Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2024 – 04:27 pm BST

PDB ID	:	2X24
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 (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:

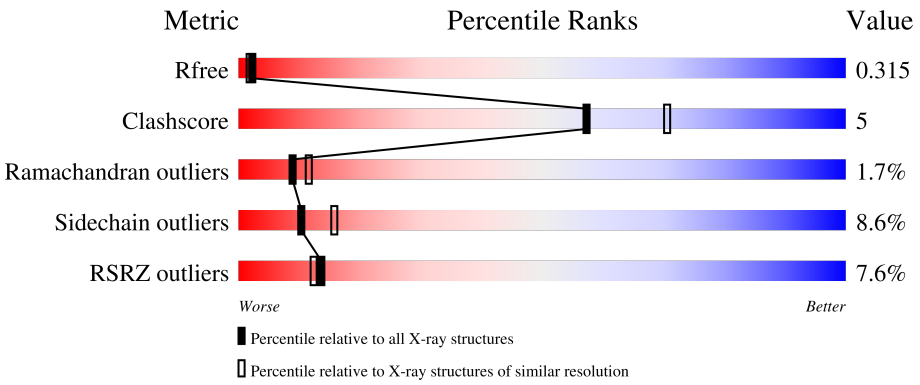
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 <=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	6% 66% 16% • 18%
1	B	793	7% 67% 15% • 16%

2 Entry composition (i)

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.

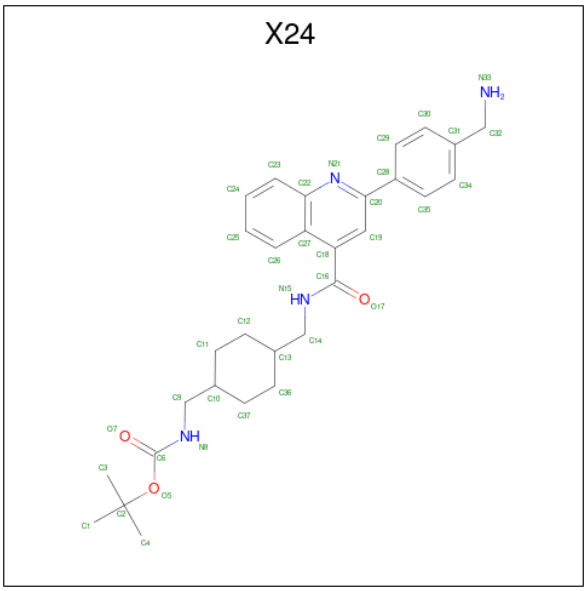
- Molecule 1 is a protein called ACETYL-COA CARBOXYLASE.

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

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 (three-letter code: X24) (formula: $C_{30}H_{38}N_4O_3$).



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

- Molecule 3 is water.

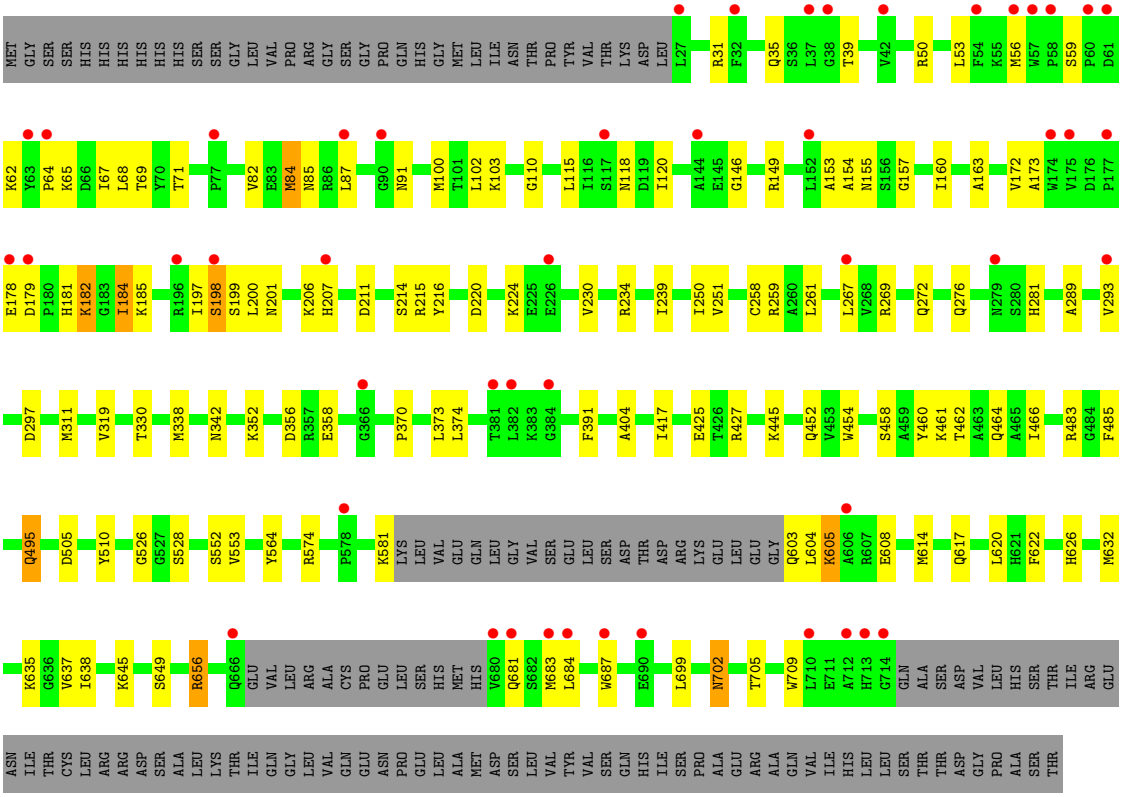
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	62	62	62	0	0
			Total	O		
3	B	84	84	84	0	0

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.

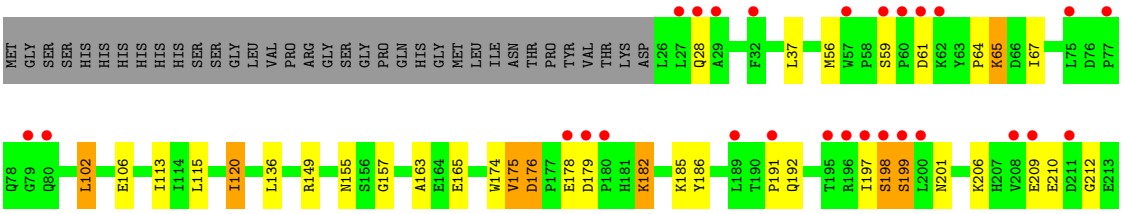
• Molecule 1: ACETYL-COA CARBOXYLASE

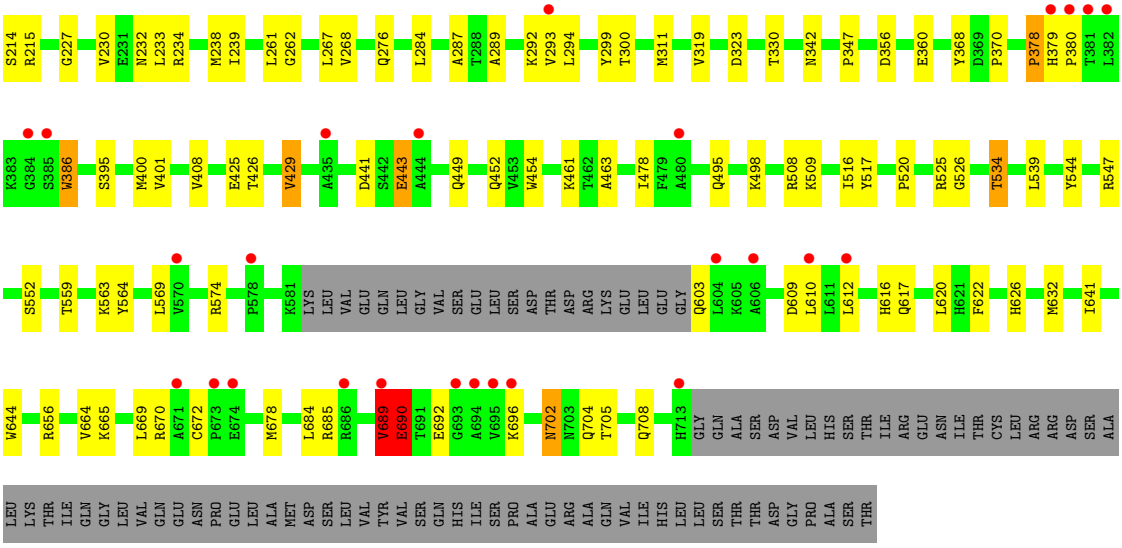
Chain A:



• Molecule 1: ACETYL-COA CARBOXYLASE

Chain B:




S214 R215 G227 V230 E231 N232 L233 R234 M238 I239 L261 G262 L267 V268 Q276 L284 A287 T288 A289 K292 V293 L294 Y299 T300 M311 V319 D323 T330 N342 P347 D356 E360 Y368 D369 P370 P378 H379 P380 T381 L382
K383 G384 S385 W386 S395 M400 V401 V408 E425 T426 V429 A435 D441 S442 E443 A444 Q449 Q452 V453 W454 K461 T462 A463 I478 F479 A480 Q495 K498 R508 K509 I516 Y517 P520 R525 G526 T534 L539 Y544 R547
S552 T559 K563 Y564 L569 V570 R574 P578 K581 LYS LEU VAL GLU GLN LEU GLY VAL SER GLU LEU SER ASP THR ASP ARG LYS GLU LEU GLU GLY Q603 L604 K605 A606 D609 L610 L611 L612 H616 Q617 L620 H621 F622 H626 M632 I641
W644 R656 V664 K665 L669 R670 A671 C672 F673 E674 M678 L684 R685 R686 V689 E690 T691 E692 G693 A694 V695 K696 N702 N703 Q704 T705 Q708 H713 GLY GLN ALA SER ASP VAL LEU HIS SER THR ILE ARG GLU ASN ILE THR CYS LEU ARG ARG ASP SER ALA
LEU LYS THR ILE GLN GLY LEU VAL GLN GLU ASN PRO GLU LEU ALA MET ASP SER LEU VAL TYR VAL SER GLN HIS ILE SER PRO ALA GLU ARG ALA GLN VAL ILE HIS LEU LEU SER THR THR ASP GLY PRO ALA SER THR

4 Data and refinement statistics (i)

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 29.49 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.70-2.40) 93.9 (29.49-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.232 , 0.283 0.251 , 0.315	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)	0.34 , 61.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	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.*

[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: 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	0.53	0/5342	0.77	2/7245 (0.0%)
1	B	0.54	0/5451	0.78	3/7395 (0.0%)
All	All	0.54	0/10793	0.78	5/14640 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	689	VAL	C-N-CA	7.91	141.48	121.70
1	A	178	GLU	C-N-CA	7.00	139.19	121.70
1	A	198	SER	C-N-CA	6.99	139.17	121.70
1	B	178	GLU	C-N-CA	6.58	138.14	121.70
1	B	198	SER	C-N-CA	6.37	137.62	121.70

There are no chirality outliers.

There are no planarity outliers.

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	5219	0	5207	56	0
1	B	5324	0	5308	56	0
2	A	37	0	38	1	0
2	B	37	0	38	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	62	0	0	0	0
3	B	84	0	0	6	0
All	All	10763	0	10591	103	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 (103) 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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:525:ARG:NH1	1:B:552:SER:OG	2.47	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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 (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	648/793 (82%)	610 (94%)	29 (4%)	9 (1%)	11 15
1	B	663/793 (84%)	614 (93%)	36 (5%)	13 (2%)	7 9
All	All	1311/1586 (83%)	1224 (93%)	65 (5%)	22 (2%)	9 11

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 (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	560/683 (82%)	514 (92%)	46 (8%)	11 17
1	B	572/683 (84%)	521 (91%)	51 (9%)	9 14
All	All	1132/1366 (83%)	1035 (91%)	97 (9%)	10 16

All (97) 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	84	MET
1	A	87	LEU
1	A	91	ASN
1	A	100	MET
1	A	115	LEU
1	A	149	ARG
1	A	184	ILE
1	A	201	ASN
1	A	206	LYS
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	342	ASN
1	A	352	LYS
1	A	356	ASP
1	A	445	LYS
1	A	454	TRP
1	A	458	SER
1	A	460	TYR
1	A	495	GLN
1	A	505	ASP
1	A	510	TYR
1	A	528	SER
1	A	552	SER
1	A	564	TYR

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Mol	Chain	Res	Type
1	A	581	LYS
1	A	603	GLN
1	A	605	LYS
1	A	614	MET
1	A	635	LYS
1	A	649	SER
1	A	656	ARG
1	A	681	GLN
1	A	683	MET
1	A	684	LEU
1	A	702	ASN
1	B	28	GLN
1	B	56	MET
1	B	61	ASP
1	B	65	LYS
1	B	102	LEU
1	B	115	LEU
1	B	120	ILE
1	B	149	ARG
1	B	165	GLU
1	B	175	VAL
1	B	176	ASP
1	B	182	LYS
1	B	192	GLN
1	B	199	SER
1	B	201	ASN
1	B	206	LYS
1	B	209	GLU
1	B	210	GLU
1	B	215	ARG
1	B	234	ARG
1	B	261	LEU
1	B	268	VAL
1	B	292	LYS
1	B	294	LEU
1	B	300	THR
1	B	323	ASP
1	B	342	ASN
1	B	356	ASP
1	B	360	GLU
1	B	386	TRP
1	B	395	SER

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Mol	Chain	Res	Type
1	B	429	VAL
1	B	441	ASP
1	B	443	GLU
1	B	454	TRP
1	B	534	THR
1	B	539	LEU
1	B	559	THR
1	B	564	TYR
1	B	574	ARG
1	B	603	GLN
1	B	609	ASP
1	B	610	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 (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	118	ASN
1	A	155	ASN
1	A	204	HIS
1	A	207	HIS
1	A	232	ASN
1	A	276	GLN
1	A	281	HIS
1	A	342	ASN
1	A	448	GLN
1	A	621	HIS
1	A	626	HIS
1	A	702	ASN
1	B	118	ASN
1	B	155	ASN
1	B	232	ASN
1	B	276	GLN
1	B	342	ASN

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Mol	Chain	Res	Type
1	B	362	GLN
1	B	405	GLN
1	B	626	HIS
1	B	702	ASN
1	B	708	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)

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	-	39,40,40	0.78	0	52,56,56	1.87	12 (23%)
2	X24	B	1714	-	39,40,40	0.73	0	52,56,56	2.73	15 (28%)

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	-	-	10/21/35/35	0/4/4/4
2	X24	B	1714	-	-	15/21/35/35	0/4/4/4

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1714	X24	O5-C6-N8	7.99	121.84	109.99
2	B	1714	X24	C18-C16-N15	7.13	125.93	116.30
2	B	1714	X24	C10-C9-N8	-6.67	100.17	112.73
2	B	1714	X24	O7-C6-N8	-6.60	114.84	124.96
2	B	1714	X24	C13-C14-N15	-6.58	100.35	112.73
2	A	1715	X24	O5-C6-N8	5.17	117.66	109.99
2	A	1715	X24	C27-C18-C16	4.66	127.43	120.68
2	A	1715	X24	C13-C14-N15	-4.57	104.12	112.73
2	B	1714	X24	C2-O5-C6	4.50	127.92	120.99
2	A	1715	X24	C2-O5-C6	4.23	127.50	120.99
2	A	1715	X24	O7-C6-N8	-3.76	119.19	124.96
2	B	1714	X24	C27-C22-N21	-3.73	119.86	123.35
2	B	1714	X24	C36-C37-C10	-3.57	106.51	112.42
2	B	1714	X24	C22-N21-C20	3.35	122.59	117.86
2	B	1714	X24	O17-C16-N15	-3.25	116.13	122.61
2	B	1714	X24	C12-C11-C10	-3.02	107.42	112.42
2	A	1715	X24	C27-C22-N21	-2.99	120.56	123.35
2	B	1714	X24	C36-C13-C12	2.95	116.54	109.33
2	A	1715	X24	C19-C18-C27	-2.81	117.60	119.97
2	B	1714	X24	O17-C16-C18	-2.75	117.92	121.72
2	A	1715	X24	C19-C18-C16	-2.72	114.84	120.16
2	A	1715	X24	C36-C37-C10	-2.68	107.98	112.42
2	A	1715	X24	C36-C13-C12	2.51	115.46	109.33
2	B	1714	X24	O5-C2-C3	2.31	116.35	107.20
2	B	1714	X24	C19-C18-C27	-2.24	118.08	119.97
2	A	1715	X24	C22-N21-C20	2.24	121.03	117.86
2	A	1715	X24	C12-C11-C10	-2.09	108.96	112.42

There are no chirality outliers.

All (25) 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

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Mol	Chain	Res	Type	Atoms
2	B	1714	X24	C36-C13-C14-N15
2	A	1715	X24	C1-C2-O5-C6
2	A	1715	X24	C3-C2-O5-C6
2	A	1715	X24	C4-C2-O5-C6
2	B	1714	X24	C1-C2-O5-C6
2	B	1714	X24	C4-C2-O5-C6
2	B	1714	X24	O7-C6-O5-C2
2	B	1714	X24	N8-C6-O5-C2
2	B	1714	X24	C3-C2-O5-C6
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	A	1715	X24	O7-C6-N8-C9
2	B	1714	X24	O7-C6-N8-C9
2	B	1714	X24	O5-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
2	B	1714	X24	N15-C16-C18-C19
2	B	1714	X24	O17-C16-C18-C19

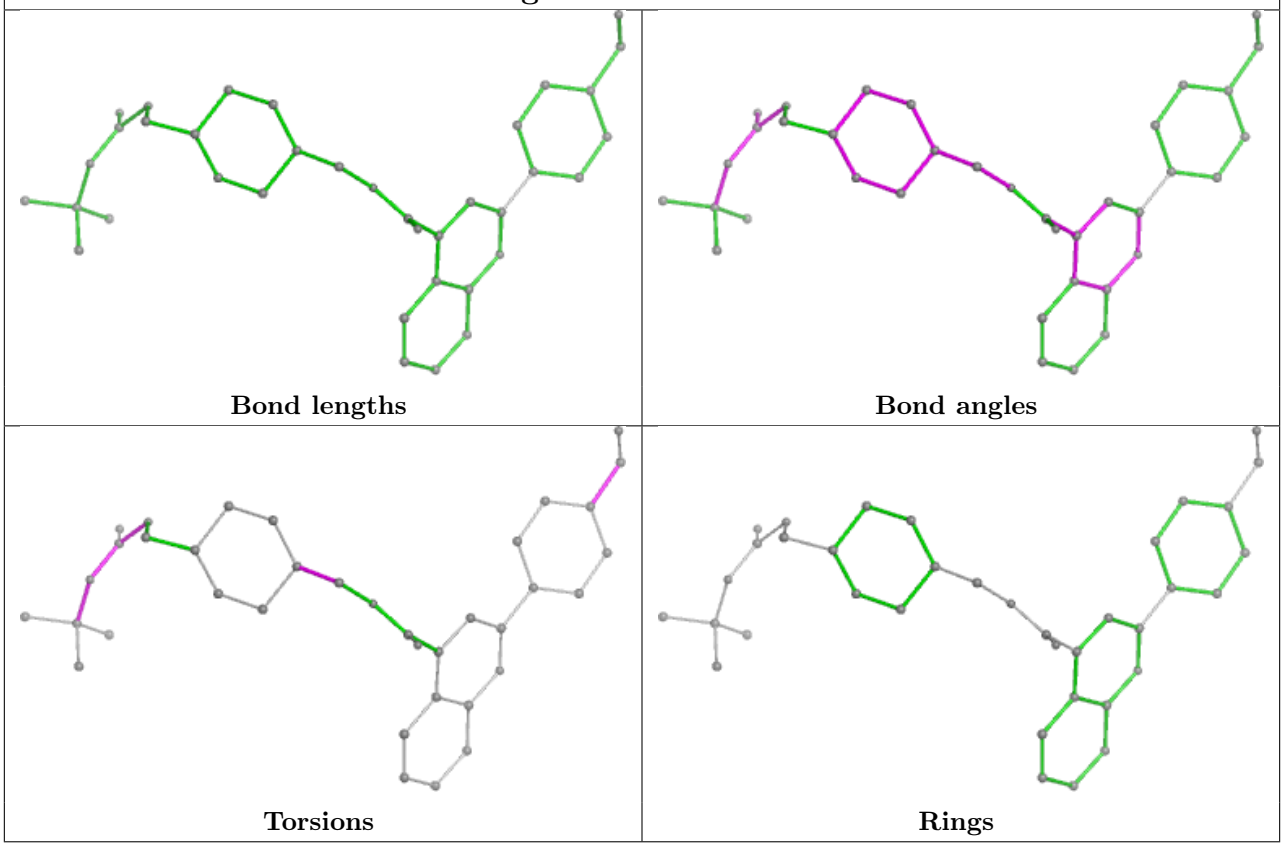
There are no ring outliers.

2 monomers are involved in 2 short contacts:

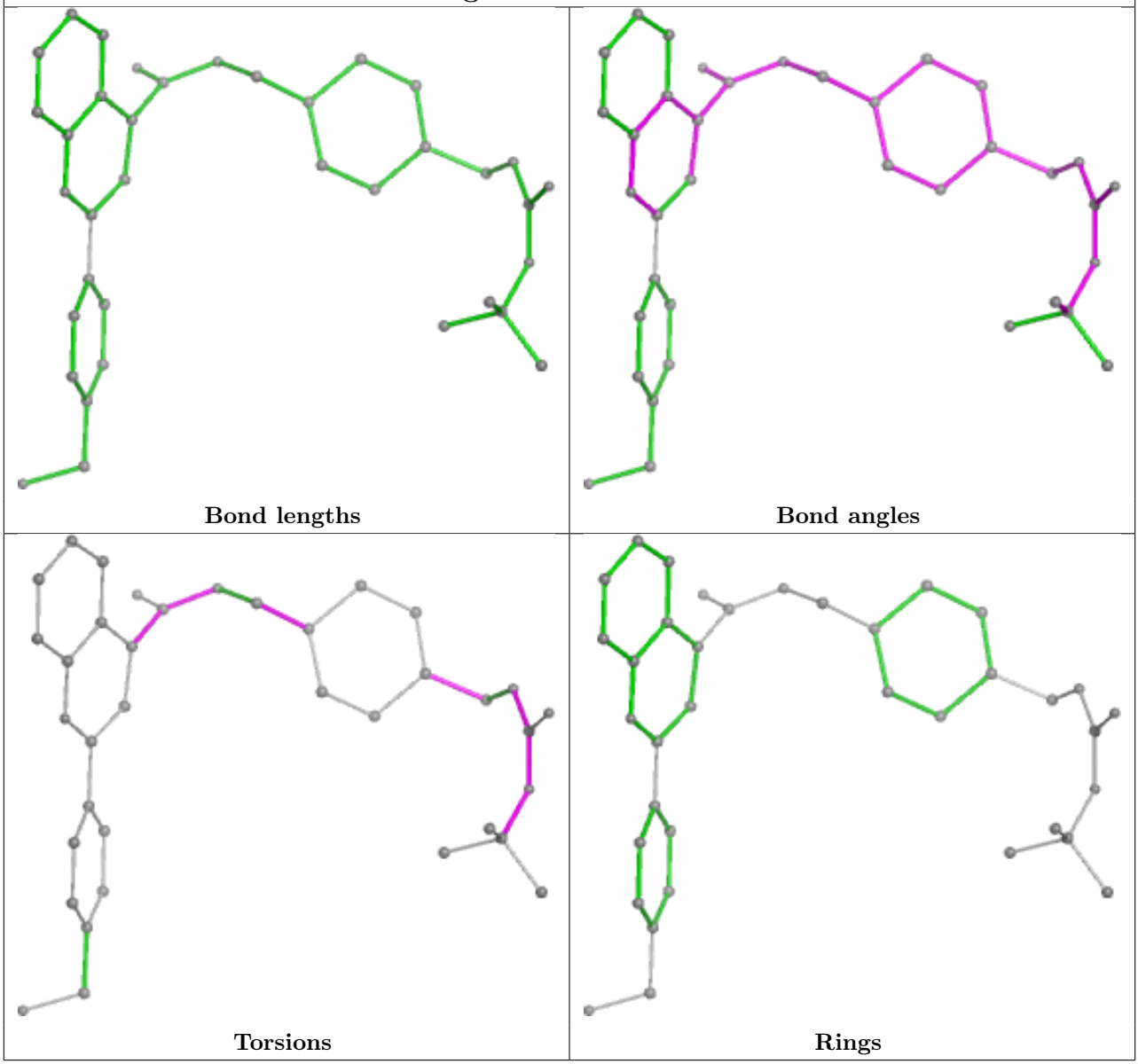
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1715	X24	1	0
2	B	1714	X24	1	0

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 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 X24 A 1715



Ligand X24 B 1714



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	654/793 (82%)	0.38	48 (7%)	15	13	15, 35, 66, 88	0
1	B	667/793 (84%)	0.38	53 (7%)	12	11	14, 34, 64, 92	0
All	All	1321/1586 (83%)	0.38	101 (7%)	13	12	14, 34, 65, 92	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	689	VAL	6.0
1	B	381	THR	5.9
1	B	196	ARG	5.7
1	B	694	ALA	5.6
1	B	671	ALA	5.4
1	A	63	TYR	5.2
1	A	687	TRP	5.0
1	A	713	HIS	4.8
1	B	695	VAL	4.5
1	A	87	LEU	4.4
1	B	211	ASP	4.3
1	B	198	SER	4.2
1	A	712	ALA	4.2
1	A	381	THR	3.9
1	B	293	VAL	3.8
1	B	59	SER	3.8
1	A	61	ASP	3.7
1	B	382	LEU	3.7
1	A	382	LEU	3.7
1	B	713	HIS	3.7
1	A	27	LEU	3.6
1	A	90	GLY	3.6
1	B	380	PRO	3.6
1	B	77	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	60	PRO	3.5
1	B	61	ASP	3.5
1	B	197	ILE	3.4
1	A	384	GLY	3.4
1	A	42	VAL	3.4
1	B	179	ASP	3.3
1	A	606	ALA	3.3
1	A	681	GLN	3.3
1	A	179	ASP	3.3
1	A	77	PRO	3.2
1	A	175	VAL	3.1
1	A	32	PHE	3.1
1	B	693	GLY	3.1
1	A	293	VAL	3.1
1	B	27	LEU	3.0
1	B	379	HIS	2.9
1	B	570	VAL	2.9
1	A	64	PRO	2.9
1	B	604	LEU	2.9
1	A	198	SER	2.8
1	A	683	MET	2.8
1	A	54	PHE	2.8
1	A	178	GLU	2.8
1	B	208	VAL	2.8
1	A	37	LEU	2.8
1	A	578	PRO	2.8
1	B	696	LYS	2.7
1	B	385	SER	2.7
1	A	666	GLN	2.7
1	B	180	PRO	2.7
1	B	199	SER	2.7
1	B	62	LYS	2.7
1	A	60	PRO	2.7
1	A	690	GLU	2.7
1	B	75	LEU	2.7
1	A	207	HIS	2.7
1	A	56	MET	2.7
1	B	686	ARG	2.6
1	B	612	LEU	2.6
1	A	714	GLY	2.6
1	A	177	PRO	2.6
1	B	178	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	267	LEU	2.5
1	B	578	PRO	2.5
1	B	384	GLY	2.5
1	B	80	GLN	2.4
1	B	28	GLN	2.4
1	A	710	LEU	2.4
1	A	174	TRP	2.3
1	A	680	VAL	2.3
1	A	226	GLU	2.3
1	A	279	ASN	2.3
1	B	32	PHE	2.3
1	B	57	TRP	2.3
1	A	196	ARG	2.2
1	B	191	PRO	2.2
1	B	195	THR	2.2
1	B	200	LEU	2.2
1	B	674	GLU	2.2
1	A	366	GLY	2.2
1	A	684	LEU	2.2
1	A	38	GLY	2.1
1	B	79	GLY	2.1
1	B	673	PRO	2.1
1	A	152	LEU	2.1
1	B	435	ALA	2.1
1	A	144	ALA	2.1
1	B	480	ALA	2.1
1	B	610	LEU	2.1
1	A	57	TRP	2.1
1	B	444	ALA	2.0
1	B	606	ALA	2.0
1	B	189	LEU	2.0
1	B	29	ALA	2.0
1	B	209	GLU	2.0
1	A	117	SER	2.0
1	A	58	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

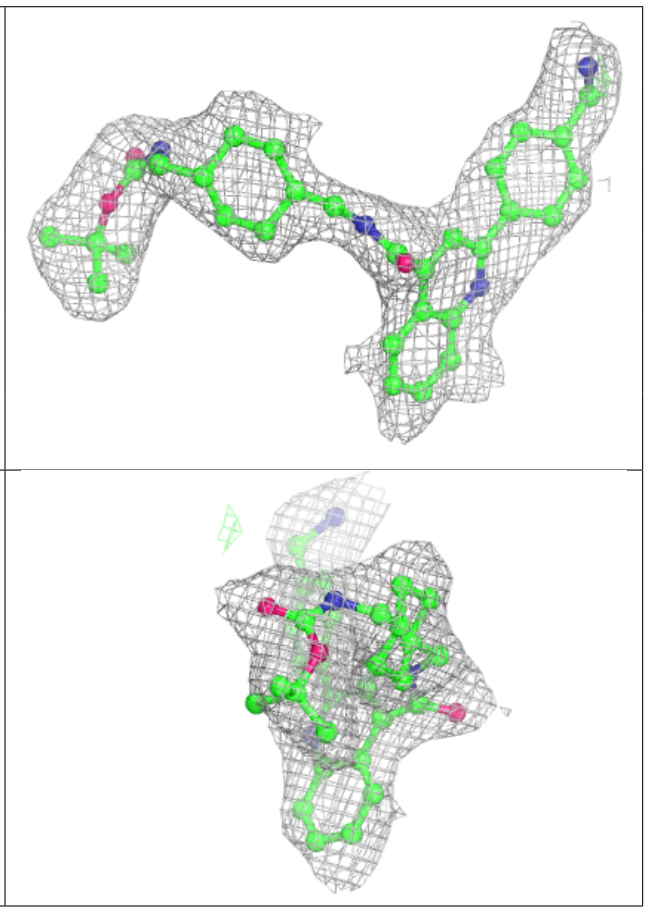
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	X24	A	1715	37/37	0.87	0.17	29,43,48,49	0
2	X24	B	1714	37/37	0.87	0.21	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.

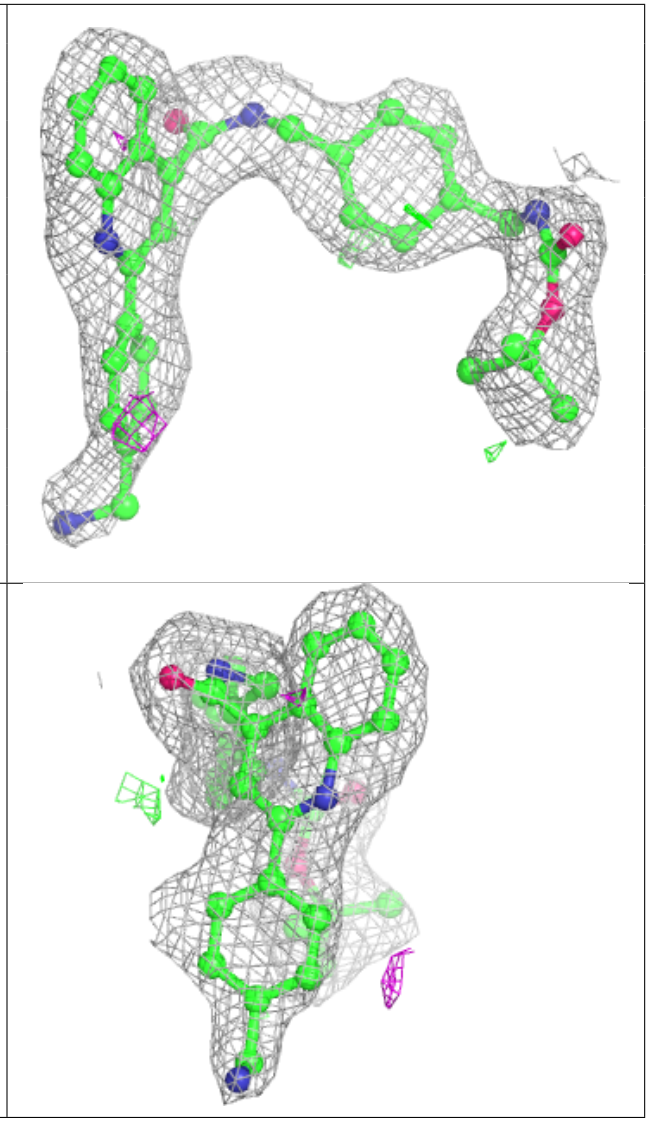
Electron density around X24 A 1715:

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.