



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:29 PM UTC

PDB ID : 8JUB / pdb_00008jub
Title : Crystal structure of glutaminase C in complex with compound 27
Authors : Wang, X.; Hanyu, S.; Tingting, D.
Deposited on : 2023-06-26
Resolution : 2.01 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

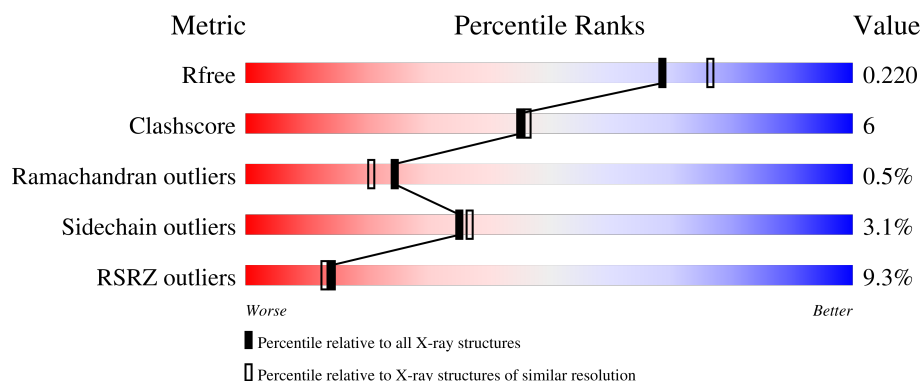
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	533	9% 65% 8% 25%
1	B	533	6% 68% 6% 25%
1	C	533	5% 66% 7% 27%
1	D	533	8% 64% 9% 26%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12868 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 Glutaminase kidney isoform, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3142	2008	530	576	28			
1	B	402	Total	C	N	O	S	0	0	0
			3147	2010	531	578	28			
1	C	391	Total	C	N	O	S	0	0	0
			3058	1950	518	562	28			
1	D	393	Total	C	N	O	S	0	0	0
			3074	1960	521	565	28			

There are 32 discrepancies between the modelled and reference sequences:

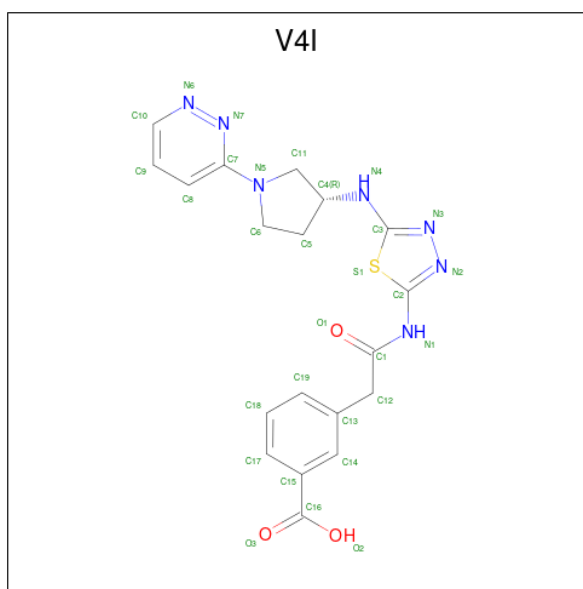
Chain	Residue	Modelled	Actual	Comment	Reference
A	63	MET	-	initiating methionine	UNP O94925
A	64	GLY	-	expression tag	UNP O94925
A	65	HIS	-	expression tag	UNP O94925
A	66	HIS	-	expression tag	UNP O94925
A	67	HIS	-	expression tag	UNP O94925
A	68	HIS	-	expression tag	UNP O94925
A	69	HIS	-	expression tag	UNP O94925
A	70	HIS	-	expression tag	UNP O94925
B	63	MET	-	initiating methionine	UNP O94925
B	64	GLY	-	expression tag	UNP O94925
B	65	HIS	-	expression tag	UNP O94925
B	66	HIS	-	expression tag	UNP O94925
B	67	HIS	-	expression tag	UNP O94925
B	68	HIS	-	expression tag	UNP O94925
B	69	HIS	-	expression tag	UNP O94925
B	70	HIS	-	expression tag	UNP O94925
C	63	MET	-	initiating methionine	UNP O94925
C	64	GLY	-	expression tag	UNP O94925
C	65	HIS	-	expression tag	UNP O94925
C	66	HIS	-	expression tag	UNP O94925
C	67	HIS	-	expression tag	UNP O94925

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Chain	Residue	Modelled	Actual	Comment	Reference
C	68	HIS	-	expression tag	UNP O94925
C	69	HIS	-	expression tag	UNP O94925
C	70	HIS	-	expression tag	UNP O94925
D	63	MET	-	initiating methionine	UNP O94925
D	64	GLY	-	expression tag	UNP O94925
D	65	HIS	-	expression tag	UNP O94925
D	66	HIS	-	expression tag	UNP O94925
D	67	HIS	-	expression tag	UNP O94925
D	68	HIS	-	expression tag	UNP O94925
D	69	HIS	-	expression tag	UNP O94925
D	70	HIS	-	expression tag	UNP O94925

- Molecule 2 is 3-[2-oxidanylidene-2-[[5-[[[(3R)-1-pyridazin-3-ylpyrrolidin-3-yl]amino]-1,3,4-thiadiazol-2-yl]amino]ethyl]benzoic acid (CCD ID: V4I) (formula: C₁₉H₁₉N₇O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			30	19	7	3	1		
2	D	1	Total	C	N	O	S	0	0
			30	19	7	3	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	73	Total	O	0	0
			73	73		

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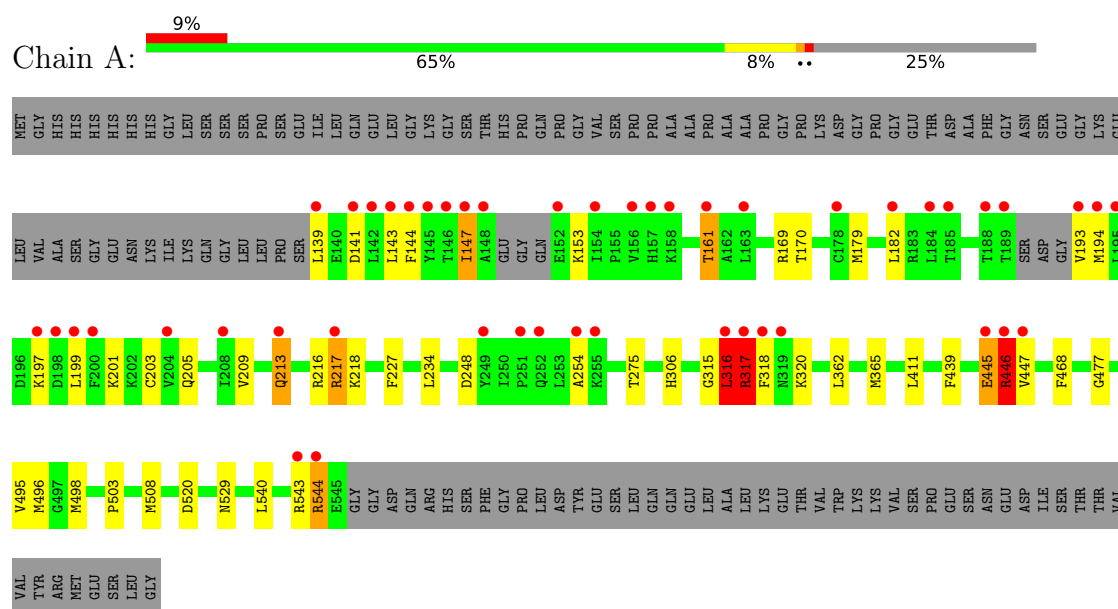
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	92	Total 92	O 92	0	0
3	C	119	Total 119	O 119	0	0
3	D	103	Total 103	O 103	0	0

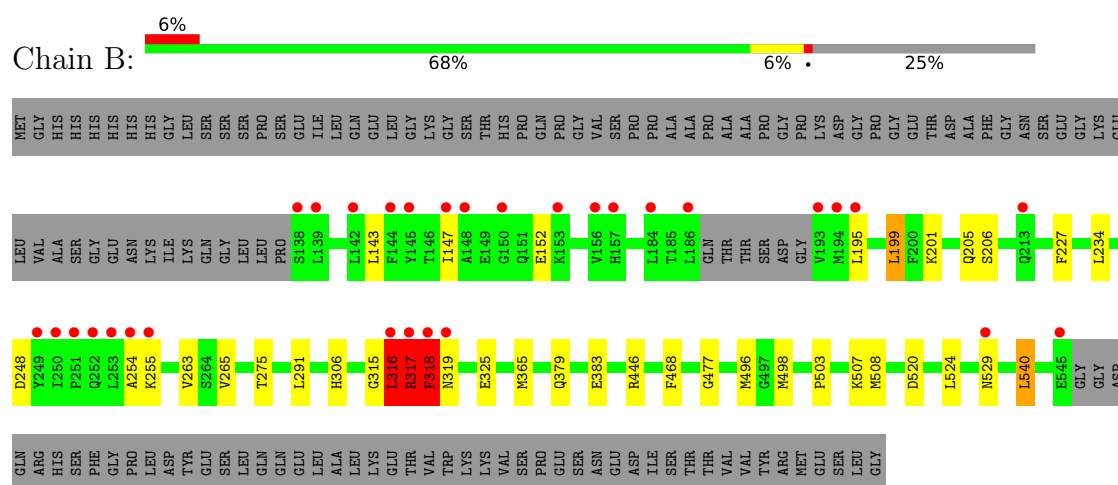
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glutaminase kidney isoform, mitochondrial



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.48Å 138.71Å 178.43Å 90.00° 93.09° 90.00°	Depositor
Resolution (Å)	89.24 – 2.01 89.24 – 2.01	Depositor EDS
% Data completeness (in resolution range)	91.2 (89.24-2.01) 91.2 (89.24-2.01)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.02Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.192 , 0.217 0.195 , 0.220	Depositor DCC
R_{free} test set	7239 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12868	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.80% 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: V4I

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	0.60	0/3211	0.99	4/4332 (0.1%)
1	B	0.60	0/3217	0.98	3/4340 (0.1%)
1	C	0.59	0/3123	0.98	4/4208 (0.1%)
1	D	0.59	0/3139	0.99	3/4231 (0.1%)
All	All	0.60	0/12690	0.98	14/17111 (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	4
1	B	0	2
1	C	0	1
1	D	0	1
All	All	0	8

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	503	PRO	N-CA-C	8.51	121.08	110.70
1	B	503	PRO	N-CA-C	8.48	121.04	110.70
1	D	503	PRO	N-CA-C	8.38	120.92	110.70
1	C	503	PRO	N-CA-C	8.11	120.59	110.70
1	C	306	HIS	CA-CB-CG	-7.21	106.59	113.80
1	B	306	HIS	CA-CB-CG	-7.13	106.67	113.80
1	B	318	PHE	CB-CA-C	-7.08	108.42	116.63
1	D	306	HIS	CA-CB-CG	-6.91	106.89	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	THR	CB-CA-C	6.84	122.15	110.79
1	A	306	HIS	CA-CB-CG	-6.12	107.68	113.80
1	C	161	THR	CB-CA-C	5.73	120.58	110.85
1	D	169	ARG	CB-CG-CD	-5.32	99.06	111.30
1	A	169	ARG	CB-CG-CD	-5.28	99.16	111.30
1	C	259	ASP	CA-CB-CG	5.22	117.82	112.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	216	ARG	Sidechain
1	A	217	ARG	Sidechain
1	A	446	ARG	Sidechain
1	A	544	ARG	Sidechain
1	B	317	ARG	Sidechain
1	B	446	ARG	Sidechain
1	C	382	ARG	Sidechain
1	D	534	ARG	Sidechain

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	3142	0	3129	40	0
1	B	3147	0	3130	35	0
1	C	3058	0	3040	22	0
1	D	3074	0	3060	53	0
2	A	30	0	0	2	0
2	D	30	0	0	1	0
3	A	73	0	0	1	0
3	B	92	0	0	0	0
3	C	119	0	0	0	0
3	D	103	0	0	1	0
All	All	12868	0	12359	147	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 6.

All (147) 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:D:496:MET:HE3	1:D:498:MET:CE	1.67	1.23
1:D:496:MET:CE	1:D:498:MET:CE	2.21	1.17
1:D:318:PHE:HB2	1:D:320:LYS:HG3	1.10	1.09
1:A:362:LEU:HD23	1:A:365:MET:HE1	1.32	1.08
1:A:362:LEU:HD23	1:A:365:MET:CE	1.85	1.06
1:D:496:MET:CE	1:D:498:MET:HE3	1.86	1.03
1:D:318:PHE:CB	1:D:320:LYS:HG3	1.88	1.02
1:D:496:MET:HE3	1:D:498:MET:HE3	1.05	1.01
1:A:362:LEU:HA	1:A:365:MET:HE3	1.44	0.99
1:D:185:THR:HG22	3:D:703:HOH:O	1.64	0.97
1:D:496:MET:CE	1:D:498:MET:HE2	1.94	0.96
1:D:538:LYS:HD3	1:D:538:LYS:H	1.28	0.94
1:B:316:LEU:C	1:B:318:PHE:H	1.76	0.94
1:D:318:PHE:HB2	1:D:320:LYS:CG	2.00	0.92
1:D:496:MET:HE1	1:D:498:MET:CE	2.02	0.90
1:C:498:MET:HE1	1:C:517:PHE:CE1	2.18	0.79
1:B:524:LEU:HD11	1:B:540:LEU:HD21	1.65	0.78
1:D:195:LEU:HD12	1:D:199:LEU:HD23	1.65	0.78
1:A:316:LEU:C	1:A:318:PHE:H	1.91	0.76
1:B:316:LEU:C	1:B:318:PHE:N	2.44	0.75
1:A:362:LEU:HD23	1:A:365:MET:HE3	1.70	0.72
1:A:227:PHE:CZ	1:A:496:MET:HE1	2.27	0.70
1:C:461:HIS:CE1	1:C:529:ASN:HD21	2.09	0.70
1:D:151:GLN:N	1:D:151:GLN:OE1	2.25	0.69
1:A:170:THR:HB	1:A:179:MET:HE2	1.74	0.68
1:B:227:PHE:CZ	1:B:496:MET:HE1	2.28	0.68
1:D:181:MET:O	1:D:185:THR:HG23	1.92	0.68
1:D:318:PHE:CD2	1:D:320:LYS:HE2	2.29	0.68
1:D:291:LEU:HD22	1:D:365:MET:HE1	1.77	0.67
1:B:507:LYS:H	1:B:507:LYS:HE2	1.61	0.66
1:A:365:MET:HG3	1:A:447:VAL:HG11	1.77	0.66
1:A:362:LEU:CD2	1:A:365:MET:HE1	2.20	0.65
1:D:316:LEU:C	1:D:318:PHE:H	2.04	0.64
1:C:498:MET:HE1	1:C:517:PHE:HE1	1.59	0.64
1:B:195:LEU:HD23	1:B:199:LEU:HD13	1.80	0.64
1:A:315:GLY:O	1:A:317:ARG:N	2.32	0.62
1:A:144:PHE:CE2	1:A:197:LYS:HG3	2.33	0.62
1:B:315:GLY:O	1:B:317:ARG:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:496:MET:HE1	1:D:498:MET:HE2	1.73	0.61
1:C:507:LYS:H	1:C:507:LYS:HE2	1.64	0.60
1:A:316:LEU:C	1:A:318:PHE:N	2.56	0.60
1:B:263:VAL:HG13	1:B:498:MET:CE	2.31	0.60
1:B:291:LEU:HD22	1:B:365:MET:HE1	1.84	0.59
1:A:193:VAL:HG12	1:A:193:VAL:O	2.02	0.59
1:B:263:VAL:CG1	1:B:498:MET:CE	2.81	0.59
1:D:144:PHE:CE2	1:D:197:LYS:HG2	2.37	0.59
1:A:143:LEU:O	1:A:147:ILE:HG22	2.03	0.58
1:B:524:LEU:HD11	1:B:540:LEU:CD2	2.34	0.58
1:B:263:VAL:HG13	1:B:498:MET:HE2	1.84	0.57
1:D:212:THR:HG23	1:D:216:ARG:HD3	1.87	0.56
1:C:380:SER:O	1:C:383:GLU:HG3	2.05	0.56
1:C:320:LYS:HZ1	2:D:601:V4I:C15	2.19	0.56
1:D:318:PHE:CG	1:D:320:LYS:HG3	2.40	0.56
1:B:477:GLY:O	1:B:529:ASN:HB2	2.06	0.56
1:B:265:VAL:CG2	1:B:498:MET:HE3	2.36	0.55
1:C:507:LYS:H	1:C:507:LYS:CE	2.19	0.55
1:C:359:MET:HE1	1:C:371:VAL:HG12	1.88	0.55
1:A:477:GLY:O	1:A:529:ASN:HB2	2.08	0.54
1:C:507:LYS:N	1:C:507:LYS:HD3	2.22	0.54
1:B:316:LEU:O	1:B:318:PHE:N	2.41	0.53
1:D:477:GLY:O	1:D:529:ASN:HB2	2.08	0.53
1:A:315:GLY:C	1:A:317:ARG:H	2.16	0.53
2:A:601:V4I:C17	1:B:317:ARG:NH2	2.71	0.53
1:C:195:LEU:HD23	1:C:199:LEU:HD23	1.89	0.53
1:A:439:PHE:HA	1:A:446:ARG:HA	1.91	0.53
1:D:142:LEU:HB3	1:D:216:ARG:HH22	1.74	0.52
1:C:507:LYS:H	1:C:507:LYS:CD	2.21	0.52
1:D:153:LYS:CB	1:D:194:MET:HE3	2.39	0.52
1:D:153:LYS:HB3	1:D:194:MET:HE3	1.91	0.52
1:A:197:LYS:HD3	1:A:197:LYS:H	1.74	0.51
1:B:325:GLU:OE2	1:D:317:ARG:HG2	2.11	0.51
1:D:193:VAL:O	1:D:193:VAL:HG12	2.09	0.51
1:B:316:LEU:HB3	1:D:325:GLU:OE2	2.10	0.51
1:B:507:LYS:H	1:B:507:LYS:CE	2.22	0.51
1:D:234:LEU:HD22	1:D:520:ASP:HB3	1.92	0.51
1:D:532:ASN:HD21	1:D:534:ARG:HB2	1.75	0.51
1:D:538:LYS:HD3	1:D:538:LYS:N	2.10	0.51
1:C:316:LEU:O	1:C:318:PHE:O	2.29	0.50
1:C:316:LEU:O	1:C:317:ARG:C	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:507:LYS:N	1:C:507:LYS:CD	2.75	0.50
1:A:153:LYS:HB3	1:A:194:MET:HE3	1.94	0.49
1:A:182:LEU:HD12	1:A:203:CYS:SG	2.52	0.49
1:A:182:LEU:CD1	1:A:203:CYS:HB3	2.42	0.49
1:A:139:LEU:HG	1:A:141:ASP:H	1.77	0.49
1:A:315:GLY:C	1:A:317:ARG:N	2.70	0.48
1:D:316:LEU:C	1:D:318:PHE:N	2.71	0.48
1:B:248:ASP:HA	1:B:254:ALA:HB2	1.94	0.48
1:D:317:ARG:HA	1:D:317:ARG:HD2	1.49	0.48
1:A:320:LYS:HD2	2:A:601:V4I:O1	2.13	0.48
1:B:507:LYS:N	1:B:507:LYS:HD3	2.29	0.48
1:B:263:VAL:CG1	1:B:498:MET:HE1	2.44	0.48
1:D:151:GLN:N	1:D:151:GLN:CD	2.72	0.48
1:A:316:LEU:O	1:A:318:PHE:N	2.47	0.47
1:B:315:GLY:C	1:B:317:ARG:H	2.22	0.47
1:C:316:LEU:O	1:C:318:PHE:N	2.47	0.47
1:C:234:LEU:HD22	1:C:520:ASP:HB3	1.97	0.47
1:A:209:VAL:O	1:A:213:GLN:HG2	2.14	0.47
1:B:143:LEU:O	1:B:147:ILE:HG12	2.15	0.47
1:D:153:LYS:HB2	1:D:194:MET:CE	2.45	0.46
1:A:153:LYS:CB	1:A:194:MET:HE3	2.45	0.46
1:C:379:GLN:O	1:C:382:ARG:HG2	2.16	0.46
1:B:507:LYS:N	1:B:507:LYS:CD	2.78	0.46
1:A:445:GLU:HG2	3:A:713:HOH:O	2.13	0.46
1:A:248:ASP:HA	1:A:254:ALA:HB2	1.97	0.46
1:B:265:VAL:HG22	1:B:498:MET:HE3	1.97	0.46
1:A:320:LYS:HE3	1:A:320:LYS:HB2	1.49	0.46
1:D:318:PHE:C	1:D:320:LYS:H	2.23	0.46
1:C:160:ILE:CG2	1:C:164:LYS:HE3	2.47	0.45
1:D:316:LEU:CD2	1:D:321:LEU:HG	2.46	0.45
1:A:153:LYS:HB2	1:A:194:MET:CE	2.46	0.45
1:B:529:ASN:ND2	1:D:529:ASN:OD1	2.44	0.45
1:B:379:GLN:O	1:B:383:GLU:HG3	2.17	0.45
1:D:536:PHE:CZ	1:D:541:ASP:HB2	2.52	0.45
1:A:234:LEU:HD22	1:A:520:ASP:HB3	1.99	0.44
1:A:439:PHE:CE2	1:A:446:ARG:HB2	2.52	0.44
1:B:524:LEU:CD1	1:B:540:LEU:HD21	2.44	0.44
1:B:265:VAL:HG23	1:B:498:MET:HE3	2.00	0.44
1:D:318:PHE:C	1:D:320:LYS:N	2.76	0.44
1:D:318:PHE:CG	1:D:320:LYS:HE2	2.52	0.44
1:D:533:LEU:HD22	1:D:533:LEU:HA	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:538:LYS:H	1:D:538:LYS:CD	2.13	0.43
1:D:142:LEU:HD12	1:D:142:LEU:H	1.83	0.43
1:C:201:LYS:O	1:C:205:GLN:HB3	2.19	0.43
1:B:315:GLY:C	1:B:317:ARG:N	2.76	0.43
1:B:201:LYS:O	1:B:205:GLN:HB3	2.19	0.43
1:B:507:LYS:H	1:B:507:LYS:CD	2.32	0.42
1:D:201:LYS:O	1:D:205:GLN:HB3	2.18	0.42
1:B:234:LEU:HD22	1:B:520:ASP:HB3	1.99	0.42
1:C:138:SER:O	1:C:142:LEU:HD13	2.19	0.42
1:A:496:MET:SD	1:A:498:MET:HE2	2.60	0.42
1:D:193:VAL:O	1:D:193:VAL:CG1	2.68	0.42
1:A:201:LYS:O	1:A:205:GLN:HB3	2.20	0.42
1:A:365:MET:HA	1:A:447:VAL:HG21	2.01	0.42
1:B:468:PHE:N	1:B:508:MET:HE3	2.35	0.42
1:C:498:MET:HE3	1:C:498:MET:HB3	1.83	0.41
1:A:317:ARG:HD3	1:A:317:ARG:HA	1.31	0.41
1:D:316:LEU:O	1:D:318:PHE:N	2.45	0.41
1:D:379:GLN:O	1:D:383:GLU:HG2	2.20	0.41
1:D:181:MET:HG2	1:D:203:CYS:HA	2.03	0.41
1:A:468:PHE:N	1:A:508:MET:HE3	2.36	0.41
1:C:411:LEU:HD23	1:C:411:LEU:HA	1.93	0.40
1:D:143:LEU:O	1:D:147:ILE:HG13	2.21	0.40
1:D:315:GLY:O	1:D:317:ARG:HD3	2.21	0.40
1:D:318:PHE:CD1	1:D:320:LYS:HB2	2.56	0.40
1:A:362:LEU:HA	1:A:365:MET:CE	2.32	0.40
1:A:495:VAL:CG2	1:A:543:ARG:HD3	2.51	0.40
1:D:534:ARG:HD2	1:D:535:HIS:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	395/533 (74%)	384 (97%)	9 (2%)	2 (0%)	24	21
1	B	398/533 (75%)	391 (98%)	5 (1%)	2 (0%)	24	21
1	C	383/533 (72%)	376 (98%)	6 (2%)	1 (0%)	36	35
1	D	385/533 (72%)	376 (98%)	6 (2%)	3 (1%)	16	11
All	All	1561/2132 (73%)	1527 (98%)	26 (2%)	8 (0%)	24	21

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	316	LEU
1	C	317	ARG
1	A	316	LEU
1	A	317	ARG
1	B	317	ARG
1	D	319	ASN
1	D	534	ARG
1	D	317	ARG

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	349/456 (76%)	335 (96%)	14 (4%)	28	27
1	B	349/456 (76%)	339 (97%)	10 (3%)	37	40
1	C	340/456 (75%)	333 (98%)	7 (2%)	47	52
1	D	342/456 (75%)	330 (96%)	12 (4%)	32	32
All	All	1380/1824 (76%)	1337 (97%)	43 (3%)	35	37

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	ILE
1	A	161	THR
1	A	199	LEU

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Mol	Chain	Res	Type
1	A	213	GLN
1	A	217	ARG
1	A	218	LYS
1	A	275	THR
1	A	316	LEU
1	A	317	ARG
1	A	411	LEU
1	A	445	GLU
1	A	446	ARG
1	A	540	LEU
1	A	544	ARG
1	B	152	GLU
1	B	199	LEU
1	B	206	SER
1	B	255	LYS
1	B	275	THR
1	B	316	LEU
1	B	317	ARG
1	B	318	PHE
1	B	319	ASN
1	B	540	LEU
1	C	152	GLU
1	C	206	SER
1	C	275	THR
1	C	319	ASN
1	C	321	LEU
1	C	350	ASN
1	C	540	LEU
1	D	206	SER
1	D	275	THR
1	D	317	ARG
1	D	318	PHE
1	D	346	LYS
1	D	507	LYS
1	D	533	LEU
1	D	534	ARG
1	D	535	HIS
1	D	538	LYS
1	D	540	LEU
1	D	544	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	GLN
1	A	347	GLN
1	A	516	HIS
1	B	213	GLN
1	B	461	HIS
1	B	519	HIS
1	C	347	GLN
1	C	461	HIS
1	C	516	HIS
1	D	187	GLN
1	D	330	HIS
1	D	347	GLN
1	D	360	GLN
1	D	516	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	V4I	A	601	-	33,33,33	1.78	3 (9%)	37,45,45	1.76	7 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	V4I	D	601	-	33,33,33	1.84	4 (12%)	37,45,45	1.86	5 (13%)

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	V4I	A	601	-	-	4/20/29/29	0/4/4/4
2	V4I	D	601	-	-	6/20/29/29	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	V4I	C2-S1	6.73	1.85	1.73
2	D	601	V4I	C3-S1	6.45	1.84	1.73
2	A	601	V4I	C3-S1	6.41	1.84	1.73
2	A	601	V4I	C2-S1	6.27	1.84	1.73
2	A	601	V4I	C2-N2	2.27	1.34	1.31
2	D	601	V4I	C3-N4	-2.09	1.31	1.34
2	D	601	V4I	C2-N2	2.01	1.34	1.31

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	V4I	C1-N1-C2	7.09	135.81	123.69
2	A	601	V4I	C1-N1-C2	5.17	132.53	123.69
2	D	601	V4I	C4-N4-C3	-4.79	116.07	124.48
2	A	601	V4I	C5-C4-C11	-4.21	95.88	103.33
2	D	601	V4I	C5-C4-C11	-3.86	96.49	103.33
2	A	601	V4I	C10-N6-N7	3.47	121.57	118.91
2	A	601	V4I	N1-C2-N2	3.44	123.89	120.81
2	A	601	V4I	C4-N4-C3	-3.40	118.51	124.48
2	D	601	V4I	N1-C2-N2	-2.86	118.26	120.81
2	D	601	V4I	C10-N6-N7	2.51	120.83	118.91
2	A	601	V4I	C2-N2-N3	2.30	114.94	112.02
2	A	601	V4I	C8-C7-N7	-2.26	120.53	123.84

There are no chirality outliers.

All (10) torsion outliers are listed below:

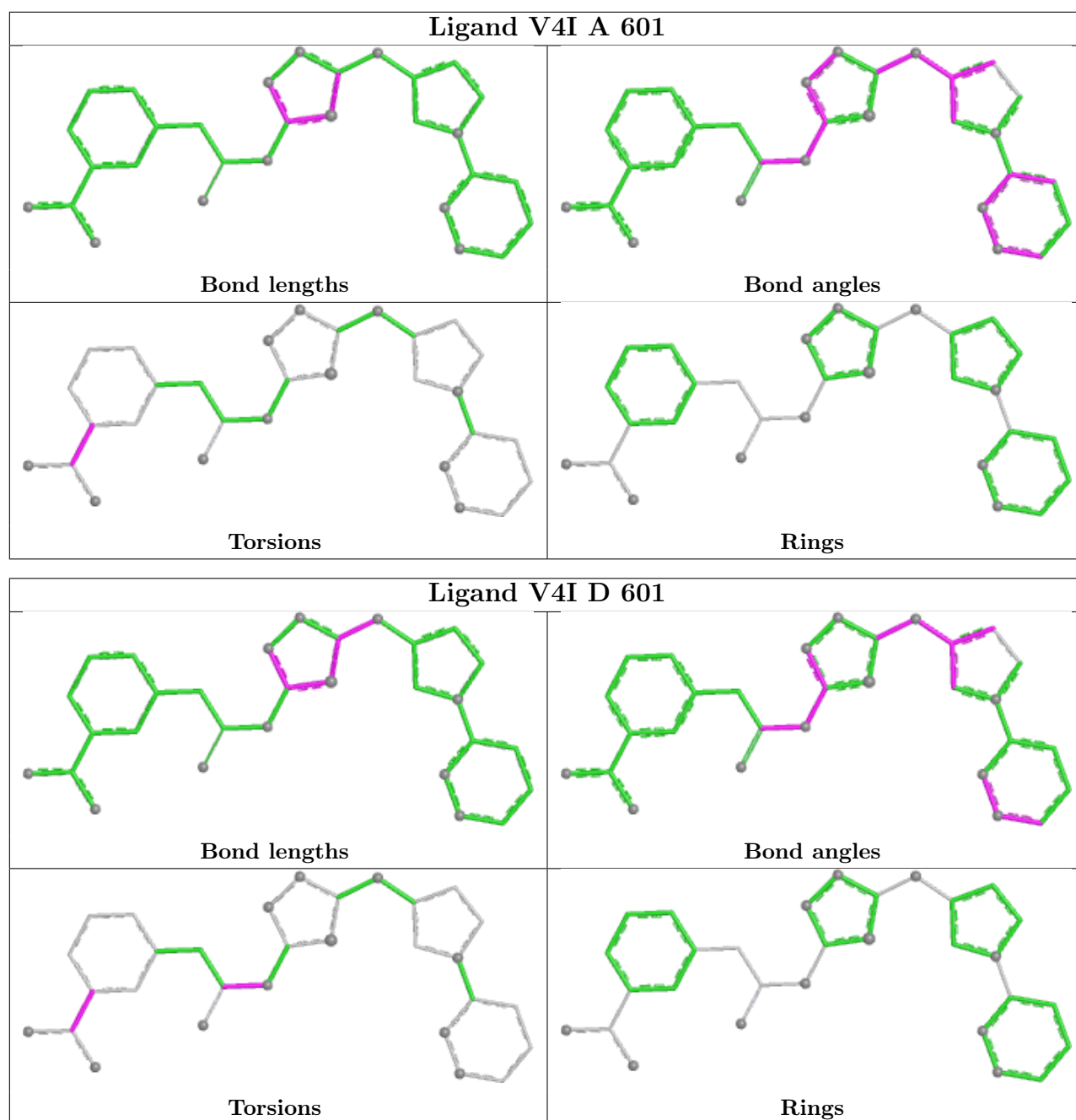
Mol	Chain	Res	Type	Atoms
2	D	601	V4I	O1-C1-N1-C2
2	D	601	V4I	C12-C1-N1-C2
2	A	601	V4I	C17-C15-C16-O3
2	D	601	V4I	C14-C15-C16-O3
2	D	601	V4I	C17-C15-C16-O3
2	A	601	V4I	C14-C15-C16-O2
2	D	601	V4I	C14-C15-C16-O2
2	D	601	V4I	C17-C15-C16-O2
2	A	601	V4I	C14-C15-C16-O3
2	A	601	V4I	C17-C15-C16-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	V4I	2	0
2	D	601	V4I	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	401/533 (75%)	0.41	47 (11%) 9 8	20, 31, 71, 110	0
1	B	402/533 (75%)	0.19	30 (7%) 20 19	20, 30, 71, 100	0
1	C	391/533 (73%)	0.24	27 (6%) 23 21	21, 31, 69, 98	0
1	D	393/533 (73%)	0.42	44 (11%) 10 9	21, 33, 72, 103	0
All	All	1587/2132 (74%)	0.32	148 (9%) 14 13	20, 31, 72, 110	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	318	PHE	8.8
1	B	316	LEU	8.7
1	C	258	PRO	8.4
1	B	318	PHE	8.0
1	D	318	PHE	7.9
1	D	534	ARG	7.7
1	D	316	LEU	7.1
1	A	193	VAL	6.8
1	C	193	VAL	6.6
1	A	139	LEU	6.5
1	B	317	ARG	6.5
1	A	316	LEU	6.4
1	D	533	LEU	6.4
1	A	319	ASN	6.1
1	A	446	ARG	6.1
1	A	544	ARG	5.8
1	B	193	VAL	5.8
1	D	319	ASN	5.7
1	A	445	GLU	5.7
1	A	317	ARG	5.4
1	C	318	PHE	5.4

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Mol	Chain	Res	Type	RSRZ
1	C	319	ASN	5.0
1	C	316	LEU	5.0
1	A	543	ARG	4.8
1	D	258	PRO	4.6
1	D	317	ARG	4.6
1	B	253	LEU	4.4
1	A	189	THR	4.4
1	D	193	VAL	4.3
1	A	144	PHE	4.3
1	B	186	LEU	4.3
1	B	254	ALA	4.2
1	C	146	THR	4.1
1	C	147	ILE	4.1
1	A	195	LEU	4.0
1	A	200	PHE	4.0
1	D	190	SER	4.0
1	D	142	LEU	3.9
1	D	145	TYR	3.8
1	A	147	ILE	3.8
1	D	195	LEU	3.8
1	A	188	THR	3.8
1	C	186	LEU	3.8
1	D	139	LEU	3.8
1	B	252	GLN	3.8
1	B	249	TYR	3.8
1	B	319	ASN	3.7
1	C	145	TYR	3.7
1	D	148	ALA	3.7
1	A	146	THR	3.7
1	A	148	ALA	3.7
1	A	447	VAL	3.5
1	D	189	THR	3.5
1	B	147	ILE	3.5
1	D	147	ILE	3.5
1	C	138	SER	3.5
1	A	145	TYR	3.5
1	B	145	TYR	3.5
1	B	250	ILE	3.4
1	C	529	ASN	3.4
1	C	150	GLY	3.4
1	D	536	PHE	3.4
1	D	532	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	156	VAL	3.4
1	D	144	PHE	3.3
1	A	154	ILE	3.3
1	D	188	THR	3.2
1	A	197	LYS	3.2
1	C	537	ALA	3.2
1	D	143	LEU	3.2
1	A	152	GLU	3.2
1	A	194	MET	3.2
1	A	254	ALA	3.1
1	D	535	HIS	3.1
1	C	248	ASP	3.1
1	D	259	ASP	3.1
1	D	154	ILE	3.0
1	A	204	VAL	3.0
1	A	213	GLN	2.9
1	B	251	PRO	2.9
1	B	194	MET	2.9
1	D	200	PHE	2.9
1	D	157	HIS	2.9
1	A	249	TYR	2.9
1	C	317	ARG	2.9
1	A	199	LEU	2.8
1	A	161	THR	2.8
1	D	247	ALA	2.8
1	A	217	ARG	2.7
1	C	348	GLY	2.7
1	D	197	LYS	2.7
1	A	182	LEU	2.7
1	B	153	LYS	2.7
1	B	138	SER	2.7
1	C	194	MET	2.7
1	D	204	VAL	2.6
1	A	143	LEU	2.6
1	B	184	LEU	2.6
1	D	199	LEU	2.6
1	D	538	LYS	2.6
1	B	150	GLY	2.6
1	D	153	LYS	2.6
1	B	213	GLN	2.5
1	A	142	LEU	2.5
1	B	139	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	144	PHE	2.5
1	C	144	PHE	2.5
1	D	225	MET	2.5
1	A	156	VAL	2.5
1	B	255	LYS	2.4
1	D	194	MET	2.4
1	A	255	LYS	2.4
1	C	153	LYS	2.4
1	B	142	LEU	2.4
1	B	195	LEU	2.4
1	B	529	ASN	2.4
1	C	320	LYS	2.3
1	C	161	THR	2.3
1	A	141	ASP	2.3
1	B	157	HIS	2.3
1	A	208	ILE	2.2
1	D	537	ALA	2.2
1	C	195	LEU	2.2
1	A	158	LYS	2.2
1	B	156	VAL	2.2
1	A	198	ASP	2.2
1	C	545	GLU	2.2
1	C	142	LEU	2.2
1	C	198	ASP	2.2
1	D	383	GLU	2.2
1	A	252	GLN	2.2
1	D	185	THR	2.2
1	A	163	LEU	2.1
1	A	184	LEU	2.1
1	D	216	ARG	2.1
1	D	348	GLY	2.1
1	D	545	GLU	2.1
1	D	178	CYS	2.1
1	A	157	HIS	2.1
1	D	181	MET	2.0
1	A	178	CYS	2.0
1	A	251	PRO	2.0
1	B	545	GLU	2.0
1	C	152	GLU	2.0
1	B	148	ALA	2.0
1	C	199	LEU	2.0
1	D	202	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	185	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

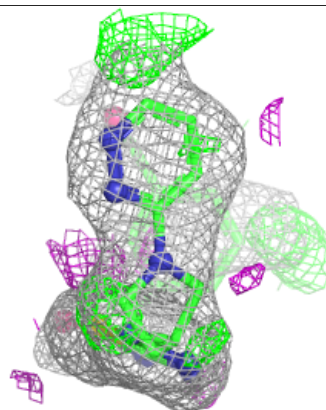
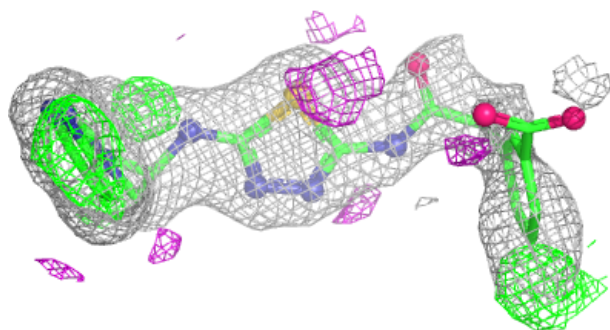
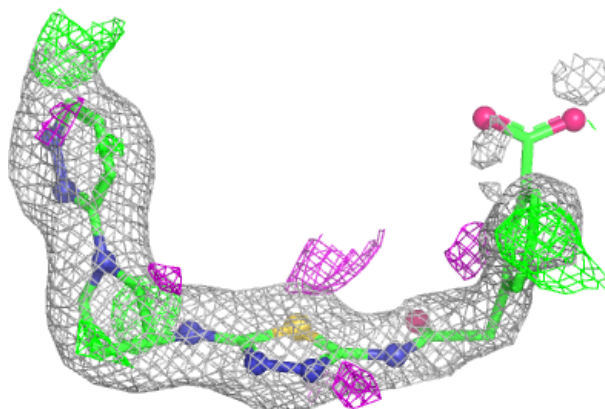
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	V4I	A	601	30/30	0.91	0.15	27,39,109,127	0
2	V4I	D	601	30/30	0.91	0.16	25,40,122,124	0

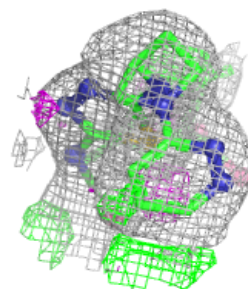
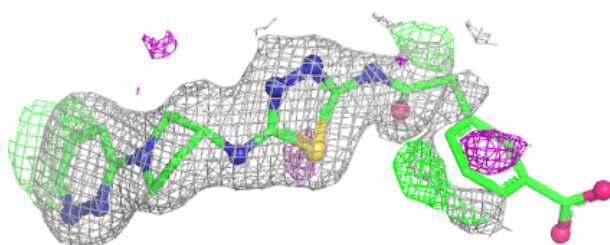
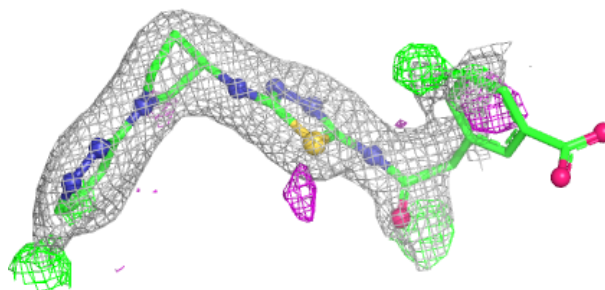
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around V4I A 601:

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

**Electron density around V4I D 601:**

$2mF_o-DF_c$ (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.