



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:03 PM UTC

PDB ID : 2X24 / pdb_00002x24
Title : bovine ACC2 CT domain in complex with inhibitor
Authors : Oster, L.; Folmer, R.; Blaho, S.; Wiberg, F.; Hallberg, K.
Deposited on : 2010-01-11
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

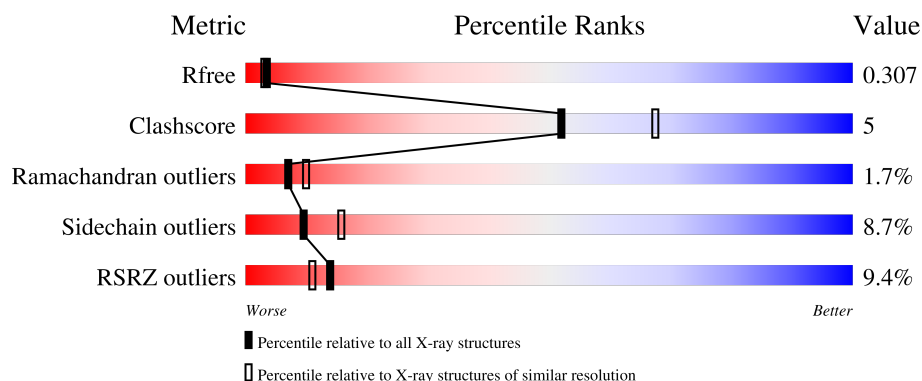
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	793	7% 64% 17% • 18%
1	B	793	8% 63% 18% • • 16%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10763 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

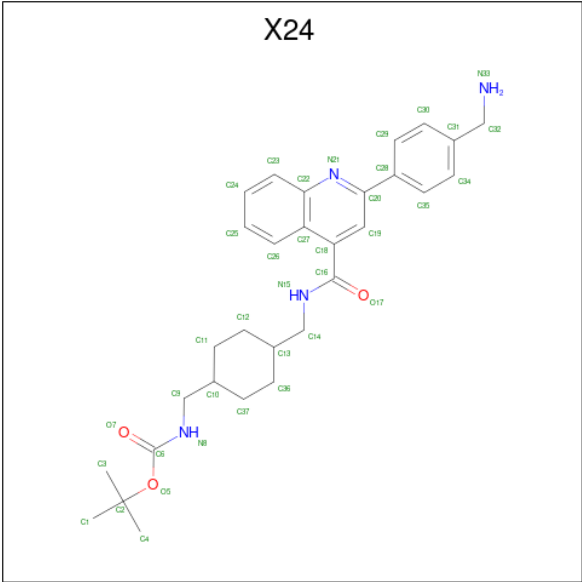
- Molecule 1 is a protein called ACETYL-COA CARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	654	Total	C	N	O	S	0	0	0
			5219	3339	899	958	23			
1	B	667	Total	C	N	O	S	0	0	0
			5324	3404	919	976	25			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	expression tag	PDB 2X24
A	-8	GLY	-	expression tag	PDB 2X24
A	-7	SER	-	expression tag	PDB 2X24
A	-6	SER	-	expression tag	PDB 2X24
A	-5	HIS	-	expression tag	PDB 2X24
A	-4	HIS	-	expression tag	PDB 2X24
A	-3	HIS	-	expression tag	PDB 2X24
A	-2	HIS	-	expression tag	PDB 2X24
A	-1	HIS	-	expression tag	PDB 2X24
A	0	HIS	-	expression tag	PDB 2X24
B	-9	MET	-	expression tag	PDB 2X24
B	-8	GLY	-	expression tag	PDB 2X24
B	-7	SER	-	expression tag	PDB 2X24
B	-6	SER	-	expression tag	PDB 2X24
B	-5	HIS	-	expression tag	PDB 2X24
B	-4	HIS	-	expression tag	PDB 2X24
B	-3	HIS	-	expression tag	PDB 2X24
B	-2	HIS	-	expression tag	PDB 2X24
B	-1	HIS	-	expression tag	PDB 2X24
B	0	HIS	-	expression tag	PDB 2X24

- Molecule 2 is TERT-BUTYL [(TRANS-4-{{(2-[4-(AMINOMETHYL)PHENYL]QUINOLIN-4-YL)CARBONYL)AMINO}METHYL}CYCLOHEXYL)METHYL]CARBAMATE (CCD ID: X24) (formula: C₃₀H₃₈N₄O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			37	30	4	3		
2	B	1	Total	C	N	O	0	0
			37	30	4	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	62	Total	O	0	0
			62	62		
3	B	84	Total	O	0	0
			84	84		

- Molecule 1: ACETYL-COA CARBOXYLASE





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	225.19Å 104.87Å 85.08Å 90.00° 95.67° 90.00°	Depositor
Resolution (Å)	29.70 – 2.40 29.70 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.70-2.40) 93.9 (29.70-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.232 , 0.283 (Not available) , 0.307	Depositor DCC
R_{free} test set	3643 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	10763	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: X24

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	0.91	0/5342	1.45	37/7245 (0.5%)
1	B	0.93	1/5451 (0.0%)	1.48	54/7395 (0.7%)
All	All	0.92	1/10793 (0.0%)	1.47	91/14640 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	496	VAL	CA-C	5.04	1.60	1.52

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	689	VAL	CA-C-N	10.99	141.48	121.70
1	B	689	VAL	C-N-CA	10.99	141.48	121.70
1	A	178	GLU	CA-C-N	9.72	139.19	121.70
1	A	178	GLU	C-N-CA	9.72	139.19	121.70
1	A	198	SER	CA-C-N	9.70	139.17	121.70
1	A	198	SER	C-N-CA	9.70	139.17	121.70
1	B	178	GLU	CA-C-N	9.13	138.14	121.70
1	B	178	GLU	C-N-CA	9.13	138.14	121.70
1	B	198	SER	CA-C-N	8.84	137.62	121.70
1	B	198	SER	C-N-CA	8.84	137.62	121.70
1	B	468	ASP	CA-CB-CG	8.53	121.13	112.60
1	B	439	ASN	CA-CB-CG	7.86	120.46	112.60
1	B	178	GLU	N-CA-C	7.63	119.38	111.14
1	B	457	ASP	CA-CB-CG	7.34	119.94	112.60
1	B	401	VAL	N-CA-CB	6.99	115.90	110.45
1	A	472	GLU	N-CA-C	-6.84	104.83	113.72
1	B	274	VAL	N-CA-C	6.73	117.60	108.17
1	B	541	ILE	N-CA-C	6.49	118.15	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	703	ASN	N-CA-C	6.49	118.15	111.14
1	A	155	ASN	N-CA-C	6.41	118.69	109.14
1	B	237	GLY	CA-C-N	6.37	129.05	120.65
1	B	237	GLY	C-N-CA	6.37	129.05	120.65
1	A	118	ASN	CA-CB-CG	6.29	118.89	112.60
1	B	352	LYS	N-CA-C	-6.21	104.76	112.90
1	B	388	SER	N-CA-C	6.17	118.95	110.24
1	B	76	ASP	CA-CB-CG	6.16	118.76	112.60
1	A	99	LYS	N-CA-C	-6.05	99.37	109.24
1	B	42	VAL	N-CA-C	6.02	117.49	110.62
1	A	259	ARG	N-CA-C	6.02	118.00	108.79
1	B	346	VAL	N-CA-CB	6.02	116.85	110.17
1	A	237	GLY	CA-C-N	5.98	128.21	120.44
1	A	237	GLY	C-N-CA	5.98	128.21	120.44
1	A	339	PRO	CA-C-N	5.96	128.58	120.54
1	A	339	PRO	C-N-CA	5.96	128.58	120.54
1	B	556	PRO	CA-C-N	5.92	129.01	120.38
1	B	556	PRO	C-N-CA	5.92	129.01	120.38
1	A	98	PHE	CA-CB-CG	5.82	119.62	113.80
1	A	304	GLN	CA-C-N	5.80	128.63	120.28
1	A	304	GLN	C-N-CA	5.80	128.63	120.28
1	B	689	VAL	CA-C-O	-5.80	113.53	120.78
1	A	457	ASP	CA-CB-CG	5.79	118.39	112.60
1	A	400	MET	CA-C-N	5.78	124.96	120.33
1	A	400	MET	C-N-CA	5.78	124.96	120.33
1	B	386	TRP	N-CA-C	5.78	117.30	108.52
1	B	297	ASP	CA-C-N	5.76	128.98	120.74
1	B	297	ASP	C-N-CA	5.76	128.98	120.74
1	A	682	SER	CA-C-N	5.76	128.00	120.28
1	A	682	SER	C-N-CA	5.76	128.00	120.28
1	B	354	PRO	N-CA-C	5.71	120.19	111.34
1	B	526	GLY	CA-C-N	5.71	126.31	119.98
1	B	526	GLY	C-N-CA	5.71	126.31	119.98
1	B	163	ALA	CA-C-N	5.68	128.46	120.28
1	B	163	ALA	C-N-CA	5.68	128.46	120.28
1	B	472	GLU	N-CA-C	-5.67	106.36	113.28
1	A	61	ASP	CA-C-N	5.62	132.28	121.54
1	A	61	ASP	C-N-CA	5.62	132.28	121.54
1	A	59	SER	N-CA-C	5.60	122.19	109.81
1	B	472	GLU	CA-C-N	5.59	130.51	122.35
1	B	472	GLU	C-N-CA	5.59	130.51	122.35
1	B	191	PRO	CA-C-N	5.57	128.53	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	191	PRO	C-N-CA	5.57	128.53	120.79
1	B	220	ASP	CA-CB-CG	5.51	118.11	112.60
1	B	178	GLU	CA-C-O	-5.49	115.05	120.70
1	B	350	THR	CB-CA-C	5.47	118.21	109.62
1	B	328	VAL	CA-C-N	5.46	128.61	120.31
1	B	328	VAL	C-N-CA	5.46	128.61	120.31
1	B	387	GLN	N-CA-C	-5.46	98.33	107.99
1	A	338	MET	N-CA-C	5.43	117.45	110.39
1	A	293	VAL	N-CA-CB	5.33	116.67	110.65
1	A	503	ILE	CA-C-N	5.32	127.46	120.60
1	A	503	ILE	C-N-CA	5.32	127.46	120.60
1	A	703	ASN	N-CA-C	5.31	116.76	111.07
1	B	617	GLN	CA-C-N	5.30	127.94	120.42
1	B	617	GLN	C-N-CA	5.30	127.94	120.42
1	A	132	ASP	CA-CB-CG	5.29	117.89	112.60
1	B	302	ASN	CA-C-N	5.29	127.89	120.28
1	B	302	ASN	C-N-CA	5.29	127.89	120.28
1	B	440	LEU	N-CA-C	5.27	117.93	111.82
1	B	436	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	198	SER	N-CA-C	5.24	116.27	108.31
1	A	533	ASP	CA-C-N	5.23	127.55	120.38
1	A	533	ASP	C-N-CA	5.23	127.55	120.38
1	A	240	ALA	CA-C-N	5.22	125.77	119.98
1	A	240	ALA	C-N-CA	5.22	125.77	119.98
1	B	100	MET	N-CA-C	5.21	117.73	109.24
1	A	480	ALA	N-CA-C	5.11	117.07	109.25
1	B	704	GLN	CA-C-N	5.11	127.08	120.44
1	B	704	GLN	C-N-CA	5.11	127.08	120.44
1	A	627	ASP	CA-CB-CG	5.11	117.71	112.60
1	B	429	VAL	N-CA-CB	5.10	117.24	110.26
1	B	59	SER	N-CA-C	5.00	120.87	109.81

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5219	0	5207	59	0
1	B	5324	0	5308	59	0
2	A	37	0	38	1	0
2	B	37	0	38	1	0
3	A	62	0	0	0	0
3	B	84	0	0	6	0
All	All	10763	0	10591	109	0

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 5.

All (109) 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:626:HIS:HE1	1:B:163:ALA:H	1.29	0.81
1:A:118:ASN:HD22	1:A:154:ALA:H	1.32	0.77
1:A:198:SER:HB3	1:A:199:SER:HB2	1.73	0.71
1:B:289:ALA:O	1:B:293:VAL:HG23	1.91	0.70
1:B:429:VAL:HG22	1:B:449:GLN:HB2	1.74	0.69
1:A:276:GLN:HE22	1:A:311:MET:HB2	1.57	0.68
1:B:155:ASN:HD22	1:B:157:GLY:H	1.44	0.66
1:A:163:ALA:H	1:B:626:HIS:HE1	1.45	0.65
1:A:198:SER:HB3	1:A:199:SER:CB	2.30	0.60
1:B:102:LEU:HD11	1:B:113:ILE:HG12	1.84	0.60
1:B:443:GLU:HA	3:B:2054:HOH:O	2.01	0.59
1:B:95:MET:HE3	1:B:135:TYR:HB2	1.84	0.58
1:A:702:ASN:HD22	1:A:705:THR:H	1.52	0.58
1:B:64:PRO:HD2	1:B:67:ILE:HD12	1.85	0.57
1:A:71:THR:HA	1:A:85:ASN:HD21	1.70	0.56
1:B:37:LEU:HD13	1:B:120:ILE:HG12	1.88	0.56
1:A:404:ALA:HB3	1:A:461:LYS:HD3	1.87	0.56
1:B:65:LYS:HD3	1:B:65:LYS:H	1.71	0.56
1:B:378:PRO:HA	1:B:386:TRP:HA	1.87	0.56
1:A:155:ASN:HD22	1:A:157:GLY:H	1.54	0.55
1:A:370:PRO:O	1:A:373:LEU:HB3	2.07	0.55
1:A:374:LEU:HD22	1:A:391:PHE:HE2	1.71	0.55
1:B:276:GLN:HE22	1:B:311:MET:HB2	1.72	0.55
1:A:319:VAL:HG21	1:A:330:THR:HG21	1.88	0.55
1:B:664:VAL:HG11	1:B:684:LEU:HD21	1.89	0.54
1:B:136:LEU:HD13	1:B:238:MET:HG2	1.89	0.54
1:B:175:VAL:HG22	1:B:182:LYS:HB3	1.90	0.53
1:A:39:THR:HG21	1:A:120:ILE:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:THR:O	1:A:466:ILE:HG13	2.10	0.52
1:A:163:ALA:H	1:B:626:HIS:CE1	2.27	0.52
1:B:517:TYR:HA	1:B:544:TYR:O	2.11	0.51
1:A:181:HIS:O	1:A:182:LYS:HB2	2.12	0.50
1:B:547:ARG:HG2	1:B:641:ILE:HG22	1.93	0.50
1:A:251:VAL:HG11	1:A:338:MET:SD	2.51	0.50
1:B:370:PRO:HG2	1:B:408:VAL:HG21	1.93	0.49
1:A:146:GLY:HA2	1:A:250:ILE:CG2	2.43	0.49
1:B:520:PRO:HG3	1:B:644:TRP:HB2	1.93	0.49
1:A:172:VAL:HG13	1:A:184:ILE:HD12	1.95	0.49
1:B:239:ILE:HD12	1:B:267:LEU:HD11	1.94	0.48
1:A:574:ARG:HD3	1:A:604:LEU:HD21	1.94	0.48
1:B:401:VAL:HG23	3:B:2030:HOH:O	2.12	0.48
1:B:227:GLY:HA2	1:B:232:ASN:HD21	1.78	0.48
1:B:622:PHE:O	1:B:626:HIS:HD2	1.97	0.48
1:A:64:PRO:HD2	1:A:67:ILE:HD12	1.95	0.47
1:A:74:VAL:HG21	1:A:84:MET:HE2	1.95	0.47
1:B:525:ARG:NH1	1:B:552:SER:OG	2.47	0.47
1:A:95:MET:HE1	1:A:127:PHE:CE2	2.50	0.47
1:A:417:ILE:HD11	1:A:656:ARG:HG2	1.96	0.46
1:A:198:SER:HB3	1:A:199:SER:CA	2.45	0.46
1:B:508:ARG:HH22	1:B:509:LYS:HE3	1.80	0.46
1:B:692:GLU:HB3	1:B:696:LYS:HD2	1.97	0.46
1:A:102:LEU:O	1:A:110:GLY:HA2	2.15	0.46
1:A:95:MET:HE3	1:A:135:TYR:HB2	1.97	0.46
1:A:269:ARG:HA	1:A:269:ARG:HD2	1.79	0.46
1:A:269:ARG:CZ	1:B:498:LYS:HG2	2.46	0.46
1:A:702:ASN:ND2	1:A:705:THR:H	2.12	0.46
1:B:478:ILE:HD12	1:B:516:ILE:HG12	1.97	0.46
1:B:617:GLN:HA	1:B:620:LEU:HD12	1.98	0.46
1:A:118:ASN:ND2	1:A:153:ALA:HA	2.30	0.46
1:B:198:SER:HB3	1:B:199:SER:HB3	1.96	0.46
1:B:704:GLN:HE21	1:B:708:GLN:NE2	2.13	0.46
1:B:370:PRO:HG3	1:B:425:GLU:HA	1.99	0.45
1:A:82:VAL:HG13	1:A:84:MET:HG2	1.97	0.45
1:B:247:TYR:OH	1:B:468:ASP:OD1	2.26	0.45
1:A:687:TRP:CD1	1:A:709:TRP:HZ2	2.34	0.45
1:B:569:LEU:HD23	1:B:612:LEU:HD23	1.99	0.45
1:B:689:VAL:HB	1:B:690:GLU:HB2	1.99	0.45
1:A:626:HIS:CE1	1:B:163:ALA:H	2.20	0.45
1:A:160:ILE:HG22	1:B:563:LYS:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:702:ASN:HD22	1:B:705:THR:H	1.66	0.44
1:A:53:LEU:HD11	1:A:102:LEU:HD23	2.00	0.44
1:A:230:VAL:HG21	1:B:632:MET:HG2	1.98	0.44
1:A:293:VAL:HG11	2:B:1714:X24:H361	2.00	0.44
1:A:358:GLU:HA	1:A:645:LYS:O	2.18	0.44
1:A:622:PHE:O	1:A:626:HIS:HD2	2.00	0.43
1:B:463:ALA:HB3	3:B:2013:HOH:O	2.19	0.43
2:A:1715:X24:H29	2:A:1715:X24:H19	1.76	0.43
1:A:452:GLN:OE1	1:A:483:ARG:HD2	2.19	0.43
1:B:400:MET:HB2	1:B:461:LYS:HE3	2.01	0.43
1:A:50:ARG:HG3	1:A:68:LEU:HB3	2.00	0.43
1:A:632:MET:HG2	1:B:230:VAL:HG11	1.99	0.43
1:B:629:ALA:HA	1:B:632:MET:HE3	2.01	0.43
1:B:426:THR:HG22	1:B:452:GLN:CG	2.49	0.43
1:A:425:GLU:OE1	1:A:427:ARG:NH2	2.32	0.42
1:A:173:ALA:HB1	1:A:185:LYS:HE3	2.01	0.42
1:A:699:LEU:HB3	1:A:705:THR:HG21	2.01	0.42
1:A:272:GLN:OE1	1:A:464:GLN:NE2	2.53	0.42
1:B:287:ALA:HB1	1:B:299:TYR:HB2	2.01	0.42
1:A:200:LEU:HD13	1:A:224:LYS:HD3	2.01	0.42
1:B:227:GLY:CA	1:B:232:ASN:HD21	2.32	0.42
1:B:319:VAL:HG21	1:B:330:THR:HG21	2.00	0.42
1:A:605:LYS:HA	1:A:608:GLU:HG2	2.02	0.42
1:B:106:GLU:HB3	1:B:347:PRO:HB2	2.01	0.42
1:A:553:VAL:HG22	1:B:233:LEU:HD21	2.01	0.41
1:B:176:ASP:HB2	1:B:182:LYS:HG3	2.02	0.41
1:A:617:GLN:HA	1:A:620:LEU:HD12	2.02	0.41
1:B:191:PRO:HD3	1:B:214:SER:O	2.20	0.41
1:B:368:TYR:HA	3:B:2037:HOH:O	2.20	0.41
1:A:239:ILE:HD12	1:A:267:LEU:HD11	2.03	0.41
1:B:174:TRP:HB3	3:B:2011:HOH:O	2.20	0.41
1:A:637:VAL:HG23	1:A:638:ILE:HG23	2.03	0.41
1:A:67:ILE:HG13	1:A:103:LYS:HB2	2.03	0.40
1:A:146:GLY:HA2	1:A:250:ILE:HG22	2.02	0.40
1:B:569:LEU:HD11	1:B:616:HIS:HA	2.03	0.40
1:A:207:HIS:HB2	1:A:216:TYR:CE1	2.56	0.40
1:A:289:ALA:O	1:A:293:VAL:HG13	2.21	0.40
1:A:485:PHE:HB2	1:B:284:LEU:HD13	2.03	0.40
1:B:185:LYS:HD2	1:B:186:TYR:HD2	1.87	0.40
1:B:534:THR:HG21	3:B:2073:HOH:O	2.21	0.40

There are no symmetry-related clashes.

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	648/793 (82%)	610 (94%)	29 (4%)	9 (1%)	9	13
1	B	663/793 (84%)	614 (93%)	36 (5%)	13 (2%)	6	7
All	All	1311/1586 (83%)	1224 (93%)	65 (5%)	22 (2%)	7	10

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	LYS
1	A	179	ASP
1	A	526	GLY
1	B	179	ASP
1	B	526	GLY
1	B	690	GLU
1	B	59	SER
1	B	197	ILE
1	A	182	LYS
1	A	197	ILE
1	A	211	ASP
1	A	258	CYS
1	B	379	HIS
1	B	380	PRO
1	B	689	VAL
1	A	495	GLN
1	B	495	GLN
1	B	669	LEU
1	A	59	SER
1	B	262	GLY
1	B	212	GLY
1	B	378	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	560/683 (82%)	517 (92%)	43 (8%)	12	20
1	B	572/683 (84%)	517 (90%)	55 (10%)	8	12
All	All	1132/1366 (83%)	1034 (91%)	98 (9%)	9	16

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ARG
1	A	35	GLN
1	A	56	MET
1	A	65	LYS
1	A	69	THR
1	A	87	LEU
1	A	91	ASN
1	A	100	MET
1	A	115	LEU
1	A	149	ARG
1	A	160	ILE
1	A	184	ILE
1	A	206	LYS
1	A	208	VAL
1	A	209	GLU
1	A	214	SER
1	A	215	ARG
1	A	220	ASP
1	A	234	ARG
1	A	259	ARG
1	A	261	LEU
1	A	281	HIS
1	A	297	ASP
1	A	298	VAL
1	A	342	ASN
1	A	356	ASP
1	A	440	LEU

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Mol	Chain	Res	Type
1	A	445	LYS
1	A	458	SER
1	A	495	GLN
1	A	505	ASP
1	A	528	SER
1	A	552	SER
1	A	581	LYS
1	A	603	GLN
1	A	605	LYS
1	A	614	MET
1	A	635	LYS
1	A	645	LYS
1	A	649	SER
1	A	656	ARG
1	A	681	GLN
1	A	684	LEU
1	B	28	GLN
1	B	56	MET
1	B	61	ASP
1	B	65	LYS
1	B	69	THR
1	B	102	LEU
1	B	115	LEU
1	B	120	ILE
1	B	143	ARG
1	B	149	ARG
1	B	160	ILE
1	B	165	GLU
1	B	175	VAL
1	B	176	ASP
1	B	182	LYS
1	B	184	ILE
1	B	192	GLN
1	B	200	LEU
1	B	206	LYS
1	B	208	VAL
1	B	209	GLU
1	B	215	ARG
1	B	225	GLU
1	B	234	ARG
1	B	261	LEU
1	B	268	VAL

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Mol	Chain	Res	Type
1	B	281	HIS
1	B	294	LEU
1	B	300	THR
1	B	342	ASN
1	B	352	LYS
1	B	355	ILE
1	B	356	ASP
1	B	360	GLU
1	B	386	TRP
1	B	395	SER
1	B	428	THR
1	B	429	VAL
1	B	441	ASP
1	B	443	GLU
1	B	534	THR
1	B	539	LEU
1	B	559	THR
1	B	574	ARG
1	B	603	GLN
1	B	610	LEU
1	B	612	LEU
1	B	656	ARG
1	B	665	LYS
1	B	670	ARG
1	B	672	CYS
1	B	678	MET
1	B	685	ARG
1	B	690	GLU
1	B	702	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	118	ASN
1	A	155	ASN
1	A	201	ASN
1	A	207	HIS
1	A	232	ASN
1	A	276	GLN
1	A	281	HIS
1	A	342	ASN

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Mol	Chain	Res	Type
1	A	439	ASN
1	A	448	GLN
1	A	464	GLN
1	A	495	GLN
1	A	626	HIS
1	A	681	GLN
1	A	702	ASN
1	B	78	GLN
1	B	91	ASN
1	B	155	ASN
1	B	201	ASN
1	B	232	ASN
1	B	276	GLN
1	B	342	ASN
1	B	393	GLN
1	B	495	GLN
1	B	626	HIS
1	B	677	HIS
1	B	702	ASN
1	B	704	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	X24	A	1715	-	40,40,40	0.75	1 (2%)	56,56,56	2.22	12 (21%)
2	X24	B	1714	-	40,40,40	0.75	0	56,56,56	2.80	15 (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	X24	A	1715	-	-	10/25/35/35	0/4/4/4
2	X24	B	1714	-	-	13/25/35/35	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1715	X24	C18-C16	-2.07	1.47	1.50

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1714	X24	O5-C6-N8	8.34	121.84	110.00
2	B	1714	X24	C18-C16-N15	7.74	125.93	116.02
2	B	1714	X24	C10-C9-N8	-7.26	100.17	112.77
2	B	1714	X24	C13-C14-N15	-7.16	100.35	112.77
2	B	1714	X24	O7-C6-N8	-6.70	114.84	124.93
2	A	1715	X24	C28-C20-N21	6.59	125.81	117.05
2	A	1715	X24	C19-C20-C28	-6.22	113.38	121.82
2	B	1714	X24	C20-N21-C22	5.70	122.59	118.12
2	A	1715	X24	O5-C6-N8	5.39	117.66	110.00
2	A	1715	X24	C13-C14-N15	-4.99	104.12	112.77
2	A	1715	X24	C27-C18-C16	4.62	127.43	120.82
2	B	1714	X24	C2-O5-C6	4.58	127.92	120.97
2	A	1715	X24	C2-O5-C6	4.31	127.50	120.97
2	A	1715	X24	O7-C6-N8	-3.81	119.19	124.93
2	A	1715	X24	C20-N21-C22	3.71	121.03	118.12
2	B	1714	X24	O17-C16-N15	-3.32	116.13	122.59
2	B	1714	X24	C36-C37-C10	-3.10	106.51	112.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1715	X24	C29-C28-C20	-3.09	116.39	121.28
2	B	1714	X24	O17-C16-C18	-2.97	117.92	121.73
2	B	1714	X24	C36-C13-C12	2.97	116.54	109.29
2	B	1714	X24	C27-C22-N21	-2.78	119.86	122.80
2	B	1714	X24	C12-C11-C10	-2.62	107.42	112.36
2	A	1715	X24	C36-C13-C12	2.52	115.46	109.29
2	A	1715	X24	C36-C37-C10	-2.32	107.98	112.36
2	B	1714	X24	O5-C2-C3	2.32	116.35	107.21
2	A	1715	X24	C27-C22-N21	-2.12	120.56	122.80
2	B	1714	X24	C9-N8-C6	2.02	124.57	121.72

There are no chirality outliers.

All (23) torsion outliers are listed below:

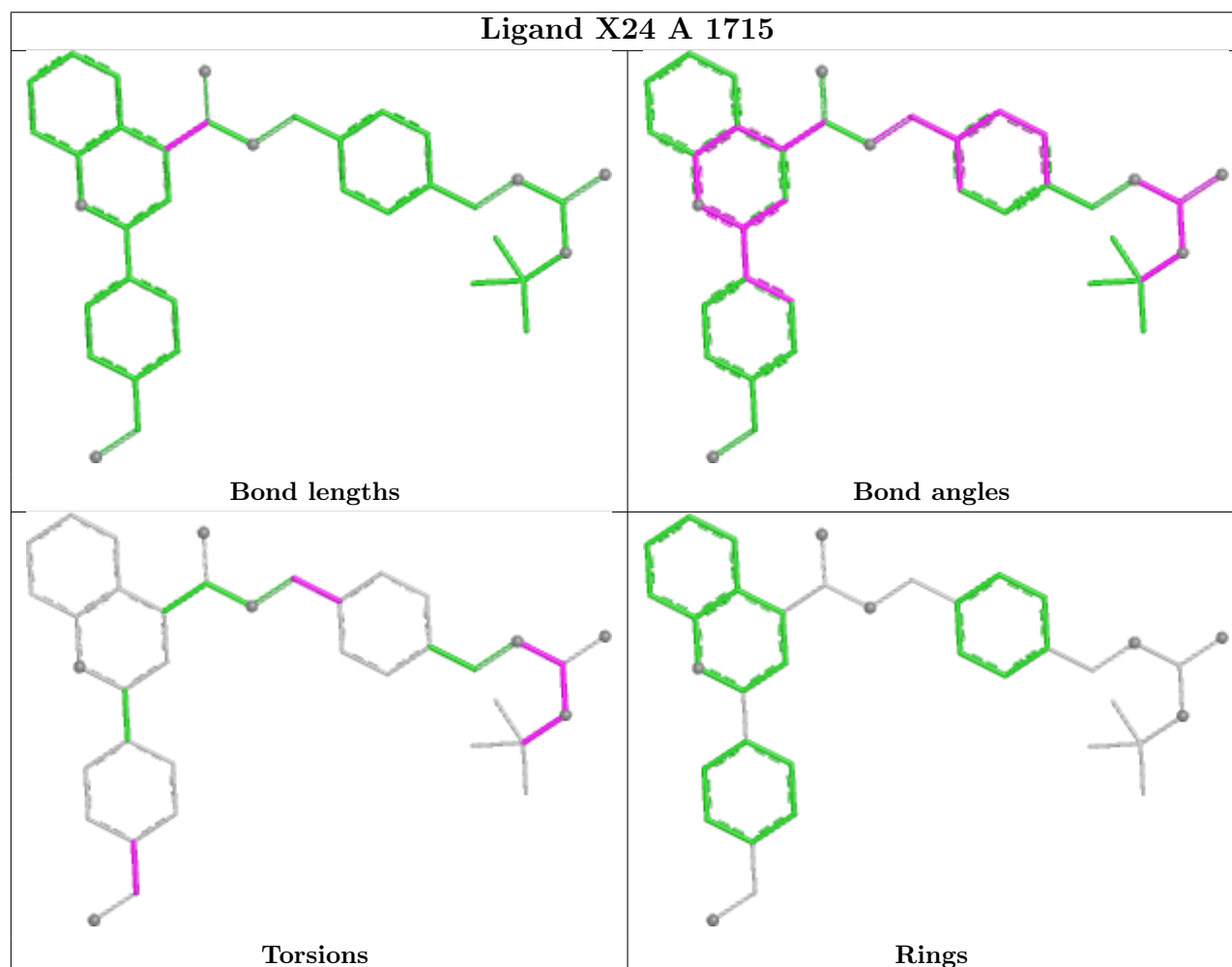
Mol	Chain	Res	Type	Atoms
2	B	1714	X24	C11-C10-C9-N8
2	B	1714	X24	C37-C10-C9-N8
2	B	1714	X24	C12-C13-C14-N15
2	B	1714	X24	C36-C13-C14-N15
2	A	1715	X24	C3-C2-O5-C6
2	A	1715	X24	C1-C2-O5-C6
2	A	1715	X24	C4-C2-O5-C6
2	B	1714	X24	O7-C6-O5-C2
2	B	1714	X24	C1-C2-O5-C6
2	B	1714	X24	C3-C2-O5-C6
2	B	1714	X24	C4-C2-O5-C6
2	B	1714	X24	N8-C6-O5-C2
2	B	1714	X24	O17-C16-N15-C14
2	B	1714	X24	C18-C16-N15-C14
2	A	1715	X24	N8-C6-O5-C2
2	A	1715	X24	O7-C6-O5-C2
2	A	1715	X24	O5-C6-N8-C9
2	B	1714	X24	O5-C6-N8-C9
2	A	1715	X24	O7-C6-N8-C9
2	B	1714	X24	O7-C6-N8-C9
2	A	1715	X24	C12-C13-C14-N15
2	A	1715	X24	C36-C13-C14-N15
2	A	1715	X24	C34-C31-C32-N33

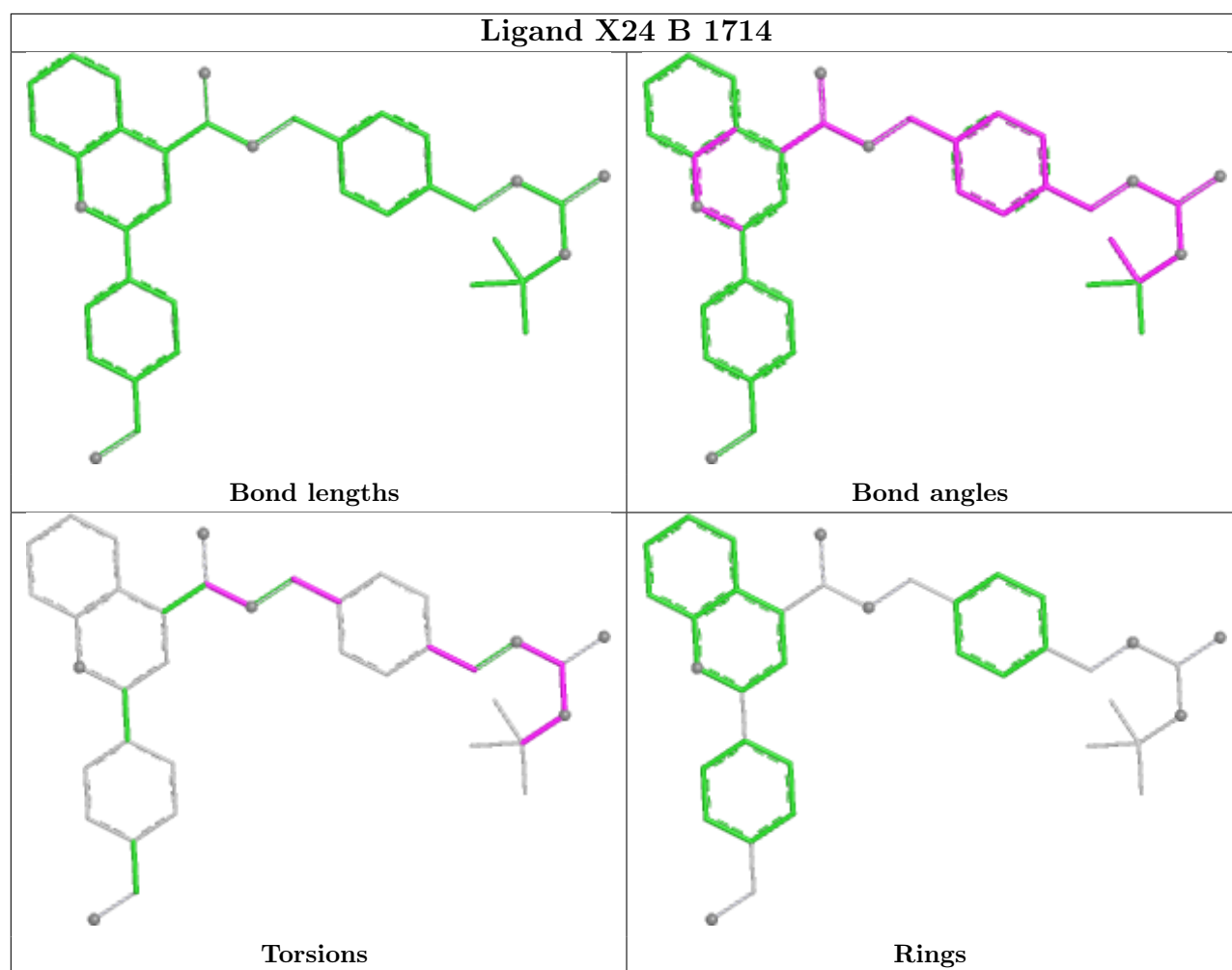
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1715	X24	1	0
2	B	1714	X24	1	0

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





5.7 Other polymers [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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	654/793 (82%)	0.73	59 (9%)	15 12	15, 35, 66, 88	0
1	B	667/793 (84%)	0.63	65 (9%)	13 10	14, 34, 64, 92	0
All	All	1321/1586 (83%)	0.68	124 (9%)	14 11	14, 34, 65, 92	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	581	LYS	6.5
1	B	689	VAL	5.7
1	B	26	LEU	5.0
1	B	383	LYS	4.6
1	B	380	PRO	4.6
1	A	687	TRP	4.6
1	B	196	ARG	4.5
1	A	581	LYS	4.4
1	A	681	GLN	4.1
1	A	381	THR	4.1
1	B	381	THR	3.9
1	B	384	GLY	3.8
1	B	208	VAL	3.7
1	B	694	ALA	3.7
1	A	63	TYR	3.7
1	B	671	ALA	3.7
1	B	198	SER	3.6
1	B	27	LEU	3.5
1	B	713	HIS	3.5
1	A	59	SER	3.5
1	A	666	GLN	3.5
1	A	713	HIS	3.5
1	A	604	LEU	3.4
1	A	60	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	680	VAL	3.4
1	A	606	ALA	3.4
1	B	179	ASP	3.3
1	A	712	ALA	3.3
1	B	197	ILE	3.3
1	B	379	HIS	3.2
1	A	124	ILE	3.2
1	A	56	MET	3.1
1	A	690	GLU	3.1
1	B	28	GLN	3.1
1	A	382	LEU	3.1
1	B	604	LEU	3.0
1	A	70	TYR	3.0
1	B	58	PRO	3.0
1	A	200	LEU	3.0
1	B	180	PRO	3.0
1	A	62	LYS	2.9
1	B	193	ASP	2.9
1	B	194	TYR	2.9
1	B	211	ASP	2.9
1	A	180	PRO	2.8
1	B	691	THR	2.8
1	B	59	SER	2.8
1	B	382	LEU	2.8
1	B	686	ARG	2.8
1	A	384	GLY	2.8
1	B	364	SER	2.8
1	A	55	LYS	2.8
1	B	229	GLY	2.8
1	A	184	ILE	2.8
1	A	87	LEU	2.8
1	A	178	GLU	2.8
1	B	60	PRO	2.7
1	B	195	THR	2.7
1	B	579	ILE	2.7
1	A	603	GLN	2.7
1	B	210	GLU	2.7
1	B	385	SER	2.6
1	B	606	ALA	2.6
1	B	57	TRP	2.6
1	A	176	ASP	2.6
1	A	27	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	610	LEU	2.5
1	A	42	VAL	2.5
1	B	448	GLN	2.5
1	A	61	ASP	2.5
1	A	226	GLU	2.5
1	A	612	LEU	2.5
1	B	63	TYR	2.5
1	A	175	VAL	2.5
1	A	179	ASP	2.5
1	B	189	LEU	2.4
1	A	32	PHE	2.4
1	A	85	ASN	2.4
1	A	198	SER	2.4
1	B	192	GLN	2.4
1	B	603	GLN	2.4
1	B	206	LYS	2.4
1	B	209	GLU	2.4
1	B	213	GLU	2.3
1	A	714	GLY	2.3
1	B	90	GLY	2.3
1	B	228	LEU	2.3
1	B	615	TYR	2.3
1	B	191	PRO	2.3
1	A	57	TRP	2.3
1	A	683	MET	2.3
1	B	343	ARG	2.3
1	A	355	ILE	2.2
1	B	214	SER	2.2
1	A	190	THR	2.2
1	A	174	TRP	2.2
1	A	173	ALA	2.2
1	A	572	THR	2.2
1	B	75	LEU	2.2
1	B	378	PRO	2.2
1	B	673	PRO	2.2
1	A	65	LYS	2.2
1	B	62	LYS	2.2
1	A	37	LEU	2.1
1	B	175	VAL	2.1
1	A	614	MET	2.1
1	A	94	GLY	2.1
1	B	612	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	435	ALA	2.1
1	B	712	ALA	2.1
1	A	196	ARG	2.1
1	A	293	VAL	2.1
1	A	578	PRO	2.1
1	B	177	PRO	2.1
1	A	122	PHE	2.0
1	A	105	LEU	2.0
1	B	201	ASN	2.0
1	B	687	TRP	2.0
1	B	698	TYR	2.0
1	A	684	LEU	2.0
1	A	605	LYS	2.0
1	B	212	GLY	2.0
1	A	77	PRO	2.0
1	A	682	SER	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

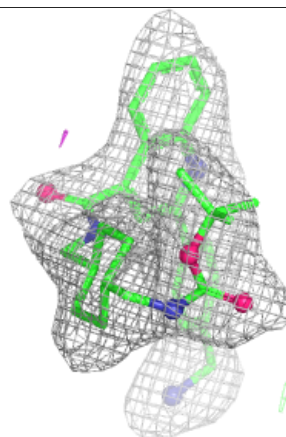
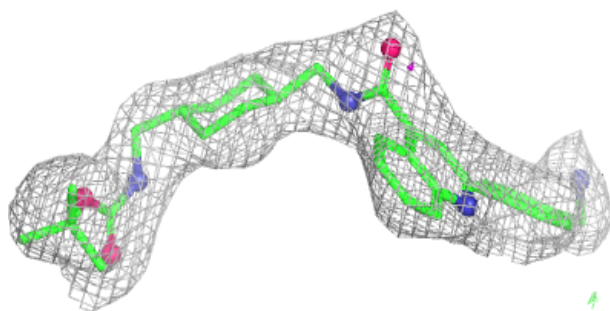
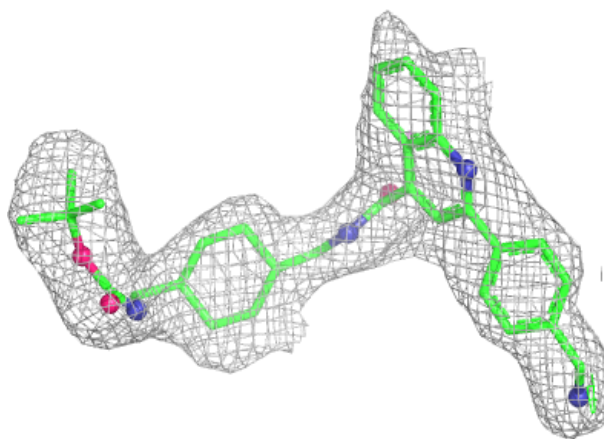
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	X24	A	1715	37/37	0.87	0.13	29,43,48,49	0
2	X24	B	1714	37/37	0.89	0.12	24,36,47,51	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.

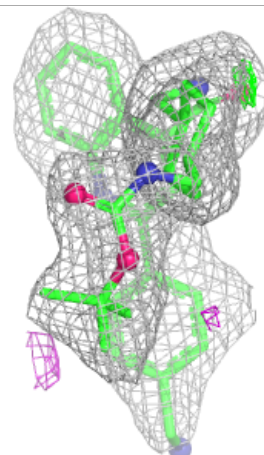
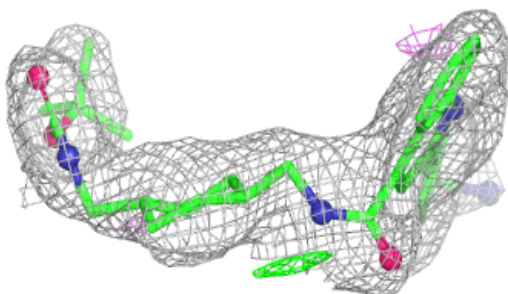
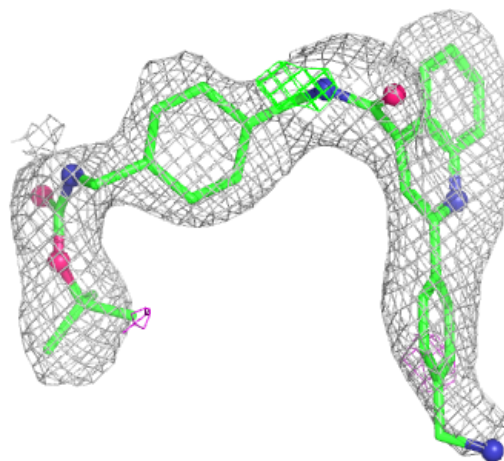
Electron density around X24 A 1715:

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



Electron density around X24 B 1714:

$2mF_o-DF_c$ (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.