



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:06 PM EDT

PDB ID : 4B73 / pdb_00004b73
Title : Discovery of an allosteric mechanism for the regulation of HCV NS3 protein function
Authors : Saalau-Bethell, S.M.; Woodhead, A.J.; Chessari, G.; Carr, M.G.; Coyle, J.; Graham, B.; Hiscock, S.D.; Murray, C.W.; Pathuri, P.; Rich, S.J.; Richardson, C.J.; Williams, P.A.; Jhoti, H.
Deposited on : 2012-08-16
Resolution : 2.50 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](#) ①) 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

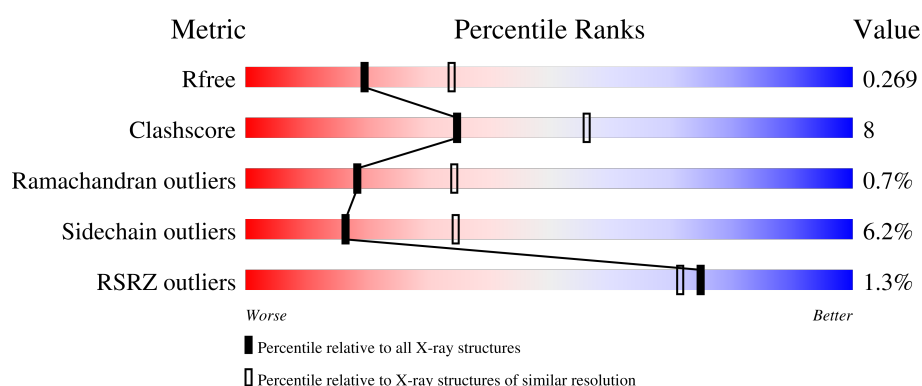
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	666	2% 78% 16% • •
1	B	666	% 81% 15% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9943 atoms, of which 46 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 NON-STRUCTURAL PROTEIN 4A, SERINE PROTEASE NS3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	645	Total	C	N	O	S	0	0	0
			4808	3026	834	918	30			
1	B	642	Total	C	N	O	S	0	0	0
			4794	3019	831	914	30			

There are 56 discrepancies between the modelled and reference sequences:

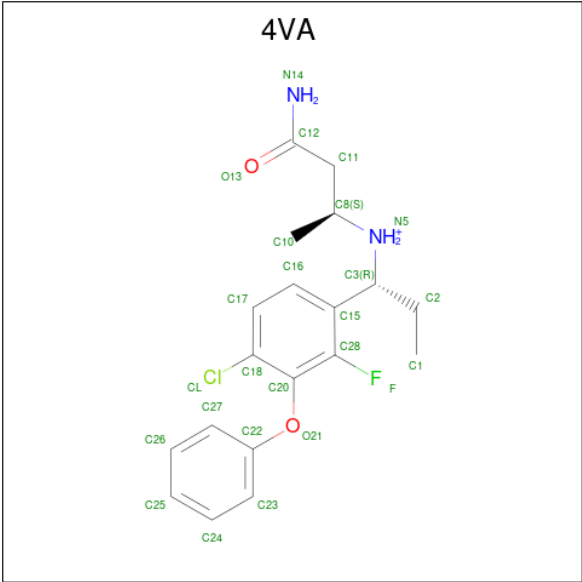
Chain	Residue	Modelled	Actual	Comment	Reference
A	684	MET	-	expression tag	UNP P26663
A	685	GLY	-	expression tag	UNP P26663
A	686	SER	-	expression tag	UNP P26663
A	687	SER	-	expression tag	UNP P26663
A	688	HIS	-	expression tag	UNP P26663
A	689	HIS	-	expression tag	UNP P26663
A	690	HIS	-	expression tag	UNP P26663
A	691	HIS	-	expression tag	UNP P26663
A	692	HIS	-	expression tag	UNP P26663
A	693	HIS	-	expression tag	UNP P26663
A	694	SER	-	expression tag	UNP P26663
A	695	SER	-	expression tag	UNP P26663
A	696	GLY	-	expression tag	UNP P26663
A	697	LEU	-	expression tag	UNP P26663
A	698	VAL	-	expression tag	UNP P26663
A	699	PRO	-	expression tag	UNP P26663
A	700	ARG	-	expression tag	UNP P26663
A	701	GLY	-	expression tag	UNP P26663
A	702	SER	-	expression tag	UNP P26663
A	703	HIS	-	expression tag	UNP P26663
A	704	MET	-	expression tag	UNP P26663
A	718	SER	-	linker	UNP P26663
A	719	GLY	-	linker	UNP P26663
A	720	SER	-	linker	UNP P26663

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Chain	Residue	Modelled	Actual	Comment	Reference
A	66	GLY	ALA	conflict	UNP P26663
A	86	GLN	PRO	conflict	UNP P26663
A	87	ALA	LYS	conflict	UNP P26663
A	147	SER	PHE	conflict	UNP P26663
B	684	MET	-	expression tag	UNP P26663
B	685	GLY	-	expression tag	UNP P26663
B	686	SER	-	expression tag	UNP P26663
B	687	SER	-	expression tag	UNP P26663
B	688	HIS	-	expression tag	UNP P26663
B	689	HIS	-	expression tag	UNP P26663
B	690	HIS	-	expression tag	UNP P26663
B	691	HIS	-	expression tag	UNP P26663
B	692	HIS	-	expression tag	UNP P26663
B	693	HIS	-	expression tag	UNP P26663
B	694	SER	-	expression tag	UNP P26663
B	695	SER	-	expression tag	UNP P26663
B	696	GLY	-	expression tag	UNP P26663
B	697	LEU	-	expression tag	UNP P26663
B	698	VAL	-	expression tag	UNP P26663
B	699	PRO	-	expression tag	UNP P26663
B	700	ARG	-	expression tag	UNP P26663
B	701	GLY	-	expression tag	UNP P26663
B	702	SER	-	expression tag	UNP P26663
B	703	HIS	-	expression tag	UNP P26663
B	704	MET	-	expression tag	UNP P26663
B	718	SER	-	linker	UNP P26663
B	719	GLY	-	linker	UNP P26663
B	720	SER	-	linker	UNP P26663
B	66	GLY	ALA	conflict	UNP P26663
B	86	GLN	PRO	conflict	UNP P26663
B	87	ALA	LYS	conflict	UNP P26663
B	147	SER	PHE	conflict	UNP P26663

- Molecule 2 is (2S)-4-amino-N-[(1R)-1-(4-chloro-2-fluoro-3-phenoxyphenyl)propyl]-4-oxobutan-2-aminium (CCD ID: 4VA) (formula: C₁₉H₂₃ClFN₂O₂).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	H	N	O	0	0
			48	19	1	1	23	2	2		
2	B	1	Total	C	Cl	F	H	N	O	0	0
			48	19	1	1	23	2	2		

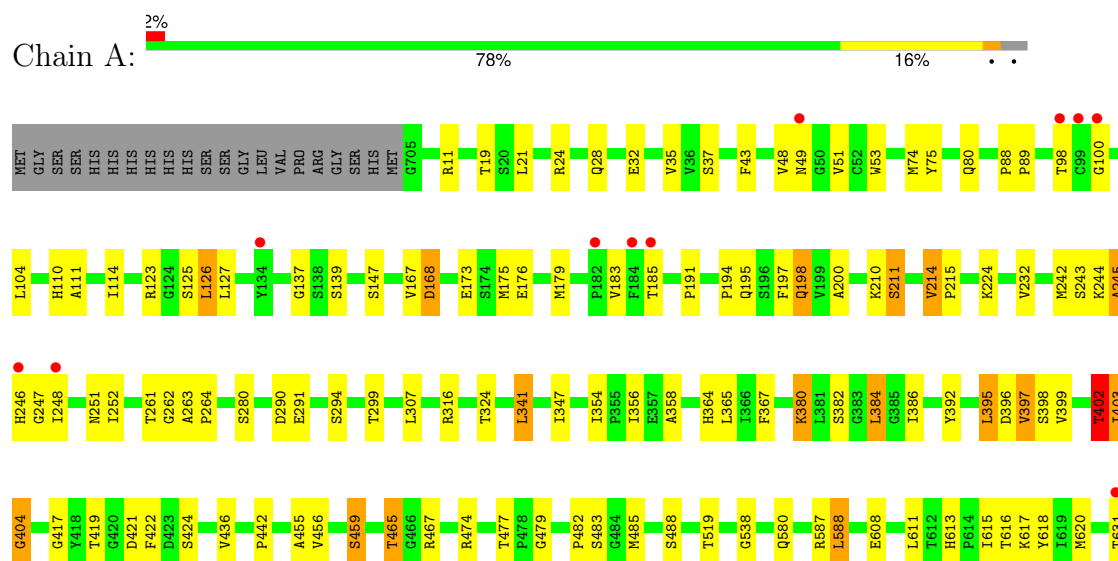
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	139	Total	O	0	0
			139	139		
3	B	106	Total	O	0	0
			106	106		

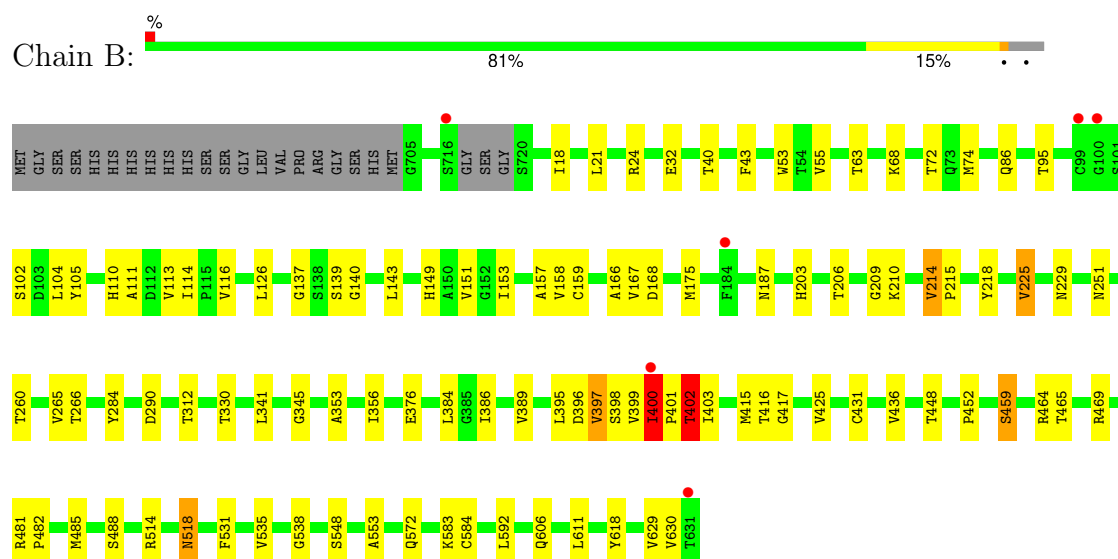
3 Residue-property plots [i](#)

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: NON-STRUCTURAL PROTEIN 4A, SERINE PROTEASE NS3



• Molecule 1: NON-STRUCTURAL PROTEIN 4A, SERINE PROTEASE NS3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.84Å 109.50Å 141.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.49 – 2.50 86.49 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.3 (86.49-2.50) 97.3 (86.49-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.6.0062	Depositor
R, R_{free}	0.183 , 0.264 0.187 , 0.269	Depositor DCC
R_{free} test set	2501 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9943	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 4VA

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	0.85	0/4917	0.93	6/6714 (0.1%)
1	B	0.81	1/4902 (0.0%)	0.94	6/6693 (0.1%)
All	All	0.83	1/9819 (0.0%)	0.94	12/13407 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	402	THR	N-CA	5.53	1.53	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	VAL	N-CA-C	-8.21	96.62	108.36
1	A	402	THR	CA-C-N	7.41	135.03	121.70
1	A	402	THR	C-N-CA	7.41	135.03	121.70
1	A	402	THR	N-CA-C	7.16	122.40	112.45
1	B	400	ILE	CA-C-N	7.13	144.12	127.00
1	B	400	ILE	C-N-CA	7.13	144.12	127.00
1	B	400	ILE	C-N-CD	-7.06	105.06	120.60
1	B	18	ILE	CB-CA-C	-5.49	104.94	111.97
1	A	114	ILE	CB-CA-C	-5.37	105.95	110.94
1	B	284	TYR	N-CA-C	5.06	117.08	109.23
1	A	49	ASN	N-CA-C	5.03	118.13	111.30
1	B	114	ILE	CB-CA-C	-5.01	105.35	110.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4808	0	4784	81	0
1	B	4794	0	4772	67	0
2	A	25	23	23	0	0
2	B	25	23	23	0	0
3	A	139	0	0	1	0
3	B	106	0	0	1	0
All	All	9897	46	9602	145	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 8.

All (145) 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:400:ILE:HG22	1:B:401:PRO:CA	1.66	1.26
1:B:400:ILE:HG22	1:B:401:PRO:C	1.82	1.03
1:B:400:ILE:CG2	1:B:402:THR:HG23	1.95	0.97
1:B:400:ILE:HG21	1:B:402:THR:HG23	1.47	0.93
1:B:400:ILE:HG22	1:B:401:PRO:HA	1.51	0.89
1:B:209:GLY:O	1:B:214:VAL:HG12	1.74	0.86
1:B:400:ILE:HG22	1:B:402:THR:N	1.93	0.83
1:A:74:MET:HE3	1:A:75:TYR:CE2	2.13	0.83
1:B:400:ILE:CG2	1:B:401:PRO:CA	2.56	0.78
1:B:400:ILE:CG2	1:B:402:THR:N	2.46	0.78
1:A:397:VAL:HG11	1:A:417:GLY:O	1.85	0.77
1:B:400:ILE:CG2	1:B:401:PRO:HA	2.15	0.76
1:A:616:THR:HG22	1:A:620:MET:HE2	1.67	0.74
1:B:400:ILE:HG22	1:B:401:PRO:N	1.98	0.74
1:A:53:TRP:NE1	1:A:175:MET:HE3	2.05	0.72
1:A:436:VAL:HG11	1:A:488:SER:HB3	1.72	0.71
1:B:400:ILE:CG2	1:B:401:PRO:C	2.61	0.70
1:B:400:ILE:HG23	1:B:402:THR:HG23	1.73	0.69
1:A:53:TRP:CD1	1:A:175:MET:HE3	2.28	0.69
1:B:209:GLY:O	1:B:214:VAL:CG1	2.42	0.67
1:A:477:THR:HG22	1:A:479:GLY:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:LEU:HD13	1:B:611:LEU:HD23	1.76	0.66
1:A:396:ASP:O	1:A:399:VAL:HG13	1.95	0.66
1:B:452:PRO:O	1:B:481:ARG:NH1	2.30	0.63
1:B:397:VAL:HG21	1:B:417:GLY:O	1.99	0.62
1:B:126:LEU:HD11	1:B:167:VAL:HG13	1.82	0.61
1:B:398:SER:HA	1:B:400:ILE:HG12	1.83	0.61
1:A:587:ARG:HG3	1:A:588:LEU:HD13	1.81	0.61
1:B:210:LYS:HA	1:B:214:VAL:HG11	1.83	0.61
1:A:245:ALA:O	1:A:247:GLY:N	2.33	0.60
1:A:347:ILE:HD11	1:A:356:ILE:HG12	1.84	0.59
1:A:380:LYS:O	1:A:384:LEU:HD13	2.04	0.58
1:A:403:ILE:O	1:A:404:GLY:O	2.22	0.58
1:B:518:ASN:HD22	1:B:518:ASN:N	2.02	0.58
1:A:51:VAL:CG2	1:A:179:MET:CE	2.81	0.58
1:A:442:PRO:HB3	1:A:611:LEU:HD22	1.87	0.57
1:B:397:VAL:O	1:B:400:ILE:HG12	2.04	0.56
1:A:19:THR:HG23	1:A:24:ARG:O	2.05	0.56
1:A:74:MET:HE3	1:A:75:TYR:CZ	2.41	0.56
1:A:403:ILE:HG22	1:A:404:GLY:N	2.21	0.55
1:A:402:THR:HG23	1:A:403:ILE:HB	1.90	0.54
1:B:553:ALA:HB1	1:B:583:LYS:HZ1	1.73	0.54
1:B:126:LEU:CD1	1:B:167:VAL:HG13	2.38	0.54
1:A:74:MET:HE3	1:A:75:TYR:HE2	1.72	0.53
1:A:110:HIS:O	1:A:111:ALA:HB3	2.10	0.52
1:A:51:VAL:HG21	1:A:179:MET:CE	2.40	0.52
1:B:531:PHE:O	1:B:535:VAL:HG23	2.10	0.51
1:B:251:ASN:HD22	1:B:260:THR:HA	1.75	0.51
1:A:436:VAL:CG1	1:A:488:SER:HB3	2.41	0.51
1:B:425:VAL:HG23	1:B:465:THR:HB	1.93	0.51
1:A:53:TRP:CE2	1:A:175:MET:HE3	2.45	0.50
1:B:345:GLY:HA3	1:B:353:ALA:HB1	1.94	0.50
1:A:214:VAL:HG22	1:A:215:PRO:HD3	1.94	0.50
1:A:214:VAL:N	1:A:215:PRO:HD2	2.27	0.50
1:A:611:LEU:HD13	1:B:611:LEU:CD2	2.41	0.49
1:B:140:GLY:HA2	1:B:153:ILE:HD12	1.94	0.49
1:B:482:PRO:HG2	1:B:485:MET:HE1	1.95	0.49
1:A:341:LEU:CD1	1:A:474:ARG:HB3	2.43	0.49
1:B:158:VAL:HB	1:B:166:ALA:HB3	1.95	0.48
1:B:225:VAL:CG1	1:B:265:VAL:HG22	2.43	0.48
1:A:482:PRO:HB2	1:A:485:MET:HE2	1.94	0.48
1:B:104:LEU:O	1:B:116:VAL:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:TRP:NE1	1:B:175:MET:HE3	2.28	0.48
1:B:210:LYS:HA	1:B:214:VAL:CG1	2.43	0.48
1:A:74:MET:CE	1:A:75:TYR:CE2	2.91	0.48
1:A:617:LYS:HA	1:A:620:MET:HE3	1.95	0.48
1:A:51:VAL:CG2	1:A:179:MET:HE2	2.44	0.48
1:A:251:ASN:HD21	1:A:262:GLY:H	1.62	0.48
1:A:364:HIS:ND1	1:A:424:SER:OG	2.38	0.48
1:B:126:LEU:HD11	1:B:167:VAL:CG1	2.44	0.48
1:B:330:THR:HG22	1:B:459:SER:HB2	1.95	0.48
1:B:436:VAL:CG1	1:B:488:SER:HB3	2.43	0.48
1:A:392:TYR:CZ	1:A:395:LEU:HD21	2.49	0.47
1:B:104:LEU:HD21	1:B:151:VAL:HG11	1.95	0.47
1:B:553:ALA:HB1	1:B:583:LYS:NZ	2.29	0.47
1:B:436:VAL:HG11	1:B:488:SER:HB3	1.96	0.47
1:B:229:ASN:HD22	1:B:290:ASP:HB3	1.80	0.47
1:B:482:PRO:HG2	1:B:485:MET:CE	2.45	0.47
1:B:538:GLY:HA3	1:B:618:TYR:CE2	2.50	0.47
1:A:53:TRP:HZ2	1:A:179:MET:HE3	1.79	0.47
1:A:382:SER:HA	1:A:386:ILE:O	2.14	0.47
1:B:43:PHE:HA	1:B:137:GLY:O	2.14	0.46
1:B:110:HIS:O	1:B:111:ALA:HB3	2.15	0.46
1:A:611:LEU:CD1	1:B:611:LEU:HD23	2.44	0.46
1:A:358:ALA:HB1	1:A:474:ARG:NH2	2.30	0.46
1:B:95:THR:OG1	1:B:149:HIS:ND1	2.49	0.46
1:B:251:ASN:HB2	1:B:266:THR:HG23	1.96	0.46
1:A:347:ILE:HD12	1:A:354:ILE:O	2.16	0.45
1:A:358:ALA:HB1	1:A:474:ARG:CZ	2.46	0.45
1:B:553:ALA:CB	1:B:583:LYS:NZ	2.80	0.45
1:A:28:GLN:OE1	1:A:28:GLN:N	2.50	0.45
1:A:538:GLY:HA3	1:A:618:TYR:CE2	2.52	0.45
1:B:398:SER:CA	1:B:400:ILE:HG12	2.47	0.45
1:A:251:ASN:HD22	1:A:261:THR:H	1.65	0.45
1:A:392:TYR:CZ	1:A:395:LEU:CD2	3.00	0.44
1:B:553:ALA:HB2	1:B:583:LYS:HZ2	1.83	0.44
1:A:294:SER:HB2	1:A:299:THR:HG21	1.99	0.44
1:B:214:VAL:HG23	1:B:218:TYR:CE2	2.53	0.44
1:A:307:LEU:HD13	1:A:519:THR:OG1	2.17	0.43
1:A:613:HIS:CE1	1:A:615:ILE:HG12	2.53	0.43
1:A:341:LEU:HD13	1:A:474:ARG:HB3	2.00	0.43
1:A:477:THR:HG22	1:A:479:GLY:N	2.31	0.43
1:A:396:ASP:O	1:A:399:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:ASN:ND2	1:B:203:HIS:CE1	2.87	0.43
1:A:421:ASP:HB3	1:A:467:ARG:HD2	2.01	0.43
1:B:514:ARG:HH11	1:B:518:ASN:HD21	1.66	0.43
1:A:53:TRP:CZ2	1:A:179:MET:HE3	2.54	0.43
1:B:74:MET:HE1	1:B:86:GLN:OE1	2.19	0.43
1:A:51:VAL:HG21	1:A:179:MET:HE2	2.01	0.43
1:A:397:VAL:O	1:A:398:SER:OG	2.34	0.43
1:B:63:THR:HG22	1:B:72:THR:HA	2.00	0.43
1:B:400:ILE:CB	1:B:401:PRO:HA	2.49	0.43
1:B:396:ASP:O	1:B:399:VAL:HG22	2.19	0.42
1:A:194:PRO:HG3	1:A:198:GLN:HB2	2.01	0.42
1:A:197:PHE:HA	1:A:316:ARG:O	2.20	0.42
1:A:263:ALA:HB1	1:A:264:PRO:HD2	2.00	0.42
1:A:48:VAL:HB	1:A:175:MET:HE1	2.00	0.42
1:A:324:THR:HB	1:A:456:VAL:HG22	2.01	0.42
1:B:214:VAL:HG22	1:B:215:PRO:HD3	2.02	0.42
1:B:24:ARG:NH2	1:B:68:LYS:O	2.53	0.42
1:B:157:ALA:HB3	1:B:629:VAL:HG23	2.01	0.42
1:A:211:SER:OG	1:A:290:ASP:OD2	2.35	0.42
1:B:415:MET:HA	1:B:464:ARG:NH2	2.35	0.42
1:A:51:VAL:HG21	1:A:179:MET:HE3	2.01	0.42
1:A:43:PHE:HA	1:A:137:GLY:O	2.20	0.42
1:B:341:LEU:HD23	3:B:2055:HOH:O	2.20	0.42
1:A:291:GLU:OE1	1:A:291:GLU:HA	2.21	0.41
1:A:402:THR:HG23	1:A:403:ILE:CG1	2.50	0.41
1:A:126:LEU:HD11	1:A:167:VAL:HG13	2.01	0.41
1:A:244:LYS:HG3	1:A:245:ALA:N	2.36	0.41
1:A:365:LEU:HD21	1:A:367:PHE:CZ	2.55	0.41
1:B:105:TYR:HB3	1:B:113:VAL:HG12	2.02	0.41
1:A:139:SER:OG	1:A:631:THR:O	2.37	0.41
1:A:243:SER:HA	1:A:248:ILE:O	2.21	0.41
1:A:88:PRO:CB	1:A:89:PRO:HD2	2.50	0.41
1:A:183:VAL:HG23	3:A:2037:HOH:O	2.19	0.41
1:A:455:ALA:HB3	1:A:483:SER:HB3	2.03	0.41
1:A:51:VAL:HG23	1:A:179:MET:CE	2.50	0.41
1:A:251:ASN:O	1:A:252:ILE:HD13	2.21	0.41
1:A:53:TRP:CD1	1:A:175:MET:CE	3.01	0.40
1:A:324:THR:HG21	1:A:459:SER:OG	2.21	0.40
1:A:422:PHE:O	1:A:465:THR:OG1	2.34	0.40
1:B:55:VAL:HG21	1:B:139:SER:HB3	2.03	0.40
1:A:123:ARG:NE	1:A:168:ASP:OD1	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:PRO:HG3	1:A:200:ALA:CB	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	643/666 (96%)	606 (94%)	32 (5%)	5 (1%)	16	31
1	B	638/666 (96%)	612 (96%)	22 (3%)	4 (1%)	21	38
All	All	1281/1332 (96%)	1218 (95%)	54 (4%)	9 (1%)	18	34

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	246	HIS
1	A	403	ILE
1	B	400	ILE
1	A	404	GLY
1	A	245	ALA
1	B	402	THR
1	B	469	ARG
1	B	584	CYS
1	A	100	GLY

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	526/544 (97%)	490 (93%)	36 (7%)	14	31
1	B	525/544 (96%)	496 (94%)	29 (6%)	19	40
All	All	1051/1088 (97%)	986 (94%)	65 (6%)	16	34

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	21	LEU
1	A	32	GLU
1	A	37	SER
1	A	80	GLN
1	A	98	THR
1	A	104	LEU
1	A	125	SER
1	A	126	LEU
1	A	127	LEU
1	A	147	SER
1	A	168	ASP
1	A	173	GLU
1	A	176	GLU
1	A	185	THR
1	A	195	GLN
1	A	198	GLN
1	A	210	LYS
1	A	211	SER
1	A	214	VAL
1	A	224	LYS
1	A	232	VAL
1	A	242	MET
1	A	280	SER
1	A	341	LEU
1	A	380	LYS
1	A	384	LEU
1	A	395	LEU
1	A	397	VAL
1	A	402	THR
1	A	419	THR
1	A	459	SER
1	A	465	THR
1	A	580	GLN

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Mol	Chain	Res	Type
1	A	588	LEU
1	A	608	GLU
1	B	21	LEU
1	B	32	GLU
1	B	40	THR
1	B	102	SER
1	B	143	LEU
1	B	159	CYS
1	B	168	ASP
1	B	206	THR
1	B	214	VAL
1	B	225	VAL
1	B	312	THR
1	B	356	ILE
1	B	376	GLU
1	B	384	LEU
1	B	386	ILE
1	B	389	VAL
1	B	395	LEU
1	B	397	VAL
1	B	403	ILE
1	B	416	THR
1	B	431	CYS
1	B	448	THR
1	B	459	SER
1	B	518	ASN
1	B	548	SER
1	B	572	GLN
1	B	592	LEU
1	B	606	GLN
1	B	630	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	73	GLN
1	A	149	HIS
1	A	195	GLN
1	A	198	GLN
1	A	246	HIS
1	A	251	ASN

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Mol	Chain	Res	Type
1	A	343	ASN
1	B	8	GLN
1	B	27	ASN
1	B	34	GLN
1	B	41	GLN
1	B	187	ASN
1	B	229	ASN
1	B	246	HIS
1	B	251	ASN
1	B	293	HIS
1	B	518	ASN
1	B	541	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	4VA	B	1721	-	26,26,26	0.92	2 (7%)	31,35,35	0.88	2 (6%)
2	4VA	A	1721	-	26,26,26	0.91	1 (3%)	31,35,35	0.82	1 (3%)

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	4VA	B	1721	-	-	3/18/18/18	0/2/2/2
2	4VA	A	1721	-	-	4/18/18/18	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1721	4VA	C3-N5	2.77	1.51	1.47
2	B	1721	4VA	C3-N5	2.57	1.50	1.47
2	B	1721	4VA	C15-C28	2.51	1.41	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1721	4VA	C22-O21-C20	3.22	123.48	118.40
2	B	1721	4VA	C22-O21-C20	3.15	123.38	118.40
2	B	1721	4VA	C20-C18-CL	2.31	121.45	118.40

There are no chirality outliers.

All (7) torsion outliers are listed below:

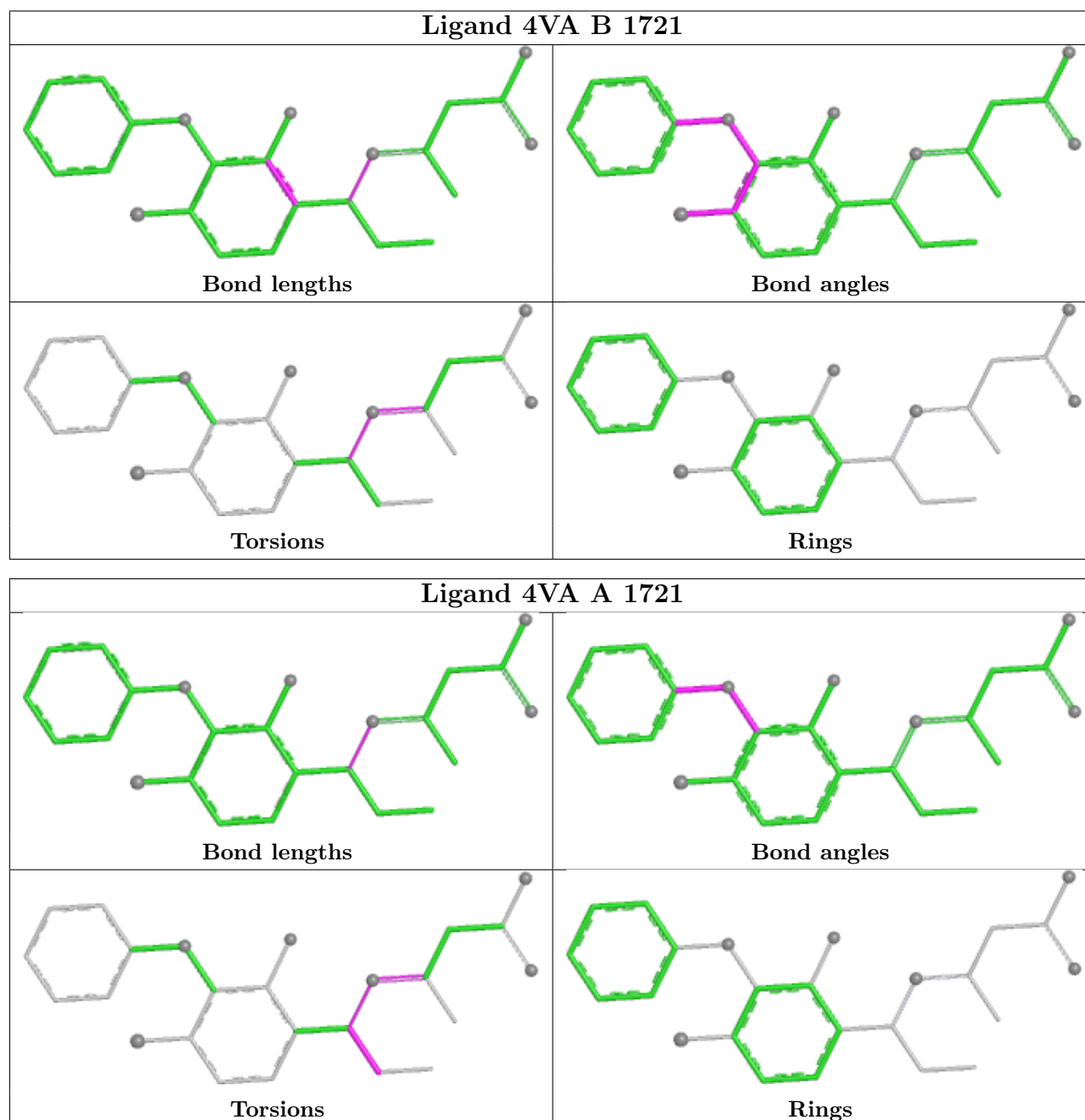
Mol	Chain	Res	Type	Atoms
2	B	1721	4VA	C15-C3-N5-C8
2	A	1721	4VA	C15-C3-N5-C8
2	A	1721	4VA	C10-C8-N5-C3
2	B	1721	4VA	C10-C8-N5-C3
2	A	1721	4VA	C1-C2-C3-N5
2	A	1721	4VA	C11-C8-N5-C3
2	B	1721	4VA	C11-C8-N5-C3

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	645/666 (96%)	-0.10	11 (1%) 69 65	24, 47, 84, 121	0
1	B	642/666 (96%)	-0.03	6 (0%) 81 78	30, 50, 80, 121	0
All	All	1287/1332 (96%)	-0.06	17 (1%) 75 71	24, 49, 82, 121	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	182	PRO	4.3
1	A	98	THR	4.1
1	A	100	GLY	3.1
1	A	248	ILE	3.1
1	A	185	THR	2.8
1	A	99	CYS	2.8
1	B	716	SER	2.7
1	B	631	THR	2.6
1	B	100	GLY	2.5
1	A	631	THR	2.5
1	B	99	CYS	2.4
1	A	184	PHE	2.4
1	A	134	TYR	2.3
1	B	184	PHE	2.2
1	A	246	HIS	2.2
1	B	400	ILE	2.1
1	A	49	ASN	2.1

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](#)

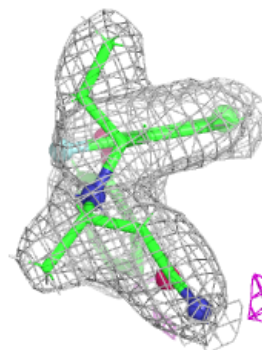
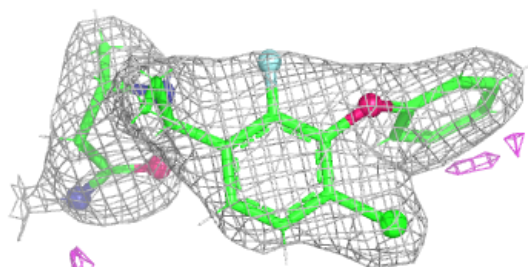
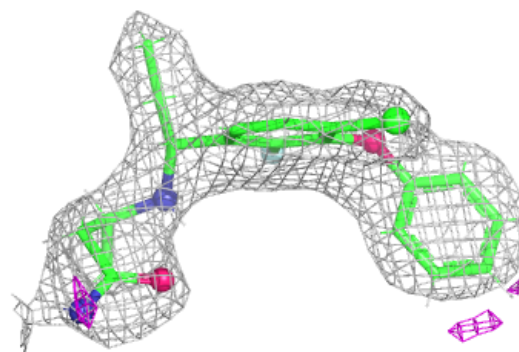
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	4VA	A	1721	25/25	0.94	0.09	22,24,30,47	48
2	4VA	B	1721	25/25	0.94	0.10	30,33,36,61	48

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.

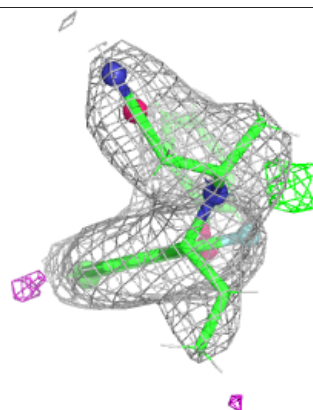
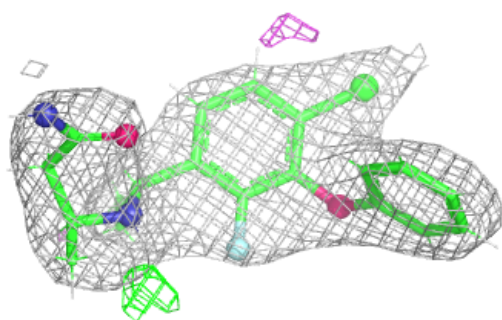
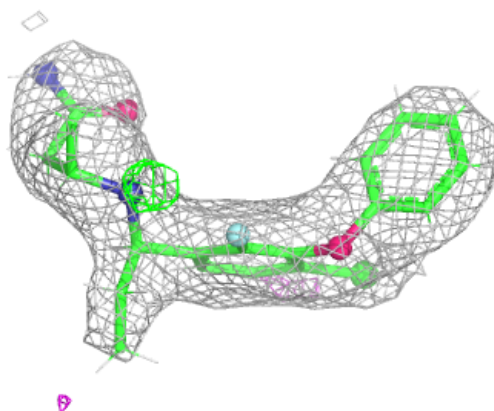
Electron density around 4VA A 1721:

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 4VA B 1721:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.