



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:10 PM UTC

PDB ID : 5RMM / pdb_00005rmm
Title : PanDDA analysis group deposition – Crystal Structure of SARS-CoV-2 heli-
case in complex with POB0066
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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 : 2.20 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)

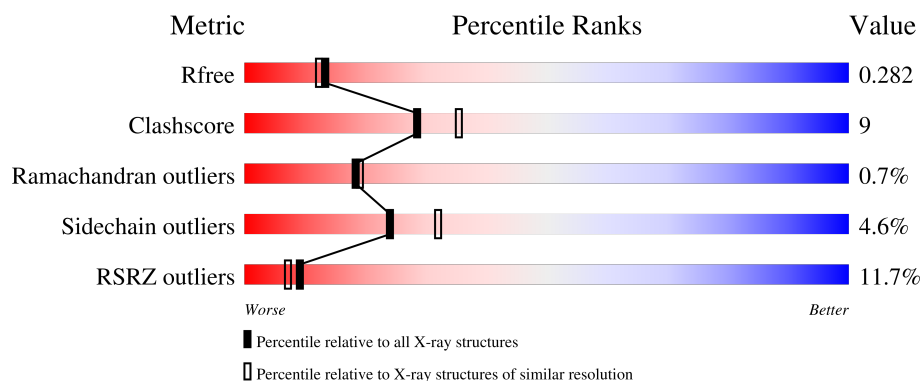
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	19% 71% 23% • 5%
1	B	601	3% 77% 19% • •

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 9421 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.

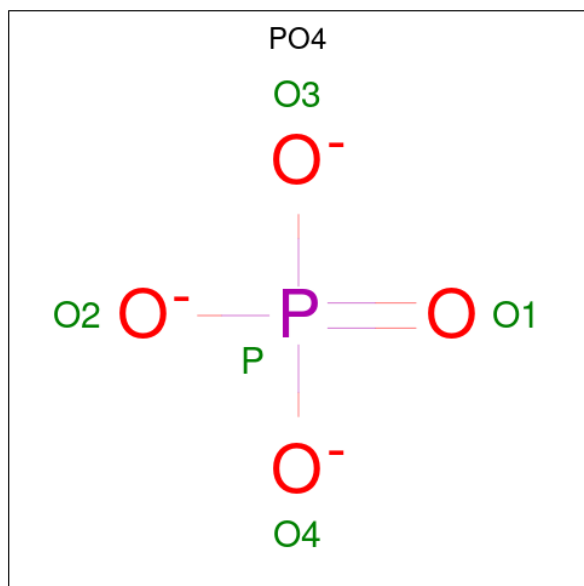
- Molecule 1 is a protein called Helicase.

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

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

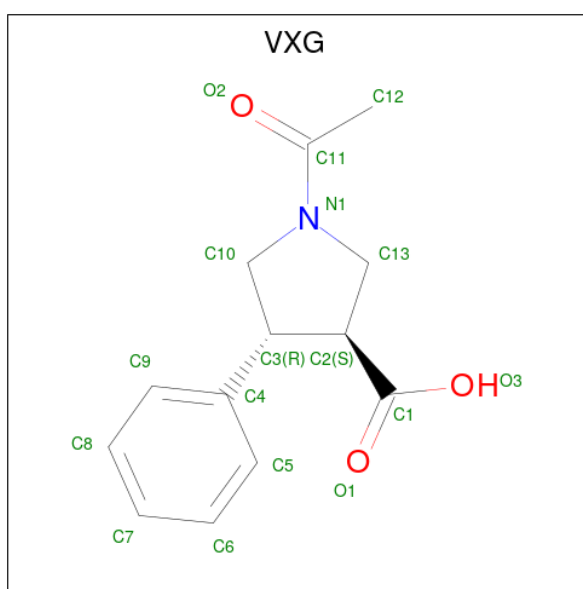
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	3	Total	Zn	0	0
			3	3		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 4 is (3S,4R)-1-acetyl-4-phenylpyrrolidine-3-carboxylic acid (CCD ID: VXG) (formula: C₁₃H₁₅NO₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 17 13 1 3	0	0

- Molecule 5 is water.

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

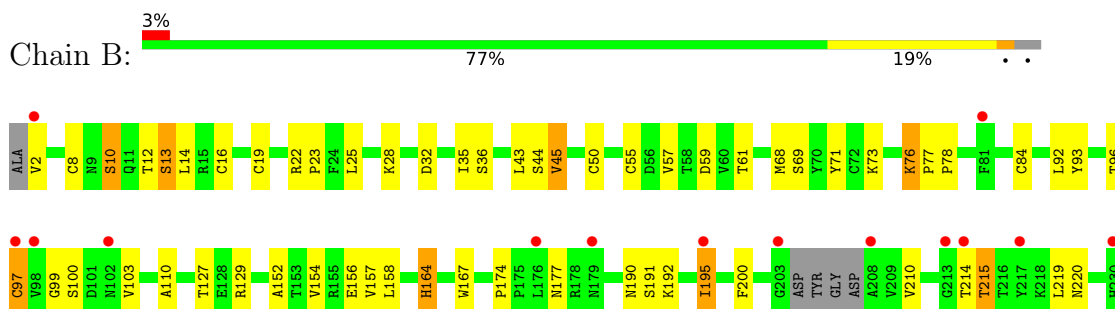
3 Residue-property plots [i](#)

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	59.01Å 70.03Å 85.75Å 103.16° 96.14° 112.25°	Depositor
Resolution (Å)	81.56 – 2.20 81.56 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.2 (81.56-2.20) 97.3 (81.56-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.212 , 0.281 0.218 , 0.282	Depositor DCC
R_{free} test set	3098 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.7	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	0.96	EDS
Total number of atoms	9421	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% 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: ZN, PO4, VXG

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	1.41	6/6156 (0.1%)
1	B	1.02	0/4610	1.38	2/6283 (0.0%)
All	All	1.04	0/9127	1.40	8/12439 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	253	TYR	CB-CA-C	6.66	118.99	110.34
1	B	415	GLY	CA-C-O	-6.21	117.26	122.29
1	A	553	ALA	CA-C-N	5.56	127.67	120.44
1	A	553	ALA	C-N-CA	5.56	127.67	120.44
1	A	289	SER	CA-C-N	5.20	127.20	120.44
1	A	289	SER	C-N-CA	5.20	127.20	120.44
1	A	591	GLU	CA-C-N	5.09	130.86	121.70
1	A	591	GLU	C-N-CA	5.09	130.86	121.70

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	4322	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4508	0	4424	72	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	10	0	0	1	0
3	B	10	0	0	0	0
4	B	17	0	0	0	0
5	A	202	0	0	9	0
5	B	251	0	0	4	0
All	All	9421	0	8746	156	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 9.

All (156) 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:12:THR:HG21	1:B:25:LEU:O	1.65	0.94
1:B:279:THR:HB	1:B:429:MET:HE2	1.60	0.83
1:B:12:THR:HG22	1:B:14:LEU:H	1.48	0.79
1:B:510:VAL:HG21	1:B:541:TYR:CD1	2.22	0.75
1:A:329:LYS:HE2	1:A:354:GLN:OE1	1.88	0.74
1:B:177:ASN:HB2	1:B:516:ASN:ND2	2.06	0.71
1:A:6:VAL:O	1:A:6:VAL:HG23	1.90	0.71
1:B:376:ILE:HG22	1:B:400:GLY:HA3	1.73	0.70
1:A:510:VAL:HG21	1:A:541:TYR:CD1	2.27	0.68
1:B:8:CYS:SG	1:B:99:GLY:C	2.77	0.67
1:A:329:LYS:CE	1:A:354:GLN:OE1	2.43	0.66
1:B:425:VAL:HG12	1:B:429:MET:HE3	1.78	0.66
1:A:44:SER:OG	1:A:45:VAL:N	2.26	0.66
1:A:351:THR:HG22	5:A:926:HOH:O	1.97	0.64
1:A:519:ASN:HB3	1:A:530:THR:HG23	1.81	0.62
1:B:280:LEU:HD11	1:B:438:LEU:HG	1.81	0.62
1:B:278:SER:HB2	1:B:436:MET:HE2	1.82	0.61
1:A:310:SER:OG	5:A:801:HOH:O	2.16	0.61
1:B:460:LYS:NZ	5:B:805:HOH:O	2.32	0.61
1:A:534:ASP:OD2	5:A:802:HOH:O	2.16	0.61
1:A:275:GLN:O	1:A:395:HIS:ND1	2.33	0.61
1:A:280:LEU:HD12	1:A:436:MET:O	2.01	0.60
1:A:64:TYR:O	1:A:70:TYR:HA	2.02	0.60
1:B:249:ILE:HD11	1:B:270:GLN:HG2	1.83	0.60
1:A:376:ILE:HG12	1:A:425:VAL:HG11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ASN:OD1	5:B:801:HOH:O	2.16	0.59
1:A:123:ALA:O	5:A:803:HOH:O	2.17	0.59
1:B:373:PHE:CE1	1:B:387:VAL:HG21	2.38	0.59
1:A:512:ILE:O	1:A:546:PHE:HA	2.05	0.56
1:B:425:VAL:CG1	1:B:429:MET:HE3	2.35	0.56
1:A:115:THR:HA	1:A:411:LEU:O	2.06	0.56
1:A:21:ARG:O	1:A:22:ARG:C	2.50	0.55
1:A:409:ARG:NH2	1:A:422:PHE:O	2.39	0.55
1:B:277:TYR:HA	1:B:396:TYR:O	2.07	0.55
1:B:8:CYS:SG	1:B:99:GLY:N	2.80	0.54
1:A:296:ALA:O	1:A:300:PRO:HA	2.08	0.53
1:B:252:LEU:HB3	1:B:299:TYR:CD1	2.43	0.53
1:B:55:CYS:SG	1:B:57:VAL:HG23	2.49	0.53
1:A:235:LEU:HD21	1:A:382:TYR:CE2	2.44	0.53
1:B:333:ILE:HB	1:B:358:CYS:SG	2.48	0.53
1:A:260:ASP:HA	1:A:263:SER:OG	2.08	0.52
1:B:50:CYS:SG	1:B:71:TYR:HA	2.50	0.52
1:A:297:LEU:HD11	1:A:324:TYR:HB3	1.92	0.52
1:B:12:THR:HG22	1:B:14:LEU:N	2.22	0.52
1:A:561:PHE:CD2	1:A:581:LEU:HD22	2.46	0.51
1:A:287:GLY:HA2	5:A:899:HOH:O	2.09	0.51
1:A:331:SER:HB2	1:A:353:GLU:HG3	1.93	0.51
1:A:519:ASN:HB3	1:A:530:THR:CG2	2.40	0.51
1:B:387:VAL:HG13	1:B:391:LEU:HD12	1.93	0.51
1:A:333:ILE:HB	1:A:358:CYS:SG	2.51	0.51
1:A:261:GLU:OE1	1:A:324:TYR:OH	2.14	0.51
1:A:6:VAL:HA	1:A:129:ARG:HD2	1.93	0.51
1:A:60:VAL:HB	5:A:900:HOH:O	2.10	0.50
1:A:238:PRO:HG3	5:A:989:HOH:O	2.10	0.50
1:B:19:CYS:SG	1:B:110:ALA:HB1	2.52	0.49
1:B:167:TRP:CZ3	1:B:174:PRO:HD2	2.47	0.49
1:A:293:ILE:HG21	1:A:320:LYS:O	2.11	0.49
1:A:280:LEU:HD11	1:A:438:LEU:HG	1.95	0.49
1:B:266:VAL:HG13	1:B:298:TYR:CE1	2.47	0.49
1:A:152:ALA:HB2	1:A:167:TRP:CZ3	2.48	0.49
1:A:284:PRO:HA	3:A:705:PO4:O2	2.13	0.48
1:B:8:CYS:SG	1:B:99:GLY:CA	3.01	0.48
1:A:332:ARG:NH2	1:A:342:CYS:SG	2.87	0.47
1:A:165:LEU:HD11	1:A:200:PHE:CE2	2.49	0.47
1:A:332:ARG:CZ	1:A:342:CYS:SG	3.03	0.47
1:B:8:CYS:HB3	1:B:10:SER:OG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:LEU:HA	1:B:43:LEU:O	2.15	0.47
1:A:503:ASN:HB3	1:A:506:TRP:CD1	2.50	0.47
1:B:510:VAL:HG21	1:B:541:TYR:CG	2.49	0.47
1:B:13:SER:O	1:B:44:SER:HA	2.15	0.47
1:A:5:CYS:SG	1:A:26:CYS:HB3	2.54	0.46
1:A:19:CYS:HB2	1:A:23:PRO:HD2	1.97	0.46
1:B:154:VAL:HG11	1:B:157:VAL:HG22	1.96	0.46
1:A:158:LEU:HD11	1:A:164:HIS:CE1	2.50	0.46
1:A:456:VAL:HG23	1:A:457:TYR:CE2	2.50	0.46
1:A:13:SER:O	1:A:44:SER:HA	2.16	0.46
1:B:371:VAL:HG23	1:B:393:ALA:HB2	1.97	0.46
1:A:6:VAL:O	1:A:6:VAL:CG2	2.61	0.46
1:A:531:GLN:HG2	1:A:536:SER:HB3	1.99	0.45
1:B:357:PHE:CD1	1:B:357:PHE:N	2.84	0.45
1:A:533:VAL:HG11	1:A:560:ARG:O	2.16	0.45
1:A:34:VAL:HA	1:A:39:HIS:O	2.16	0.45
1:A:251:GLY:HA3	1:A:394:LYS:HD3	1.99	0.45
1:A:59:ASP:CG	1:A:61:THR:HG1	2.23	0.45
1:A:139:LYS:HG2	1:A:232:VAL:HG22	1.99	0.45
1:B:73:LYS:HA	1:B:76:LYS:HD3	1.99	0.45
1:B:195:ILE:HG23	1:B:195:ILE:O	2.15	0.45
1:B:368:ALA:O	1:B:393:ALA:HA	2.16	0.45
1:B:512:ILE:O	1:B:546:PHE:HA	2.17	0.45
1:B:127:THR:HG23	5:B:930:HOH:O	2.16	0.45
1:B:445:PRO:HD2	1:B:448:ILE:HD12	1.99	0.45
1:A:405:LEU:HD13	1:A:534:ASP:OD1	2.17	0.45
1:B:200:PHE:HA	1:B:210:VAL:O	2.16	0.45
1:B:156:GLU:HB3	1:B:164:HIS:HB2	1.99	0.44
1:A:5:CYS:HA	1:A:24:PHE:O	2.17	0.44
1:A:549:THR:HG22	1:A:550:THR:HG23	1.99	0.44
1:B:561:PHE:CZ	1:B:585:LEU:HD21	2.52	0.44
1:B:152:ALA:HB2	1:B:167:TRP:CZ3	2.52	0.44
1:A:367:THR:HG22	1:A:392:ARG:HB3	2.00	0.44
1:A:368:ALA:O	1:A:393:ALA:HA	2.18	0.44
1:A:140:ALA:HA	1:A:232:VAL:HG21	1.98	0.44
1:B:16:CYS:O	1:B:22:ARG:HA	2.17	0.44
1:A:130:LEU:HD23	1:A:130:LEU:HA	1.88	0.44
1:A:214:THR:HG22	1:A:340:VAL:HG12	1.99	0.44
1:A:276:LYS:O	1:A:395:HIS:HA	2.18	0.44
1:A:388:ASN:HB3	5:A:978:HOH:O	2.18	0.44
1:B:377:SER:O	1:B:406:PRO:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ARG:O	1:A:23:PRO:N	2.51	0.43
1:B:2:VAL:N	5:B:826:HOH:O	2.51	0.43
1:B:97:CYS:O	1:B:97:CYS:SG	2.76	0.43
1:A:366:THR:OG1	1:A:367:THR:N	2.52	0.43
1:B:32:ASP:O	1:B:36:SER:OG	2.33	0.43
1:B:511:PHE:O	1:B:530:THR:HA	2.18	0.43
1:A:303:ARG:NH1	1:A:353:GLU:O	2.52	0.43
1:A:59:ASP:OD1	1:A:61:THR:OG1	2.29	0.43
1:A:456:VAL:HG23	1:A:457:TYR:CD2	2.54	0.43
1:B:13:SER:HB3	1:B:92:LEU:HB2	2.01	0.43
1:A:241:VAL:HG13	5:A:816:HOH:O	2.18	0.43
1:A:451:THR:HG21	1:A:585:LEU:HD23	2.00	0.43
1:B:28:LYS:CB	1:B:97:CYS:SG	3.07	0.42
1:B:284:PRO:HG2	1:B:566:THR:HG21	2.01	0.42
1:A:390:ARG:O	1:A:391:LEU:HD23	2.18	0.42
1:B:533:VAL:HG11	1:B:560:ARG:O	2.20	0.42
1:A:18:ALA:HB3	1:A:39:HIS:ND1	2.35	0.42
1:A:457:TYR:O	1:A:458:ASP:C	2.62	0.42
1:B:8:CYS:SG	1:B:99:GLY:O	2.78	0.42
1:B:77:PRO:HB2	1:B:78:PRO:HD2	2.02	0.42
1:A:279:THR:HB	1:A:429:MET:HE2	2.02	0.42
1:A:331:SER:HA	1:A:347:LYS:O	2.20	0.42
1:B:177:ASN:HB2	1:B:516:ASN:HD21	1.83	0.42
1:B:477:LYS:NZ	1:B:551:GLU:OE2	2.50	0.42
1:A:544:VAL:O	1:A:572:ILE:HA	2.20	0.42
1:B:129:ARG:HA	1:B:129:ARG:HD2	1.81	0.42
1:B:258:ILE:HG13	1:B:259:SER:N	2.34	0.41
1:A:63:LEU:HB3	1:A:83:LEU:HD12	2.02	0.41
1:A:127:THR:O	1:A:131:LYS:HG3	2.20	0.41
1:B:263:SER:HA	1:B:266:VAL:HG23	2.01	0.41
1:B:419:PRO:HA	1:B:422:PHE:CE1	2.56	0.41
1:A:435:ASP:C	1:A:436:MET:HG3	2.45	0.41
1:A:512:ILE:HA	1:A:531:GLN:O	2.19	0.41
1:B:12:THR:CG2	1:B:14:LEU:H	2.26	0.41
1:B:19:CYS:HB2	1:B:23:PRO:HD2	2.00	0.41
1:A:120:TYR:CE2	1:A:409:ARG:HG2	2.56	0.41
1:B:61:THR:HG22	1:B:84:CYS:SG	2.61	0.41
1:B:262:PHE:CE2	1:B:297:LEU:HD12	2.55	0.41
1:A:252:LEU:HD21	1:A:369:ASP:HB3	2.02	0.41
1:B:214:THR:O	1:B:215:THR:HB	2.21	0.41
1:B:512:ILE:HA	1:B:531:GLN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:HIS:ND1	1:A:275:GLN:HG2	2.35	0.41
1:B:44:SER:O	1:B:45:VAL:C	2.63	0.41
1:B:249:ILE:HG23	1:B:273:GLY:HA3	2.01	0.41
1:A:76:LYS:HD2	1:A:80:SER:OG	2.21	0.41
1:B:59:ASP:OD1	1:B:59:ASP:C	2.63	0.41
1:A:521:VAL:HG12	1:A:525:ILE:HD12	2.03	0.40
1:A:139:LYS:O	1:A:143:GLU:HG2	2.21	0.40
1:B:92:LEU:HB3	1:B:93:TYR:CD2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	564/601 (94%)	515 (91%)	43 (8%)	6 (1%)	11	10
1	B	580/601 (96%)	542 (93%)	36 (6%)	2 (0%)	36	42
All	All	1144/1202 (95%)	1057 (92%)	79 (7%)	8 (1%)	18	19

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	215	THR
1	B	45	VAL
1	A	484	VAL
1	A	208	ALA
1	A	283	PRO
1	A	195	ILE
1	A	6	VAL
1	A	249	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%)	467 (96%)	18 (4%)	30	41
1	B	498/523 (95%)	471 (95%)	27 (5%)	20	25
All	All	983/1046 (94%)	938 (95%)	45 (5%)	24	32

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	26	CYS
1	A	44	SER
1	A	46	ASN
1	A	81	PHE
1	A	86	ASN
1	A	156	GLU
1	A	163	LEU
1	A	173	ARG
1	A	209	VAL
1	A	226	VAL
1	A	255	THR
1	A	392	ARG
1	A	424	SER
1	A	502	ARG
1	A	530	THR
1	A	531	GLN
1	A	592	ILE
1	B	10	SER
1	B	13	SER
1	B	35	ILE
1	B	68	MET
1	B	69	SER
1	B	76	LYS
1	B	96	THR
1	B	97	CYS
1	B	100	SER

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Mol	Chain	Res	Type
1	B	103	VAL
1	B	158	LEU
1	B	164	HIS
1	B	190	ASN
1	B	191	SER
1	B	192	LYS
1	B	195	ILE
1	B	219	LEU
1	B	220	ASN
1	B	247	VAL
1	B	258	ILE
1	B	275	GLN
1	B	278	SER
1	B	350	SER
1	B	353	GLU
1	B	458	ASP
1	B	484	VAL
1	B	592	ILE

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	11	GLN
1	A	116	ASN
1	A	179	ASN
1	A	275	GLN
1	A	404	GLN
1	A	459	ASN
1	A	503	ASN
1	A	516	ASN
1	B	46	ASN
1	B	51	ASN
1	B	75	HIS
1	B	88	GLN
1	B	179	ASN
1	B	268	ASN
1	B	404	GLN
1	B	459	ASN
1	B	470	GLN
1	B	516	ASN
1	B	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 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$
3	PO4	A	704	-	4,4,4	0.99	0	6,6,6	0.64	0
3	PO4	B	705	-	4,4,4	1.08	0	6,6,6	0.43	0
4	VXG	B	701	-	18,18,18	0.81	1 (5%)	21,25,25	0.81	0
3	PO4	B	706	-	4,4,4	0.86	0	6,6,6	0.42	0
3	PO4	A	705	-	4,4,4	0.82	0	6,6,6	0.51	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	VXG	B	701	-	-	0/12/24/24	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	701	VXG	O3-C1	-3.21	1.20	1.30

There are no bond angle outliers.

There are no chirality outliers.

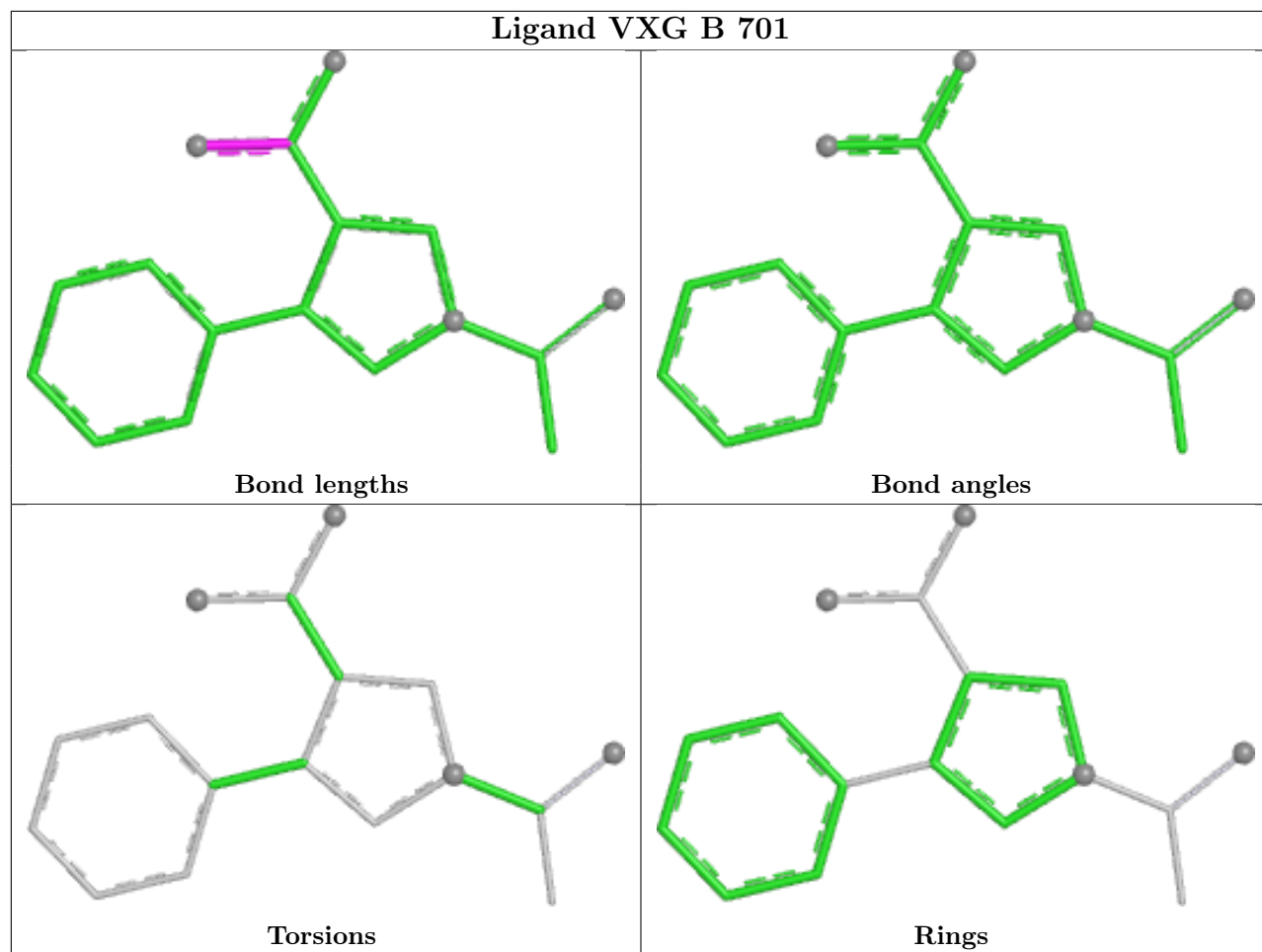
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	705	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%)	0.90	117 (20%) 2 2	27, 69, 156, 231	0
1	B	585/601 (97%)	0.12	18 (3%) 51 48	20, 46, 96, 137	1 (0%)
All	All	1157/1202 (96%)	0.51	135 (11%) 9 7	20, 55, 130, 231	1 (0%)

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	592	ILE	5.5
1	A	169	VAL	4.7
1	A	225	PHE	4.6
1	A	151	ILE	4.4
1	B	102	ASN	4.0
1	A	6	VAL	4.0
1	A	45	VAL	3.9
1	A	340	VAL	3.8
1	A	258	ILE	3.8
1	A	84	CYS	3.8
1	A	149	TYR	3.7
1	A	154	VAL	3.8
1	A	296	ALA	3.7
1	A	334	ILE	3.6
1	A	2	VAL	3.6
1	A	224	TYR	3.6
1	A	7	LEU	3.5
1	B	217	TYR	3.4
1	A	305	VAL	3.3
1	A	170	GLY	3.3
1	A	209	VAL	3.3
1	A	226	VAL	3.3
1	A	181	VAL	3.3
1	A	103	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	25	LEU	3.2
1	A	132	LEU	3.2
1	A	235	LEU	3.2
1	A	182	PHE	3.2
1	B	203	GLY	3.2
1	A	200	PHE	3.1
1	A	165	LEU	3.1
1	A	167	TRP	3.1
1	A	355	TYR	3.1
1	A	300	PRO	3.1
1	A	387	VAL	3.1
1	B	208	ALA	3.0
1	A	393	ALA	3.0
1	B	336	ALA	2.9
1	A	256	LEU	2.9
1	A	249	ILE	2.9
1	A	176	LEU	2.9
1	A	157	VAL	2.9
1	A	371	VAL	2.9
1	A	184	GLY	2.9
1	A	1	ALA	2.9
1	A	252	LEU	2.9
1	A	210	VAL	2.8
1	A	153	THR	2.8
1	A	272	VAL	2.8
1	A	92	LEU	2.7
1	A	221	VAL	2.7
1	A	277	TYR	2.7
1	A	396	TYR	2.7
1	A	328	ASP	2.7
1	A	195	ILE	2.7
1	A	240	LEU	2.7
1	A	326	PRO	2.7
1	A	43	LEU	2.7
1	A	232	VAL	2.6
1	B	592	ILE	2.6
1	A	145	PHE	2.6
1	B	98	VAL	2.6
1	A	370	ILE	2.6
1	A	215	THR	2.6
1	A	152	ALA	2.5
1	A	247	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	340	VAL	2.5
1	A	227	LEU	2.5
1	A	318	CYS	2.5
1	A	49	VAL	2.5
1	A	266	VAL	2.5
1	B	214	THR	2.5
1	A	163	LEU	2.5
1	B	81	PHE	2.4
1	A	155	ARG	2.4
1	A	254	PRO	2.4
1	A	273	GLY	2.4
1	A	304	ILE	2.4
1	A	183	THR	2.4
1	A	416	THR	2.4
1	A	70	TYR	2.3
1	A	217	TYR	2.3
1	A	306	TYR	2.3
1	A	91	GLY	2.3
1	A	4	ALA	2.3
1	A	144	THR	2.3
1	A	219	LEU	2.3
1	A	198	TYR	2.3
1	A	338	ALA	2.3
1	A	485	SER	2.3
1	B	2	VAL	2.3
1	A	9	ASN	2.3
1	A	185	TYR	2.3
1	A	214	THR	2.3
1	A	297	LEU	2.2
1	A	352	LEU	2.2
1	A	428	LEU	2.2
1	A	178	ARG	2.2
1	A	196	GLY	2.2
1	A	299	TYR	2.2
1	A	325	LEU	2.2
1	B	176	LEU	2.2
1	A	245	HIS	2.2
1	A	351	THR	2.2
1	A	93	TYR	2.2
1	A	333	ILE	2.2
1	B	213	GLY	2.2
1	B	230	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	255	THR	2.2
1	A	180	TYR	2.2
1	A	356	VAL	2.2
1	B	179	ASN	2.2
1	A	307	THR	2.2
1	A	179	ASN	2.1
1	A	237	ALA	2.1
1	A	94	LYS	2.1
1	A	172	PRO	2.1
1	A	346	PHE	2.1
1	A	228	THR	2.1
1	A	229	SER	2.1
1	A	324	TYR	2.1
1	B	195	ILE	2.1
1	A	81	PHE	2.1
1	A	336	ALA	2.1
1	B	256	LEU	2.1
1	A	24	PHE	2.1
1	A	147	LEU	2.0
1	A	220	ASN	2.0
1	A	161	ARG	2.0
1	A	301	SER	2.0
1	A	292	ALA	2.0
1	A	27	CYS	2.0
1	B	97	CYS	2.0
1	A	335	PRO	2.0
1	A	171	LYS	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.

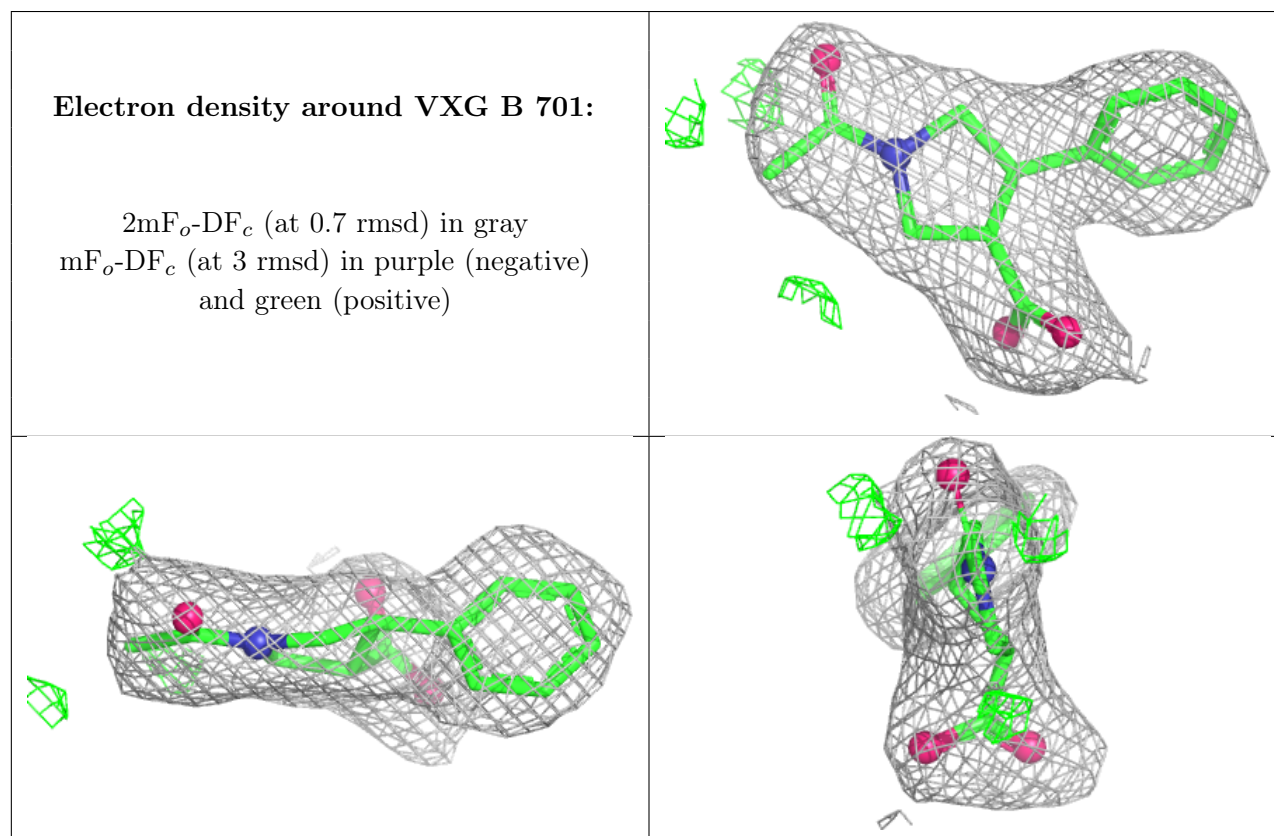
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
4	VXG	B	701	17/17	0.93	0.09	33,44,48,49	17
3	PO4	A	705	5/5	0.97	0.06	37,40,44,45	0
3	PO4	B	705	5/5	0.97	0.05	37,39,42,50	0
2	ZN	A	703	1/1	0.97	0.06	84,84,84,84	0
3	PO4	A	704	5/5	0.98	0.06	39,41,43,49	0
2	ZN	A	702	1/1	0.98	0.04	58,58,58,58	0
2	ZN	B	703	1/1	0.99	0.02	57,57,57,57	0
2	ZN	B	704	1/1	0.99	0.03	83,83,83,83	0
3	PO4	B	706	5/5	0.99	0.04	33,33,35,36	0
2	ZN	A	701	1/1	0.99	0.02	56,56,56,56	0
2	ZN	B	702	1/1	1.00	0.01	42,42,42,42	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.