Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 11:00 PM EDT

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 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 (i) 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 (i)) were used in the production of this report:

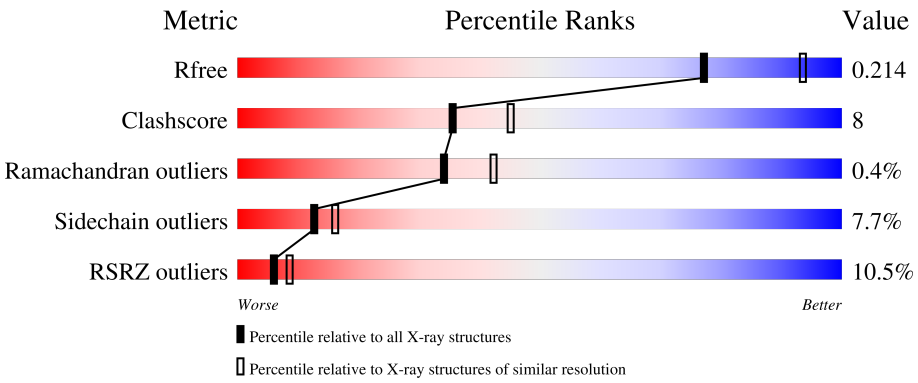
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 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	758	8% 75% 13% • 9%
1	B	758	10% 71% 15% • 10%
1	C	758	10% 73% 14% • • 11%

2 Entry composition (i)

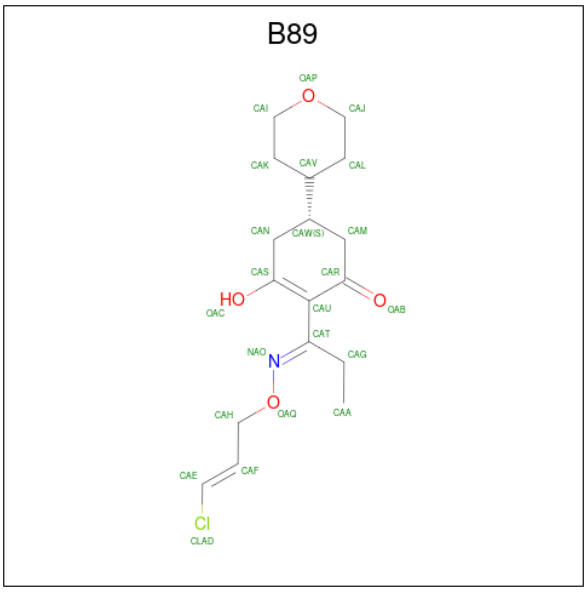
There are 3 unique types of molecules in this entry. The entry contains 17693 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- 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: $C_{17}H_{24}ClNO_4$).



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

Continued on next page...

Continued from previous page...

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

- Molecule 3 is water.

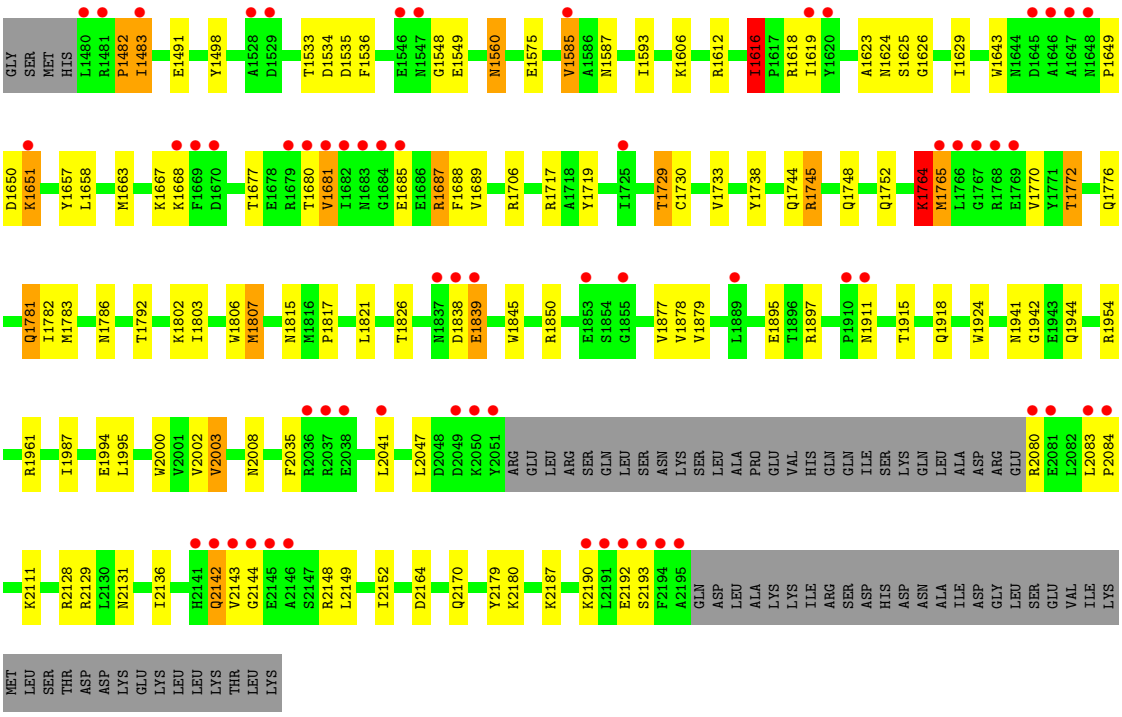
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	483	483	483	0	0
			Total	O		
3	B	415	415	415	0	0
			Total	O		
3	C	405	405	405	0	0

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.

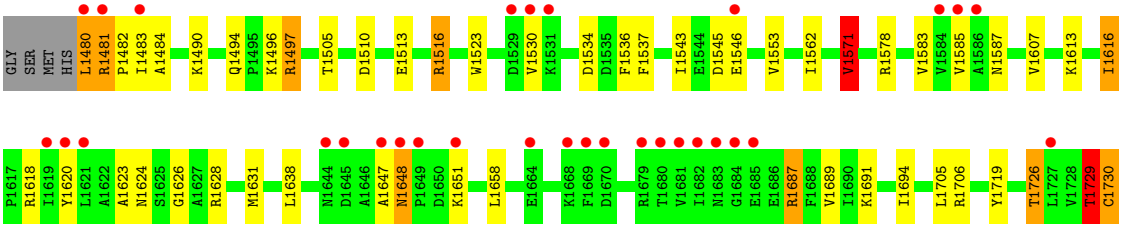
• Molecule 1: Acetyl-CoA carboxylase

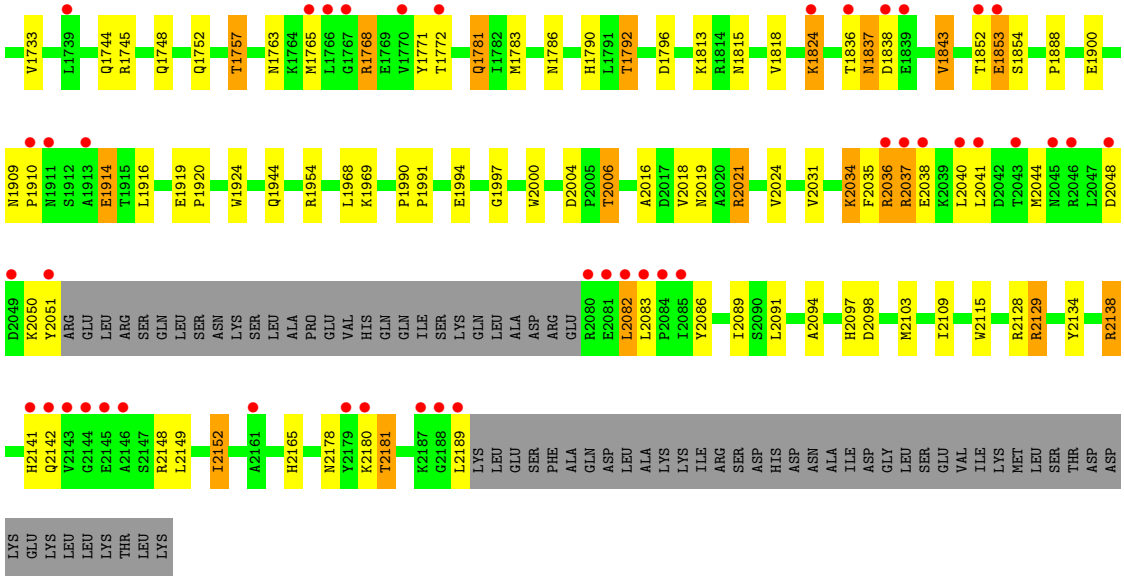
Chain A:



• Molecule 1: Acetyl-CoA carboxylase

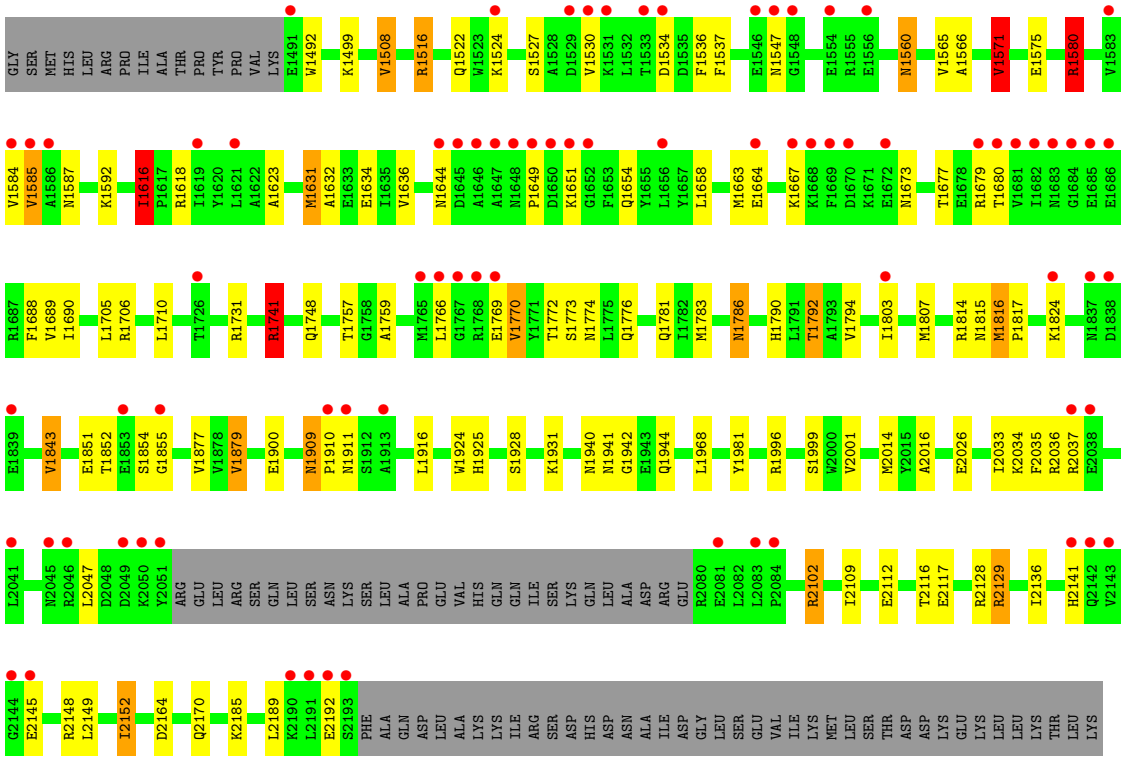
Chain B:





- Molecule 1: Acetyl-CoA carboxylase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	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) 98.7 (29.93-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.24 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.187 , 0.221 0.181 , 0.214	Depositor DCC
R_{free} test set	9659 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	33.1	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 54.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17693	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[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 (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(^{o})	Ideal(^{o})
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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 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	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

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 8.

All (264) 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: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:1513:GLU:OE2	1:B:1516:ARG:NH1	2.04	0.91
1:B:2138:ARG:HG2	1:B:2138:ARG:HH11	1.36	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1792:THR:HG22	3:B:195:HOH:O	1.72	0.89
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
1:B:1480:LEU:O	1:B:1481:ARG:HG2	1.74	0.86
2:B:2:B89:HAJA	3:C:1276:HOH:O	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:H	1:A:1560:ASN:HD22	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:H	1:B:1837:ASN:ND2	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:H	1:B:1781:GLN:HE21	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2033:ILE:HG22	1:C:2034:LYS:HD3	1.75	0.68
1:A:1651:LYS:HD2	1:A:1651:LYS:O	1.93	0.68
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:2040:LEU:HD11	1:B:2086:TYR:O	1.99	0.63
1:B:2041:LEU:HA	1:B:2044:MET:HE2	1.80	0.63
1:C:1759:ALA:H	1:C:1774:ASN:ND2	1.95	0.63
1:C:1792:THR:CG2	3:C:317:HOH:O	2.46	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:H	1:C:1560:ASN:ND2	1.95	0.62
1:C:1644:ASN:HD21	1:C:1654:GLN:CG	2.13	0.61
1:A:2142:GLN:HG2	1:A:2143:VAL:H	1.66	0.61
1:B:1768:ARG:HH11	1:B:1768:ARG:CG	2.12	0.61
1:C:1772:THR:N	1:C:1776:GLN:HE22	1.95	0.61
1:B:1768:ARG:HH11	1:B:1768:ARG:HB2	1.66	0.60
1:B:1687:ARG:HG3	1:B:1687:ARG:HH11	1.65	0.60
1:A:1560:ASN:H	1:A:1560:ASN:ND2	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:A:1624:ASN:HD21	1:A:1733:VAL:H	1.50	0.58
1:C:1852:THR:HB	1:C:1855:GLY:O	2.03	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1768:ARG:HH11	1:B:1768:ARG:CB	2.17	0.57
1:C:2129:ARG:CD	3:C:1240:HOH:O	2.41	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:B:1836:THR:HG22	1:B:1838:ASP:H	1.70	0.56
1:C:1772:THR:N	1:C:1776:GLN:NE2	2.53	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
1:A:1815:ASN:ND2	1:A:1944:GLN:HE22	2.05	0.55
1:B:1494:GLN:HE21	1:B:1496:LYS:N	1.96	0.55
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.53	0.55
2:C:3:B89:HAAA	3:C:266:HOH:O	2.06	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:A:2131:ASN:ND2	1:A:2179:TYR:OH	2.40	0.55
1:B:1513:GLU:OE1	1:B:1516:ARG:NH1	2.20	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:H	1:B:1837:ASN:HD22	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:1483:ILE:HD12	3:A:662:HOH:O	2.09	0.52
1:A:1815:ASN:HD22	1:A:1944:GLN:HE22	1.57	0.52
3:B:1287:HOH:O	1:C:1649:PRO:HG2	2.10	0.52
1:B:1616:ILE:HD11	3:B:473:HOH:O	2.09	0.51
1:B:1954:ARG:NH1	1:B:1994:GLU:OE1	2.43	0.51
1:A:1845:TRP:CD2	1:A:1850:ARG:HD3	2.45	0.51
1:B:2082:LEU:H	1:B:2082:LEU:CD2	2.24	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1821:LEU:HD22	3:A:1310:HOH:O	2.09	0.51
1:B:1768:ARG:HH11	1:B:1768:ARG:HG3	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
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:HH11	1:B:2138:ARG:CG	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:1505:THR:HB	1:B:1730:CYS:HB2	1.95	0.48
1:B:2016:ALA:HB2	1:B:2103:MET:CE	2.20	0.48
1:A:1533:THR:HG22	1:A:1535:ASP:H	1.79	0.47
1:B:1748:GLN:HE22	1:B:1783:MET:HB2	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: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:B:2006:THR:CG2	1:C:1710:LEU:HA	2.44	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:1757:THR:HG22	2:C:3:B89:HAL	1.97	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:1545:ASP:HB2	3:B:1288:HOH:O	2.15	0.46
1:B:2006:THR:CG2	1:C:1710:LEU:CA	2.93	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1587:ASN:HD22	1:A:1623:ALA:H	1.63	0.46
1:A:1803:ILE:O	1:A:1807:MET:HG2	2.15	0.46
1:B:1687:ARG:HH11	1:B:1687:ARG:CG	2.29	0.46
1:A:1483:ILE:H	1:A:1483:ILE:CD1	2.28	0.46
1:A:2041:LEU:HD11	1:A:2080:ARG:HH21	1.80	0.45
1:B:1523:TRP:HB3	1:B:1530:VAL:HG11	1.97	0.45
1:B:1990:PRO:HB2	1:B:1991:PRO:HD2	1.98	0.45
1:C:1537:PHE:HD2	1:C:1571:VAL:CG1	2.28	0.45
1:B:1969:LYS:HA	1:C:1741:ARG:HD2	1.98	0.45
1:A:1781:GLN:H	1:A:1781:GLN:HE21	1.65	0.45
1:B:2034:LYS:HA	1:B:2034:LYS:HD2	1.83	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: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
2:B:2:B89:HAGA	1:C:2001:VAL:HG21	1.98	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:O	1:A:1629:ILE:HG13	2.16	0.44
1:B:2000:TRP:CD1	1:C:1705:LEU:HB3	2.51	0.44
1:C:1663:MET:HE3	1:C:1688:PHE:HB3	1.99	0.44
1:A:1560:ASN:ND2	1:A:1560:ASN:N	2.64	0.44
1:A:1593:ILE:HG22	1:A:1625:SER:OG	2.17	0.44
1:B:1480:LEU:O	1:B:1481:ARG:HD2	2.18	0.44
1:B:1994:GLU:HA	1:B:2021:ARG:O	2.18	0.44
1:A:1987:ILE:HD12	1:A:2003:VAL:HG22	1.99	0.44
1:B:1768:ARG:CB	1:B:1768:ARG:NH1	2.79	0.44
1:B:2006:THR:HG21	1:C:1710:LEU:HB2	2.00	0.44
1:B:2129:ARG:NH2	3:B:597:HOH:O	2.42	0.44
1:B:1585:VAL:HB	1:B:1607:VAL:HG11	2.00	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: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:1838:ASP:O	1:A:1839:GLU:HB2	2.17	0.43
1:B:1730:CYS:CA	1:B:1752:GLN:HE21	2.29	0.43
1:B:2103:MET:HE2	1:B:2103:MET:HB3	1.89	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1677:THR:HA	1:A:1689:VAL:O	2.19	0.43
1:B:1545:ASP:OD2	1:B:1545:ASP:C	2.57	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
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:A:1764:LYS:O	1:A:1765:MET:C	2.56	0.42
1:C:1925:HIS:HE1	3:C:659:HOH:O	2.01	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:A:1792:THR:O	1:A:1802:LYS:HE2	2.19	0.42
1:A:1995:LEU:HG	1:A:2000:TRP:HA	2.01	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:1548:GLY:O	1:A:1606:LYS:HE2	2.20	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:1668:LYS:HD3	1:A:1668:LYS:HA	1.83	0.41
1:B:2037:ARG:HB3	1:B:2037:ARG:NH1	2.35	0.41
1:B:1620:TYR:HB3	1:B:1726:THR:HB	2.02	0.41
1:B:1624:ASN:HD22	1:B:1626:GLY:H	1.66	0.41
1:B:1914:GLU:O	1:B:1914:GLU:HG2	2.20	0.41
1:B:1543:ILE:HD11	1:B:1553:VAL:HG11	2.03	0.41
1:B:1694:ILE:HA	1:C:2102:ARG:CD	2.46	0.41
1:A:1575:GLU:HB3	3:A:1310:HOH:O	2.20	0.41
1:A:1738:TYR:CD1	2:A:1:B89:CAF	3.03	0.41
1:B:1909:ASN:HA	1:B:1910:PRO:HD3	1.91	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:A:1491:GLU:HB3	1:A:1498:TYR:HB2	2.03	0.41
1:B:1705:LEU:HD23	2:B:2:B89:HAA	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1537:PHE:CD2	1:B:1571:VAL:HG13	2.55	0.40
1:A:1719:TYR:CE2	1:A:1744:GLN:HG3	2.56	0.40
1:B:1631:MET:HE2	1:C:2034:LYS:HB3	2.03	0.40
1:B:1719:TYR:CE2	1:B:1744:GLN:HG3	2.57	0.40
1:B:1792:THR:HG21	3:B:859:HOH:O	2.21	0.40
1:C:2016:ALA:O	1:C:2112:GLU:HA	2.22	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	Interatomic distance (Å)	Clash overlap (Å)
3:A:241:HOH:O	3:A:1113:HOH:O[2_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	684/758 (90%)	656 (96%)	24 (4%)	4 (1%)	25	31
1	B	678/758 (89%)	639 (94%)	36 (5%)	3 (0%)	34	42
1	C	671/758 (88%)	645 (96%)	24 (4%)	2 (0%)	41	50
All	All	2033/2274 (89%)	1940 (95%)	84 (4%)	9 (0%)	34	42

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1765	MET
1	A	1839	GLU
1	B	2142	GLN
1	B	2141	HIS

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	584/648 (90%)	547 (94%)	37 (6%)	18	24
1	B	579/648 (89%)	531 (92%)	48 (8%)	11	14
1	C	573/648 (88%)	524 (91%)	49 (9%)	10	12
All	All	1736/1944 (89%)	1602 (92%)	134 (8%)	13	16

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Sometimes 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 (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)

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	B	2	-	22,24,24	1.78	8 (36%)	23,31,31	2.06	5 (21%)
2	B89	A	1	-	22,24,24	1.71	6 (27%)	23,31,31	2.01	5 (21%)
2	B89	C	3	-	22,24,24	2.01	7 (31%)	23,31,31	1.88	6 (26%)

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	B	2	-	-	5/14/40/40	0/2/2/2
2	B89	A	1	-	-	6/14/40/40	0/2/2/2
2	B89	C	3	-	-	4/14/40/40	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	B89	CAT-NAO	4.99	1.33	1.28
2	B	2	B89	CAT-NAO	3.70	1.32	1.28
2	A	1	B89	OAB-CAR	3.47	1.30	1.23
2	C	3	B89	CAN-CAS	3.41	1.53	1.49
2	A	1	B89	OAQ-NAO	-3.29	1.36	1.42
2	B	2	B89	OAB-CAR	3.25	1.29	1.23
2	C	3	B89	OAQ-NAO	-3.22	1.36	1.42
2	C	3	B89	CAU-CAR	3.11	1.53	1.45
2	C	3	B89	OAB-CAR	3.06	1.29	1.23
2	A	1	B89	CAU-CAR	3.04	1.53	1.45
2	A	1	B89	CAT-NAO	2.73	1.31	1.28
2	B	2	B89	OAQ-NAO	-2.65	1.37	1.42
2	B	2	B89	CAU-CAR	2.63	1.52	1.45
2	C	3	B89	CAH-CAF	-2.53	1.39	1.49
2	B	2	B89	CAH-CAF	-2.52	1.39	1.49
2	B	2	B89	CAG-CAT	2.39	1.55	1.50
2	B	2	B89	OAC-CAS	2.31	1.39	1.32
2	A	1	B89	CAH-CAF	-2.20	1.40	1.49
2	B	2	B89	CAM-CAR	2.03	1.54	1.50
2	A	1	B89	CAG-CAT	2.02	1.54	1.50
2	C	3	B89	OAC-CAS	2.02	1.38	1.32

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	B89	CAH-OAQ-NAO	6.47	114.74	107.94
2	A	1	B89	CAH-OAQ-NAO	6.26	114.52	107.94
2	B	2	B89	CAS-CAU-CAT	-4.46	118.16	121.10
2	A	1	B89	OAP-CAJ-CAL	-4.38	104.17	111.74
2	C	3	B89	OAC-CAS-CAN	3.99	119.86	113.29
2	C	3	B89	CAH-OAQ-NAO	3.91	112.06	107.94
2	C	3	B89	CAS-CAU-CAT	-3.50	118.79	121.10
2	C	3	B89	OAQ-NAO-CAT	3.40	116.55	111.47
2	A	1	B89	CAJ-CAL-CAV	-2.97	106.90	110.73
2	C	3	B89	OAC-CAS-CAU	-2.72	116.61	121.95
2	C	3	B89	CAM-CAR-CAU	2.71	121.38	115.98
2	A	1	B89	CAS-CAU-CAT	-2.51	119.44	121.10
2	B	2	B89	CAM-CAR-CAU	2.48	120.92	115.98
2	B	2	B89	OAB-CAR-CAU	-2.43	118.82	122.77
2	A	1	B89	OAC-CAS-CAN	2.34	117.14	113.29
2	B	2	B89	OAC-CAS-CAN	2.19	116.90	113.29

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	B89	CAA-CAG-CAT-NAO
2	A	1	B89	CAG-CAT-CAU-CAR
2	A	1	B89	CAG-CAT-CAU-CAS
2	A	1	B89	NAO-CAT-CAU-CAS
2	B	2	B89	CAA-CAG-CAT-NAO
2	B	2	B89	CAG-CAT-CAU-CAR
2	B	2	B89	CAG-CAT-CAU-CAS
2	B	2	B89	NAO-CAT-CAU-CAS
2	C	3	B89	CAG-CAT-CAU-CAR
2	C	3	B89	CAG-CAT-CAU-CAS
2	C	3	B89	NAO-CAT-CAU-CAS
2	A	1	B89	CAA-CAG-CAT-CAU
2	B	2	B89	CAA-CAG-CAT-CAU
2	C	3	B89	CAF-CAH-OAQ-NAO
2	A	1	B89	CAF-CAH-OAQ-NAO

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	B89	3	0

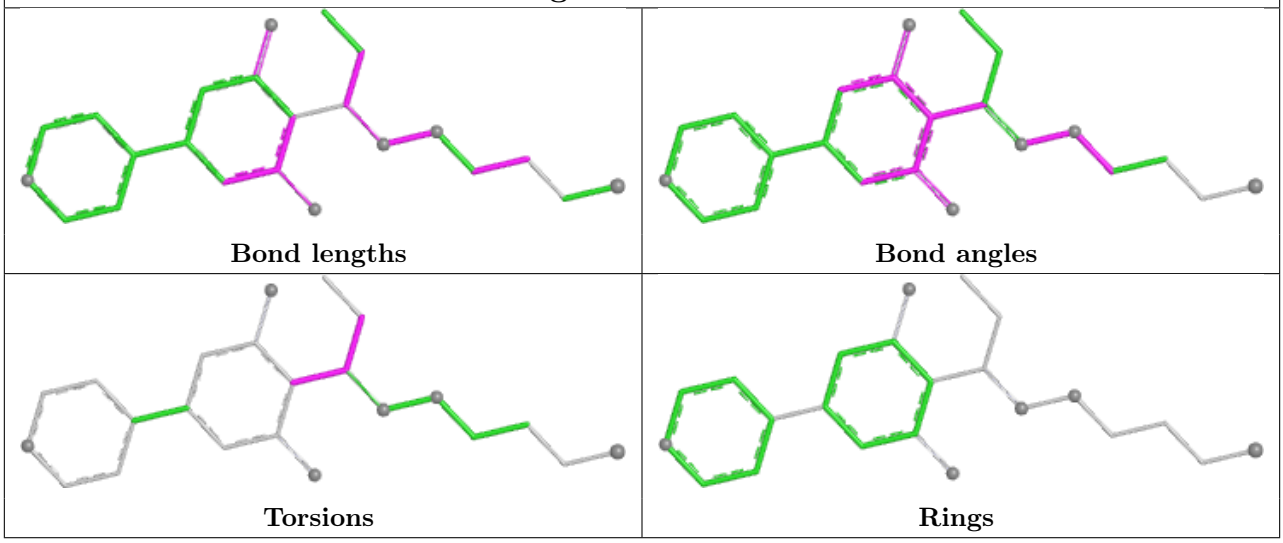
Continued on next page...

Continued from previous page...

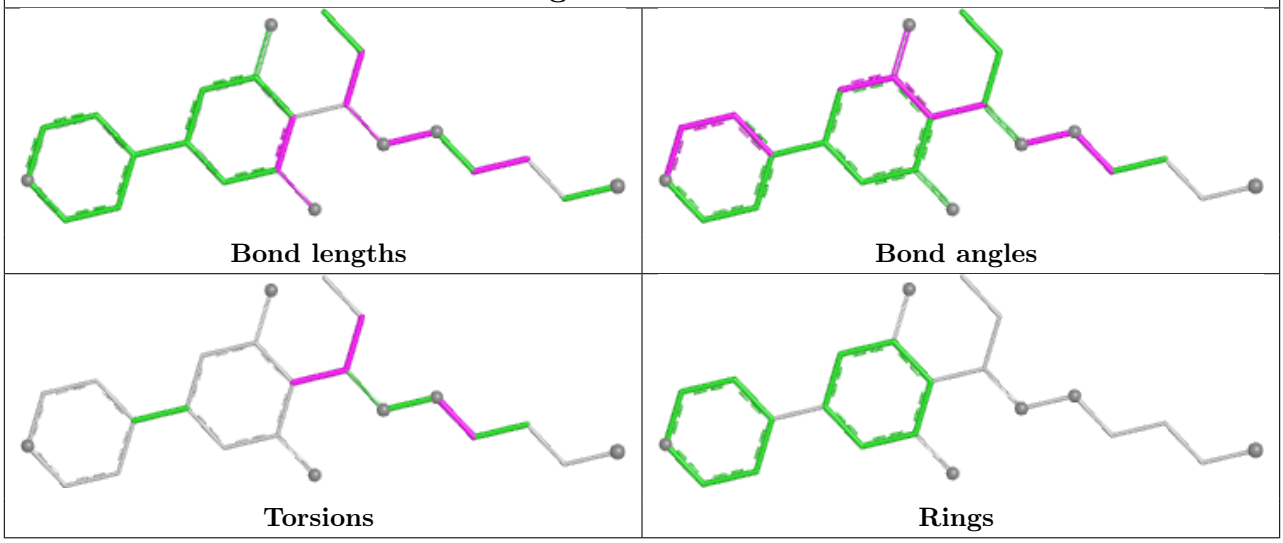
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	B89	1	0
2	C	3	B89	2	0

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.

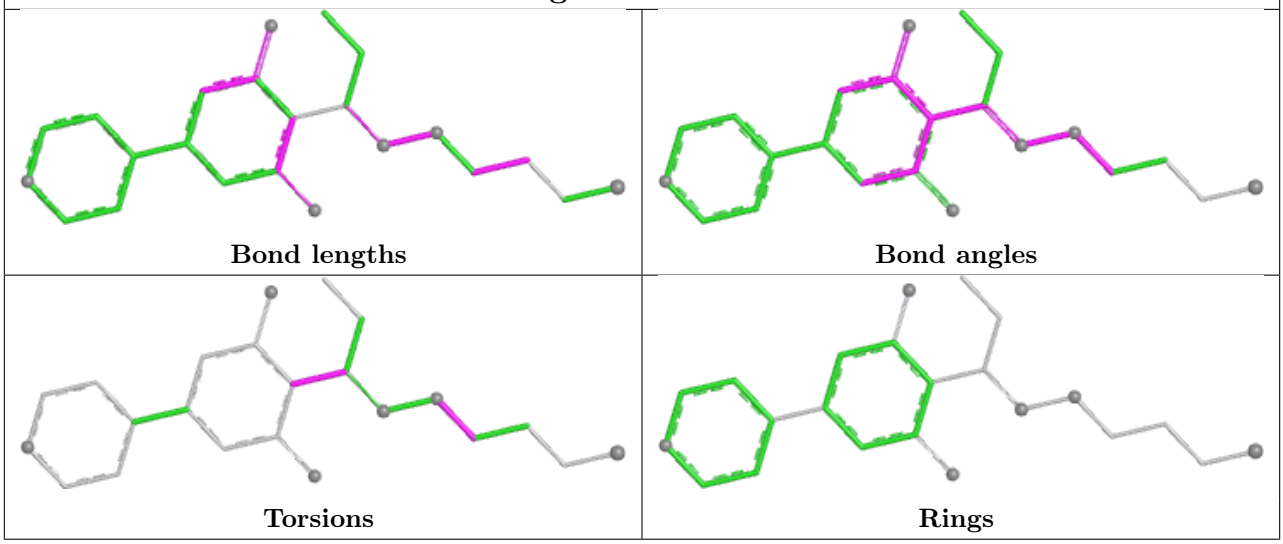
Ligand B89 B 2



Ligand B89 A 1



Ligand B89 C 3



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	688/758 (90%)	0.19	62 (9%)	9	12	17, 29, 75, 99	0
1	B	682/758 (89%)	0.34	75 (10%)	5	7	16, 33, 85, 103	0
1	C	675/758 (89%)	0.25	78 (11%)	4	6	17, 33, 83, 101	0
All	All	2045/2274 (89%)	0.26	215 (10%)	6	8	16, 31, 81, 103	0

All (215) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2143	VAL	10.5
1	A	2143	VAL	10.0
1	B	2143	VAL	9.3
1	B	2144	GLY	8.1
1	A	2194	PHE	7.9
1	C	2144	GLY	7.2
1	A	2144	GLY	7.1
1	B	2083	LEU	6.9
1	A	1685	GLU	6.5
1	B	1684	GLY	6.4
1	B	1681	VAL	6.2
1	C	1648	ASN	6.2
1	C	1647	ALA	6.1
1	B	1682	ILE	6.1
1	B	1480	LEU	6.0
1	C	1682	ILE	6.0
1	A	2191	LEU	5.9
1	C	2191	LEU	5.8
1	B	2082	LEU	5.7
1	B	2041	LEU	5.6
1	A	1684	GLY	5.4
1	B	1648	ASN	5.3
1	B	1838	ASP	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	2193	SER	5.3
1	A	1480	LEU	5.3
1	B	2084	PRO	5.2
1	B	1669	PHE	5.1
1	B	2189	LEU	5.0
1	A	1683	ASN	4.9
1	B	2085	ILE	4.9
1	B	2037	ARG	4.8
1	A	1910	PRO	4.8
1	B	2051	TYR	4.6
1	B	2145	GLU	4.6
1	B	1647	ALA	4.6
1	C	1646	ALA	4.6
1	B	2046	ARG	4.6
1	C	1679	ARG	4.6
1	A	1669	PHE	4.5
1	A	1838	ASP	4.5
1	B	1767	GLY	4.5
1	C	1669	PHE	4.5
1	A	1767	GLY	4.5
1	C	1911	ASN	4.5
1	C	1683	ASN	4.4
1	C	1685	GLU	4.4
1	B	1679	ARG	4.4
1	C	1546	GLU	4.4
1	C	1651	LYS	4.3
1	A	1911	ASN	4.2
1	B	2187	LYS	4.1
1	B	2036	ARG	4.1
1	C	2037	ARG	4.1
1	A	1681	VAL	4.0
1	B	1685	GLU	4.0
1	C	1681	VAL	3.9
1	A	1668	LYS	3.9
1	B	2188	GLY	3.9
1	A	1647	ALA	3.8
1	C	1680	THR	3.8
1	A	2141	HIS	3.8
1	B	1649	PRO	3.8
1	B	1651	LYS	3.8
1	A	2041	LEU	3.7
1	A	1648	ASN	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	2142	GLN	3.7
1	B	1839	GLU	3.7
1	C	1650	ASP	3.7
1	B	2081	GLU	3.6
1	C	1530	VAL	3.6
1	A	2145	GLU	3.6
1	C	1668	LYS	3.5
1	A	1645	ASP	3.5
1	C	1838	ASP	3.5
1	B	2142	GLN	3.5
1	A	1855	GLY	3.4
1	A	1481	ARG	3.4
1	C	1684	GLY	3.4
1	A	1646	ALA	3.4
1	C	1910	PRO	3.4
1	A	1682	ILE	3.4
1	A	1839	GLU	3.4
1	B	1911	ASN	3.4
1	C	1584	VAL	3.4
1	B	1483	ILE	3.3
1	C	1644	ASN	3.3
1	A	1546	GLU	3.3
1	C	2141	HIS	3.3
1	C	2145	GLU	3.3
1	C	1670	ASP	3.3
1	A	2081	GLU	3.3
1	A	1547	ASN	3.3
1	C	1547	ASN	3.2
1	B	1586	ALA	3.2
1	A	2193	SER	3.2
1	A	2190	LYS	3.2
1	A	1529	ASP	3.2
1	A	2049	ASP	3.2
1	A	2080	ARG	3.2
1	C	1548	GLY	3.2
1	B	1683	ASN	3.2
1	C	1839	GLU	3.1
1	C	2041	LEU	3.1
1	B	2045	ASN	3.1
1	C	1853	GLU	3.1
1	A	1853	GLU	3.1
1	B	2180	LYS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1483	ILE	3.0
1	B	1765	MET	3.0
1	B	1546	GLU	3.0
1	B	1680	THR	3.0
1	B	1910	PRO	3.0
1	B	1621	LEU	3.0
1	B	2049	ASP	3.0
1	C	1619	ILE	3.0
1	A	2037	ARG	3.0
1	B	1853	GLU	3.0
1	A	2036	ARG	3.0
1	C	1529	ASP	2.9
1	A	1766	LEU	2.9
1	A	2051	TYR	2.9
1	B	2146	ALA	2.9
1	A	1679	ARG	2.9
1	C	2051	TYR	2.9
1	C	1837	ASN	2.8
1	B	1585	VAL	2.8
1	C	1913	ALA	2.8
1	C	2192	GLU	2.8
1	B	1770	VAL	2.8
1	B	1913	ALA	2.8
1	C	1766	LEU	2.8
1	C	1767	GLY	2.8
1	C	1585	VAL	2.7
1	A	2038	GLU	2.7
1	A	1768	ARG	2.7
1	C	1621	LEU	2.7
1	A	1769	GLU	2.7
1	C	1855	GLY	2.7
1	B	2080	ARG	2.6
1	C	1491	GLU	2.6
1	B	1772	THR	2.6
1	A	2083	LEU	2.6
1	A	2142	GLN	2.6
1	C	1765	MET	2.6
1	B	1645	ASP	2.6
1	B	2038	GLU	2.6
1	C	1726	THR	2.5
1	B	1530	VAL	2.5
1	B	1664	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1824	LYS	2.5
1	A	2146	ALA	2.5
1	C	1769	GLU	2.5
1	B	1584	VAL	2.5
1	B	1481	ARG	2.5
1	C	1824	LYS	2.5
1	A	1680	THR	2.4
1	C	2083	LEU	2.4
1	A	2084	PRO	2.4
1	A	1670	ASP	2.4
1	C	1534	ASP	2.4
1	C	1554	GLU	2.4
1	C	2038	GLU	2.4
1	A	1837	ASN	2.4
1	C	1556	GLU	2.4
1	A	1651	LYS	2.4
1	C	1664	GLU	2.4
1	C	1656	LEU	2.4
1	C	1649	PRO	2.4
1	C	2084	PRO	2.4
1	A	2050	LYS	2.4
1	B	1529	ASP	2.4
1	A	2195	ALA	2.4
1	B	1852	THR	2.4
1	C	1531	LYS	2.3
1	C	1667	LYS	2.3
1	A	1765	MET	2.3
1	A	1725	ILE	2.3
1	C	2050	LYS	2.3
1	C	2045	ASN	2.3
1	C	1533	THR	2.3
1	B	2141	HIS	2.3
1	C	2046	ARG	2.3
1	C	1583	VAL	2.3
1	C	1586	ALA	2.3
1	B	1727	LEU	2.2
1	B	2043	THR	2.2
1	A	1585	VAL	2.2
1	B	1620	TYR	2.2
1	C	2081	GLU	2.2
1	C	1652	GLY	2.2
1	B	1739	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1670	ASP	2.1
1	B	2048	ASP	2.1
1	C	2190	LYS	2.1
1	C	1672	GLU	2.1
1	B	1644	ASN	2.1
1	A	2192	GLU	2.1
1	C	1686	GLU	2.1
1	C	2049	ASP	2.1
1	B	1766	LEU	2.1
1	B	2179	TYR	2.1
1	B	1668	LYS	2.1
1	B	2040	LEU	2.1
1	A	1620	TYR	2.1
1	A	1889	LEU	2.1
1	B	1619	ILE	2.1
1	C	1768	ARG	2.1
1	B	2161	ALA	2.1
1	C	1645	ASP	2.0
1	B	1836	THR	2.0
1	A	1528	ALA	2.0
1	B	1531	LYS	2.0
1	A	1619	ILE	2.0
1	C	1803	ILE	2.0
1	C	1524	LYS	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)

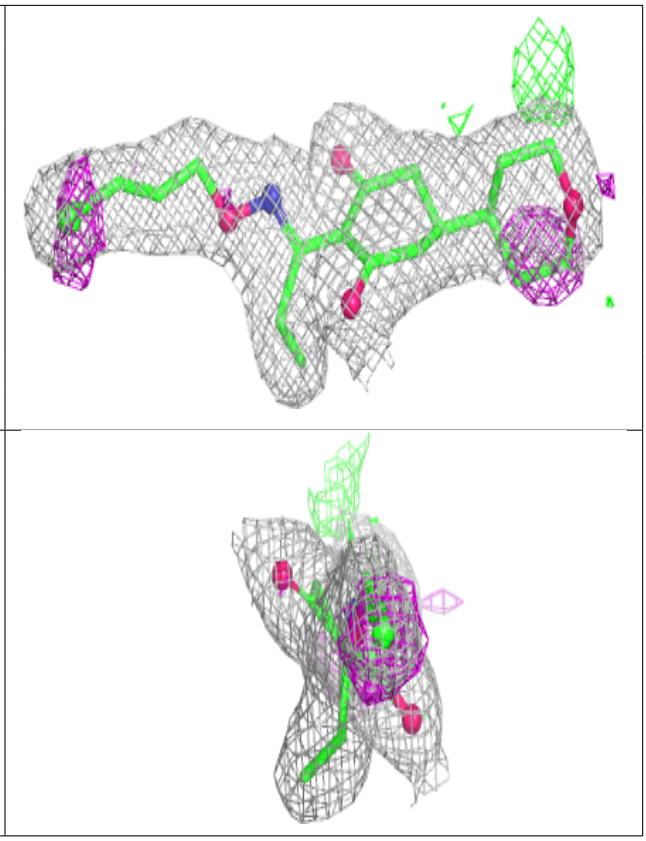
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	B89	A	1	23/23	0.90	0.15	29,38,49,52	0
2	B89	C	3	23/23	0.91	0.17	43,52,59,64	0
2	B89	B	2	23/23	0.93	0.15	28,37,46,50	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.

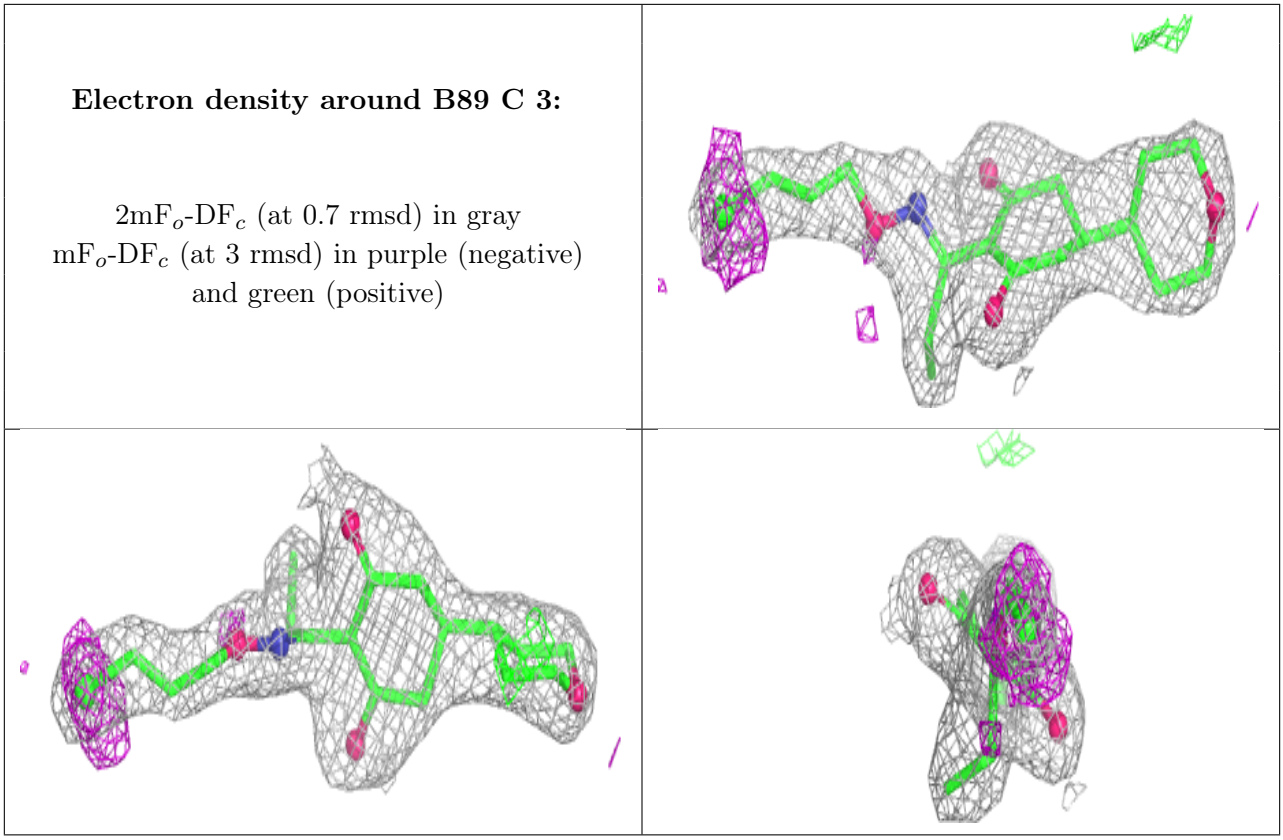
Electron density around B89 A 1:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



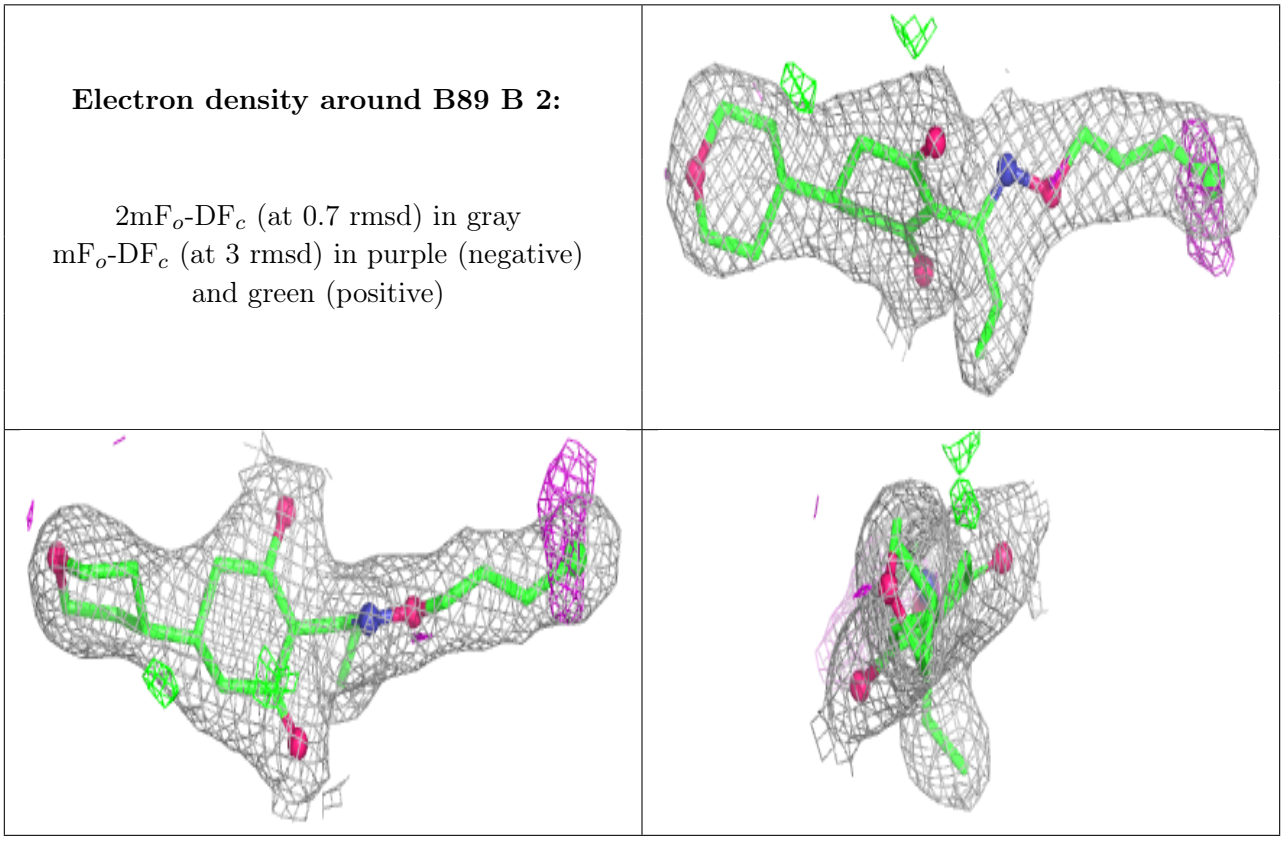
Electron density around B89 C 3:

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



Electron density around B89 B 2:

$2mF_o$-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.