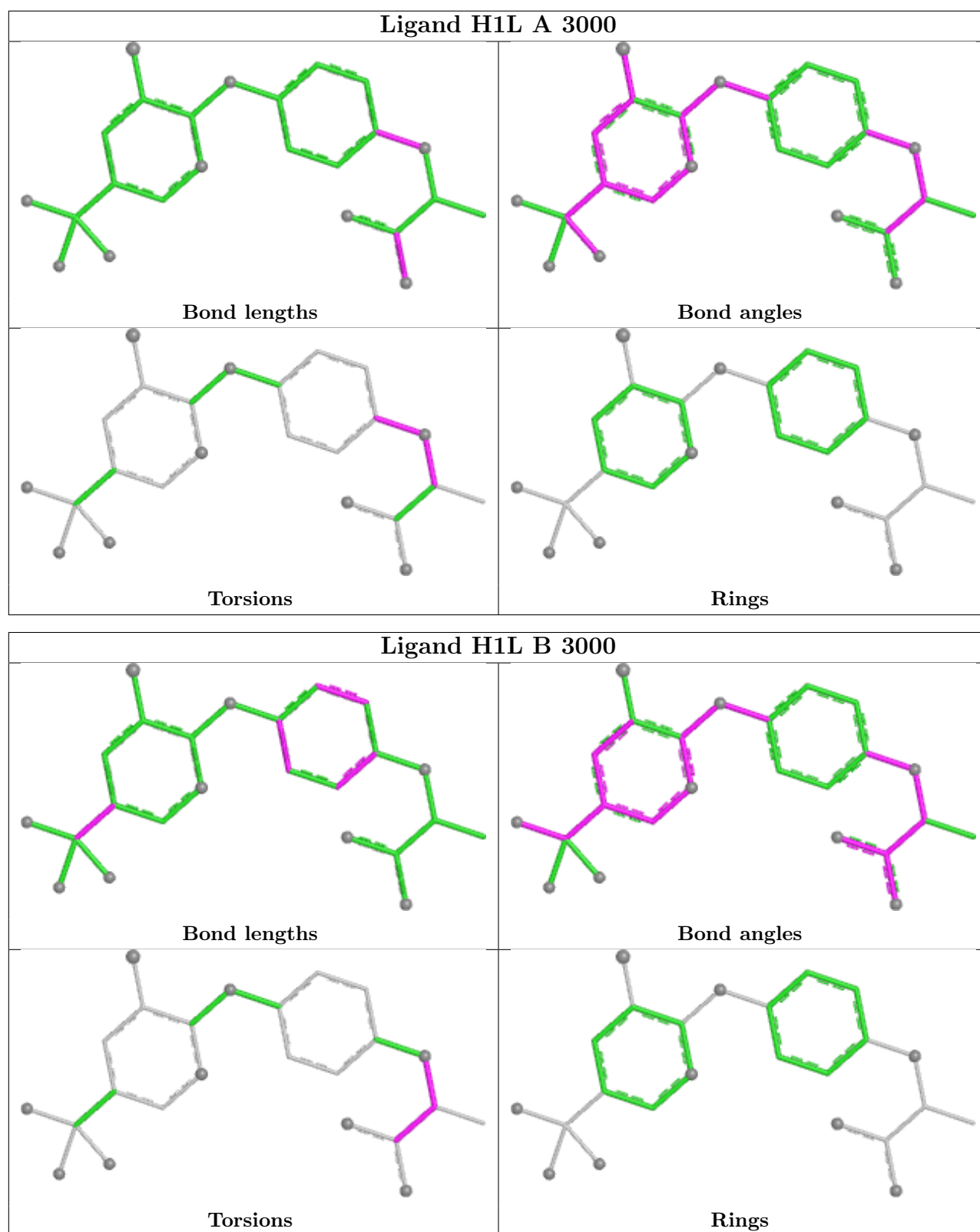
There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3000	H1L	6	0
2	B	3000	H1L	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

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	654/737 (88%)	0.42	90 (13%) 6 5	13, 32, 98, 100	0
1	B	654/737 (88%)	0.57	107 (16%) 4 3	15, 37, 99, 100	0
1	C	644/737 (87%)	0.55	103 (15%) 5 4	14, 37, 100, 100	0
All	All	1952/2211 (88%)	0.52	300 (15%) 5 4	13, 36, 100, 100	0

All (300) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2047	LEU	8.7
1	C	2047	LEU	7.8
1	B	2047	LEU	7.8
1	C	1913	ALA	6.7
1	B	1908	ALA	6.6
1	C	1758	GLY	6.2
1	B	1646	ALA	6.1
1	A	2143	VAL	6.0
1	C	1908	ALA	5.8
1	B	1907	PRO	5.5
1	B	1683	ASN	5.3
1	B	1904	PRO	5.2
1	B	2187	LYS	5.2
1	A	1680	THR	5.1
1	C	1685	GLU	4.9
1	A	1905	ALA	4.8
1	B	2043	THR	4.8
1	C	2143	VAL	4.8
1	C	1677	THR	4.7
1	B	1903	ILE	4.7
1	B	1905	ALA	4.7
1	A	1758	GLY	4.7
1	B	1659	THR	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	2082	LEU	4.6
1	A	2046	ARG	4.6
1	A	2145	GLU	4.6
1	B	1682	ILE	4.6
1	C	1681	VAL	4.6
1	B	2085	ILE	4.5
1	B	1913	ALA	4.5
1	C	2082	LEU	4.5
1	B	1681	VAL	4.5
1	C	1645	ASP	4.4
1	C	1680	THR	4.4
1	A	1762	ILE	4.4
1	B	1910	PRO	4.4
1	A	1910	PRO	4.3
1	B	1761	ALA	4.3
1	C	1682	ILE	4.3
1	C	1773	SER	4.2
1	B	1658	LEU	4.2
1	C	1910	PRO	4.2
1	C	1669	PHE	4.2
1	A	1683	ASN	4.2
1	B	2041	LEU	4.1
1	B	1644	ASN	4.1
1	A	1766	LEU	4.0
1	A	1838	ASP	4.0
1	B	1647	ALA	4.0
1	C	1916	LEU	4.0
1	A	1641	VAL	4.0
1	A	1913	ALA	4.0
1	A	1839	GLU	4.0
1	C	1770	VAL	4.0
1	A	1761	ALA	3.9
1	B	1669	PHE	3.9
1	B	1684	GLY	3.9
1	C	1679	ARG	3.9
1	A	1908	ALA	3.9
1	A	1771	TYR	3.8
1	C	1775	LEU	3.8
1	B	1686	GLU	3.8
1	C	1906	ASP	3.8
1	A	1915	THR	3.8
1	A	1643	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	1911	ASN	3.7
1	C	1644	ASN	3.7
1	A	2036	ARG	3.7
1	A	1907	PRO	3.7
1	B	1906	ASP	3.7
1	C	1650	ASP	3.7
1	B	2045	ASN	3.7
1	B	1758	GLY	3.7
1	B	1729	THR	3.7
1	A	1645	ASP	3.7
1	A	1649	PRO	3.6
1	C	1768	ARG	3.6
1	C	2081	GLU	3.6
1	B	1766	LEU	3.6
1	A	2084	PRO	3.6
1	C	1646	ALA	3.6
1	A	1912	SER	3.6
1	C	1762	ILE	3.6
1	B	2081	GLU	3.6
1	C	1905	ALA	3.5
1	C	1640	GLN	3.5
1	C	2190	LYS	3.5
1	B	2046	ARG	3.5
1	C	1676	LEU	3.5
1	A	1757	THR	3.5
1	C	1772	THR	3.5
1	B	2084	PRO	3.4
1	C	1907	PRO	3.4
1	C	1683	ASN	3.4
1	C	1675	VAL	3.4
1	C	1767	GLY	3.4
1	A	2081	GLU	3.4
1	C	1838	ASP	3.4
1	A	1903	ILE	3.4
1	C	1909	ASN	3.4
1	C	1764	LYS	3.4
1	C	2041	LEU	3.3
1	A	2045	ASN	3.3
1	C	1647	ALA	3.3
1	C	1660	SER	3.3
1	B	1901	ASN	3.3
1	A	1681	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	1770	VAL	3.3
1	B	2083	LEU	3.3
1	B	1912	SER	3.3
1	B	1764	LYS	3.2
1	B	1645	ASP	3.2
1	C	1759	ALA	3.2
1	A	1646	ALA	3.2
1	C	1771	TYR	3.2
1	B	2144	GLY	3.2
1	C	1492	TRP	3.2
1	C	2085	ILE	3.2
1	A	1965	ASN	3.1
1	B	2188	GLY	3.1
1	A	1685	GLU	3.1
1	C	2144	GLY	3.1
1	A	2043	THR	3.1
1	B	1664	GLU	3.1
1	C	1678	GLU	3.1
1	C	2037	ARG	3.1
1	B	1680	THR	3.1
1	B	1915	THR	3.0
1	A	1648	ASN	3.0
1	B	1965	ASN	3.0
1	A	2082	LEU	3.0
1	C	1554	GLU	3.0
1	C	1665	THR	3.0
1	B	1679	ARG	3.0
1	A	1916	LEU	3.0
1	B	1660	SER	3.0
1	C	1761	ALA	3.0
1	C	1643	TRP	3.0
1	B	1657	TYR	3.0
1	B	1768	ARG	3.0
1	C	1648	ASN	3.0
1	B	2180	LYS	2.9
1	C	1902	LEU	2.9
1	A	1760	PRO	2.9
1	B	1760	PRO	2.9
1	B	1772	THR	2.9
1	B	2149	LEU	2.9
1	C	1674	SER	2.9
1	A	1651	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	1772	THR	2.9
1	B	1655	TYR	2.9
1	A	1901	ASN	2.9
1	A	1764	LYS	2.9
1	A	2141	HIS	2.9
1	C	1654	GLN	2.9
1	C	1769	GLU	2.9
1	B	1650	ASP	2.9
1	B	1757	THR	2.9
1	A	1682	ILE	2.9
1	B	2189	LEU	2.9
1	C	1632	ALA	2.8
1	C	1766	LEU	2.8
1	B	1730	CYS	2.8
1	A	1904	PRO	2.8
1	B	1762	ILE	2.8
1	B	1533	THR	2.8
1	A	2142	GLN	2.8
1	B	2145	GLU	2.8
1	C	2045	ASN	2.8
1	C	2083	LEU	2.8
1	A	1658	LEU	2.8
1	A	1906	ASP	2.8
1	B	1637	PRO	2.8
1	A	2026	GLU	2.7
1	A	1958	GLY	2.7
1	C	2038	GLU	2.7
1	C	1653	PHE	2.7
1	B	2086	TYR	2.7
1	B	2042	ASP	2.7
1	B	2037	ARG	2.7
1	B	1916	LEU	2.7
1	A	1482	PRO	2.7
1	A	1687	ARG	2.7
1	B	2181	THR	2.7
1	C	1904	PRO	2.7
1	A	1650	ASP	2.7
1	A	1914	GLU	2.7
1	B	1919	GLU	2.7
1	B	2142	GLN	2.7
1	C	1531	LYS	2.6
1	C	1912	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	1531	LYS	2.6
1	B	1667	LYS	2.6
1	A	1678	GLU	2.6
1	B	1653	PHE	2.6
1	B	1771	TYR	2.6
1	B	2190	LYS	2.6
1	C	1903	ILE	2.6
1	B	1838	ASP	2.6
1	A	2031	VAL	2.5
1	A	2019	ASN	2.5
1	C	1687	ARG	2.5
1	C	2046	ARG	2.5
1	C	1651	LYS	2.5
1	A	1777	LEU	2.5
1	C	2087	GLY	2.5
1	C	1672	GLU	2.5
1	A	1911	ASN	2.5
1	B	1668	LYS	2.5
1	C	1917	ILE	2.5
1	A	2189	LEU	2.5
1	C	1957	SER	2.5
1	A	1769	GLU	2.5
1	A	1826	THR	2.5
1	C	1671	LYS	2.5
1	C	1649	PRO	2.4
1	A	1657	TYR	2.4
1	B	1824	LYS	2.4
1	A	1837	ASN	2.4
1	A	1768	ARG	2.4
1	B	1643	TRP	2.4
1	B	1852	THR	2.4
1	A	2190	LYS	2.4
1	A	1494	GLN	2.4
1	B	1654	GLN	2.4
1	A	1655	TYR	2.4
1	A	1659	THR	2.4
1	A	2086	TYR	2.4
1	A	1531	LYS	2.3
1	A	1679	ARG	2.3
1	B	1651	LYS	2.3
1	B	1770	VAL	2.3
1	A	1778	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	1642	ALA	2.3
1	C	2084	PRO	2.3
1	B	2141	HIS	2.3
1	B	1649	PRO	2.3
1	C	1760	PRO	2.3
1	C	1530	VAL	2.3
1	A	2144	GLY	2.3
1	B	1638	LEU	2.3
1	A	1729	THR	2.3
1	B	2143	VAL	2.3
1	C	1958	GLY	2.3
1	A	1759	ALA	2.2
1	C	1853	GLU	2.2
1	B	1918	GLN	2.2
1	A	1653	PHE	2.2
1	A	1686	GLU	2.2
1	B	1769	GLU	2.2
1	B	1648	ASN	2.2
1	C	2141	HIS	2.2
1	A	2083	LEU	2.2
1	A	2085	ILE	2.2
1	C	2036	ARG	2.2
1	C	1689	VAL	2.2
1	A	1773	SER	2.2
1	A	1647	ALA	2.2
1	C	1839	GLU	2.2
1	C	1914	GLU	2.2
1	B	2134	TYR	2.2
1	B	2140	SER	2.2
1	C	1688	PHE	2.2
1	C	2040	LEU	2.2
1	B	1917	ILE	2.1
1	C	1684	GLY	2.1
1	A	1688	PHE	2.1
1	C	1686	GLU	2.1
1	C	1667	LYS	2.1
1	B	1677	THR	2.1
1	A	1902	LEU	2.1
1	B	1777	LEU	2.1
1	B	2036	ARG	2.1
1	C	2086	TYR	2.1
1	B	1853	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1644	ASN	2.1
1	C	1658	LEU	2.1
1	C	1915	THR	2.1
1	B	1687	ARG	2.1
1	B	2138	ARG	2.1
1	C	1763	ASN	2.1
1	B	2186	LEU	2.1
1	C	2149	LEU	2.1
1	A	1684	GLY	2.1
1	B	2035	PHE	2.1
1	C	1655	TYR	2.1
1	B	2034	LYS	2.0
1	C	2142	GLN	2.0
1	C	1641	VAL	2.0
1	B	1920	PRO	2.0
1	C	1638	LEU	2.0
1	B	2089	ILE	2.0
1	C	1661	GLU	2.0
1	C	1657	TYR	2.0
1	A	1483	ILE	2.0
1	C	1898	THR	2.0
1	B	1685	GLU	2.0
1	A	1689	VAL	2.0
1	B	1675	VAL	2.0
1	B	1689	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

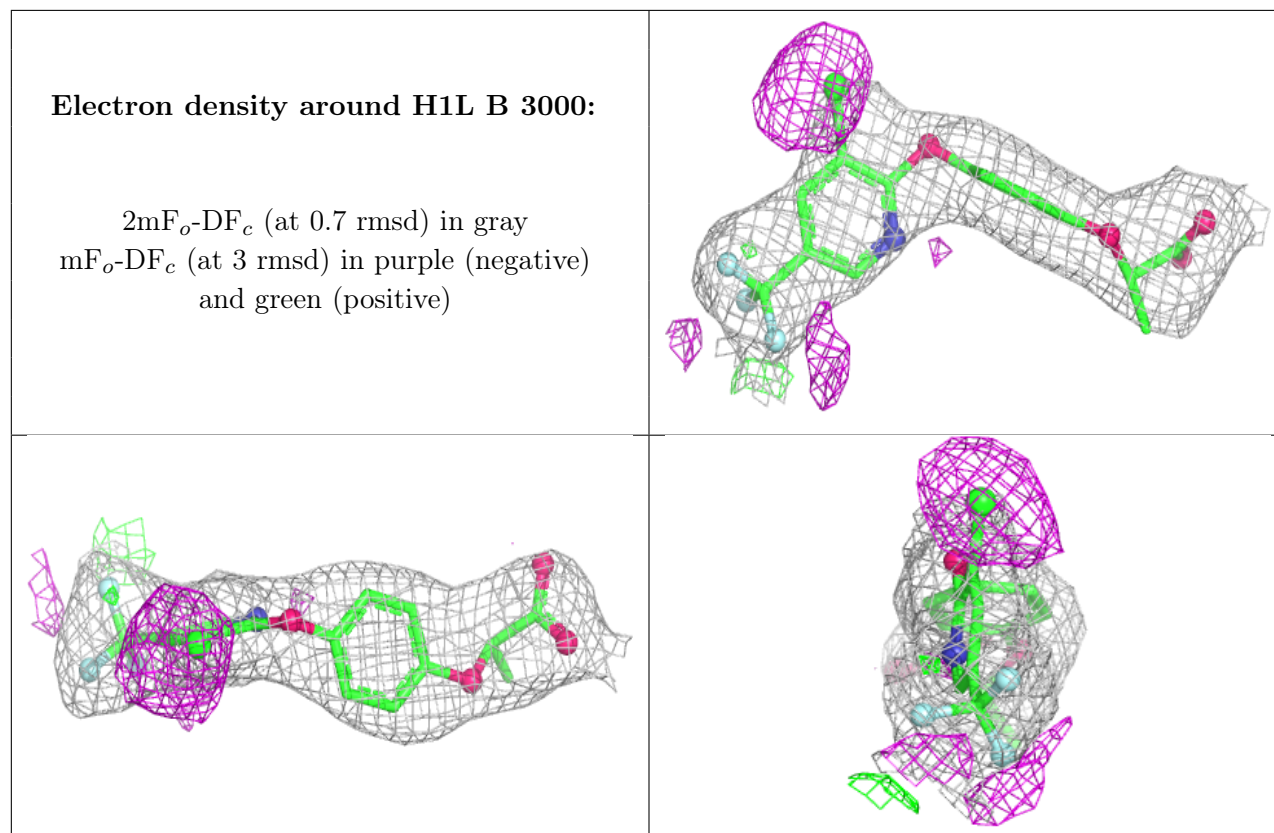
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

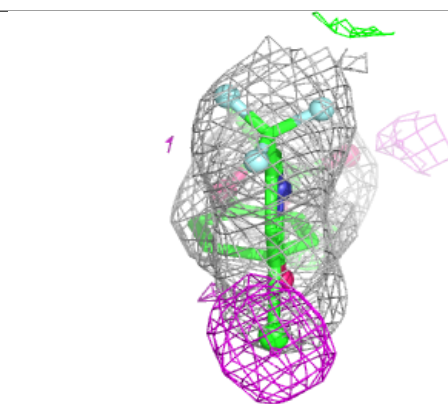
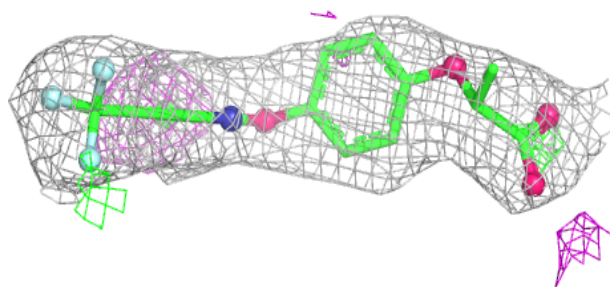
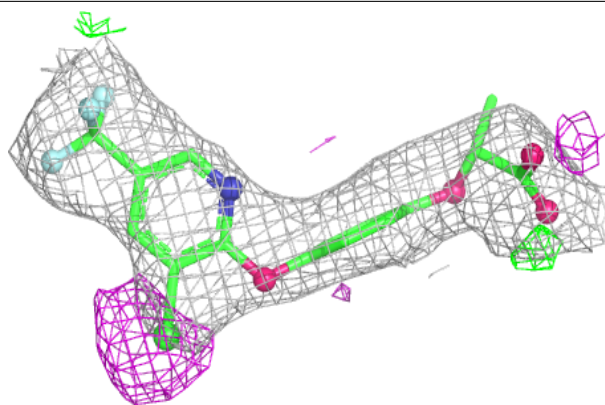
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	H1L	B	3000	24/24	0.86	0.17	44,49,59,71	0
2	H1L	C	3000	24/24	0.86	0.17	52,55,60,71	0
2	H1L	A	3000	24/24	0.90	0.13	29,38,45,54	0

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

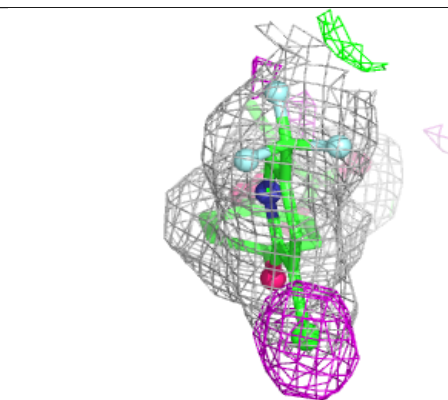
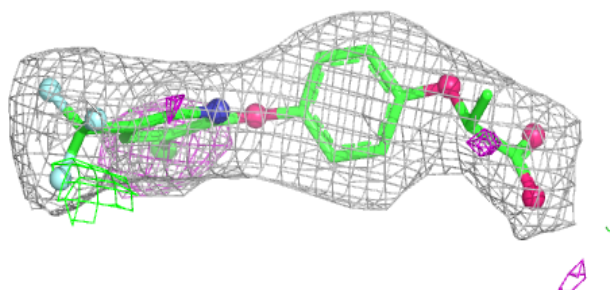
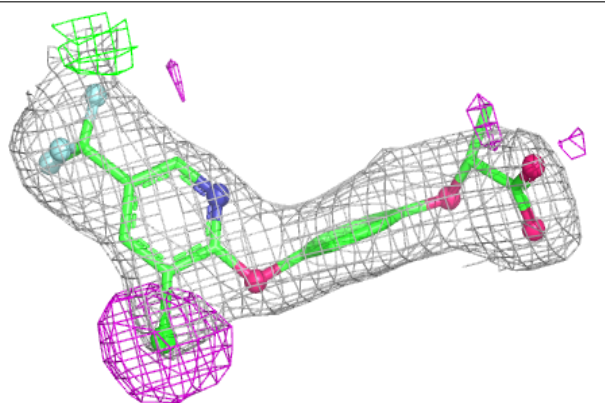


Electron density around H1L C 3000:

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

**Electron density around H1L 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.