Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2023 – 12:59 PM EDT

PDB ID	:	6UEL
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:

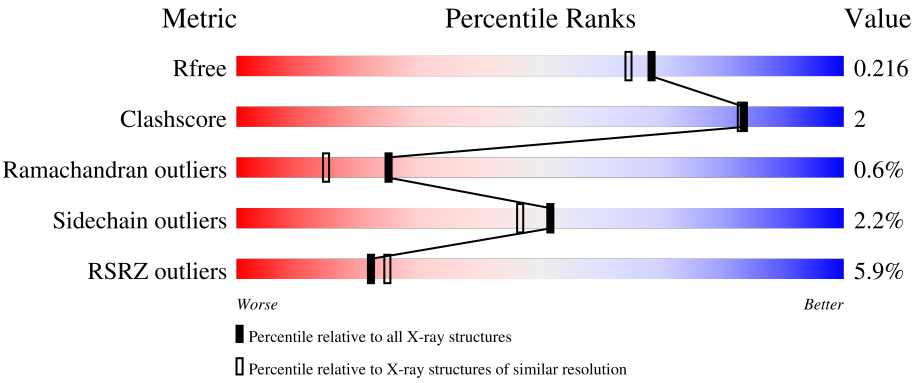
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 <=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	6% 81% 7% • 11%
1	B	1500	4% 82% 6% • 11%

2 Entry composition

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.

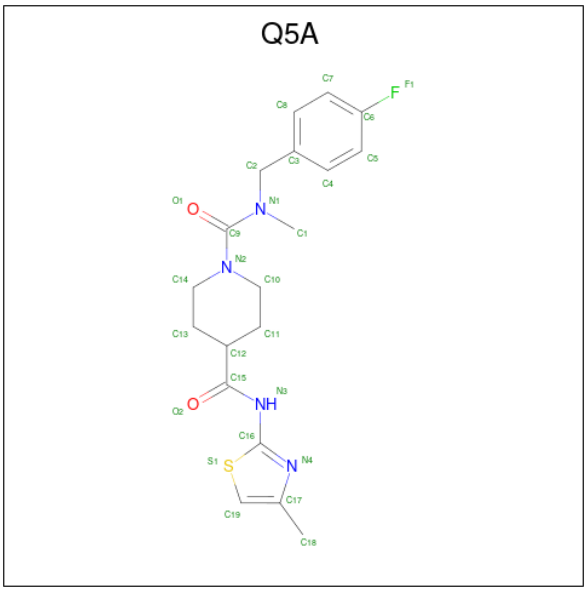
- Molecule 1 is a protein called Carbamoyl-phosphate synthase [ammonia], mitochondrial.

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 (three-letter code: 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)piperidine-1,4-dicarboxamide (three-letter code: Q5A) (formula: $C_{19}H_{23}FN_4O_2S$) (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.

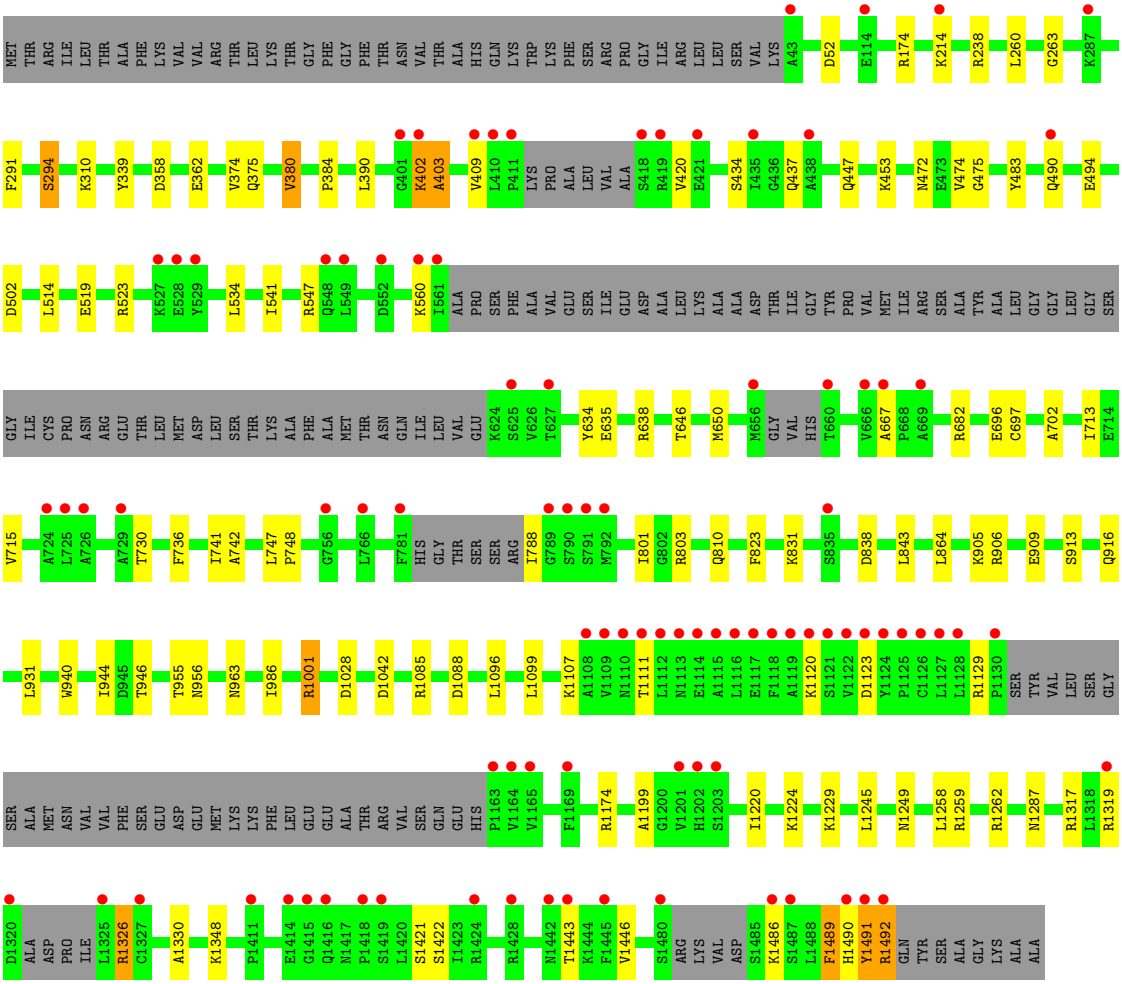
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	786	Total	O	0	0
			786	786		
4	B	836	Total	O	0	0
			836	836		

3 Residue-property plots (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.

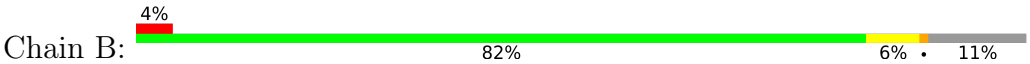
• Molecule 1: Carbamoyl-phosphate synthase [ammonia], mitochondrial

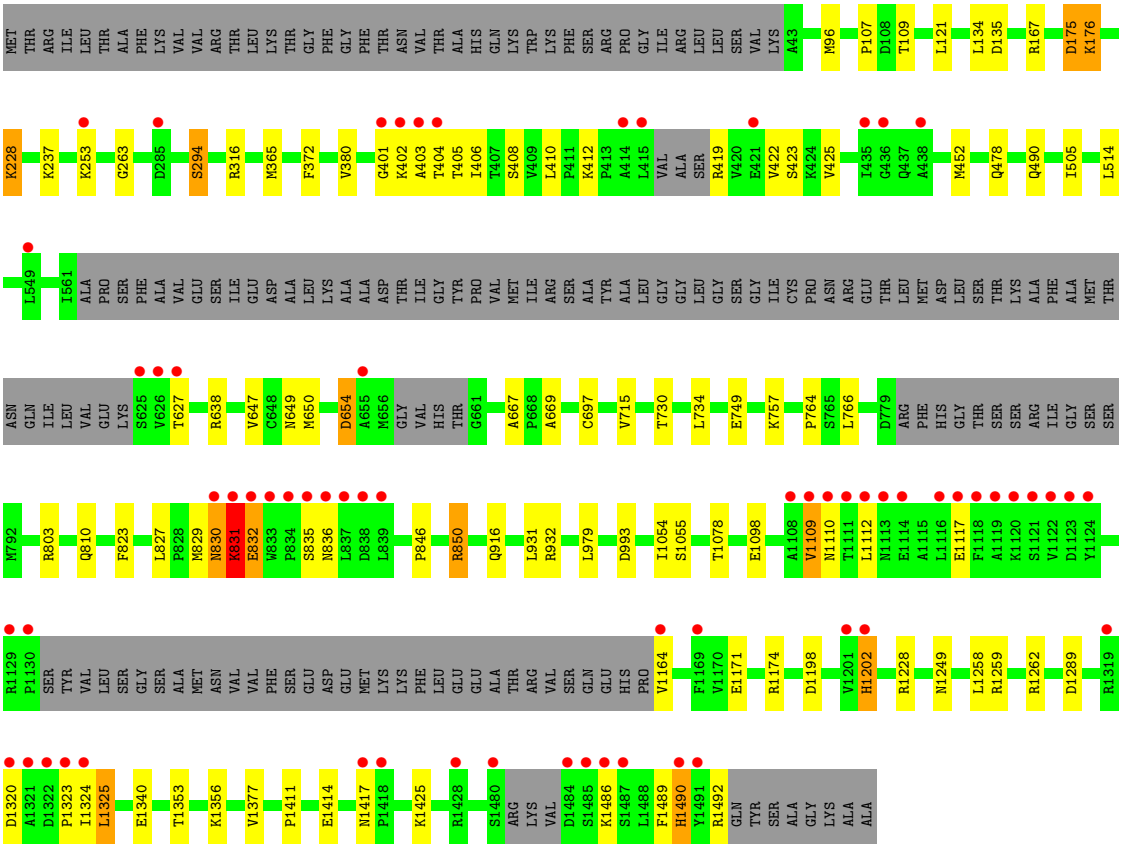
Chain A:



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

Chain B:




MET THR ARG ILE LEU THR ALA PHE LYS VAL VAL ARG THR LEU LYS THR GLY PHE GLY PHE THR ASN VAL THR ALA HIS GLN LYS TRP LYS PHE SER ARG PRO GLY ILE ARG LEU LEU SER VAL LYS A43 M96 P107 D108 T109 L121 L134 D135 R167 D175 K176
K228 K237 K253 G263 D285 S294 R316 M365 F372 V380 G401 K402 A403 T404 T405 I406 T407 S408 V409 L410 P411 K412 P413 A414 L415 VAL ALA SER R419 V420 E421 V422 S423 K424 V425 I435 G436 Q437 A438 M452 Q478 Q490 I505 L514
L549 I561 ALA PRO SER PHE ALA VAL GLU SER ILE GLU ASP ALA LEU LYS ALA ALA ASP THR ILE GLY TYR PRO VAL MET ILE ARG SER ALA TYR ALA LEU GLY GLY LEU GLY SER GLY ILE CYS PRO ASN ARG GLU THR LEU MET ASP LEU SER THR LYS ALA PHE ALA MET THR
ASN GLN ILE LEU VAL GLU LYS S625 V626 T627 R638 V647 G648 N649 M650 D654 A655 M656 GLY VAL HIS THR G661 A667 P668 A669 C697 V715 T730 L734 E749 K757 P764 S765 L766 D779 ARG PHE HIS GLY THR SER SER ARG ILE GLY SER SER
M792 R803 Q810 F823 L827 P828 M829 N830 K831 E832 W833 P834 S835 N836 L837 D838 L839 P846 R850 Q916 L931 R932 L979 D993 I1054 S1055 T1078 E1098 A1108 V1109 N1110 T1111 L1112 N1113 E1114 A1115 L1116 E1117 F1118 A1119 K1120 S1121 V1122 D1123 Y1124
R1129 P1130 SER TYR VAL LEU SER GLY SER ALA MET ASN VAL VAL PHE SER GLU ASP GLU MET LYS LYS PHE LEU GLU GLU ALA THR ARG VAL SER GLN GLU HIS PRO V1164 F1169 V1170 E1171 R1174 D1198 V1201 H1202 R1228 N1249 L1258 R1259 R1262 D1289 R1319
D1320 A1321 D1322 P1323 I1324 L1325 E1340 T1353 K1356 V1377 P1411 E1414 N1417 P1418 K1425 R1428 S1480 ARG LYS VAL D1484 S1485 K1486 S1487 L1488 F1489 H1490 Y1491 R1492 GLN TYR SER ALA GLY LYS ALA ALA

4 Data and refinement statistics (i)

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 57.22 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (139.03-1.90) 100.0 (57.22-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[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

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	0.92	1/10511 (0.0%)	0.94	24/14235 (0.2%)
1	B	0.95	4/10508 (0.0%)	0.92	21/14236 (0.1%)
All	All	0.93	5/21019 (0.0%)	0.93	45/28471 (0.2%)

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

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1490	HIS	N-CA	7.16	1.60	1.46
1	B	1490	HIS	CA-C	6.37	1.69	1.52
1	A	940	TRP	CE3-CZ3	6.21	1.49	1.38
1	B	1340	GLU	CD-OE1	5.38	1.31	1.25
1	B	654	ASP	C-O	5.09	1.33	1.23

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1174	ARG	NE-CZ-NH1	13.35	126.98	120.30
1	A	1001	ARG	NE-CZ-NH2	-13.28	113.66	120.30
1	A	1174	ARG	NE-CZ-NH2	-11.77	114.41	120.30
1	B	850	ARG	NE-CZ-NH2	-10.72	114.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	850	ARG	NE-CZ-NH1	9.53	125.07	120.30
1	A	1001	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	B	803	ARG	NE-CZ-NH2	-9.03	115.78	120.30
1	B	1174	ARG	NE-CZ-NH2	-8.59	116.00	120.30
1	B	932	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	B	1174	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	A	1492	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	A	1259	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	A	906	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	B	316	ARG	NE-CZ-NH1	-6.53	117.03	120.30
1	B	96	MET	CG-SD-CE	-6.22	90.25	100.20
1	A	1085	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	B	1289	ASP	CB-CG-OD1	6.16	123.84	118.30
1	B	175	ASP	CB-CG-OD1	6.10	123.79	118.30
1	B	228	LYS	CD-CE-NZ	-6.08	97.71	111.70
1	A	358	ASP	CB-CG-OD1	6.07	123.76	118.30
1	B	167	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	A	906	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	1088	ASP	CB-CG-OD1	5.92	123.62	118.30
1	B	1259	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	B	638	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	A	1085	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	1262	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B	993	ASP	CB-CG-OD1	5.44	123.19	118.30
1	A	638	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	838	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	B	1490	HIS	N-CA-C	5.28	125.25	111.00
1	B	1228	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	B	1198	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	B	1489	PHE	N-CA-C	5.22	125.09	111.00
1	B	1198	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	838	ASP	CB-CG-OD1	5.21	122.98	118.30
1	A	52	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	1492	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	1326	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	A	1317	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	A	238	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	1042	ASP	CB-CG-OD1	5.06	122.86	118.30
1	A	682	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	B	803	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	174	ARG	NE-CZ-NH2	-5.01	117.80	120.30

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 (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	10313	0	10369	48	0
1	B	10309	0	10374	45	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	12	1
All	All	22300	0	20743	98	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 (98) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:A:1602:Q5A:O2	3:A:1602:Q5A:S1	2.72	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:452:MET:CE	1:B:505:ILE:HD11	2.45	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG22	1:B:1353:THR:O	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:175:ASP:C	1:B:176:LYS:HD3	2.38	0.43
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:A:490:GLN:NE2	1:A:1486:LYS:HB2	2.34	0.43
1:B:514:LEU:HD23	1:B:514:LEU:C	2.39	0.43
1:B:452:MET:HE2	1:B:505:ILE:HD11	2.00	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:A:374:VAL:HG11	1:A:390:LEU:HD13	2.02	0.42
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:422:VAL:HG11	1:B:425:VAL:HG22	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	34 24
1	B	1318/1500 (88%)	1272 (96%)	35 (3%)	11 (1%)	19 9
All	All	2635/3000 (88%)	2552 (97%)	67 (2%)	16 (1%)	25 15

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

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Mol	Chain	Res	Type
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 (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	1136/1274 (89%)	1112 (98%)	24 (2%)	53	48
1	B	1136/1274 (89%)	1110 (98%)	26 (2%)	50	45
All	All	2272/2548 (89%)	2222 (98%)	50 (2%)	52	47

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	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	560	LYS
1	A	788	ILE
1	A	831	LYS
1	A	843	LEU
1	A	864	LEU
1	A	1096	LEU
1	A	1107	LYS
1	A	1111	THR

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Mol	Chain	Res	Type
1	A	1120	LYS
1	A	1129	ARG
1	A	1249	ASN
1	A	1258	LEU
1	A	1287	ASN
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	423	SER
1	B	627	THR
1	B	757	LYS
1	B	827	LEU
1	B	832	GLU
1	B	835	SER
1	B	836	ASN
1	B	1098	GLU
1	B	1109	VAL
1	B	1110	ASN
1	B	1112	LEU
1	B	1117	GLU
1	B	1171	GLU
1	B	1202	HIS
1	B	1249	ASN
1	B	1356	LYS
1	B	1417	ASN
1	B	1425	LYS
1	B	1490	HIS
1	B	1492	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	GLN
1	A	276	GLN
1	A	320	GLN

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Mol	Chain	Res	Type
1	A	437	GLN
1	A	447	GLN
1	A	490	GLN
1	A	810	GLN
1	A	916	GLN
1	A	963	ASN
1	A	970	ASN
1	B	490	GLN
1	B	649	ASN
1	B	810	GLN
1	B	836	ASN
1	B	886	ASN
1	B	1062	ASN
1	B	1417	ASN

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)

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	-	24,29,29	1.24	3 (12%)	31,40,40	2.19	8 (25%)
3	Q5A	B	1602	-	24,29,29	1.79	6 (25%)	31,40,40	2.33	10 (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	-	-	1/18/30/30	0/3/3/3
3	Q5A	B	1602	-	-	0/18/30/30	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1602	Q5A	C2-C3	-3.96	1.44	1.51
3	B	1602	Q5A	F1-C6	-3.92	1.26	1.36
3	A	1602	Q5A	C11-C10	-3.16	1.43	1.52
3	B	1602	Q5A	C11-C12	-3.09	1.45	1.53
3	B	1602	Q5A	C15-N3	-2.72	1.29	1.35
3	B	1602	Q5A	C12-C15	2.48	1.56	1.51
3	A	1602	Q5A	C2-C3	-2.41	1.47	1.51
3	B	1602	Q5A	C16-N3	-2.14	1.33	1.36
3	A	1602	Q5A	C11-C12	-2.02	1.47	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1602	Q5A	C11-C10-N2	7.96	122.92	110.82
3	B	1602	Q5A	C11-C10-N2	6.95	121.39	110.82
3	B	1602	Q5A	C16-N3-C15	-4.67	118.63	129.02
3	B	1602	Q5A	C14-C13-C12	-4.30	103.27	110.41
3	A	1602	Q5A	C16-N3-C15	-3.51	121.22	129.02
3	A	1602	Q5A	C14-C13-C12	-3.27	104.97	110.41
3	B	1602	Q5A	N1-C9-N2	3.17	123.73	116.23
3	A	1602	Q5A	C11-C12-C15	-3.05	103.98	110.69
3	A	1602	Q5A	C2-C3-C8	3.04	126.49	120.77
3	B	1602	Q5A	C2-C3-C8	3.01	126.43	120.77
3	A	1602	Q5A	N1-C9-N2	2.87	123.03	116.23
3	B	1602	Q5A	O1-C9-N2	-2.80	117.64	123.80
3	B	1602	Q5A	C10-C11-C12	2.52	114.61	110.41
3	B	1602	Q5A	C7-C6-C5	-2.45	119.57	122.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1602	Q5A	C18-C17-C19	-2.41	122.69	129.06
3	B	1602	Q5A	C12-C15-N3	-2.41	111.49	115.02
3	B	1602	Q5A	C13-C14-N2	-2.32	107.29	110.82
3	A	1602	Q5A	C3-C2-N1	-2.06	109.00	112.98

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

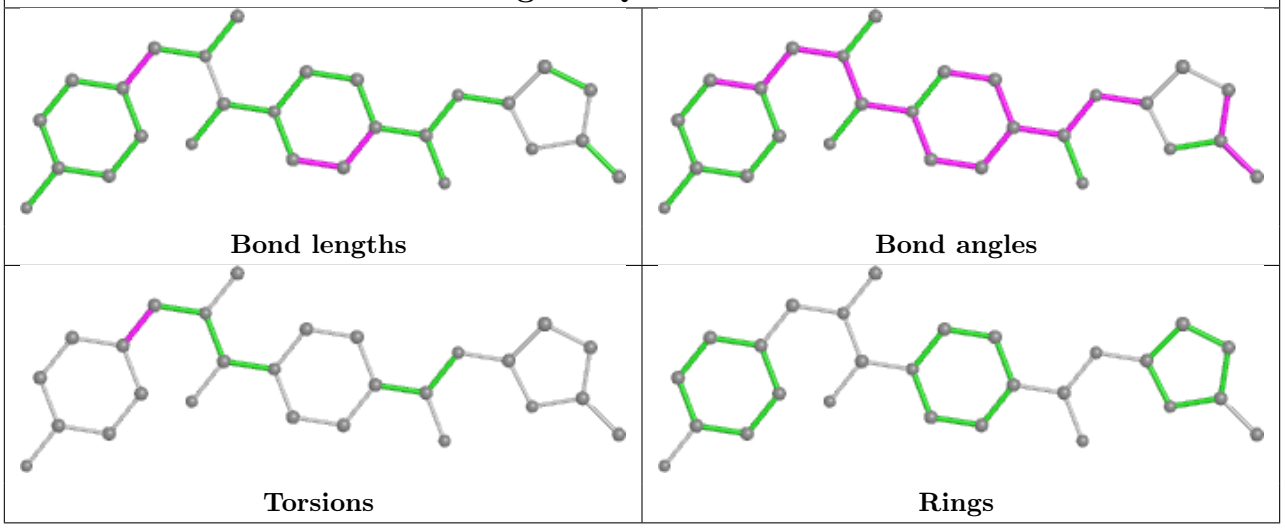
There are no ring outliers.

2 monomers are involved in 5 short contacts:

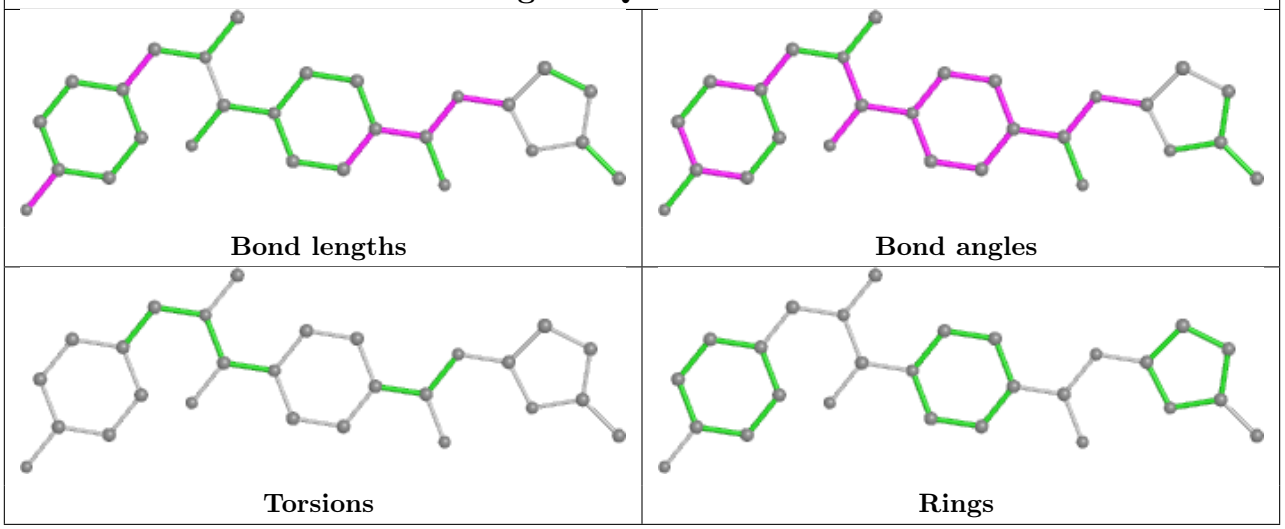
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1602	Q5A	3	0
3	B	1602	Q5A	2	0

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 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 Q5A A 1602



Ligand Q5A B 1602



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, 95^{th} 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%)	0.07	92 (6%)	16	19	15, 26, 66, 108	0
1	B	1332/1500 (88%)	-0.05	65 (4%)	29	33	13, 24, 68, 130	0
All	All	2665/3000 (88%)	0.01	157 (5%)	22	25	13, 25, 67, 130	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1321	ALA	13.9
1	B	403	ALA	8.3
1	A	790	SER	8.1
1	A	1491	TYR	7.0
1	A	1122	VAL	6.9
1	A	1116	LEU	6.5
1	B	1324	ILE	6.4
1	A	1124	TYR	6.4
1	B	402	LYS	6.2
1	A	1112	LEU	6.0
1	B	1201	VAL	5.9
1	B	1124	TYR	5.9
1	A	1320	ASP	5.8
1	B	1322	ASP	5.8
1	B	1320	ASP	5.7
1	A	1118	PHE	5.4
1	A	1164	VAL	5.4
1	A	1113	ASN	5.1
1	A	1418	PRO	5.1
1	A	1130	PRO	5.0
1	B	414	ALA	4.9
1	B	837	LEU	4.9
1	B	1123	ASP	4.8
1	B	1122	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	1111	THR	4.6
1	A	1115	ALA	4.6
1	B	1164	VAL	4.6
1	A	1415	GLY	4.5
1	A	1123	ASP	4.4
1	B	401	GLY	4.4
1	A	1490	HIS	4.3
1	B	1484	ASP	4.2
1	A	1121	SER	4.1
1	A	1128	LEU	4.1
1	A	789	GLY	4.1
1	B	435	ILE	4.1
1	B	1112	LEU	4.1
1	A	438	ALA	4.0
1	A	418	SER	4.0
1	A	1119	ALA	4.0
1	B	415	LEU	4.0
1	A	1163	PRO	3.9
1	A	1125	PRO	3.9
1	B	836	ASN	3.9
1	B	1202	HIS	3.8
1	A	1109	VAL	3.8
1	A	1120	LYS	3.8
1	A	409	VAL	3.7
1	A	435	ILE	3.7
1	B	1113	ASN	3.6
1	B	831	LYS	3.6
1	B	625	SER	3.6
1	A	410	LEU	3.6
1	A	781	PHE	3.5
1	B	655	ALA	3.5
1	B	285	ASP	3.5
1	A	1319	ARG	3.5
1	A	1487	SER	3.4
1	A	411	PRO	3.4
1	A	1127	LEU	3.4
1	B	1109	VAL	3.4
1	B	1116	LEU	3.4
1	A	1117	GLU	3.3
1	A	1165	VAL	3.3
1	A	1110	ASN	3.3
1	A	791	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	1428	ARG	3.3
1	B	835	SER	3.2
1	B	1490	HIS	3.2
1	A	1201	VAL	3.2
1	B	838	ASP	3.1
1	A	792	MET	3.0
1	A	1202	HIS	3.0
1	B	404	THR	3.0
1	B	1118	PHE	3.0
1	B	1130	PRO	3.0
1	A	1416	GLN	3.0
1	A	402	LYS	2.9
1	A	835	SER	2.9
1	B	832	GLU	2.9
1	A	1428	ARG	2.9
1	B	438	ALA	2.9
1	B	1319	ARG	2.9
1	A	1114	GLU	2.8
1	B	1114	GLU	2.8
1	A	1108	ALA	2.8
1	B	830	ASN	2.8
1	B	1110	ASN	2.8
1	A	401	GLY	2.8
1	B	1323	PRO	2.8
1	A	560	LYS	2.8
1	A	1169	PHE	2.8
1	A	1445	PHE	2.8
1	A	1486	LYS	2.7
1	B	1119	ALA	2.7
1	A	625	SER	2.7
1	B	1485	SER	2.6
1	A	756	GLY	2.6
1	A	1492	ARG	2.6
1	B	1121	SER	2.6
1	B	1129	ARG	2.6
1	B	1169	PHE	2.5
1	A	1442	ASN	2.5
1	B	627	THR	2.5
1	B	436	GLY	2.5
1	B	833	TRP	2.5
1	B	1111	THR	2.5
1	B	834	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	527	LYS	2.4
1	B	1418	PRO	2.4
1	A	529	TYR	2.4
1	B	1117	GLU	2.4
1	A	552	ASP	2.4
1	A	421	GLU	2.4
1	A	490	GLN	2.4
1	B	1491	TYR	2.4
1	A	419	ARG	2.3
1	A	43	ALA	2.3
1	B	1480	SER	2.3
1	A	549	LEU	2.3
1	B	626	VAL	2.3
1	B	1486	LYS	2.3
1	A	1443	THR	2.3
1	A	726	ALA	2.3
1	A	114	GLU	2.3
1	A	528	GLU	2.3
1	A	1419	SER	2.2
1	B	1417	ASN	2.2
1	A	561	ILE	2.2
1	A	1414	GLU	2.2
1	A	656	MET	2.2
1	B	1487	SER	2.2
1	B	1108	ALA	2.2
1	A	766	LEU	2.2
1	A	287	LYS	2.2
1	B	253	LYS	2.2
1	A	1203	SER	2.1
1	A	627	THR	2.1
1	A	669	ALA	2.1
1	A	214	LYS	2.1
1	A	666	VAL	2.1
1	A	548	GLN	2.1
1	A	660	THR	2.1
1	A	729	ALA	2.1
1	A	724	ALA	2.1
1	A	725	LEU	2.1
1	B	839	LEU	2.1
1	A	1424	ARG	2.1
1	B	1120	LYS	2.1
1	A	1480	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1126	CYS	2.1
1	B	549	LEU	2.1
1	A	1411	PRO	2.0
1	B	421	GLU	2.0
1	A	667	ALA	2.0
1	A	1325	LEU	2.0
1	A	1327	CYS	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)

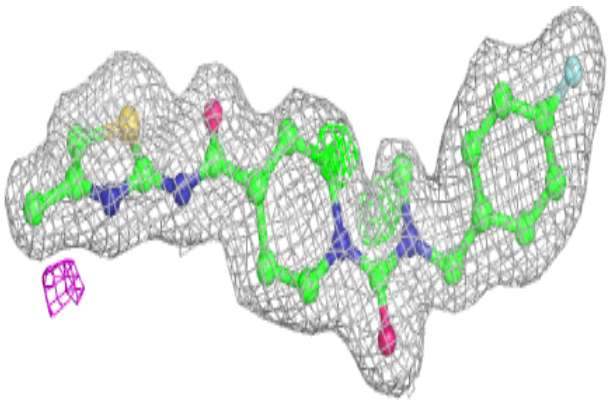
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

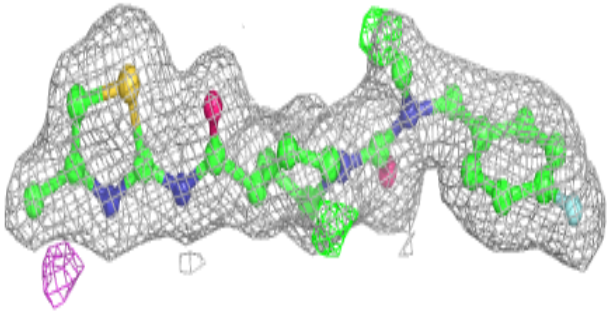
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	Q5A	A	1602	27/27	0.97	0.09	20,24,27,30	0
3	Q5A	B	1602	27/27	0.97	0.07	21,24,27,31	0
2	ZN	A	1601	1/1	1.00	0.05	23,23,23,23	0
2	ZN	B	1601	1/1	1.00	0.05	21,21,21,21	0

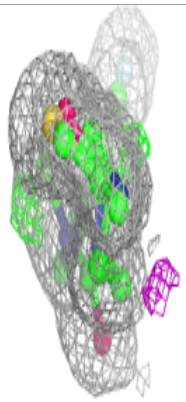
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

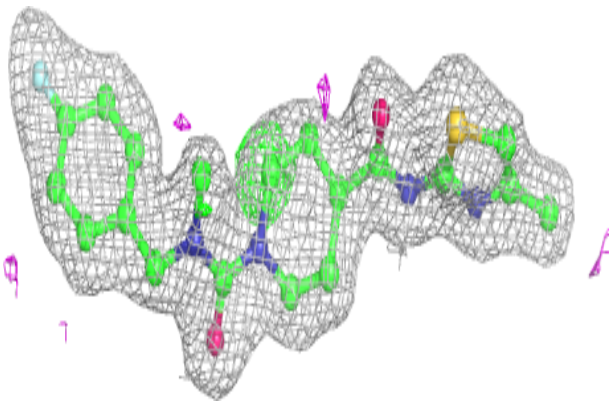


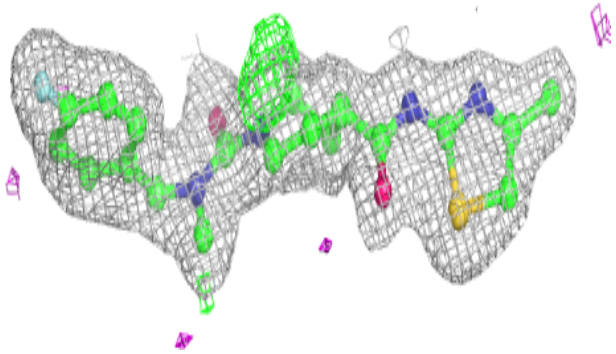


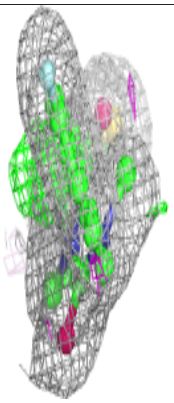


Electron density around Q5A B 1602:

$2mF_o$-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.