



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 1, 2022 – 01:47 PM EDT

PDB ID : 5RML
Title : PanDDA analysis group deposition – Crystal Structure of SARS-CoV-2 heli-
case in complex with Z85956652
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 : 2.43 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.29
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

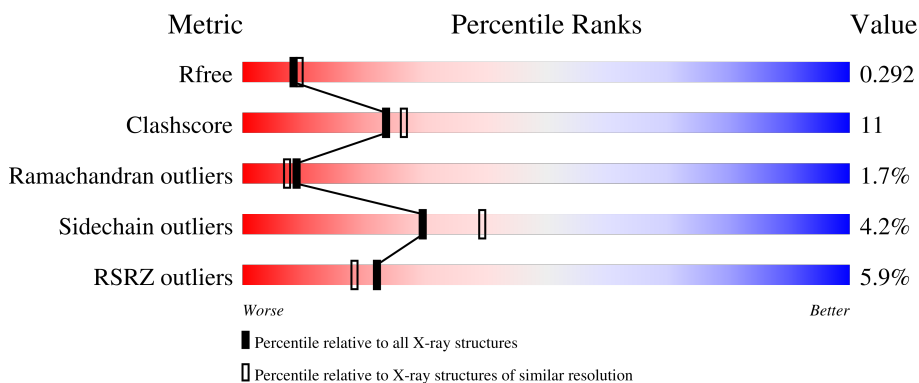
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 23%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 10px;">9% 71% 23% • 5%</p>
1	B	601	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 25%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 10px;">2% 71% 25% ••</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	B	702	-	-	X	-
4	VXD	A	701	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9417 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.

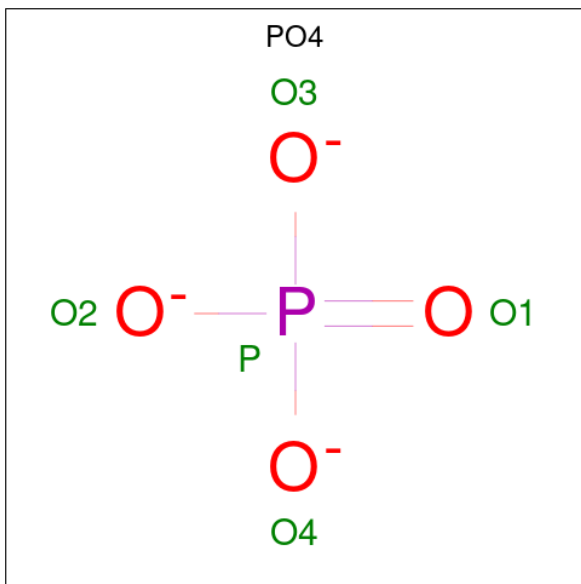
- Molecule 1 is a protein called Helicase.

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

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

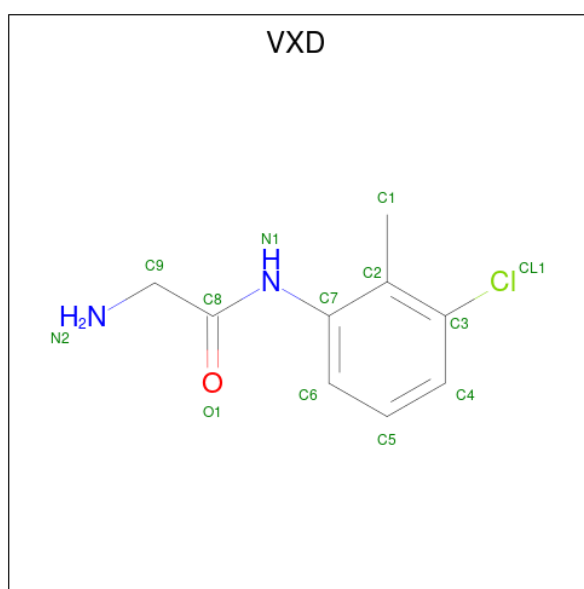
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total 3	Zn 3	0	0
2	A	3	Total 3	Zn 3	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 4 is N-(3-chloro-2-methylphenyl)glycinamide (three-letter code: VXD) (formula: C₉H₁₁ClN₂O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C Cl N O 13 9 1 2 1	0	0

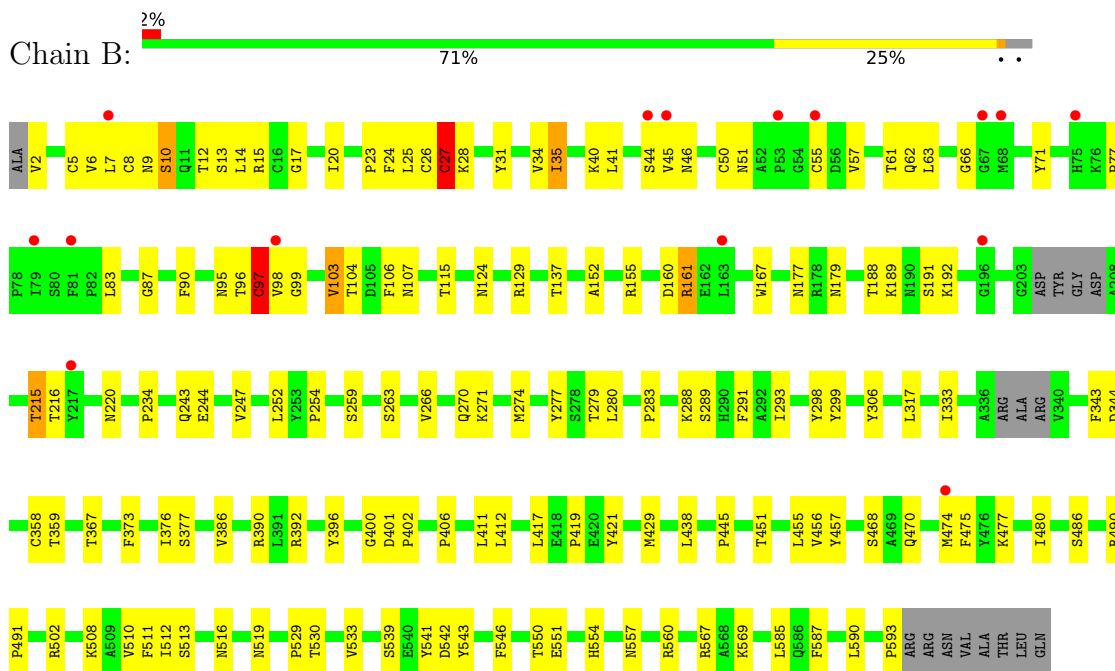
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	251	Total O 251 251	0	0
5	A	202	Total O 202 202	0	0

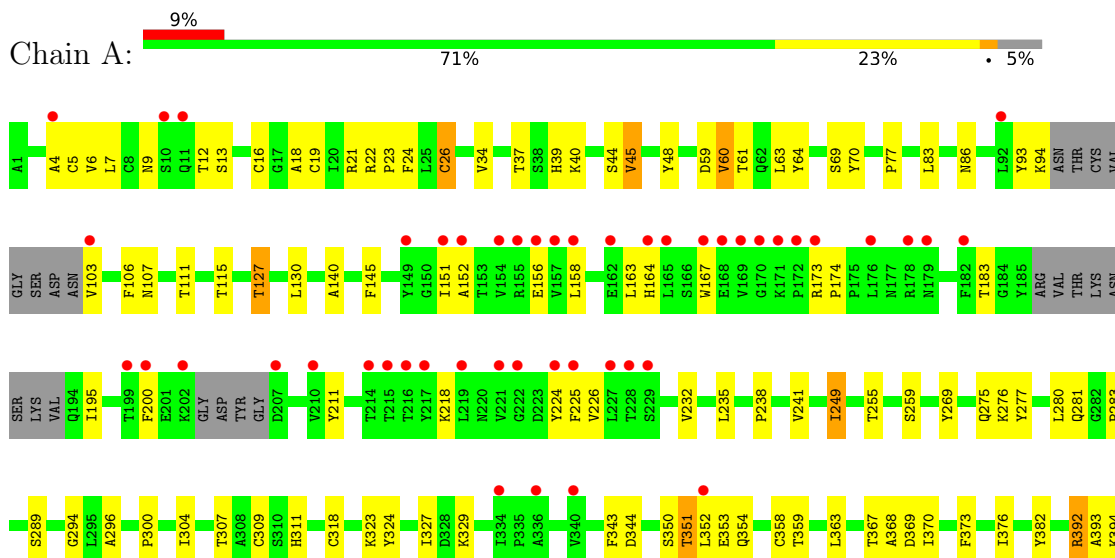
3 Residue-property plots [i](#)

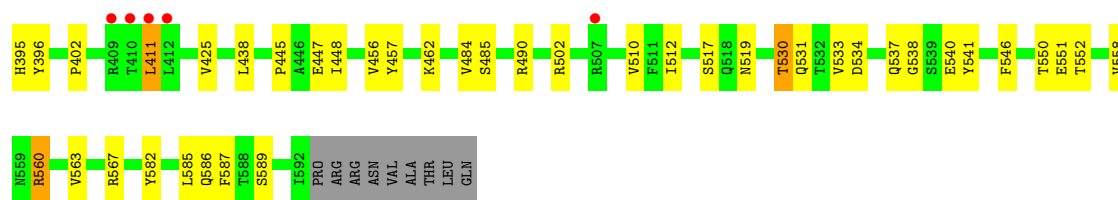
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 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	58.94Å 70.10Å 85.45Å 102.81° 95.84° 112.42°	Depositor
Resolution (Å)	81.52 – 2.43 81.52 – 2.43	Depositor EDS
% Data completeness (in resolution range)	97.0 (81.52-2.43) 97.0 (81.52-2.43)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.42Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.207 , 0.288 0.220 , 0.292	Depositor DCC
R_{free} test set	2298 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtrriage
Anisotropy	0.055	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9417	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% 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: PO4, VXD, ZN

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	0.73	0/4517	0.88	1/6156 (0.0%)
1	B	0.72	0/4610	0.90	0/6283
All	All	0.72	0/9127	0.89	1/12439 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	560	ARG	NE-CZ-NH1	5.48	123.04	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4417	0	4321	95	0
1	B	4508	0	4425	105	0
2	A	3	0	0	0	0
2	B	3	0	0	2	0
3	A	10	0	0	1	0
3	B	10	0	0	0	0
4	A	13	0	0	3	0
5	A	202	0	0	18	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	251	0	0	16	2
All	All	9417	0	8746	198	2

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 11.

All (198) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ASP:OD1	1:A:61:THR:OG1	1.83	0.96
1:B:5:CYS:HG	2:B:702:ZN:ZN	0.61	0.91
1:A:145:PHE:HD2	4:A:701:VXD:CL1	2.01	0.80
1:A:534:ASP:OD2	5:A:802:HOH:O	2.01	0.79
1:B:401:ASP:OD2	1:B:457:TYR:OH	2.01	0.78
1:B:5:CYS:SG	2:B:702:ZN:ZN	1.73	0.76
1:B:12:THR:CG2	1:B:26:CYS:HA	2.14	0.76
1:A:368:ALA:O	1:A:393:ALA:HA	1.86	0.75
1:A:447:GLU:HA	5:A:945:HOH:O	1.87	0.75
1:A:13:SER:OG	1:A:44:SER:HB2	1.89	0.73
1:B:8:CYS:SG	1:B:99:GLY:N	2.54	0.73
1:B:12:THR:HG21	1:B:25:LEU:O	1.89	0.72
1:B:12:THR:HG21	1:B:26:CYS:HA	1.70	0.72
1:B:7:LEU:HD12	1:B:103:VAL:HG22	1.71	0.71
1:B:508:LYS:HD3	5:B:920:HOH:O	1.90	0.70
1:B:124:ASN:HD22	1:B:421:TYR:HA	1.57	0.69
1:A:224:TYR:OH	5:A:801:HOH:O	1.99	0.69
1:B:34:VAL:O	1:B:40:LYS:NZ	2.22	0.69
1:B:177:ASN:HB3	1:B:516:ASN:ND2	2.08	0.69
1:B:7:LEU:CD1	1:B:103:VAL:HG22	2.25	0.67
1:B:2:VAL:N	5:B:805:HOH:O	2.29	0.66
1:B:376:ILE:HG22	1:B:400:GLY:HA3	1.78	0.65
1:A:269:TYR:OH	1:A:294:GLY:HA3	1.97	0.65
1:A:411:LEU:HD21	4:A:701:VXD:C1	2.27	0.65
1:A:327:ILE:O	5:A:803:HOH:O	2.15	0.65
1:A:200:PHE:N	5:A:804:HOH:O	2.21	0.64
1:B:44:SER:N	1:B:46:ASN:O	2.29	0.64
1:A:60:VAL:HB	5:A:906:HOH:O	1.98	0.63
1:A:145:PHE:CD2	4:A:701:VXD:CL1	2.87	0.63
1:A:235:LEU:HD21	1:A:382:TYR:CE2	2.34	0.62
1:B:474[B]:MET:HG2	1:B:590:LEU:HB2	1.81	0.62
1:B:377:SER:O	1:B:406:PRO:HA	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:LEU:HB3	1:B:299:TYR:CD1	2.35	0.61
1:B:333:ILE:HB	1:B:358:CYS:SG	2.40	0.61
1:B:306:TYR:HB3	1:B:317:LEU:HD13	1.83	0.61
1:B:542:ASP:OD1	1:B:569:LYS:HE3	2.01	0.60
1:A:350:SER:O	1:A:352:LEU:N	2.34	0.60
1:B:417:LEU:HA	5:B:881:HOH:O	2.00	0.60
1:B:344:ASP:HB3	5:B:968:HOH:O	2.02	0.60
1:B:14:LEU:HB2	1:B:25:LEU:O	2.02	0.59
1:B:61:THR:O	1:B:62:GLN:NE2	2.36	0.59
1:B:277:TYR:HA	1:B:396:TYR:O	2.02	0.59
1:A:519:ASN:HB3	1:A:530:THR:HG23	1.84	0.59
1:B:83:LEU:O	1:B:90:PHE:N	2.33	0.58
1:B:270:GLN:O	1:B:274:MET:HG3	2.03	0.58
1:B:510:VAL:HG21	1:B:541:TYR:CD1	2.38	0.58
1:A:519:ASN:HB3	1:A:530:THR:CG2	2.34	0.58
1:B:271:LYS:NZ	5:B:802:HOH:O	2.27	0.57
1:A:275:GLN:O	1:A:395:HIS:ND1	2.38	0.57
1:B:50:CYS:SG	1:B:71:TYR:HA	2.45	0.56
1:A:296:ALA:O	1:A:300:PRO:HA	2.05	0.56
1:A:510:VAL:HG21	1:A:541:TYR:CD1	2.41	0.56
1:A:276:LYS:O	1:A:395:HIS:HA	2.05	0.55
1:A:367:THR:HA	1:A:392:ARG:O	2.06	0.55
1:A:537:GLN:OE1	1:A:563:VAL:HG21	2.07	0.55
1:B:8:CYS:C	1:B:10:SER:H	2.10	0.55
1:A:4:ALA:O	1:A:24:PHE:HB2	2.07	0.55
1:A:512:ILE:O	1:A:546:PHE:HA	2.07	0.55
1:A:163:LEU:HD23	1:A:211:TYR:CD2	2.43	0.54
1:A:249:ILE:O	1:A:249:ILE:HG22	2.09	0.53
1:A:370:ILE:HA	1:A:395:HIS:O	2.08	0.53
1:B:470:GLN:NE2	1:B:543:TYR:OH	2.40	0.53
1:B:510:VAL:HG21	1:B:541:TYR:CG	2.44	0.53
1:A:585:LEU:HD22	1:A:587:PHE:CZ	2.44	0.52
1:A:281:GLN:HG3	1:A:402:PRO:HD2	1.91	0.52
1:B:280:LEU:HD11	1:B:438:LEU:HG	1.92	0.52
1:B:502:ARG:NH2	5:B:826:HOH:O	2.42	0.52
1:A:277:TYR:HA	1:A:396:TYR:O	2.10	0.52
1:A:323:LYS:HG2	1:A:324:TYR:CE1	2.45	0.52
1:B:17:GLY:HA3	1:B:41:LEU:HD23	1.92	0.51
1:B:35:ILE:O	1:B:35:ILE:HD12	2.11	0.51
1:B:480:ILE:HD13	1:B:550:THR:HG22	1.93	0.50
1:B:519:ASN:CB	5:B:869:HOH:O	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:GLY:HA2	3:A:706:PO4:O4	2.10	0.50
1:A:7:LEU:HD13	1:A:103:VAL:HG22	1.94	0.50
1:A:37:THR:OG1	1:A:39:HIS:HB2	2.11	0.50
1:A:64:TYR:O	1:A:70:TYR:HA	2.12	0.50
1:B:6:VAL:CG1	5:B:978:HOH:O	2.60	0.50
1:A:411:LEU:HD23	1:A:411:LEU:N	2.27	0.50
1:A:533:VAL:HG11	1:A:560:ARG:HG3	1.94	0.50
1:B:593:PRO:HG2	5:B:826:HOH:O	2.12	0.49
1:B:15:ARG:HA	1:B:23:PRO:O	2.12	0.49
1:B:455:LEU:HG	1:B:456:VAL:HG13	1.94	0.49
1:A:4:ALA:O	1:A:24:PHE:CB	2.60	0.49
1:B:27:CYS:HB3	5:B:966:HOH:O	2.12	0.49
1:A:63:LEU:HB3	1:A:83:LEU:HD12	1.95	0.49
1:A:558:VAL:HG13	5:A:954:HOH:O	2.13	0.49
1:B:115:THR:HA	1:B:411:LEU:O	2.12	0.49
1:A:5:CYS:SG	1:A:26:CYS:HB3	2.53	0.49
1:A:369:ASP:O	1:A:394:LYS:HB2	2.13	0.49
1:B:66:GLY:HA3	1:B:77:PRO:CG	2.43	0.49
1:B:44:SER:C	1:B:46:ASN:N	2.66	0.49
1:A:167:TRP:CZ3	1:A:174:PRO:HD2	2.48	0.48
1:A:586:GLN:NE2	5:A:818:HOH:O	2.42	0.48
1:B:8:CYS:SG	1:B:98:VAL:HB	2.54	0.48
1:B:288:LYS:O	1:B:291:PHE:HB3	2.13	0.48
1:A:462:LYS:HA	5:A:852:HOH:O	2.14	0.48
1:B:343:PHE:HA	5:B:814:HOH:O	2.14	0.48
1:A:289:SER:HB2	5:A:811:HOH:O	2.13	0.48
1:B:12:THR:HG21	1:B:26:CYS:CA	2.40	0.48
1:A:19:CYS:HB2	1:A:23:PRO:HD2	1.96	0.48
1:A:130:LEU:HD12	5:A:933:HOH:O	2.13	0.48
1:A:376:ILE:HG12	1:A:425:VAL:HG11	1.95	0.48
1:B:7:LEU:HD12	1:B:103:VAL:CG2	2.41	0.47
1:B:160:ASP:O	1:B:161:ARG:CB	2.61	0.47
1:A:151:ILE:HG12	1:A:226:VAL:HG22	1.97	0.47
1:B:551:GLU:HB3	5:B:873:HOH:O	2.14	0.47
1:A:351:THR:HG22	5:A:849:HOH:O	2.13	0.47
1:B:585:LEU:HD22	1:B:587:PHE:CE2	2.50	0.47
1:A:238:PRO:CB	5:A:904:HOH:O	2.63	0.47
1:B:31:TYR:CE2	1:B:87:GLY:HA2	2.50	0.47
1:B:220:ASN:N	1:B:220:ASN:OD1	2.48	0.47
1:A:18:ALA:O	1:A:39:HIS:CE1	2.68	0.47
1:B:7:LEU:HD21	1:B:106:PHE:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:CYS:HB3	1:A:343:PHE:CD2	2.50	0.46
1:A:550:THR:HB	1:A:552:THR:HG23	1.97	0.46
1:A:235:LEU:HD21	1:A:382:TYR:CZ	2.50	0.46
1:A:367:THR:HG22	1:A:392:ARG:HB3	1.96	0.46
1:B:71:TYR:CD2	1:B:77:PRO:HD3	2.49	0.46
1:B:152:ALA:HB2	1:B:167:TRP:CZ3	2.50	0.46
1:A:34:VAL:HA	1:A:39:HIS:O	2.15	0.46
1:B:13:SER:O	1:B:44:SER:HA	2.15	0.46
1:A:585:LEU:HD22	1:A:587:PHE:CE2	2.51	0.46
1:B:477:LYS:NZ	1:B:551:GLU:OE2	2.32	0.46
1:B:9:ASN:O	1:B:10:SER:C	2.55	0.46
1:A:152:ALA:HB2	1:A:167:TRP:CE3	2.51	0.46
1:A:152:ALA:HB2	1:A:167:TRP:CZ3	2.51	0.45
1:B:215:THR:OG1	1:B:216:THR:N	2.49	0.45
1:A:44:SER:O	1:A:45:VAL:C	2.54	0.45
1:B:234:PRO:HD3	1:A:352:LEU:CD1	2.47	0.45
1:B:55:CYS:SG	1:B:57:VAL:HG23	2.57	0.45
1:A:280:LEU:HD11	1:A:438:LEU:HG	1.98	0.45
1:A:307:THR:HA	1:A:358:CYS:O	2.17	0.45
1:B:15:ARG:HD3	1:B:24:PHE:CE2	2.51	0.45
1:B:263:SER:HA	1:B:266:VAL:HG23	1.98	0.45
1:A:158:LEU:HD11	1:A:164:HIS:CE1	2.52	0.45
1:A:140:ALA:HA	1:A:232:VAL:HG21	1.98	0.44
1:A:93:TYR:O	1:A:94:LYS:O	2.36	0.44
1:B:27:CYS:CB	5:B:966:HOH:O	2.66	0.44
1:A:490:ARG:HD2	5:A:990:HOH:O	2.18	0.44
1:B:533:VAL:HG11	1:B:560:ARG:HG3	2.00	0.44
1:A:106:PHE:HD1	1:A:130:LEU:HD21	1.83	0.44
1:B:475:PHE:CZ	1:B:477:LYS:HE2	2.53	0.43
1:B:26:CYS:O	1:B:27:CYS:C	2.55	0.43
1:B:511:PHE:HB3	1:B:530:THR:HG22	2.00	0.43
1:B:279:THR:HB	1:B:429:MET:HE3	2.00	0.43
1:B:554:HIS:ND1	5:B:815:HOH:O	2.36	0.43
1:A:309:CYS:HB3	5:A:978:HOH:O	2.18	0.43
1:A:456:VAL:HG23	1:A:457:TYR:CE2	2.54	0.43
1:B:490:ARG:N	1:B:491:PRO:CD	2.83	0.42
1:A:200:PHE:HZ	1:A:225:PHE:CD2	2.37	0.42
1:A:358:CYS:HB3	1:A:363:LEU:HD23	2.00	0.42
1:B:557:ASN:HB2	5:B:985:HOH:O	2.18	0.42
1:A:304:ILE:HA	1:A:370:ILE:O	2.19	0.42
1:A:127:THR:HG22	1:A:130:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:LYS:HE2	1:A:354:GLN:OE1	2.19	0.42
1:B:234:PRO:CD	1:A:352:LEU:HD11	2.49	0.42
1:B:254:PRO:HB3	1:B:298:TYR:CE2	2.55	0.42
1:A:115:THR:HA	1:A:411:LEU:O	2.20	0.42
1:A:582:TYR:OH	1:A:589:SER:HB2	2.20	0.42
1:B:14:LEU:O	1:B:24:PHE:HA	2.20	0.42
1:B:63:LEU:HB3	1:B:83:LEU:HD12	2.02	0.42
1:B:103:VAL:HG12	1:B:107:ASN:ND2	2.34	0.42
1:B:367:THR:HA	1:B:392:ARG:O	2.20	0.42
1:B:376:ILE:HG21	1:B:429:MET:HE1	2.02	0.42
1:A:311:HIS:ND1	1:A:359:THR:HG21	2.35	0.42
1:A:445:PRO:HD2	1:A:448:ILE:HD12	2.02	0.42
1:B:512:ILE:O	1:B:546:PHE:HA	2.20	0.41
1:B:115:THR:O	1:B:412:LEU:HD12	2.21	0.41
1:B:129:ARG:HD2	1:B:129:ARG:HA	1.86	0.41
1:B:179:ASN:HD22	1:B:179:ASN:HA	1.72	0.41
1:B:451:THR:HG21	1:B:585:LEU:HD23	2.02	0.41
1:A:107:ASN:O	1:A:111:THR:OG1	2.32	0.41
1:A:353:GLU:HA	1:A:353:GLU:OE2	2.19	0.41
1:B:402:PRO:O	1:B:419:PRO:HB3	2.20	0.41
1:A:350:SER:O	1:A:353:GLU:HG2	2.20	0.41
1:B:386:VAL:O	1:B:390:ARG:HG2	2.19	0.41
1:A:34:VAL:O	1:A:40:LYS:NZ	2.33	0.41
1:A:241:VAL:HG12	5:A:992:HOH:O	2.19	0.41
1:A:456:VAL:HG23	1:A:457:TYR:CD2	2.55	0.41
1:B:31:TYR:CZ	1:B:87:GLY:HA2	2.56	0.41
1:B:480:ILE:HD11	5:B:927:HOH:O	2.20	0.41
1:B:243:GLN:HG3	1:B:244:GLU:N	2.36	0.41
1:B:279:THR:HB	1:B:429:MET:CE	2.50	0.41
1:A:16:CYS:O	1:A:22:ARG:HA	2.21	0.41
1:A:540:GLU:HA	1:A:567:ARG:O	2.21	0.41
1:B:28:LYS:CB	1:B:97:CYS:SG	3.09	0.40
1:A:77:PRO:HB2	5:A:937:HOH:O	2.19	0.40
1:B:9:ASN:O	1:B:10:SER:O	2.39	0.40
1:B:539:SER:O	1:B:567:ARG:HD3	2.20	0.40
1:B:12:THR:HG22	1:B:13:SER:N	2.36	0.40
1:A:21:ARG:O	1:A:22:ARG:HB2	2.21	0.40
1:A:238:PRO:HG3	5:A:904:HOH:O	2.21	0.40
1:B:8:CYS:HB3	1:B:10:SER:HB2	2.02	0.40
1:B:20:ILE:HD11	1:B:137:THR:O	2.21	0.40
1:B:152:ALA:HB2	1:B:167:TRP:CH2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:PRO:HB3	1:B:468:SER:HB3	2.04	0.40
1:A:585:LEU:HD23	1:A:585:LEU:HA	1.95	0.40

All (2) 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:1008:HOH:O	5:A:975:HOH:O[1_556]	1.83	0.37
5:B:1001:HOH:O	5:A:873:HOH:O[1_556]	2.10	0.10

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%)	508 (90%)	45 (8%)	11 (2%)	7 5
1	B	580/601 (96%)	540 (93%)	32 (6%)	8 (1%)	11 10
All	All	1144/1202 (95%)	1048 (92%)	77 (7%)	19 (2%)	9 7

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	10	SER
1	B	27	CYS
1	A	249	ILE
1	A	351	THR
1	B	97	CYS
1	B	189	LYS
1	A	6	VAL
1	A	195	ILE
1	A	484	VAL
1	B	51	ASN

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Mol	Chain	Res	Type
1	B	161	ARG
1	A	45	VAL
1	A	48	TYR
1	A	218	LYS
1	B	45	VAL
1	A	9	ASN
1	B	283	PRO
1	A	60	VAL
1	A	283	PRO

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	485/523 (93%)	465 (96%)	20 (4%)	30	40
1	B	498/523 (95%)	477 (96%)	21 (4%)	30	39
All	All	983/1046 (94%)	942 (96%)	41 (4%)	30	39

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	27	CYS
1	B	35	ILE
1	B	95	ASN
1	B	96	THR
1	B	97	CYS
1	B	103	VAL
1	B	104	THR
1	B	155	ARG
1	B	188	THR
1	B	191	SER
1	B	192	LYS
1	B	215	THR
1	B	247	VAL
1	B	259	SER

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Mol	Chain	Res	Type
1	B	289	SER
1	B	293	ILE
1	B	359	THR
1	B	373	PHE
1	B	486	SER
1	B	513	SER
1	B	529	PRO
1	A	12	THR
1	A	26	CYS
1	A	69	SER
1	A	86	ASN
1	A	127	THR
1	A	156	GLU
1	A	173	ARG
1	A	183	THR
1	A	255	THR
1	A	259	SER
1	A	344	ASP
1	A	373	PHE
1	A	392	ARG
1	A	411	LEU
1	A	485	SER
1	A	502	ARG
1	A	517	SER
1	A	530	THR
1	A	531	GLN
1	A	551	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	46	ASN
1	B	62	GLN
1	B	179	ASN
1	B	268	ASN
1	B	404	GLN
1	B	470	GLN
1	B	516	ASN
1	A	179	ASN
1	A	257	ASN
1	A	531	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 monosaccharides 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
3	PO4	B	704	-	4,4,4	1.10	0	6,6,6	0.49	0
3	PO4	A	705	-	4,4,4	0.78	0	6,6,6	0.87	0
3	PO4	B	705	-	4,4,4	2.17	2 (50%)	6,6,6	0.37	0
3	PO4	A	706	-	4,4,4	0.99	0	6,6,6	0.52	0
4	VXD	A	701	-	12,13,13	0.33	0	15,17,17	0.54	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
4	VXD	A	701	-	-	2/6/6/6	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	705	PO4	P-O1	3.55	1.59	1.50
3	B	705	PO4	P-O3	-2.12	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

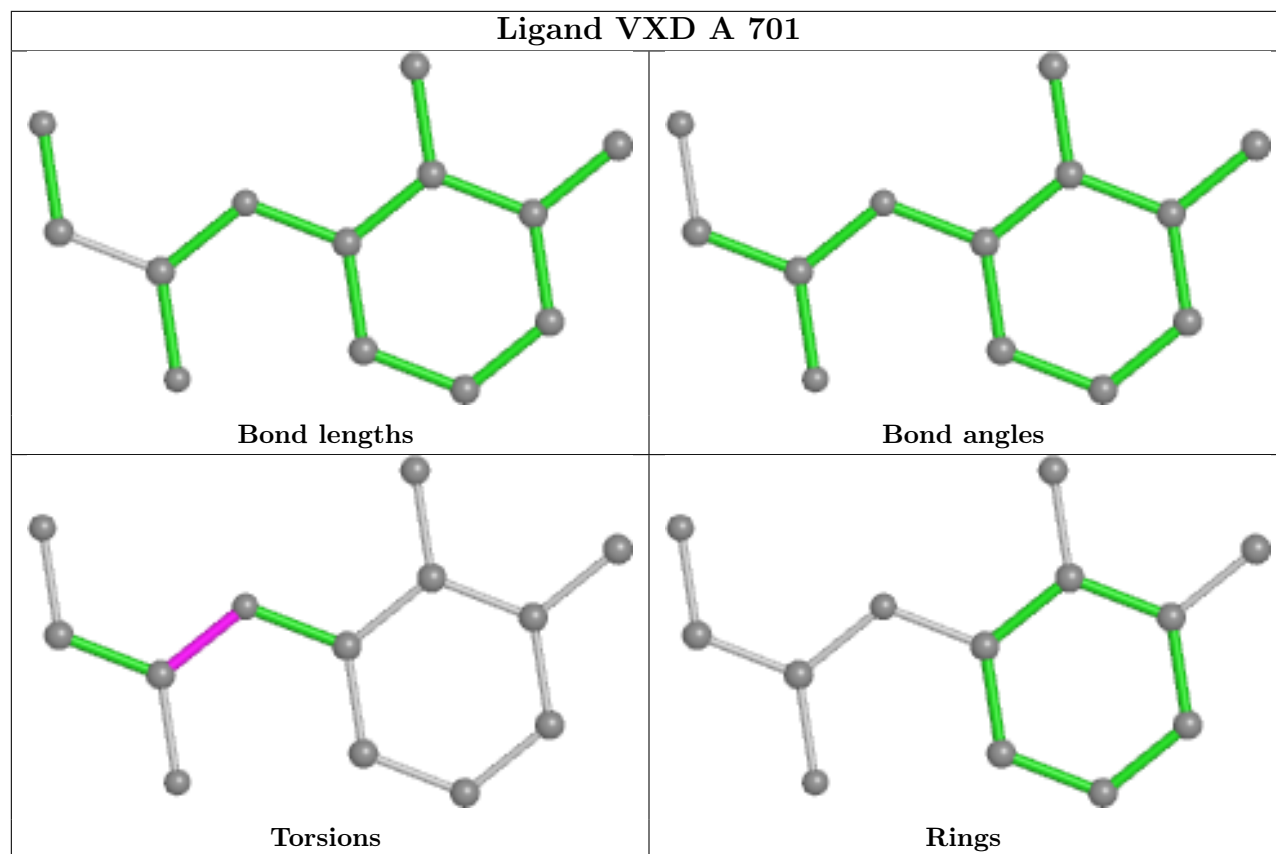
Mol	Chain	Res	Type	Atoms
4	A	701	VXD	C9-C8-N1-C7
4	A	701	VXD	O1-C8-N1-C7

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	706	PO4	1	0
4	A	701	VXD	3	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%)	0.36	53 (9%) 8 6	31, 66, 134, 179	4 (0%)
1	B	585/601 (97%)	-0.09	15 (2%) 56 52	29, 51, 104, 128	1 (0%)
All	All	1157/1202 (96%)	0.13	68 (5%) 22 18	29, 58, 121, 179	5 (0%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	167	TRP	11.1
1	A	202	LYS	10.2
1	A	225	PHE	8.8
1	A	169	VAL	7.8
1	A	200	PHE	7.7
1	A	411	LEU	7.7
1	A	410	THR	7.4
1	A	149	TYR	7.0
1	A	412	LEU	6.5
1	A	228	THR	6.2
1	A	178	ARG	6.1
1	A	221	VAL	6.1
1	A	215	THR	5.5
1	B	45	VAL	5.1
1	B	474[A]	MET	5.1
1	A	409	ARG	5.0
1	A	336	ALA	4.6
1	A	176	LEU	4.4
1	A	179	ASN	4.3
1	A	156	GLU	4.2
1	A	164	HIS	4.0
1	A	10	SER	3.9
1	B	196	GLY	3.9
1	A	219	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	170	GLY	3.9
1	B	68	MET	3.9
1	A	224	TYR	3.6
1	A	229	SER	3.6
1	B	67	GLY	3.5
1	A	207	ASP	3.4
1	A	210	VAL	3.2
1	A	222	GLY	3.2
1	A	158	LEU	3.1
1	A	103	VAL	3.1
1	A	217	TYR	3.0
1	A	168	GLU	3.0
1	A	11	GLN	3.0
1	B	79	ILE	2.9
1	A	157	VAL	2.8
1	B	98	VAL	2.7
1	A	334	ILE	2.7
1	B	44	SER	2.7
1	B	53	PRO	2.7
1	A	352	LEU	2.7
1	A	154	VAL	2.6
1	B	75	HIS	2.6
1	A	92	LEU	2.5
1	B	81	PHE	2.5
1	A	171	LYS	2.5
1	B	217	TYR	2.5
1	A	151	ILE	2.5
1	A	340	VAL	2.4
1	A	162	GLU	2.4
1	A	173	ARG	2.4
1	A	199	THR	2.4
1	B	163	LEU	2.4
1	B	7	LEU	2.3
1	A	4	ALA	2.3
1	A	227	LEU	2.3
1	A	216	THR	2.3
1	A	507	ARG	2.3
1	A	152	ALA	2.3
1	A	165	LEU	2.2
1	A	172	PRO	2.2
1	A	182	PHE	2.2
1	A	214	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	55	CYS	2.1
1	A	155	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](#)

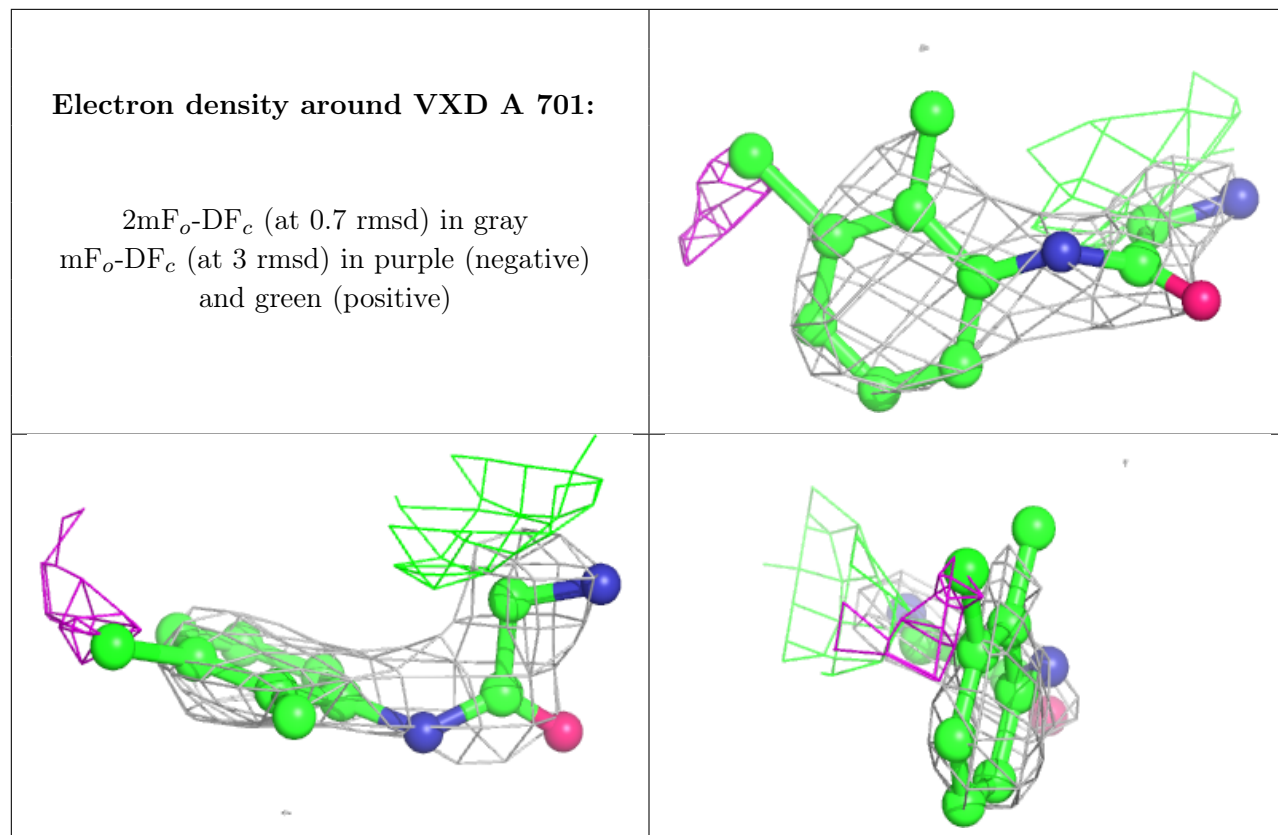
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(Å ²)	Q<0.9
4	VXD	A	701	13/13	0.62	0.44	36,40,45,56	13
2	ZN	B	703	1/1	0.95	0.11	92,92,92,92	0
2	ZN	A	704	1/1	0.96	0.06	87,87,87,87	0
2	ZN	A	703	1/1	0.96	0.12	65,65,65,65	0
3	PO4	B	704	5/5	0.98	0.13	34,43,49,49	0
3	PO4	B	705	5/5	0.98	0.12	36,38,43,45	0
3	PO4	A	706	5/5	0.98	0.13	50,50,61,62	0
2	ZN	A	702	1/1	0.98	0.12	68,68,68,68	0
3	PO4	A	705	5/5	0.99	0.14	43,43,44,50	0
2	ZN	B	701	1/1	0.99	0.11	44,44,44,44	0
2	ZN	B	702	1/1	0.99	0.11	56,56,56,56	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.