



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:54 PM GMT

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

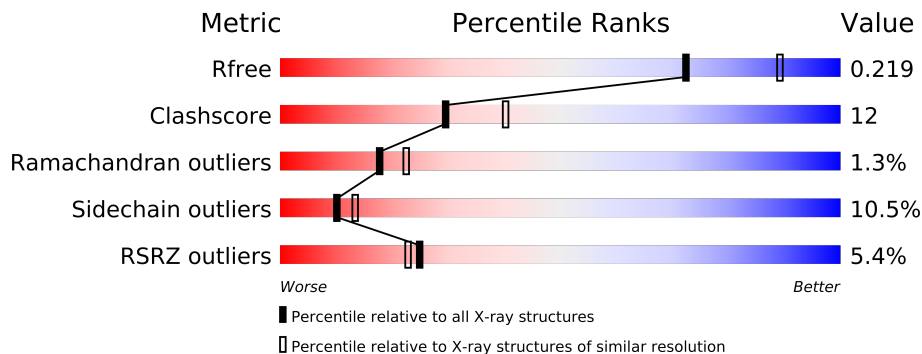
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2989 (2.48-2.40)
Clashscore	79885	3698 (2.48-2.40)
Ramachandran outliers	78287	3639 (2.48-2.40)
Sidechain outliers	78261	3640 (2.48-2.40)
RSRZ outliers	66119	2993 (2.48-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	769	
1	B	769	
1	C	769	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	A	2	-	X
2	SO4	C	3	-	X
3	B38	B	102[A]	-	X
3	B38	B	102[B]	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18770 atoms, of which 0 are hydrogen and 0 are deuterium.

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:

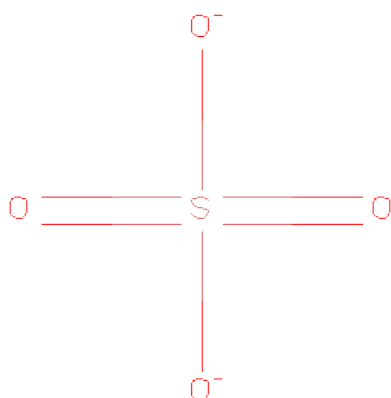
Chain	Residue	Modelled	Actual	Comment	Reference
A	1473	MET	-	EXPRESSION TAG	UNP Q00955
A	1474	ALA	-	EXPRESSION TAG	UNP Q00955
A	1475	SER	-	EXPRESSION TAG	UNP Q00955
A	2234	LEU	-	EXPRESSION TAG	UNP Q00955
A	2235	GLU	-	EXPRESSION TAG	UNP Q00955
A	2236	HIS	-	EXPRESSION TAG	UNP Q00955
A	2237	HIS	-	EXPRESSION 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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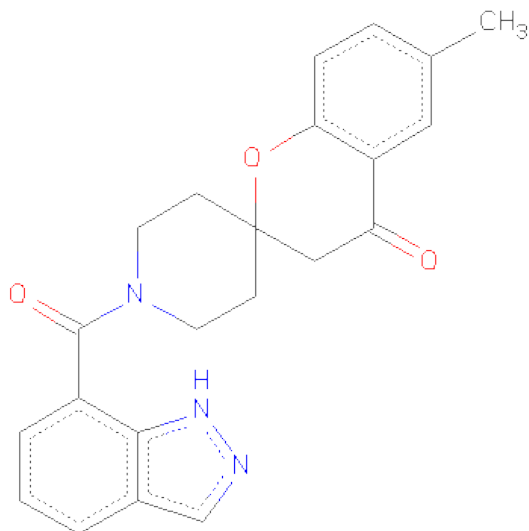
Chain	Residue	Modelled	Actual	Comment	Reference
C	1474	ALA	-	EXPRESSION TAG	UNP Q00955
C	1475	SER	-	EXPRESSION TAG	UNP Q00955
C	2234	LEU	-	EXPRESSION TAG	UNP Q00955
C	2235	GLU	-	EXPRESSION TAG	UNP Q00955
C	2236	HIS	-	EXPRESSION TAG	UNP Q00955
C	2237	HIS	-	EXPRESSION TAG	UNP Q00955
C	2238	HIS	-	EXPRESSION 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: O₄S).



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

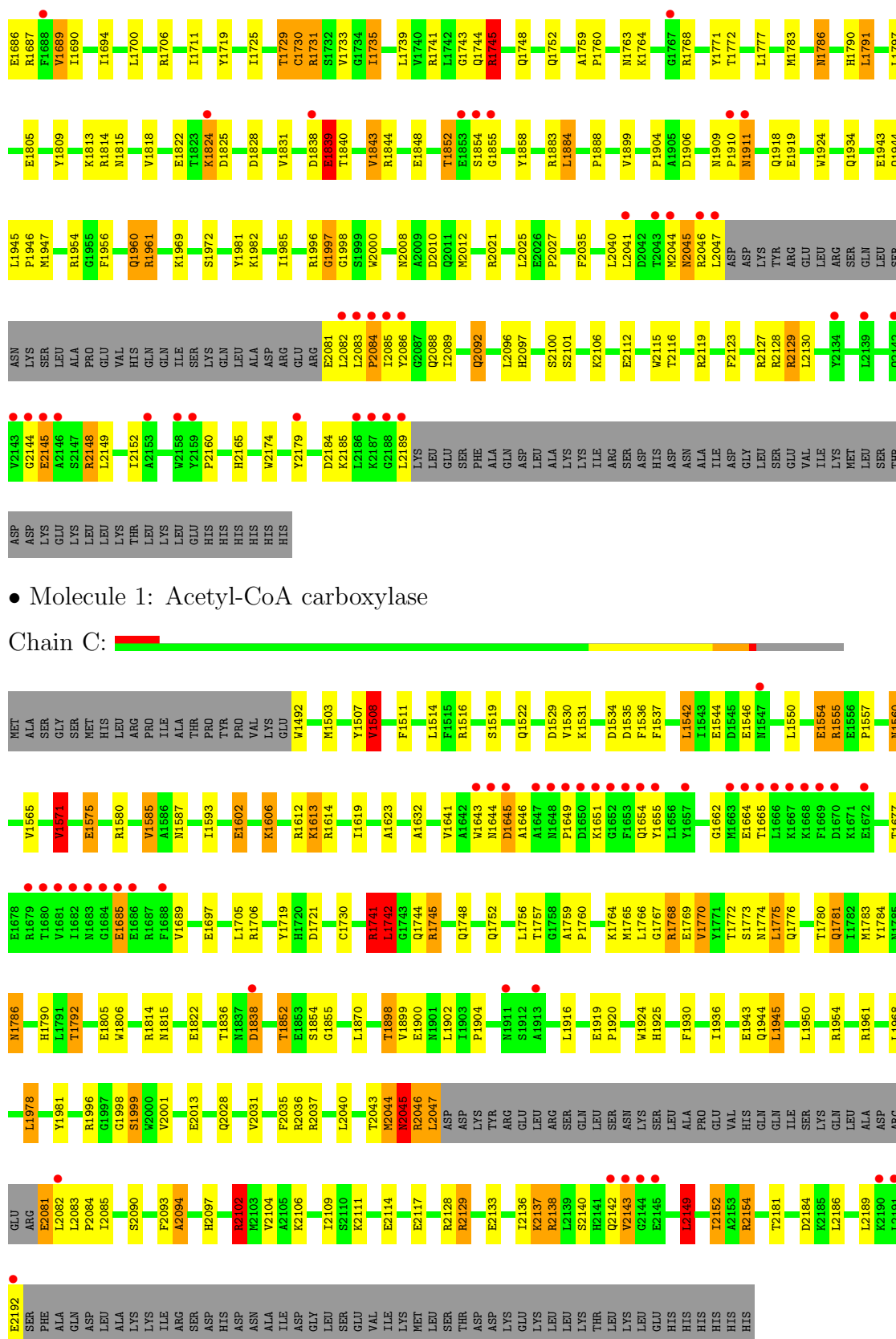
- Molecule 3 is 1'-(1H-INDAZOL-7-YLCARBONYL)-6-METHYLSPIRO[CHROMENE-2,4'-PIPERIDIN]-4(3H)-ONE (three-letter code: B38) (formula: C₂₂H₂₁N₃O₃).



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

- Molecule 4 is water.

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



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.160 , 0.218 0.169 , 0.219	Depositor DCC
R_{free} test set	15829 reflections (11.04%)	DCC
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 , 53.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 159203 reflections	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.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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(°)	Ideal(°)
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(°)	Ideal(°)
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(°)	Ideal(°)
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(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	28	0	21	1	0
4	A	861	0	0	58	9
4	B	762	0	0	60	0
4	C	780	0	0	60	4
All	All	18770	0	16124	396	9

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (396) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:C:1706:ARG:HD3	4:C:743:HOH:O	1.65	0.97
1:A:1772:THR:H	1:A:1776:GLN:HE22	1.11	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:OG1	1:B:1729:THR:O	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	Distance(Å)	Clash(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
1:B:2089:ILE:HD13	1:C:1641:VAL:HG21	1.77	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:HD22	1:A:1560:ASN:H	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:1729:THR:O	1:A:1729:THR:OG1	2.14	0.64
1:A:1683:ASN:HD22	1:A:1684:GLY:H	1.45	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:B:1843:VAL:HB	4:B:1205:HOH:O	2.00	0.60
1:B:1763:ASN:HD21	1:B:1771:TYR:H	1.49	0.60
1:A:2080:ARG:O	4:A:1172:HOH:O	2.16	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:HD3	1:A:2055:ARG:N	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:C	1:B:1545:ASP:OD2	2.42	0.57
1:B:1602:GLU:OE2	1:B:1606:LYS:CE	2.53	0.57
1:C:1998:GLY:HA2	1:C:2001:VAL:HG13	1.87	0.57
1:B:1839:GLU:HG2	4:B:2340:HOH:O	2.03	0.57
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.53	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1772:THR:HB	4:A:2340:HOH:O	2.05	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:B:1748:GLN:HE22	1:B:1783:MET:HB2	1.69	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:A:1499:LYS:NZ	4:A:2287:HOH:O	2.38	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:2081:GLU:N	4:C:995:HOH:O	2.40	0.55
1:C:1537:PHE:HD2	1:C:1571:VAL:HG13	1.70	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:C:1492:TRP:CA	4:C:1063:HOH:O	2.50	0.54
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: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:B:2184:ASP:HB2	4:B:2333:HOH:O	2.08	0.54
1:A:1961:ARG:HD3	4:A:1436:HOH:O	2.07	0.54
1:A:2054:LEU:C	1:A:2055:ARG:HD3	2.28	0.54
1:C:1529:ASP:HB2	4:C:2293:HOH:O	2.08	0.54
1:B:2045:ASN:HD22	1:B:2045:ASN:N	2.05	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:2111:LYS:HD3	4:C:2488:HOH:O	2.07	0.53
1:C:1790:HIS:HA	1:C:1870:LEU:HD23	1.90	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:C:2046:ARG:HG3	4:C:2425:HOH:O	2.09	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:A:1726:THR:HG21	1:A:1740:VAL:HG22	1.91	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: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:A:1592:LYS:NZ	4:A:968:HOH:O	2.42	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:C:1503:MET:CE	4:C:1065:HOH:O	2.59	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:2081:GLU:N	4:C:2426:HOH:O	2.43	0.50
1:B:1652:GLY:HA2	1:C:2085:ILE:HD11	1.93	0.50
1:C:1662:GLY:HA3	4:C:1148:HOH:O	2.10	0.50
1:B:1960:GLN:CD	4:B:605:HOH:O	2.41	0.50
1:A:1812:ALA:HB3	1:A:1816:MET:HE1	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:1981:TYR:CG	1:B:1985:ILE:HD11	2.47	0.49
1:A:1895:GLU:OE1	1:A:1897:ARG:HD3	2.12	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:C:1773:SER:H	1:C:1776:GLN:HE21	1.57	0.49
1:A:2137:LYS:CE	4:A:394:HOH:O	2.60	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:C:1780:THR:O	1:C:1784:TYR:HB3	2.13	0.48
1:B:1665:THR:O	1:B:1669:PHE:HD1	1.95	0.48
1:A:1576:TYR:CZ	1:A:1812:ALA:HB2	2.48	0.48
1:A:1900:GLU:HB3	1:A:1916:LEU:HD11	1.94	0.48
1:A:1662:GLY:HA3	4:A:2552:HOH:O	2.12	0.48
1:A:1731:ARG:HD3	4:A:2350:HOH:O	2.14	0.48
1:C:2097:HIS:O	1:C:2102:ARG:HG3	2.13	0.48
1:A:1812:ALA:HB3	1:A:1816:MET:CE	2.43	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:A:1643:TRP:CZ3	1:A:1649:PRO:HB3	2.49	0.48
1:B:1649:PRO:C	1:B:1651:LYS:N	2.67	0.48
1:B:2129:ARG:NE	4:B:959:HOH:O	2.17	0.47
1:B:2116:THR:HB	4:B:326:HOH:O	2.14	0.47
1:A:1575:GLU:CG	4:A:960:HOH:O	2.61	0.47
1:B:1480:LEU:N	4:B:1457:HOH:O	2.46	0.47
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:1794:VAL:HG21	4:A:2249:HOH:O	2.14	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1677:THR:HA	1:C:1689:VAL:O	2.14	0.47
1:C:1781:GLN:NE2	2:C:3:SO4:O1	2.41	0.47
1:A:1790:HIS:HD2	4:A:61:HOH:O	1.98	0.47
1:C:2047:LEU:CD2	4:C:2422:HOH:O	2.62	0.47
1:B:1676:LEU:HG	1:B:1694:ILE:HD11	1.97	0.47
1:C:2093:PHE:HA	4:C:2427:HOH:O	2.15	0.47
1:B:1657:TYR:CD2	1:B:1687:ARG:HG2	2.50	0.47
1:B:2083:LEU:HB2	1:B:2084:PRO:HD3	1.95	0.47
1:C:1904:PRO:HG3	4:C:2503:HOH:O	2.15	0.46
1:A:2008:ASN:C	1:A:2008:ASN:HD22	2.17	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:2047:LEU:HD21	1:A:2079:GLU:CG	2.45	0.46
1:C:1697:GLU:HG3	4:C:2446:HOH:O	2.14	0.46
1:B:1483:ILE:O	1:B:1484:ALA:HB3	2.16	0.46
1:A:1545:ASP:C	1:A:1545:ASP:OD2	2.53	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:B:1575:GLU:HB3	4:B:1430:HOH:O	2.16	0.46
1:A:1741:ARG:HH22	1:A:1934:GLN:NE2	2.13	0.46
1:B:2101:SER:N	4:B:931:HOH:O	2.48	0.46
1:A:1527:SER:O	1:A:1530:VAL:HG22	2.15	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:1820:ILE:HD12	4:A:2539:HOH:O	2.17	0.45
1:A:1480:LEU:HA	1:A:1492:TRP:CD1	2.51	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:1819:PRO:O	1:A:1883[B]:ARG:NH1	2.40	0.45
1:B:1730:CYS:CA	1:B:1752:GLN:HE21	2.22	0.45
1:A:1624:ASN:HD22	1:A:1626:GLY:H	1.63	0.45
1:C:1593:ILE:HG22	4:C:1065:HOH:O	2.16	0.45
1:A:1981:TYR:CG	1:A:1985:ILE:HD11	2.51	0.45
1:B:1815:ASN:H	1:B:1944:GLN:NE2	2.01	0.45
1:C:1936:ILE:HD13	1:C:1978:LEU:HD13	1.99	0.45
1:C:1898:THR:HG22	4:C:225:HOH:O	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2137:LYS:HE2	4:A:394:HOH:O	2.16	0.45
1:A:1836:THR:OG1	1:A:1839:GLU:HG3	2.16	0.45
1:A:1745:ARG:NH2	4:A:243:HOH:O	2.23	0.45
1:C:1554:GLU:OE2	4:C:2498:HOH:O	2.21	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:1744:GLN:O	1:C:1790:HIS:CE1	2.70	0.45
1:A:1679:ARG:HG2	4:A:2577:HOH:O	2.17	0.45
1:C:1900:GLU:HB3	1:C:1916:LEU:HD11	1.99	0.45
1:B:1719:TYR:CE2	1:B:1744:GLN:HG3	2.52	0.45
1:C:2093:PHE:CA	4:C:2427:HOH:O	2.64	0.44
1:B:1690:ILE:HG12	4:B:2285:HOH:O	2.18	0.44
1:B:1602:GLU:OE2	1:B:1606:LYS:HE2	2.16	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:A:1899:VAL:HB	1:A:1919:GLU:HB2	1.99	0.44
1:B:1822:GLU:N	4:B:1168:HOH:O	2.49	0.44
1:C:2104:VAL:HG23	1:C:2109:ILE:HD11	1.99	0.44
1:B:2097:HIS:CE1	1:C:1632:ALA:H	2.26	0.44
1:B:1831:VAL:HG11	1:B:2115:TRP:CZ2	2.52	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:2134:TYR:CD2	1:A:2135:LEU:HD13	2.51	0.44
1:A:1854:SER:OG	4:A:1269:HOH:O	2.21	0.44
1:B:1852:THR:HG22	1:B:1855:GLY:O	2.17	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:A:1756:LEU:HA	1:A:1756:LEU:HD12	1.94	0.44
1:C:2140:SER:C	1:C:2142:GLN:H	2.21	0.44
1:C:2081:GLU:O	1:C:2081:GLU:OE1	2.36	0.43
1:B:1711:ILE:HD11	1:B:1735:ILE:HD12	1.99	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
1:C:1530:VAL:CG2	4:C:1191:HOH:O	2.63	0.43
1:C:1519:SER:O	1:C:1522:GLN:HB2	2.17	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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1549:GLU:CD	1:A:1606:LYS:HZ1	2.22	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:HG23	1:B:1682:ILE:O	2.19	0.42
1:C:2149:LEU:HD13	1:C:2149:LEU:C	2.40	0.42
1:C:1619:ILE:N	1:C:1619:ILE:HD12	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:B:2179:TYR:HE2	4:B:1279:HOH:O	2.02	0.42
1:A:1781:GLN:HB2	1:A:1781:GLN:HE21	1.53	0.42
1:C:1619:ILE:CD1	1:C:1619:ILE:N	2.83	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:B:2101:SER:CA	4:B:931:HOH:O	2.59	0.42
1:B:1480:LEU:HA	1:B:1492:TRP:CD1	2.54	0.42
1:A:2041:LEU:HD23	1:A:2044:MET:HE3	2.01	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:B:2010:ASP:CG	1:B:2148:ARG:HD2	2.40	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:1818:VAL:HB	1:B:1888:PRO:HG2	2.02	0.42
1:C:2044:MET:C	1:C:2046:ARG:H	2.22	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:B:1522:GLN:HG2	4:B:2246:HOH:O	2.19	0.42
1:A:2048:ASP:HA	4:A:892:HOH:O	2.20	0.42
1:A:1481:ARG:HB2	4:A:2526:HOH:O	2.20	0.42
1:A:2164:ASP:H	1:A:2170:GLN:NE2	2.18	0.42
1:A:1575:GLU:HB3	1:A:1819:PRO:HB2	2.01	0.41
1:C:1898:THR:HB	1:C:1920:PRO:HA	2.02	0.41
1:B:1513:GLU:OE2	1:B:1516:ARG:HD3	2.20	0.41
1:C:1719:TYR:CE2	1:C:1744:GLN:HG3	2.55	0.41
1:B:1516:ARG:NH2	4:B:2436:HOH:O	2.53	0.41
1:A:1827:TRP:HZ3	1:A:2120:ARG:HG2	1.84	0.41
1:C:1790:HIS:HD2	4:C:37:HOH:O	2.02	0.41
1:C:1748:GLN:HE22	1:C:1783:MET:HB2	1.85	0.41
1:A:1813:LYS:HG2	1:A:1816:MET:HE3	2.03	0.41
1:B:1505:THR:HB	1:B:1730:CYS:HB2	2.03	0.41
1:A:2152:ILE:HG21	4:A:2564:HOH:O	2.20	0.41
1:B:2106:LYS:HD2	1:B:2106:LYS:HA	1.88	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1675:VAL:HG22	1:A:1690:ILE:HG23	2.02	0.41
1:C:2181:THR:O	1:C:2184:ASP:HB2	2.21	0.41
1:A:1657:TYR:CE2	1:A:1687:ARG:HD2	2.55	0.41
1:B:1790:HIS:O	1:B:1791:LEU:HD13	2.20	0.41
1:A:1675:VAL:HG13	1:A:1677:THR:HG23	2.02	0.41
1:A:1774:ASN:HA	1:A:1774:ASN:HD22	1.66	0.41
1:A:1892:ILE:HD12	1:A:1947:MET:HE1	2.03	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:B:1633:GLU:HA	1:B:1633:GLU:OE1	2.20	0.41
1:A:1879:VAL:HG13	1:A:1931:LYS:HE2	2.03	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: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:B:1677:THR:HA	1:B:1689:VAL:O	2.21	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:B:1690:ILE:CG2	4:B:2285:HOH:O	2.53	0.40
1:C:1852:THR:HG21	4:C:604:HOH:O	2.20	0.40
1:A:2011:GLN:O	1:A:2129:ARG:NH2	2.51	0.40
1:B:1745:ARG:HD3	1:B:1943:GLU:OE2	2.21	0.40
1:B:1497:ARG:HD3	1:B:1510:ASP:OD1	2.21	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	Distance(Å)	Clash(Å)
4:A:81:HOH:O	4:A:2568:HOH:O[2_555]	1.72	0.48
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

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	690/769 (90%)	645 (94%)	38 (6%)	7 (1%)	22	30
1	B	673/769 (88%)	622 (92%)	42 (6%)	9 (1%)	18	22
1	C	664/769 (86%)	620 (93%)	34 (5%)	10 (2%)	15	19
All	All	2027/2307 (88%)	1887 (93%)	114 (6%)	26 (1%)	18	22

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
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

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Mol	Chain	Res	Type
1	B	2144	GLY

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	589/658 (90%)	536 (91%)	53 (9%)	14	19
1	B	574/658 (87%)	508 (88%)	66 (12%)	8	10
1	C	566/658 (86%)	504 (89%)	62 (11%)	9	11
All	All	1729/1974 (88%)	1548 (90%)	181 (10%)	10	13

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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

Some 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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	A	101	-	32,32,32	2.46	11 (34%)	46,48,48	3.31	12 (26%)
2	SO4	A	2	-	4,4,4	0.48	0	6,6,6	0.71	0
3	B38	B	102[A]	-	12,12,32	1.69	3 (25%)	11,16,48	6.61	3 (27%)
3	B38	B	102[B]	-	12,12,32	1.50	2 (16%)	11,16,48	6.39	2 (18%)
2	SO4	C	1	-	4,4,4	0.18	0	6,6,6	0.59	0
3	B38	C	100	-	32,32,32	2.49	13 (40%)	46,48,48	3.22	9 (19%)
2	SO4	C	3	-	4,4,4	0.21	0	6,6,6	0.35	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	A	101	-	-	0/8/34/34	0/1/5/5
2	SO4	A	2	-	-	0/0/0/0	0/0/0/0
3	B38	B	102[A]	-	-	0/0/2/34	0/0/2/5
3	B38	B	102[B]	-	-	0/0/2/34	0/0/2/5
2	SO4	C	1	-	-	0/0/0/0	0/0/0/0
3	B38	C	100	-	-	0/8/34/34	0/1/5/5
2	SO4	C	3	-	-	0/0/0/0	0/0/0/0

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	100	B38	C11-C14	6.31	1.50	1.38
3	C	100	B38	C13-C15	6.14	1.50	1.38
3	A	101	B38	C11-C14	6.08	1.50	1.38
3	A	101	B38	C13-C10	-5.00	1.31	1.39
3	A	101	B38	C10-C6	4.45	1.49	1.40
3	C	100	B38	C10-C6	4.42	1.49	1.40
3	A	101	B38	C13-C15	4.37	1.47	1.38
3	C	100	B38	C13-C10	-4.27	1.32	1.39
3	A	101	B38	C11-C6	-4.01	1.31	1.39
3	C	100	B38	O2-C6	-3.91	1.31	1.37
3	A	101	B38	C5-C1	3.71	1.57	1.52
3	B	102[A]	B38	C20-C26	3.58	1.53	1.41
3	A	101	B38	O2-C6	-3.37	1.32	1.37
3	C	100	B38	C11-C6	-3.20	1.32	1.39
3	B	102[B]	B38	N23-N24	-2.88	1.32	1.37
3	B	102[B]	B38	C20-C26	2.68	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	102[A]	B38	N23-N24	-2.66	1.32	1.37
3	A	101	B38	C4-C1	2.46	1.55	1.52
3	C	100	B38	C4-C1	2.44	1.55	1.52
3	C	100	B38	C20-C26	2.42	1.53	1.50
3	C	100	B38	C4-C8	2.25	1.55	1.52
3	A	101	B38	C19-C20	2.24	1.41	1.37
3	B	102[A]	B38	O28-C26	2.22	1.24	1.17
3	C	100	B38	C19-C20	2.20	1.41	1.37
3	C	100	B38	O12-C7	2.17	1.26	1.22
3	A	101	B38	C4-C8	2.11	1.55	1.52
3	C	100	B38	C26-N27	2.07	1.39	1.34
3	A	101	B38	O12-C7	2.05	1.26	1.22
3	C	100	B38	C5-C1	2.02	1.55	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	102[A]	B38	C25-N24-N23	21.55	110.31	104.27
3	B	102[B]	B38	C25-N24-N23	21.01	110.16	104.27
3	A	101	B38	C25-N24-N23	19.06	109.61	104.27
3	C	100	B38	C25-N24-N23	18.43	109.44	104.27
3	C	100	B38	C4-C1-C3	-6.08	106.26	111.92
3	A	101	B38	O2-C1-C5	5.50	116.97	106.22
3	A	101	B38	C4-C1-C3	-3.91	108.28	111.92
3	A	101	B38	C9-C5-C1	3.77	115.47	112.38
3	C	100	B38	O2-C1-C5	3.48	113.04	106.22
3	A	101	B38	C5-C1-C3	-3.30	108.84	111.92
3	C	100	B38	C4-C8-N27	-3.23	106.35	110.94
3	C	100	B38	C3-C7-C10	-3.10	111.51	116.56
3	C	100	B38	C5-C1-C4	-2.86	105.77	109.54
3	A	101	B38	C13-C10-C6	2.77	122.29	118.20
3	A	101	B38	C3-C7-C10	-2.76	112.05	116.56
3	A	101	B38	C20-C26-N27	2.74	121.63	118.21
3	A	101	B38	C1-O2-C6	-2.57	114.69	117.78
3	C	100	B38	C6-C10-C7	-2.52	118.41	119.89
3	A	101	B38	O28-C26-C20	-2.42	116.80	121.20
3	A	101	B38	O2-C1-C3	-2.37	106.84	109.35
3	B	102[A]	B38	C19-C20-C22	-2.32	117.49	119.99
3	B	102[A]	B38	C21-C25-N24	-2.19	107.32	113.99
3	B	102[B]	B38	C21-C25-N24	-2.15	107.44	113.99
3	C	100	B38	C25-C21-C22	2.10	106.58	104.80
3	A	101	B38	C21-C25-N24	-2.10	107.59	113.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	100	B38	O2-C6-C10	2.08	124.44	121.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	693/769 (90%)	-0.15	29 (4%)	35	33	30, 45, 98, 125	0
1	B	677/769 (88%)	0.00	38 (5%)	24	22	29, 49, 101, 125	0
1	C	668/769 (86%)	-0.07	43 (6%)	19	17	29, 48, 109, 131	0
All	All	2038/2307 (88%)	-0.07	110 (5%)	25	23	29, 47, 102, 131	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2194	PHE	6.7
1	B	2082	LEU	6.3
1	C	1644	ASN	5.7
1	B	2086	TYR	5.3
1	C	1669	PHE	5.2
1	C	2143	VAL	5.1
1	B	2143	VAL	5.0
1	C	1681	VAL	4.7
1	B	2083	LEU	4.6
1	B	2085	ILE	4.4
1	C	1647	ALA	4.4
1	A	2144	GLY	4.4
1	B	2084	PRO	4.4
1	A	2195	ALA	4.2
1	B	2144	GLY	4.2
1	C	1685	GLU	4.2
1	B	2044	MET	4.0
1	A	2143	VAL	3.8
1	C	1655	TYR	3.8
1	B	2142	GLN	3.7
1	C	1682	ILE	3.6
1	C	1680	THR	3.6
1	C	1645	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	2142	GLN	3.5
1	C	1650	ASP	3.5
1	A	2052	ARG	3.4
1	B	2187	LYS	3.4
1	B	2047	LEU	3.4
1	A	2191	LEU	3.4
1	B	2041	LEU	3.4
1	C	1657	TYR	3.4
1	C	1666	LEU	3.4
1	C	1665	THR	3.4
1	A	1682	ILE	3.2
1	C	2144	GLY	3.2
1	C	2190	LYS	3.2
1	A	2145	GLU	3.2
1	B	1681	VAL	3.2
1	B	2145	GLU	3.1
1	C	1651	LYS	3.1
1	C	2192	GLU	3.1
1	B	2186	LEU	3.0
1	C	1668	LYS	3.0
1	B	1854	SER	3.0
1	A	1679	ARG	3.0
1	A	2051	TYR	3.0
1	C	2082	LEU	2.9
1	C	1649	PRO	2.9
1	C	1663	MET	2.9
1	C	1652	GLY	2.8
1	C	1653	PHE	2.8
1	B	2046	ARG	2.7
1	B	2179	TYR	2.7
1	B	2158	TRP	2.7
1	C	1688	PHE	2.7
1	C	1643	TRP	2.7
1	A	2193	SER	2.6
1	B	1767	GLY	2.6
1	A	2049	ASP	2.5
1	A	2083	LEU	2.5
1	A	2192	GLU	2.5
1	B	2189	LEU	2.5
1	B	1838	ASP	2.5
1	C	1913	ALA	2.5
1	A	1685	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1855	GLY	2.5
1	B	1853	GLU	2.4
1	B	1855	GLY	2.4
1	A	1681	VAL	2.4
1	C	2191	LEU	2.4
1	A	1684	GLY	2.4
1	B	2188	GLY	2.4
1	C	1686	GLU	2.4
1	A	1651	LYS	2.4
1	C	1547	ASN	2.4
1	A	2189	LEU	2.4
1	A	1911	ASN	2.3
1	A	1669	PHE	2.3
1	A	1853	GLU	2.3
1	B	1911	ASN	2.3
1	C	1683	ASN	2.3
1	C	1679	ARG	2.3
1	C	1670	ASP	2.3
1	A	2190	LYS	2.3
1	A	1838	ASP	2.3
1	B	2134	TYR	2.3
1	A	2079	GLU	2.3
1	B	1648	ASN	2.3
1	B	1688	PHE	2.2
1	B	1682	ILE	2.2
1	B	2043	THR	2.2
1	C	1667	LYS	2.2
1	C	2142	GLN	2.2
1	B	1647	ALA	2.2
1	C	1911	ASN	2.1
1	B	2146	ALA	2.1
1	B	2153	ALA	2.1
1	A	1644	ASN	2.1
1	C	1672	GLU	2.1
1	C	1654	GLN	2.1
1	A	1683	ASN	2.1
1	C	2145	GLU	2.1
1	B	2159	TYR	2.1
1	C	1664	GLU	2.1
1	B	2139	LEU	2.1
1	C	1648	ASN	2.0
1	B	1824	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	1838	ASP	2.0
1	C	1684	GLY	2.0
1	B	1910	PRO	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	C	3	5/5	0.37	9.51	120,120,121,122	0
2	SO4	A	2	5/5	0.28	6.26	85,86,88,91	0
3	B38	B	102[B]	11/28	0.26	3.52	89,90,91,91	11
3	B38	B	102[A]	11/28	0.26	3.52	87,87,88,88	11
3	B38	C	100	28/28	0.16	1.07	67,78,82,83	0
2	SO4	C	1	5/5	0.20	1.07	81,82,83,84	0
3	B38	A	101	28/28	0.15	0.52	71,80,90,91	0

6.5 Other polymers ⓘ

There are no such residues in this entry.