Full wwPDB X-ray Structure Validation Report (i)

Sep 1, 2022 – 12:37 PM EDT

PDB ID	:	5RMM
Title	:	PanDDA analysis group deposition – Crystal Structure of SARS-CoV-2 helicase in complex with POB0066
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	:	2.20 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 (i) 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:

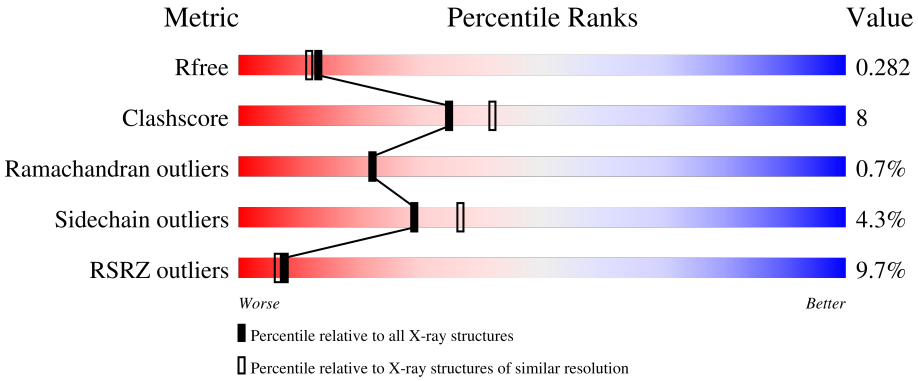
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 <=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	16% 72% 22% • 5%
1	B	601	2% 78% 18% • •

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.

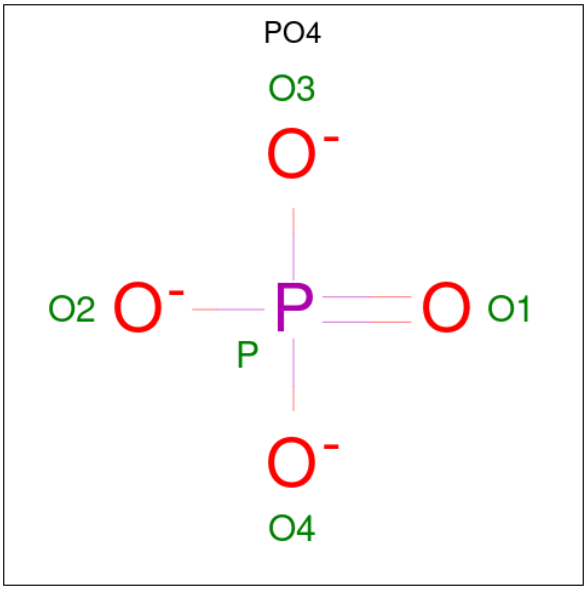
- Molecule 1 is a protein called Helicase.

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 (three-letter code: ZN) (formula: Zn).

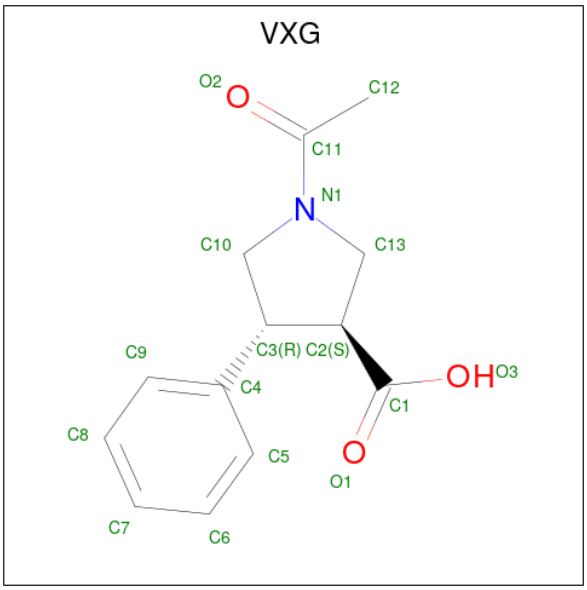
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	3	Total	Zn	0	0
			3	3		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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 (three-letter code: VXG) (formula: $C_{13}H_{15}NO_3$) (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.

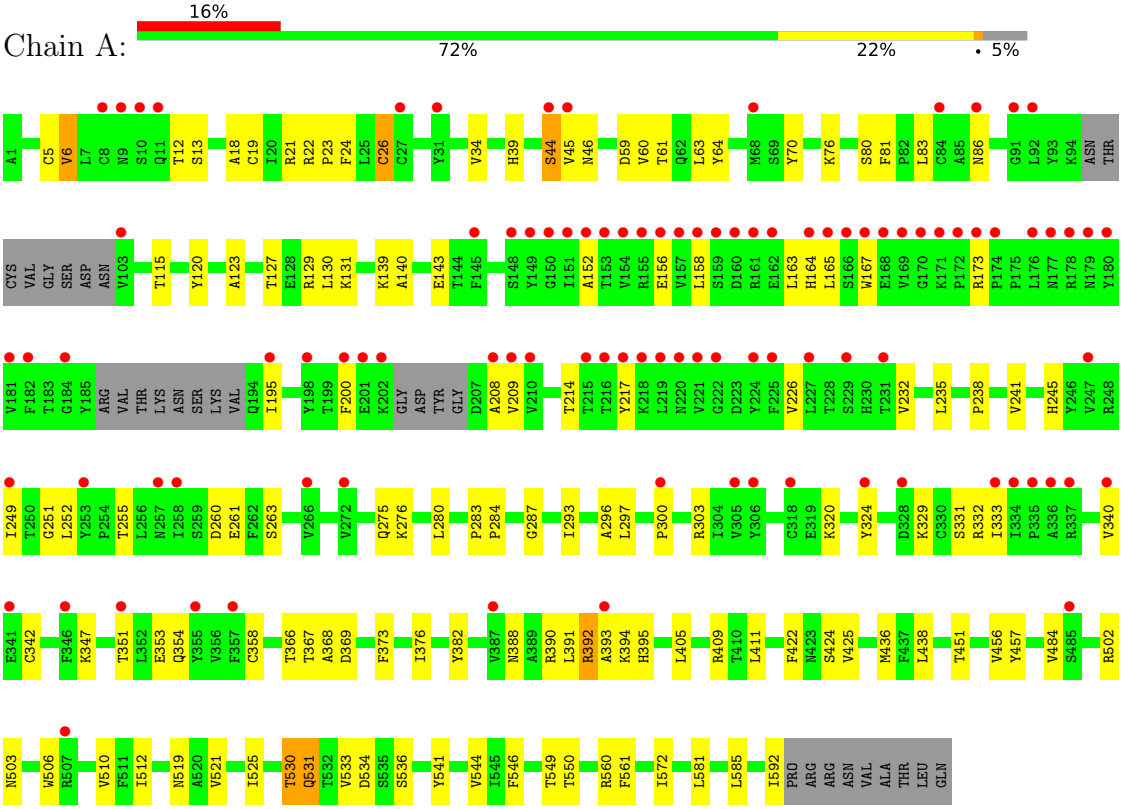
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	202	Total O 202 202	0	0
5	B	251	Total O 251 251	0	0

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.

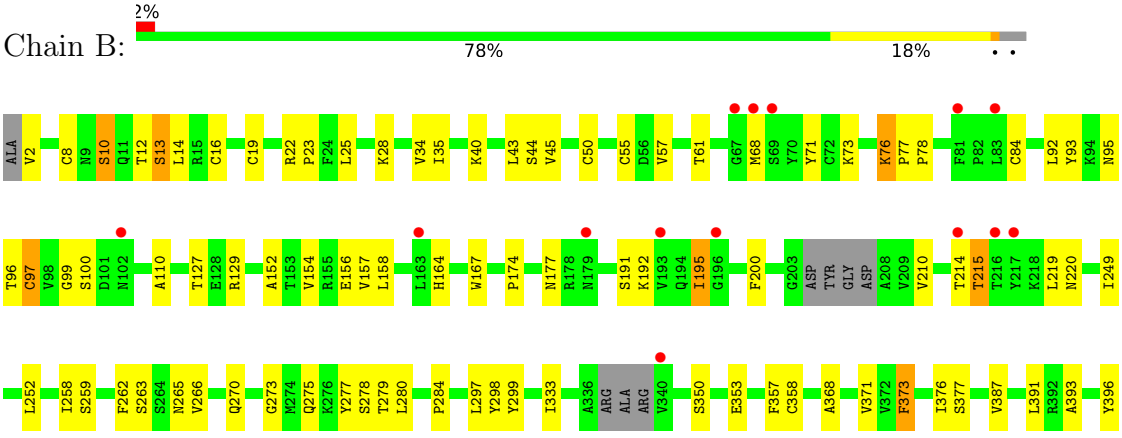
• Molecule 1: Helicase

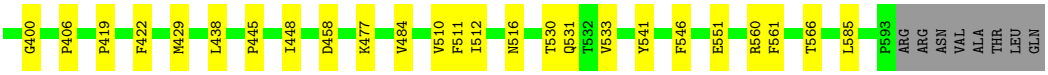
Chain A:



• Molecule 1: Helicase

Chain B:




G400
P406
P419
F422
M429
L438
P445
I448
D458
K477
V484
V510
F511
I512
N516
T530
Q531
T532
V533
Y541
F546
E551
R560
F561
T566
L585
P593
ARG
ARG
ASN
VAL
ALA
THR
LEU
GLN

4 Data and refinement statistics (i)

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) 97.2 (81.56-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.18%)	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 , 47.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PO4, VXG, 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	0.69	0/4517	0.81	0/6156
1	B	0.66	0/4610	0.82	0/6283
All	All	0.68	0/9127	0.81	0/12439

There are no bond length outliers.

There are no bond angle outliers.

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	79	0
1	B	4508	0	4424	68	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	8	0
5	B	251	0	0	3	0
All	All	9421	0	8746	147	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 8.

All (147) 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: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:A:329:LYS:CE	1:A:354:GLN:OE1	2.43	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:B:8:CYS:SG	1:B:99:GLY:C	2.77	0.63
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: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
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:279:THR:HB	1:B:429:MET:HE2	1.88	0.56
1:A:115:THR:HA	1:A:411:LEU:O	2.06	0.56
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:21:ARG:O	1:A:22:ARG:C	2.50	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:59:ASP:OD1	1:A:61:THR:OG1	2.29	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
1:B:14:LEU:HA	1:B:43:LEU:O	2.15	0.47
1:B:376:ILE:HG21	1:B:429:MET:HE3	1.95	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:B:34:VAL:O	1:B:40:LYS:NZ	2.46	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:B:195:ILE:HG23	1:B:195:ILE:O	2.15	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:279:THR:HB	1:B:429:MET:CE	2.47	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
1:B:477:LYS:NZ	1:B:551:GLU:OE2	2.50	0.44
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: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: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:B:8:CYS:SG	1:B:99:GLY:O	2.78	0.42
1:A:390:ARG:O	1:A:391:LEU:HD23	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:77:PRO:HB2	1:B:78:PRO:HD2	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: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: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
1:A:245:HIS:ND1	1:A:275:GLN:HG2	2.35	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: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 (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%)	515 (91%)	43 (8%)	6 (1%)	14 12
1	B	580/601 (96%)	542 (93%)	36 (6%)	2 (0%)	41 46
All	All	1144/1202 (95%)	1057 (92%)	79 (7%)	8 (1%)	22 22

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 (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 39
1	B	498/523 (95%)	476 (96%)	22 (4%)	28 35
All	All	983/1046 (94%)	941 (96%)	42 (4%)	29 36

All (42) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	173	ARG
1	A	209	VAL
1	A	217	TYR
1	A	226	VAL
1	A	255	THR
1	A	373	PHE
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	76	LYS
1	B	95	ASN
1	B	96	THR
1	B	97	CYS
1	B	100	SER
1	B	158	LEU
1	B	191	SER
1	B	192	LYS
1	B	195	ILE
1	B	219	LEU
1	B	220	ASN
1	B	275	GLN
1	B	278	SER
1	B	350	SER
1	B	353	GLU
1	B	373	PHE
1	B	458	ASP
1	B	484	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	ASN
1	A	179	ASN
1	A	404	GLN
1	A	503	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	51	ASN
1	B	88	GLN
1	B	179	ASN
1	B	268	ASN
1	B	470	GLN
1	B	516	ASN
1	B	531	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	VXG	B	701	-	18,18,18	0.79	1 (5%)	21,25,25	0.80	0
3	PO4	A	705	-	4,4,4	0.77	0	6,6,6	0.47	0
3	PO4	B	706	-	4,4,4	0.84	0	6,6,6	0.40	0
3	PO4	B	705	-	4,4,4	1.03	0	6,6,6	0.41	0
3	PO4	A	704	-	4,4,4	0.94	0	6,6,6	0.60	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	-3.09	1.20	1.30

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

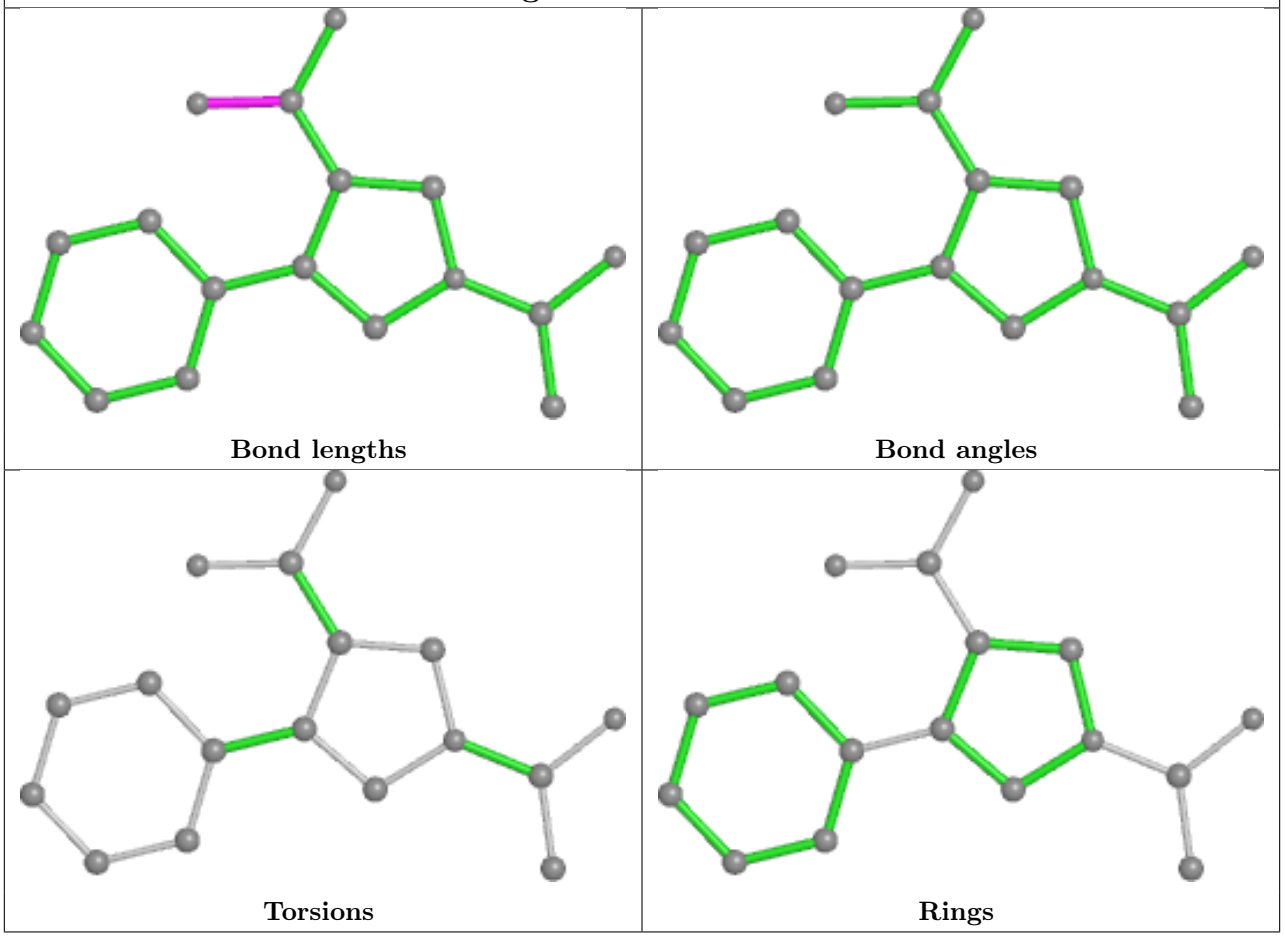
There are no ring outliers.

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 then 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.

Ligand VXG B 701



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, 95^{th} 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%)	0.77	98 (17%) 1 1	27, 69, 156, 231	0
1	B	585/601 (97%)	-0.10	14 (2%) 59 56	26, 46, 96, 137	0
All	All	1157/1202 (96%)	0.33	112 (9%) 7 6	26, 55, 130, 231	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	178	ARG	13.1
1	A	149	TYR	12.7
1	A	167	TRP	11.6
1	A	156	GLU	10.6
1	A	170	GLY	9.6
1	A	154	VAL	9.2
1	A	225	PHE	9.2
1	A	169	VAL	8.7
1	A	182	PHE	8.0
1	A	152	ALA	8.0
1	A	229	SER	7.9
1	A	165	LEU	6.9
1	A	202	LYS	6.6
1	A	157	VAL	6.6
1	A	210	VAL	6.3
1	A	221	VAL	5.9
1	B	217	TYR	5.7
1	A	9	ASN	5.6
1	A	215	THR	5.6
1	A	217	TYR	5.5
1	A	340	VAL	5.4
1	B	81	PHE	5.1
1	A	176	LEU	5.1
1	A	224	TYR	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	153	THR	4.7
1	A	200	PHE	4.7
1	B	340	VAL	4.6
1	A	334	ILE	4.6
1	B	67	GLY	4.5
1	A	184	GLY	4.4
1	A	219	LEU	4.3
1	A	168	GLU	4.3
1	A	218	LYS	4.2
1	A	328	ASP	4.2
1	A	272	VAL	4.1
1	A	45	VAL	4.1
1	A	86	ASN	4.1
1	A	164	HIS	3.9
1	A	336	ALA	3.9
1	A	181	VAL	3.8
1	A	266	VAL	3.7
1	A	180	TYR	3.7
1	B	214	THR	3.7
1	A	247	VAL	3.6
1	A	166	SER	3.6
1	A	220	ASN	3.5
1	A	249	ILE	3.5
1	A	155	ARG	3.5
1	A	84	CYS	3.4
1	A	162	GLU	3.4
1	A	172	PRO	3.4
1	A	216	THR	3.4
1	A	257	ASN	3.3
1	A	161	ARG	3.3
1	A	258	ILE	3.2
1	A	198	TYR	3.2
1	A	387	VAL	3.2
1	A	208	ALA	3.2
1	A	103	VAL	3.2
1	A	151	ILE	3.1
1	A	195	ILE	3.1
1	A	335	PRO	3.0
1	A	300	PRO	3.0
1	A	341	GLU	2.9
1	A	209	VAL	2.9
1	A	305	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	222	GLY	2.8
1	A	179	ASN	2.8
1	A	159	SER	2.8
1	A	174	PRO	2.7
1	A	357	PHE	2.7
1	A	158	LEU	2.7
1	B	68	MET	2.6
1	A	351	THR	2.6
1	A	10	SER	2.6
1	A	201	GLU	2.6
1	A	324	TYR	2.6
1	B	196	GLY	2.6
1	A	177	ASN	2.5
1	A	92	LEU	2.5
1	B	69	SER	2.5
1	A	171	LYS	2.5
1	A	507	ARG	2.5
1	A	231	THR	2.4
1	A	145	PHE	2.3
1	A	346	PHE	2.3
1	A	337	ARG	2.3
1	A	355	TYR	2.3
1	A	485	SER	2.3
1	B	83	LEU	2.2
1	A	8	CYS	2.2
1	A	91	GLY	2.2
1	A	150	GLY	2.2
1	A	148	SER	2.2
1	A	333	ILE	2.2
1	A	173	ARG	2.1
1	A	27	CYS	2.1
1	A	160	ASP	2.1
1	A	44	SER	2.1
1	A	318	CYS	2.1
1	A	306	TYR	2.1
1	A	11	GLN	2.1
1	A	227	LEU	2.1
1	B	163	LEU	2.1
1	A	68	MET	2.1
1	A	393	ALA	2.1
1	B	179	ASN	2.1
1	B	193	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	31	TYR	2.1
1	A	253	TYR	2.1
1	B	102	ASN	2.0
1	B	216	THR	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)

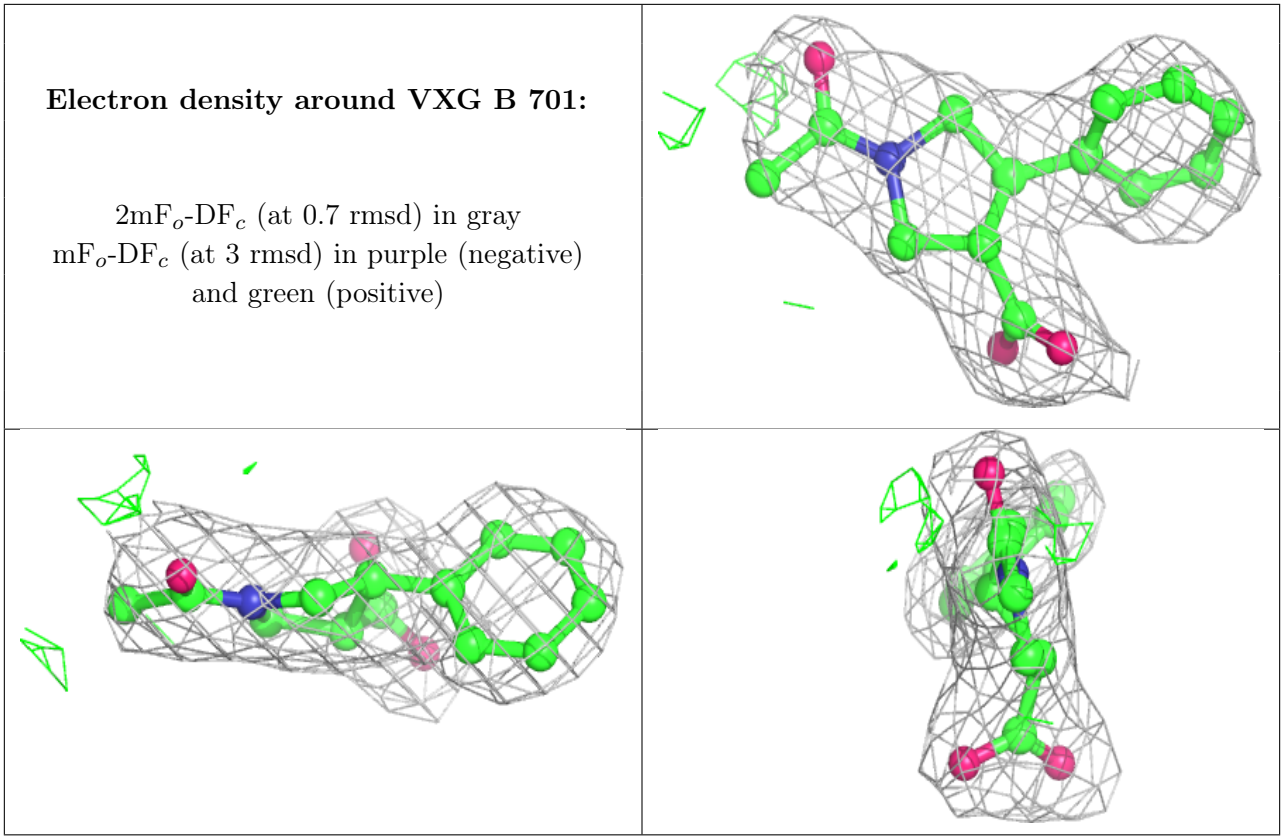
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	ZN	A	703	1/1	0.95	0.05	84,84,84,84	0
4	VXG	B	701	17/17	0.95	0.14	33,44,48,49	17
2	ZN	B	704	1/1	0.96	0.07	83,83,83,83	0
2	ZN	A	702	1/1	0.96	0.09	58,58,58,58	0
3	PO4	B	705	5/5	0.98	0.13	37,39,42,50	0
2	ZN	A	701	1/1	0.99	0.12	56,56,56,56	0
3	PO4	A	704	5/5	0.99	0.09	39,41,43,49	0
3	PO4	A	705	5/5	0.99	0.12	37,40,44,45	0
2	ZN	B	702	1/1	0.99	0.11	42,42,42,42	0
3	PO4	B	706	5/5	0.99	0.13	33,33,35,36	0
2	ZN	B	703	1/1	0.99	0.12	57,57,57,57	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 VXG 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.