Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 12:30 PM EDT

PDB ID	:	3H0S
Title	:	Crystal structure of the carboxyltransferase domain of acetyl-coenzyme A carboxylase in complex with compound 7
Authors	:	Vajdos, F.
Deposited on	:	2009-04-10
Resolution	:	2.43 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:

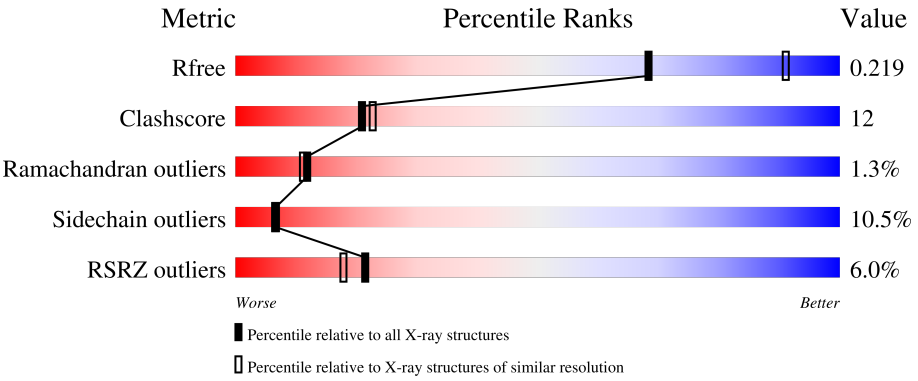
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.43 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}	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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

Mol	Chain	Length	Quality of chain
1	A	769	4% 65% 20% 5% • 10%
1	B	769	6% 62% 21% • • 12%
1	C	769	6% 65% 17% 5% • 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	C	3	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 18770 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	693	Total	C	N	O	S	0	1	0
			5538	3525	957	1037	19			
1	B	677	Total	C	N	O	S	0	0	0
			5395	3439	928	1009	19			
1	C	668	Total	C	N	O	S	0	0	0
			5324	3391	916	998	19			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1473	MET	-	expression tag	UNP Q00955
A	1474	ALA	-	expression tag	UNP Q00955
A	1475	SER	-	expression tag	UNP Q00955
A	2234	LEU	-	expression tag	UNP Q00955
A	2235	GLU	-	expression tag	UNP Q00955
A	2236	HIS	-	expression tag	UNP Q00955
A	2237	HIS	-	expression tag	UNP Q00955
A	2238	HIS	-	expression tag	UNP Q00955
A	2239	HIS	-	expression tag	UNP Q00955
A	2240	HIS	-	expression tag	UNP Q00955
A	2241	HIS	-	expression tag	UNP Q00955
B	1473	MET	-	expression tag	UNP Q00955
B	1474	ALA	-	expression tag	UNP Q00955
B	1475	SER	-	expression tag	UNP Q00955
B	2234	LEU	-	expression tag	UNP Q00955
B	2235	GLU	-	expression tag	UNP Q00955
B	2236	HIS	-	expression tag	UNP Q00955
B	2237	HIS	-	expression tag	UNP Q00955
B	2238	HIS	-	expression tag	UNP Q00955
B	2239	HIS	-	expression tag	UNP Q00955
B	2240	HIS	-	expression tag	UNP Q00955
B	2241	HIS	-	expression tag	UNP Q00955
C	1473	MET	-	expression tag	UNP Q00955

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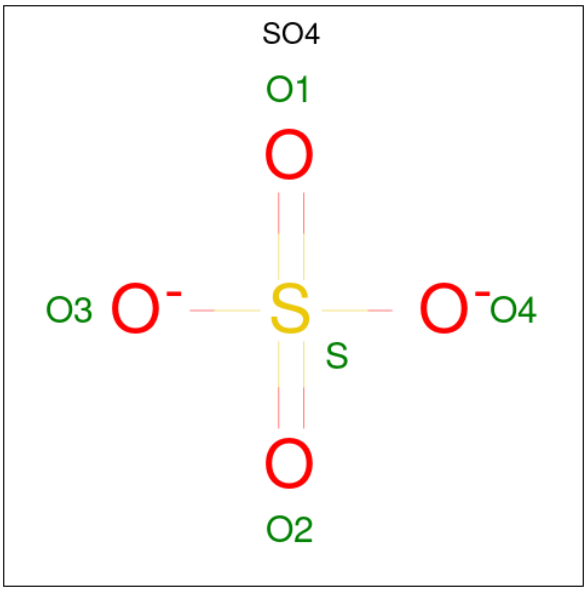
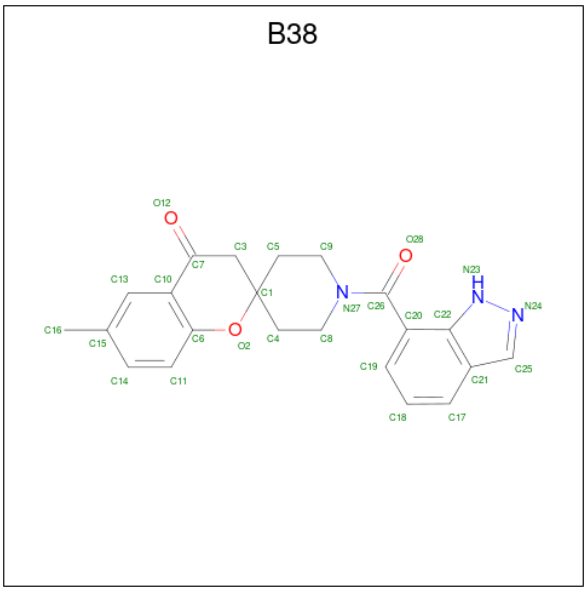
Chain	Residue	Modelled	Actual	Comment	Reference
C	1474	ALA	-	expression tag	UNP Q00955
C	1475	SER	-	expression tag	UNP Q00955
C	2234	LEU	-	expression tag	UNP Q00955
C	2235	GLU	-	expression tag	UNP Q00955
C	2236	HIS	-	expression tag	UNP Q00955
C	2237	HIS	-	expression tag	UNP Q00955
C	2238	HIS	-	expression tag	UNP Q00955
C	2239	HIS	-	expression tag	UNP Q00955
C	2240	HIS	-	expression tag	UNP Q00955
C	2241	HIS	-	expression tag	UNP Q00955

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

- Molecule 3 is 1'-(1H-indazol-7-ylcarbonyl)-6-methylspiro[chromene-2,4'-piperidin]-4(3H)-one (three-letter code: B38) (formula: $C_{22}H_{21}N_3O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 28 22 3 3	0	0
3	B	1	Total C N O 39 30 5 4	0	1
3	C	1	Total C N O 28 22 3 3	0	0

- Molecule 4 is water.

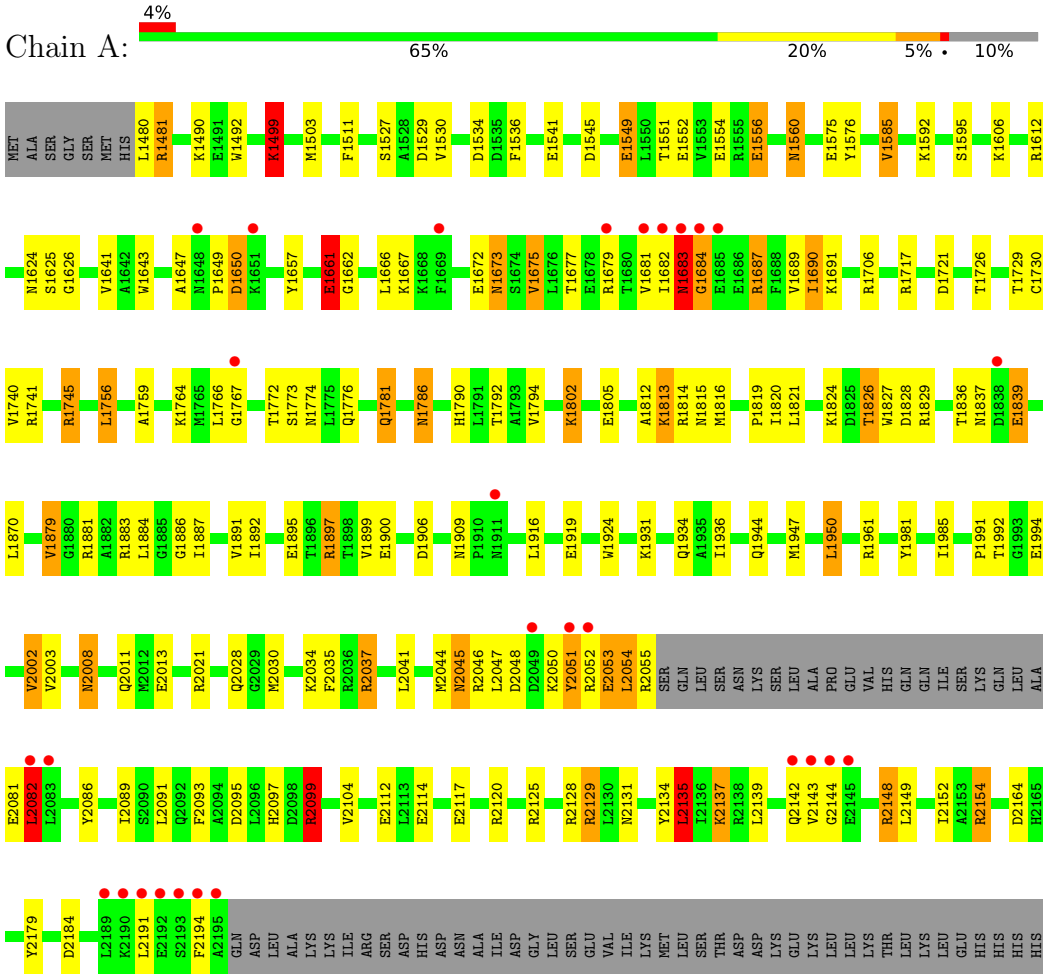
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	861	Total O 861 861	0	0
4	B	762	Total O 762 762	0	0
4	C	780	Total O 780 780	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

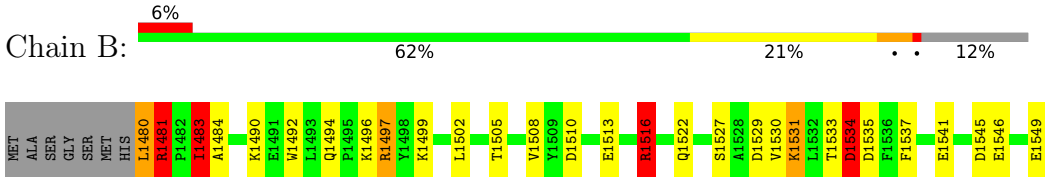
• Molecule 1: Acetyl-CoA carboxylase

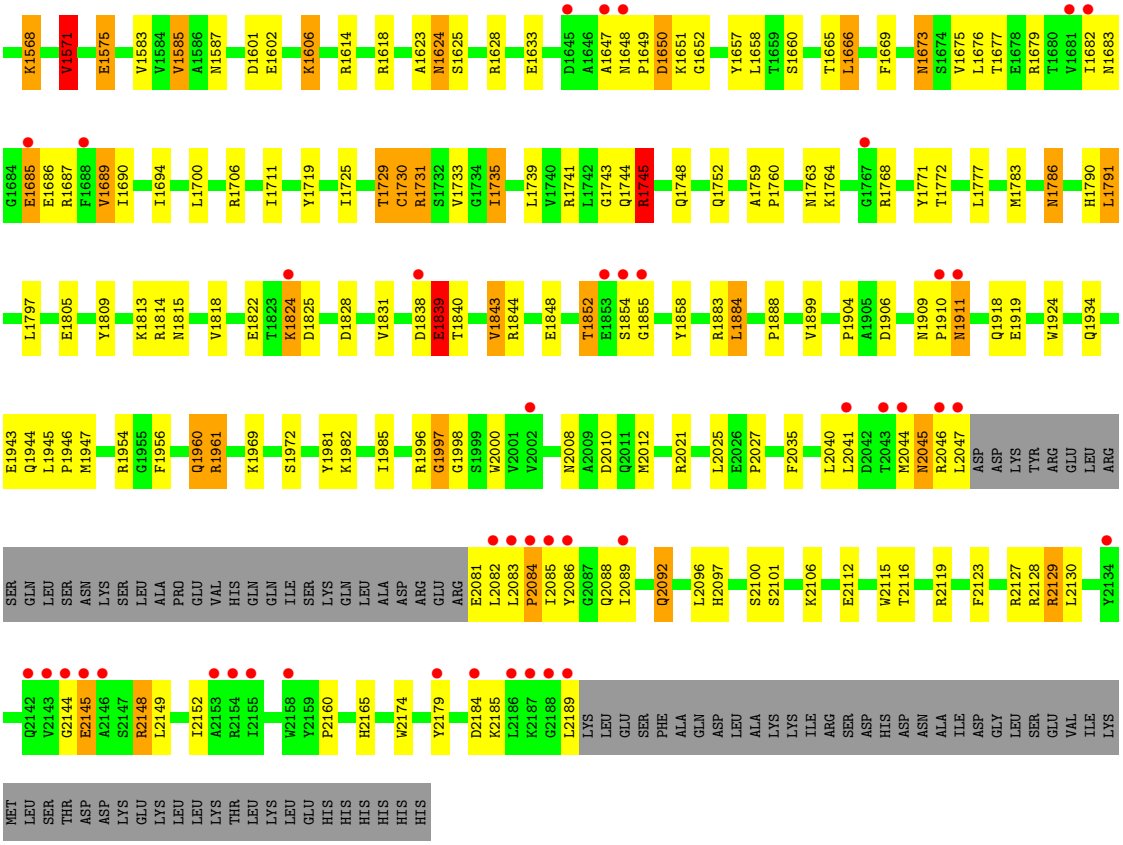
Chain A:



• Molecule 1: Acetyl-CoA carboxylase

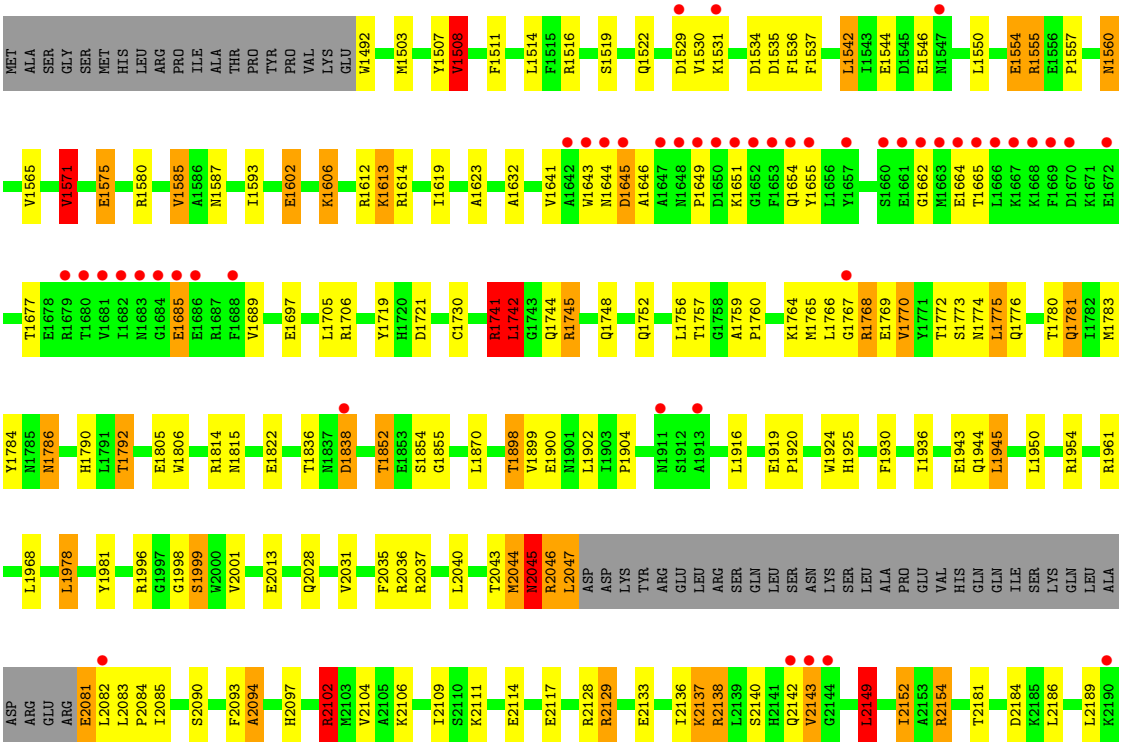
Chain B:

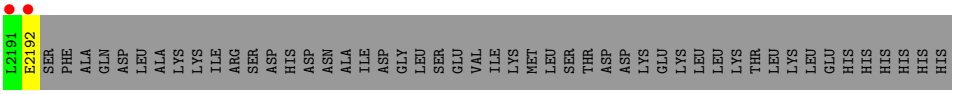




• Molecule 1: Acetyl-CoA carboxylase

Chain C:




L2191
E2192
SER
PHE
ALA
GLN
ASP
LEU
ALA
LYS
LYS
ILE
ARG
SER
ASP
HIS
ASP
ASN
ALA
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LEU
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4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	246.72Å 121.68Å 145.99Å 90.00° 94.23° 90.00°	Depositor
Resolution (Å)	40.70 – 2.43 40.70 – 2.43	Depositor EDS
% Data completeness (in resolution range)	98.5 (40.70-2.43) 98.5 (40.70-2.43)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 2.42Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.160 , 0.218 0.169 , 0.219	Depositor DCC
R_{free} test set	15829 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å^2)	45.4	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 58.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	18770	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, B38

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.18	20/5668 (0.4%)	1.10	34/7676 (0.4%)
1	B	1.15	14/5516 (0.3%)	1.09	34/7475 (0.5%)
1	C	1.13	13/5441 (0.2%)	1.07	31/7369 (0.4%)
All	All	1.16	47/16625 (0.3%)	1.09	99/22520 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
All	All	0	6

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1554	GLU	CG-CD	11.50	1.69	1.51
1	C	1575	GLU	CD-OE2	9.50	1.36	1.25
1	A	2117	GLU	CD-OE1	9.17	1.35	1.25
1	B	1575	GLU	CD-OE2	8.64	1.35	1.25
1	A	1805	GLU	CG-CD	8.26	1.64	1.51
1	A	1786	ASN	CB-CG	-7.53	1.33	1.51
1	C	2013	GLU	CB-CG	-7.50	1.37	1.52
1	B	1839	GLU	CG-CD	7.44	1.63	1.51
1	C	1786	ASN	CB-CG	-7.39	1.34	1.51
1	A	1805	GLU	CD-OE1	7.17	1.33	1.25
1	A	2114	GLU	CG-CD	7.15	1.62	1.51
1	A	1556	GLU	CG-CD	7.12	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1568	LYS	CE-NZ	7.06	1.66	1.49
1	C	1613	LYS	CD-CE	7.00	1.68	1.51
1	A	2137	LYS	CD-CE	6.65	1.67	1.51
1	C	2117	GLU	CG-CD	6.46	1.61	1.51
1	B	1546	GLU	CB-CG	6.41	1.64	1.52
1	A	2013	GLU	CB-CG	-6.31	1.40	1.52
1	B	1745	ARG	CD-NE	-6.25	1.35	1.46
1	A	1554	GLU	CB-CG	6.00	1.63	1.52
1	B	1805	GLU	CD-OE1	5.97	1.32	1.25
1	C	1981	TYR	CD1-CE1	-5.95	1.30	1.39
1	A	1992	THR	N-CA	5.95	1.58	1.46
1	B	1745	ARG	CG-CD	5.77	1.66	1.51
1	B	1575	GLU	CG-CD	5.64	1.60	1.51
1	A	1891	VAL	CB-CG1	5.49	1.64	1.52
1	C	2114	GLU	CG-CD	5.43	1.60	1.51
1	A	2117	GLU	CG-CD	5.43	1.60	1.51
1	C	1507	TYR	CD2-CE2	-5.38	1.31	1.39
1	B	1839	GLU	CB-CG	5.37	1.62	1.52
1	A	2129	ARG	CZ-NH1	5.36	1.40	1.33
1	C	1721	ASP	CB-CG	-5.34	1.40	1.51
1	C	1805	GLU	CD-OE2	5.30	1.31	1.25
1	A	1549	GLU	CG-CD	5.29	1.59	1.51
1	B	1568	LYS	CD-CE	5.28	1.64	1.51
1	A	2002	VAL	CB-CG1	-5.24	1.41	1.52
1	A	2166	GLU	CD-OE1	5.23	1.31	1.25
1	C	1575	GLU	CD-OE1	5.23	1.31	1.25
1	B	2129	ARG	CZ-NH1	5.22	1.39	1.33
1	A	1499	LYS	CD-CE	5.22	1.64	1.51
1	B	1549	GLU	CG-CD	5.20	1.59	1.51
1	C	1685	GLU	CB-CG	5.18	1.61	1.52
1	A	1661	GLU	CG-CD	5.16	1.59	1.51
1	A	1839	GLU	CG-CD	5.15	1.59	1.51
1	B	1805	GLU	CG-CD	5.11	1.59	1.51
1	C	1575	GLU	CG-CD	5.03	1.59	1.51
1	B	1786	ASN	CB-CG	-5.01	1.39	1.51

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1717	ARG	NE-CZ-NH2	-18.02	111.29	120.30
1	B	1745	ARG	NE-CZ-NH2	-16.24	112.18	120.30
1	A	1717	ARG	NE-CZ-NH1	15.14	127.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1745	ARG	NE-CZ-NH1	14.42	127.51	120.30
1	A	1745	ARG	NE-CZ-NH2	-14.02	113.29	120.30
1	B	1516	ARG	NE-CZ-NH2	-12.69	113.96	120.30
1	C	1745	ARG	NE-CZ-NH2	-11.60	114.50	120.30
1	A	1745	ARG	NE-CZ-NH1	11.25	125.92	120.30
1	C	2102	ARG	NE-CZ-NH2	-10.76	114.92	120.30
1	B	2119	ARG	NE-CZ-NH2	-10.66	114.97	120.30
1	C	1745	ARG	NE-CZ-NH1	10.52	125.56	120.30
1	A	2099	ARG	NE-CZ-NH2	-10.14	115.23	120.30
1	C	1814	ARG	NE-CZ-NH1	10.06	125.33	120.30
1	C	1814	ARG	NE-CZ-NH2	-9.44	115.58	120.30
1	C	1961	ARG	NE-CZ-NH2	-9.26	115.67	120.30
1	C	2102	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	A	1786	ASN	CB-CA-C	-9.15	92.09	110.40
1	B	1745	ARG	CD-NE-CZ	9.15	136.41	123.60
1	C	2129	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	A	1991	PRO	C-N-CA	-8.75	99.82	121.70
1	B	2129	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	C	2036	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	B	1555	ARG	NE-CZ-NH1	8.59	124.60	120.30
1	B	2129	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	B	1730	CYS	N-CA-C	-8.24	88.76	111.00
1	A	2099	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	B	1571	VAL	CB-CA-C	-8.11	95.99	111.40
1	A	1706	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	B	1516	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	C	2154	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	C	2138	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	C	1612	ARG	NE-CZ-NH1	7.55	124.07	120.30
1	C	1741	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	B	1961	ARG	NE-CZ-NH2	-7.49	116.55	120.30
1	C	2138	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	B	1786	ASN	CB-CA-C	-7.31	95.77	110.40
1	C	1786	ASN	CB-CA-C	-7.28	95.84	110.40
1	A	1706	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	B	1706	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	A	2125	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	B	1814	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	C	1516	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	A	2046	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	A	1897	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	C	1571	VAL	CB-CA-C	-6.80	98.48	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	2154	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	B	1585	VAL	CB-CA-C	-6.51	99.03	111.40
1	B	1516	ARG	CG-CD-NE	-6.48	98.19	111.80
1	B	1481	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	B	1961	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	A	2148	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	C	2149	LEU	CA-CB-CG	6.22	129.61	115.30
1	B	1883	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	B	1706	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	1881	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	C	2013	GLU	CG-CD-OE2	-6.01	106.28	118.30
1	A	1585	VAL	CB-CA-C	-5.97	100.06	111.40
1	A	1991	PRO	O-C-N	-5.94	113.20	122.70
1	A	1717	ARG	CG-CD-NE	-5.94	99.33	111.80
1	C	1612	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	1614	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	B	2119	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	1814	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	B	1497	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	B	1555	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	A	2082	LEU	CA-CB-CG	5.77	128.58	115.30
1	A	2099	ARG	CG-CD-NE	-5.74	99.74	111.80
1	A	1814	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	B	1568	LYS	CD-CE-NZ	5.68	124.77	111.70
1	B	2021	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	C	1542	LEU	CA-CB-CG	5.61	128.21	115.30
1	C	1614	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	C	1508	VAL	CB-CA-C	-5.58	100.79	111.40
1	B	1601	ASP	CB-CG-OD1	5.58	123.32	118.30
1	C	1585	VAL	CB-CA-C	-5.50	100.96	111.40
1	B	1481	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	C	1745	ARG	CD-NE-CZ	5.46	131.25	123.60
1	B	1628	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	B	2021	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	B	1828	ASP	CB-CG-OD1	-5.37	113.47	118.30
1	A	2154	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	C	1742	LEU	CA-CB-CG	5.34	127.59	115.30
1	A	1881	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	A	1612	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	2167	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	1717	ARG	CD-NE-CZ	5.27	130.97	123.60
1	A	1721	ASP	CB-CG-OD2	-5.25	113.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1614	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	1745	ARG	CD-NE-CZ	5.20	130.88	123.60
1	C	2013	GLU	CB-CA-C	-5.18	100.04	110.40
1	C	1721	ASP	N-CA-CB	-5.17	101.30	110.60
1	A	1829	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	C	2129	ARG	CG-CD-NE	-5.13	101.03	111.80
1	B	1483	ILE	CB-CA-C	5.11	121.83	111.60
1	B	1947	MET	CG-SD-CE	5.11	108.38	100.20
1	C	1580	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	1950	LEU	CA-CB-CG	5.05	126.91	115.30
1	A	1612	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	2135	LEU	CB-CG-CD1	5.04	119.57	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1786	ASN	Mainchain
1	A	2081	GLU	Peptide
1	B	1745	ARG	Sidechain
1	B	1997	GLY	Peptide
1	C	2044	MET	Peptide
1	C	2045	ASN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5538	0	5469	137	0
1	B	5395	0	5339	144	0
1	C	5324	0	5264	125	0
2	A	5	0	0	0	0
2	C	10	0	0	2	0
3	A	28	0	21	1	0
3	B	39	0	10	2	0
3	C	28	0	21	1	0
4	A	861	0	0	58	9

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	762	0	0	60	0
4	C	780	0	0	60	4
All	All	18770	0	16124	396	9

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 12.

All (396) 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:1625:SER:HB2	4:A:974:HOH:O	1.37	1.23
1:B:1534:ASP:N	4:B:2475:HOH:O	1.75	1.17
1:A:1556:GLU:HG2	4:A:2327:HOH:O	1.52	1.07
1:B:1960:GLN:HG3	4:B:605:HOH:O	1.54	1.05
1:C:1555:ARG:N	4:C:2372:HOH:O	1.87	1.05
1:C:2094:ALA:N	4:C:2427:HOH:O	1.81	1.04
1:A:1575:GLU:OE1	4:A:2483:HOH:O	1.76	1.04
1:A:1821:LEU:HD22	4:A:960:HOH:O	1.59	1.02
1:A:2154:ARG:HD3	4:A:216:HOH:O	1.61	1.01
1:A:1820:ILE:HG23	4:A:2539:HOH:O	1.56	1.01
1:C:2082:LEU:HA	4:C:308:HOH:O	1.59	1.01
1:A:2052:ARG:O	1:A:2053:GLU:HG3	1.64	0.98
1:A:1772:THR:H	1:A:1776:GLN:HE22	1.11	0.97
1:C:1706:ARG:HD3	4:C:743:HOH:O	1.65	0.97
1:C:1575:GLU:OE1	4:C:975:HOH:O	1.86	0.91
1:A:1886:GLY:C	4:A:2539:HOH:O	2.10	0.90
1:A:2047:LEU:O	1:A:2051:TYR:HB2	1.71	0.90
1:B:1815:ASN:H	1:B:1944:GLN:HE22	1.19	0.90
1:B:1533:THR:C	4:B:2475:HOH:O	2.05	0.89
1:A:1772:THR:H	1:A:1776:GLN:NE2	1.72	0.87
1:A:2184:ASP:OD1	1:B:1481:ARG:NH2	2.07	0.87
1:B:1729:THR:O	1:B:1729:THR:OG1	1.91	0.87
1:B:1843:VAL:HG12	4:B:1205:HOH:O	1.75	0.87
1:C:2046:ARG:HA	4:C:2425:HOH:O	1.75	0.86
1:C:2090:SER:O	1:C:2093:PHE:O	1.95	0.85
1:C:2133:GLU:OE2	4:C:2458:HOH:O	1.95	0.85
1:A:1824:LYS:CA	4:A:934:HOH:O	2.23	0.84
1:C:1836:THR:HB	4:C:2489:HOH:O	1.76	0.84
1:B:2008:ASN:N	1:B:2012:MET:CE	2.41	0.84
1:B:1575:GLU:OE1	4:B:1430:HOH:O	1.95	0.83
1:A:1511:PHE:HZ	4:A:830:HOH:O	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1690:ILE:HG23	4:B:2285:HOH:O	1.79	0.83
1:C:2137:LYS:NZ	4:C:981:HOH:O	2.13	0.82
1:B:1494:GLN:HE21	1:B:1496:LYS:H	1.28	0.81
1:B:1730:CYS:HA	1:B:1752:GLN:HE21	1.42	0.81
1:C:1772:THR:H	1:C:1776:GLN:HE22	1.26	0.80
1:A:1677:THR:HG22	4:A:2376:HOH:O	1.83	0.78
1:A:2149:LEU:HD12	4:A:1146:HOH:O	1.83	0.78
1:B:1904:PRO:HG2	4:C:1432:HOH:O	1.84	0.77
1:A:1650:ASP:HA	4:A:2408:HOH:O	1.85	0.76
1:C:1492:TRP:HA	4:C:1063:HOH:O	1.86	0.76
1:C:1492:TRP:O	4:C:2455:HOH:O	2.04	0.75
1:A:1759:ALA:H	1:A:1774:ASN:HD21	1.35	0.75
1:B:1683:ASN:HB2	4:B:2278:HOH:O	1.86	0.75
1:B:1660:SER:OG	1:B:1686:GLU:OE2	2.05	0.74
1:C:1759:ALA:H	1:C:1774:ASN:ND2	1.85	0.74
1:B:1960:GLN:CG	4:B:605:HOH:O	2.21	0.73
1:B:1606:LYS:HD2	4:B:267:HOH:O	1.87	0.73
1:A:2052:ARG:O	1:A:2053:GLU:CG	2.36	0.73
1:A:1690:ILE:HD13	4:A:2376:HOH:O	1.87	0.72
1:C:1613:LYS:HG2	4:C:2267:HOH:O	1.89	0.72
1:B:1649:PRO:O	1:B:1651:LYS:N	2.23	0.72
1:B:1675:VAL:HB	4:B:2285:HOH:O	1.90	0.71
1:B:2097:HIS:HE1	1:C:1632:ALA:H	1.38	0.71
1:A:1661:GLU:HB2	4:A:2410:HOH:O	1.91	0.71
1:B:1843:VAL:CG1	4:B:1205:HOH:O	2.36	0.71
1:C:2044:MET:SD	4:C:2479:HOH:O	2.49	0.71
1:A:1826:THR:HG21	4:A:1351:HOH:O	1.90	0.70
1:A:1667:LYS:HD3	1:A:1672:GLU:HG2	1.73	0.70
1:B:1530:VAL:HB	4:B:2535:HOH:O	1.89	0.70
1:B:1960:GLN:OE1	4:B:605:HOH:O	2.10	0.70
1:B:2008:ASN:H	1:B:2012:MET:CE	2.03	0.70
1:C:1759:ALA:H	1:C:1774:ASN:HD21	1.40	0.70
1:B:1625:SER:HB2	4:B:2511:HOH:O	1.91	0.69
1:C:1773:SER:H	1:C:1776:GLN:NE2	1.89	0.69
1:B:1997:GLY:HA2	1:B:2000:TRP:HB3	1.75	0.69
1:C:1575:GLU:HB3	4:C:975:HOH:O	1.94	0.68
1:A:1503:MET:HE1	4:A:601:HOH:O	1.92	0.68
1:B:1906:ASP:OD1	4:B:2482:HOH:O	2.11	0.68
1:C:2046:ARG:NH1	4:C:2321:HOH:O	2.27	0.67
1:A:1759:ALA:H	1:A:1774:ASN:ND2	1.92	0.67
1:A:1677:THR:HA	1:A:1689:VAL:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2089:ILE:HD13	1:C:1641:VAL:HG21	1.77	0.67
1:A:2044:MET:C	1:A:2045:ASN:HD22	1.98	0.66
1:B:1490:LYS:NZ	4:B:261:HOH:O	2.22	0.66
1:B:2101:SER:HA	4:B:931:HOH:O	1.94	0.66
1:A:1560:ASN:H	1:A:1560:ASN:HD22	1.42	0.66
1:B:1954:ARG:O	1:B:1996:ARG:HB2	1.97	0.65
1:B:1843:VAL:CB	4:B:1205:HOH:O	2.44	0.65
1:A:2137:LYS:HG3	4:A:394:HOH:O	1.96	0.65
1:A:1731:ARG:N	4:A:2478:HOH:O	2.29	0.65
1:B:2008:ASN:N	1:B:2012:MET:HE1	2.11	0.64
1:C:1792:THR:HG21	4:C:343:HOH:O	1.97	0.64
1:A:1683:ASN:HD22	1:A:1684:GLY:H	1.45	0.64
1:A:1729:THR:O	1:A:1729:THR:OG1	2.14	0.64
1:B:1899:VAL:HB	1:B:1919:GLU:HB2	1.80	0.63
1:B:1541:GLU:OE1	1:B:1555:ARG:HD3	1.98	0.63
1:B:1683:ASN:HB2	4:B:327:HOH:O	1.99	0.63
1:A:1624:ASN:HD21	1:A:1733:VAL:H	1.44	0.62
1:B:1666:LEU:HD23	4:B:2259:HOH:O	1.99	0.62
1:B:1606:LYS:CD	4:B:267:HOH:O	2.44	0.62
1:C:1530:VAL:HG22	4:C:1191:HOH:O	2.00	0.62
1:B:1624:ASN:HD21	1:B:1733:VAL:H	1.47	0.62
1:B:1730:CYS:HA	1:B:1752:GLN:NE2	2.13	0.62
1:A:2047:LEU:HD23	1:A:2050:LYS:HB3	1.82	0.61
1:A:1815:ASN:ND2	1:A:1944:GLN:HE22	1.98	0.61
1:B:1972:SER:HB3	1:C:1742:LEU:HD13	1.83	0.60
1:A:2080:ARG:O	4:A:1172:HOH:O	2.16	0.60
1:B:1763:ASN:HD21	1:B:1771:TYR:H	1.49	0.60
1:B:1843:VAL:HB	4:B:1205:HOH:O	2.00	0.60
1:C:2046:ARG:CZ	4:C:2321:HOH:O	2.49	0.60
1:A:1624:ASN:ND2	1:A:1733:VAL:H	2.00	0.59
1:A:1996:ARG:O	1:A:1999:SER:HB2	2.03	0.59
1:A:2055:ARG:N	1:A:2055:ARG:HD3	2.18	0.58
1:B:1529:ASP:C	4:B:276:HOH:O	2.42	0.58
1:A:2045:ASN:HD22	1:A:2045:ASN:N	2.02	0.58
1:A:2047:LEU:HD23	1:A:2050:LYS:CB	2.34	0.57
1:B:1624:ASN:ND2	1:B:1733:VAL:H	2.02	0.57
1:C:1925:HIS:HE1	4:C:664:HOH:O	1.87	0.57
1:B:1759:ALA:HB3	1:B:1760:PRO:HD3	1.87	0.57
1:B:1545:ASP:OD2	1:B:1545:ASP:C	2.42	0.57
1:B:1602:GLU:OE2	1:B:1606:LYS:CE	2.53	0.57
1:B:1839:GLU:HG2	4:B:2340:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1998:GLY:HA2	1:C:2001:VAL:HG13	1.87	0.57
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.53	0.57
1:A:1772:THR:HB	4:A:2340:HOH:O	2.05	0.56
1:B:1748:GLN:HE22	1:B:1783:MET:HB2	1.69	0.56
1:B:2008:ASN:N	1:B:2012:MET:HE2	2.21	0.56
1:C:1852:THR:HB	1:C:1855:GLY:O	2.05	0.56
1:A:1499:LYS:NZ	4:A:2287:HOH:O	2.38	0.56
1:A:2047:LEU:HD22	1:A:2082:LEU:HD21	1.86	0.56
1:A:2144:GLY:HA2	4:A:2311:HOH:O	2.05	0.56
1:B:1673:ASN:ND2	4:B:870:HOH:O	2.38	0.56
1:B:1675:VAL:CG1	4:B:2285:HOH:O	2.53	0.56
1:B:1649:PRO:C	1:B:1651:LYS:H	2.09	0.56
1:B:2047:LEU:HD11	4:B:2431:HOH:O	2.05	0.56
1:A:1815:ASN:HD22	1:A:1944:GLN:HE22	1.54	0.56
1:A:2134:TYR:HD2	1:A:2135:LEU:HD13	1.71	0.55
1:B:2040:LEU:HD11	1:B:2086:TYR:O	2.06	0.55
1:A:2037:ARG:HD2	4:A:2456:HOH:O	2.04	0.55
1:C:1554:GLU:HG3	4:C:2383:HOH:O	2.06	0.55
1:C:1537:PHE:HD2	1:C:1571:VAL:HG13	1.70	0.55
1:C:2081:GLU:N	4:C:995:HOH:O	2.40	0.55
1:C:2047:LEU:C	4:C:895:HOH:O	2.45	0.55
1:A:2143:VAL:HG11	1:A:2154:ARG:NH1	2.22	0.55
1:B:1969:LYS:HA	1:C:1741:ARG:HD2	1.87	0.55
1:A:2143:VAL:CG1	4:A:2465:HOH:O	2.55	0.55
1:C:1838:ASP:HA	4:C:1406:HOH:O	2.06	0.55
1:B:1683:ASN:CB	4:B:2278:HOH:O	2.50	0.54
1:B:2112:GLU:CD	4:B:931:HOH:O	2.46	0.54
1:C:1492:TRP:CA	4:C:1063:HOH:O	2.50	0.54
1:C:1560:ASN:HD22	1:C:1560:ASN:H	1.55	0.54
1:A:1994:GLU:HA	1:A:2021:ARG:O	2.07	0.54
1:C:1587:ASN:HD22	1:C:1623:ALA:H	1.55	0.54
4:B:2538:HOH:O	1:C:2028:GLN:HG2	2.06	0.54
1:A:1961:ARG:HD3	4:A:1436:HOH:O	2.07	0.54
1:B:2184:ASP:HB2	4:B:2333:HOH:O	2.08	0.54
1:A:2054:LEU:C	1:A:2055:ARG:HD3	2.28	0.54
1:B:2045:ASN:N	1:B:2045:ASN:HD22	2.05	0.54
1:C:1529:ASP:HB2	4:C:2293:HOH:O	2.08	0.54
1:C:1766:LEU:HD12	1:C:1770:VAL:HG11	1.89	0.54
1:A:1647:ALA:HB2	4:A:2345:HOH:O	2.07	0.54
1:A:1575:GLU:HG3	4:A:960:HOH:O	2.08	0.54
1:B:1884:LEU:HD13	1:B:2123:PHE:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1535:ASP:HB3	4:B:2374:HOH:O	2.09	0.53
1:A:1772:THR:N	1:A:1776:GLN:NE2	2.49	0.53
1:B:1568:LYS:HD3	4:B:2322:HOH:O	2.07	0.53
1:C:1790:HIS:HA	1:C:1870:LEU:HD23	1.90	0.53
1:C:2111:LYS:HD3	4:C:2488:HOH:O	2.07	0.53
1:C:1925:HIS:HD2	4:C:86:HOH:O	1.92	0.53
1:B:1725:ILE:HA	4:B:2308:HOH:O	2.08	0.53
1:C:1646:ALA:N	4:C:2414:HOH:O	2.41	0.53
1:A:1887:ILE:N	4:A:2539:HOH:O	2.35	0.53
1:A:1726:THR:HG21	1:A:1740:VAL:HG22	1.91	0.53
1:B:2100:SER:C	4:B:931:HOH:O	2.46	0.53
1:C:1623:ALA:HA	1:C:1730:CYS:HB3	1.91	0.53
1:C:2046:ARG:HG3	4:C:2425:HOH:O	2.09	0.53
1:C:2129:ARG:NH1	4:C:714:HOH:O	2.34	0.53
1:A:1836:THR:HG22	4:A:2381:HOH:O	2.08	0.53
1:A:2095:ASP:O	1:A:2099:ARG:HD3	2.09	0.53
1:A:2047:LEU:HD13	4:A:2364:HOH:O	2.08	0.52
1:B:2089:ILE:CD1	1:C:1641:VAL:HG21	2.38	0.52
1:B:2129:ARG:NH2	4:B:959:HOH:O	2.37	0.52
1:C:1643:TRP:C	1:C:1645:ASP:H	2.12	0.52
1:C:1655:TYR:CE1	1:C:1689:VAL:HG22	2.45	0.52
1:C:1554:GLU:C	4:C:2372:HOH:O	2.35	0.52
1:A:1826:THR:CG2	4:A:1351:HOH:O	2.55	0.52
1:B:1537:PHE:HD2	1:B:1571:VAL:HG13	1.74	0.52
1:A:1549:GLU:OE1	1:A:1606:LYS:NZ	2.43	0.52
1:A:1592:LYS:NZ	4:A:968:HOH:O	2.42	0.52
1:A:1826:THR:HG22	1:A:1828:ASP:H	1.75	0.52
1:C:1606:LYS:NZ	4:C:1452:HOH:O	2.43	0.52
1:C:1780:THR:OG1	2:C:3:SO4:O2	2.08	0.52
1:B:1694:ILE:HA	1:C:2102:ARG:CD	2.40	0.52
1:C:2045:ASN:O	4:C:2425:HOH:O	2.18	0.51
1:A:1595:SER:HB3	4:A:974:HOH:O	2.10	0.51
1:A:1773:SER:H	1:A:1776:GLN:HE21	1.59	0.51
1:A:2131:ASN:ND2	1:A:2179:TYR:OH	2.42	0.51
1:B:1741:ARG:HH22	1:B:1934:GLN:NE2	2.09	0.51
1:A:1906:ASP:OD2	4:A:2573:HOH:O	2.19	0.51
1:A:1730:CYS:O	1:A:1731:ARG:C	2.48	0.51
1:A:1764:LYS:HE3	4:A:2554:HOH:O	2.11	0.51
1:B:1685:GLU:HB2	4:B:1100:HOH:O	2.10	0.51
1:C:1503:MET:CE	4:C:1065:HOH:O	2.59	0.51
1:B:1652:GLY:HA2	1:C:2085:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2081:GLU:N	4:C:2426:HOH:O	2.43	0.50
1:C:1662:GLY:HA3	4:C:1148:HOH:O	2.10	0.50
1:A:1812:ALA:HB3	1:A:1816:MET:HE1	1.93	0.50
1:B:1960:GLN:CD	4:B:605:HOH:O	2.41	0.50
1:C:1537:PHE:CD2	1:C:1571:VAL:HG13	2.46	0.50
1:C:1899:VAL:HB	1:C:1919:GLU:HB2	1.94	0.50
1:C:1557:PRO:HG3	4:C:2387:HOH:O	2.11	0.50
1:A:2030:MET:HE2	4:A:2578:HOH:O	2.11	0.50
1:A:2086:TYR:HA	1:A:2089:ILE:HD12	1.92	0.50
1:A:2093:PHE:O	1:A:2097:HIS:CD2	2.65	0.50
1:A:1511:PHE:CZ	4:A:830:HOH:O	2.46	0.50
1:A:1895:GLU:OE1	1:A:1897:ARG:HD3	2.12	0.49
1:B:1981:TYR:CG	1:B:1985:ILE:HD11	2.47	0.49
1:A:2104:VAL:HG21	1:A:2112:GLU:HG2	1.95	0.49
1:C:2102:ARG:O	1:C:2106:LYS:HG2	2.11	0.49
1:B:1530:VAL:CG1	4:B:946:HOH:O	2.59	0.49
1:B:1673:ASN:C	1:B:1673:ASN:HD22	2.16	0.49
1:A:2137:LYS:CE	4:A:394:HOH:O	2.60	0.49
1:C:1773:SER:H	1:C:1776:GLN:HE21	1.57	0.49
1:C:1815:ASN:ND2	1:C:1944:GLN:HE22	2.10	0.49
1:C:1606:LYS:HD3	4:C:220:HOH:O	2.12	0.49
1:C:1822:GLU:HB3	4:C:632:HOH:O	2.12	0.49
1:B:1531:LYS:HA	4:B:2486:HOH:O	2.12	0.49
1:B:1956:PHE:HB2	1:C:1756:LEU:HD13	1.95	0.49
1:B:1665:THR:O	1:B:1669:PHE:HD1	1.95	0.48
1:C:1780:THR:O	1:C:1784:TYR:HB3	2.13	0.48
1:A:1576:TYR:CZ	1:A:1812:ALA:HB2	2.48	0.48
1:A:1662:GLY:HA3	4:A:2552:HOH:O	2.12	0.48
1:A:1900:GLU:HB3	1:A:1916:LEU:HD11	1.94	0.48
1:A:1731:ARG:HD3	4:A:2350:HOH:O	2.14	0.48
1:A:1812:ALA:HB3	1:A:1816:MET:CE	2.43	0.48
1:C:2097:HIS:O	1:C:2102:ARG:HG3	2.13	0.48
1:A:1643:TRP:CZ3	1:A:1649:PRO:HB3	2.49	0.48
1:B:2008:ASN:H	1:B:2012:MET:HE2	1.75	0.48
1:B:2092:GLN:O	1:B:2096:LEU:HD12	2.13	0.48
1:B:1649:PRO:C	1:B:1651:LYS:N	2.67	0.48
1:B:2116:THR:HB	4:B:326:HOH:O	2.14	0.47
1:B:2129:ARG:NE	4:B:959:HOH:O	2.17	0.47
1:A:1575:GLU:CG	4:A:960:HOH:O	2.61	0.47
1:A:1794:VAL:HG21	4:A:2249:HOH:O	2.14	0.47
1:B:1480:LEU:N	4:B:1457:HOH:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1997:GLY:HA3	1:C:1705:LEU:HD22	1.96	0.47
1:C:2028:GLN:NE2	4:C:2390:HOH:O	2.46	0.47
1:A:2044:MET:O	1:A:2045:ASN:ND2	2.47	0.47
1:B:1647:ALA:O	1:B:1648:ASN:HB2	2.15	0.47
1:A:2137:LYS:CG	4:A:394:HOH:O	2.61	0.47
1:C:1677:THR:HA	1:C:1689:VAL:O	2.14	0.47
1:A:1790:HIS:HD2	4:A:61:HOH:O	1.98	0.47
1:C:1781:GLN:NE2	2:C:3:SO4:O1	2.41	0.47
1:B:1676:LEU:HG	1:B:1694:ILE:HD11	1.97	0.47
1:C:2047:LEU:CD2	4:C:2422:HOH:O	2.62	0.47
1:B:1657:TYR:CD2	1:B:1687:ARG:HG2	2.50	0.47
1:C:2093:PHE:HA	4:C:2427:HOH:O	2.15	0.47
1:B:2083:LEU:HB2	1:B:2084:PRO:HD3	1.95	0.47
1:A:2008:ASN:C	1:A:2008:ASN:HD22	2.17	0.46
1:C:1904:PRO:HG3	4:C:2503:HOH:O	2.15	0.46
1:C:2093:PHE:O	1:C:2094:ALA:HB3	2.15	0.46
1:A:1490:LYS:NZ	4:A:192:HOH:O	2.30	0.46
1:A:1545:ASP:OD2	1:A:1545:ASP:C	2.53	0.46
1:A:2047:LEU:HD21	1:A:2079:GLU:CG	2.45	0.46
1:B:1483:ILE:O	1:B:1484:ALA:HB3	2.16	0.46
1:C:1697:GLU:HG3	4:C:2446:HOH:O	2.14	0.46
3:A:101:B38:H16B	4:A:453:HOH:O	2.16	0.46
1:B:2041:LEU:HD23	1:B:2044:MET:CE	2.46	0.46
1:B:1839:GLU:CG	4:B:2340:HOH:O	2.60	0.46
1:B:1982:LYS:HD2	4:B:1122:HOH:O	2.16	0.46
1:C:1508:VAL:HG22	4:C:122:HOH:O	2.16	0.46
1:C:2093:PHE:O	1:C:2094:ALA:CB	2.63	0.46
1:A:1741:ARG:HH22	1:A:1934:GLN:NE2	2.13	0.46
1:B:1575:GLU:HB3	4:B:1430:HOH:O	2.16	0.46
1:A:1527:SER:O	1:A:1530:VAL:HG22	2.15	0.46
1:B:2101:SER:N	4:B:931:HOH:O	2.48	0.46
1:A:2143:VAL:HG11	1:A:2154:ARG:HH12	1.80	0.45
1:C:1775:LEU:O	1:C:1781:GLN:OE1	2.34	0.45
1:A:1480:LEU:HA	1:A:1492:TRP:CD1	2.51	0.45
1:A:1820:ILE:HD12	4:A:2539:HOH:O	2.17	0.45
1:A:1606:LYS:HE3	4:A:154:HOH:O	2.16	0.45
1:B:1844:ARG:O	1:B:1848:GLU:HG2	2.17	0.45
1:C:1544:GLU:OE1	1:C:1602:GLU:OE2	2.34	0.45
1:C:1954:ARG:O	3:C:100:B38:H4A	2.16	0.45
1:A:1624:ASN:HD22	1:A:1626:GLY:H	1.63	0.45
1:A:1819:PRO:O	1:A:1883[B]:ARG:NH1	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1981:TYR:CG	1:A:1985:ILE:HD11	2.51	0.45
1:B:1730:CYS:CA	1:B:1752:GLN:HE21	2.22	0.45
1:C:1593:ILE:HG22	4:C:1065:HOH:O	2.16	0.45
1:B:1815:ASN:H	1:B:1944:GLN:NE2	2.01	0.45
1:C:1898:THR:HG22	4:C:225:HOH:O	2.16	0.45
1:C:1936:ILE:HD13	1:C:1978:LEU:HD13	1.99	0.45
1:A:1745:ARG:NH2	4:A:243:HOH:O	2.23	0.45
1:A:1836:THR:OG1	1:A:1839:GLU:HG3	2.16	0.45
1:A:2137:LYS:HE2	4:A:394:HOH:O	2.16	0.45
1:B:1480:LEU:O	1:B:1481:ARG:O	2.35	0.45
1:B:1735:ILE:HD13	1:B:1739:LEU:HG	1.98	0.45
1:C:1554:GLU:OE2	4:C:2498:HOH:O	2.21	0.45
1:A:1679:ARG:HG2	4:A:2577:HOH:O	2.17	0.45
1:C:1744:GLN:O	1:C:1790:HIS:CE1	2.70	0.45
1:B:1719:TYR:CE2	1:B:1744:GLN:HG3	2.52	0.45
1:C:1900:GLU:HB3	1:C:1916:LEU:HD11	1.99	0.45
1:A:1899:VAL:HB	1:A:1919:GLU:HB2	1.99	0.44
1:B:1602:GLU:OE2	1:B:1606:LYS:HE2	2.16	0.44
1:B:1690:ILE:HG12	4:B:2285:HOH:O	2.18	0.44
1:B:1822:GLU:N	4:B:1168:HOH:O	2.49	0.44
4:B:796:HOH:O	1:C:1757:THR:HG23	2.17	0.44
1:C:1852:THR:HG21	4:C:2335:HOH:O	2.16	0.44
1:C:2093:PHE:CA	4:C:2427:HOH:O	2.64	0.44
1:C:2104:VAL:HG23	1:C:2109:ILE:HD11	1.99	0.44
1:B:1831:VAL:HG11	1:B:2115:TRP:CZ2	2.52	0.44
1:B:2097:HIS:CE1	1:C:1632:ALA:H	2.26	0.44
1:B:2047:LEU:HD13	1:B:2047:LEU:C	2.37	0.44
1:B:1527:SER:O	1:B:1530:VAL:HG12	2.18	0.44
1:A:1790:HIS:HA	1:A:1870:LEU:HD23	1.99	0.44
1:C:1954:ARG:HD2	4:C:1013:HOH:O	2.16	0.44
1:A:1854:SER:OG	4:A:1269:HOH:O	2.21	0.44
1:A:2134:TYR:CD2	1:A:2135:LEU:HD13	2.51	0.44
1:B:1852:THR:HG22	1:B:1855:GLY:O	2.17	0.44
1:A:1756:LEU:HD12	1:A:1756:LEU:HA	1.94	0.44
1:B:1730:CYS:O	1:B:1731:ARG:C	2.57	0.44
1:B:2000:TRP:CD1	1:C:1705:LEU:HB3	2.53	0.44
1:C:2140:SER:C	1:C:2142:GLN:H	2.21	0.44
1:B:1711:ILE:HD11	1:B:1735:ILE:HD12	1.99	0.43
1:C:2081:GLU:OE1	1:C:2081:GLU:O	2.36	0.43
1:B:1909:ASN:HD21	1:B:1911:ASN:HD22	1.66	0.43
3:B:102[B]:B38:C17	1:C:1757:THR:HG22	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1519:SER:O	1:C:1522:GLN:HB2	2.17	0.43
1:C:1530:VAL:CG2	4:C:1191:HOH:O	2.63	0.43
1:C:1535:ASP:HB2	4:C:471:HOH:O	2.18	0.43
1:B:1998:GLY:HA3	4:B:39:HOH:O	2.17	0.43
1:B:1675:VAL:CB	4:B:2285:HOH:O	2.56	0.43
1:A:1549:GLU:CD	1:A:1606:LYS:HZ1	2.22	0.43
1:A:1677:THR:CG2	4:A:2376:HOH:O	2.52	0.43
1:A:1690:ILE:HA	4:A:2376:HOH:O	2.19	0.43
1:B:1824:LYS:NZ	1:B:1858:TYR:OH	2.34	0.43
1:A:1936:ILE:HG12	1:A:1947:MET:CE	2.48	0.43
1:B:1694:ILE:HA	1:C:2102:ARG:HD3	2.01	0.43
1:B:1682:ILE:O	1:B:1682:ILE:HG23	2.19	0.42
1:B:2179:TYR:HE2	4:B:1279:HOH:O	2.02	0.42
1:C:1619:ILE:HD12	1:C:1619:ILE:N	2.34	0.42
1:C:1745:ARG:HG2	1:C:1806:TRP:CZ2	2.53	0.42
1:C:2136:ILE:HD11	1:C:2152:ILE:HG23	2.01	0.42
1:C:2149:LEU:HD13	1:C:2149:LEU:C	2.40	0.42
1:A:1781:GLN:HE21	1:A:1781:GLN:HB2	1.53	0.42
1:A:1541:GLU:O	1:A:1552:GLU:HA	2.18	0.42
1:C:1534:ASP:HB3	4:C:2473:HOH:O	2.18	0.42
1:C:1619:ILE:N	1:C:1619:ILE:CD1	2.83	0.42
1:B:2101:SER:CA	4:B:931:HOH:O	2.59	0.42
1:A:2041:LEU:HD23	1:A:2044:MET:HE3	2.01	0.42
1:B:1480:LEU:HA	1:B:1492:TRP:CD1	2.54	0.42
1:B:1743:GLY:O	4:B:2308:HOH:O	2.22	0.42
1:B:2160:PRO:HD3	1:B:2174:TRP:CZ2	2.54	0.42
1:A:1529:ASP:HB2	4:A:1378:HOH:O	2.18	0.42
1:A:1792:THR:O	1:A:1802:LYS:HE2	2.20	0.42
1:B:2010:ASP:CG	1:B:2148:ARG:HD2	2.40	0.42
1:B:1818:VAL:HB	1:B:1888:PRO:HG2	2.02	0.42
1:A:1481:ARG:HB2	4:A:2526:HOH:O	2.20	0.42
1:A:2048:ASP:HA	4:A:892:HOH:O	2.20	0.42
1:A:2164:ASP:H	1:A:2170:GLN:NE2	2.18	0.42
1:B:1522:GLN:HG2	4:B:2246:HOH:O	2.19	0.42
3:B:102[B]:B38:H17	4:C:417:HOH:O	2.19	0.42
1:C:1730:CYS:HA	1:C:1752:GLN:OE1	2.19	0.42
1:C:2044:MET:C	1:C:2046:ARG:H	2.22	0.42
1:A:1575:GLU:HB3	1:A:1819:PRO:HB2	2.01	0.41
1:B:1513:GLU:OE2	1:B:1516:ARG:HD3	2.20	0.41
1:C:1898:THR:HB	1:C:1920:PRO:HA	2.02	0.41
1:A:1827:TRP:HZ3	1:A:2120:ARG:HG2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1516:ARG:NH2	4:B:2436:HOH:O	2.53	0.41
1:C:1719:TYR:CE2	1:C:1744:GLN:HG3	2.55	0.41
1:C:1748:GLN:HE22	1:C:1783:MET:HB2	1.85	0.41
1:C:1790:HIS:HD2	4:C:37:HOH:O	2.02	0.41
1:A:1813:LYS:HG2	1:A:1816:MET:HE3	2.03	0.41
1:A:2152:ILE:HG21	4:A:2564:HOH:O	2.20	0.41
1:B:1505:THR:HB	1:B:1730:CYS:HB2	2.03	0.41
1:B:2106:LYS:HA	1:B:2106:LYS:HD2	1.88	0.41
1:A:1657:TYR:CE2	1:A:1687:ARG:HD2	2.55	0.41
1:A:1675:VAL:HG22	1:A:1690:ILE:HG23	2.02	0.41
1:B:1790:HIS:O	1:B:1791:LEU:HD13	2.20	0.41
1:C:2181:THR:O	1:C:2184:ASP:HB2	2.21	0.41
1:A:1675:VAL:HG13	1:A:1677:THR:HG23	2.02	0.41
1:A:1774:ASN:HD22	1:A:1774:ASN:HA	1.66	0.41
1:A:1879:VAL:HG13	1:A:1931:LYS:HE2	2.03	0.41
1:A:1892:ILE:HD12	1:A:1947:MET:HE1	2.03	0.41
1:B:1633:GLU:HA	1:B:1633:GLU:OE1	2.20	0.41
1:B:1809:TYR:O	1:B:1945:LEU:HD21	2.21	0.41
1:C:1996:ARG:O	1:C:1999:SER:HB2	2.21	0.41
1:C:1759:ALA:N	1:C:1774:ASN:HD21	2.15	0.41
1:C:1766:LEU:O	1:C:1768:ARG:N	2.54	0.41
1:B:1625:SER:CB	4:B:2511:HOH:O	2.59	0.40
1:B:1677:THR:HA	1:B:1689:VAL:O	2.21	0.40
1:C:1759:ALA:O	1:C:1760:PRO:C	2.59	0.40
1:C:2081:GLU:C	4:C:2426:HOH:O	2.59	0.40
1:A:1575:GLU:H	1:A:1575:GLU:CD	2.24	0.40
1:A:1821:LEU:O	1:A:1886:GLY:HA2	2.21	0.40
1:A:2011:GLN:O	1:A:2129:ARG:NH2	2.51	0.40
1:B:1497:ARG:HD3	1:B:1510:ASP:OD1	2.21	0.40
1:B:1690:ILE:CG2	4:B:2285:HOH:O	2.53	0.40
1:B:1745:ARG:HD3	1:B:1943:GLU:OE2	2.21	0.40
1:C:1852:THR:HG21	4:C:604:HOH:O	2.20	0.40
1:C:1943:GLU:HB3	1:C:1945:LEU:HD22	2.03	0.40
1:B:1910:PRO:HA	4:B:2325:HOH:O	2.20	0.40
1:B:1946:PRO:HG3	1:B:2130:LEU:HD21	2.02	0.40

All (9) 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)
4:A:81:HOH:O	4:A:2568:HOH:O[2_555]	1.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:307:HOH:O	4:A:2586:HOH:O[2_555]	1.88	0.32
4:A:1181:HOH:O	4:C:126:HOH:O[4_555]	2.04	0.16
4:A:81:HOH:O	4:A:2477:HOH:O[2_555]	2.05	0.15
4:A:1181:HOH:O	4:C:2445:HOH:O[4_555]	2.05	0.15
4:A:545:HOH:O	4:A:2474:HOH:O[2_555]	2.14	0.06
4:A:1414:HOH:O	4:A:1414:HOH:O[2_555]	2.18	0.02
4:A:2599:HOH:O	4:C:408:HOH:O[4_555]	2.18	0.02
4:A:2309:HOH:O	4:C:289:HOH:O[4_555]	2.19	0.01

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	690/769 (90%)	645 (94%)	38 (6%)	7 (1%)	15 16
1	B	673/769 (88%)	622 (92%)	42 (6%)	9 (1%)	12 11
1	C	664/769 (86%)	620 (93%)	34 (5%)	10 (2%)	10 9
All	All	2027/2307 (88%)	1887 (93%)	114 (6%)	26 (1%)	12 11

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1650	ASP
1	A	1673	ASN
1	A	1683	ASN
1	B	1481	ARG
1	B	1650	ASP
1	B	1731	ARG
1	B	2046	ARG
1	B	2145	GLU
1	C	2094	ALA
1	C	2143	VAL
1	B	1534	ASP

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Mol	Chain	Res	Type
1	C	1555	ARG
1	C	1644	ASN
1	C	1767	GLY
1	B	1825	ASP
1	C	1764	LYS
1	C	1765	MET
1	A	1684	GLY
1	A	2053	GLU
1	C	2084	PRO
1	A	1731	ARG
1	B	2084	PRO
1	C	1649	PRO
1	C	2045	ASN
1	A	1767	GLY
1	B	2144	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	589/658 (90%)	536 (91%)	53 (9%)	9 10
1	B	574/658 (87%)	508 (88%)	66 (12%)	5 5
1	C	566/658 (86%)	504 (89%)	62 (11%)	6 5
All	All	1729/1974 (88%)	1548 (90%)	181 (10%)	7 6

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1481	ARG
1	A	1499	LYS
1	A	1534	ASP
1	A	1536	PHE
1	A	1551	THR
1	A	1560	ASN
1	A	1585	VAL

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Mol	Chain	Res	Type
1	A	1618	ARG
1	A	1641	VAL
1	A	1661	GLU
1	A	1666	LEU
1	A	1673	ASN
1	A	1675	VAL
1	A	1681	VAL
1	A	1682	ILE
1	A	1683	ASN
1	A	1687	ARG
1	A	1690	ILE
1	A	1691	LYS
1	A	1756	LEU
1	A	1766	LEU
1	A	1781	GLN
1	A	1802	LYS
1	A	1813	LYS
1	A	1826	THR
1	A	1837	ASN
1	A	1854	SER
1	A	1879	VAL
1	A	1884	LEU
1	A	1909	ASN
1	A	1924	TRP
1	A	1950	LEU
1	A	2002	VAL
1	A	2003	VAL
1	A	2008	ASN
1	A	2028	GLN
1	A	2034	LYS
1	A	2035	PHE
1	A	2037	ARG
1	A	2045	ASN
1	A	2051	TYR
1	A	2054	LEU
1	A	2080	ARG
1	A	2082	LEU
1	A	2091	LEU
1	A	2099	ARG
1	A	2128	ARG
1	A	2135	LEU
1	A	2139	LEU

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Mol	Chain	Res	Type
1	A	2142	GLN
1	A	2148	ARG
1	A	2191	LEU
1	A	2194	PHE
1	B	1480	LEU
1	B	1481	ARG
1	B	1483	ILE
1	B	1499	LYS
1	B	1502	LEU
1	B	1508	VAL
1	B	1516	ARG
1	B	1531	LYS
1	B	1534	ASP
1	B	1555	ARG
1	B	1565	VAL
1	B	1571	VAL
1	B	1583	VAL
1	B	1585	VAL
1	B	1606	LYS
1	B	1618	ARG
1	B	1624	ASN
1	B	1650	ASP
1	B	1658	LEU
1	B	1666	LEU
1	B	1673	ASN
1	B	1679	ARG
1	B	1685	GLU
1	B	1689	VAL
1	B	1700	LEU
1	B	1729	THR
1	B	1735	ILE
1	B	1764	LYS
1	B	1768	ARG
1	B	1772	THR
1	B	1777	LEU
1	B	1786	ASN
1	B	1791	LEU
1	B	1797	LEU
1	B	1813	LYS
1	B	1824	LYS
1	B	1838	ASP
1	B	1839	GLU

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Mol	Chain	Res	Type
1	B	1840	THR
1	B	1843	VAL
1	B	1852	THR
1	B	1854	SER
1	B	1884	LEU
1	B	1911	ASN
1	B	1918	GLN
1	B	1924	TRP
1	B	1960	GLN
1	B	1961	ARG
1	B	2025	LEU
1	B	2027	PRO
1	B	2035	PHE
1	B	2045	ASN
1	B	2081	GLU
1	B	2082	LEU
1	B	2085	ILE
1	B	2088	GLN
1	B	2092	GLN
1	B	2127	ARG
1	B	2128	ARG
1	B	2145	GLU
1	B	2148	ARG
1	B	2149	LEU
1	B	2152	ILE
1	B	2165	HIS
1	B	2185	LYS
1	B	2189	LEU
1	C	1508	VAL
1	C	1511	PHE
1	C	1514	LEU
1	C	1531	LYS
1	C	1536	PHE
1	C	1542	LEU
1	C	1546	GLU
1	C	1550	LEU
1	C	1554	GLU
1	C	1560	ASN
1	C	1565	VAL
1	C	1571	VAL
1	C	1585	VAL
1	C	1602	GLU

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Mol	Chain	Res	Type
1	C	1606	LYS
1	C	1645	ASP
1	C	1651	LYS
1	C	1654	GLN
1	C	1664	GLU
1	C	1665	THR
1	C	1685	GLU
1	C	1741	ARG
1	C	1742	LEU
1	C	1768	ARG
1	C	1769	GLU
1	C	1770	VAL
1	C	1775	LEU
1	C	1781	GLN
1	C	1786	ASN
1	C	1792	THR
1	C	1838	ASP
1	C	1852	THR
1	C	1854	SER
1	C	1898	THR
1	C	1902	LEU
1	C	1924	TRP
1	C	1930	PHE
1	C	1945	LEU
1	C	1950	LEU
1	C	1968	LEU
1	C	1978	LEU
1	C	1999	SER
1	C	2031	VAL
1	C	2035	PHE
1	C	2037	ARG
1	C	2040	LEU
1	C	2043	THR
1	C	2046	ARG
1	C	2047	LEU
1	C	2081	GLU
1	C	2083	LEU
1	C	2102	ARG
1	C	2128	ARG
1	C	2137	LYS
1	C	2138	ARG
1	C	2143	VAL

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Mol	Chain	Res	Type
1	C	2149	LEU
1	C	2152	ILE
1	C	2154	ARG
1	C	2186	LEU
1	C	2189	LEU
1	C	2192	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1547	ASN
1	A	1560	ASN
1	A	1587	ASN
1	A	1624	ASN
1	A	1640	GLN
1	A	1683	ASN
1	A	1748	GLN
1	A	1774	ASN
1	A	1776	GLN
1	A	1781	GLN
1	A	1790	HIS
1	A	1815	ASN
1	A	1909	ASN
1	A	1918	GLN
1	A	1934	GLN
1	A	2008	ASN
1	A	2045	ASN
1	A	2097	HIS
1	A	2131	ASN
1	A	2170	GLN
1	B	1494	GLN
1	B	1517	GLN
1	B	1522	GLN
1	B	1581	GLN
1	B	1587	ASN
1	B	1605	ASN
1	B	1624	ASN
1	B	1673	ASN
1	B	1748	GLN
1	B	1752	GLN
1	B	1763	ASN
1	B	1786	ASN

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Mol	Chain	Res	Type
1	B	1815	ASN
1	B	1911	ASN
1	B	1934	GLN
1	B	1941	ASN
1	B	1944	GLN
1	B	1960	GLN
1	B	2045	ASN
1	B	2097	HIS
1	B	2131	ASN
1	C	1517	GLN
1	C	1522	GLN
1	C	1560	ASN
1	C	1587	ASN
1	C	1605	ASN
1	C	1640	GLN
1	C	1683	ASN
1	C	1748	GLN
1	C	1774	ASN
1	C	1776	GLN
1	C	1781	GLN
1	C	1786	ASN
1	C	1790	HIS
1	C	1815	ASN
1	C	1911	ASN
1	C	1918	GLN
1	C	1925	HIS
1	C	1941	ASN
1	C	2011	GLN
1	C	2092	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

7 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	$\#\|Z\| > 2$
3	B38	B	102[B]	-	32,32,32	2.64	13 (40%)	32,48,48	1.51	5 (15%)
2	SO4	A	2	-	4,4,4	0.28	0	6,6,6	0.84	0
2	SO4	C	3	-	4,4,4	0.13	0	6,6,6	0.47	0
3	B38	B	102[A]	-	32,32,32	2.67	13 (40%)	32,48,48	1.56	5 (15%)
3	B38	A	101	-	32,32,32	2.54	13 (40%)	32,48,48	1.25	3 (9%)
3	B38	C	100	-	32,32,32	2.58	11 (34%)	32,48,48	1.39	4 (12%)
2	SO4	C	1	-	4,4,4	0.23	0	6,6,6	0.71	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	B38	B	102[B]	-	-	4/8/34/34	0/5/5/5
3	B38	C	100	-	-	0/8/34/34	0/5/5/5
3	B38	B	102[A]	-	-	0/8/34/34	0/5/5/5
3	B38	A	101	-	-	0/8/34/34	0/5/5/5

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	102[A]	B38	C13-C15	6.86	1.50	1.39
3	B	102[B]	B38	C13-C15	6.86	1.50	1.39
3	C	100	B38	C13-C15	6.80	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	100	B38	C14-C11	6.67	1.50	1.38
3	A	101	B38	C14-C11	6.43	1.50	1.38
3	B	102[A]	B38	C14-C11	6.25	1.50	1.38
3	B	102[B]	B38	C14-C11	6.25	1.50	1.38
3	A	101	B38	C13-C10	-5.26	1.31	1.39
3	A	101	B38	C13-C15	4.83	1.47	1.39
3	B	102[A]	B38	C10-C6	4.75	1.49	1.40
3	B	102[B]	B38	C10-C6	4.75	1.49	1.40
3	C	100	B38	C13-C10	-4.49	1.32	1.39
3	A	101	B38	C10-C6	4.47	1.49	1.40
3	C	100	B38	C10-C6	4.45	1.49	1.40
3	B	102[A]	B38	C13-C10	-4.22	1.33	1.39
3	B	102[B]	B38	C13-C10	-4.22	1.33	1.39
3	A	101	B38	C11-C6	-4.14	1.31	1.39
3	C	100	B38	O2-C6	-4.11	1.31	1.37
3	B	102[A]	B38	O2-C6	-3.72	1.32	1.37
3	B	102[B]	B38	O2-C6	-3.72	1.32	1.37
3	A	101	B38	O2-C6	-3.54	1.32	1.37
3	A	101	B38	C5-C1	3.45	1.57	1.52
3	B	102[A]	B38	C3-C7	3.33	1.55	1.50
3	B	102[B]	B38	C3-C7	3.33	1.55	1.50
3	C	100	B38	C11-C6	-3.30	1.32	1.39
3	B	102[A]	B38	C11-C6	-3.12	1.33	1.39
3	B	102[B]	B38	C11-C6	-3.12	1.33	1.39
3	A	101	B38	C3-C1	2.77	1.55	1.53
3	B	102[B]	B38	N24-N23	-2.69	1.32	1.37
3	B	102[A]	B38	O12-C7	2.51	1.26	1.22
3	B	102[B]	B38	O12-C7	2.51	1.26	1.22
3	B	102[A]	B38	N24-N23	-2.50	1.32	1.37
3	C	100	B38	O12-C7	2.44	1.26	1.22
3	B	102[A]	B38	C3-C1	2.44	1.55	1.53
3	B	102[B]	B38	C3-C1	2.44	1.55	1.53
3	B	102[A]	B38	C5-C1	2.38	1.56	1.52
3	B	102[B]	B38	C5-C1	2.38	1.56	1.52
3	B	102[A]	B38	C26-N27	2.33	1.39	1.34
3	C	100	B38	C26-N27	2.33	1.39	1.34
3	B	102[B]	B38	C21-C22	-2.32	1.39	1.43
3	A	101	B38	O12-C7	2.30	1.26	1.22
3	A	101	B38	C4-C1	2.26	1.55	1.52
3	C	100	B38	C20-C26	2.25	1.53	1.50
3	C	100	B38	C4-C1	2.24	1.55	1.52
3	B	102[B]	B38	C20-C22	-2.24	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	101	B38	C3-C7	2.09	1.53	1.50
3	A	101	B38	C19-C20	2.07	1.41	1.38
3	B	102[A]	B38	C19-C20	2.06	1.41	1.38
3	C	100	B38	C19-C20	2.03	1.41	1.38
3	A	101	B38	C14-C15	-2.03	1.33	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	100	B38	C3-C7-C10	-3.60	111.51	116.49
3	B	102[A]	B38	O2-C1-C3	-3.33	105.53	109.64
3	B	102[B]	B38	O2-C1-C3	-3.33	105.53	109.64
3	B	102[A]	B38	C6-C10-C7	-3.32	117.94	119.85
3	B	102[B]	B38	C6-C10-C7	-3.32	117.94	119.85
3	B	102[A]	B38	C5-C1-C4	-3.28	105.31	109.56
3	B	102[B]	B38	C5-C1-C4	-3.28	105.31	109.56
3	A	101	B38	C3-C7-C10	-3.21	112.05	116.49
3	B	102[A]	B38	O12-C7-C3	3.08	125.40	121.16
3	B	102[B]	B38	O12-C7-C3	3.08	125.40	121.16
3	C	100	B38	C5-C1-C4	-2.93	105.77	109.56
3	A	101	B38	C13-C10-C6	2.86	122.29	118.29
3	B	102[A]	B38	C3-C7-C10	-2.62	112.86	116.49
3	B	102[B]	B38	C3-C7-C10	-2.62	112.86	116.49
3	C	100	B38	C6-C10-C7	-2.52	118.41	119.85
3	C	100	B38	C4-C8-N27	-2.32	106.35	110.92
3	A	101	B38	O2-C1-C3	-2.27	106.84	109.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	102[B]	B38	C20-C26-N27-C9
3	B	102[B]	B38	O28-C26-N27-C9
3	B	102[B]	B38	C20-C26-N27-C8
3	B	102[B]	B38	O28-C26-N27-C8

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	102[B]	B38	2	0

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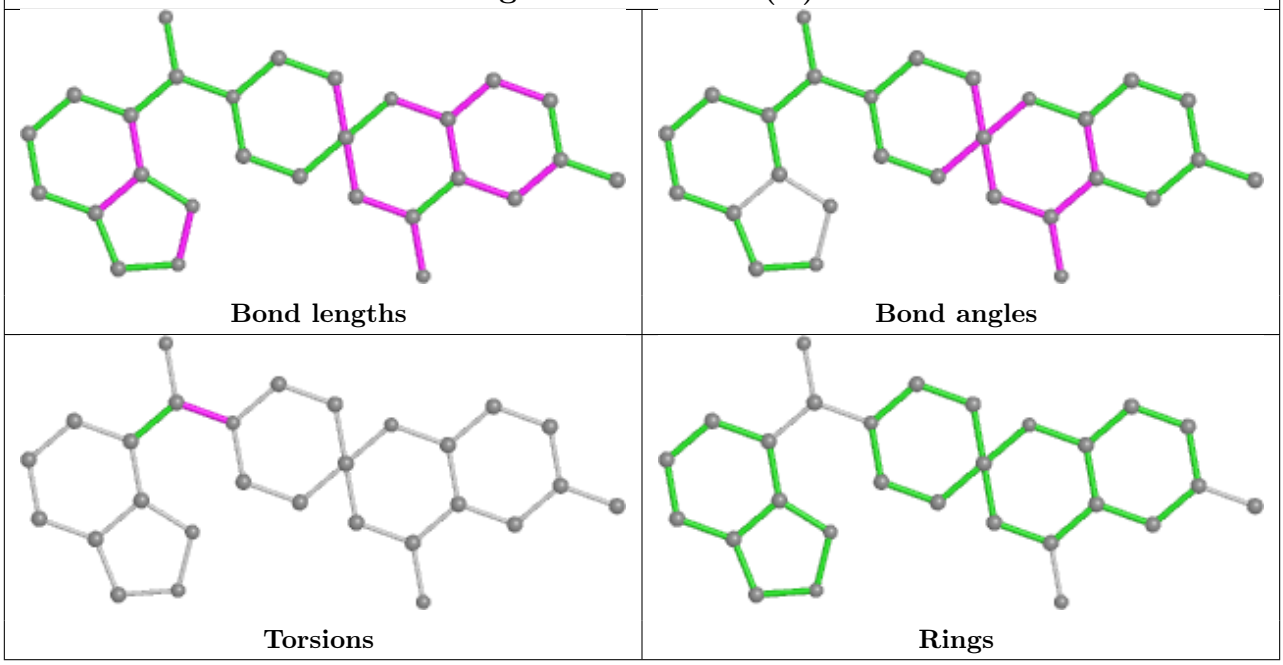
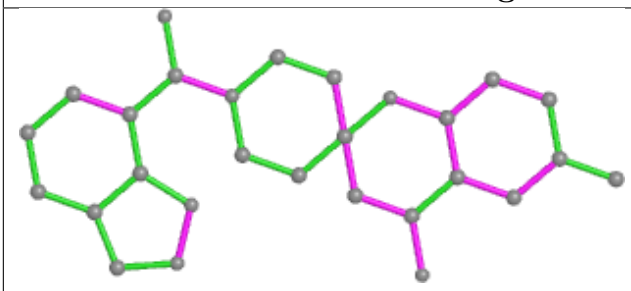
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	SO4	2	0
3	A	101	B38	1	0
3	C	100	B38	1	0

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

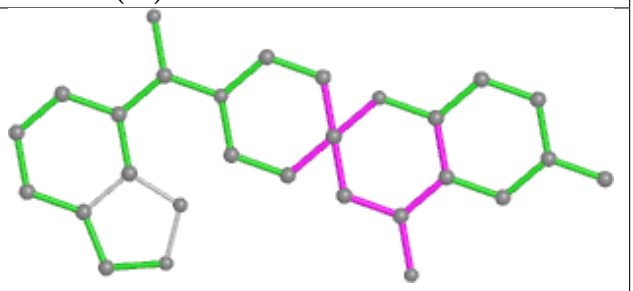
Ligand B38 B 102 (B)



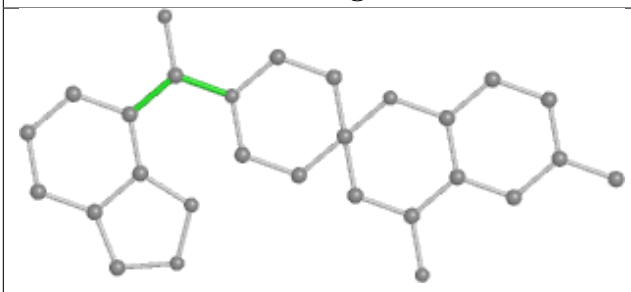
Ligand B38 B 102 (A)



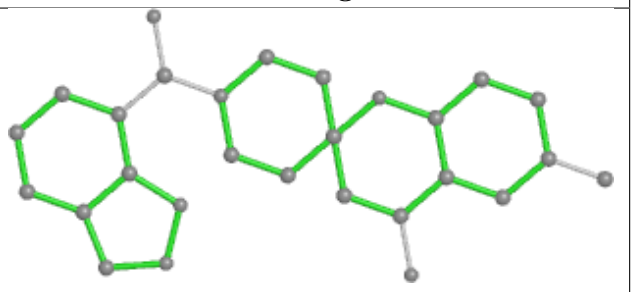
Bond lengths



Bond angles

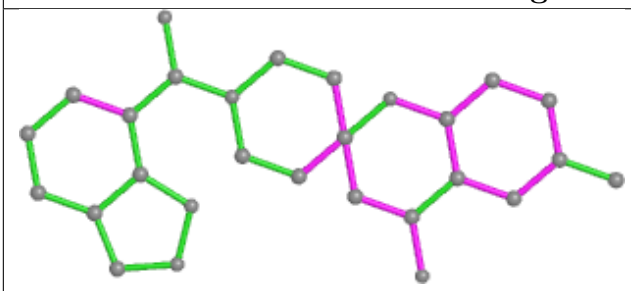


Torsions

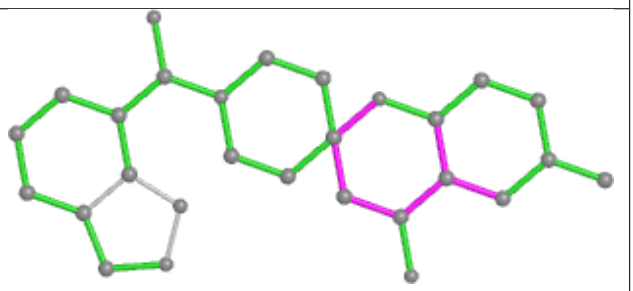


Rings

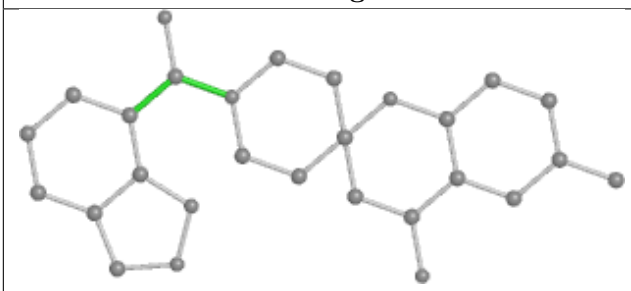
Ligand B38 A 101



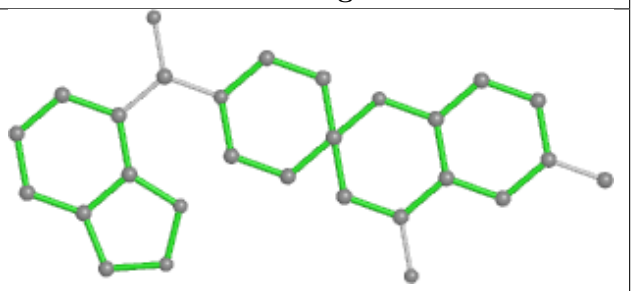
Bond lengths



Bond angles

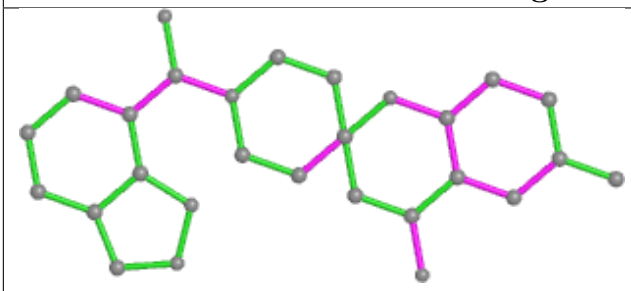


Torsions

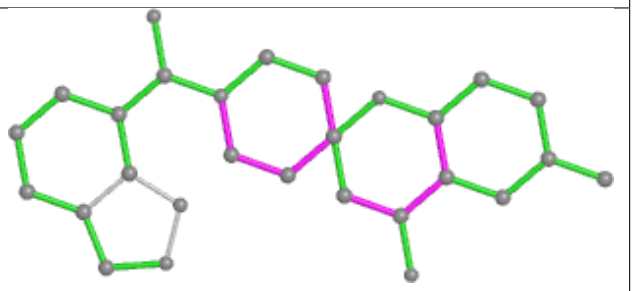


Rings

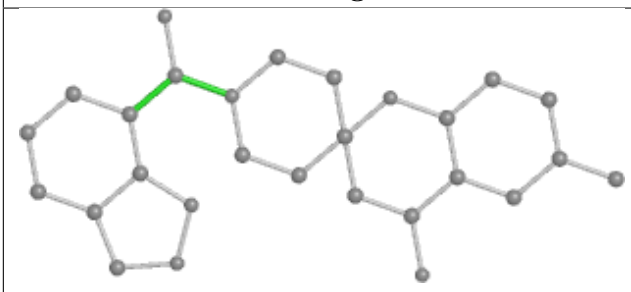
Ligand B38 C 100



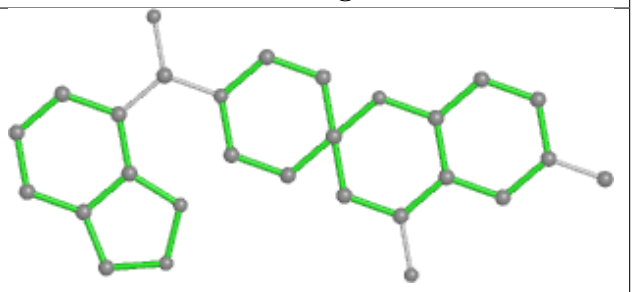
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	693/769 (90%)	-0.16	31 (4%)	33	30	30, 45, 98, 125	0
1	B	677/769 (88%)	-0.00	43 (6%)	19	16	29, 49, 101, 125	0
1	C	668/769 (86%)	-0.07	49 (7%)	15	11	29, 48, 109, 131	0
All	All	2038/2307 (88%)	-0.08	123 (6%)	21	18	29, 47, 102, 131	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2194	PHE	7.4
1	B	2082	LEU	6.3
1	C	1644	ASN	5.8
1	B	2086	TYR	5.7
1	C	2143	VAL	5.3
1	B	2085	ILE	5.3
1	C	1669	PHE	5.2
1	B	2143	VAL	5.1
1	C	1647	ALA	5.0
1	C	1681	VAL	5.0
1	C	1685	GLU	4.9
1	B	2084	PRO	4.8
1	B	2083	LEU	4.7
1	A	2144	GLY	4.5
1	C	1680	THR	4.3
1	B	2144	GLY	4.2
1	B	2044	MET	4.2
1	A	2195	ALA	4.2
1	C	1645	ASP	4.1
1	A	2143	VAL	4.1
1	C	1650	ASP	3.9
1	C	1655	TYR	3.9
1	C	1665	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	2052	ARG	3.8
1	C	1682	ILE	3.8
1	A	2142	GLN	3.8
1	C	1666	LEU	3.8
1	B	2041	LEU	3.7
1	B	1681	VAL	3.7
1	C	1657	TYR	3.7
1	A	1682	ILE	3.7
1	B	2142	GLN	3.6
1	B	2145	GLU	3.6
1	B	2047	LEU	3.5
1	C	1663	MET	3.5
1	C	1649	PRO	3.4
1	A	2145	GLU	3.4
1	B	2187	LYS	3.3
1	C	2144	GLY	3.3
1	A	2191	LEU	3.3
1	C	2190	LYS	3.2
1	C	2192	GLU	3.2
1	C	1651	LYS	3.2
1	B	2046	ARG	3.2
1	B	2186	LEU	3.2
1	C	2082	LEU	3.1
1	A	1679	ARG	3.0
1	C	1668	LYS	3.0
1	A	1684	GLY	3.0
1	C	1688	PHE	3.0
1	B	1854	SER	2.9
1	A	2051	TYR	2.9
1	A	2193	SER	2.9
1	B	1682	ILE	2.9
1	A	1681	VAL	2.9
1	A	1855	GLY	2.9
1	B	2179	TYR	2.9
1	C	1652	GLY	2.9
1	A	2192	GLU	2.8
1	A	1911	ASN	2.7
1	B	1855	GLY	2.7
1	C	1643	TRP	2.7
1	B	2188	GLY	2.7
1	C	1679	ARG	2.7
1	A	2049	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	1648	ASN	2.7
1	A	1685	GLU	2.7
1	C	1683	ASN	2.7
1	C	2191	LEU	2.7
1	B	1838	ASP	2.7
1	B	2146	ALA	2.7
1	B	2158	TRP	2.6
1	C	1662	GLY	2.6
1	C	1670	ASP	2.6
1	B	2153	ALA	2.6
1	B	1853	GLU	2.6
1	C	1654	GLN	2.6
1	C	1648	ASN	2.5
1	C	1686	GLU	2.5
1	A	1853	GLU	2.5
1	C	1653	PHE	2.5
1	C	1664	GLU	2.5
1	C	1547	ASN	2.5
1	A	1669	PHE	2.5
1	A	1767	GLY	2.5
1	B	2189	LEU	2.4
1	C	1913	ALA	2.4
1	B	1767	GLY	2.4
1	B	1911	ASN	2.4
1	B	2134	TYR	2.4
1	A	2190	LYS	2.3
1	B	1688	PHE	2.3
1	A	2083	LEU	2.3
1	C	1684	GLY	2.3
1	C	1911	ASN	2.3
1	A	2082	LEU	2.3
1	C	1660	SER	2.3
1	B	1645	ASP	2.3
1	A	1838	ASP	2.3
1	A	2189	LEU	2.3
1	A	1651	LYS	2.2
1	B	2043	THR	2.2
1	A	1648	ASN	2.2
1	B	1824	LYS	2.2
1	C	1667	LYS	2.2
1	B	2154	ARG	2.2
1	B	1647	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	2079	GLU	2.2
1	C	2142	GLN	2.2
1	B	2155	ILE	2.2
1	A	1683	ASN	2.1
1	C	1531	LYS	2.1
1	B	2184	ASP	2.1
1	C	1672	GLU	2.1
1	C	1767	GLY	2.1
1	C	1642	ALA	2.1
1	C	1529	ASP	2.0
1	C	1838	ASP	2.0
1	B	2002	VAL	2.0
1	B	2089	ILE	2.0
1	B	1685	GLU	2.0
1	C	1661	GLU	2.0
1	B	1910	PRO	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 monosaccharides in this entry.

6.4 Ligands (i)

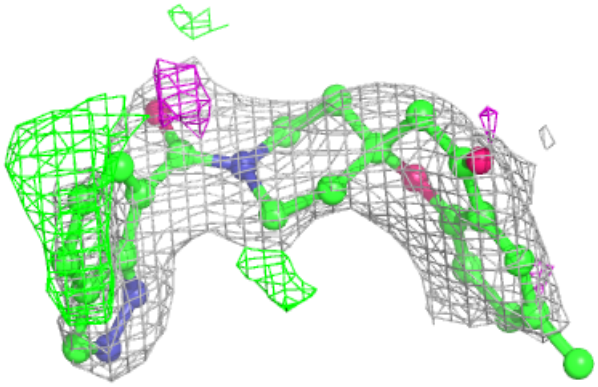
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

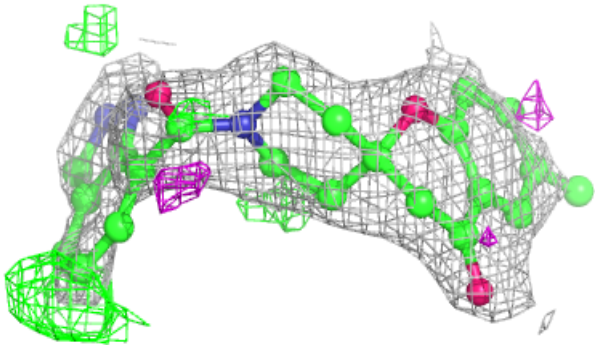
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	B38	B	102[A]	28/28	0.85	0.26	83,88,91,92	11
3	B38	B	102[B]	28/28	0.85	0.26	83,90,91,92	11
3	B38	C	100	28/28	0.88	0.17	67,78,82,83	0
3	B38	A	101	28/28	0.90	0.16	71,80,90,91	0
2	SO4	A	2	5/5	0.96	0.28	85,86,88,91	0
2	SO4	C	3	5/5	0.96	0.38	120,120,121,122	0
2	SO4	C	1	5/5	0.98	0.20	81,82,83,84	0

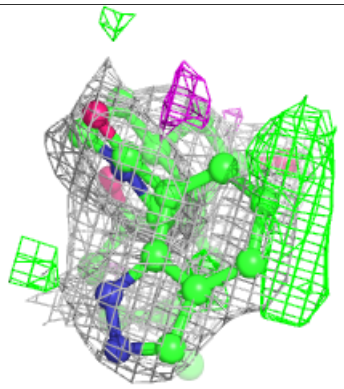
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B38 B 102 (A):

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

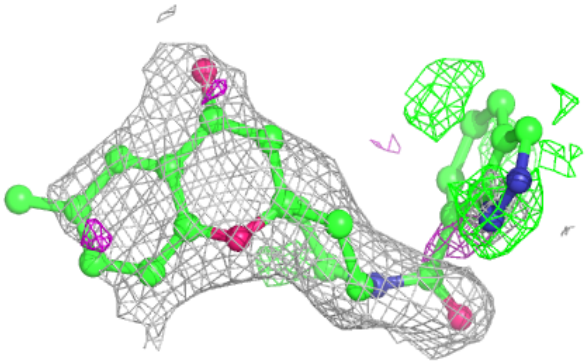


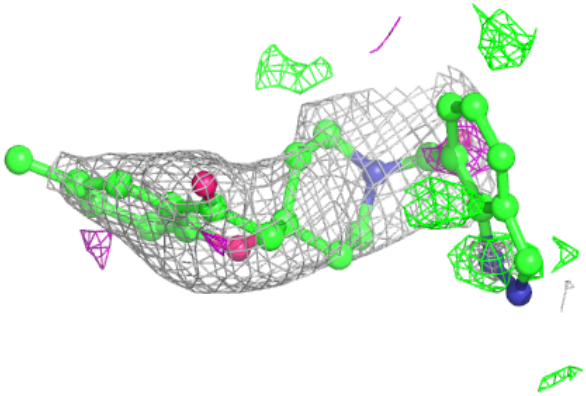


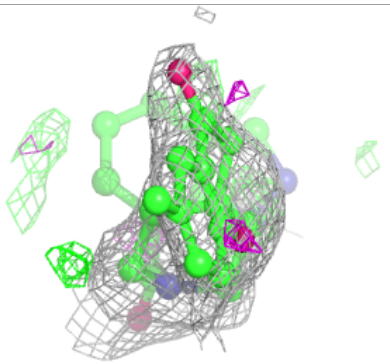


Electron density around B38 B 102 (B):

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

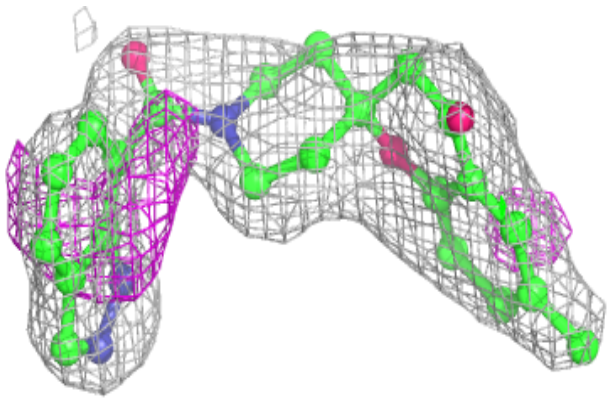


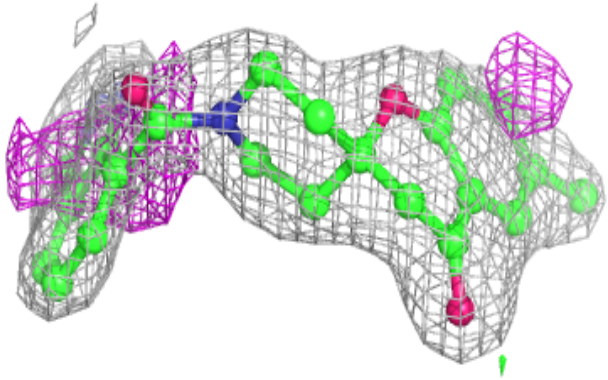


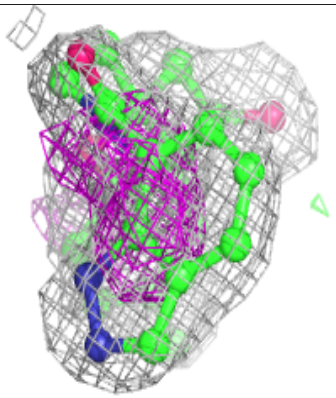


Electron density around B38 C 100:

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

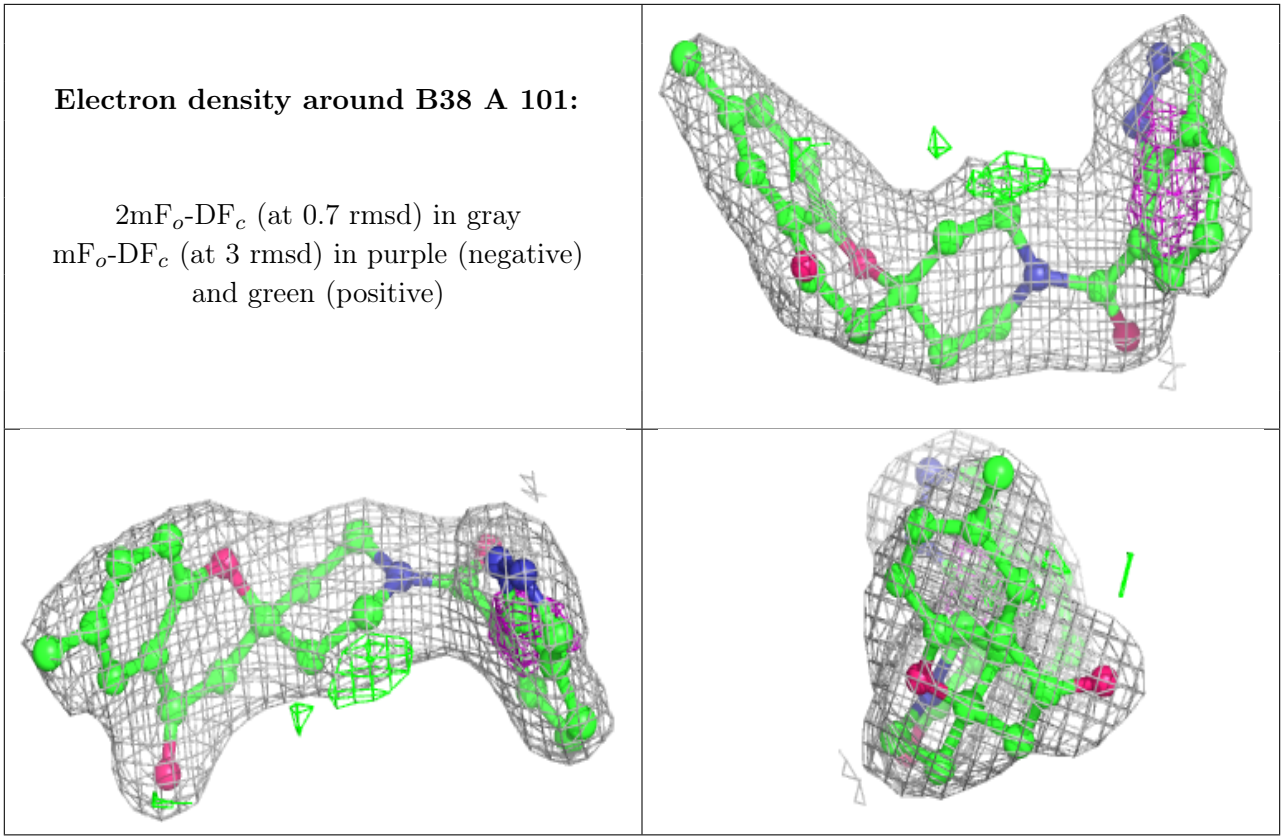






Electron density around B38 A 101:

$2mF_o$-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.