



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2024 – 03:52 AM EST

PDB ID : 1C4G  
Title : PHOSPHOGLUCOMUTASE VANADATE BASED TRANSITION STATE ANALOG COMPLEX  
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Deposited on : 1999-08-24  
Resolution : 2.70 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

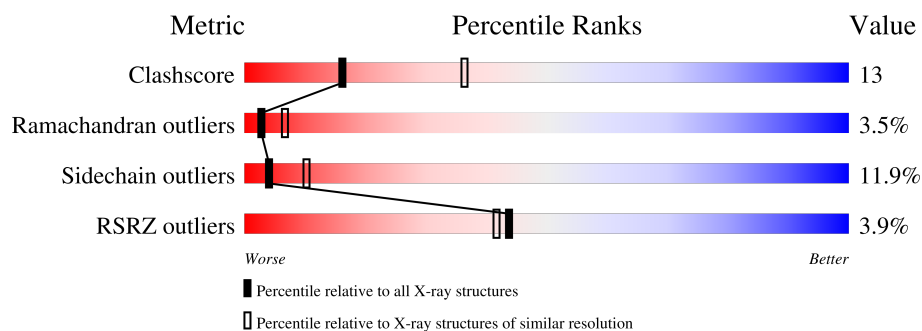
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	561	 6% 63% 29% 7%
1	B	561	 2% 67% 28% 5%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8877 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.

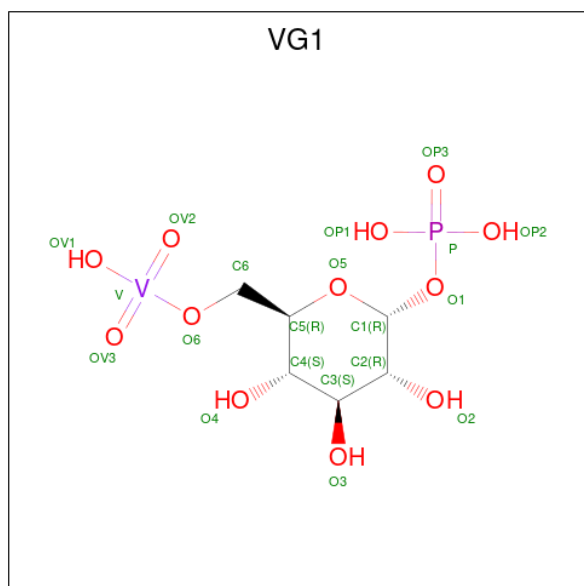
- Molecule 1 is a protein called PROTEIN (ALPHA-D-GLUCOSE 1-PHOSPHATE PHOSPHOGLUCOMUTASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	561	Total	C	N	O	S	0	0	0
			4329	2753	743	817	16			
1	B	561	Total	C	N	O	S	0	0	0
			4329	2753	743	817	16			

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Co	0	0
			1	1		

- Molecule 3 is ALPHA-D-GLUCOSE-1-PHOSPHATE-6-VANADATE (three-letter code: VG1) (formula: C<sub>6</sub>H<sub>13</sub>O<sub>12</sub>PV).

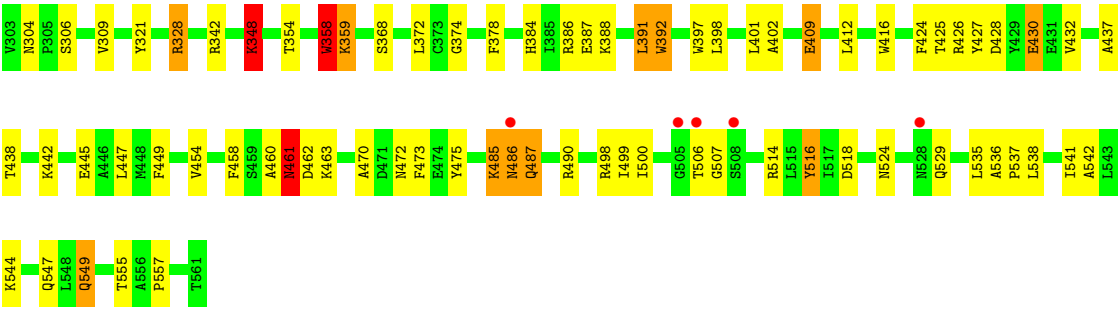


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	O	P	V	0	0
			20	6	12	1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	84	Total	O	0	0
			84	84		
4	B	114	Total	O	0	0
			114	114		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	174.42Å 174.42Å 101.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.70 6.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	85.9 (6.00-2.70) 74.2 (6.00-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.10 (at 2.71Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.192 , 0.290 0.255 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.2	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 100.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	8877	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CO, VG1

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	1.22	4/4416 (0.1%)	1.06	16/5969 (0.3%)
1	B	1.11	3/4416 (0.1%)	1.05	17/5969 (0.3%)
All	All	1.16	7/8832 (0.1%)	1.05	33/11938 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
All	All	0	4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	416	TRP	CG-CD2	-5.72	1.33	1.43
1	A	488	GLY	N-CA	5.65	1.54	1.46
1	A	239	GLU	CD-OE1	-5.64	1.19	1.25
1	B	392	TRP	CG-CD2	-5.24	1.34	1.43
1	A	445	GLU	CG-CD	5.19	1.59	1.51
1	A	476	HIS	CB-CG	5.19	1.59	1.50
1	B	358	TRP	CG-CD2	-5.18	1.34	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	397	TRP	CD1-CG-CD2	13.96	117.47	106.30
1	B	358	TRP	CD1-CG-CD2	13.45	117.06	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	416	TRP	CD1-CG-CD2	13.44	117.06	106.30
1	B	392	TRP	CD1-CG-CD2	13.30	116.94	106.30
1	B	397	TRP	CD1-CG-CD2	13.21	116.87	106.30
1	B	416	TRP	CD1-CG-CD2	13.09	116.77	106.30
1	A	392	TRP	CD1-CG-CD2	13.05	116.74	106.30
1	A	392	TRP	CE2-CD2-CG	-8.93	100.15	107.30
1	A	397	TRP	CE2-CD2-CG	-8.39	100.59	107.30
1	B	358	TRP	CE2-CD2-CG	-8.37	100.60	107.30
1	B	392	TRP	CE2-CD2-CG	-8.30	100.66	107.30
1	B	397	TRP	CE2-CD2-CG	-8.10	100.82	107.30
1	A	416	TRP	CE2-CD2-CG	-7.89	100.99	107.30
1	B	416	TRP	CE2-CD2-CG	-7.78	101.08	107.30
1	A	397	TRP	CG-CD1-NE1	-7.10	103.00	110.10
1	B	397	TRP	CG-CD1-NE1	-7.07	103.03	110.10
1	A	392	TRP	CB-CG-CD1	-6.90	118.03	127.00
1	A	397	TRP	CB-CG-CD1	-6.85	118.09	127.00
1	A	392	TRP	CG-CD1-NE1	-6.72	103.38	110.10
1	A	416	TRP	CG-CD1-NE1	-6.66	103.44	110.10
1	B	416	TRP	CG-CD1-NE1	-6.64	103.46	110.10
1	B	392	TRP	CB-CG-CD1	-6.63	118.38	127.00
1	B	358	TRP	CB-CG-CD1	-6.45	118.62	127.00
1	B	397	TRP	CB-CG-CD1	-6.19	118.95	127.00
1	B	392	TRP	CG-CD1-NE1	-6.18	103.92	110.10
1	A	392	TRP	CG-CD2-CE3	5.97	139.27	133.90
1	B	358	TRP	CG-CD1-NE1	-5.92	104.18	110.10
1	A	386	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	A	397	TRP	CG-CD2-CE3	5.32	138.68	133.90
1	A	416	TRP	CB-CG-CD1	-5.20	120.24	127.00
1	B	63	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	A	487	GLN	N-CA-C	5.14	124.88	111.00
1	B	392	TRP	CG-CD2-CE3	5.09	138.48	133.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	321	TYR	Sidechain
1	A	427	TYR	Sidechain
1	A	520	TYR	Sidechain
1	B	516	TYR	Sidechain

## 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	4329	0	4332	108	0
1	B	4329	0	4333	115	0
2	A	1	0	0	0	0
3	A	20	0	10	3	0
4	A	84	0	0	4	0
4	B	114	0	0	10	0
All	All	8877	0	8675	223	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 13.

All (223) 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:70:ILE:HG21	1:A:166:LEU:HD21	1.34	1.09
1:B:40:GLN:HG3	1:B:156:TYR:HB2	1.47	0.96
1:B:63:ARG:HH22	1:B:115:ALA:HB2	1.35	0.91
1:A:441:MET:SD	1:A:501:PHE:HB3	2.15	0.86
1:B:391:LEU:HD23	4:B:573:HOH:O	1.77	0.85
1:B:118:ASN:HD22	1:B:119:PRO:HD2	1.44	0.81
1:A:116:SER:HB3	3:A:563:VG1:OV2	1.81	0.80
1:A:287:ASP:HB2	1:A:292:ARG:HB2	1.61	0.80
1:A:429:TYR:HB2	1:A:513:ILE:HB	1.66	0.78
1:A:7:LYS:HD3	1:A:155:GLU:HB3	1.62	0.78
1:A:309:VAL:HG13	1:A:380:THR:HG23	1.65	0.76
1:B:427:TYR:CD1	1:B:557:PRO:HG3	2.21	0.75
1:B:224:MET:SD	1:B:286:PHE:O	2.51	0.69
1:B:168:VAL:HG23	4:B:563:HOH:O	1.92	0.68
1:B:148:GLN:HA	1:B:151:LYS:HE3	1.76	0.67
1:A:447:LEU:HD23	1:A:448:MET:N	2.11	0.66
1:A:356:THR:HG21	1:A:502:ARG:NH2	2.11	0.66
1:A:356:THR:CG2	1:A:502:ARG:NH2	2.59	0.66
1:A:95:THR:HG22	1:A:112:ILE:HD13	1.78	0.65
1:A:436:GLY:HA3	1:A:552:THR:HG23	1.78	0.65
1:B:63:ARG:NH2	1:B:115:ALA:HB2	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ARG:HD3	1:B:120:GLY:HA3	1.78	0.64
1:B:256:PHE:HD1	1:B:261:PRO:HG3	1.63	0.64
1:B:358:TRP:NE1	1:B:388:LYS:HG3	2.13	0.62
1:A:356:THR:CG2	1:A:502:ARG:HH22	2.13	0.61
1:B:426:ARG:NH2	4:B:672:HOH:O	2.33	0.61
1:A:473:PHE:HB2	1:A:490:ARG:CZ	2.31	0.60
1:B:384:HIS:HB3	4:B:614:HOH:O	2.00	0.60
1:A:450:ASP:HB3	1:A:453:PHE:CE1	2.36	0.60
1:B:261:PRO:HB2	1:B:287:ASP:HA	1.83	0.60
1:B:458:PHE:HB3	1:B:541:ILE:HD13	1.83	0.60
1:A:303:VAL:HG13	1:A:412:LEU:HD11	1.84	0.60
1:A:383:ASP:HB2	1:A:386:ARG:HH21	1.66	0.59
1:B:228:VAL:HG12	4:B:583:HOH:O	2.03	0.59
1:B:14:GLN:HE21	1:B:150:SER:HB2	1.67	0.59
1:B:198:LEU:HD22	1:B:202:PHE:HE2	1.66	0.59
1:A:316:ILE:HD13	1:A:327:VAL:HG22	1.84	0.58
1:A:431:GLU:OE2	1:A:510:GLY:HA3	2.04	0.58
1:B:233:LYS:HE3	1:B:247:ALA:HB3	1.85	0.58
1:B:60:GLY:HA3	1:B:66:MET:SD	2.43	0.57
1:A:388:LYS:NZ	3:A:563:VG1:OV1	2.38	0.57
1:B:387:GLU:HG3	1:B:388:LYS:H	1.71	0.56
1:A:548:LEU:HD12	1:A:548:LEU:H	1.70	0.56
1:B:25:VAL:HG22	1:B:126:PHE:HB2	1.87	0.56
1:A:383:ASP:HB2	1:A:386:ARG:NH2	2.21	0.56
1:B:102:ILE:HD11	1:B:110:GLY:HA3	1.88	0.56
1:B:263:PRO:HB3	1:B:294:MET:HB2	1.88	0.56
1:B:88:GLY:HA3	1:B:93:LEU:HD13	1.87	0.56
1:A:335:PRO:HA	1:A:500:ILE:CD1	2.36	0.56
1:B:255:ASP:O	1:B:256:PHE:HB2	2.07	0.55
1:A:63:ARG:HD2	1:A:125:ASP:O	2.06	0.55
1:A:164:VAL:HG22	1:A:174:PHE:CZ	2.41	0.55
1:B:309:VAL:HG21	1:B:374:GLY:HA3	1.87	0.55
1:B:536:ALA:HB3	1:B:537:PRO:HD3	1.88	0.55
1:B:265:LEU:HD12	1:B:294:MET:SD	2.47	0.54
1:B:427:TYR:CE1	1:B:557:PRO:HG3	2.42	0.54
1:B:358:TRP:HE1	1:B:388:LYS:HG3	1.71	0.54
1:A:291:ASP:OD2	1:A:388:LYS:HG3	2.08	0.54
1:B:236:LEU:HA	1:B:240:LEU:HD12	1.89	0.54
1:B:256:PHE:CD1	1:B:261:PRO:HG3	2.43	0.53
1:B:460:ALA:HB3	1:B:537:PRO:HB3	1.89	0.53
1:A:4:VAL:HG12	1:A:160:PRO:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ARG:HB3	1:B:256:PHE:HE2	1.73	0.53
1:A:264:ASN:HD21	1:A:267:TYR:HD2	1.54	0.53
1:B:275:MET:SD	1:B:283:GLY:HA3	2.49	0.53
1:B:70:ILE:O	1:B:74:VAL:HG13	2.09	0.53
1:B:61:ASP:HB3	1:B:114:THR:HG22	1.91	0.53
1:B:63:ARG:HH12	1:B:115:ALA:CB	2.22	0.53
1:A:89:GLN:O	1:A:90:ASN:HB2	2.09	0.53
1:B:210:LEU:HG	1:B:402:ALA:HB2	1.90	0.53
1:A:469:LYS:O	1:A:470:ALA:HB2	2.09	0.53
1:B:24:ARG:O	1:B:27:VAL:HG12	2.09	0.52
1:A:89:GLN:HE21	1:A:169:LEU:HG	1.74	0.52
1:A:355:PRO:HD3	1:A:475:TYR:CG	2.45	0.52
1:A:472:ASN:ND2	1:A:489:LEU:HD23	2.24	0.52
1:B:432:VAL:CG1	1:B:437:ALA:HB2	2.40	0.52
1:A:365:MET:CE	1:A:373:CYS:SG	2.98	0.52
1:B:230:PRO:HD3	1:B:252:PRO:HD3	1.91	0.52
1:B:101:ILE:O	1:B:105:ILE:HG12	2.10	0.52
1:B:426:ARG:HD3	1:B:428:ASP:OD2	2.09	0.52
1:A:335:PRO:HA	1:A:500:ILE:HD12	1.92	0.52
1:B:147:PHE:O	1:B:151:LYS:HG2	2.10	0.52
1:B:473:PHE:O	1:B:487:GLN:HB2	2.10	0.52
1:A:489:LEU:O	1:A:500:ILE:HA	2.11	0.51
1:B:95:THR:CG2	1:B:387:GLU:HG2	2.40	0.51
1:B:432:VAL:HG11	1:B:437:ALA:HB2	1.93	0.51
1:A:473:PHE:HB2	1:A:490:ARG:NE	2.26	0.51
1:A:92:ILE:HG23	1:A:227:VAL:HG23	1.93	0.50
1:A:559:VAL:HG22	4:A:583:HOH:O	2.09	0.50
1:B:291:ASP:HB2	1:B:388:LYS:CB	2.41	0.50
1:A:264:ASN:HB2	1:A:561:THR:HG23	1.94	0.50
1:B:176:LEU:HD11	1:B:183:PHE:HB2	1.92	0.50
1:A:321:TYR:CZ	1:A:325:THR:HG21	2.47	0.50
1:A:335:PRO:O	1:A:424:PHE:HE2	1.95	0.50
1:A:309:VAL:HG13	1:A:380:THR:CG2	2.37	0.50
1:B:425:THR:CG2	1:B:535:LEU:HD13	2.41	0.50
1:A:108:ILE:HG23	4:A:618:HOH:O	2.12	0.49
1:A:272:VAL:HG22	1:A:296:LEU:HD21	1.95	0.49
1:A:432:VAL:HG23	1:A:433:GLU:H	1.76	0.49
1:A:536:ALA:HB3	1:A:537:PRO:HD3	1.93	0.49
1:A:306:SER:OG	1:A:336:THR:HG23	2.12	0.49
1:B:425:THR:HG22	1:B:535:LEU:HD13	1.93	0.49
1:B:291:ASP:OD1	1:B:388:LYS:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:LYS:O	1:B:149:ILE:HG13	2.12	0.49
1:A:356:THR:HG23	1:A:502:ARG:HH22	1.76	0.48
1:B:23:LYS:HB3	1:B:27:VAL:HG11	1.94	0.48
1:B:291:ASP:HB2	1:B:388:LYS:HB3	1.96	0.48
1:A:157:ALA:HB2	4:A:633:HOH:O	2.13	0.48
1:A:356:THR:HG23	1:A:502:ARG:NH2	2.28	0.48
1:B:32:THR:O	1:B:33:ASN:HB2	2.14	0.48
1:B:445:GLU:HG2	1:B:449:PHE:CE2	2.49	0.48
1:B:472:ASN:HD21	1:B:486:ASN:HA	1.78	0.48
1:A:3:ILE:HD11	1:A:176:LEU:HD12	1.95	0.47
1:A:514:ARG:NH2	3:A:563:VG1:OP1	2.43	0.47
1:B:55:THR:HA	1:B:84:ARG:O	2.14	0.47
1:A:151:LYS:HE2	1:A:152:THR:HG23	1.96	0.47
1:A:356:THR:HG21	1:A:502:ARG:HH22	1.76	0.47
1:B:260:HIS:HB2	1:B:267:TYR:HE2	1.79	0.47
1:A:201:ILE:HG23	1:A:321:TYR:HB2	1.97	0.47
1:B:270:ASP:O	1:B:274:THR:HG23	2.14	0.47
1:A:365:MET:HB3	1:A:386:ARG:CZ	2.45	0.47
1:A:404:ARG:O	1:A:405:LYS:HB2	2.14	0.47
1:B:398:LEU:HA	1:B:401:LEU:HD12	1.95	0.47
1:B:176:LEU:N	1:B:176:LEU:HD12	2.29	0.47
1:B:265:LEU:HD11	1:B:302:PHE:CD1	2.51	0.46
1:A:92:ILE:HG23	1:A:227:VAL:CG2	2.46	0.46
1:B:260:HIS:H	1:B:260:HIS:CD2	2.34	0.45
1:B:201:ILE:HG21	1:B:392:TRP:HE1	1.81	0.45
1:B:498:ARG:NH1	1:B:500:ILE:HD11	2.31	0.45
1:B:538:LEU:HD12	1:B:538:LEU:HA	1.79	0.45
1:B:328:ARG:H	1:B:328:ARG:HG2	1.57	0.45
1:A:489:LEU:HG	4:A:606:HOH:O	2.17	0.45
1:B:301:PHE:CD1	1:B:409:GLU:HG2	2.52	0.45
1:B:485:LYS:O	1:B:486:ASN:HB2	2.16	0.45
1:A:197:MET:SD	1:A:384:HIS:HD2	2.39	0.45
1:B:63:ARG:HB3	1:B:256:PHE:CE2	2.52	0.45
1:B:119:PRO:HA	4:B:585:HOH:O	2.15	0.45
1:A:3:ILE:HG12	1:A:159:CYS:SG	2.57	0.45
1:A:291:ASP:HB2	1:A:388:LYS:O	2.17	0.45
1:A:121:GLY:HA2	1:A:255:ASP:HA	1.98	0.45
1:A:477:ASP:HA	1:A:478:PRO:HD3	1.83	0.45
1:A:95:THR:HG22	1:A:112:ILE:HG21	1.99	0.45
1:A:329:GLY:HA3	1:A:369:LYS:O	2.17	0.45
1:A:445:GLU:O	1:A:446:ALA:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:GLY:O	1:A:554:ARG:HG2	2.17	0.45
1:B:14:GLN:NE2	1:B:150:SER:HB2	2.30	0.45
1:B:92:ILE:HG23	1:B:227:VAL:HG23	1.98	0.45
1:B:224:MET:SD	1:B:286:PHE:N	2.90	0.44
1:B:438:THR:O	1:B:442:LYS:HG3	2.17	0.44
1:B:499:ILE:HD13	1:B:542:ALA:HB2	1.99	0.44
1:B:549:GLN:OE1	1:B:555:THR:HG22	2.17	0.44
1:B:43:ILE:HD11	1:B:76:ILE:HG22	2.00	0.44
1:B:293:ASN:HD22	1:B:295:ILE:HD11	1.82	0.44
1:B:15:LYS:HD3	1:B:147:PHE:CD1	2.52	0.44
1:A:535:LEU:HB3	1:A:539:ILE:HD11	1.99	0.44
1:B:348:LYS:HA	1:B:348:LYS:HD2	1.57	0.44
1:A:204:PHE:CD2	1:A:240:LEU:HD11	2.52	0.44
1:A:210:LEU:HD11	1:A:217:LEU:HD22	1.99	0.44
1:A:334:MET:SD	1:A:500:ILE:HD13	2.58	0.44
1:B:538:LEU:HB2	4:B:632:HOH:O	2.17	0.44
1:A:271:LEU:HD22	1:A:285:ALA:HB2	2.00	0.44
1:A:358:TRP:CD1	1:A:388:LYS:HE2	2.53	0.44
1:B:33:ASN:O	1:B:37:ASN:HB2	2.18	0.44
1:A:416:TRP:HB3	1:A:527:ILE:HG21	1.99	0.43
1:B:176:LEU:HD11	1:B:183:PHE:CB	2.48	0.43
1:A:335:PRO:O	1:A:424:PHE:CE2	2.71	0.43
1:A:86:VAL:HG22	1:A:186:GLU:HB3	1.99	0.43
1:A:513:ILE:HG22	1:A:515:LEU:HD13	2.01	0.43
1:B:260:HIS:CD2	1:B:260:HIS:N	2.86	0.43
1:A:39:ILE:HG22	1:A:76:ILE:HG21	1.99	0.43
1:B:61:ASP:OD2	1:B:63:ARG:HG2	2.19	0.43
1:A:180:PHE:HB3	1:A:181:LYS:HD2	2.01	0.43
1:B:368:SER:HA	4:B:607:HOH:O	2.19	0.43
1:A:15:LYS:HB2	1:A:147:PHE:CE2	2.54	0.43
1:A:486:ASN:N	1:A:486:ASN:OD1	2.52	0.43
1:A:502:ARG:HD2	1:A:516:TYR:HE2	1.84	0.43
1:B:224:MET:SD	1:B:285:ALA:HB1	2.59	0.43
1:A:293:ASN:HB3	1:A:390:GLY:HA2	2.00	0.43
1:B:247:ALA:HB1	1:B:250:CYS:SG	2.59	0.43
1:B:198:LEU:HD22	1:B:202:PHE:CE2	2.51	0.43
1:A:228:VAL:HG11	1:A:286:PHE:CG	2.54	0.42
1:B:63:ARG:HH12	1:B:115:ALA:HB3	1.84	0.42
1:A:378:PHE:CD2	1:A:378:PHE:N	2.87	0.42
1:B:29:GLN:NE2	1:B:64:PHE:HE2	2.17	0.42
1:A:59:GLY:O	1:A:113:LEU:HD23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ILE:HG22	1:A:312:ILE:O	2.19	0.42
1:B:158:ILE:HG12	1:B:159:CYS:N	2.34	0.42
1:B:304:ASN:ND2	4:B:593:HOH:O	2.51	0.42
1:B:424:PHE:HD2	1:B:518:ASP:HB2	1.84	0.42
1:A:458:PHE:HZ	1:A:541:ILE:HD12	1.84	0.42
1:B:63:ARG:HH12	1:B:115:ALA:HB2	1.85	0.42
1:B:176:LEU:HD12	1:B:176:LEU:H	1.84	0.42
1:B:201:ILE:HG23	1:B:321:TYR:HB2	2.02	0.42
1:B:461:ASN:HB3	1:B:462:ASP:H	1.69	0.42
1:A:94:SER:HB3	1:A:96:PRO:HD2	2.02	0.41
1:A:456:LYS:H	1:A:467:VAL:HG21	1.84	0.41
1:B:138:ALA:HA	1:B:139:PRO:HD3	1.85	0.41
1:B:342:ARG:HG3	4:B:616:HOH:O	2.20	0.41
1:A:95:THR:N	1:A:96:PRO:HD2	2.35	0.41
1:A:176:LEU:HD23	1:A:176:LEU:N	2.35	0.41
1:A:440:MET:HG3	1:A:441:MET:N	2.35	0.41
1:A:468:GLU:HB2	1:A:494:ALA:HA	2.02	0.41
1:A:15:LYS:HA	1:A:16:PRO:HD3	1.89	0.41
1:A:485:LYS:HB2	1:A:487:GLN:NE2	2.36	0.41
1:A:138:ALA:HB1	1:A:142:ILE:HB	2.02	0.41
1:A:213:GLY:HA3	1:A:214:PRO:HD2	1.90	0.41
1:A:441:MET:CE	1:A:501:PHE:HB3	2.50	0.41
1:A:475:TYR:H	1:A:484:SER:HB2	1.85	0.41
1:B:426:ARG:HG3	1:B:516:TYR:CD1	2.56	0.41
1:B:524:ASN:N	1:B:524:ASN:HD22	2.18	0.41
1:B:113:LEU:HD22	1:B:113:LEU:N	2.36	0.41
1:B:219:ILE:HG22	1:B:282:PHE:HB3	2.03	0.41
1:A:530:ASP:HA	1:A:531:PRO:HD3	1.73	0.40
1:B:141:ALA:HB3	1:B:142:ILE:HD12	2.03	0.40
1:B:354:THR:HG22	1:B:475:TYR:CZ	2.56	0.40
1:B:470:ALA:HA	1:B:490:ARG:O	2.21	0.40
1:A:221:ILE:O	1:A:248:VAL:HG22	2.21	0.40
1:A:546:SER:O	1:A:547:GLN:HB2	2.22	0.40
1:A:556:ALA:HA	1:A:557:PRO:HD2	1.84	0.40
1:B:292:ARG:HG2	1:B:378:PHE:O	2.22	0.40
1:A:63:ARG:HG3	1:A:64:PHE:N	2.35	0.40
1:A:117:HIS:HB2	1:A:262:ASP:HB2	2.03	0.40
1:B:137:PRO:HB2	1:B:359:LYS:HE3	2.04	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	559/561 (100%)	461 (82%)	73 (13%)	25 (4%)	2	4
1	B	559/561 (100%)	506 (90%)	39 (7%)	14 (2%)	4	12
All	All	1118/1122 (100%)	967 (86%)	112 (10%)	39 (4%)	3	7

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	446	ALA
1	A	470	ALA
1	A	486	ASN
1	A	487	GLN
1	A	531	PRO
1	A	545	VAL
1	B	29	GLN
1	B	348	LYS
1	B	461	ASN
1	A	32	THR
1	A	431	GLU
1	A	437	ALA
1	A	548	LEU
1	B	32	THR
1	B	33	ASN
1	B	192	GLU
1	B	430	GLU
1	A	50	GLN
1	A	192	GLU
1	A	463	LYS
1	A	468	GLU
1	A	471	ASP
1	A	501	PHE
1	B	507	GLY
1	A	12	PRO

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Mol	Chain	Res	Type
1	A	313	ALA
1	A	348	LYS
1	A	557	PRO
1	B	486	ASN
1	A	455	GLY
1	B	65	TYR
1	B	252	PRO
1	A	105	ILE
1	A	530	ASP
1	B	487	GLN
1	B	454	VAL
1	B	263	PRO
1	A	312	ILE
1	A	214	PRO

### 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	462/462 (100%)	404 (87%)	58 (13%)	3	9
1	B	462/462 (100%)	410 (89%)	52 (11%)	4	11
All	All	924/924 (100%)	814 (88%)	110 (12%)	4	10

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	31	SER
1	A	50	GLN
1	A	68	GLU
1	A	82	ILE
1	A	116	SER
1	A	140	GLU
1	A	142	ILE
1	A	148	GLN

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Mol	Chain	Res	Type
1	A	162	LEU
1	A	172	GLN
1	A	176	LEU
1	A	177	GLU
1	A	181	LYS
1	A	197	MET
1	A	199	ARG
1	A	207	LEU
1	A	220	ARG
1	A	271	LEU
1	A	308	SER
1	A	309	VAL
1	A	348	LYS
1	A	356	THR
1	A	361	PHE
1	A	375	GLU
1	A	380	THR
1	A	382	SER
1	A	388	LYS
1	A	406	GLN
1	A	426	ARG
1	A	427	TYR
1	A	428	ASP
1	A	430	GLU
1	A	433	GLU
1	A	439	LYS
1	A	440	MET
1	A	443	ASP
1	A	445	GLU
1	A	447	LEU
1	A	451	ARG
1	A	458	PHE
1	A	462	ASP
1	A	485	LYS
1	A	490	ARG
1	A	492	ILE
1	A	495	ASP
1	A	497	SER
1	A	498	ARG
1	A	514	ARG
1	A	515	LEU
1	A	517	ILE

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Mol	Chain	Res	Type
1	A	523	ASP
1	A	529	GLN
1	A	532	GLN
1	A	535	LEU
1	A	539	ILE
1	A	546	SER
1	A	555	THR
1	B	6	VAL
1	B	24	ARG
1	B	37	ASN
1	B	40	GLN
1	B	41	SER
1	B	43	ILE
1	B	52	GLN
1	B	53	GLU
1	B	63	ARG
1	B	67	LYS
1	B	95	THR
1	B	104	LYS
1	B	117	HIS
1	B	118	ASN
1	B	125	ASP
1	B	133	SER
1	B	156	TYR
1	B	162	LEU
1	B	163	LYS
1	B	169	LEU
1	B	175	ASP
1	B	207	LEU
1	B	210	LEU
1	B	215	ASN
1	B	217	LEU
1	B	260	HIS
1	B	271	LEU
1	B	275	MET
1	B	276	LYS
1	B	291	ASP
1	B	298	LYS
1	B	306	SER
1	B	328	ARG
1	B	348	LYS
1	B	358	TRP

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Mol	Chain	Res	Type
1	B	359	LYS
1	B	372	LEU
1	B	386	ARG
1	B	391	LEU
1	B	409	GLU
1	B	412	LEU
1	B	430	GLU
1	B	447	LEU
1	B	461	ASN
1	B	463	LYS
1	B	485	LYS
1	B	506	THR
1	B	514	ARG
1	B	529	GLN
1	B	544	LYS
1	B	547	GLN
1	B	549	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	89	GLN
1	A	245	ASN
1	A	280	HIS
1	A	293	ASN
1	A	304	ASN
1	A	323	GLN
1	A	363	ASN
1	A	384	HIS
1	A	406	GLN
1	A	417	HIS
1	A	487	GLN
1	A	532	GLN
1	B	14	GLN
1	B	118	ASN
1	B	260	HIS
1	B	264	ASN
1	B	280	HIS
1	B	293	ASN
1	B	406	GLN
1	B	472	ASN

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Mol	Chain	Res	Type
1	B	487	GLN
1	B	524	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	VG1	A	563	2,1	14,20,20	1.84	2 (14%)	24,31,31	1.50	4 (16%)

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
3	VG1	A	563	2,1	-	2/7/31/31	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	563	VG1	P-O1	-5.37	1.50	1.59
3	A	563	VG1	O5-C5	2.43	1.50	1.44

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	563	VG1	O5-C5-C6	3.45	113.54	106.69
3	A	563	VG1	P-O1-C1	-2.72	116.25	123.54
3	A	563	VG1	O5-C5-C4	-2.05	106.00	109.70
3	A	563	VG1	O5-C1-C2	-2.01	106.24	110.37

There are no chirality outliers.

All (2) torsion outliers are listed below:

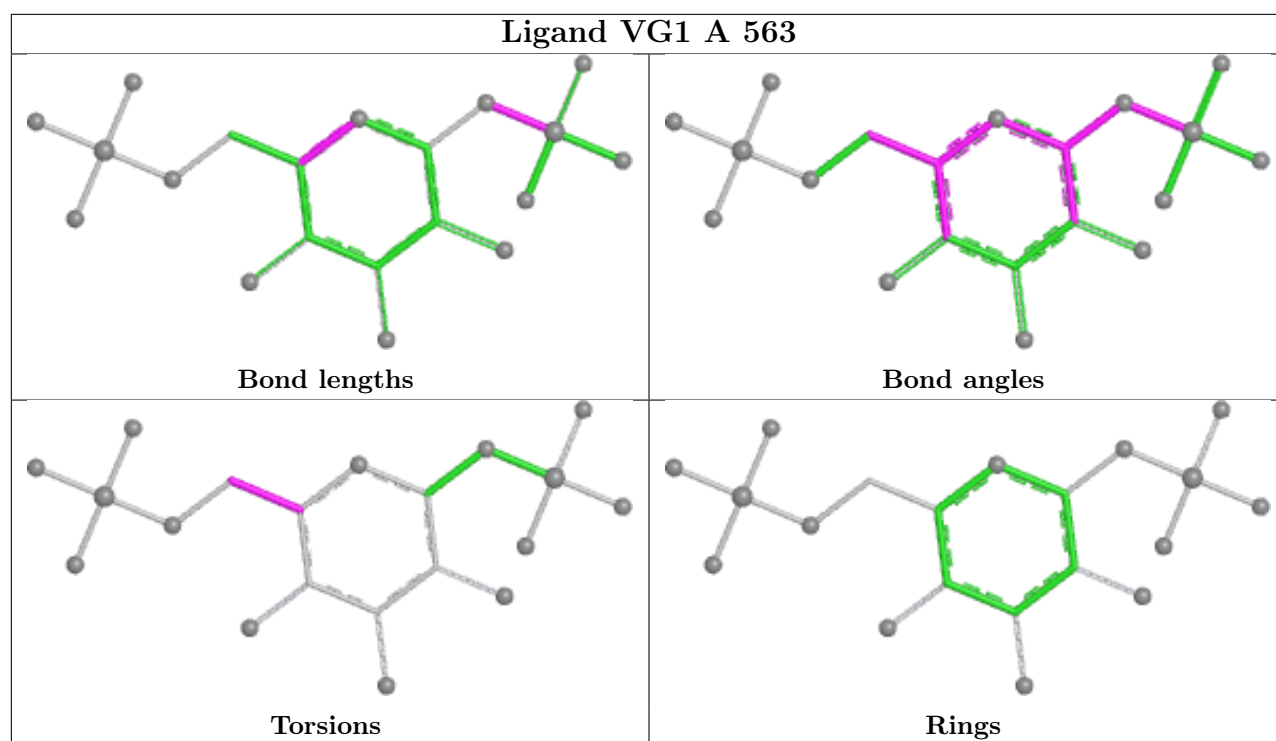
Mol	Chain	Res	Type	Atoms
3	A	563	VG1	O5-C5-C6-O6
3	A	563	VG1	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	563	VG1	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 ⓘ

**Warning:** The R factor obtained from EDS is 0.2479, which does not match the depositor's R factor of 0.192. Please interpret the results in this section carefully.

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<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	561/561 (100%)	0.05	33 (5%)	29 27	2, 20, 38, 56	0
1	B	561/561 (100%)	-0.36	11 (1%)	64 64	2, 12, 43, 58	0
All	All	1122/1122 (100%)	-0.16	44 (3%)	44 42	2, 17, 40, 58	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	455	GLY	5.6
1	A	559	VAL	5.0
1	A	508	SER	4.9
1	A	437	ALA	4.8
1	A	454	VAL	4.7
1	A	510	GLY	4.1
1	A	536	ALA	4.1
1	B	505	GLY	4.0
1	A	509	ALA	3.9
1	A	443	ASP	3.7
1	B	508	SER	3.6
1	A	496	GLY	3.6
1	A	541	ILE	3.5
1	A	540	SER	3.5
1	A	428	ASP	3.4
1	A	555	THR	3.3
1	A	501	PHE	3.3
1	B	261	PRO	3.2
1	A	459	SER	3.1
1	A	546	SER	3.0
1	A	435	GLU	3.0
1	A	449	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	30	SER	2.9
1	A	513	ILE	2.6
1	B	506	THR	2.5
1	A	214	PRO	2.5
1	A	473	PHE	2.4
1	A	470	ALA	2.4
1	A	539	ILE	2.4
1	A	561	THR	2.3
1	B	116	SER	2.3
1	A	553	GLY	2.3
1	A	464	VAL	2.3
1	A	460	ALA	2.3
1	A	438	THR	2.3
1	B	528	ASN	2.2
1	B	32	THR	2.2
1	A	471	ASP	2.2
1	B	115	ALA	2.2
1	A	557	PRO	2.1
1	B	264	ASN	2.1
1	A	537	PRO	2.1
1	A	439	LYS	2.1
1	B	486	ASN	2.1

## 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<sup>th</sup> 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.

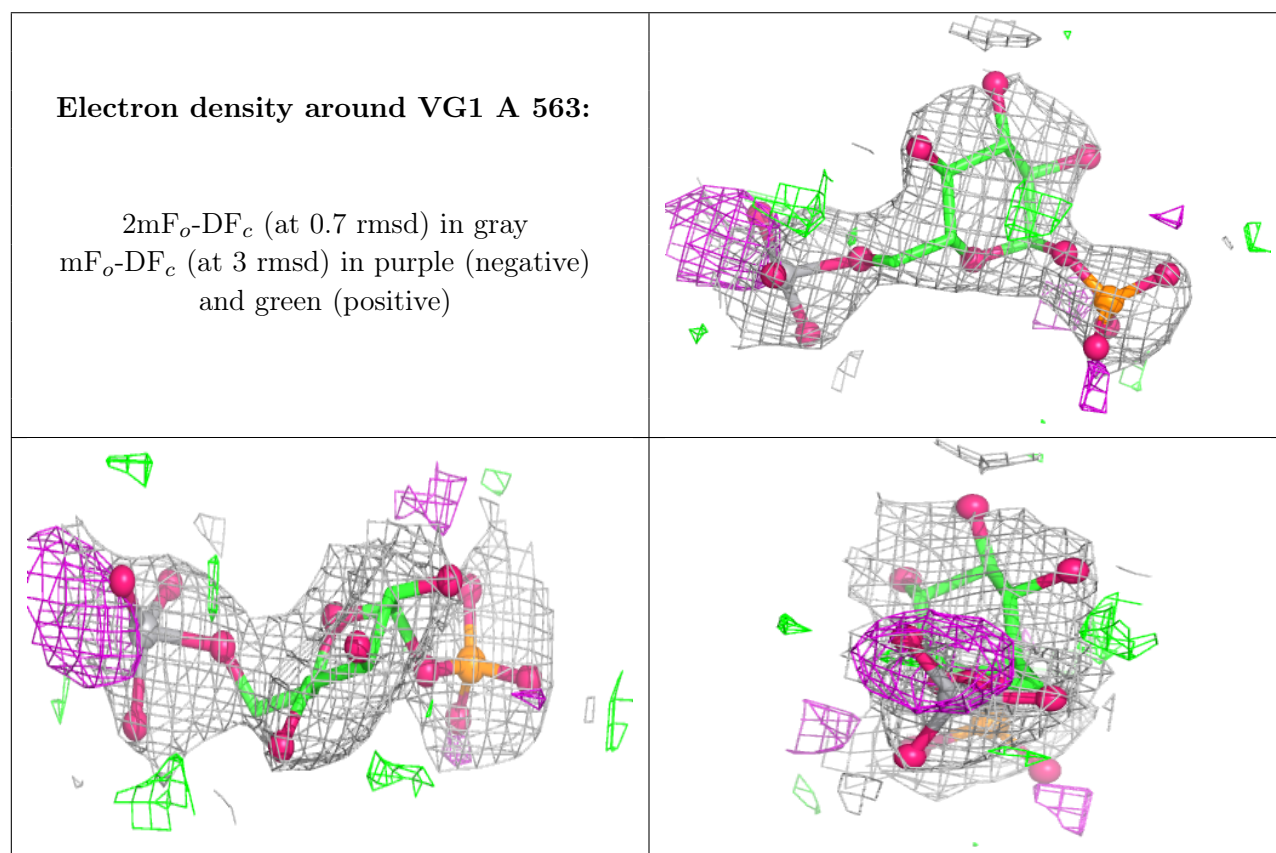
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	CO	A	562	1/1	0.85	0.21	2,2,2,2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	VG1	A	563	20/20	0.86	0.14	17,27,38,42	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.