



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 06:19 PM BST

PDB ID : 2BX8
Title : Human serum albumin complexed with azapropazone
Authors : Ghuman, J.; Zunszain, P.A.; Petitpas, I.; Bhattacharya, A.A.; Curry, S.
Deposited on : 2005-07-25
Resolution : 2.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

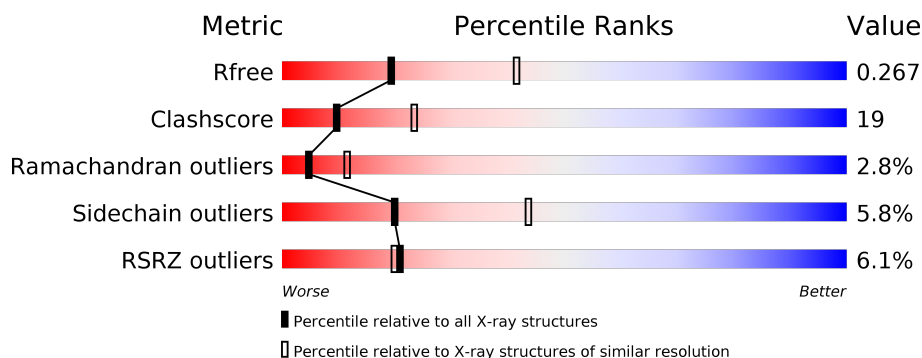
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	585	<div> <div>5%</div> <div> <div></div> <div>64%</div> <div>31%</div> <div>..</div> </div> </div>
1	B	585	<div> <div>7%</div> <div> <div></div> <div>65%</div> <div>30%</div> <div>...</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AZQ	A	2001	X	-	-	-
2	AZQ	A	2002	X	-	-	-
2	AZQ	B	2001	X	-	-	-
2	AZQ	B	2002	X	-	-	-

2 Entry composition [i](#)

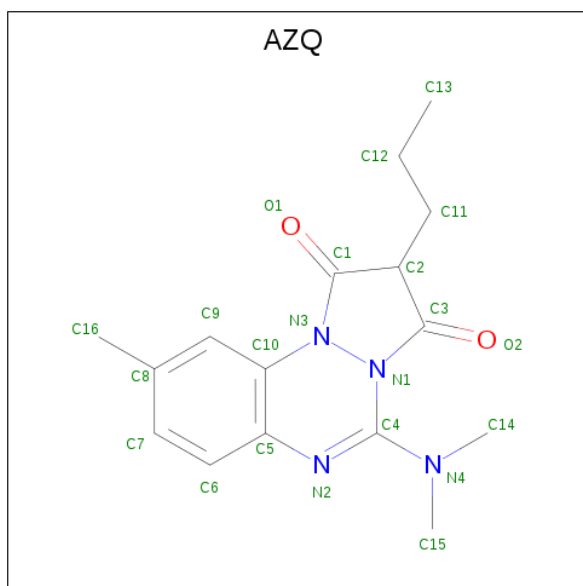
There are 2 unique types of molecules in this entry. The entry contains 8669 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SERUM ALBUMIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	578	Total	C	N	O	S	0	0	0
			4324	2735	716	832	41			
1	B	578	Total	C	N	O	S	0	0	0
			4257	2684	714	820	39			

- Molecule 2 is AZAPROPAZONE (three-letter code: AZQ) (formula: $C_{16}H_{20}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			22	16	4	2		
2	A	1	Total	C	N	O	0	0
			22	16	4	2		
2	B	1	Total	C	N	O	0	0
			22	16	4	2		
2	B	1	Total	C	N	O	0	0
			22	16	4	2		

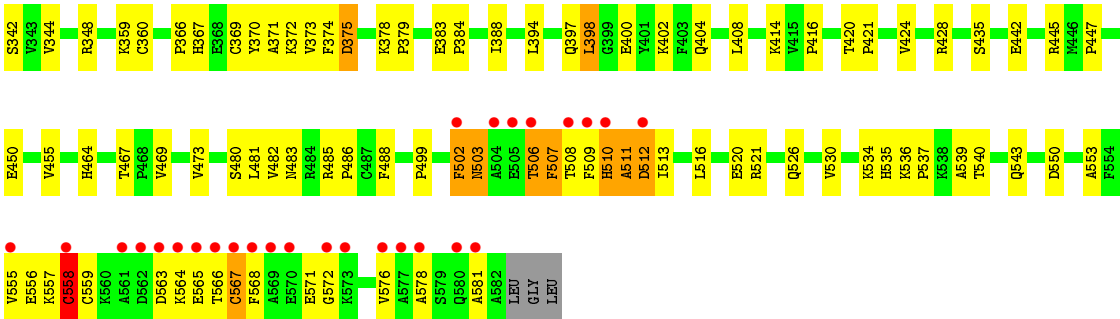
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

Chain A:

Chain B:

7% 65% 30%

ASP ALA HIS LYS SS R9 D13 L14 G15 F19 L22 V23 A26 F27 Y30 L31 Q32 Q33 C34 P35 F36 E37 D38 H39 V40 K41 L42 V43 V46 T47 E48 F49 A50 K51 T52 C53 V54 A55 D56 E57 S58 A59 E60 N61 G62 D63 K64 F70 V77 A78 T79 L80 R81 E82 R83 T83 Y84 G85 R86 M87 A88 D89 C90 R98 N99 E100 C101 F102 L103 Q104 H105 K106 P110 F127 H128 D129 L139 Y140 E141 R144 R145 H146 P147 Y148 F149 Y150 A151 P152 E153 L154 L155 F156 F157 A158 C168 C169 G177 L178 L179 P180 L185 R186 C189 K190 A194 K195 Q196 F206 K212 E244 L250 R257 S272 S273 K274 L275 K276 E277 C278 C279 E280 L283 L284 E285 K286 S287 I290 V293 E294 D296 A300 V310 V315 K323 D324 E333 R336 V374



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.20Å 54.95Å 119.90Å 81.21° 91.07° 64.75°	Depositor
Resolution (Å)	41.45 – 2.70 41.44 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.5 (41.45-2.70) 95.7 (41.44-2.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.237 , 0.273 0.232 , 0.267	Depositor DCC
R_{free} test set	1592 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	65.1	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 69.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8669	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% 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: AZQ

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	0.47	0/4410	0.70	2/6001 (0.0%)
1	B	0.45	0/4339	0.68	3/5912 (0.1%)
All	All	0.46	0/8749	0.69	5/11913 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	558	CYS	CA-CB-SG	8.80	129.84	114.00
1	A	558	CYS	CA-CB-SG	8.18	128.73	114.00
1	A	567	CYS	CA-CB-SG	-6.08	103.06	114.00
1	B	222	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	B	567	CYS	CA-CB-SG	-5.11	104.80	114.00

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	4324	0	3978	173	0
1	B	4257	0	3862	148	0
2	A	44	0	34	9	0
2	B	44	0	34	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8669	0	7908	321	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 19.

All (321) 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:547:VAL:HG12	1:A:551:PHE:HE1	1.33	0.94
1:B:151:ALA:HB3	1:B:152:PRO:HD3	1.53	0.90
1:A:551:PHE:HA	1:A:554:PHE:HD1	1.37	0.86
1:B:39:HIS:O	1:B:43:VAL:HG23	1.76	0.85
1:A:551:PHE:HA	1:A:554:PHE:CD1	2.11	0.84
1:A:189:GLY:HA3	2:A:2002:AZQ:H7	1.59	0.83
1:A:547:VAL:HG12	1:A:551:PHE:CE1	2.14	0.82
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.61	0.81
1:B:106:LYS:HD3	1:B:147:PRO:HB2	1.63	0.80
1:A:257:ARG:HE	2:A:2001:AZQ:H6	1.46	0.77
1:A:424:VAL:O	1:A:428:ARG:HG3	1.83	0.77
1:B:424:VAL:O	1:B:428:ARG:HG3	1.85	0.77
1:A:225:LYS:HG2	1:A:299:PRO:HG3	1.66	0.77
1:A:373:VAL:HG13	1:A:374:PHE:HD1	1.50	0.77
1:B:564:LYS:O	1:B:566:THR:N	2.18	0.76
1:A:503:ASN:HB3	1:A:506:THR:H	1.51	0.76
1:A:150:TYR:OH	1:A:257:ARG:HG3	1.85	0.75
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.69	0.74
1:B:503:ASN:HB3	1:B:506:THR:H	1.53	0.73
1:A:283:LEU:HG	1:A:284:LEU:HD23	1.69	0.73
1:A:378:LYS:HB3	1:A:379:PRO:HD3	1.71	0.73
1:B:81:ARG:HE	1:B:88:ALA:HB3	1.53	0.73
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.70	0.72
1:B:61:ASN:HB3	1:B:64:LYS:HD2	1.71	0.71
1:A:39:HIS:O	1:A:43:VAL:HG23	1.90	0.71
1:B:503:ASN:HB2	1:B:506:THR:OG1	1.91	0.70
1:B:48:GLU:O	1:B:48:GLU:HG2	1.90	0.69
1:A:507:PHE:CZ	1:A:509:PHE:HZ	2.10	0.69
1:A:503:ASN:HB2	1:A:506:THR:OG1	1.93	0.69
1:A:414:LYS:O	1:A:472:ARG:NH1	2.27	0.68
1:B:52:THR:HA	1:B:56:ASP:OD2	1.94	0.67
1:A:23:VAL:O	1:A:27:PHE:HD1	1.77	0.67
1:B:206:PHE:CE2	1:B:481:LEU:HD13	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:GLY:O	1:A:576:VAL:HG23	1.96	0.66
1:B:189:GLY:HA3	2:B:2002:AZQ:C7	2.26	0.66
1:A:23:VAL:HG13	1:A:70:PHE:HE2	1.61	0.65
1:B:572:GLY:O	1:B:576:VAL:HG23	1.96	0.65
1:B:276:LYS:HE3	1:B:280:GLU:OE2	1.96	0.65
1:B:483:ASN:O	1:B:486:PRO:HD2	1.96	0.65
1:B:81:ARG:NE	1:B:88:ALA:HB3	2.12	0.65
1:A:117:ARG:HB2	1:A:123:MET:CE	2.27	0.64
1:B:383:GLU:HB3	1:B:384:PRO:HD3	1.78	0.64
1:A:408:LEU:HD11	1:A:526:GLN:HB3	1.80	0.64
1:A:120:VAL:HG21	1:A:175:ALA:HA	1.80	0.64
1:A:26:ALA:HB2	1:A:250:LEU:HD12	1.79	0.63
1:A:150:TYR:CE2	2:A:2001:AZQ:H7	2.34	0.63
1:A:567:CYS:O	1:A:571:GLU:HB2	1.99	0.63
1:A:373:VAL:HG13	1:A:374:PHE:CD1	2.32	0.62
1:A:139:LEU:HD21	1:A:158:ALA:HB2	1.81	0.62
1:A:564:LYS:O	1:A:566:THR:N	2.27	0.62
1:A:61:ASN:HD22	1:A:64:LYS:HE3	1.65	0.62
1:B:190:LYS:HE3	2:B:2002:AZQ:H12	1.82	0.62
1:B:408:LEU:HD22	1:B:530:VAL:CG2	2.30	0.62
1:B:42:LEU:O	1:B:46:VAL:HG23	1.99	0.61
1:B:408:LEU:HD11	1:B:526:GLN:HB3	1.80	0.61
1:A:550:ASP:HB3	1:A:554:PHE:HE1	1.64	0.61
1:A:117:ARG:HB2	1:A:123:MET:HE3	1.82	0.61
1:A:464:HIS:CE1	1:A:469:VAL:H	2.18	0.61
1:B:568:PHE:O	1:B:572:GLY:HA3	2.00	0.61
1:B:483:ASN:C	1:B:486:PRO:HD2	2.21	0.61
1:A:420:THR:O	1:A:424:VAL:HG23	1.99	0.61
1:B:516:LEU:O	1:B:521:ARG:NH2	2.32	0.61
1:B:420:THR:HB	1:B:421:PRO:HD3	1.83	0.60
1:B:279:CYS:HA	1:B:286:LYS:HD2	1.83	0.60
1:A:224:PRO:HB2	1:A:299:PRO:HD3	1.83	0.60
1:A:568:PHE:O	1:A:572:GLY:HA3	2.02	0.60
1:B:567:CYS:O	1:B:571:GLU:HB2	2.02	0.59
1:B:372:LYS:O	1:B:375:ASP:HB2	2.02	0.59
1:B:511:ALA:C	1:B:513:ILE:H	2.05	0.59
1:A:146:HIS:CE1	2:A:2002:AZQ:H161	2.38	0.59
1:B:36:PHE:O	1:B:40:VAL:HG23	2.03	0.59
1:A:551:PHE:CA	1:A:554:PHE:HD1	2.12	0.58
1:A:384:PRO:O	1:A:388:ILE:HG12	2.03	0.58
1:A:38:ASP:O	1:A:42:LEU:HG	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ALA:O	1:A:513:ILE:N	2.37	0.58
1:B:30:TYR:HE1	1:B:103:LEU:HD23	1.69	0.58
1:A:106:LYS:HD3	1:A:147:PRO:HB2	1.84	0.58
1:B:373:VAL:HG13	1:B:374:PHE:HD1	1.69	0.58
1:A:306:ALA:HA	1:A:310:VAL:HG22	1.85	0.57
1:B:57:GLU:OE1	1:B:57:GLU:HA	2.05	0.57
1:A:502:PHE:CE1	1:A:507:PHE:CZ	2.92	0.57
1:A:408:LEU:HD22	1:A:530:VAL:CG2	2.34	0.57
1:A:376:GLU:O	1:A:379:PRO:HD2	2.05	0.56
1:B:98:ARG:O	1:B:101:CYS:HB3	2.05	0.56
1:B:564:LYS:C	1:B:566:THR:H	2.06	0.56
1:B:257:ARG:HE	2:B:2001:AZQ:H6	1.69	0.56
1:A:168:CYS:SG	1:A:177:CYS:C	2.85	0.56
1:B:168:CYS:SG	1:B:177:CYS:C	2.85	0.56
1:B:81:ARG:HE	1:B:88:ALA:CB	2.18	0.56
1:A:265:CYS:SG	1:A:286:LYS:HD2	2.46	0.55
1:B:14:LEU:HD13	1:B:22:LEU:HD12	1.88	0.55
1:B:348:ARG:NH2	1:B:450:GLU:OE2	2.36	0.55
1:A:42:LEU:O	1:A:46:VAL:HG23	2.06	0.55
1:A:153:GLU:O	1:A:157:PHE:HD1	1.90	0.55
1:B:511:ALA:O	1:B:513:ILE:N	2.35	0.55
1:A:388:ILE:HD12	1:A:449:ALA:CB	2.37	0.55
1:A:503:ASN:CB	1:A:506:THR:HB	2.37	0.55
1:B:206:PHE:CD2	1:B:481:LEU:HD22	2.42	0.55
1:B:257:ARG:CZ	1:B:287:SER:HB3	2.36	0.55
1:B:50:ALA:O	1:B:54:VAL:HG23	2.07	0.55
1:B:394:LEU:O	1:B:397:GLN:HG2	2.07	0.54
1:B:464:HIS:CG	1:B:473:VAL:HG11	2.42	0.54
1:B:540:THR:OG1	1:B:543:GLN:HG2	2.07	0.54
1:A:179:LEU:HB2	1:A:180:PRO:HD3	1.89	0.54
1:B:555:VAL:O	1:B:559:CYS:HB2	2.08	0.54
1:B:553:ALA:O	1:B:556:GLU:HG2	2.07	0.54
1:A:503:ASN:HB3	1:A:506:THR:N	2.20	0.54
1:B:189:GLY:HA3	2:B:2002:AZQ:H7	1.89	0.54
1:A:547:VAL:CG1	1:A:551:PHE:HE1	2.14	0.53
1:B:151:ALA:CB	1:B:152:PRO:HD3	2.33	0.53
1:A:95:GLU:OE1	1:A:96:PRO:HA	2.09	0.53
1:A:553:ALA:O	1:A:556:GLU:HG2	2.09	0.53
1:B:373:VAL:HG13	1:B:374:PHE:N	2.23	0.53
1:A:507:PHE:O	1:A:507:PHE:CD2	2.61	0.53
1:B:508:THR:HG22	1:B:509:PHE:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:PHE:O	1:A:572:GLY:N	2.42	0.53
1:A:512:ASP:O	1:A:515:THR:HG22	2.09	0.52
1:A:563:ASP:OD1	1:A:567:CYS:HB3	2.10	0.52
1:B:22:LEU:HD21	1:B:155:LEU:HD11	1.90	0.52
1:B:485:ARG:HB3	1:B:486:PRO:HD3	1.91	0.52
1:A:418:VAL:HG12	1:A:423:LEU:HG	1.91	0.52
1:B:367:HIS:O	1:B:371:ALA:HB2	2.10	0.52
1:A:503:ASN:HB2	1:A:506:THR:CB	2.39	0.52
1:A:189:GLY:HA3	2:A:2002:AZQ:C7	2.37	0.52
1:B:141:GLU:OE1	1:B:144:ARG:HD3	2.10	0.51
1:A:150:TYR:HB2	1:A:196:GLN:HG2	1.93	0.51
1:B:464:HIS:CE1	1:B:469:VAL:H	2.27	0.51
1:B:503:ASN:CB	1:B:506:THR:HB	2.40	0.51
1:A:146:HIS:NE2	2:A:2002:AZQ:H161	2.25	0.51
1:A:502:PHE:HE1	1:A:507:PHE:CZ	2.27	0.51
1:A:325:VAL:HG12	1:A:329:MET:HE2	1.93	0.51
1:B:503:ASN:HB3	1:B:506:THR:N	2.24	0.51
1:B:378:LYS:HB2	1:B:379:PRO:HD3	1.93	0.51
1:A:511:ALA:C	1:A:513:ILE:H	2.14	0.50
1:B:509:PHE:O	1:B:510:HIS:C	2.50	0.50
1:A:377:PHE:O	1:A:381:VAL:HG23	2.10	0.50
1:A:564:LYS:C	1:A:566:THR:H	2.12	0.50
1:B:283:LEU:HG	1:B:284:LEU:N	2.26	0.50
1:A:49:PHE:O	1:A:49:PHE:HD2	1.94	0.50
1:B:398:LEU:O	1:B:402:LYS:HB2	2.11	0.50
1:A:61:ASN:C	1:A:63:ASP:H	2.15	0.50
1:B:503:ASN:HB2	1:B:506:THR:CB	2.42	0.50
1:A:325:VAL:HG12	1:A:329:MET:CE	2.42	0.49
1:A:408:LEU:HD22	1:A:530:VAL:HG22	1.94	0.49
1:A:503:ASN:CB	1:A:506:THR:CB	2.90	0.49
1:B:26:ALA:HB2	1:B:250:LEU:HD12	1.94	0.49
1:B:563:ASP:OD1	1:B:567:CYS:HB3	2.12	0.49
1:B:507:PHE:N	1:B:507:PHE:CD2	2.80	0.49
1:A:151:ALA:CB	1:A:152:PRO:HD3	2.39	0.49
1:A:66:LEU:HB3	1:A:70:PHE:CE1	2.48	0.49
1:B:290:ILE:O	1:B:293:VAL:HG12	2.12	0.49
1:A:568:PHE:O	1:A:572:GLY:CA	2.60	0.48
1:B:375:ASP:O	1:B:378:LYS:HG3	2.13	0.48
1:A:257:ARG:HH21	2:A:2001:AZQ:C7	2.26	0.48
1:A:430:LEU:O	1:A:433:VAL:HG12	2.12	0.48
1:B:240:LYS:HE2	1:B:244:GLU:OE2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:GLU:CD	1:B:37:GLU:H	2.16	0.48
1:A:282:PRO:HB2	1:A:285:GLU:OE1	2.14	0.48
1:A:370:TYR:CD1	1:A:370:TYR:C	2.87	0.48
1:B:57:GLU:O	1:B:58:SER:C	2.50	0.48
1:B:286:LYS:O	1:B:290:ILE:HG13	2.14	0.48
1:B:507:PHE:N	1:B:507:PHE:HD2	2.11	0.48
1:A:519:LYS:O	1:A:523:ILE:HG13	2.14	0.48
1:B:186:ARG:O	1:B:190:LYS:HG3	2.14	0.48
1:B:384:PRO:O	1:B:388:ILE:HG12	2.14	0.48
1:B:416:PRO:O	1:B:534:LYS:HE3	2.14	0.48
1:B:54:VAL:HG12	1:B:55:ALA:N	2.29	0.48
1:B:221:GLN:NE2	1:B:341:TYR:O	2.47	0.48
1:A:257:ARG:CZ	1:A:287:SER:HB3	2.44	0.47
1:B:568:PHE:O	1:B:572:GLY:CA	2.62	0.47
1:B:139:LEU:HD21	1:B:158:ALA:HB2	1.95	0.47
1:B:168:CYS:SG	1:B:178:LEU:N	2.87	0.47
1:A:206:PHE:CE2	1:A:481:LEU:HD13	2.49	0.47
1:A:547:VAL:CG1	1:A:551:PHE:CE1	2.92	0.47
1:A:150:TYR:HD2	1:A:153:GLU:HB2	1.79	0.47
1:A:279:CYS:HA	1:A:286:LYS:CD	2.44	0.47
1:B:293:VAL:HG22	1:B:294:GLU:N	2.29	0.47
1:B:272:SER:HB3	1:B:275:LEU:HG	1.96	0.47
1:B:222:ARG:HD3	1:B:293:VAL:HG13	1.95	0.47
1:B:310:VAL:HG21	1:B:374:PHE:CE1	2.49	0.47
1:A:189:GLY:C	2:A:2002:AZQ:H163	2.34	0.47
1:B:348:ARG:HG3	1:B:482:VAL:HG12	1.95	0.47
1:A:464:HIS:HE1	1:A:470:SER:H	1.63	0.47
1:A:509:PHE:O	1:A:510:HIS:C	2.53	0.47
1:B:81:ARG:HG2	1:B:88:ALA:CB	2.43	0.47
1:B:196:GLN:HA	1:B:196:GLN:NE2	2.30	0.47
1:B:276:LYS:HG3	1:B:277:GLU:N	2.27	0.47
1:B:442:GLU:HA	1:B:445:ARG:HD2	1.97	0.47
1:B:503:ASN:CB	1:B:506:THR:CB	2.92	0.47
1:A:23:VAL:O	1:A:27:PHE:CD1	2.65	0.47
1:A:109:ASN:HA	1:A:109:ASN:HD22	1.55	0.46
1:A:333:GLU:O	1:A:336:ARG:HG2	2.14	0.46
1:B:81:ARG:HG2	1:B:88:ALA:HB3	1.97	0.46
1:B:568:PHE:O	1:B:572:GLY:N	2.48	0.46
1:A:223:PHE:CD1	1:A:272:SER:HB2	2.51	0.46
1:B:536:LYS:O	1:B:539:ALA:HB3	2.15	0.46
1:A:502:PHE:HE1	1:A:507:PHE:HZ	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LEU:HG	1:A:284:LEU:N	2.31	0.46
1:A:517:SER:O	1:A:521:ARG:HG3	2.15	0.46
1:A:110:PRO:HB2	1:A:112:LEU:HG	1.97	0.46
1:B:510:HIS:O	1:B:512:ASP:N	2.49	0.46
1:A:49:PHE:CD2	1:A:49:PHE:C	2.88	0.46
1:A:348:ARG:HG3	1:A:482:VAL:HG12	1.98	0.45
1:B:38:ASP:O	1:B:42:LEU:HG	2.16	0.45
1:A:25:ILE:O	1:A:29:GLN:HG3	2.15	0.45
1:B:408:LEU:HD22	1:B:530:VAL:HG22	1.97	0.45
1:A:306:ALA:CA	1:A:310:VAL:HG22	2.45	0.45
1:B:503:ASN:HA	1:B:503:ASN:HD22	1.56	0.45
1:B:153:GLU:O	1:B:157:PHE:HD1	1.98	0.45
1:A:117:ARG:HB2	1:A:123:MET:HE1	1.97	0.45
1:A:525:LYS:HE2	1:A:552:ALA:HA	1.97	0.45
1:A:157:PHE:HE2	1:A:188:GLU:HG2	1.81	0.45
1:A:290:ILE:O	1:A:293:VAL:HG12	2.15	0.45
1:B:342:SER:HA	1:B:447:PRO:HA	1.99	0.45
1:A:508:THR:HG22	1:A:509:PHE:N	2.32	0.45
1:A:392:CYS:O	1:A:396:GLU:HG3	2.17	0.45
1:B:179:LEU:HB2	1:B:180:PRO:HD3	1.99	0.45
1:A:115:LEU:HD22	1:A:145:ARG:NH1	2.32	0.45
1:A:61:ASN:C	1:A:63:ASP:N	2.71	0.45
1:B:370:TYR:C	1:B:370:TYR:CD1	2.90	0.45
1:A:372:LYS:O	1:A:375:ASP:HB2	2.17	0.44
1:A:61:ASN:HB3	1:A:64:LYS:HD2	1.98	0.44
1:B:30:TYR:CE1	1:B:103:LEU:HD23	2.50	0.44
1:A:551:PHE:O	1:A:555:VAL:HG23	2.16	0.44
1:B:366:PRO:O	1:B:369:CYS:N	2.50	0.44
1:B:323:LYS:HG3	1:B:324:ASP:N	2.32	0.44
1:B:194:ALA:HB1	1:B:455:VAL:HG13	1.99	0.44
1:B:578:ALA:O	1:B:581:ALA:HB3	2.17	0.44
1:B:499:PRO:HB3	1:B:535:HIS:O	2.18	0.44
1:A:156:PHE:HE1	1:A:285:GLU:HG3	1.83	0.44
1:B:146:HIS:CE1	2:B:2002:AZQ:H161	2.52	0.44
1:A:543:GLN:O	1:A:547:VAL:HG23	2.17	0.44
1:A:61:ASN:O	1:A:63:ASP:N	2.51	0.44
1:B:185:LEU:HD23	1:B:185:LEU:HA	1.84	0.44
1:B:279:CYS:HA	1:B:286:LYS:CD	2.47	0.44
1:B:408:LEU:HD21	1:B:424:VAL:HA	2.00	0.44
1:A:257:ARG:NH1	1:A:287:SER:HB3	2.33	0.43
1:A:178:LEU:O	1:A:179:LEU:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:PRO:O	1:A:369:CYS:HB3	2.18	0.43
1:B:274:LYS:HE2	1:B:296:ASP:HA	2.00	0.43
1:B:333:GLU:HA	1:B:336:ARG:HD2	1.99	0.43
1:B:9:HIS:CD2	1:B:13:ASP:OD2	2.71	0.43
1:B:103:LEU:C	1:B:105:HIS:H	2.22	0.43
1:A:141:GLU:OE1	1:A:141:GLU:HA	2.18	0.43
1:A:417:GLN:H	1:A:417:GLN:CD	2.22	0.43
1:A:578:ALA:O	1:A:581:ALA:HB3	2.18	0.43
1:B:100:GLU:O	1:B:104:GLN:HG3	2.18	0.43
1:B:70:PHE:CD1	1:B:70:PHE:N	2.87	0.43
1:A:511:ALA:C	1:A:513:ILE:N	2.71	0.43
1:A:532:LEU:HD23	1:A:532:LEU:HA	1.87	0.43
1:A:6:GLU:O	1:A:9:HIS:HB3	2.19	0.43
1:A:39:HIS:HD2	1:A:140:TYR:CE1	2.36	0.43
1:A:485:ARG:HB3	1:A:486:PRO:CD	2.46	0.43
1:B:32:GLN:NE2	1:B:110:PRO:HG3	2.34	0.43
1:B:23:VAL:O	1:B:27:PHE:CD1	2.72	0.43
1:A:464:HIS:CG	1:A:473:VAL:HG11	2.54	0.43
1:A:540:THR:O	1:A:544:LEU:HG	2.18	0.43
1:B:333:GLU:O	1:B:336:ARG:HG2	2.19	0.43
1:B:400:GLU:O	1:B:404:GLN:HG3	2.19	0.43
1:A:563:ASP:OD2	1:A:567:CYS:N	2.52	0.43
1:B:511:ALA:C	1:B:513:ILE:N	2.71	0.43
1:A:507:PHE:CE1	1:A:509:PHE:HZ	2.37	0.42
1:A:464:HIS:HE1	1:A:469:VAL:H	1.66	0.42
1:A:510:HIS:O	1:A:512:ASP:N	2.52	0.42
1:A:78:ALA:C	1:A:80:LEU:H	2.23	0.42
1:B:190:LYS:CE	2:B:2002:AZQ:H12	2.49	0.42
1:A:179:LEU:CB	1:A:180:PRO:HD3	2.49	0.42
1:B:367:HIS:HA	1:B:370:TYR:CZ	2.54	0.42
1:A:206:PHE:CD2	1:A:481:LEU:HD22	2.55	0.42
1:A:157:PHE:CE2	1:A:188:GLU:HG2	2.55	0.42
1:A:281:LYS:HB2	1:A:282:PRO:CD	2.49	0.42
1:B:149:PHE:HE2	2:B:2002:AZQ:H162	1.84	0.42
1:B:516:LEU:HD22	1:B:520:GLU:CB	2.50	0.42
1:A:39:HIS:CD2	1:A:140:TYR:HE1	2.38	0.42
1:B:34:CYS:HA	1:B:35:PRO:HD3	1.91	0.42
1:B:509:PHE:O	1:B:510:HIS:O	2.38	0.42
1:A:23:VAL:HG13	1:A:27:PHE:HE1	1.84	0.42
1:A:310:VAL:O	1:A:370:TYR:HE1	2.02	0.42
1:A:49:PHE:HD2	1:A:49:PHE:C	2.24	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:VAL:O	1:B:469:VAL:HG22	2.20	0.42
1:A:131:GLU:O	1:A:132:GLU:C	2.59	0.41
1:A:259:ASP:HA	1:A:262:LYS:HE2	2.02	0.41
1:B:537:PRO:C	1:B:539:ALA:N	2.73	0.41
1:A:137:LYS:O	1:A:141:GLU:HG2	2.20	0.41
1:A:502:PHE:CE1	1:A:507:PHE:HZ	2.38	0.41
1:A:81:ARG:HA	1:A:84:TYR:O	2.21	0.41
1:A:264:ILE:HD12	2:A:2001:AZQ:H151	2.03	0.41
1:A:483:ASN:O	1:A:486:PRO:HD2	2.21	0.41
1:A:78:ALA:C	1:A:80:LEU:N	2.73	0.41
1:B:149:PHE:CE2	2:B:2002:AZQ:H162	2.56	0.41
1:B:359:LYS:CG	1:B:360:CYS:N	2.83	0.41
1:A:141:GLU:OE1	1:A:144:ARG:HD3	2.20	0.41
1:A:214:TRP:CD1	1:A:343:VAL:HG11	2.56	0.41
1:B:194:ALA:O	1:B:195:LYS:C	2.59	0.41
1:B:218:ARG:HG2	2:B:2001:AZQ:H131	2.01	0.41
1:A:34:CYS:HA	1:A:35:PRO:HD3	1.65	0.41
1:A:39:HIS:HD2	1:A:140:TYR:HE1	1.66	0.41
1:A:342:SER:HA	1:A:447:PRO:HA	2.03	0.41
1:A:464:HIS:CE1	1:A:470:SER:H	2.38	0.41
1:A:66:LEU:HD13	1:A:66:LEU:N	2.35	0.41
1:A:95:GLU:OE1	1:A:99:ASN:HB2	2.20	0.41
1:A:518:GLU:OE1	1:A:521:ARG:HD2	2.21	0.41
1:A:387:LEU:HD22	1:A:485:ARG:NH1	2.36	0.41
1:A:87:MET:O	1:A:90:CYS:HB2	2.20	0.41
1:A:366:PRO:O	1:A:367:HIS:C	2.58	0.41
1:B:15:GLY:O	1:B:19:PHE:HB3	2.20	0.41
1:B:359:LYS:HG3	1:B:360:CYS:N	2.35	0.41
1:A:557:LYS:O	1:A:560:LYS:N	2.44	0.40
1:A:66:LEU:O	1:A:70:PHE:HD1	2.04	0.40
1:B:414:LYS:HE3	1:B:488:PHE:O	2.20	0.40
1:B:81:ARG:HA	1:B:84:TYR:O	2.21	0.40
1:B:482:VAL:O	1:B:482:VAL:HG12	2.21	0.40
1:A:117:ARG:HA	1:A:118:PRO:HD3	1.88	0.40
1:A:274:LYS:HE3	1:A:296:ASP:HA	2.02	0.40
1:A:388:ILE:HD12	1:A:449:ALA:HB3	2.02	0.40
1:B:564:LYS:C	1:B:566:THR:N	2.71	0.40
1:B:502:PHE:HE2	1:B:507:PHE:CZ	2.40	0.40
1:A:116:VAL:HG22	1:A:117:ARG:N	2.36	0.40
1:B:51:LYS:C	1:B:53:CYS:H	2.25	0.40
1:B:70:PHE:HD1	1:B:70:PHE:N	2.18	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:MET:O	1:B:90:CYS:HB2	2.22	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	576/585 (98%)	506 (88%)	54 (9%)	16 (3%)	5	11
1	B	576/585 (98%)	509 (88%)	51 (9%)	16 (3%)	5	11
All	All	1152/1170 (98%)	1015 (88%)	105 (9%)	32 (3%)	5	11

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	ALA
1	A	300	ALA
1	A	510	HIS
1	A	511	ALA
1	B	54	VAL
1	B	60	GLU
1	B	300	ALA
1	B	510	HIS
1	B	511	ALA
1	B	565	GLU
1	A	150	TYR
1	A	512	ASP
1	A	557	LYS
1	A	565	GLU
1	B	58	SER
1	B	85	GLY
1	B	512	ASP

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Mol	Chain	Res	Type
1	B	557	LYS
1	B	558	CYS
1	A	58	SER
1	A	558	CYS
1	A	62	CYS
1	A	538	LYS
1	A	307	ALA
1	B	86	GLU
1	B	129	ASP
1	A	179	LEU
1	B	77	VAL
1	B	179	LEU
1	A	180	PRO
1	A	315	VAL
1	B	315	VAL

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	435/511 (85%)	410 (94%)	25 (6%)	20	44
1	B	417/511 (82%)	393 (94%)	24 (6%)	20	43
All	All	852/1022 (83%)	803 (94%)	49 (6%)	20	43

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	TYR
1	A	37	GLU
1	A	38	ASP
1	A	49	PHE
1	A	66	LEU
1	A	79	THR
1	A	83	THR
1	A	109	ASN

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Mol	Chain	Res	Type
1	A	179	LEU
1	A	245	CYS
1	A	257	ARG
1	A	281	LYS
1	A	284	LEU
1	A	323	LYS
1	A	334	TYR
1	A	375	ASP
1	A	435	SER
1	A	467	THR
1	A	471	ASP
1	A	498	VAL
1	A	503	ASN
1	A	506	THR
1	A	507	PHE
1	A	550	ASP
1	A	558	CYS
1	B	34	CYS
1	B	38	ASP
1	B	56	ASP
1	B	57	GLU
1	B	58	SER
1	B	82	GLU
1	B	83	THR
1	B	105	HIS
1	B	179	LEU
1	B	212	LYS
1	B	283	LEU
1	B	323	LYS
1	B	344	VAL
1	B	375	ASP
1	B	398	LEU
1	B	435	SER
1	B	467	THR
1	B	480	SER
1	B	502	PHE
1	B	503	ASN
1	B	506	THR
1	B	507	PHE
1	B	550	ASP
1	B	558	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	61	ASN
1	A	99	ASN
1	A	109	ASN
1	A	196	GLN
1	A	338	HIS
1	A	385	GLN
1	A	464	HIS
1	A	483	ASN
1	A	503	ASN
1	B	111	ASN
1	B	196	GLN
1	B	385	GLN
1	B	464	HIS
1	B	483	ASN
1	B	503	ASN
1	B	543	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](#)

4 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	AZQ	A	2001	-	17,24,24	3.23	10 (58%)	21,36,36	3.03	9 (42%)
2	AZQ	A	2002	-	17,24,24	2.92	7 (41%)	21,36,36	2.57	8 (38%)
2	AZQ	B	2002	-	17,24,24	3.13	6 (35%)	21,36,36	2.64	8 (38%)
2	AZQ	B	2001	-	17,24,24	3.41	11 (64%)	21,36,36	3.12	8 (38%)

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	AZQ	A	2001	-	1/1/4/4	5/7/23/23	0/3/3/3
2	AZQ	A	2002	-	1/1/4/4	6/7/23/23	0/3/3/3
2	AZQ	B	2002	-	1/1/4/4	6/7/23/23	0/3/3/3
2	AZQ	B	2001	-	1/1/4/4	4/7/23/23	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	AZQ	C2-C1	-8.12	1.37	1.52
2	B	2001	AZQ	C2-C1	-7.82	1.37	1.52
2	B	2002	AZQ	C2-C3	-7.73	1.38	1.52
2	A	2002	AZQ	C2-C3	-7.47	1.38	1.52
2	B	2002	AZQ	C2-C1	-7.40	1.38	1.52
2	A	2002	AZQ	C2-C1	-6.61	1.40	1.52
2	A	2001	AZQ	C2-C3	-5.66	1.41	1.52
2	B	2001	AZQ	C2-C3	-5.61	1.42	1.52
2	B	2001	AZQ	C6-C7	4.83	1.46	1.36
2	B	2002	AZQ	C5-N2	4.31	1.44	1.37
2	A	2001	AZQ	C6-C7	3.93	1.44	1.36
2	B	2001	AZQ	C9-C8	3.84	1.44	1.37
2	B	2001	AZQ	C5-N2	3.65	1.43	1.37
2	A	2001	AZQ	C9-C8	3.50	1.44	1.37
2	A	2001	AZQ	C5-N2	3.31	1.43	1.37
2	A	2002	AZQ	C5-N2	3.21	1.42	1.37
2	B	2001	AZQ	C9-C10	3.11	1.46	1.40
2	B	2001	AZQ	C13-C12	-3.10	1.24	1.49
2	B	2001	AZQ	C4-N2	3.04	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	AZQ	C12-C11	3.04	1.68	1.51
2	A	2001	AZQ	C12-C11	2.97	1.68	1.51
2	B	2002	AZQ	C13-C12	-2.88	1.26	1.49
2	A	2002	AZQ	C13-C12	-2.87	1.26	1.49
2	A	2001	AZQ	C13-C12	-2.84	1.26	1.49
2	A	2002	AZQ	C12-C11	2.82	1.67	1.51
2	B	2002	AZQ	C12-C11	2.76	1.66	1.51
2	B	2002	AZQ	C6-C7	2.65	1.42	1.36
2	A	2001	AZQ	C4-N2	2.61	1.37	1.32
2	A	2002	AZQ	C6-C7	2.60	1.42	1.36
2	A	2001	AZQ	C6-C5	-2.49	1.37	1.41
2	A	2001	AZQ	C9-C10	2.38	1.45	1.40
2	B	2001	AZQ	C14-N4	2.23	1.50	1.45
2	A	2002	AZQ	C9-C8	2.20	1.41	1.37
2	B	2001	AZQ	C6-C5	-2.10	1.38	1.41

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	AZQ	O2-C3-C2	8.78	135.05	126.89
2	A	2001	AZQ	O2-C3-C2	8.32	134.62	126.89
2	B	2002	AZQ	O2-C3-C2	7.27	133.65	126.89
2	A	2002	AZQ	O2-C3-C2	7.22	133.60	126.89
2	A	2001	AZQ	O1-C1-C2	7.18	133.56	126.89
2	B	2001	AZQ	O1-C1-C2	6.93	133.34	126.89
2	B	2002	AZQ	O1-C1-C2	5.27	131.79	126.89
2	A	2002	AZQ	O1-C1-C2	4.95	131.49	126.89
2	B	2001	AZQ	C10-C5-N2	-3.95	116.58	122.12
2	A	2002	AZQ	O2-C3-N1	-3.70	120.12	124.33
2	B	2002	AZQ	O2-C3-N1	-3.67	120.16	124.33
2	A	2001	AZQ	O2-C3-N1	-3.64	120.19	124.33
2	A	2002	AZQ	O1-C1-N3	-3.63	120.20	124.33
2	B	2002	AZQ	O1-C1-N3	-3.60	120.23	124.33
2	A	2001	AZQ	C9-C10-N3	3.57	126.40	122.05
2	B	2001	AZQ	O1-C1-N3	-3.54	120.31	124.33
2	B	2001	AZQ	C9-C10-N3	3.37	126.16	122.05
2	A	2001	AZQ	C10-C5-N2	-3.24	117.57	122.12
2	B	2001	AZQ	C2-C3-N1	-3.11	103.97	107.55
2	B	2001	AZQ	O2-C3-N1	-3.01	120.91	124.33
2	B	2002	AZQ	N2-C4-N4	2.87	122.04	117.26
2	A	2002	AZQ	C9-C10-N3	2.85	125.52	122.05
2	B	2001	AZQ	C7-C8-C9	-2.80	114.94	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2002	AZQ	C7-C6-C5	-2.69	117.46	120.84
2	B	2002	AZQ	C10-C5-N2	-2.63	118.43	122.12
2	A	2001	AZQ	C2-C1-N3	-2.52	104.65	107.55
2	A	2001	AZQ	C7-C8-C9	-2.41	115.42	118.40
2	A	2002	AZQ	C10-C5-N2	-2.41	118.74	122.12
2	A	2001	AZQ	O1-C1-N3	-2.24	121.78	124.33
2	A	2002	AZQ	C7-C6-C5	-2.20	118.07	120.84
2	A	2001	AZQ	C2-C3-N1	-2.09	105.15	107.55
2	A	2002	AZQ	C13-C12-C11	-2.07	103.28	113.29
2	B	2002	AZQ	C6-C5-N2	2.01	121.75	118.69

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2001	AZQ	C2
2	A	2002	AZQ	C2
2	B	2002	AZQ	C2
2	B	2001	AZQ	C2

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	AZQ	C12-C11-C2-C3
2	A	2001	AZQ	N1-C4-N4-C15
2	A	2001	AZQ	N2-C4-N4-C15
2	A	2002	AZQ	C12-C11-C2-C3
2	A	2002	AZQ	N1-C4-N4-C14
2	A	2002	AZQ	N1-C4-N4-C15
2	A	2002	AZQ	N2-C4-N4-C14
2	A	2002	AZQ	N2-C4-N4-C15
2	B	2002	AZQ	N1-C4-N4-C14
2	B	2002	AZQ	N1-C4-N4-C15
2	B	2002	AZQ	N2-C4-N4-C14
2	B	2002	AZQ	N2-C4-N4-C15
2	B	2001	AZQ	C12-C11-C2-C3
2	B	2001	AZQ	N1-C4-N4-C15
2	B	2001	AZQ	N2-C4-N4-C15
2	A	2001	AZQ	N2-C4-N4-C14
2	B	2001	AZQ	N2-C4-N4-C14
2	B	2002	AZQ	C2-C11-C12-C13
2	A	2001	AZQ	C2-C11-C12-C13
2	B	2002	AZQ	C12-C11-C2-C1

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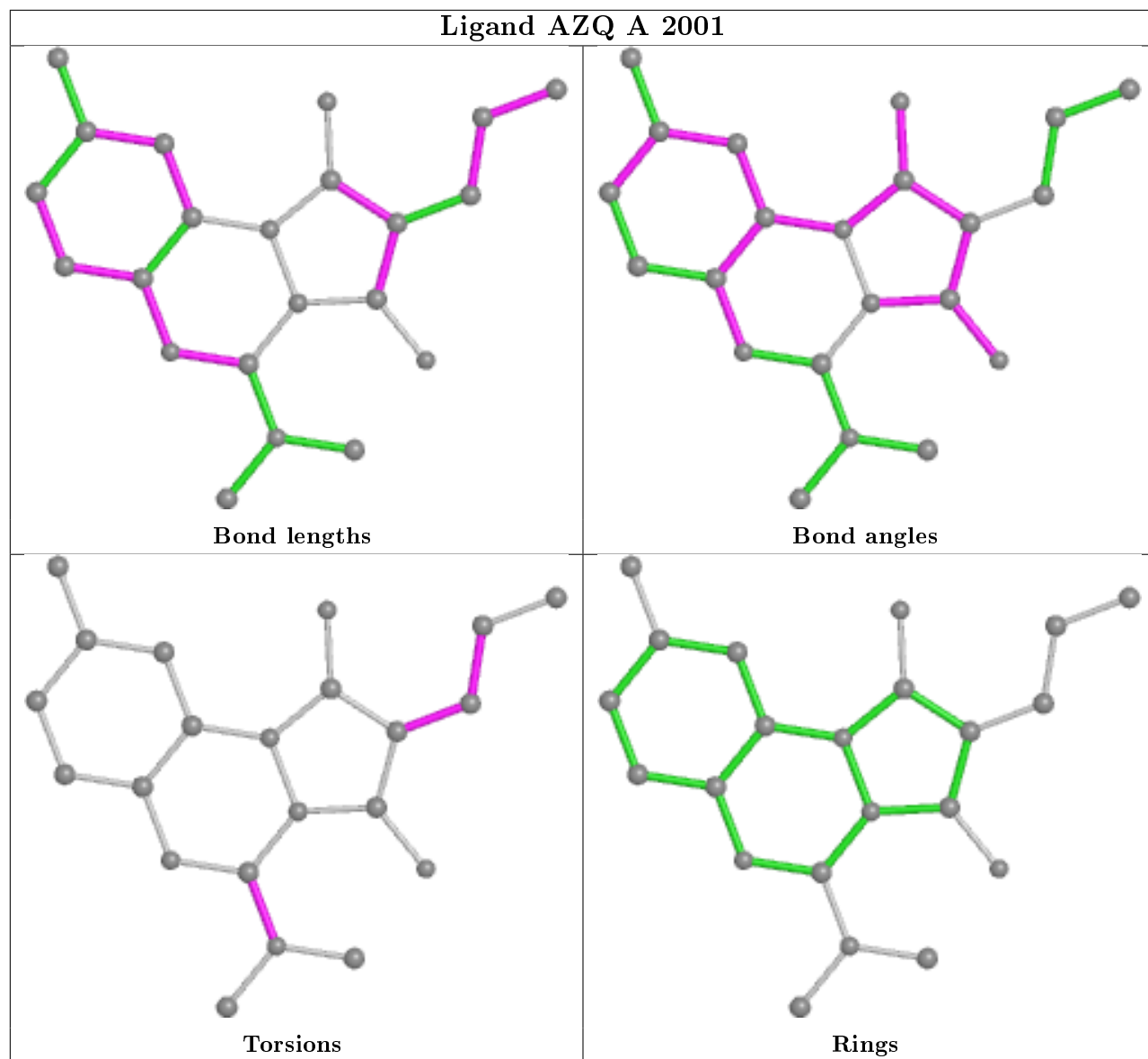
Mol	Chain	Res	Type	Atoms
2	A	2002	AZQ	C2-C11-C12-C13

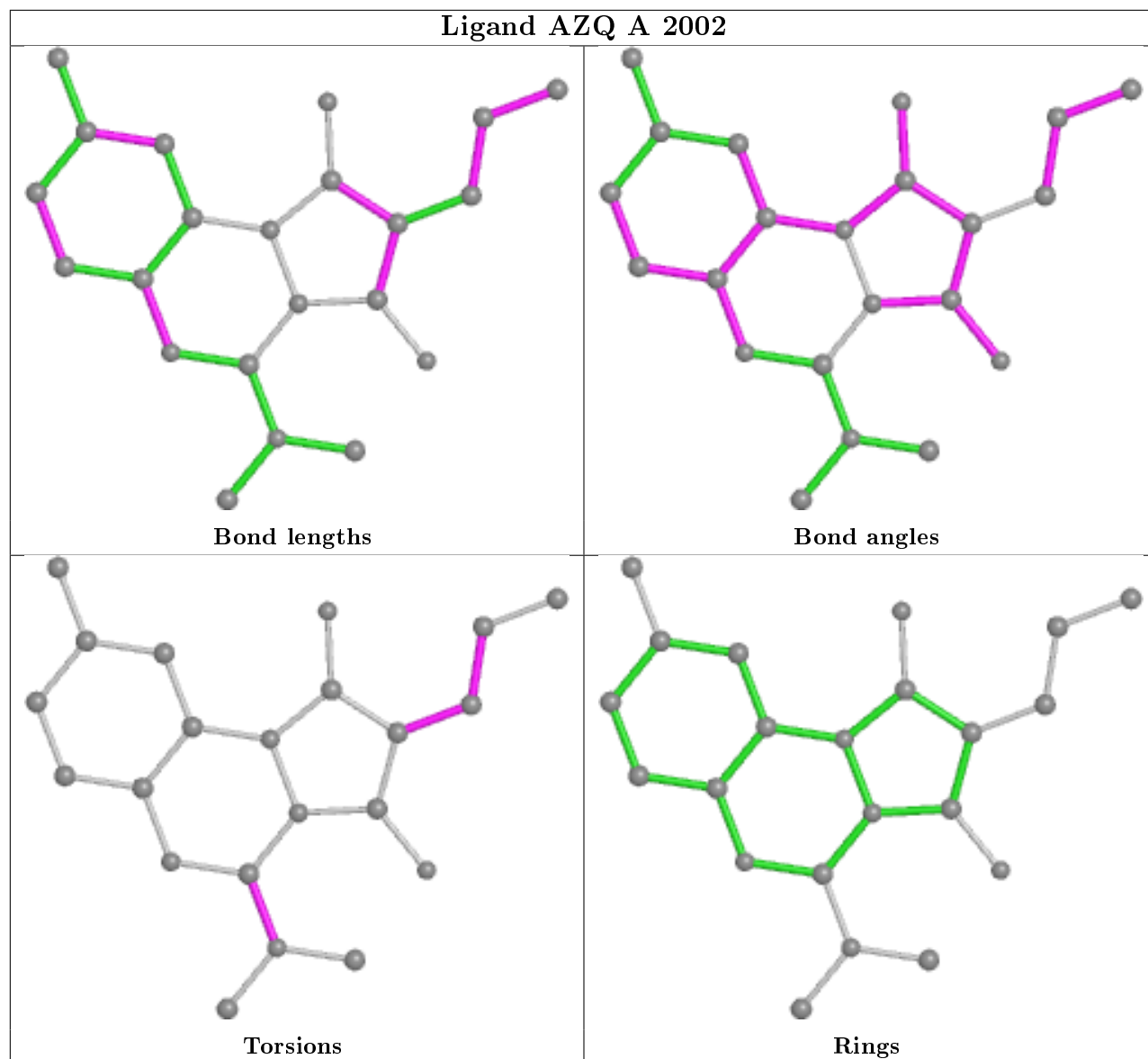
There are no ring outliers.

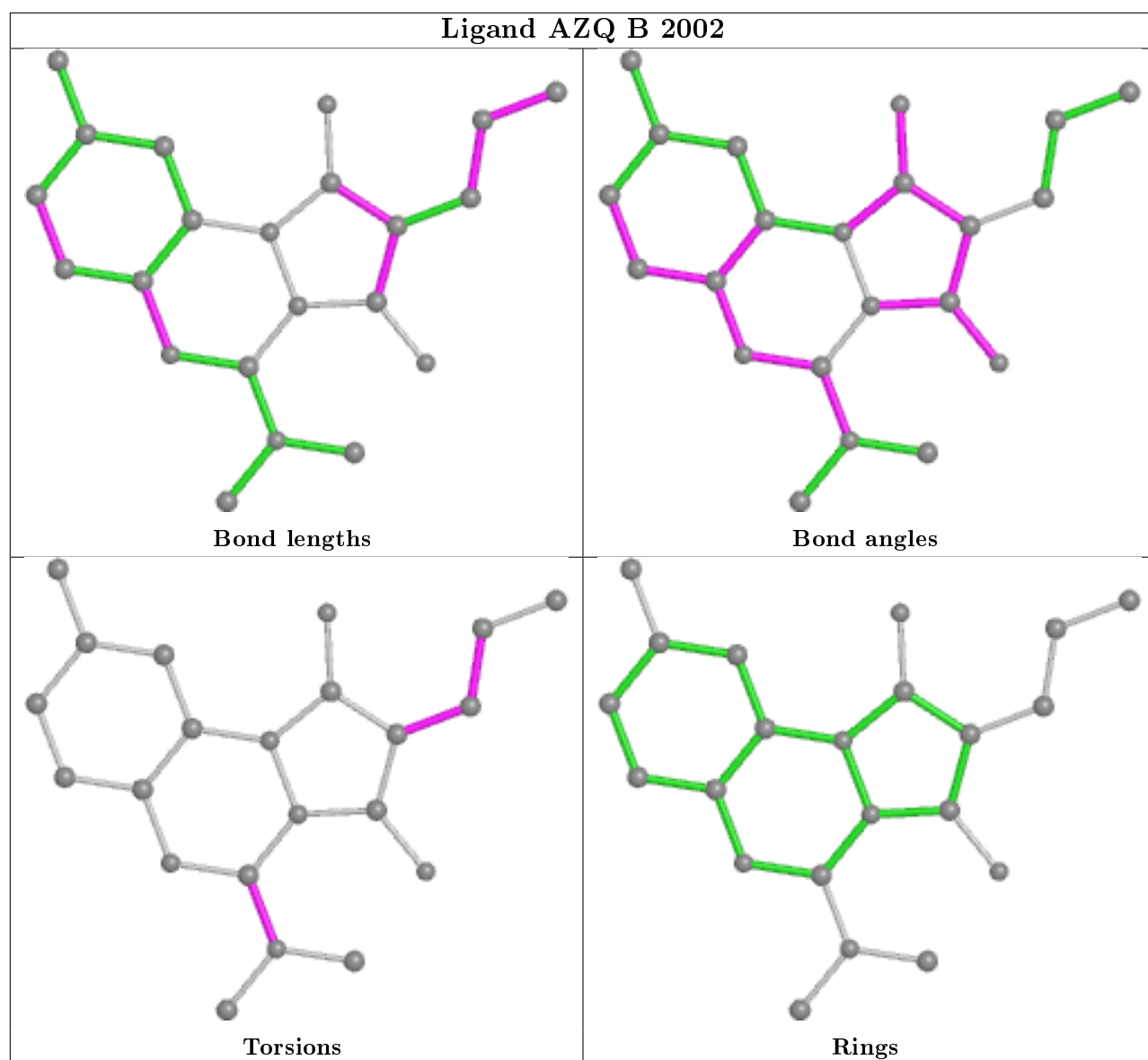
4 monomers are involved in 18 short contacts:

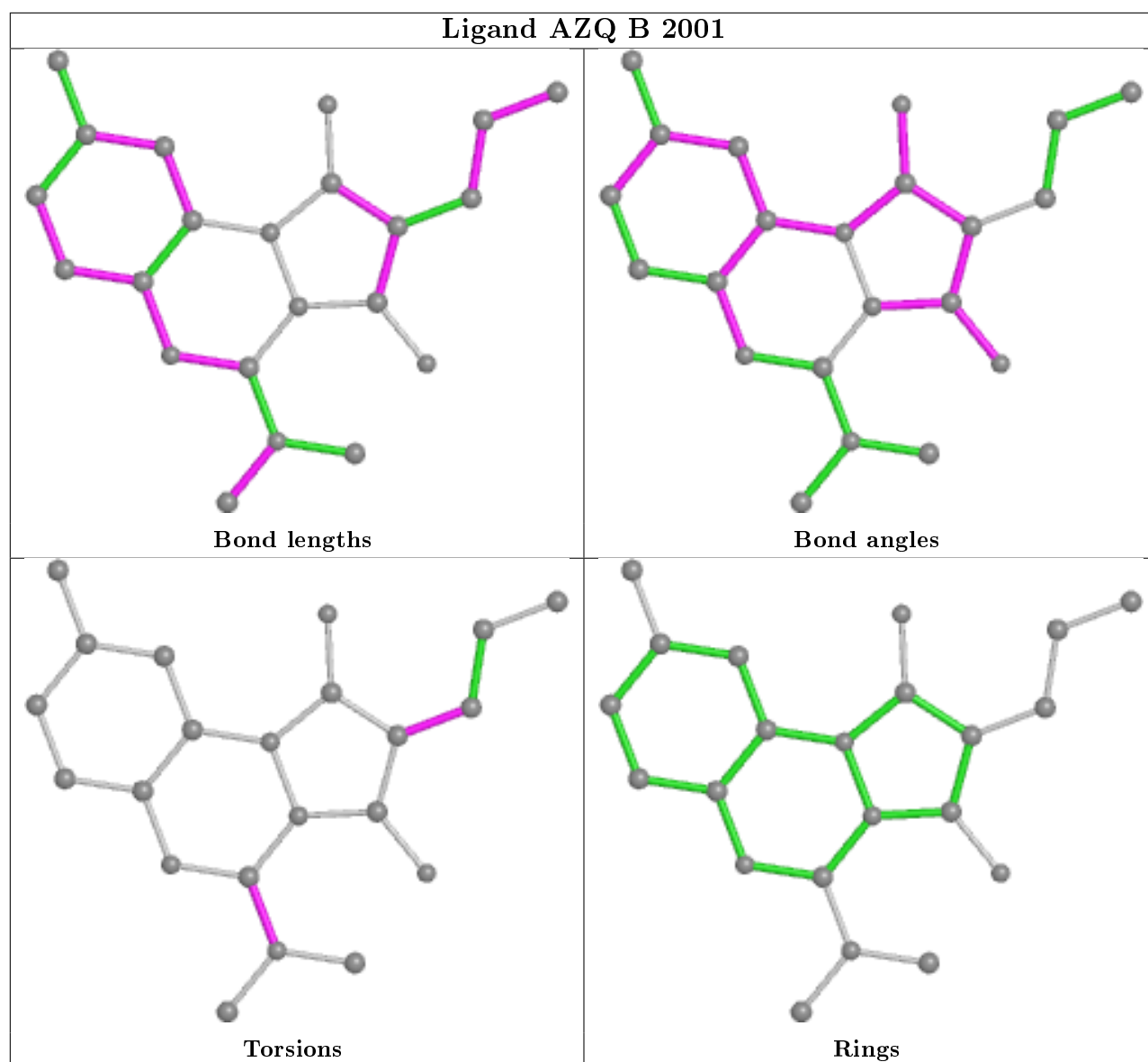
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	AZQ	4	0
2	A	2002	AZQ	5	0
2	B	2002	AZQ	7	0
2	B	2001	AZQ	2	0

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 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	578/585 (98%)	0.03	29 (5%)	28 27	34, 71, 140, 159	0
1	B	578/585 (98%)	0.20	42 (7%)	15 13	30, 76, 145, 162	0
All	All	1156/1170 (98%)	0.12	71 (6%)	21 20	30, 73, 142, 162	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	83	THR	11.7
1	A	510	HIS	8.2
1	B	569	ALA	7.9
1	B	577	ALA	6.5
1	B	510	HIS	6.3
1	A	569	ALA	6.0
1	B	79	THR	5.8
1	B	84	TYR	5.7
1	A	54	VAL	5.5
1	B	562	ASP	5.3
1	B	566	THR	5.3
1	B	564	LYS	5.2
1	A	578	ALA	5.1
1	A	511	ALA	5.1
1	B	573	LYS	5.0
1	B	82	GLU	4.9
1	A	505	GLU	4.8
1	A	79	THR	4.8
1	A	566	THR	4.8
1	B	87	MET	4.7
1	B	80	LEU	4.7
1	A	581	ALA	4.6
1	A	83	THR	4.5
1	B	508	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	581	ALA	4.3
1	A	508	THR	4.3
1	B	81	ARG	3.9
1	A	564	LYS	3.9
1	A	57	GLU	3.9
1	B	578	ALA	3.8
1	B	565	GLU	3.8
1	B	505	GLU	3.7
1	B	63	ASP	3.7
1	B	561	ALA	3.5
1	B	580	GLN	3.4
1	A	85	GLY	3.4
1	B	558	CYS	3.3
1	B	563	ASP	3.3
1	B	504	ALA	3.2
1	B	576	VAL	3.2
1	A	561	ALA	3.1
1	B	570	GLU	3.1
1	A	87	MET	3.1
1	B	568	PHE	3.1
1	B	502	PHE	2.9
1	A	559	CYS	2.9
1	B	512	ASP	2.9
1	A	84	TYR	2.8
1	A	568	PHE	2.8
1	B	555	VAL	2.8
1	A	56	ASP	2.7
1	B	58	SER	2.7
1	B	509	PHE	2.7
1	B	5	SER	2.7
1	B	572	GLY	2.5
1	B	78	ALA	2.5
1	A	171	ALA	2.4
1	B	506	THR	2.4
1	B	77	VAL	2.4
1	B	127	PHE	2.4
1	B	567	CYS	2.4
1	A	560	LYS	2.3
1	A	551	PHE	2.3
1	A	558	CYS	2.3
1	A	572	GLY	2.1
1	B	169	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	57	GLU	2.1
1	A	552	ALA	2.1
1	A	82	GLU	2.1
1	A	573	LYS	2.0
1	A	80	LEU	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](#)

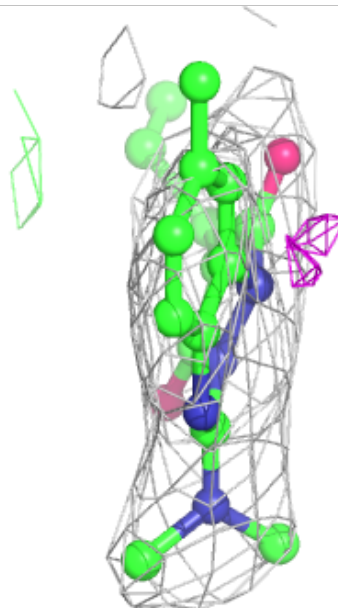
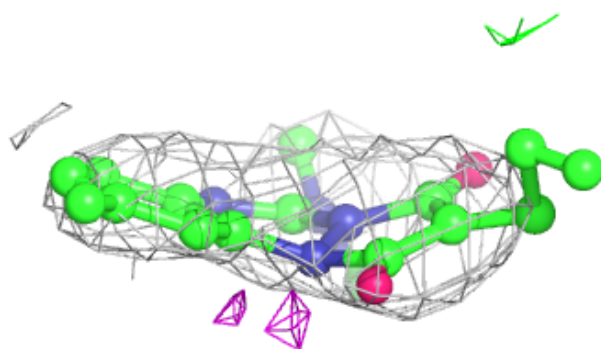
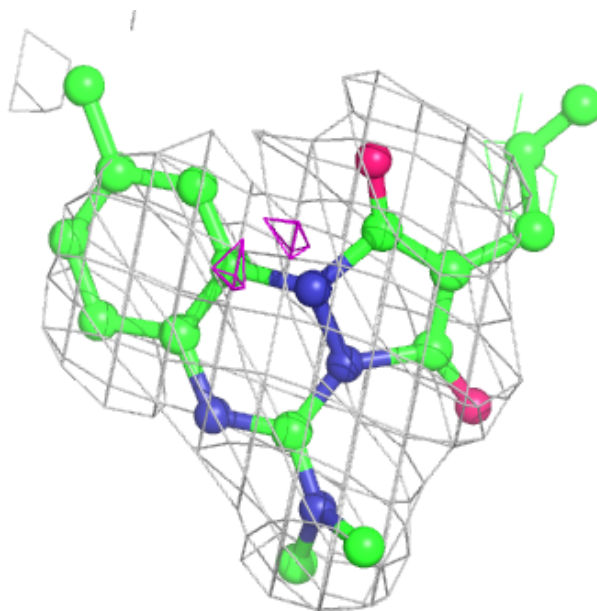
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	AZQ	A	2002	22/22	0.86	0.26	98,101,103,104	0
2	AZQ	B	2002	22/22	0.87	0.22	96,100,101,101	0
2	AZQ	B	2001	22/22	0.90	0.31	99,102,104,105	0
2	AZQ	A	2001	22/22	0.91	0.27	95,96,99,102	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.

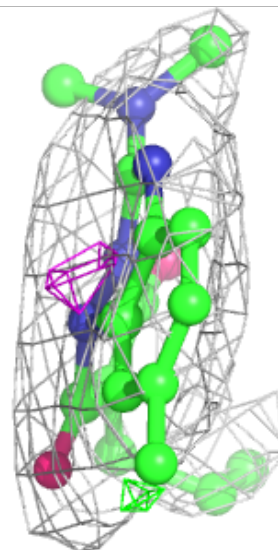
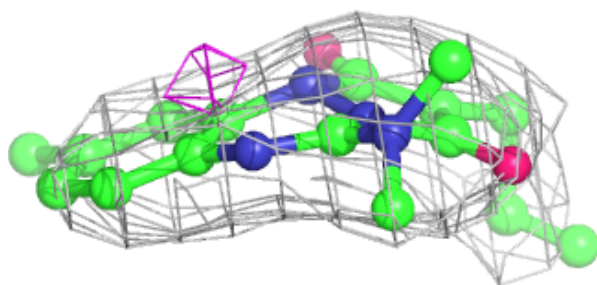
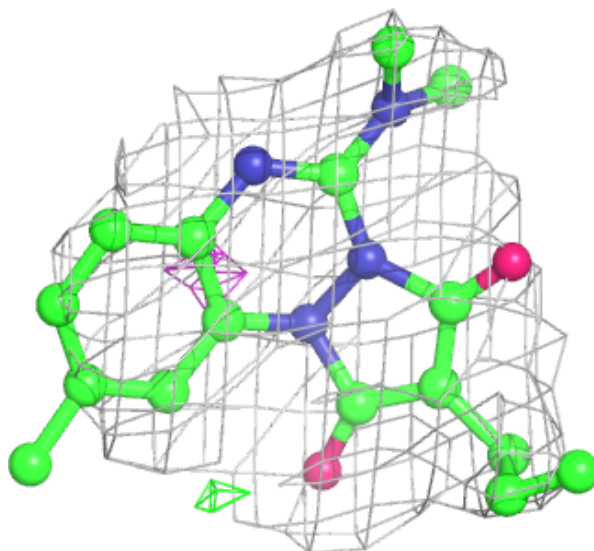
Electron density around AZQ A 2002:

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



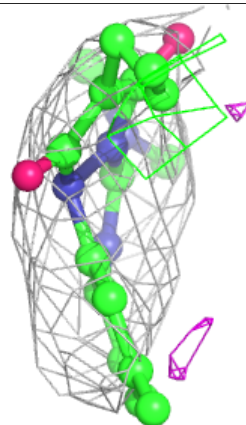
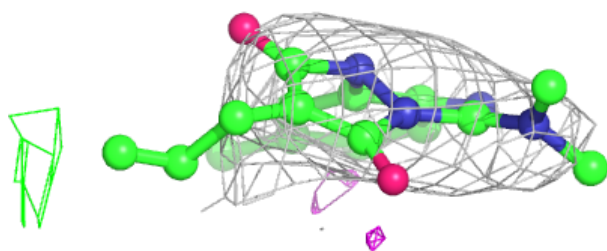
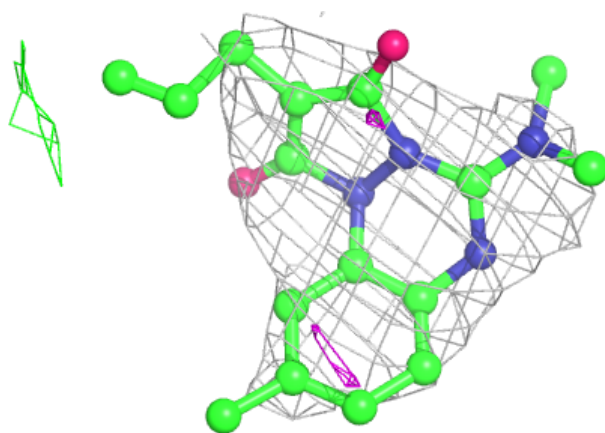
Electron density around AZQ B 2002:

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



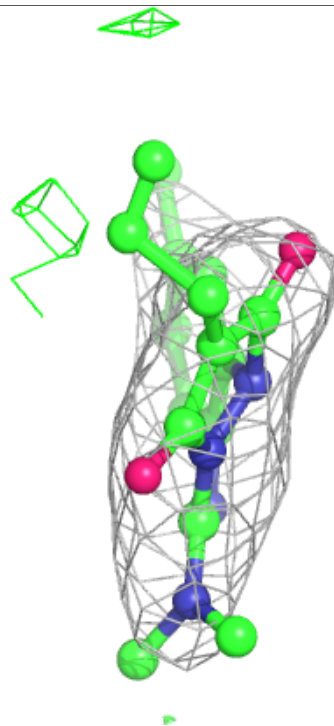
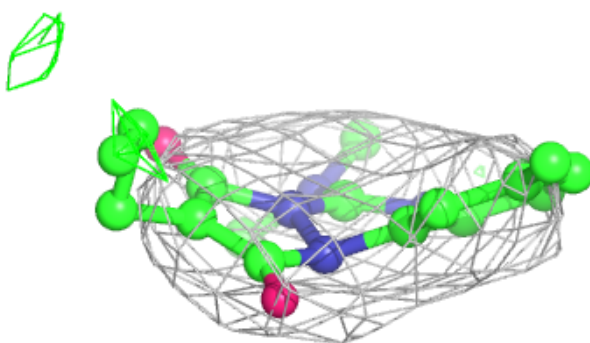
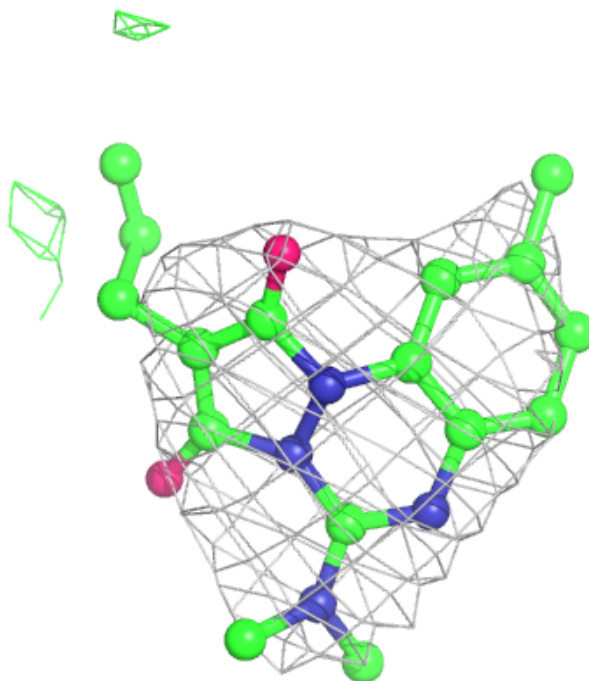
Electron density around AZQ B 2001:

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



Electron density around AZQ A 2001:

$2mF_o-DF_c$ (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.