



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:48 AM UTC

PDB ID : 5RLG / pdb_00005rlg
Title : PanDDA analysis group deposition – Crystal Structure of SARS-CoV-2 heli-
case in complex with Z19739650
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 : 1.96 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)

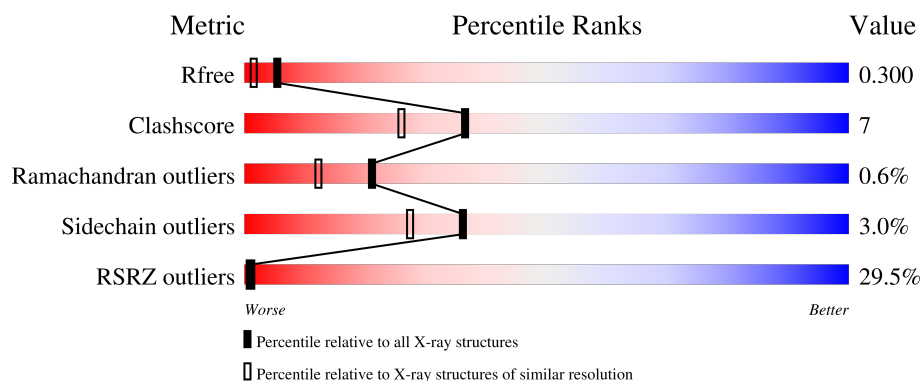
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	38% 76% 19% 5%
1	B	601	19% 81% 14% 5%

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

2 Entry composition [i](#)

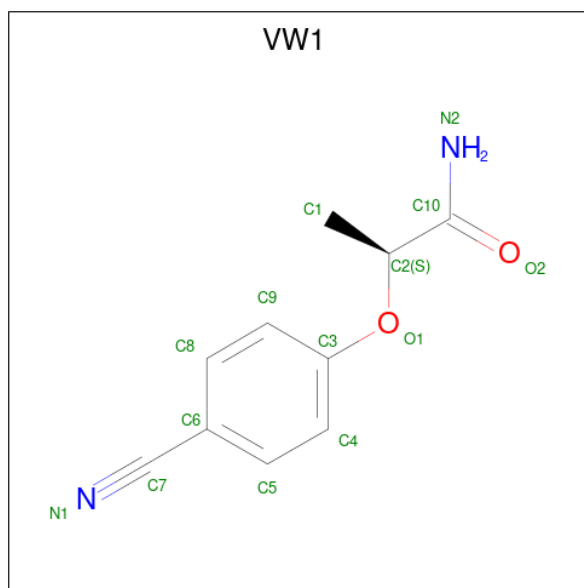
There are 5 unique types of molecules in this entry. The entry contains 9418 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (2S)-2-(4-cyanophenoxy)propanamide (CCD ID: VW1) (formula: $C_{10}H_{10}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	10	2	2		

- 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		

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

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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		

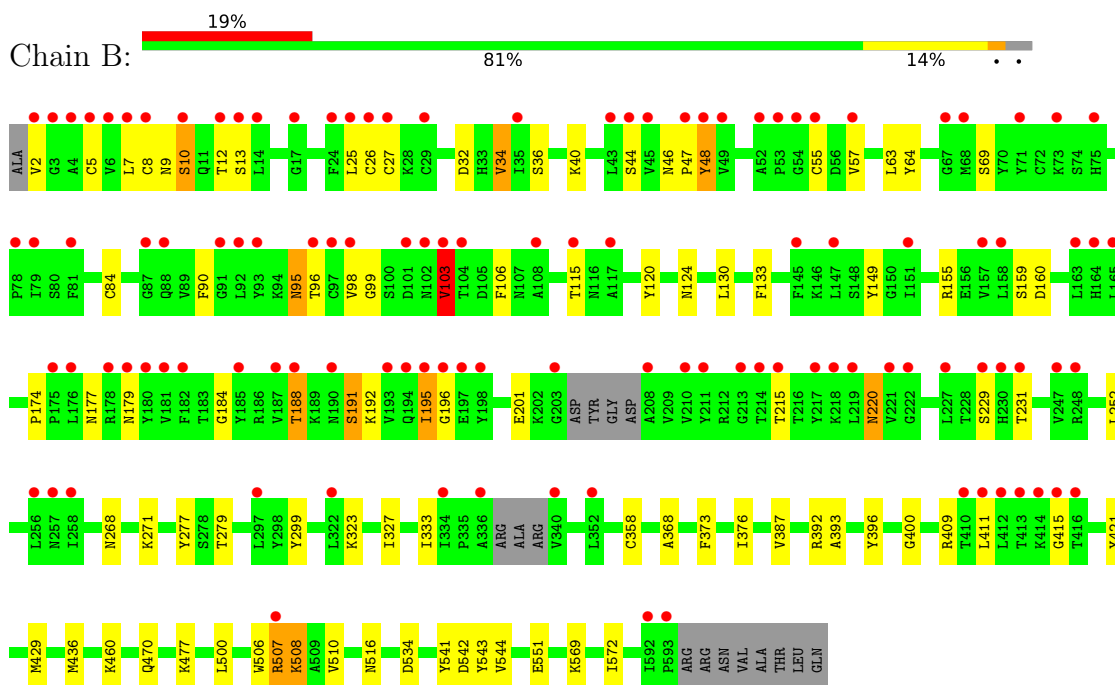
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	250	Total	O	0	0
			250	250		
5	A	203	Total	O	0	0
			203	203		

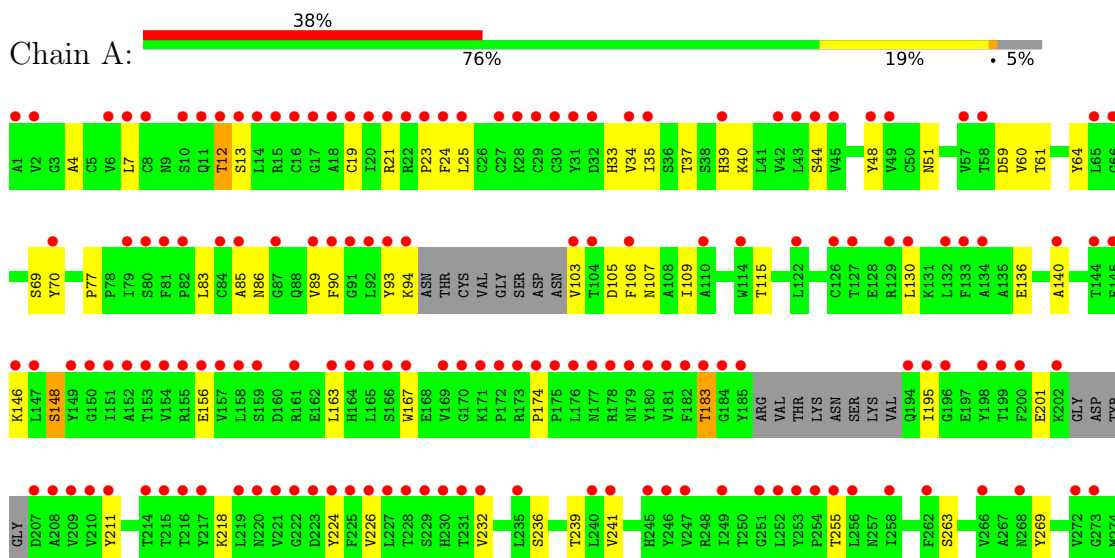
3 Residue-property plots [i](#)

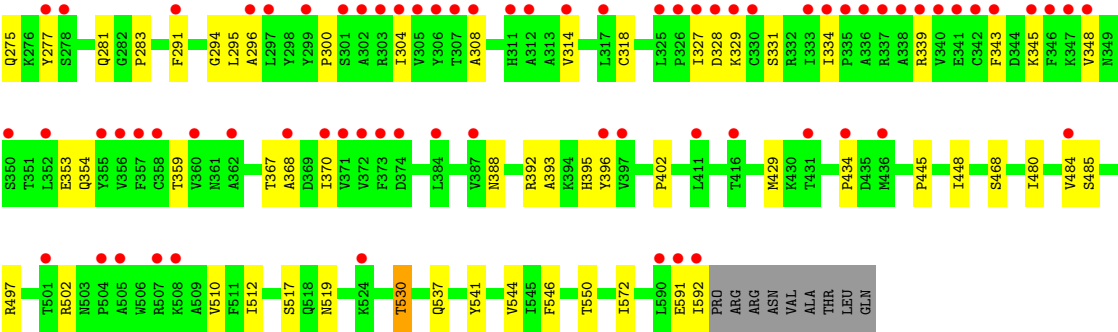
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	59.18Å 70.31Å 85.68Å 103.01° 96.26° 112.07°	Depositor
Resolution (Å)	81.54 – 1.96 81.54 – 1.96	Depositor EDS
% Data completeness (in resolution range)	94.0 (81.54-1.96) 94.1 (81.54-1.96)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.246 , 0.286 0.263 , 0.300	Depositor DCC
R_{free} test set	4460 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 31.6	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	0.93	EDS
Total number of atoms	9418	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, VW1, 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	1.11	0/4517	1.42	3/6156 (0.0%)
1	B	1.06	0/4610	1.37	6/6283 (0.1%)
All	All	1.09	0/9127	1.40	9/12439 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	415	GLY	CA-C-O	-5.71	118.29	122.23
1	B	133	PHE	CA-C-O	-5.50	115.04	120.82
1	B	196	GLY	CA-C-O	-5.49	117.85	122.29
1	A	115	THR	N-CA-C	-5.48	106.64	113.38
1	B	534	ASP	CB-CA-C	5.22	119.46	110.79
1	A	314	VAL	CA-C-N	5.18	128.18	120.31
1	A	314	VAL	C-N-CA	5.18	128.18	120.31
1	B	34	VAL	CA-C-O	-5.06	115.48	120.85
1	B	103	VAL	N-CA-C	-5.00	107.59	112.29

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	4321	61	0
1	B	4508	0	4426	67	0
2	B	14	0	0	5	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	0	0
5	A	203	0	0	11	1
5	B	250	0	0	10	1
All	All	9418	0	8747	128	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 (128) 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:956:HOH:O	1.99	1.15
1:B:47:PRO:O	5:B:801:HOH:O	1.79	1.01
1:A:60:VAL:HB	5:A:920:HOH:O	1.68	0.93
1:B:8:CYS:SG	1:B:99:GLY:N	2.43	0.91
1:B:2:VAL:N	5:B:803:HOH:O	2.03	0.90
1:B:271:LYS:NZ	5:B:802:HOH:O	1.95	0.85
1:A:224:TYR:OH	5:A:801:HOH:O	1.98	0.81
1:B:392:ARG:CB	5:B:1040:HOH:O	2.35	0.74
1:A:368:ALA:O	1:A:393:ALA:HA	1.87	0.73
1:B:12:THR:HG21	1:B:26:CYS:HA	1.69	0.73
1:B:376:ILE:HG22	1:B:400:GLY:HA3	1.71	0.72
1:A:510:VAL:HG21	1:A:541:TYR:CD1	2.26	0.70
1:A:537:GLN:O	5:A:802:HOH:O	2.10	0.69
1:B:508:LYS:HG2	2:B:701:VW1:N1	2.10	0.67
1:B:460:LYS:NZ	5:B:807:HOH:O	2.25	0.65
1:B:12:THR:HG21	1:B:25:LEU:O	1.96	0.65
1:A:334:ILE:HD12	1:A:348:VAL:HG13	1.79	0.65
1:A:13:SER:OG	1:A:44:SER:HB2	1.97	0.65
1:B:12:THR:CG2	1:B:26:CYS:HA	2.27	0.65
1:A:468:SER:O	5:A:803:HOH:O	2.15	0.65
1:A:331:SER:HB2	1:A:353:GLU:HG3	1.79	0.65
1:B:115:THR:HA	1:B:411:LEU:O	1.99	0.63
1:B:510:VAL:HG21	1:B:541:TYR:CD1	2.36	0.61
1:B:48:TYR:OH	1:B:90:PHE:O	2.08	0.60
1:B:201:GLU:OE2	5:B:804:HOH:O	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:SER:O	1:B:44:SER:HA	2.02	0.59
1:A:163:LEU:HD23	1:A:211:TYR:CD2	2.38	0.59
1:B:477:LYS:NZ	1:B:551:GLU:OE2	2.30	0.59
1:A:497:ARG:HG2	5:A:883:HOH:O	2.05	0.57
1:B:7:LEU:HD12	1:B:103:VAL:HG22	1.87	0.57
1:A:367:THR:HA	1:A:392:ARG:O	2.05	0.56
1:B:44:SER:N	1:B:46:ASN:O	2.35	0.56
1:B:8:CYS:SG	1:B:99:GLY:O	2.64	0.55
1:A:480:ILE:HG12	1:A:550:THR:HG22	1.88	0.55
1:B:184:GLY:C	1:B:195:ILE:HG22	2.31	0.55
1:A:269:TYR:OH	1:A:294:GLY:HA3	2.07	0.54
1:B:7:LEU:CD1	1:B:103:VAL:HG22	2.38	0.54
1:A:7:LEU:HD13	1:A:103:VAL:HG22	1.89	0.54
1:A:519:ASN:HB3	1:A:530:THR:HG23	1.90	0.54
1:A:140:ALA:HA	1:A:232:VAL:HG21	1.90	0.53
1:A:269:TYR:CD1	1:A:295:LEU:HD13	2.44	0.53
1:B:508:LYS:HG2	2:B:701:VW1:C7	2.40	0.52
1:B:252:LEU:HB3	1:B:299:TYR:CD1	2.44	0.52
1:B:508:LYS:CG	2:B:701:VW1:N1	2.72	0.52
1:A:93:TYR:O	1:A:94:LYS:O	2.27	0.52
1:B:188:THR:HG1	1:B:191:SER:H	1.59	0.51
1:B:279:THR:HB	1:B:429:MET:HE2	1.93	0.51
1:B:277:TYR:HA	1:B:396:TYR:O	2.11	0.50
1:A:4:ALA:O	1:A:24:PHE:HB2	2.12	0.50
1:B:34:VAL:O	1:B:40:LYS:NZ	2.37	0.50
1:B:103:VAL:CG1	1:B:103:VAL:O	2.59	0.50
1:B:323:LYS:O	1:B:323:LYS:HG2	2.11	0.50
1:A:130:LEU:HD12	5:A:874:HOH:O	2.11	0.50
1:B:177:ASN:HB3	1:B:516:ASN:ND2	2.26	0.50
1:A:277:TYR:HA	1:A:396:TYR:O	2.12	0.49
1:B:220:ASN:N	1:B:220:ASN:OD1	2.45	0.49
1:A:519:ASN:HB3	1:A:530:THR:CG2	2.42	0.49
1:A:296:ALA:O	1:A:300:PRO:HA	2.13	0.49
1:B:506:TRP:HA	2:B:701:VW1:N1	2.28	0.48
1:A:304:ILE:HG12	1:A:370:ILE:HB	1.95	0.48
1:A:291:PHE:C	1:A:291:PHE:CD1	2.92	0.47
1:B:279:THR:HB	1:B:429:MET:CE	2.45	0.47
1:B:368:ALA:O	1:B:393:ALA:HA	2.15	0.47
1:B:500:LEU:HB3	1:B:507:ARG:HD2	1.97	0.47
1:B:120:TYR:CE2	1:B:409:ARG:HG2	2.50	0.46
1:A:318:CYS:HB3	1:A:343:PHE:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LEU:O	1:A:89:VAL:HA	2.16	0.46
1:A:269:TYR:OH	1:A:294:GLY:C	2.59	0.46
1:B:32:ASP:O	1:B:36:SER:OG	2.23	0.46
1:A:329:LYS:HE2	1:A:354:GLN:OE1	2.16	0.46
1:B:551:GLU:HG3	5:B:938:HOH:O	2.15	0.45
1:A:241:VAL:HG12	5:A:999:HOH:O	2.16	0.45
1:B:7:LEU:HD21	1:B:106:PHE:HB2	1.99	0.45
1:B:7:LEU:CD2	1:B:130:LEU:HD21	2.47	0.45
1:B:8:CYS:SG	1:B:98:VAL:HB	2.57	0.45
1:B:506:TRP:HA	2:B:701:VW1:C7	2.47	0.45
1:A:591:GLU:O	1:A:592:ILE:HB	2.17	0.45
1:A:445:PRO:HD2	1:A:448:ILE:HD12	1.98	0.45
1:A:34:VAL:O	1:A:40:LYS:NZ	2.35	0.44
1:A:7:LEU:HD21	1:A:106:PHE:HB2	2.00	0.44
1:A:77:PRO:HB2	5:A:914:HOH:O	2.17	0.44
1:A:512:ILE:O	1:A:546:PHE:HA	2.17	0.44
1:A:183:THR:N	1:A:226:VAL:O	2.40	0.44
1:A:239:THR:O	1:A:388:ASN:ND2	2.51	0.44
1:B:9:ASN:O	1:B:10:SER:C	2.61	0.44
1:B:159:SER:OG	1:B:160:ASP:O	2.35	0.44
1:B:333:ILE:HB	1:B:358:CYS:SG	2.58	0.44
1:A:48:TYR:OH	1:A:90:PHE:O	2.23	0.44
1:A:339:ARG:NH2	5:A:828:HOH:O	2.50	0.43
1:A:105:ASP:O	1:A:109:ILE:HG13	2.17	0.43
1:A:59:ASP:OD1	1:A:61:THR:OG1	2.35	0.43
1:A:269:TYR:OH	1:A:294:GLY:CA	2.66	0.43
1:A:308:ALA:O	1:A:359:THR:HA	2.19	0.43
1:A:281:GLN:HG3	1:A:402:PRO:HD2	2.01	0.43
1:A:327:ILE:HD11	1:A:345:LYS:O	2.19	0.42
1:A:85:ALA:O	1:A:86:ASN:C	2.62	0.42
1:B:268:ASN:ND2	1:B:436:MET:HG2	2.34	0.42
1:A:12:THR:HG21	1:A:25:LEU:O	2.19	0.42
1:A:37:THR:OG1	1:A:39:HIS:HB2	2.18	0.42
1:A:328:ASP:HA	5:A:870:HOH:O	2.20	0.42
1:A:64:TYR:O	1:A:70:TYR:HA	2.19	0.42
1:A:544:VAL:O	1:A:572:ILE:HA	2.20	0.42
1:B:470:GLN:NE2	1:B:543:TYR:OH	2.53	0.42
1:B:106:PHE:CD2	1:B:106:PHE:C	2.98	0.42
1:B:7:LEU:HD21	1:B:130:LEU:HD21	2.02	0.41
1:B:95:ASN:OD1	1:B:95:ASN:N	2.48	0.41
1:B:516:ASN:ND2	5:B:833:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ARG:NE	1:A:136:GLU:OE2	2.47	0.41
1:A:167:TRP:CZ3	1:A:174:PRO:HD2	2.55	0.41
1:B:149:TYR:HB3	1:B:174:PRO:HD3	2.02	0.41
1:B:542:ASP:OD1	1:B:569:LYS:HE3	2.20	0.41
1:A:19:CYS:HB2	1:A:23:PRO:HD2	2.01	0.41
1:B:5:CYS:HB2	1:B:26:CYS:HB3	2.03	0.41
1:B:124:ASN:HD22	1:B:421:TYR:HA	1.85	0.41
1:B:373:PHE:CE1	1:B:387:VAL:HG21	2.56	0.41
1:A:146:LYS:C	1:A:148:SER:H	2.29	0.41
1:B:55:CYS:SG	1:B:57:VAL:HG23	2.60	0.41
1:A:33:HIS:HA	1:A:107:ASN:OD1	2.21	0.41
1:B:179:ASN:HD22	1:B:179:ASN:HA	1.76	0.41
1:B:195:ILE:O	1:B:195:ILE:HG23	2.21	0.41
1:B:544:VAL:O	1:B:572:ILE:HA	2.21	0.41
1:B:48:TYR:CZ	1:B:90:PHE:O	2.74	0.41
1:B:8:CYS:SG	1:B:99:GLY:CA	3.08	0.40
1:A:429:MET:HG2	1:A:434:PRO:HB3	2.03	0.40
1:B:63:LEU:C	1:B:64:TYR:CD1	2.99	0.40
1:A:275:GLN:O	1:A:395:HIS:ND1	2.48	0.40
1:A:263:SER:N	5:A:830:HOH:O	2.53	0.40
1:B:84:CYS:HB3	5:B:929:HOH:O	2.20	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)
5:B:1021:HOH:O	5:A:835:HOH:O[1_556]	2.09	0.11

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	564/601 (94%)	528 (94%)	32 (6%)	4 (1%)	18	10
1	B	580/601 (96%)	540 (93%)	37 (6%)	3 (0%)	24	16
All	All	1144/1202 (95%)	1068 (93%)	69 (6%)	7 (1%)	21	12

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	ILE
1	A	218	LYS
1	A	484	VAL
1	B	10	SER
1	B	48	TYR
1	A	283	PRO
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	485/523 (93%)	471 (97%)	14 (3%)	37	29
1	B	498/523 (95%)	483 (97%)	15 (3%)	36	27
All	All	983/1046 (94%)	954 (97%)	29 (3%)	36	27

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	69	SER
1	B	95	ASN
1	B	96	THR
1	B	103	VAL
1	B	155	ARG
1	B	188	THR
1	B	191	SER
1	B	192	LYS
1	B	215	THR

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Mol	Chain	Res	Type
1	B	220	ASN
1	B	229	SER
1	B	231	THR
1	B	327	ILE
1	B	507	ARG
1	B	508	LYS
1	A	12	THR
1	A	35	ILE
1	A	51	ASN
1	A	69	SER
1	A	148	SER
1	A	156	GLU
1	A	183	THR
1	A	201	GLU
1	A	236	SER
1	A	255	THR
1	A	485	SER
1	A	502	ARG
1	A	517	SER
1	A	530	THR

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

Mol	Chain	Res	Type
1	B	46	ASN
1	B	51	ASN
1	B	179	ASN
1	B	245	HIS
1	B	268	ASN
1	B	404	GLN
1	B	459	ASN
1	B	470	GLN
1	B	516	ASN
1	A	11	GLN
1	A	86	ASN
1	A	177	ASN
1	A	275	GLN
1	A	586	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 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	705	-	4,4,4	1.14	0	6,6,6	0.62	0
4	PO4	A	704	-	4,4,4	0.69	0	6,6,6	0.70	0
4	PO4	B	705	-	4,4,4	1.40	1 (25%)	6,6,6	0.35	0
4	PO4	B	706	-	4,4,4	1.21	0	6,6,6	0.57	0
2	VW1	B	701	-	14,14,14	0.24	0	18,18,18	0.71	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	VW1	B	701	-	-	0/10/10/10	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	705	PO4	P-O1	2.11	1.55	1.50

There are no bond angle outliers.

There are no chirality outliers.

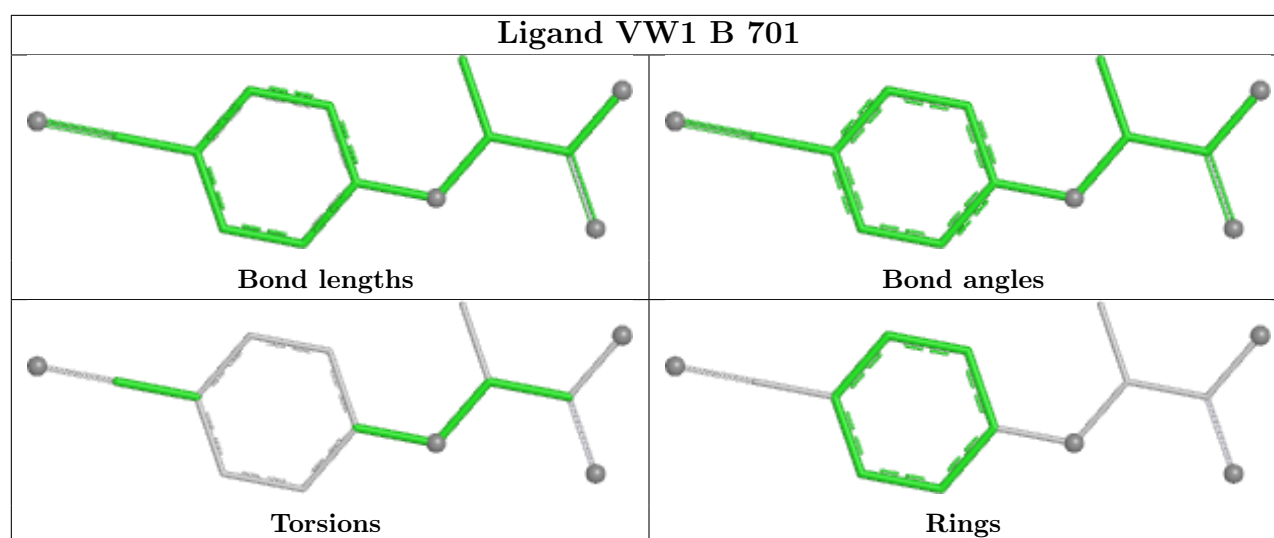
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	VW1	5	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 ⓘ

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

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%)	1.75	227 (39%)	1 0	28, 57, 136, 177	0
1	B	585/601 (97%)	1.07	114 (19%)	3 3	21, 43, 94, 128	1 (0%)
All	All	1157/1202 (96%)	1.41	341 (29%)	1 1	21, 50, 120, 177	1 (0%)

All (341) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	45	VAL	7.4
1	A	169	VAL	6.8
1	A	592	ILE	6.7
1	B	193	VAL	6.5
1	A	152	ALA	6.3
1	A	151	ILE	6.0
1	A	219	LEU	5.9
1	A	225	PHE	5.8
1	B	98	VAL	5.7
1	A	247	VAL	5.7
1	A	185	TYR	5.6
1	A	7	LEU	5.6
1	A	181	VAL	5.6
1	A	167	TRP	5.6
1	B	12	THR	5.5
1	B	2	VAL	5.5
1	A	6	VAL	5.5
1	A	221	VAL	5.4
1	B	214	THR	5.4
1	A	227	LEU	5.3
1	A	81	PHE	5.2
1	A	336	ALA	5.2
1	A	210	VAL	5.2
1	B	14	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	149	TYR	5.1
1	A	208	ALA	5.0
1	B	217	TYR	5.0
1	B	196	GLY	5.0
1	A	200	PHE	4.9
1	A	43	LEU	4.8
1	A	226	VAL	4.8
1	B	592	ILE	4.8
1	A	352	LEU	4.8
1	A	334	ILE	4.7
1	A	195	ILE	4.7
1	B	7	LEU	4.7
1	B	413	THR	4.6
1	A	176	LEU	4.6
1	B	340	VAL	4.5
1	A	182	PHE	4.5
1	A	25	LEU	4.5
1	A	387	VAL	4.4
1	B	97	CYS	4.4
1	B	593	PRO	4.4
1	A	305	VAL	4.3
1	A	1	ALA	4.3
1	A	154	VAL	4.3
1	A	306	TYR	4.3
1	A	217	TYR	4.2
1	A	229	SER	4.2
1	B	57	VAL	4.2
1	A	165	LEU	4.1
1	A	222	GLY	4.1
1	B	415	GLY	4.1
1	A	370	ILE	4.1
1	A	371	VAL	4.1
1	A	224	TYR	4.1
1	A	14	LEU	4.1
1	A	157	VAL	4.0
1	A	209	VAL	4.0
1	A	304	ILE	4.0
1	A	256	LEU	4.0
1	A	45	VAL	4.0
1	B	53	PRO	4.0
1	A	2	VAL	4.0
1	A	92	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	158	LEU	3.9
1	B	195	ILE	3.9
1	A	198	TYR	3.9
1	B	6	VAL	3.9
1	A	12	THR	3.8
1	A	103	VAL	3.8
1	B	102	ASN	3.8
1	B	44	SER	3.8
1	A	174	PRO	3.8
1	A	228	THR	3.8
1	B	81	PHE	3.8
1	A	93	TYR	3.7
1	A	147	LEU	3.7
1	B	203	GLY	3.7
1	B	47	PRO	3.7
1	A	338	ALA	3.7
1	A	180	TYR	3.6
1	A	94	LYS	3.6
1	A	170	GLY	3.6
1	A	235	LEU	3.6
1	A	155	ARG	3.6
1	B	221	VAL	3.6
1	A	397	VAL	3.6
1	A	253	TYR	3.5
1	B	26	CYS	3.5
1	B	101	ASP	3.5
1	A	153	THR	3.5
1	A	258	ILE	3.4
1	A	333	ILE	3.4
1	A	232	VAL	3.4
1	A	348	VAL	3.4
1	A	90	PHE	3.4
1	A	183	THR	3.4
1	A	199	THR	3.4
1	A	214	THR	3.4
1	A	215	THR	3.4
1	A	246	TYR	3.3
1	B	78	PRO	3.3
1	A	396	TYR	3.3
1	A	178	ARG	3.3
1	B	79	ILE	3.3
1	B	103	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	210	VAL	3.3
1	B	163	LEU	3.3
1	B	8	CYS	3.3
1	A	329	LYS	3.3
1	B	336	ALA	3.3
1	A	372	VAL	3.3
1	A	343	PHE	3.3
1	B	414	LYS	3.2
1	A	340	VAL	3.2
1	A	362	ALA	3.2
1	A	241	VAL	3.2
1	A	268	ASN	3.2
1	A	346	PHE	3.2
1	B	96	THR	3.2
1	B	227	LEU	3.2
1	A	145	PHE	3.2
1	A	27	CYS	3.2
1	B	180	TYR	3.1
1	A	355	TYR	3.1
1	B	43	LEU	3.1
1	B	49	VAL	3.1
1	B	334	ILE	3.1
1	A	82	PRO	3.1
1	B	211	TYR	3.1
1	B	256	LEU	3.1
1	A	133	PHE	3.1
1	A	373	PHE	3.1
1	A	184	GLY	3.1
1	A	70	TYR	3.1
1	A	330	CYS	3.1
1	B	52	ALA	3.1
1	A	524	LYS	3.0
1	B	187	VAL	3.0
1	A	89	VAL	3.0
1	A	179	ASN	3.0
1	A	357	PHE	3.0
1	A	164	HIS	3.0
1	A	335	PRO	3.0
1	B	176	LEU	3.0
1	B	181	VAL	3.0
1	B	208	ALA	3.0
1	A	65	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	31	TYR	3.0
1	A	42	VAL	3.0
1	A	202	LYS	3.0
1	B	54	GLY	3.0
1	A	303	ARG	3.0
1	A	505	ALA	3.0
1	A	35	ILE	3.0
1	B	25	LEU	2.9
1	A	277	TYR	2.9
1	A	230	HIS	2.9
1	B	219	LEU	2.9
1	A	223	ASP	2.9
1	A	255	THR	2.9
1	A	172	PRO	2.9
1	B	164	HIS	2.9
1	A	11	GLN	2.9
1	A	79	ILE	2.9
1	B	92	LEU	2.9
1	B	147	LEU	2.9
1	A	297	LEU	2.9
1	A	177	ASN	2.9
1	A	44	SER	2.9
1	B	68	MET	2.9
1	B	151	ILE	2.9
1	B	412	LEU	2.8
1	A	163	LEU	2.8
1	A	411	LEU	2.8
1	A	345	LYS	2.8
1	A	368	ALA	2.8
1	B	27	CYS	2.8
1	A	19	CYS	2.8
1	B	222	GLY	2.8
1	A	132	LEU	2.8
1	A	194	GLN	2.8
1	A	272	VAL	2.8
1	A	207	ASP	2.8
1	A	252	LEU	2.8
1	A	49	VAL	2.8
1	A	311	HIS	2.7
1	A	301	SER	2.7
1	B	257	ASN	2.7
1	B	4	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	91	GLY	2.7
1	B	145	PHE	2.7
1	A	13	SER	2.7
1	A	171	LYS	2.7
1	B	352	LEU	2.7
1	A	166	SER	2.7
1	A	254	PRO	2.7
1	A	28	LYS	2.7
1	A	296	ALA	2.6
1	A	358	CYS	2.6
1	A	231	THR	2.6
1	A	327	ILE	2.6
1	A	15	ARG	2.6
1	A	328	ASP	2.6
1	B	231	THR	2.6
1	A	16	CYS	2.6
1	A	356	VAL	2.6
1	A	127	THR	2.6
1	B	29	CYS	2.6
1	A	30	CYS	2.6
1	B	297	LEU	2.6
1	A	251	GLY	2.6
1	A	140	ALA	2.6
1	A	266	VAL	2.6
1	A	302	ALA	2.6
1	A	211	TYR	2.5
1	B	24	PHE	2.5
1	A	240	LEU	2.5
1	A	249	ILE	2.5
1	A	278	SER	2.5
1	B	48	TYR	2.5
1	B	198	TYR	2.5
1	A	299	TYR	2.5
1	A	374	ASP	2.5
1	A	130	LEU	2.5
1	B	67	GLY	2.5
1	B	35	ILE	2.5
1	A	114	TRP	2.5
1	A	104	THR	2.5
1	B	5	CYS	2.5
1	B	185	TYR	2.5
1	A	384	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	179	ASN	2.5
1	A	161	ARG	2.5
1	A	216	THR	2.5
1	A	29	CYS	2.4
1	B	182	PHE	2.4
1	B	411	LEU	2.4
1	A	122	LEU	2.4
1	B	197	GLU	2.4
1	B	258	ILE	2.4
1	A	144	THR	2.4
1	A	175	PRO	2.4
1	B	158	LEU	2.4
1	B	165	LEU	2.4
1	A	317	LEU	2.4
1	A	24	PHE	2.4
1	B	218	LYS	2.4
1	B	104	THR	2.4
1	B	108	ALA	2.4
1	B	248	ARG	2.4
1	A	337	ARG	2.4
1	A	507	ARG	2.4
1	B	175	PRO	2.4
1	A	23	PRO	2.4
1	A	504	PRO	2.4
1	B	87	GLY	2.4
1	A	84	CYS	2.4
1	A	325	LEU	2.4
1	B	410	THR	2.4
1	A	20	ILE	2.4
1	A	21	ARG	2.4
1	A	22	ARG	2.4
1	A	85	ALA	2.4
1	B	10	SER	2.4
1	A	339	ARG	2.3
1	A	590	LEU	2.3
1	A	18	ALA	2.3
1	A	326	PRO	2.3
1	B	229	SER	2.3
1	A	126	CYS	2.3
1	B	93	TYR	2.3
1	A	307	THR	2.3
1	B	213	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	66	GLY	2.3
1	A	156	GLU	2.3
1	B	190	ASN	2.3
1	B	215	THR	2.3
1	A	48	TYR	2.3
1	A	508	LYS	2.3
1	A	87	GLY	2.3
1	A	32	ASP	2.3
1	B	230	HIS	2.3
1	A	347	LYS	2.3
1	A	17	GLY	2.2
1	A	150	GLY	2.2
1	A	291	PHE	2.2
1	B	88	GLN	2.2
1	A	245	HIS	2.2
1	A	416	THR	2.2
1	A	591	GLU	2.2
1	A	110	ALA	2.2
1	B	507	ARG	2.2
1	A	57	VAL	2.2
1	A	501	THR	2.2
1	A	159	SER	2.2
1	A	350	SER	2.2
1	B	117	ALA	2.2
1	B	247	VAL	2.2
1	A	484	VAL	2.2
1	A	8	CYS	2.2
1	A	146	LYS	2.2
1	A	173	ARG	2.2
1	B	71	TYR	2.1
1	B	55	CYS	2.1
1	A	342	CYS	2.1
1	B	178	ARG	2.1
1	A	436	MET	2.1
1	A	308	ALA	2.1
1	A	312	ALA	2.1
1	A	58	THR	2.1
1	B	3	GLY	2.1
1	B	91	GLY	2.1
1	B	157	VAL	2.1
1	A	360	VAL	2.1
1	B	73	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	341	GLU	2.1
1	B	322	LEU	2.1
1	B	188	THR	2.1
1	B	17	GLY	2.1
1	A	220	ASN	2.1
1	B	194	GLN	2.1
1	A	434	PRO	2.1
1	A	106	PHE	2.0
1	A	262	PHE	2.0
1	B	13	SER	2.0
1	A	80	SER	2.0
1	B	115	THR	2.0
1	B	416	THR	2.0
1	A	431	THR	2.0
1	A	196	GLY	2.0
1	A	314	VAL	2.0
1	A	134	ALA	2.0
1	A	10	SER	2.0
1	B	75	HIS	2.0
1	A	39	HIS	2.0
1	A	273	GLY	2.0
1	A	34	VAL	2.0
1	A	129	ARG	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.

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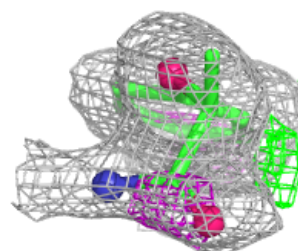
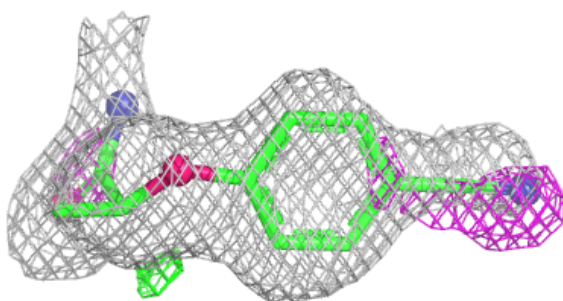
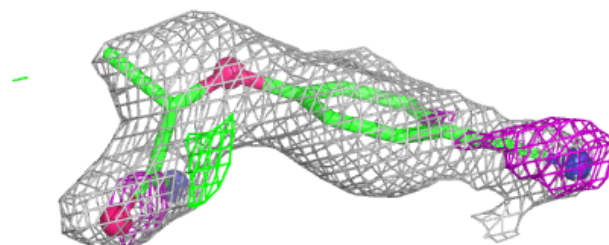
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	VW1	B	701	14/14	0.79	0.12	20,20,20,20	14
4	PO4	B	705	5/5	0.94	0.08	38,39,42,49	0
4	PO4	A	705	5/5	0.94	0.08	34,39,48,49	0
4	PO4	A	704	5/5	0.95	0.07	36,40,42,47	0
4	PO4	B	706	5/5	0.95	0.09	39,40,45,51	0
3	ZN	B	703	1/1	0.96	0.06	59,59,59,59	0
3	ZN	A	703	1/1	0.96	0.05	96,96,96,96	0
3	ZN	A	702	1/1	0.97	0.06	48,48,48,48	0
3	ZN	B	704	1/1	0.97	0.05	76,76,76,76	0
3	ZN	B	702	1/1	0.99	0.02	42,42,42,42	0
3	ZN	A	701	1/1	0.99	0.03	53,53,53,53	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 VW1 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 [i](#)

There are no such residues in this entry.