



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 04:22 AM GMT

PDB ID : 3K8X  
Title : Crystal structure of the carboxyltransferase domain of acetyl-coenzyme A carboxylase in complex with tepraloxydim  
Authors : Xiang, S.; Callaghan, M.M.; Watson, K.G.; Tong, L.  
Deposited on : 2009-10-15  
Resolution : 2.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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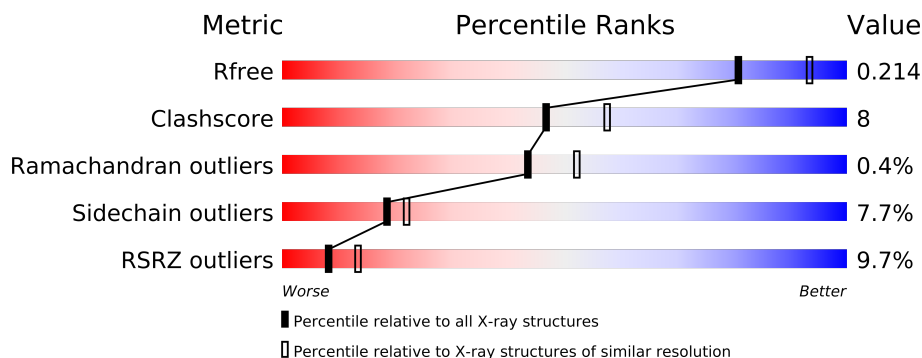
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	758	
1	B	758	
1	C	758	

## 2 Entry composition i

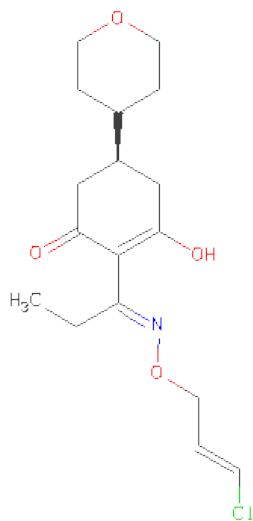
There are 3 unique types of molecules in this entry. The entry contains 17693 atoms, of which 0 are hydrogen and 0 are deuterium.

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	688	Total	C	N	O	S	0	0	0
			5491	3500	944	1028	19			
1	B	682	Total	C	N	O	S	0	0	0
			5443	3468	937	1019	19			
1	C	675	Total	C	N	O	S	0	0	0
			5387	3428	927	1013	19			

- Molecule 2 is (5S)-2-[(1E)-N-{[(2E)-3-CHLOROPROP-2-EN-1-YL]OXY}PROPANIMIDOYL]-3-HYDROXY-5-(TETRAHYDRO-2H-PYRAN-4-YL)CYCLOHEX-2-EN-1-ONE (three-letter code: B89) (formula: C<sub>17</sub>H<sub>24</sub>ClNO<sub>4</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			23	17	1	1	4		
2	B	1	Total	C	Cl	N	O	0	0
			23	17	1	1	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Cl	N	O	0	0
			23	17	1	1	4		

- Molecule 3 is water.

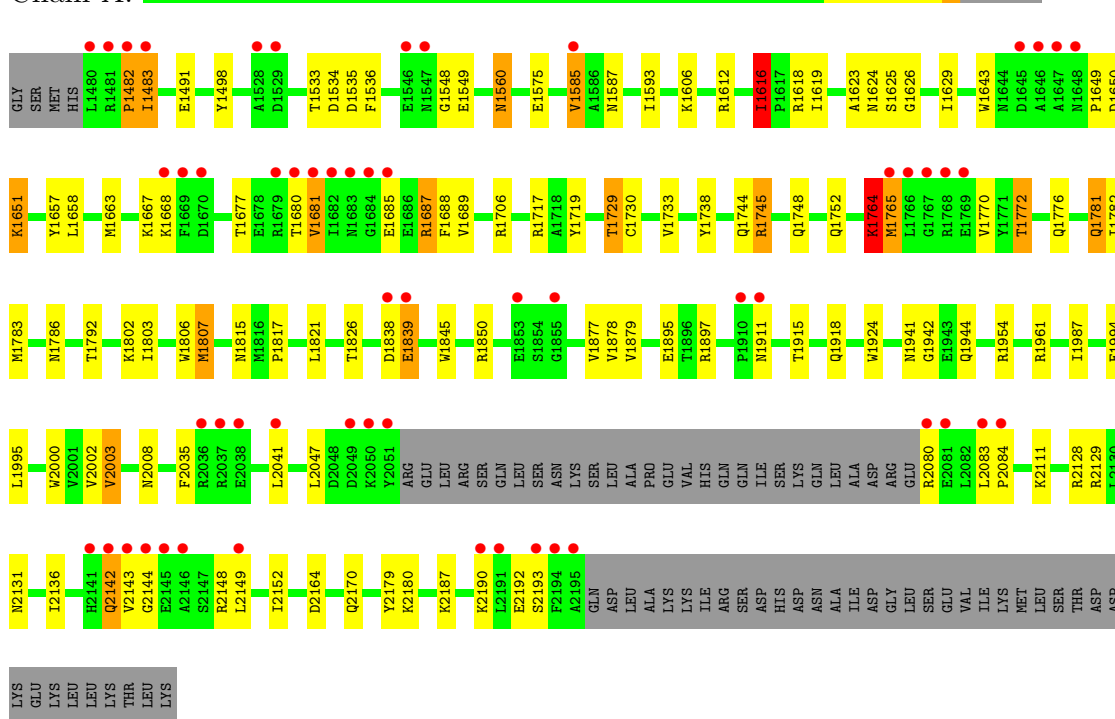
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	483	Total	O	0	0
			483	483		
3	B	415	Total	O	0	0
			415	415		
3	C	405	Total	O	0	0
			405	405		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

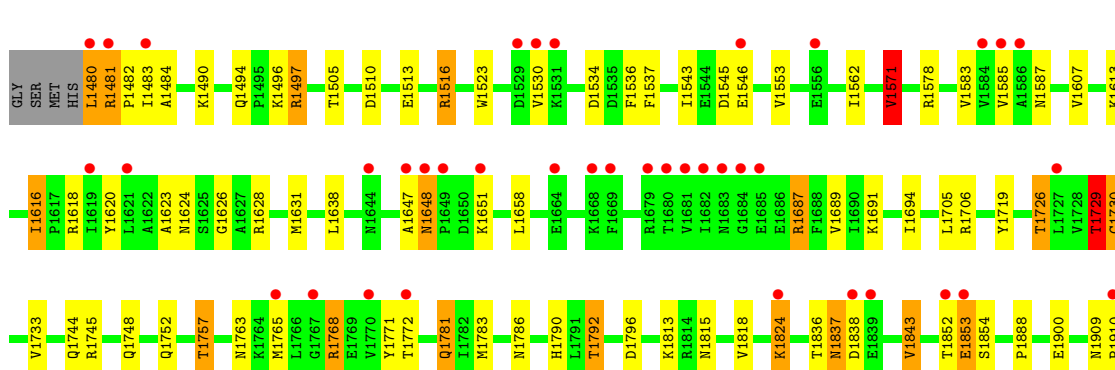
- Molecule 1: Acetyl-CoA carboxylase

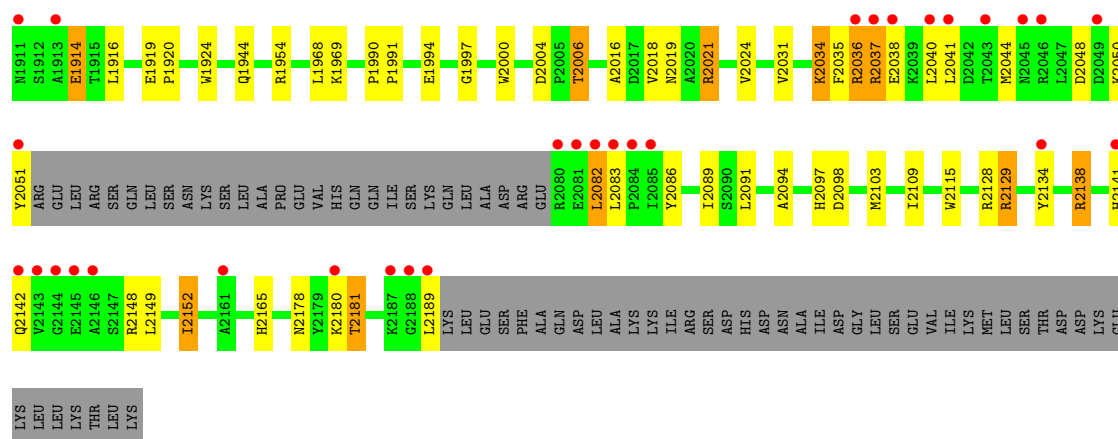
Chain A:



- Molecule 1: Acetyl-CoA carboxylase

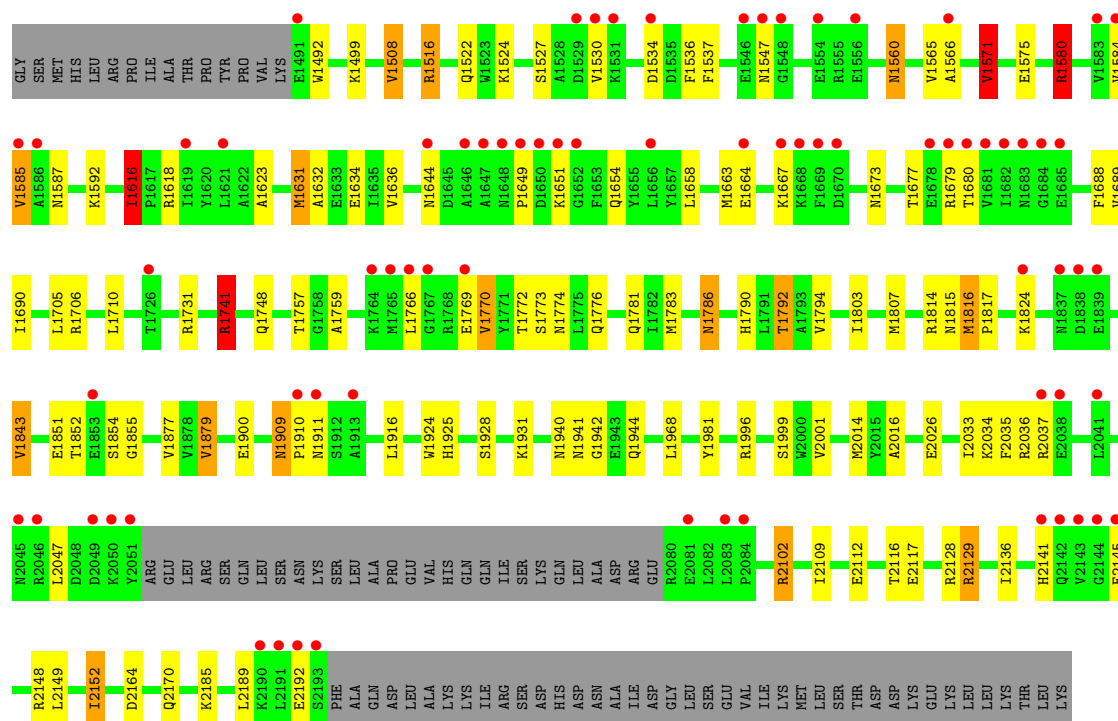
Chain B:





• Molecule 1: Acetyl-CoA carboxylase

Chain C:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	247.30Å 124.80Å 145.37Å 90.00° 94.32° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 29.93 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (30.00-2.30) 98.8 (29.93-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.24 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.187 , 0.221 0.182 , 0.214	Depositor DCC
$R_{free}$ test set	9659 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.1	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 40.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 192187 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17693	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: B89

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.73	2/5614 (0.0%)	0.82	16/7605 (0.2%)
1	B	0.70	0/5565	0.79	15/7540 (0.2%)
1	C	0.70	1/5505 (0.0%)	0.78	14/7454 (0.2%)
All	All	0.71	3/16684 (0.0%)	0.80	45/22599 (0.2%)

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	1
1	B	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1942	GLY	N-CA	7.12	1.56	1.46
1	A	1786	ASN	CB-CG	-6.26	1.36	1.51
1	C	1942	GLY	N-CA	6.21	1.55	1.46

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1745	ARG	NE-CZ-NH2	-15.32	112.64	120.30
1	A	1717	ARG	NE-CZ-NH2	-14.52	113.04	120.30
1	A	1745	ARG	NE-CZ-NH2	-12.81	113.89	120.30
1	A	1941	ASN	C-N-CA	-10.64	99.95	122.30
1	C	1741	ARG	NE-CZ-NH1	10.34	125.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1745	ARG	NE-CZ-NH1	9.49	125.04	120.30
1	C	1941	ASN	C-N-CA	-8.88	103.64	122.30
1	C	1741	ARG	NE-CZ-NH2	-8.80	115.90	120.30
1	B	1497	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	B	2129	ARG	NE-CZ-NH2	-8.07	116.27	120.30
1	A	1717	ARG	NE-CZ-NH1	7.97	124.29	120.30
1	A	1585	VAL	CB-CA-C	-7.28	97.57	111.40
1	B	2129	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	B	1571	VAL	CB-CA-C	-7.13	97.86	111.40
1	A	1786	ASN	CB-CA-C	-6.96	96.48	110.40
1	B	1786	ASN	CB-CA-C	-6.93	96.54	110.40
1	C	2102	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	B	1497	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	B	1745	ARG	CG-CD-NE	-6.58	97.99	111.80
1	A	1717	ARG	CG-CD-NE	-6.55	98.05	111.80
1	C	2102	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	1745	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	C	1585	VAL	CB-CA-C	-6.23	99.56	111.40
1	C	1843	VAL	CB-CA-C	-5.97	100.05	111.40
1	C	2129	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	C	1571	VAL	CB-CA-C	-5.90	100.18	111.40
1	C	1928	SER	N-CA-CB	-5.76	101.86	110.50
1	B	1516	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	C	1814	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	2129	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	B	1843	VAL	CB-CA-C	-5.49	100.97	111.40
1	A	1941	ASN	O-C-N	-5.47	113.90	123.20
1	B	1706	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	1729	THR	CB-CA-C	-5.42	96.97	111.60
1	C	1616	ILE	CG1-CB-CG2	5.40	123.28	111.40
1	B	1571	VAL	CG1-CB-CG2	5.36	119.48	110.90
1	A	1745	ARG	CG-CD-NE	-5.34	100.59	111.80
1	A	1616	ILE	CA-CB-CG2	5.27	121.44	110.90
1	A	1729	THR	N-CA-C	5.27	125.22	111.00
1	C	1508	VAL	CB-CA-C	-5.25	101.43	111.40
1	A	1706	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	B	1628	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	C	1580	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	1961	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	1612	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1482	PRO	Peptide
1	B	1481	ARG	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	5491	0	5431	72	0
1	B	5443	0	5382	127	0
1	C	5387	0	5318	77	0
2	A	23	0	24	1	0
2	B	23	0	24	3	0
2	C	23	0	24	2	0
3	A	483	0	0	9	1
3	B	415	0	0	16	0
3	C	405	0	0	20	0
All	All	17693	0	16203	264	1

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 8.

All (264) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1482:PRO:HB2	3:A:1267:HOH:O	1.40	1.15
1:B:2024:VAL:HG13	3:C:266:HOH:O	1.54	1.06
1:B:2016:ALA:HB2	1:B:2103:MET:HE3	1.46	0.97
1:A:1772:THR:H	1:A:1776:GLN:HE22	1.06	0.94
1:B:1815:ASN:H	1:B:1944:GLN:HE22	1.09	0.93
1:B:1757:THR:HG21	3:C:1242:HOH:O	1.67	0.93
1:B:1494:GLN:HE21	1:B:1496:LYS:H	1.16	0.93
1:B:2138:ARG:HH11	1:B:2138:ARG:HG2	1.36	0.91
1:B:1513:GLU:OE2	1:B:1516:ARG:NH1	2.04	0.91
1:C:2129:ARG:HD2	3:C:1240:HOH:O	1.70	0.91
1:C:1772:THR:H	1:C:1776:GLN:HE22	1.18	0.89
1:B:1792:THR:HG22	3:B:195:HOH:O	1.72	0.89

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2016:ALA:CB	1:B:2103:MET:CE	2.50	0.89
1:B:2004:ASP:OD2	1:B:2006:THR:HB	1.75	0.86
2:B:2:B89:HAJA	3:C:1276:HOH:O	1.74	0.86
1:B:1480:LEU:O	1:B:1481:ARG:HG2	1.74	0.86
1:B:2016:ALA:CB	1:B:2103:MET:HE3	2.06	0.86
1:C:1852:THR:HG22	1:C:1854:SER:H	1.43	0.84
1:A:1772:THR:H	1:A:1776:GLN:NE2	1.76	0.84
1:A:2142:GLN:HG2	1:A:2143:VAL:N	1.91	0.82
1:B:1480:LEU:C	1:B:1481:ARG:HG2	2.00	0.82
1:C:1644:ASN:HD21	1:C:1654:GLN:HG2	1.41	0.81
1:B:1513:GLU:CD	1:B:1516:ARG:HH12	1.83	0.81
1:B:1513:GLU:CD	1:B:1516:ARG:NH1	2.35	0.80
1:A:1560:ASN:HD22	1:A:1560:ASN:H	1.28	0.80
1:A:1730:CYS:HA	1:A:1752:GLN:HE21	1.47	0.79
1:B:1729:THR:CG2	1:B:1796:ASP:OD1	2.30	0.79
1:A:1954:ARG:NH1	1:A:1994:GLU:OE1	2.15	0.79
1:B:1481:ARG:HG3	3:B:1309:HOH:O	1.82	0.79
1:B:2016:ALA:CB	1:B:2103:MET:HE1	2.13	0.79
1:B:2103:MET:HE2	1:B:2109:ILE:HD13	1.64	0.78
1:C:1560:ASN:HD22	1:C:1560:ASN:H	1.32	0.78
1:B:1483:ILE:HG13	3:B:382:HOH:O	1.83	0.78
1:B:1483:ILE:HA	3:B:1265:HOH:O	1.82	0.77
1:B:2097:HIS:HE1	1:C:1632:ALA:H	1.33	0.77
1:B:1624:ASN:HD21	1:B:1733:VAL:H	1.32	0.76
1:B:1729:THR:HG22	1:B:1796:ASP:OD1	1.87	0.75
1:C:1766:LEU:HD12	1:C:1770:VAL:HG11	1.69	0.74
1:B:1578:ARG:HD3	3:B:1013:HOH:O	1.86	0.74
1:C:1772:THR:H	1:C:1776:GLN:NE2	1.87	0.72
1:B:2016:ALA:HB3	1:B:2103:MET:HE1	1.72	0.72
1:B:2044:MET:SD	1:B:2082:LEU:HD21	2.30	0.72
1:B:2016:ALA:HB3	1:B:2103:MET:CE	2.20	0.71
1:B:1837:ASN:ND2	1:B:1837:ASN:H	1.86	0.71
1:B:1852:THR:HG22	3:B:520:HOH:O	1.89	0.71
1:B:1480:LEU:O	1:B:1481:ARG:CG	2.38	0.70
1:B:1694:ILE:HA	1:C:2102:ARG:HD3	1.73	0.70
1:B:1730:CYS:HA	1:B:1752:GLN:HE21	1.55	0.70
1:B:1726:THR:CG2	3:B:5:HOH:O	2.38	0.70
1:B:1781:GLN:HE21	1:B:1781:GLN:H	1.38	0.70
1:B:1781:GLN:H	1:B:1781:GLN:NE2	1.89	0.69
1:C:1580:ARG:HD3	3:C:36:HOH:O	1.92	0.68
1:C:2033:ILE:HG22	1:C:2034:LYS:HD3	1.75	0.68
1:A:1651:LYS:O	1:A:1651:LYS:HD2	1.93	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1658:LEU:HG	1:C:1690:ILE:HD11	1.75	0.68
1:A:1658:LEU:HB2	1:A:1663:MET:HE1	1.77	0.67
1:C:1587:ASN:HD22	1:C:1623:ALA:H	1.43	0.67
1:C:1792:THR:HG23	3:C:317:HOH:O	1.94	0.67
1:C:1644:ASN:ND2	1:C:1654:GLN:HG2	2.10	0.66
1:B:1763:ASN:HD21	1:B:1771:TYR:H	1.44	0.65
1:C:1537:PHE:CD2	1:C:1571:VAL:HG13	2.32	0.65
1:A:1729:THR:O	1:A:1729:THR:OG1	2.15	0.64
1:B:1624:ASN:ND2	1:B:1733:VAL:H	1.95	0.64
1:B:2006:THR:HG23	1:C:1710:LEU:HA	1.79	0.64
1:C:1616:ILE:HD11	3:C:336:HOH:O	1.98	0.64
1:C:1658:LEU:HD12	1:C:1663:MET:HE1	1.80	0.64
1:B:2041:LEU:HA	1:B:2044:MET:HE2	1.80	0.63
1:B:2040:LEU:HD11	1:B:2086:TYR:O	1.99	0.63
1:C:1792:THR:CG2	3:C:317:HOH:O	2.46	0.63
1:C:1759:ALA:H	1:C:1774:ASN:ND2	1.95	0.63
1:B:1494:GLN:NE2	1:B:1496:LYS:H	1.93	0.63
1:A:2111:LYS:HE3	3:A:1129:HOH:O	1.98	0.63
1:A:2164:ASP:H	1:A:2170:GLN:NE2	1.97	0.62
1:A:1658:LEU:HB2	1:A:1663:MET:CE	2.30	0.62
1:B:1726:THR:HG23	3:B:5:HOH:O	1.97	0.62
1:C:1560:ASN:ND2	1:C:1560:ASN:H	1.95	0.62
1:C:1644:ASN:HD21	1:C:1654:GLN:CG	2.13	0.61
1:C:1772:THR:N	1:C:1776:GLN:HE22	1.95	0.61
1:A:2142:GLN:HG2	1:A:2143:VAL:H	1.66	0.61
1:B:1768:ARG:CG	1:B:1768:ARG:HH11	2.12	0.61
1:B:1768:ARG:HB2	1:B:1768:ARG:HH11	1.66	0.60
1:B:1687:ARG:HH11	1:B:1687:ARG:HG3	1.65	0.60
1:A:1560:ASN:ND2	1:A:1560:ASN:H	1.96	0.60
1:A:2136:ILE:HD11	1:A:2152:ILE:HD13	1.85	0.59
1:A:1895:GLU:OE1	1:A:1897:ARG:HD3	2.04	0.58
1:B:1497:ARG:HD3	1:B:1510:ASP:OD1	2.03	0.58
1:C:1852:THR:HB	1:C:1855:GLY:O	2.03	0.58
1:A:1624:ASN:HD21	1:A:1733:VAL:H	1.50	0.58
1:C:1900:GLU:HB3	1:C:1916:LEU:HD11	1.84	0.58
1:C:1816:MET:HG3	1:C:1817:PRO:HD2	1.85	0.58
1:A:1776:GLN:O	1:A:1782:ILE:HD11	2.04	0.57
1:B:2021:ARG:HG3	1:B:2098:ASP:O	2.03	0.57
1:B:2048:ASP:OD2	1:B:2050:LYS:HG2	2.04	0.57
1:C:1706:ARG:HD3	3:C:361:HOH:O	2.03	0.57
1:A:2142:GLN:NE2	1:A:2144:GLY:O	2.38	0.57
1:C:2129:ARG:CD	3:C:1240:HOH:O	2.41	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1768:ARG:HH11	1:B:1768:ARG:CB	2.17	0.57
1:B:2103:MET:CE	1:B:2109:ILE:HD13	2.34	0.57
1:C:1592:LYS:HE2	3:C:633:HOH:O	2.03	0.57
1:C:1537:PHE:HD2	1:C:1571:VAL:HG13	1.68	0.57
1:A:1748:GLN:HE22	1:A:1783:MET:HB2	1.69	0.57
1:B:1638:LEU:HD12	1:B:1658:LEU:HD22	1.85	0.57
1:C:1772:THR:N	1:C:1776:GLN:NE2	2.53	0.56
1:B:1836:THR:HG22	1:B:1838:ASP:H	1.70	0.56
1:B:1991:PRO:O	1:B:2019:ASN:O	2.23	0.56
1:B:1537:PHE:HD2	1:B:1571:VAL:HG13	1.71	0.56
1:B:1480:LEU:O	1:B:1481:ARG:CD	2.53	0.56
1:A:2164:ASP:H	1:A:2170:GLN:HE22	1.54	0.55
1:B:1900:GLU:HB3	1:B:1916:LEU:HD11	1.88	0.55
2:C:3:B89:HAAA	3:C:266:HOH:O	2.06	0.55
1:B:1494:GLN:HE21	1:B:1496:LYS:N	1.96	0.55
1:A:1815:ASN:ND2	1:A:1944:GLN:HE22	2.05	0.55
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.53	0.55
1:C:1748:GLN:HE22	1:C:1783:MET:HB2	1.71	0.55
1:B:2082:LEU:HD23	1:B:2082:LEU:H	1.70	0.55
1:B:1513:GLU:OE1	1:B:1516:ARG:NH1	2.20	0.55
1:A:2131:ASN:ND2	1:A:2179:TYR:OH	2.40	0.55
1:A:1624:ASN:ND2	1:A:1733:VAL:H	2.05	0.54
1:C:2136:ILE:HD11	1:C:2152:ILE:HG23	1.88	0.54
1:A:1730:CYS:HA	1:A:1752:GLN:NE2	2.20	0.54
1:B:2178:ASN:HD22	1:B:2181:THR:HG21	1.73	0.54
1:A:1624:ASN:HD22	1:A:1626:GLY:H	1.56	0.54
1:B:2097:HIS:CE1	1:C:1632:ALA:H	2.19	0.53
1:B:1837:ASN:HD22	1:B:1837:ASN:H	1.57	0.53
1:C:1996:ARG:O	1:C:1999:SER:HB2	2.09	0.53
1:C:2026:GLU:HB2	3:C:1197:HOH:O	2.10	0.52
1:C:1925:HIS:HD2	3:C:279:HOH:O	1.92	0.52
1:A:1815:ASN:HD22	1:A:1944:GLN:HE22	1.57	0.52
1:A:1483:ILE:HD12	3:A:662:HOH:O	2.09	0.52
3:B:1287:HOH:O	1:C:1649:PRO:HG2	2.10	0.52
1:B:1954:ARG:NH1	1:B:1994:GLU:OE1	2.43	0.51
1:B:1616:ILE:HD11	3:B:473:HOH:O	2.09	0.51
1:B:2082:LEU:CD2	1:B:2082:LEU:H	2.24	0.51
1:A:1845:TRP:CD2	1:A:1850:ARG:HD3	2.45	0.51
1:A:1821:LEU:HD22	3:A:1310:HOH:O	2.09	0.51
1:B:1768:ARG:HG3	1:B:1768:ARG:HH11	1.74	0.51
1:B:1997:GLY:HA2	3:C:266:HOH:O	2.11	0.50
1:C:1516:ARG:NH1	3:C:1112:HOH:O	2.44	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1768:ARG:HB2	1:B:1768:ARG:NH1	2.26	0.50
1:C:2189:LEU:O	1:C:2192:GLU:HG3	2.12	0.50
1:C:1673:ASN:H	1:C:1673:ASN:ND2	2.10	0.50
1:A:1649:PRO:O	1:A:1651:LYS:N	2.44	0.50
1:A:1680:THR:HG22	1:A:1681:VAL:N	2.26	0.50
1:A:1730:CYS:CA	1:A:1752:GLN:HE21	2.23	0.49
1:C:1527:SER:O	1:C:1530:VAL:HG22	2.12	0.49
1:A:2180:LYS:HG2	1:B:1482:PRO:HD3	1.95	0.48
1:B:2138:ARG:CG	1:B:2138:ARG:HH11	2.17	0.48
1:A:1657:TYR:CE2	1:A:1687:ARG:HD2	2.49	0.48
1:C:1909:ASN:HD22	1:C:1910:PRO:HD2	1.79	0.48
1:B:1790:HIS:HD2	3:B:70:HOH:O	1.97	0.48
1:B:2134:TYR:CZ	1:B:2138:ARG:HD2	2.48	0.48
1:C:1773:SER:H	1:C:1776:GLN:HE21	1.60	0.48
1:B:2016:ALA:HB2	1:B:2103:MET:CE	2.20	0.48
1:B:1505:THR:HB	1:B:1730:CYS:HB2	1.95	0.48
1:B:1748:GLN:HE22	1:B:1783:MET:HB2	1.79	0.47
1:A:1533:THR:HG22	1:A:1535:ASP:H	1.79	0.47
3:A:386:HOH:O	1:B:1490:LYS:HE2	2.13	0.47
1:C:1815:ASN:ND2	1:C:1944:GLN:HE22	2.11	0.47
1:B:1818:VAL:HB	1:B:1888:PRO:HG2	1.96	0.47
1:B:2006:THR:CG2	1:C:1710:LEU:HA	2.44	0.47
1:A:1680:THR:HG22	1:A:1681:VAL:H	1.78	0.47
1:A:2190:LYS:C	1:A:2192:GLU:H	2.18	0.47
1:C:1757:THR:HG22	2:C:3:B89:HAL	1.97	0.47
1:A:1772:THR:N	1:A:1776:GLN:NE2	2.56	0.47
1:B:1730:CYS:HA	1:B:1752:GLN:NE2	2.25	0.47
1:C:1524:LYS:HA	1:C:1524:LYS:HD3	1.76	0.47
1:A:1772:THR:N	1:A:1776:GLN:HE22	1.91	0.47
1:B:2152:ILE:H	1:B:2152:ILE:HG13	1.58	0.47
1:B:1546:GLU:HG2	3:B:1288:HOH:O	2.14	0.46
1:B:2006:THR:CG2	1:C:1710:LEU:CA	2.93	0.46
1:B:1545:ASP:HB2	3:B:1288:HOH:O	2.15	0.46
1:C:1575:GLU:HG2	3:C:84:HOH:O	2.16	0.46
1:B:1480:LEU:C	1:B:1481:ARG:CG	2.77	0.46
1:A:2142:GLN:CG	1:A:2143:VAL:N	2.70	0.46
1:C:2164:ASP:H	1:C:2170:GLN:NE2	2.14	0.46
1:B:1687:ARG:CG	1:B:1687:ARG:HH11	2.29	0.46
1:A:1803:ILE:O	1:A:1807:MET:HG2	2.15	0.46
1:A:1587:ASN:HD22	1:A:1623:ALA:H	1.63	0.46
1:A:1483:ILE:CD1	1:A:1483:ILE:H	2.28	0.46
1:A:2041:LEU:HD11	1:A:2080:ARG:HH21	1.80	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1523:TRP:HB3	1:B:1530:VAL:HG11	1.97	0.45
1:C:1537:PHE:HD2	1:C:1571:VAL:CG1	2.28	0.45
1:B:1990:PRO:HB2	1:B:1991:PRO:HD2	1.98	0.45
1:B:1969:LYS:HA	1:C:1741:ARG:HD2	1.98	0.45
1:C:1783:MET:HA	1:C:1786:ASN:HB2	1.97	0.45
1:C:1815:ASN:HD22	1:C:1944:GLN:HE22	1.64	0.45
1:A:1781:GLN:H	1:A:1781:GLN:HE21	1.65	0.45
1:B:2034:LYS:HD2	1:B:2034:LYS:HA	1.83	0.45
2:B:2:B89:HAGA	1:C:2001:VAL:HG21	1.98	0.45
1:B:2050:LYS:HG3	1:B:2051:TYR:N	2.31	0.45
1:B:2094:ALA:HB2	1:C:1631:MET:CE	2.47	0.45
1:C:1566:ALA:HA	1:C:1584:VAL:O	2.17	0.45
1:A:2143:VAL:HB	1:A:2193:SER:HB3	1.98	0.45
1:A:1838:ASP:HB2	3:A:780:HOH:O	2.15	0.45
1:C:1909:ASN:HD22	1:C:1910:PRO:CD	2.29	0.44
1:A:1629:ILE:HG13	1:A:1629:ILE:O	2.16	0.44
1:C:1663:MET:HE3	1:C:1688:PHE:HB3	1.99	0.44
1:B:2000:TRP:CD1	1:C:1705:LEU:HB3	2.51	0.44
1:A:1560:ASN:ND2	1:A:1560:ASN:N	2.64	0.44
1:B:1480:LEU:O	1:B:1481:ARG:HD2	2.18	0.44
1:A:1593:ILE:HG22	1:A:1625:SER:OG	2.17	0.44
1:B:1994:GLU:HA	1:B:2021:ARG:O	2.18	0.44
1:B:2006:THR:HG21	1:C:1710:LEU:HB2	2.00	0.44
1:B:1768:ARG:CB	1:B:1768:ARG:NH1	2.79	0.44
1:B:2129:ARG:NH2	3:B:597:HOH:O	2.42	0.44
1:A:1987:ILE:HD12	1:A:2003:VAL:HG22	1.99	0.44
1:B:1585:VAL:HB	1:B:1607:VAL:HG11	2.00	0.44
1:B:2134:TYR:OH	1:B:2138:ARG:HD2	2.17	0.44
1:B:2138:ARG:HG2	1:B:2138:ARG:NH1	2.15	0.44
1:A:1745:ARG:HG2	1:A:1806:TRP:CZ2	2.52	0.44
1:B:1919:GLU:HA	1:B:1920:PRO:HD2	1.89	0.44
1:B:2103:MET:HB3	1:B:2103:MET:HE2	1.89	0.43
1:B:1730:CYS:CA	1:B:1752:GLN:HE21	2.29	0.43
1:A:1838:ASP:O	1:A:1839:GLU:HB2	2.17	0.43
1:B:1647:ALA:O	1:B:1648:ASN:ND2	2.51	0.43
1:B:1852:THR:HG22	1:B:1853:GLU:N	2.33	0.43
1:A:1616:ILE:HD11	3:A:542:HOH:O	2.17	0.43
1:A:1575:GLU:OE1	3:A:1310:HOH:O	2.21	0.43
1:B:1545:ASP:C	1:B:1545:ASP:OD2	2.57	0.43
1:A:1677:THR:HA	1:A:1689:VAL:O	2.19	0.43
1:C:2148:ARG:HG3	3:C:1027:HOH:O	2.18	0.43
1:C:1790:HIS:HD2	3:C:32:HOH:O	2.02	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2148:ARG:O	1:B:2152:ILE:HG13	2.19	0.43
1:A:1817:PRO:HD3	1:B:1484:ALA:HB1	2.00	0.43
1:C:1677:THR:HG22	1:C:1690:ILE:HD13	2.01	0.42
1:B:2036:ARG:O	1:B:2038:GLU:N	2.51	0.42
1:C:1879:VAL:HG13	1:C:1931:LYS:HE2	2.01	0.42
1:C:1925:HIS:HE1	3:C:659:HOH:O	2.01	0.42
1:A:1764:LYS:O	1:A:1765:MET:C	2.56	0.42
1:A:2083:LEU:HB2	1:A:2084:PRO:HD3	2.01	0.42
1:B:1824:LYS:HB2	3:B:799:HOH:O	2.19	0.42
1:C:2014:MET:CG	1:C:2109:ILE:HG22	2.50	0.42
1:B:1616:ILE:HD12	1:B:1813:LYS:HG2	2.02	0.42
1:C:2116:THR:HG22	1:C:2117:GLU:OE2	2.19	0.42
1:C:1677:THR:HA	1:C:1689:VAL:O	2.19	0.42
1:C:1786:ASN:HD22	1:C:1786:ASN:HA	1.37	0.42
1:A:1995:LEU:HG	1:A:2000:TRP:HA	2.01	0.42
1:A:1792:THR:O	1:A:1802:LYS:HE2	2.19	0.42
1:A:1663:MET:HE1	1:A:1688:PHE:HB2	2.02	0.42
1:C:1803:ILE:O	1:C:1807:MET:HG3	2.20	0.42
1:A:1548:GLY:O	1:A:1606:LYS:HE2	2.20	0.42
1:A:1668:LYS:HA	1:A:1668:LYS:HD3	1.83	0.41
1:B:2037:ARG:NH1	1:B:2037:ARG:HB3	2.35	0.41
1:B:1624:ASN:HD22	1:B:1626:GLY:H	1.66	0.41
1:B:1620:TYR:HB3	1:B:1726:THR:HB	2.02	0.41
1:B:1914:GLU:O	1:B:1914:GLU:HG2	2.20	0.41
1:B:1694:ILE:HA	1:C:2102:ARG:CD	2.46	0.41
1:B:1543:ILE:HD11	1:B:1553:VAL:HG11	2.03	0.41
1:A:1575:GLU:HB3	3:A:1310:HOH:O	2.20	0.41
1:B:1909:ASN:HA	1:B:1910:PRO:HD3	1.91	0.41
1:A:1738:TYR:CD1	2:A:1:B89:CAF	3.03	0.41
1:B:1991:PRO:HG3	1:B:2115:TRP:CG	2.55	0.41
1:C:1940:ASN:HB2	1:C:1981:TYR:CE1	2.56	0.41
1:B:1705:LEU:HD23	2:B:2:B89:HAA	2.03	0.41
1:A:1491:GLU:HB3	1:A:1498:TYR:HB2	2.03	0.41
1:B:2031:VAL:HG21	1:B:2091:LEU:HD23	2.02	0.41
1:A:1643:TRP:CZ3	1:A:1649:PRO:HB3	2.56	0.40
1:B:1537:PHE:CD2	1:B:1571:VAL:HG13	2.55	0.40
1:B:1792:THR:HG21	3:B:859:HOH:O	2.21	0.40
1:B:1631:MET:HE2	1:C:2034:LYS:HB3	2.03	0.40
1:C:2016:ALA:O	1:C:2112:GLU:HA	2.22	0.40
1:A:1719:TYR:CE2	1:A:1744:GLN:HG3	2.56	0.40
1:B:1719:TYR:CE2	1:B:1744:GLN:HG3	2.57	0.40
1:A:2142:GLN:CG	1:A:2143:VAL:H	2.32	0.40



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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:241:HOH:O	3:A:1113:HOH:O[2_555]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	684/758 (90%)	656 (96%)	24 (4%)	4 (1%)	33	39
1	B	678/758 (89%)	639 (94%)	36 (5%)	3 (0%)	43	52
1	C	671/758 (88%)	645 (96%)	24 (4%)	2 (0%)	50	60
All	All	2033/2274 (89%)	1940 (95%)	84 (4%)	9 (0%)	43	52

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1650	ASP
1	A	1764	LYS
1	B	2037	ARG
1	C	1492	TRP
1	C	2141	HIS
1	A	1765	MET
1	A	1839	GLU
1	B	2142	GLN
1	B	2141	HIS

### 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	584/648 (90%)	547 (94%)	37 (6%)	25	32
1	B	579/648 (89%)	531 (92%)	48 (8%)	16	19
1	C	573/648 (88%)	524 (91%)	49 (9%)	15	17
All	All	1736/1944 (89%)	1602 (92%)	134 (8%)	18	22

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1483	ILE
1	A	1534	ASP
1	A	1536	PHE
1	A	1549	GLU
1	A	1560	ASN
1	A	1585	VAL
1	A	1616	ILE
1	A	1618	ARG
1	A	1619	ILE
1	A	1651	LYS
1	A	1667	LYS
1	A	1681	VAL
1	A	1685	GLU
1	A	1687	ARG
1	A	1764	LYS
1	A	1770	VAL
1	A	1772	THR
1	A	1781	GLN
1	A	1807	MET
1	A	1826	THR
1	A	1877	VAL
1	A	1878	VAL
1	A	1879	VAL
1	A	1911	ASN
1	A	1915	THR
1	A	1918	GLN
1	A	1924	TRP
1	A	2002	VAL
1	A	2003	VAL
1	A	2008	ASN
1	A	2035	PHE
1	A	2047	LEU
1	A	2128	ARG
1	A	2142	GLN

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Mol	Chain	Res	Type
1	A	2148	ARG
1	A	2149	LEU
1	A	2187	LYS
1	B	1480	LEU
1	B	1534	ASP
1	B	1536	PHE
1	B	1562	ILE
1	B	1571	VAL
1	B	1583	VAL
1	B	1613	LYS
1	B	1616	ILE
1	B	1618	ARG
1	B	1648	ASN
1	B	1651	LYS
1	B	1687	ARG
1	B	1689	VAL
1	B	1691	LYS
1	B	1726	THR
1	B	1729	THR
1	B	1730	CYS
1	B	1757	THR
1	B	1765	MET
1	B	1768	ARG
1	B	1772	THR
1	B	1781	GLN
1	B	1792	THR
1	B	1824	LYS
1	B	1837	ASN
1	B	1843	VAL
1	B	1853	GLU
1	B	1854	SER
1	B	1914	GLU
1	B	1924	TRP
1	B	1968	LEU
1	B	2006	THR
1	B	2018	VAL
1	B	2021	ARG
1	B	2034	LYS
1	B	2035	PHE
1	B	2036	ARG
1	B	2082	LEU
1	B	2083	LEU

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Mol	Chain	Res	Type
1	B	2089	ILE
1	B	2128	ARG
1	B	2138	ARG
1	B	2149	LEU
1	B	2152	ILE
1	B	2165	HIS
1	B	2180	LYS
1	B	2181	THR
1	B	2189	LEU
1	C	1499	LYS
1	C	1508	VAL
1	C	1516	ARG
1	C	1522	GLN
1	C	1534	ASP
1	C	1536	PHE
1	C	1547	ASN
1	C	1560	ASN
1	C	1565	VAL
1	C	1571	VAL
1	C	1580	ARG
1	C	1585	VAL
1	C	1616	ILE
1	C	1618	ARG
1	C	1631	MET
1	C	1634	GLU
1	C	1636	VAL
1	C	1651	LYS
1	C	1664	GLU
1	C	1667	LYS
1	C	1679	ARG
1	C	1680	THR
1	C	1731	ARG
1	C	1741	ARG
1	C	1769	GLU
1	C	1770	VAL
1	C	1781	GLN
1	C	1786	ASN
1	C	1792	THR
1	C	1794	VAL
1	C	1816	MET
1	C	1824	LYS
1	C	1843	VAL

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Mol	Chain	Res	Type
1	C	1851	GLU
1	C	1877	VAL
1	C	1879	VAL
1	C	1909	ASN
1	C	1911	ASN
1	C	1924	TRP
1	C	1968	LEU
1	C	2035	PHE
1	C	2036	ARG
1	C	2037	ARG
1	C	2047	LEU
1	C	2128	ARG
1	C	2145	GLU
1	C	2149	LEU
1	C	2152	ILE
1	C	2185	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1560	ASN
1	A	1581	GLN
1	A	1587	ASN
1	A	1624	ASN
1	A	1644	ASN
1	A	1673	ASN
1	A	1683	ASN
1	A	1744	GLN
1	A	1748	GLN
1	A	1752	GLN
1	A	1776	GLN
1	A	1781	GLN
1	A	1790	HIS
1	A	1815	ASN
1	A	1837	ASN
1	A	1934	GLN
1	A	1965	ASN
1	A	2008	ASN
1	A	2045	ASN
1	A	2097	HIS
1	A	2131	ASN
1	A	2142	GLN

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Mol	Chain	Res	Type
1	A	2170	GLN
1	B	1494	GLN
1	B	1517	GLN
1	B	1587	ASN
1	B	1599	GLN
1	B	1624	ASN
1	B	1644	ASN
1	B	1648	ASN
1	B	1748	GLN
1	B	1752	GLN
1	B	1763	ASN
1	B	1781	GLN
1	B	1790	HIS
1	B	1815	ASN
1	B	1837	ASN
1	B	1934	GLN
1	B	1941	ASN
1	B	1944	GLN
1	B	2097	HIS
1	B	2131	ASN
1	B	2178	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	1644	ASN
1	C	1648	ASN
1	C	1673	ASN
1	C	1748	GLN
1	C	1774	ASN
1	C	1776	GLN
1	C	1786	ASN
1	C	1790	HIS
1	C	1815	ASN
1	C	1909	ASN
1	C	1911	ASN
1	C	1918	GLN
1	C	1941	ASN
1	C	2011	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 ⓘ

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	B89	A	1	-	24,24,24	1.65	6 (25%)	31,31,31	1.66	5 (16%)
2	B89	B	2	-	24,24,24	1.68	8 (33%)	31,31,31	1.86	6 (19%)
2	B89	C	3	-	24,24,24	1.87	8 (33%)	31,31,31	1.83	7 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	B89	A	1	-	-	0/15/40/40	0/2/2/2
2	B89	B	2	-	-	0/15/40/40	0/2/2/2
2	B89	C	3	-	-	0/15/40/40	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	B89	CAT-NAO	4.13	1.33	1.28
2	C	3	B89	CAE-CAF	3.19	1.39	1.30
2	A	1	B89	CAE-CAF	3.14	1.39	1.30
2	C	3	B89	CAN-CAS	3.10	1.53	1.49
2	B	2	B89	CAT-NAO	3.04	1.32	1.28
2	B	2	B89	CAE-CAF	3.00	1.38	1.30
2	A	1	B89	OAB-CAR	2.99	1.30	1.23
2	A	1	B89	OAQ-NAO	-2.90	1.36	1.42
2	C	3	B89	OAQ-NAO	-2.83	1.36	1.42
2	C	3	B89	CAU-CAR	2.81	1.53	1.45
2	B	2	B89	OAB-CAR	2.80	1.29	1.23
2	A	1	B89	CAU-CAR	2.74	1.53	1.45
2	C	3	B89	CAH-CAF	-2.66	1.39	1.49
2	B	2	B89	CAH-CAF	-2.65	1.39	1.49
2	C	3	B89	OAB-CAR	2.63	1.29	1.23
2	B	2	B89	OAC-CAS	2.40	1.39	1.32
2	B	2	B89	CAU-CAR	2.37	1.52	1.45
2	B	2	B89	OAQ-NAO	-2.34	1.37	1.42
2	A	1	B89	CAH-CAF	-2.32	1.40	1.49
2	A	1	B89	CAT-NAO	2.22	1.31	1.28
2	C	3	B89	OAC-CAS	2.10	1.38	1.32
2	B	2	B89	CAM-CAR	2.05	1.54	1.50

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	B89	CAH-OAQ-NAO	6.05	114.74	107.97
2	A	1	B89	CAH-OAQ-NAO	5.85	114.52	107.97
2	C	3	B89	OAC-CAS-CAN	4.91	119.86	113.28
2	B	2	B89	CAG-CAT-NAO	-4.38	116.94	124.72
2	C	3	B89	CAG-CAT-NAO	-3.86	117.86	124.72
2	C	3	B89	CAH-OAQ-NAO	3.65	112.06	107.97
2	C	3	B89	OAQ-NAO-CAT	3.63	116.55	111.56
2	A	1	B89	CAG-CAT-NAO	-3.54	118.42	124.72
2	A	1	B89	OAC-CAS-CAN	2.88	117.14	113.28
2	B	2	B89	CAU-CAT-NAO	2.78	118.66	114.71
2	B	2	B89	OAC-CAS-CAN	2.70	116.90	113.28
2	C	3	B89	CAU-CAT-NAO	2.51	118.27	114.71
2	C	3	B89	CAM-CAR-CAU	2.47	121.38	116.18
2	A	1	B89	CAW-CAN-CAS	-2.34	111.02	114.43
2	C	3	B89	OAC-CAS-CAU	-2.33	116.61	121.65
2	B	2	B89	CAM-CAR-CAU	2.25	120.92	116.18
2	A	1	B89	OAP-CAJ-CAL	-2.18	104.17	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	B89	CAR-CAU-CAT	2.12	124.07	120.12

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	688/758 (90%)	0.13	57 (8%)	11 18	17, 29, 75, 99	0
1	B	682/758 (89%)	0.30	69 (10%)	7 12	16, 33, 85, 103	0
1	C	675/758 (89%)	0.22	73 (10%)	6 10	17, 33, 83, 101	0
All	All	2045/2274 (89%)	0.21	199 (9%)	8 13	16, 31, 81, 103	0

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2143	VAL	11.1
1	B	2143	VAL	10.5
1	A	2143	VAL	9.2
1	B	2144	GLY	8.3
1	B	2083	LEU	7.9
1	C	2144	GLY	7.6
1	A	2194	PHE	7.4
1	B	1480	LEU	7.0
1	B	2082	LEU	6.8
1	A	2144	GLY	6.7
1	A	1685	GLU	6.5
1	A	2191	LEU	6.1
1	B	2189	LEU	6.1
1	B	2041	LEU	5.8
1	C	1647	ALA	5.7
1	C	1682	ILE	5.6
1	B	2084	PRO	5.6
1	B	1684	GLY	5.6
1	C	2191	LEU	5.5
1	B	1838	ASP	5.5
1	B	1682	ILE	5.5
1	A	1480	LEU	5.4
1	B	1681	VAL	5.4

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Mol	Chain	Res	Type	RSRZ
1	C	1648	ASN	5.4
1	B	1669	PHE	5.3
1	C	2193	SER	5.2
1	B	1648	ASN	5.1
1	A	1838	ASP	4.9
1	A	1684	GLY	4.8
1	A	1910	PRO	4.8
1	C	1679	ARG	4.7
1	B	2037	ARG	4.7
1	C	1683	ASN	4.6
1	C	1685	GLU	4.5
1	B	1647	ALA	4.5
1	B	2046	ARG	4.5
1	A	1683	ASN	4.4
1	B	2085	ILE	4.4
1	B	2051	TYR	4.4
1	C	1546	GLU	4.3
1	C	1669	PHE	4.3
1	C	1651	LYS	4.3
1	B	2145	GLU	4.3
1	C	1911	ASN	4.3
1	B	1651	LYS	4.2
1	C	1646	ALA	4.2
1	A	1669	PHE	4.2
1	A	1481	ARG	4.1
1	B	1767	GLY	4.1
1	A	1911	ASN	4.0
1	B	2188	GLY	4.0
1	A	1681	VAL	3.9
1	B	2187	LYS	3.9
1	C	2037	ARG	3.9
1	C	1684	GLY	3.8
1	C	1681	VAL	3.8
1	C	1644	ASN	3.8
1	C	1838	ASP	3.8
1	C	1680	THR	3.8
1	A	1767	GLY	3.8
1	A	2041	LEU	3.8
1	B	1839	GLU	3.7
1	B	1649	PRO	3.7
1	B	1679	ARG	3.7
1	B	1685	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	2141	HIS	3.6
1	A	1646	ALA	3.6
1	C	1668	LYS	3.6
1	A	1647	ALA	3.5
1	A	2081	GLU	3.5
1	A	1668	LYS	3.5
1	C	2141	HIS	3.4
1	C	2142	GLN	3.4
1	B	2142	GLN	3.4
1	B	1483	ILE	3.4
1	C	2145	GLU	3.4
1	C	1839	GLU	3.4
1	A	2145	GLU	3.3
1	A	1648	ASN	3.3
1	B	1770	VAL	3.3
1	A	1682	ILE	3.3
1	A	1529	ASP	3.3
1	B	2036	ARG	3.3
1	A	2080	ARG	3.3
1	B	1911	ASN	3.3
1	B	2081	GLU	3.3
1	C	1584	VAL	3.2
1	A	1853	GLU	3.2
1	A	1645	ASP	3.2
1	B	1683	ASN	3.2
1	A	2051	TYR	3.2
1	C	1547	ASN	3.2
1	C	1853	GLU	3.1
1	C	1530	VAL	3.1
1	C	1650	ASP	3.1
1	A	1855	GLY	3.1
1	A	1547	ASN	3.1
1	A	2049	ASP	3.0
1	C	2041	LEU	3.0
1	C	1910	PRO	3.0
1	A	1483	ILE	3.0
1	A	2037	ARG	3.0
1	A	1839	GLU	3.0
1	B	1546	GLU	3.0
1	B	1586	ALA	3.0
1	A	1546	GLU	2.9
1	B	2049	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	1679	ARG	2.9
1	B	2045	ASN	2.9
1	B	1680	THR	2.9
1	B	2080	ARG	2.9
1	C	1767	GLY	2.9
1	B	1772	THR	2.9
1	C	1491	GLU	2.9
1	C	1837	ASN	2.9
1	C	1670	ASP	2.9
1	B	1910	PRO	2.8
1	B	1530	VAL	2.8
1	A	2036	ARG	2.8
1	C	2083	LEU	2.8
1	C	1619	ILE	2.8
1	A	2038	GLU	2.7
1	A	2195	ALA	2.7
1	C	1548	GLY	2.7
1	C	1766	LEU	2.7
1	A	1769	GLU	2.7
1	C	2192	GLU	2.7
1	A	2050	LYS	2.7
1	B	1585	VAL	2.7
1	C	1529	ASP	2.7
1	C	2051	TYR	2.7
1	C	1824	LYS	2.7
1	C	1652	GLY	2.6
1	C	1765	MET	2.6
1	B	1621	LEU	2.6
1	B	2180	LYS	2.6
1	B	1853	GLU	2.6
1	A	2190	LYS	2.6
1	B	1481	ARG	2.6
1	C	1585	VAL	2.5
1	C	1913	ALA	2.5
1	B	1765	MET	2.5
1	B	2146	ALA	2.5
1	C	1556	GLU	2.5
1	C	1534	ASP	2.5
1	B	1913	ALA	2.5
1	B	1584	VAL	2.5
1	C	1554	GLU	2.4
1	A	2146	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	1649	PRO	2.4
1	A	2193	SER	2.4
1	A	2083	LEU	2.4
1	B	1664	GLU	2.4
1	B	2038	GLU	2.4
1	B	1824	LYS	2.4
1	A	2149	LEU	2.4
1	A	1585	VAL	2.4
1	C	2045	ASN	2.4
1	C	1664	GLU	2.4
1	B	1529	ASP	2.3
1	C	1621	LEU	2.3
1	A	1768	ARG	2.3
1	A	1766	LEU	2.3
1	C	1726	THR	2.3
1	C	2050	LYS	2.3
1	B	2043	THR	2.3
1	B	2141	HIS	2.3
1	B	2161	ALA	2.3
1	B	2040	LEU	2.3
1	C	2049	ASP	2.2
1	A	1680	THR	2.2
1	B	1727	LEU	2.2
1	A	1765	MET	2.2
1	A	1670	ASP	2.2
1	A	2142	GLN	2.2
1	C	2046	ARG	2.2
1	B	2134	TYR	2.2
1	A	2084	PRO	2.2
1	C	1764	LYS	2.2
1	C	1566	ALA	2.2
1	C	2084	PRO	2.1
1	C	1656	LEU	2.1
1	B	1668	LYS	2.1
1	C	1667	LYS	2.1
1	C	1678	GLU	2.1
1	C	1583	VAL	2.1
1	C	1586	ALA	2.1
1	C	2081	GLU	2.1
1	B	1644	ASN	2.1
1	B	1531	LYS	2.1
1	C	1531	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	2038	GLU	2.1
1	A	1482	PRO	2.0
1	C	2190	LYS	2.0
1	B	1619	ILE	2.0
1	A	1528	ALA	2.0
1	B	1556	GLU	2.0
1	C	1769	GLU	2.0
1	B	1852	THR	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	B89	C	3	23/23	0.16	1.70	43,52,59,64	0
2	B89	A	1	23/23	0.14	0.80	29,38,49,52	0
2	B89	B	2	23/23	0.15	0.65	28,37,46,50	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.