



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:32 PM UTC

PDB ID : 6UEL / pdb_00006uel
Title : CPS1 bound to allosteric inhibitor H3B-193
Authors : Larsen, N.A.; Nguyen, T.V.
Deposited on : 2019-09-21
Resolution : 1.90 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

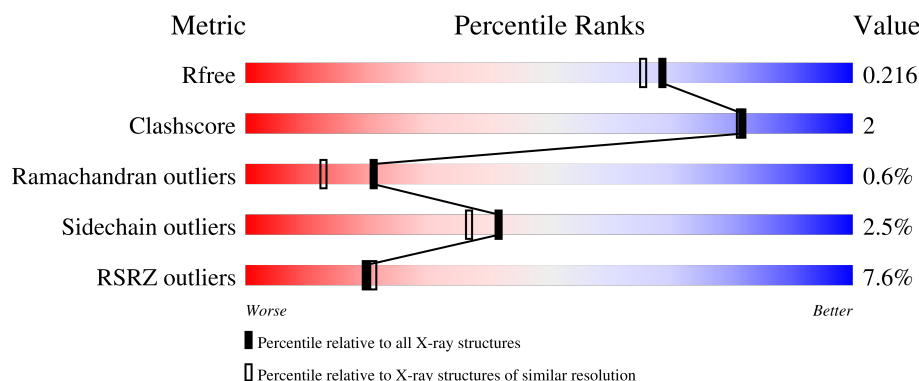
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	1500	7% 81% 7% 11%
1	B	1500	7% 81% 7% 11%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 22300 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.

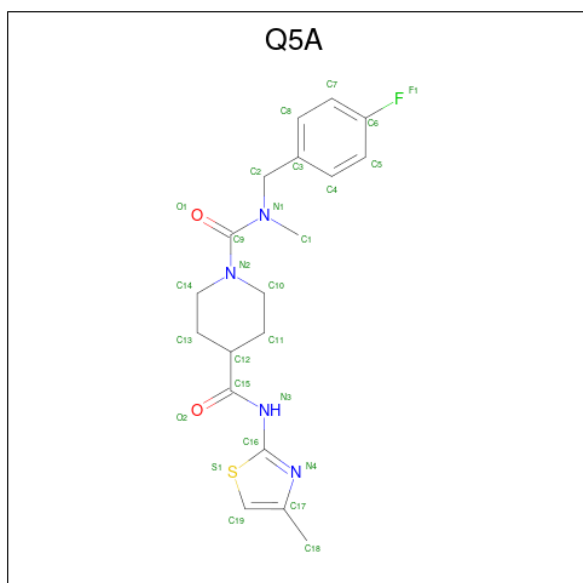
- Molecule 1 is a protein called Carbamoyl-phosphate synthase [ammonia], mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1333	Total	C	N	O	S	0	0	0
			10313	6555	1746	1959	53			
1	B	1332	Total	C	N	O	S	0	0	0
			10309	6554	1743	1959	53			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is N 1 -[(4-fluorophenyl)methyl]-N 1 -methyl-N 4 -(4-methyl-1,3-thiazol-2-yl)pi peridine-1,4-dicarboxamide (CCD ID: Q5A) (formula: C₁₉H₂₃FN₄O₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			27	19	1	4	2	1		
3	B	1	Total	C	F	N	O	S	0	0
			27	19	1	4	2	1		

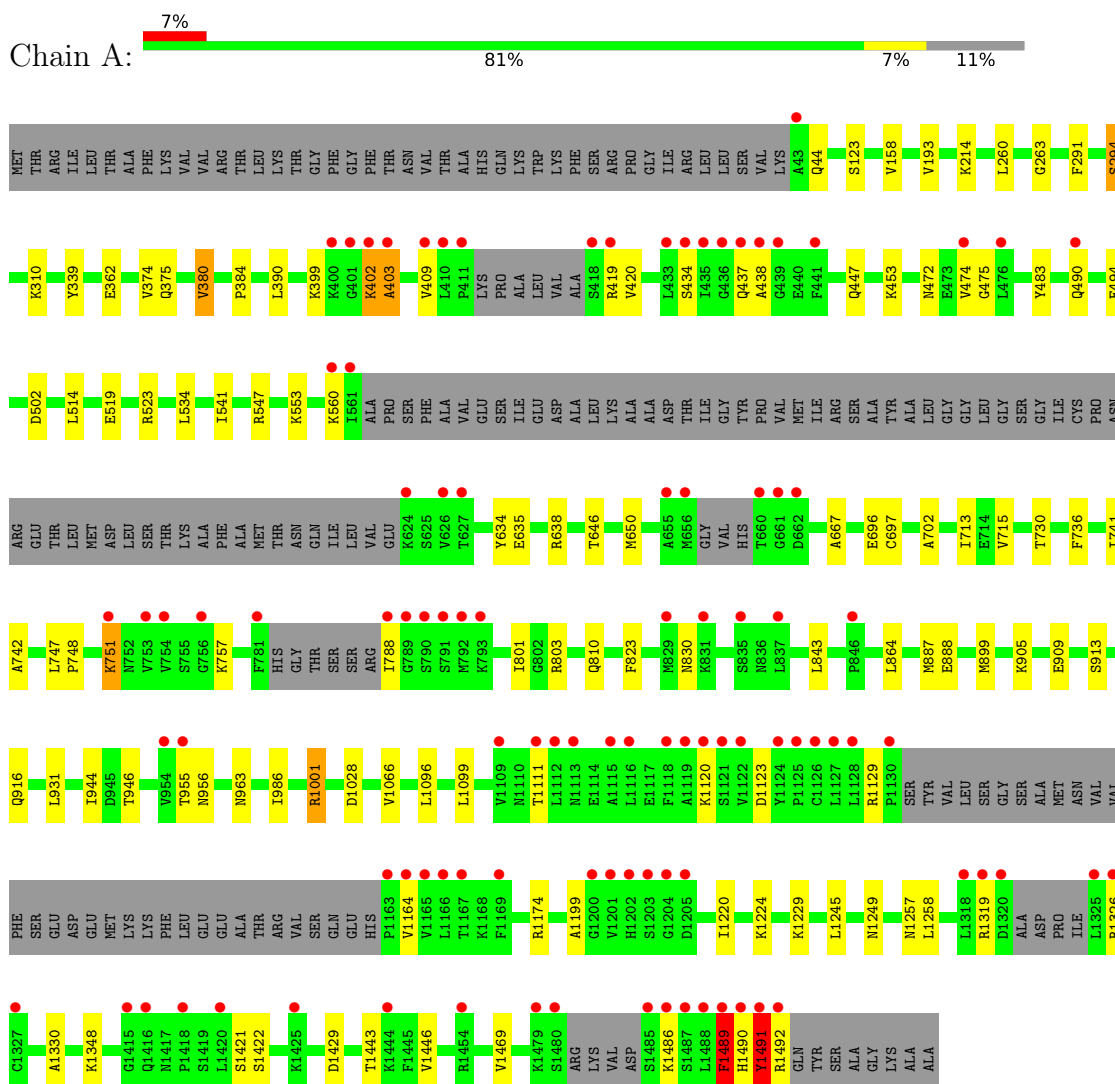
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	786	Total	O	0	0
			786	786		
4	B	836	Total	O	0	0
			836	836		

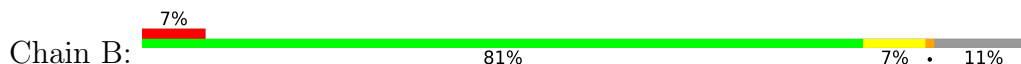
3 Residue-property plots

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: Carbamoyl-phosphate synthase [ammonia], mitochondrial



- Molecule 1: Carbamoyl-phosphate synthase [ammonia], mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.59Å 132.34Å 142.44Å 90.00° 102.57° 90.00°	Depositor
Resolution (Å)	139.03 – 1.90 139.03 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (139.03-1.90) 99.9 (139.03-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.172 , 0.209 0.181 , 0.216	Depositor DCC
R_{free} test set	14084 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22300	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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: ZN, Q5A

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	1.23	14/10511 (0.1%)	1.08	10/14235 (0.1%)
1	B	1.27	23/10508 (0.2%)	1.09	12/14236 (0.1%)
All	All	1.25	37/21019 (0.2%)	1.08	22/28471 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1490	HIS	CA-C	13.24	1.69	1.53
1	B	1490	HIS	N-CA	10.16	1.60	1.46
1	A	751	LYS	CA-C	7.66	1.62	1.52
1	B	654	ASP	C-O	7.29	1.33	1.23
1	B	1489	PHE	N-CA	7.26	1.54	1.45
1	B	381	THR	CA-CB	7.20	1.57	1.52
1	B	1491	TYR	N-CA	7.20	1.56	1.46
1	B	1491	TYR	CA-C	7.09	1.62	1.52
1	B	751	LYS	CA-C	6.69	1.61	1.52
1	B	485	LEU	CA-C	-6.66	1.45	1.52
1	A	1066	VAL	CA-C	6.36	1.59	1.52
1	A	888	GLU	CA-C	6.30	1.60	1.52
1	B	381	THR	C-O	-6.26	1.21	1.23
1	B	1489	PHE	CA-C	6.25	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	638	ARG	C-O	5.88	1.30	1.24
1	A	1491	TYR	N-CA	5.84	1.53	1.46
1	A	193	VAL	C-O	5.77	1.29	1.24
1	A	1469	VAL	N-CA	-5.65	1.39	1.46
1	A	887	MET	C-O	5.63	1.30	1.24
1	B	1489	PHE	C-N	5.62	1.40	1.33
1	B	771	THR	CA-C	-5.61	1.46	1.52
1	B	842	GLU	C-O	-5.59	1.17	1.24
1	A	1174	ARG	CD-NE	-5.54	1.38	1.46
1	B	496	ILE	CA-C	5.52	1.59	1.52
1	B	1263	SER	N-CA	-5.41	1.39	1.46
1	B	1490	HIS	CA-CB	5.38	1.60	1.53
1	B	231	VAL	N-CA	-5.36	1.40	1.46
1	A	158	VAL	C-O	-5.33	1.18	1.24
1	B	172	ILE	N-CA	5.30	1.52	1.46
1	A	123	SER	N-CA	5.28	1.52	1.46
1	A	751	LYS	N-CA	5.16	1.52	1.46
1	A	899	MET	N-CA	5.12	1.52	1.46
1	B	972	ASP	C-O	-5.12	1.17	1.24
1	B	560	LYS	C-O	5.05	1.30	1.23
1	B	645	VAL	N-CA	5.05	1.51	1.46
1	A	1257	ASN	N-CA	5.03	1.52	1.46
1	B	497	LYS	N-CA	5.02	1.52	1.46

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1490	HIS	N-CA-C	12.89	125.25	108.24
1	B	1491	TYR	N-CA-C	9.84	122.73	108.86
1	A	751	LYS	N-CA-C	9.47	124.21	110.10
1	B	1489	PHE	N-CA-C	9.46	125.09	110.42
1	A	1489	PHE	N-CA-C	8.48	123.01	109.86
1	B	420	VAL	N-CA-C	-6.75	100.24	109.55
1	B	653	VAL	N-CA-C	-6.51	104.50	110.82
1	B	1479	LYS	N-CA-C	6.27	117.78	111.07
1	B	344	THR	N-CA-C	6.24	118.97	107.99
1	A	1001	ARG	NE-CZ-NH2	-6.16	113.66	119.20
1	A	1257	ASN	N-CA-C	-5.87	98.84	108.41
1	B	1180	ALA	N-CA-C	5.79	117.59	108.96
1	A	830	ASN	N-CA-C	5.78	119.64	112.47
1	A	438	ALA	N-CA-C	5.64	118.16	111.33
1	B	816	CYS	N-CA-C	5.62	117.41	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	861	ASN	N-CA-C	5.55	119.64	112.86
1	A	419	ARG	N-CA-C	5.55	117.01	111.07
1	B	1478	GLN	N-CA-C	-5.51	105.18	111.07
1	A	1174	ARG	NE-CZ-NH1	5.48	126.98	121.50
1	A	1164	VAL	N-CA-C	5.39	116.24	108.48
1	A	1174	ARG	NE-CZ-NH2	-5.32	114.41	119.20
1	B	644	CYS	CB-CA-C	5.04	117.98	110.62

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1319	ARG	Peptide
1	A	1489	PHE	Peptide
1	B	831	LYS	Peptide

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	10313	0	10369	49	0
1	B	10309	0	10374	48	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	0	3	0
3	B	27	0	0	2	0
4	A	786	0	0	3	1
4	B	836	0	0	13	1
All	All	22300	0	20743	102	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (102) 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:B:452:MET:HE3	1:B:505:ILE:HD11	1.52	0.88
1:A:913:SER:H	1:A:916:GLN:HE21	1.29	0.80
1:B:810:GLN:HE21	1:B:823:PHE:H	1.37	0.73
1:A:913:SER:H	1:A:916:GLN:NE2	1.95	0.65
3:B:1602:Q5A:C1	3:B:1602:Q5A:C10	2.77	0.62
1:A:697:CYS:SG	1:A:715:VAL:HG13	2.40	0.62
1:B:419:ARG:NH2	1:B:749:GLU:OE1	2.33	0.61
1:B:135:ASP:OD2	4:B:1701:HOH:O	2.16	0.61
1:A:810:GLN:HE21	1:A:823:PHE:H	1.47	0.61
1:B:830:ASN:OD1	1:B:832:GLU:N	2.33	0.60
1:B:810:GLN:HE22	1:B:916:GLN:HE22	1.49	0.60
1:A:634:TYR:HD2	1:A:646:THR:HG21	1.67	0.60
3:B:1602:Q5A:S1	3:B:1602:Q5A:O2	2.59	0.59
1:B:404:THR:HG22	1:B:408:SER:OG	2.05	0.56
1:B:697:CYS:SG	1:B:715:VAL:HG13	2.45	0.56
1:B:109:THR:HG22	4:B:2455:HOH:O	2.05	0.56
1:A:490:GLN:HE21	1:A:1486:LYS:HB2	1.70	0.56
1:B:107:PRO:HD2	4:B:2455:HOH:O	2.06	0.56
1:A:635:GLU:OE1	1:A:696:GLU:OE2	2.23	0.55
1:B:372:PHE:HB3	1:B:406:ILE:HG12	1.87	0.55
1:B:650:MET:HG3	4:B:2397:HOH:O	2.06	0.54
3:A:1602:Q5A:C1	3:A:1602:Q5A:C10	2.86	0.54
1:B:830:ASN:O	1:B:831:LYS:CB	2.55	0.53
1:A:310:LYS:HD3	1:A:339:TYR:CZ	2.44	0.53
1:A:1491:TYR:CG	1:A:1492:ARG:N	2.77	0.53
1:A:650:MET:HG2	1:A:667:ALA:HB2	1.91	0.53
1:B:406:ILE:HD12	4:B:1991:HOH:O	2.09	0.52
1:A:453:LYS:HG3	4:A:1738:HOH:O	2.08	0.52
1:B:135:ASP:OD1	4:B:1702:HOH:O	2.19	0.52
1:A:741:ILE:HD11	1:A:747:LEU:HD21	1.91	0.51
1:B:931:LEU:HD12	4:B:2134:HOH:O	2.10	0.51
1:B:365:MET:HB2	1:B:406:ILE:HD13	1.92	0.51
1:B:121:LEU:HD21	4:B:2455:HOH:O	2.09	0.51
1:A:380:VAL:HG11	1:A:384:PRO:O	2.12	0.50
1:B:405:THR:HG23	1:B:408:SER:H	1.76	0.50
1:A:730:THR:O	1:A:946:THR:HG22	2.11	0.50
1:B:263:GLY:O	1:B:294:SER:HB3	2.11	0.50
1:B:830:ASN:O	1:B:831:LYS:HB2	2.12	0.50
3:A:1602:Q5A:C1	3:A:1602:Q5A:C8	2.89	0.49
1:A:447:GLN:HE21	1:A:736:PHE:HB2	1.77	0.49
1:A:747:LEU:HB2	1:A:748:PRO:HD3	1.94	0.49
1:B:175:ASP:C	1:B:176:LYS:HD3	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1602:Q5A:O2	3:A:1602:Q5A:S1	2.72	0.48
1:B:514:LEU:HD23	1:B:514:LEU:C	2.39	0.48
1:A:483:TYR:CD2	1:A:1491:TYR:HB2	2.47	0.48
1:A:310:LYS:HD3	1:A:339:TYR:CE2	2.49	0.48
1:B:810:GLN:NE2	1:B:823:PHE:H	2.08	0.47
1:B:649:ASN:ND2	1:B:669:ALA:H	2.11	0.47
1:A:519:GLU:OE2	1:A:523:ARG:HD3	2.15	0.47
1:B:1078:THR:HG21	1:B:1258:LEU:HD13	1.97	0.47
1:A:1220:ILE:HG22	1:A:1224:LYS:HE2	1.97	0.47
1:B:490:GLN:HE21	1:B:1486:LYS:HB2	1.80	0.47
1:B:979:LEU:HD12	1:B:1054:ILE:HG22	1.96	0.46
1:A:472:ASN:O	1:A:1001:ARG:NH2	2.47	0.46
1:B:1377:VAL:HG23	4:B:1747:HOH:O	2.16	0.46
1:A:905:LYS:HD2	4:A:2453:HOH:O	2.16	0.46
1:A:519:GLU:O	1:A:523:ARG:HG3	2.17	0.45
1:A:1443:THR:HA	1:A:1446:VAL:HG23	1.97	0.45
1:A:494:GLU:HG3	1:A:1486:LYS:HD3	1.98	0.45
1:A:1348:LYS:HE3	1:A:1489:PHE:CD1	2.51	0.45
1:A:909:GLU:HB3	1:A:963:ASN:HD21	1.81	0.45
1:A:986:ILE:HD13	1:A:1330:ALA:HB1	1.98	0.45
1:B:401:GLY:O	1:B:403:ALA:N	2.49	0.44
1:B:1055:SER:HB3	4:B:1729:HOH:O	2.17	0.44
1:B:1353:THR:O	1:B:1353:THR:HG22	2.17	0.44
1:A:453:LYS:NZ	1:A:475:GLY:O	2.46	0.44
1:A:514:LEU:HD11	1:A:541:ILE:HD13	1.99	0.44
1:A:1099:LEU:HD13	1:A:1229:LYS:HB3	1.98	0.44
1:A:702:ALA:HB2	1:A:713:ILE:HD11	1.99	0.44
1:A:931:LEU:HD12	4:A:2203:HOH:O	2.17	0.44
1:B:647:VAL:HG21	1:B:734:LEU:HD21	2.00	0.43
1:B:1411:PRO:O	1:B:1414:GLU:HG3	2.19	0.43
1:B:401:GLY:O	1:B:402:LYS:C	2.62	0.43
1:A:490:GLN:NE2	1:A:1486:LYS:HB2	2.34	0.43
1:A:1429:ASP:OD1	1:A:1429:ASP:C	2.61	0.43
1:A:803:ARG:HB2	1:A:963:ASN:HB2	2.00	0.43
1:A:1490:HIS:NE2	1:A:1492:ARG:NH2	2.66	0.43
1:A:402:LYS:O	1:A:403:ALA:HB2	2.19	0.42
1:B:1109:VAL:HG12	1:B:1164:VAL:HG13	2.01	0.42
1:B:478:GLN:HG3	4:B:2387:HOH:O	2.19	0.42
1:B:134:LEU:HD23	1:B:135:ASP:HB2	2.02	0.42
1:B:829:MET:O	1:B:830:ASN:C	2.62	0.42
1:A:374:VAL:HG11	1:A:390:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:944:ILE:O	1:A:955:THR:HG21	2.18	0.42
1:B:650:MET:HG2	1:B:667:ALA:HB2	2.00	0.42
1:B:862:MET:HE3	1:B:862:MET:HB2	1.89	0.42
1:B:422:VAL:HG11	1:B:425:VAL:HG22	2.01	0.42
1:B:772:LYS:NZ	4:B:1774:HOH:O	2.53	0.42
1:A:263:GLY:O	1:A:294:SER:HB3	2.19	0.41
1:B:654:ASP:OD2	1:B:850:ARG:HD3	2.20	0.41
1:A:534:LEU:HB3	1:A:742:ALA:HB1	2.02	0.41
1:A:362:GLU:HA	1:A:375:GLN:HB3	2.02	0.41
1:B:730:THR:HG22	1:B:766:LEU:HD11	2.01	0.41
1:A:1199:ALA:CB	1:A:1245:LEU:CD2	2.98	0.41
1:B:647:VAL:HA	1:B:764:PRO:HD2	2.02	0.41
1:B:1323:PRO:O	1:B:1325:LEU:N	2.47	0.41
1:A:986:ILE:CD1	1:A:1330:ALA:HB1	2.51	0.41
1:B:1262:ARG:HD3	4:B:2259:HOH:O	2.20	0.41
1:A:260:LEU:HA	1:A:291:PHE:O	2.21	0.41
1:A:801:ILE:HD13	1:A:944:ILE:HD11	2.02	0.40
1:A:502:ASP:OD1	1:A:502:ASP:N	2.53	0.40
1:A:956:ASN:HB2	1:A:1028:ASP:O	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1975:HOH:O	4:B:2363:HOH:O[2_656]	2.08	0.12

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	1317/1500 (88%)	1280 (97%)	32 (2%)	5 (0%)	30 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1318/1500 (88%)	1272 (96%)	35 (3%)	11 (1%)	16	8
All	All	2635/3000 (88%)	2552 (97%)	67 (2%)	16 (1%)	21	13

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	402	LYS
1	B	830	ASN
1	B	831	LYS
1	A	402	LYS
1	A	403	ALA
1	B	829	MET
1	A	294	SER
1	A	380	VAL
1	B	380	VAL
1	B	846	PRO
1	B	1202	HIS
1	A	1123	ASP
1	B	1320	ASP
1	B	294	SER
1	B	1325	LEU
1	B	1324	ILE

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	1136/1274 (89%)	1110 (98%)	26 (2%)	44	40
1	B	1136/1274 (89%)	1105 (97%)	31 (3%)	39	34
All	All	2272/2548 (89%)	2215 (98%)	57 (2%)	42	37

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	214	LYS
1	A	399	LYS
1	A	409	VAL
1	A	420	VAL
1	A	434	SER
1	A	437	GLN
1	A	474	VAL
1	A	547	ARG
1	A	553	LYS
1	A	560	LYS
1	A	751	LYS
1	A	757	LYS
1	A	788	ILE
1	A	843	LEU
1	A	864	LEU
1	A	1096	LEU
1	A	1111	THR
1	A	1120	LYS
1	A	1129	ARG
1	A	1249	ASN
1	A	1258	LEU
1	A	1326	ARG
1	A	1421	SER
1	A	1422	SER
1	A	1491	TYR
1	B	176	LYS
1	B	228	LYS
1	B	237	LYS
1	B	253	LYS
1	B	410	LEU
1	B	412	LYS
1	B	420	VAL
1	B	422	VAL
1	B	423	SER
1	B	560	LYS
1	B	627	THR
1	B	827	LEU
1	B	832	GLU
1	B	835	SER
1	B	836	ASN
1	B	1098	GLU
1	B	1109	VAL

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Mol	Chain	Res	Type
1	B	1110	ASN
1	B	1112	LEU
1	B	1117	GLU
1	B	1127	LEU
1	B	1128	LEU
1	B	1176	VAL
1	B	1202	HIS
1	B	1249	ASN
1	B	1356	LYS
1	B	1417	ASN
1	B	1421	SER
1	B	1488	LEU
1	B	1490	HIS
1	B	1492	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	ASN
1	A	276	GLN
1	A	437	GLN
1	A	447	GLN
1	A	490	GLN
1	A	548	GLN
1	A	700	GLN
1	A	810	GLN
1	A	916	GLN
1	A	963	ASN
1	A	985	HIS
1	A	1046	GLN
1	A	1059	GLN
1	A	1298	HIS
1	A	1401	ASN
1	A	1440	ASN
1	B	437	GLN
1	B	490	GLN
1	B	674	ASN
1	B	704	HIS
1	B	716	ASN
1	B	810	GLN
1	B	836	ASN
1	B	886	ASN

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Mol	Chain	Res	Type
1	B	936	ASN
1	B	974	HIS
1	B	985	HIS
1	B	1062	ASN
1	B	1213	GLN
1	B	1298	HIS
1	B	1380	GLN
1	B	1413	GLN
1	B	1416	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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
3	Q5A	A	1602	-	28,29,29	1.62	7 (25%)	37,40,40	2.30	12 (32%)
3	Q5A	B	1602	-	28,29,29	2.04	8 (28%)	37,40,40	2.24	12 (32%)

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
3	Q5A	A	1602	-	-	1/20/30/30	0/3/3/3
3	Q5A	B	1602	-	-	0/20/30/30	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1602	Q5A	C17-N4	-4.34	1.32	1.38
3	A	1602	Q5A	C17-N4	-4.06	1.32	1.38
3	B	1602	Q5A	F1-C6	-3.94	1.26	1.36
3	B	1602	Q5A	C15-N3	-3.93	1.29	1.36
3	B	1602	Q5A	C2-C3	-3.92	1.44	1.51
3	B	1602	Q5A	C16-N3	-3.40	1.33	1.38
3	A	1602	Q5A	C11-C10	-3.21	1.43	1.52
3	B	1602	Q5A	C11-C12	-3.17	1.45	1.53
3	A	1602	Q5A	C16-N3	-3.02	1.33	1.38
3	A	1602	Q5A	C15-N3	-2.78	1.31	1.36
3	B	1602	Q5A	C18-C17	2.62	1.54	1.50
3	A	1602	Q5A	C16-S1	2.57	1.77	1.74
3	B	1602	Q5A	C12-C15	2.53	1.56	1.51
3	A	1602	Q5A	C2-C3	-2.38	1.47	1.51
3	A	1602	Q5A	C11-C12	-2.07	1.47	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1602	Q5A	C11-C10-N2	6.26	122.92	110.66
3	B	1602	Q5A	C11-C10-N2	5.48	121.39	110.66
3	A	1602	Q5A	C19-C17-N4	5.38	118.15	114.51
3	B	1602	Q5A	C15-N3-C16	-4.86	118.63	124.54
3	B	1602	Q5A	C14-C13-C12	-4.59	103.27	110.54
3	A	1602	Q5A	C17-C19-S1	-3.83	108.55	111.23
3	B	1602	Q5A	S1-C16-N4	-3.75	111.75	115.69
3	A	1602	Q5A	S1-C16-N4	-3.72	111.78	115.69
3	A	1602	Q5A	C18-C17-C19	-3.57	122.69	126.42
3	A	1602	Q5A	C14-C13-C12	-3.51	104.97	110.54
3	A	1602	Q5A	C11-C12-C15	-3.23	103.98	110.79
3	B	1602	Q5A	N1-C9-N2	3.17	123.73	116.23
3	A	1602	Q5A	C2-C3-C8	3.12	126.49	120.75
3	B	1602	Q5A	C2-C3-C8	3.09	126.43	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1602	Q5A	O1-C9-N2	-3.00	117.64	124.05
3	B	1602	Q5A	C17-C19-S1	-2.98	109.14	111.23
3	A	1602	Q5A	N1-C9-N2	2.87	123.03	116.23
3	A	1602	Q5A	C15-N3-C16	-2.73	121.22	124.54
3	B	1602	Q5A	C10-C11-C12	2.57	114.61	110.54
3	B	1602	Q5A	C7-C6-C5	-2.46	119.57	122.80
3	A	1602	Q5A	S1-C16-N3	2.43	127.63	123.29
3	B	1602	Q5A	S1-C16-N3	2.25	127.30	123.29
3	A	1602	Q5A	C3-C2-N1	-2.13	109.00	113.02
3	B	1602	Q5A	C11-C12-C15	-2.10	106.37	110.79

There are no chirality outliers.

All (1) torsion outliers are listed below:

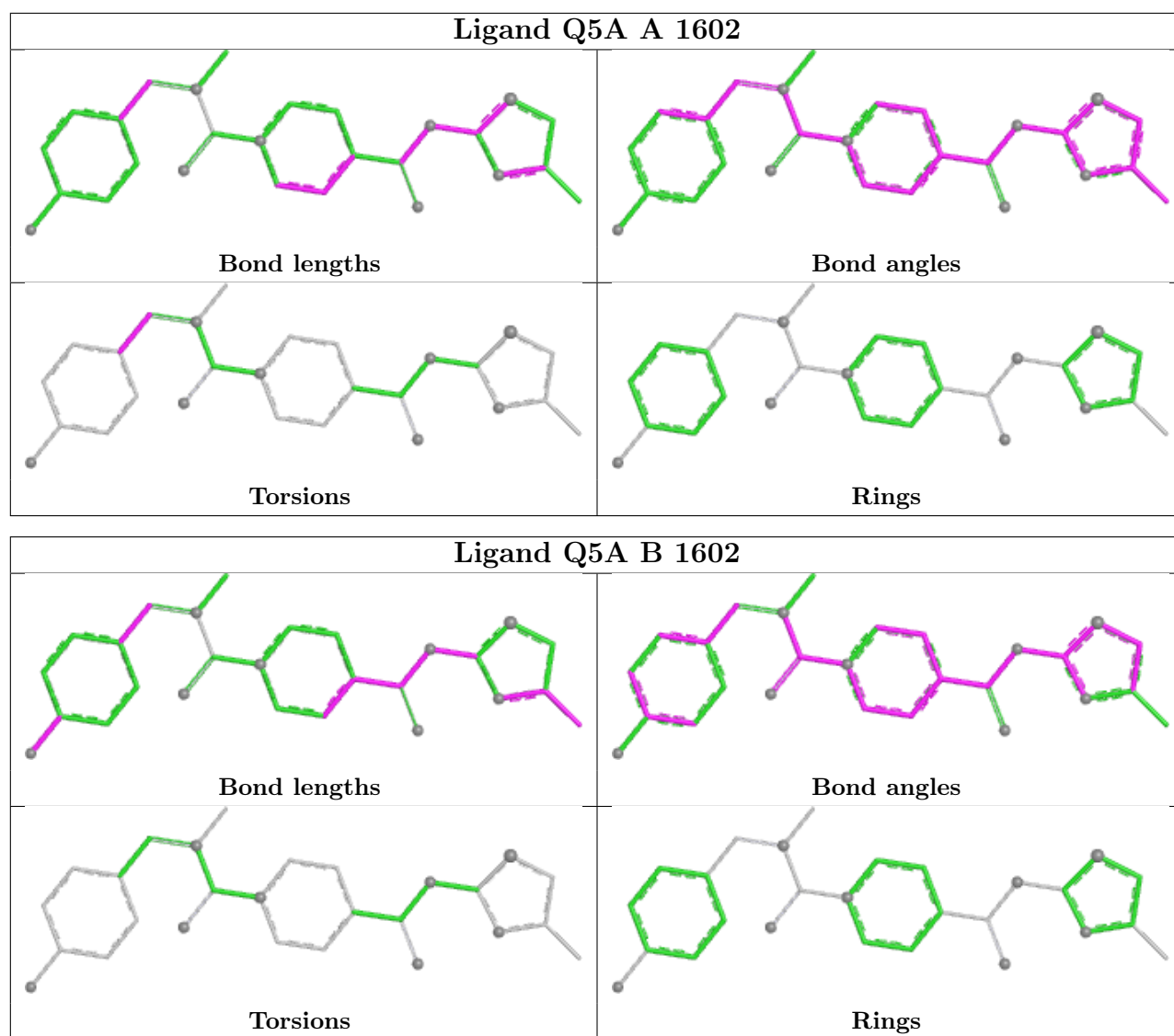
Mol	Chain	Res	Type	Atoms
3	A	1602	Q5A	N1-C2-C3-C8

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1602	Q5A	3	0
3	B	1602	Q5A	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	1333/1500 (88%)	0.19	101 (7%)	20 21	15, 26, 66, 108	0
1	B	1332/1500 (88%)	0.14	101 (7%)	20 21	13, 24, 68, 130	0
All	All	2665/3000 (88%)	0.16	202 (7%)	20 21	13, 25, 67, 130	0

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	403	ALA	7.0
1	B	655	ALA	6.8
1	A	781	PHE	6.7
1	A	792	MET	6.7
1	A	1122	VAL	6.6
1	A	1163	PRO	6.6
1	B	1202	HIS	6.5
1	B	1201	VAL	6.5
1	B	1324	ILE	6.4
1	A	788	ILE	6.2
1	B	415	LEU	6.1
1	B	438	ALA	5.8
1	A	1491	TYR	5.8
1	A	410	LEU	5.7
1	A	1201	VAL	5.7
1	B	1124	TYR	5.6
1	B	1122	VAL	5.5
1	B	1490	HIS	5.5
1	A	1124	TYR	5.4
1	B	1130	PRO	5.3
1	A	438	ALA	5.1
1	B	435	ILE	5.1
1	B	1164	VAL	5.1
1	A	1112	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	1130	PRO	5.1
1	A	411	PRO	5.0
1	A	1202	HIS	5.0
1	A	1490	HIS	5.0
1	A	403	ALA	4.9
1	B	1321	ALA	4.9
1	A	753	VAL	4.8
1	B	439	GLY	4.8
1	B	656	MET	4.7
1	B	1313	PHE	4.6
1	A	791	SER	4.6
1	A	1486	LYS	4.5
1	B	1169	PHE	4.5
1	A	409	VAL	4.4
1	B	1488	LEU	4.3
1	B	626	VAL	4.3
1	B	1116	LEU	4.3
1	B	1127	LEU	4.3
1	B	1491	TYR	4.3
1	B	1119	ALA	4.2
1	A	1127	LEU	4.2
1	B	1128	LEU	4.2
1	B	433	LEU	4.1
1	B	792	MET	4.1
1	A	1164	VAL	4.0
1	B	1125	PRO	4.0
1	A	656	MET	4.0
1	B	404	THR	4.0
1	A	435	ILE	4.0
1	A	1119	ALA	3.9
1	B	1112	LEU	3.9
1	A	418	SER	3.9
1	A	1125	PRO	3.9
1	B	1109	VAL	3.9
1	A	441	PHE	3.9
1	B	402	LYS	3.9
1	A	1418	PRO	3.8
1	B	1323	PRO	3.8
1	B	561	ILE	3.8
1	A	1204	GLY	3.8
1	A	402	LYS	3.8
1	B	1129	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	1109	VAL	3.7
1	B	1486	LYS	3.7
1	A	43	ALA	3.7
1	B	1203	SER	3.7
1	A	626	VAL	3.7
1	A	1325	LEU	3.6
1	B	1108	ALA	3.6
1	B	1492	ARG	3.6
1	A	1169	PHE	3.6
1	A	560	LYS	3.6
1	A	1116	LEU	3.6
1	A	1492	ARG	3.5
1	A	1115	ALA	3.5
1	B	414	ALA	3.5
1	A	1416	GLN	3.5
1	A	954	VAL	3.5
1	A	1118	PHE	3.5
1	A	1487	SER	3.4
1	B	1485	SER	3.4
1	A	751	LYS	3.4
1	A	1320	ASP	3.4
1	A	846	PRO	3.4
1	A	1165	VAL	3.4
1	A	1113	ASN	3.4
1	B	177	GLY	3.4
1	B	830	ASN	3.4
1	B	837	LEU	3.3
1	B	1487	SER	3.3
1	A	1111	THR	3.3
1	A	1203	SER	3.3
1	B	43	ALA	3.3
1	A	661	GLY	3.3
1	B	625	SER	3.2
1	B	1327	CYS	3.2
1	A	655	ALA	3.2
1	B	1126	CYS	3.2
1	A	1479	LYS	3.1
1	B	1110	ASN	3.1
1	B	846	PRO	3.1
1	A	1128	LEU	3.1
1	B	1118	PHE	3.1
1	B	627	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	790	SER	3.1
1	A	1326	ARG	3.1
1	A	1420	LEU	3.1
1	B	441	PHE	3.1
1	B	831	LYS	3.1
1	B	1120	LYS	3.1
1	A	754	VAL	3.0
1	B	1489	PHE	3.0
1	B	1166	LEU	3.0
1	A	1205	ASP	3.0
1	A	401	GLY	3.0
1	A	789	GLY	3.0
1	B	1115	ALA	3.0
1	B	954	VAL	2.9
1	A	1167	THR	2.9
1	B	1322	ASP	2.9
1	A	1126	CYS	2.8
1	A	1488	LEU	2.8
1	B	401	GLY	2.8
1	A	436	GLY	2.8
1	B	1165	VAL	2.8
1	B	662	ASP	2.8
1	B	437	GLN	2.7
1	A	1120	LYS	2.7
1	B	1114	GLU	2.7
1	B	829	MET	2.7
1	A	662	ASP	2.7
1	A	1480	SER	2.7
1	B	1113	ASN	2.7
1	A	1200	GLY	2.6
1	A	829	MET	2.6
1	B	1443	THR	2.6
1	A	434	SER	2.6
1	B	793	LYS	2.6
1	A	433	LEU	2.6
1	B	436	GLY	2.6
1	A	660	THR	2.6
1	A	756	GLY	2.6
1	B	1111	THR	2.6
1	B	1205	ASP	2.5
1	A	400	LYS	2.5
1	B	176	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	1123	ASP	2.5
1	A	476	LEU	2.5
1	A	1319	ARG	2.5
1	B	138	LYS	2.4
1	A	627	THR	2.4
1	B	1424	ARG	2.4
1	B	343	ASN	2.4
1	A	561	ILE	2.4
1	A	437	GLN	2.4
1	B	412	LYS	2.4
1	B	1428	ARG	2.3
1	B	834	PRO	2.3
1	A	793	LYS	2.3
1	B	661	GLY	2.3
1	B	1121	SER	2.3
1	B	474	VAL	2.3
1	A	1327	CYS	2.3
1	B	313	MET	2.3
1	A	419	ARG	2.3
1	B	1415	GLY	2.3
1	B	1480	SER	2.3
1	A	831	LYS	2.3
1	A	837	LEU	2.3
1	A	1444	LYS	2.3
1	A	1454	ARG	2.2
1	A	1485	SER	2.2
1	B	1319	ARG	2.2
1	A	1166	LEU	2.2
1	B	1479	LYS	2.2
1	B	838	ASP	2.2
1	B	1484	ASP	2.2
1	A	1318	LEU	2.2
1	A	624	LYS	2.2
1	A	1425	LYS	2.2
1	A	490	GLN	2.1
1	A	955	THR	2.1
1	B	420	VAL	2.1
1	A	439	GLY	2.1
1	B	1204	GLY	2.1
1	B	1417	ASN	2.1
1	A	1121	SER	2.1
1	A	1415	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1489	PHE	2.1
1	B	757	LYS	2.1
1	B	1418	PRO	2.1
1	B	1420	LEU	2.1
1	A	835	SER	2.0
1	B	1444	LYS	2.0
1	B	406	ILE	2.0
1	B	1447	HIS	2.0
1	B	952	PRO	2.0
1	A	474	VAL	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](#)

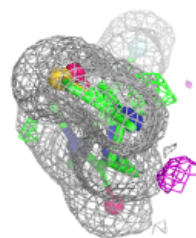
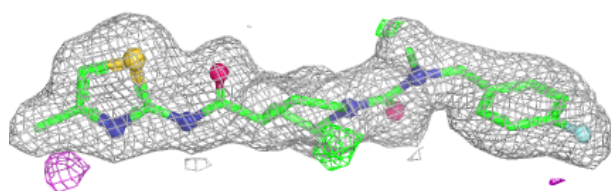
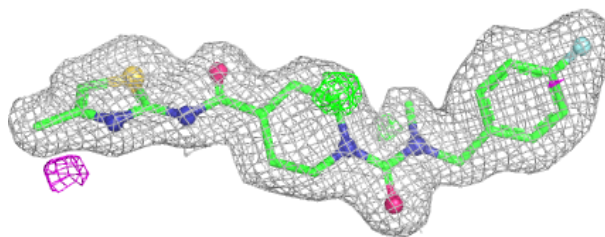
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	Q5A	A	1602	27/27	0.97	0.06	20,24,27,30	0
3	Q5A	B	1602	27/27	0.97	0.06	21,24,27,31	0
2	ZN	A	1601	1/1	1.00	0.03	23,23,23,23	0
2	ZN	B	1601	1/1	1.00	0.02	21,21,21,21	0

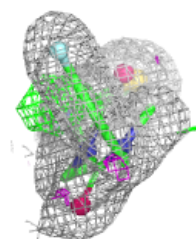
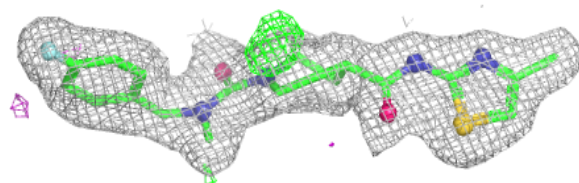
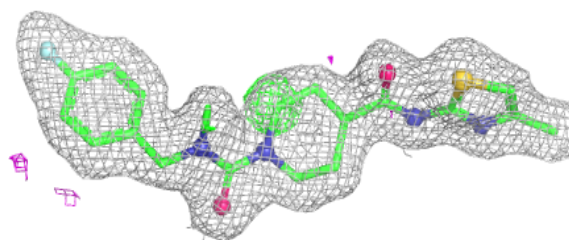
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Q5A A 1602:

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

**Electron density around Q5A B 1602:**

$2mF_o-DF_c$ (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.