



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:52 PM UTC

PDB ID : 5RL7 / pdb_00005rl7
Title : PanDDA analysis group deposition – Crystal Structure of SARS-CoV-2 heli-
case in complex with Z364321922
Authors : Newman, J.A.; Yosaatmadja, Y.; Douangamath, A.; Aimon, A.; Powell, A.J.;
Dias, A.; Fearon, D.; Dunnett, L.; Brandao-Neto, J.; Krojer, T.; Skyner, R.;
Gorrie-Stone, T.; Thompson, W.; von Delft, F.; Arrowsmith, C.H.; Edwards,
A.; Bountra, C.; Gileadi, O.
Deposited on : 2020-09-16
Resolution : 1.89 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)

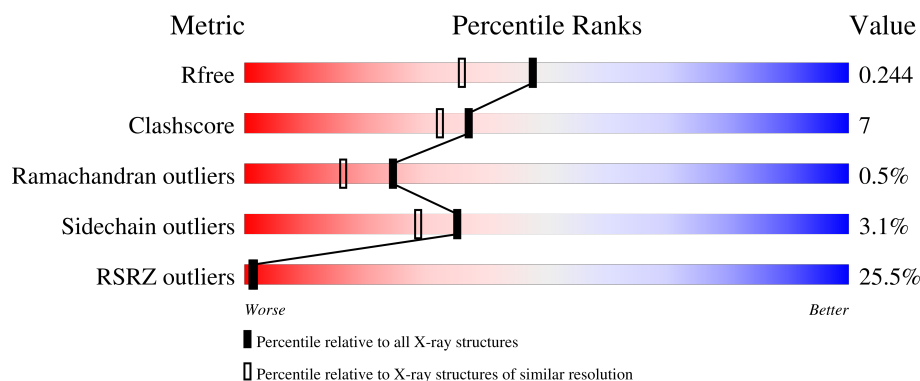
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	601	33% 78% 16% • 5%
1	B	601	16% 81% 16% •

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition [i](#)

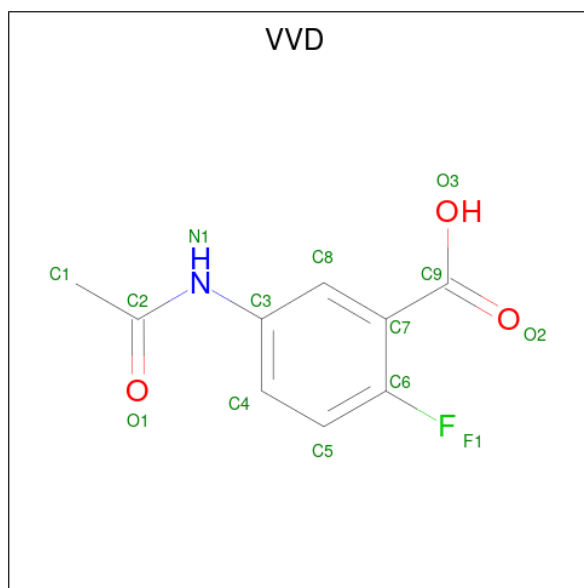
There are 5 unique types of molecules in this entry. The entry contains 9433 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	585	Total	C	N	O	S	0	1	0
			4508	2875	750	848	35			
1	A	572	Total	C	N	O	S	0	0	0
			4417	2816	737	832	32			

- Molecule 2 is 5-(acetylamino)-2-fluorobenzoic acid (CCD ID: VVD) (formula: $C_9H_8FNO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	F	N	O	0	0
			14	9	1	1	3		
2	A	1	Total	C	F	N	O	0	0
			14	9	1	1	3		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Zn	0	0
			3	3		
3	A	3	Total	Zn	0	0
			3	3		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		

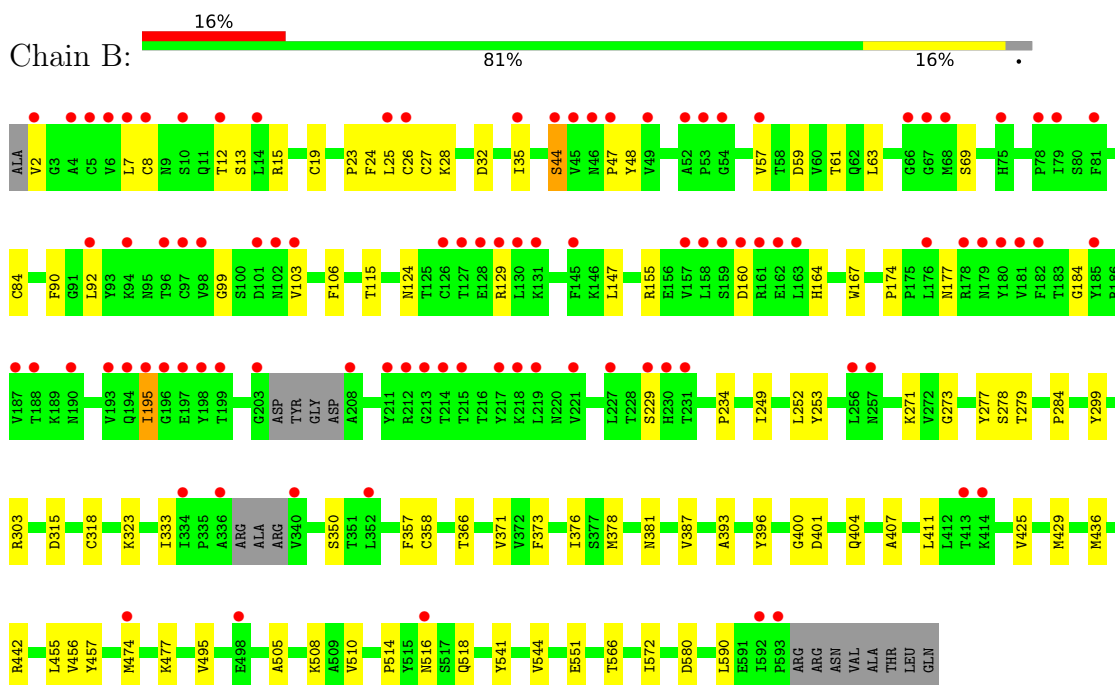
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	251	Total	O	0	0
			251	251		
5	A	203	Total	O	0	0
			203	203		

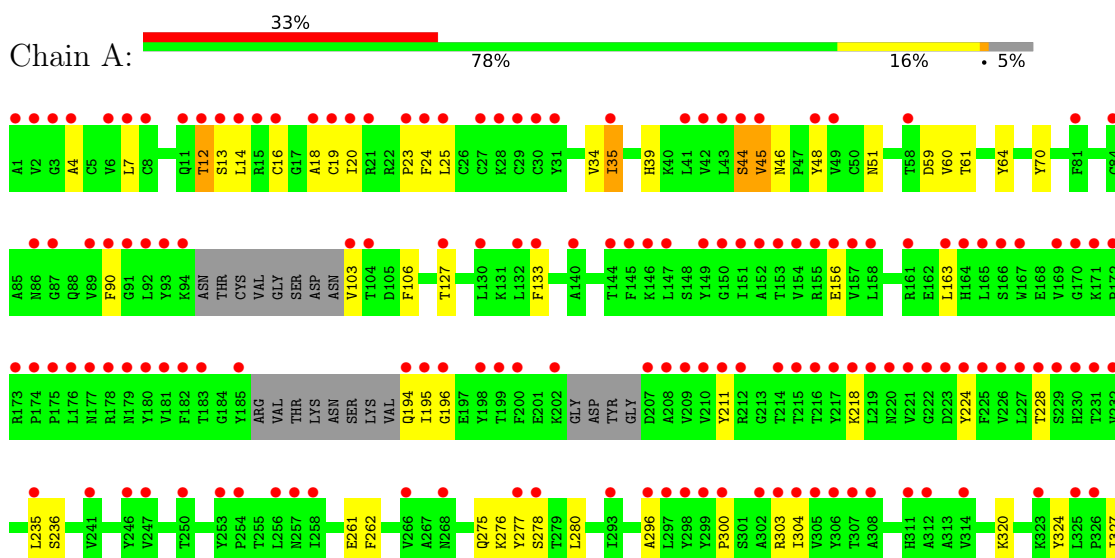
3 Residue-property plots [i](#)

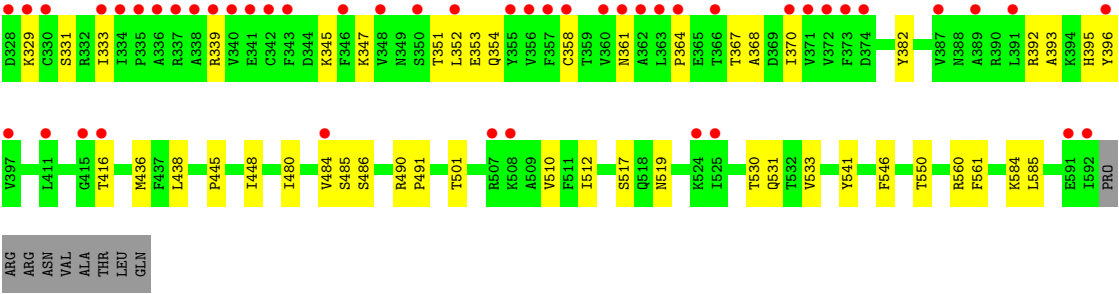
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Helicase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.15Å 70.28Å 85.59Å 102.73° 96.54° 112.33°	Depositor
Resolution (Å)	81.45 – 1.89 81.45 – 1.89	Depositor EDS
% Data completeness (in resolution range)	95.9 (81.45-1.89) 96.0 (81.45-1.89)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.227 , 0.269 (Not available) , 0.244	Depositor DCC
R_{free} test set	4992 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 28.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9433	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 5.79% 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: VVD, ZN, PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.06	0/4517	1.40	3/6156 (0.0%)
1	B	1.03	1/4610 (0.0%)	1.39	5/6283 (0.1%)
All	All	1.05	1/9127 (0.0%)	1.39	8/12439 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	514	PRO	C-O	-5.07	1.17	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	580	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	262	PHE	CA-C-N	5.26	127.64	120.54
1	A	262	PHE	C-N-CA	5.26	127.64	120.54
1	B	350	SER	CA-C-N	5.25	127.32	120.28
1	B	350	SER	C-N-CA	5.25	127.32	120.28
1	A	416	THR	CB-CA-C	5.12	118.57	109.72
1	B	253	TYR	CB-CA-C	5.08	118.48	110.71
1	B	44	SER	O-C-N	5.02	125.69	122.03

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	4417	0	4322	59	1
1	B	4508	0	4424	67	1
2	A	14	0	0	0	0
2	B	14	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	10	0	0	0	0
4	B	10	0	0	1	0
5	A	203	0	0	7	0
5	B	251	0	0	8	0
All	All	9433	0	8746	125	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 7.

All (125) 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:27:CYS:SG	5:B:839:HOH:O	1.93	1.21
1:B:12:THR:HG21	1:B:25:LEU:O	1.66	0.95
1:B:279:THR:HB	1:B:429:MET:HE2	1.63	0.79
1:B:510:VAL:HG21	1:B:541:TYR:CD1	2.18	0.79
1:B:13:SER:O	1:B:44:SER:HA	1.85	0.77
1:B:508:LYS:HD3	5:B:995:HOH:O	1.86	0.75
1:A:584:LYS:NZ	5:A:802:HOH:O	2.18	0.72
1:B:8:CYS:SG	1:B:99:GLY:O	2.50	0.69
1:A:510:VAL:HG21	1:A:541:TYR:CD1	2.28	0.69
1:B:47:PRO:O	5:B:801:HOH:O	2.11	0.68
1:B:129:ARG:O	1:B:129:ARG:HD3	1.93	0.68
1:B:184:GLY:C	1:B:195:ILE:HG22	2.19	0.67
1:B:425:VAL:CG1	1:B:429:MET:HE3	2.26	0.65
1:B:425:VAL:HG12	1:B:429:MET:HE3	1.77	0.65
1:B:8:CYS:SG	1:B:99:GLY:N	2.70	0.65
1:A:368:ALA:O	1:A:393:ALA:HA	1.97	0.65
1:B:474[A]:MET:SD	1:B:495:VAL:HG11	2.37	0.65
1:A:486:SER:OG	1:A:517:SER:OG	2.07	0.64
1:A:275:GLN:O	1:A:395:HIS:ND1	2.29	0.64
1:A:7:LEU:HD13	1:A:103:VAL:HG22	1.80	0.63
1:A:339:ARG:NH2	5:A:808:HOH:O	2.31	0.63
1:A:320:LYS:NZ	5:A:811:HOH:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:LYS:NZ	5:B:807:HOH:O	2.32	0.62
1:A:7:LEU:HD21	1:A:106:PHE:HB2	1.82	0.62
1:A:261:GLU:OE1	1:A:324:TYR:OH	2.12	0.61
1:A:59:ASP:OD1	1:A:61:THR:OG1	2.15	0.61
1:B:7:LEU:HD21	1:B:106:PHE:HB2	1.85	0.59
1:B:278:SER:HB2	1:B:436:MET:HE2	1.83	0.59
1:B:315:ASP:O	1:B:318:CYS:HB2	2.04	0.57
1:B:7:LEU:CD1	1:B:103:VAL:HG22	2.35	0.57
1:A:44:SER:OG	1:A:45:VAL:N	2.37	0.57
1:A:16:CYS:SG	1:A:18:ALA:HB3	2.45	0.57
1:A:277:TYR:HA	1:A:396:TYR:O	2.04	0.57
1:A:64:TYR:O	1:A:70:TYR:HA	2.05	0.56
1:B:474[B]:MET:HG2	1:B:590:LEU:HB2	1.88	0.55
1:A:13:SER:OG	1:A:44:SER:HB2	2.06	0.55
1:A:235:LEU:HD21	1:A:382:TYR:CE2	2.42	0.54
1:B:8:CYS:SG	1:B:99:GLY:CA	2.96	0.54
1:B:333:ILE:HB	1:B:358:CYS:SG	2.48	0.54
1:A:224:TYR:OH	5:A:801:HOH:O	2.07	0.53
1:A:34:VAL:HA	1:A:39:HIS:O	2.08	0.53
1:B:2:VAL:N	5:B:817:HOH:O	2.42	0.53
1:A:194:GLN:O	1:A:196:GLY:N	2.35	0.53
1:B:129:ARG:HD3	1:B:129:ARG:C	2.32	0.52
1:B:277:TYR:HA	1:B:396:TYR:O	2.11	0.51
1:A:327:ILE:HD11	1:A:345:LYS:O	2.09	0.51
1:B:48:TYR:O	5:B:803:HOH:O	2.19	0.51
1:B:8:CYS:SG	1:B:99:GLY:C	2.94	0.51
1:A:367:THR:HA	1:A:392:ARG:O	2.11	0.50
1:A:106:PHE:CE1	1:A:133:PHE:CE2	3.00	0.50
1:A:296:ALA:O	1:A:300:PRO:HA	2.11	0.50
1:A:304:ILE:HG12	1:A:370:ILE:HB	1.93	0.50
1:B:13:SER:HB2	1:B:92:LEU:HB2	1.94	0.49
1:B:323:LYS:O	1:B:323:LYS:HG2	2.13	0.49
1:A:4:ALA:O	1:A:24:PHE:HB2	2.13	0.48
1:A:519:ASN:HB3	1:A:530:THR:HG23	1.95	0.48
1:B:167:TRP:CZ3	1:B:174:PRO:HD2	2.48	0.48
1:B:28:LYS:O	1:B:32:ASP:OD1	2.30	0.48
1:A:20:ILE:HG22	5:A:888:HOH:O	2.13	0.48
1:B:252:LEU:HB3	1:B:299:TYR:CD1	2.49	0.48
1:B:249:ILE:HG23	1:B:273:GLY:HA3	1.96	0.47
1:A:512:ILE:O	1:A:546:PHE:HA	2.15	0.47
1:A:561:PHE:CZ	1:A:585:LEU:HD21	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ARG:HG3	1:B:24:PHE:CD2	2.50	0.47
1:B:103:VAL:CG1	1:B:103:VAL:O	2.63	0.47
1:B:371:VAL:HG23	1:B:393:ALA:HB2	1.96	0.47
1:B:401:ASP:OD2	1:B:457:TYR:OH	2.24	0.47
1:A:361:ASN:OD1	5:A:803:HOH:O	2.21	0.46
1:B:477:LYS:NZ	1:B:551:GLU:OE2	2.40	0.46
1:A:280:LEU:HD11	1:A:438:LEU:HG	1.98	0.46
1:A:35:ILE:O	1:A:35:ILE:HG12	2.16	0.46
1:A:48:TYR:OH	1:A:90:PHE:O	2.23	0.46
1:A:12:THR:HG21	1:A:25:LEU:O	2.15	0.46
1:B:35:ILE:C	1:B:35:ILE:HD12	2.41	0.46
1:B:147:LEU:HD21	1:B:229:SER:OG	2.16	0.46
1:A:445:PRO:HD2	1:A:448:ILE:HD12	1.98	0.46
1:B:195:ILE:HG23	1:B:195:ILE:O	2.15	0.46
1:A:261:GLU:OE1	1:A:324:TYR:CZ	2.69	0.45
1:B:59:ASP:OD1	1:B:59:ASP:C	2.59	0.45
1:A:331:SER:HB2	1:A:353:GLU:HG3	1.98	0.45
1:B:234:PRO:CD	1:A:352:LEU:HD11	2.46	0.45
1:B:61:THR:HG22	1:B:84:CYS:SG	2.57	0.44
1:A:19:CYS:HB2	1:A:23:PRO:HD2	1.99	0.44
1:A:278:SER:HB2	1:A:436:MET:HE2	1.97	0.44
1:B:13:SER:O	1:B:44:SER:CA	2.63	0.44
1:B:357:PHE:CD1	1:B:357:PHE:N	2.86	0.44
1:B:510:VAL:HG21	1:B:541:TYR:CG	2.53	0.44
1:A:331:SER:HA	1:A:347:LYS:O	2.18	0.44
1:B:124:ASN:OD1	1:B:381:ASN:ND2	2.48	0.43
1:B:19:CYS:HB2	1:B:23:PRO:HD2	2.00	0.43
1:B:376:ILE:HG22	1:B:400:GLY:HA3	1.99	0.43
1:B:373:PHE:CE1	1:B:387:VAL:HG21	2.54	0.43
1:A:163:LEU:HD23	1:A:211:TYR:CD2	2.53	0.43
1:B:48:TYR:OH	1:B:90:PHE:O	2.30	0.43
1:B:57:VAL:HG12	1:B:63:LEU:HD21	2.00	0.43
1:A:512:ILE:HA	1:A:531:GLN:O	2.18	0.43
1:B:177:ASN:C	5:B:895:HOH:O	2.61	0.42
1:A:60:VAL:HB	5:A:929:HOH:O	2.20	0.42
1:B:516:ASN:ND2	5:B:831:HOH:O	2.52	0.42
1:A:276:LYS:O	1:A:395:HIS:HA	2.20	0.42
1:A:329:LYS:HE2	1:A:354:GLN:OE1	2.19	0.42
1:A:333:ILE:HB	1:A:358:CYS:SG	2.59	0.42
1:B:378:MET:O	1:B:407:ALA:HB2	2.20	0.42
1:A:351:THR:HG23	1:A:364:PRO:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:GLN:NE2	4:B:706:PO4:O2	2.47	0.42
1:B:12:THR:CG2	1:B:26:CYS:HA	2.50	0.42
1:B:455:LEU:HG	1:B:456:VAL:HG13	2.02	0.42
1:B:284:PRO:HG2	1:B:566:THR:HG21	2.02	0.41
1:B:505:ALA:O	1:B:508:LYS:HG2	2.20	0.41
1:B:518:GLN:HA	1:B:518:GLN:OE1	2.20	0.41
1:B:7:LEU:HD12	1:B:103:VAL:HG22	2.02	0.41
1:B:303:ARG:NH2	1:B:366:THR:OG1	2.53	0.41
1:A:303:ARG:NH1	1:A:353:GLU:O	2.53	0.41
1:B:103:VAL:O	1:B:103:VAL:HG13	2.21	0.41
1:A:275:GLN:O	1:A:395:HIS:CE1	2.73	0.41
1:A:490:ARG:HB2	1:A:491:PRO:HD3	2.03	0.41
1:B:115:THR:HA	1:B:411:LEU:O	2.20	0.41
1:A:12:THR:HG22	1:A:14:LEU:H	1.86	0.41
1:A:519:ASN:HB3	1:A:530:THR:CG2	2.51	0.41
1:A:533:VAL:HG11	1:A:560:ARG:O	2.21	0.41
1:A:353:GLU:OE2	1:A:353:GLU:HA	2.21	0.41
1:A:480:ILE:HG21	1:A:550:THR:HG22	2.03	0.41
1:A:486:SER:CB	1:A:517:SER:OG	2.70	0.40
1:B:544:VAL:O	1:B:572:ILE:HA	2.21	0.40
1:A:278:SER:HB2	1:A:436:MET:CE	2.51	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)
1:B:442:ARG:NH1	1:A:501:THR:O[1_666]	2.13	0.07

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	564/601 (94%)	528 (94%)	31 (6%)	5 (1%)	14	6
1	B	580/601 (96%)	545 (94%)	34 (6%)	1 (0%)	43	36
All	All	1144/1202 (95%)	1073 (94%)	65 (6%)	6 (0%)	24	16

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	ILE
1	A	218	LYS
1	A	484	VAL
1	A	228	THR
1	A	45	VAL
1	B	195	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	252/523 (48%)	243 (96%)	9 (4%)	31	23
1	B	167/523 (32%)	163 (98%)	4 (2%)	43	38
All	All	419/1046 (40%)	406 (97%)	13 (3%)	35	29

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	69	SER
1	B	155	ARG
1	B	160	ASP
1	B	164	HIS
1	A	12	THR
1	A	35	ILE
1	A	44	SER
1	A	46	ASN
1	A	51	ASN
1	A	127	THR

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Mol	Chain	Res	Type
1	A	156	GLU
1	A	236	SER
1	A	485	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	46	ASN
1	B	88	GLN
1	B	516	ASN
1	A	179	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\# Z > 2$
4	PO4	A	706	-	4,4,4	1.38	0	6,6,6	0.48	0
2	VVD	A	701	-	14,14,14	0.56	0	19,19,19	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	VVD	B	701	-	14,14,14	0.69	0	19,19,19	0.59	0
4	PO4	B	705	-	4,4,4	0.54	0	6,6,6	0.57	0
4	PO4	A	705	-	4,4,4	0.83	0	6,6,6	0.48	0
4	PO4	B	706	-	4,4,4	1.38	1 (25%)	6,6,6	0.64	0

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	VVD	A	701	-	-	6/8/8/8	0/1/1/1
2	VVD	B	701	-	-	2/8/8/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	706	PO4	P-O3	-2.18	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	VVD	C1-C2-N1-C3
2	B	701	VVD	O1-C2-N1-C3
2	A	701	VVD	C6-C7-C9-O2
2	A	701	VVD	C6-C7-C9-O3
2	A	701	VVD	C4-C3-N1-C2
2	A	701	VVD	C8-C7-C9-O3
2	A	701	VVD	C8-C7-C9-O2
2	A	701	VVD	C8-C3-N1-C2

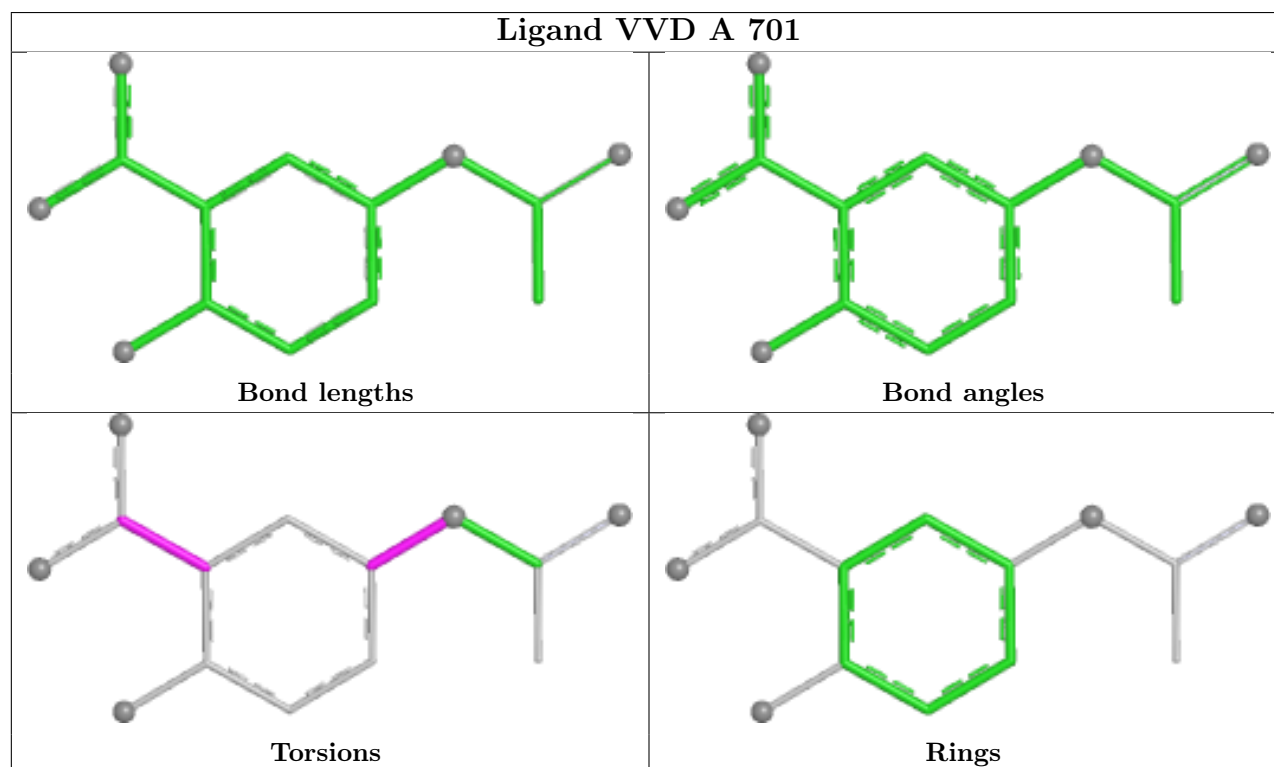
There are no ring outliers.

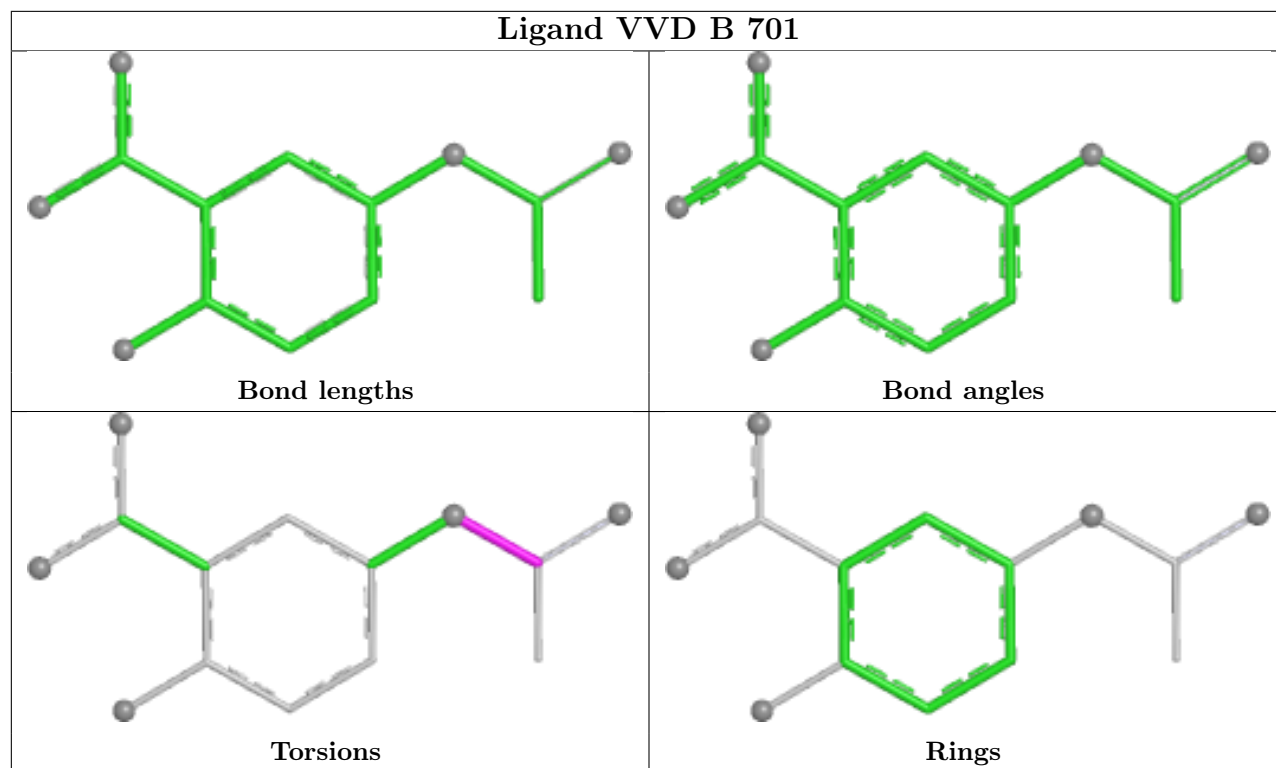
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	706	PO4	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	572/601 (95%)	1.60	200 (34%) 1 0	24, 50, 134, 175	0
1	B	585/601 (97%)	0.81	95 (16%) 4 4	6, 39, 84, 131	7 (1%)
All	All	1157/1202 (96%)	1.20	295 (25%) 1 1	6, 45, 114, 175	7 (0%)

All (295) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	219	LEU	7.6
1	A	592	ILE	7.5
1	B	127	THR	7.5
1	A	152	ALA	7.4
1	A	149	TYR	7.4
1	A	229	SER	7.2
1	B	126	CYS	7.1
1	B	193	VAL	6.8
1	A	151	ILE	6.6
1	A	209	VAL	6.5
1	A	169	VAL	6.4
1	B	474[A]	MET	6.4
1	A	7	LEU	6.4
1	B	130	LEU	6.2
1	A	181	VAL	6.0
1	A	210	VAL	5.8
1	A	247	VAL	5.7
1	A	6	VAL	5.4
1	A	170	GLY	5.4
1	A	179	ASN	5.4
1	A	167	TRP	5.4
1	A	336	ALA	5.4
1	A	81	PHE	5.3
1	A	208	ALA	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	185	TYR	5.2
1	A	226	VAL	5.2
1	A	227	LEU	5.2
1	B	45	VAL	5.2
1	A	176	LEU	5.0
1	A	217	TYR	5.0
1	A	158	LEU	5.0
1	B	131	LYS	5.0
1	A	45	VAL	4.9
1	A	221	VAL	4.9
1	A	224	TYR	4.9
1	B	203	GLY	4.8
1	B	129	ARG	4.8
1	A	305	VAL	4.7
1	B	2	VAL	4.7
1	A	154	VAL	4.7
1	B	214	THR	4.7
1	A	200	PHE	4.6
1	B	97	CYS	4.6
1	A	222	GLY	4.6
1	B	217	TYR	4.5
1	A	352	LEU	4.5
1	A	145	PHE	4.5
1	A	195	ILE	4.5
1	A	256	LEU	4.5
1	A	153	THR	4.5
1	A	387	VAL	4.4
1	B	195	ILE	4.4
1	A	94	LYS	4.3
1	A	103	VAL	4.2
1	B	340	VAL	4.2
1	A	180	TYR	4.2
1	A	25	LEU	4.2
1	A	157	VAL	4.1
1	B	53	PRO	4.1
1	A	334	ILE	4.1
1	A	165	LEU	4.1
1	A	12	THR	4.0
1	B	79	ILE	4.0
1	A	232	VAL	4.0
1	B	128	GLU	4.0
1	B	592	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	300	PRO	4.0
1	A	215	THR	3.9
1	A	230	HIS	3.9
1	B	78	PRO	3.9
1	B	593	PRO	3.9
1	A	225	PHE	3.9
1	A	202	LYS	3.9
1	B	198	TYR	3.9
1	A	198	TYR	3.9
1	A	43	LEU	3.9
1	A	127	THR	3.9
1	A	296	ALA	3.9
1	A	178	ARG	3.8
1	A	258	ILE	3.8
1	B	6	VAL	3.8
1	B	102	ASN	3.7
1	A	177	ASN	3.7
1	B	219	LEU	3.7
1	B	194	GLN	3.6
1	A	8	CYS	3.6
1	B	218	LYS	3.6
1	A	155	ARG	3.6
1	A	326	PRO	3.6
1	B	208	ALA	3.6
1	B	187	VAL	3.6
1	A	132	LEU	3.6
1	B	196	GLY	3.6
1	A	164	HIS	3.6
1	A	356	VAL	3.6
1	A	257	ASN	3.5
1	A	199	THR	3.5
1	B	98	VAL	3.5
1	B	336	ALA	3.5
1	A	27	CYS	3.5
1	A	362	ALA	3.5
1	B	12	THR	3.5
1	A	241	VAL	3.5
1	B	96	THR	3.4
1	A	146	LYS	3.4
1	A	92	LEU	3.4
1	A	304	ILE	3.4
1	A	370	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	147	LEU	3.4
1	A	231	THR	3.4
1	A	246	TYR	3.4
1	A	328	ASP	3.4
1	A	42	VAL	3.4
1	B	176	LEU	3.4
1	A	182	PHE	3.4
1	A	311	HIS	3.3
1	A	306	TYR	3.3
1	A	163	LEU	3.3
1	B	81	PHE	3.3
1	A	335	PRO	3.3
1	B	52	ALA	3.3
1	A	253	TYR	3.3
1	A	333	ILE	3.3
1	A	1	ALA	3.3
1	A	183	THR	3.3
1	A	216	THR	3.3
1	B	4	ALA	3.2
1	A	235	LEU	3.2
1	A	214	THR	3.2
1	A	348	VAL	3.2
1	A	144	THR	3.1
1	A	312	ALA	3.1
1	A	361	ASN	3.1
1	A	254	PRO	3.1
1	A	14	LEU	3.1
1	A	166	SER	3.1
1	B	57	VAL	3.1
1	A	223	ASP	3.1
1	A	90	PHE	3.1
1	B	68	MET	3.1
1	A	340	VAL	3.1
1	A	372	VAL	3.1
1	A	228	THR	3.1
1	B	67	GLY	3.1
1	A	374	ASP	3.0
1	A	2	VAL	3.0
1	A	49	VAL	3.0
1	A	268	ASN	3.0
1	A	307	THR	3.0
1	A	218	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	212	ARG	3.0
1	B	221	VAL	2.9
1	A	211	TYR	2.9
1	A	484	VAL	2.9
1	A	35	ILE	2.9
1	B	54	GLY	2.9
1	B	181	VAL	2.9
1	A	371	VAL	2.9
1	B	180	TYR	2.9
1	A	396	TYR	2.9
1	A	357	PHE	2.9
1	B	8	CYS	2.9
1	A	29	CYS	2.9
1	B	215	THR	2.8
1	A	18	ALA	2.8
1	A	133	PHE	2.8
1	B	159	SER	2.8
1	A	150	GLY	2.8
1	A	416	THR	2.8
1	A	174	PRO	2.8
1	B	211	TYR	2.8
1	A	350	SER	2.8
1	A	24	PHE	2.8
1	A	524	LYS	2.8
1	B	158	LEU	2.8
1	B	256	LEU	2.8
1	A	297	LEU	2.8
1	A	172	PRO	2.8
1	A	16	CYS	2.7
1	A	366	THR	2.7
1	B	92	LEU	2.7
1	A	308	ALA	2.7
1	B	163	LEU	2.7
1	A	330	CYS	2.7
1	A	337	ARG	2.7
1	A	325	LEU	2.7
1	B	179	ASN	2.7
1	A	329	LYS	2.7
1	A	4	ALA	2.6
1	A	508	LYS	2.6
1	B	352	LEU	2.6
1	B	101	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	338	ALA	2.6
1	B	413	THR	2.6
1	B	212	ARG	2.6
1	A	156	GLU	2.6
1	B	26	CYS	2.5
1	A	19	CYS	2.5
1	A	48	TYR	2.5
1	A	13	SER	2.5
1	A	44	SER	2.5
1	A	161	ARG	2.5
1	A	303	ARG	2.5
1	A	507	ARG	2.5
1	A	355	TYR	2.5
1	B	414	LYS	2.5
1	B	7	LEU	2.5
1	A	363	LEU	2.5
1	B	257	ASN	2.5
1	A	266	VAL	2.5
1	B	5	CYS	2.5
1	A	358	CYS	2.5
1	A	93	TYR	2.5
1	A	3	GLY	2.5
1	A	91	GLY	2.5
1	A	339	ARG	2.5
1	A	360	VAL	2.5
1	A	397	VAL	2.5
1	A	28	LYS	2.5
1	A	220	ASN	2.4
1	A	299	TYR	2.4
1	B	145	PHE	2.4
1	A	346	PHE	2.4
1	A	11	GLN	2.4
1	B	199	THR	2.4
1	B	49	VAL	2.4
1	B	103	VAL	2.4
1	A	87	GLY	2.4
1	A	411	LEU	2.4
1	B	190	ASN	2.4
1	A	194	GLN	2.4
1	A	207	ASP	2.4
1	B	229	SER	2.4
1	B	227	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	15	ARG	2.3
1	B	188	THR	2.3
1	B	197	GLU	2.3
1	A	591	GLU	2.3
1	A	278	SER	2.3
1	A	314	VAL	2.3
1	A	341	GLU	2.3
1	B	185	TYR	2.3
1	A	389	ALA	2.3
1	A	41	LEU	2.3
1	A	104	THR	2.3
1	A	373	PHE	2.3
1	A	23	PRO	2.3
1	A	302	ALA	2.3
1	A	84	CYS	2.3
1	A	130	LEU	2.3
1	A	250	THR	2.3
1	B	178	ARG	2.2
1	A	277	TYR	2.2
1	A	364	PRO	2.2
1	A	89	VAL	2.2
1	B	161	ARG	2.2
1	B	14	LEU	2.2
1	A	175	PRO	2.2
1	A	415	GLY	2.2
1	B	516	ASN	2.2
1	A	171	LYS	2.2
1	A	342	CYS	2.2
1	B	46	ASN	2.2
1	B	75	HIS	2.2
1	B	231	THR	2.2
1	A	30	CYS	2.2
1	B	213	GLY	2.2
1	B	498	GLU	2.1
1	A	20	ILE	2.1
1	B	44	SER	2.1
1	A	323	LYS	2.1
1	A	86	ASN	2.1
1	A	31	TYR	2.1
1	A	293	ILE	2.1
1	A	525	ILE	2.1
1	B	10	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	66	GLY	2.1
1	A	196	GLY	2.1
1	B	25	LEU	2.1
1	B	35	ILE	2.1
1	B	160	ASP	2.1
1	A	21	ARG	2.1
1	A	173	ARG	2.1
1	B	230	HIS	2.1
1	A	391	LEU	2.1
1	A	140	ALA	2.1
1	B	94	LYS	2.0
1	B	162	GLU	2.0
1	B	182	PHE	2.0
1	B	334	ILE	2.0
1	B	157	VAL	2.0
1	A	343	PHE	2.0
1	A	58	THR	2.0
1	A	298	TYR	2.0
1	B	47	PRO	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	VVD	A	701	14/14	0.78	0.13	52,59,64,66	0
2	VVD	B	701	14/14	0.81	0.17	71,82,94,96	0
4	PO4	B	705	5/5	0.94	0.08	38,40,42,44	0
3	ZN	A	703	1/1	0.96	0.06	54,54,54,54	0

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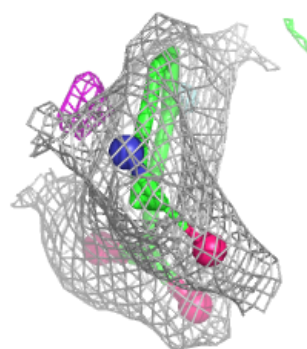
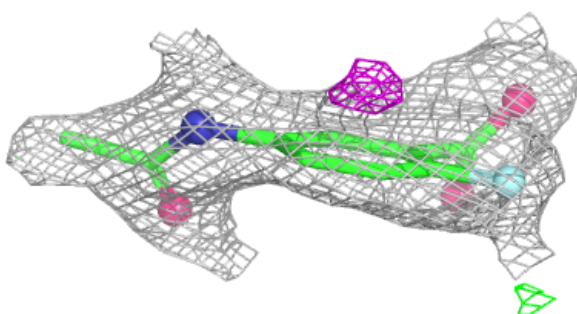
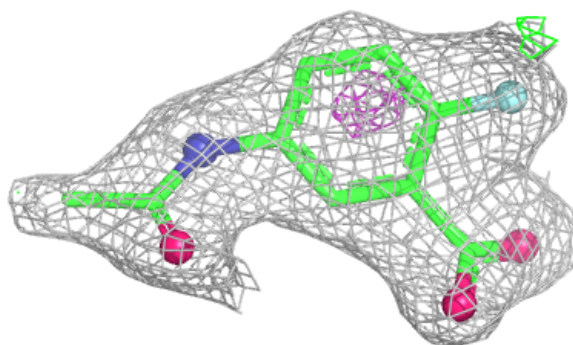
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PO4	B	706	5/5	0.96	0.08	35,36,38,49	0
3	ZN	B	703	1/1	0.97	0.05	52,52,52,52	0
3	ZN	A	704	1/1	0.97	0.05	79,79,79,79	0
3	ZN	B	704	1/1	0.98	0.05	72,72,72,72	0
4	PO4	A	705	5/5	0.98	0.06	34,35,40,41	0
4	PO4	A	706	5/5	0.98	0.06	30,36,38,43	0
3	ZN	B	702	1/1	0.99	0.02	36,36,36,36	0
3	ZN	A	702	1/1	0.99	0.03	44,44,44,44	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.

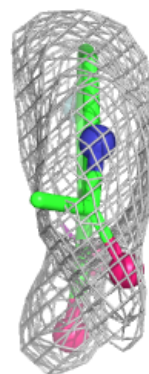
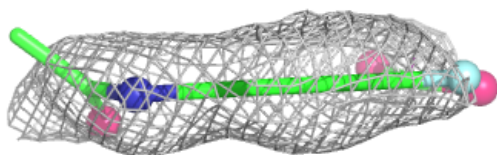
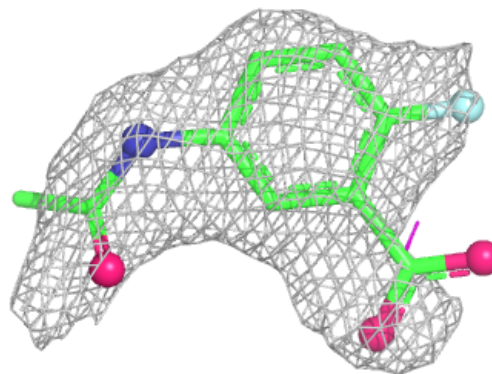
Electron density around VVD A 701:

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 VVD B 701:

$2mF_o-DF_c$ (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.