Full wwPDB X-ray Structure Validation Report (i)

Aug 2, 2023 – 08:12 AM EDT

PDB ID	:	1C47
Title	:	BINDING DRIVEN STRUCTURAL CHANGES IN CRYSTALINE PHOSPHOGLUCOMUTASE ASSOCIATED WITH CHEMICAL REACTION
Authors	:	Baranidharan, S.; Ray Jr., W.J.
Deposited on	:	1999-08-11
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*
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 (i)) were used in the production of this report:

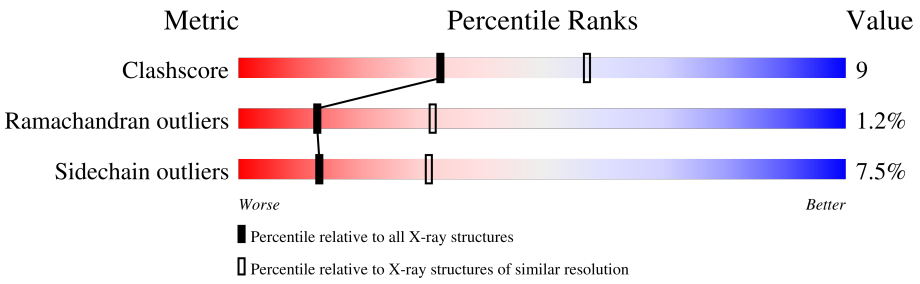
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.70 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	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (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 >=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%

Mol	Chain	Length	Quality of chain
1	A	561	72% 25% • •
1	B	561	72% 25% •

2 Entry composition (i)

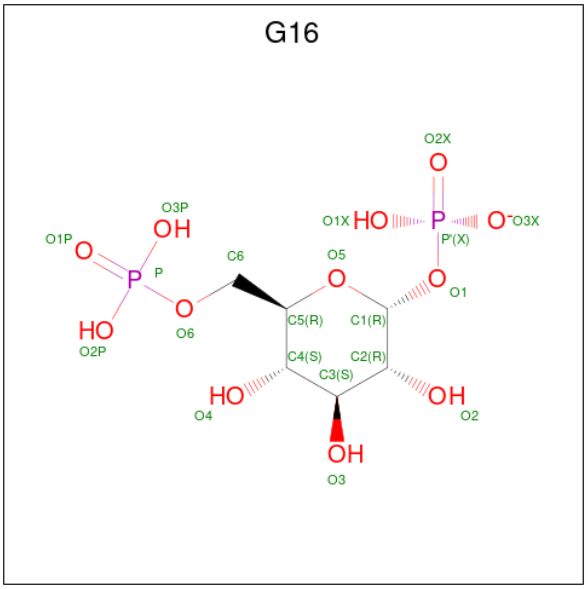
There are 4 unique types of molecules in this entry. The entry contains 8828 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALPHA-D-GLUCOSE 1,6-BISPHOSPHATE PHOSPHOTRANSFERASE.

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

- Molecule 2 is 1,6-di-O-phosphono-alpha-D-glucopyranose (three-letter code: G16) (formula: $C_6H_{13}O_{12}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	20	6	12	2	0	0

- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cd		
3	A	1	1	1	0	0
			Total	Cd		
3	B	1	1	1	0	0

- Molecule 4 is water.

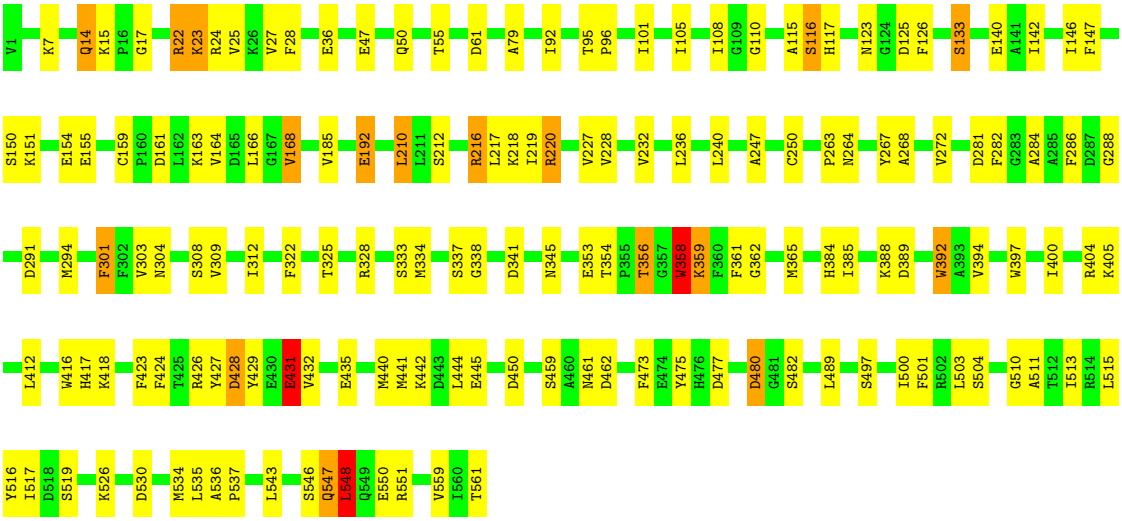
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	59	59	59	0	0
			Total	O		
4	B	89	89	89	0	0

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. 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. 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.

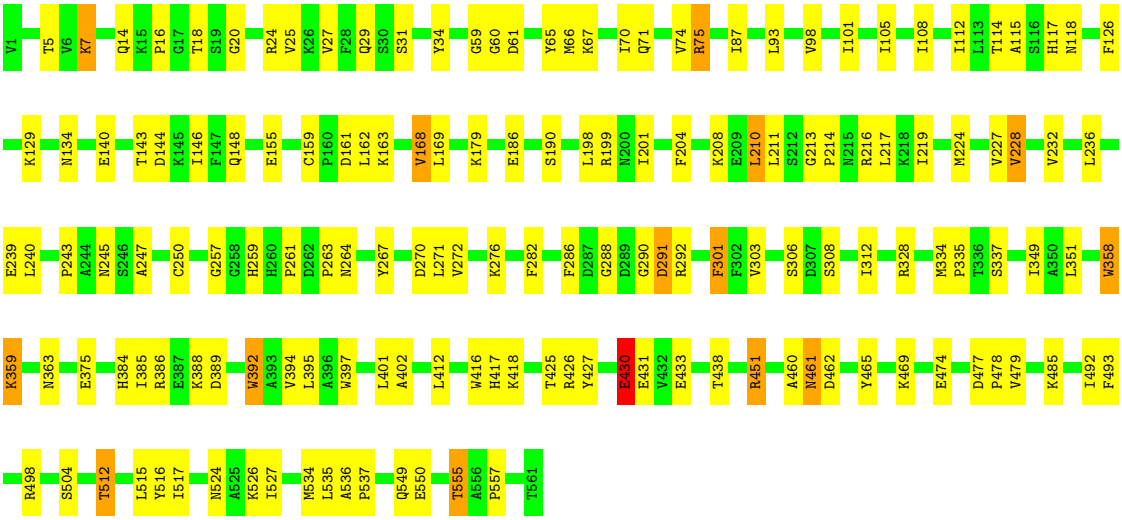
• Molecule 1: ALPHA-D-GLUCOSE 1,6-BISPHOSPHATE PHOSPHOTRANSFERASE

Chain A:



• Molecule 1: ALPHA-D-GLUCOSE 1,6-BISPHOSPHATE PHOSPHOTRANSFERASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	174.42Å 174.42Å 101.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.70 48.55 – 2.57	Depositor EDS
% Data completeness (in resolution range)	96.5 (6.00-2.70) 90.8 (48.55-2.57)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 2.58Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.183 , 0.248 0.256 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	30.7	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	8828	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: G16, CD

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	1.47	15/4416 (0.3%)	0.94	12/5969 (0.2%)
1	B	1.54	21/4416 (0.5%)	1.00	17/5969 (0.3%)
All	All	1.51	36/8832 (0.4%)	0.97	29/11938 (0.2%)

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	550	GLU	CD-OE2	-8.27	1.16	1.25
1	B	308	SER	CB-OG	-8.17	1.31	1.42
1	A	36	GLU	CD-OE1	-7.92	1.17	1.25
1	B	312	ILE	C-O	-7.23	1.09	1.23
1	B	186	GLU	CG-CD	-7.22	1.41	1.51
1	A	133	SER	CB-OG	7.12	1.51	1.42
1	B	358	TRP	CG-CD2	-6.77	1.32	1.43
1	B	351	LEU	C-O	-6.59	1.10	1.23
1	B	375	GLU	CG-CD	6.56	1.61	1.51
1	B	555	THR	CA-C	6.29	1.69	1.52
1	B	397	TRP	CG-CD2	-6.23	1.33	1.43
1	B	65	TYR	CG-CD1	6.06	1.47	1.39
1	A	308	SER	CB-OG	-6.00	1.34	1.42
1	A	192	GLU	N-CA	5.97	1.58	1.46
1	B	87	ILE	C-O	-5.95	1.12	1.23
1	B	416	TRP	CG-CD2	-5.77	1.33	1.43
1	A	416	TRP	CG-CD2	-5.74	1.33	1.43
1	B	498	ARG	CZ-NH2	-5.70	1.25	1.33
1	A	140	GLU	CG-CD	5.64	1.60	1.51
1	B	550	GLU	CD-OE1	-5.61	1.19	1.25
1	A	322	PHE	CG-CD2	5.58	1.47	1.38
1	A	397	TRP	CG-CD2	-5.53	1.34	1.43
1	A	220	ARG	CZ-NH1	5.47	1.40	1.33
1	B	385	ILE	CA-C	5.46	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	361	PHE	CE1-CZ	5.44	1.47	1.37
1	B	201	ILE	C-O	5.34	1.33	1.23
1	B	186	GLU	CB-CG	-5.30	1.42	1.52
1	A	110	GLY	C-O	-5.22	1.15	1.23
1	A	353	GLU	CD-OE1	-5.21	1.20	1.25
1	B	384	HIS	CG-ND1	-5.19	1.27	1.38
1	B	358	TRP	CD1-NE1	-5.18	1.29	1.38
1	A	362	GLY	CA-C	-5.14	1.43	1.51
1	A	475	TYR	CG-CD2	5.14	1.45	1.39
1	B	213	GLY	CA-C	5.14	1.60	1.51
1	B	306	SER	CB-OG	-5.05	1.35	1.42
1	A	359	LYS	N-CA	5.00	1.56	1.46

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	392	TRP	CD1-CG-CD2	14.56	117.95	106.30
1	B	416	TRP	CD1-CG-CD2	14.15	117.62	106.30
1	B	397	TRP	CD1-CG-CD2	13.73	117.29	106.30
1	B	358	TRP	CD1-CG-CD2	13.63	117.21	106.30
1	A	416	TRP	CD1-CG-CD2	13.57	117.15	106.30
1	A	397	TRP	CD1-CG-CD2	13.38	117.00	106.30
1	A	392	TRP	CD1-CG-CD2	13.21	116.87	106.30
1	B	358	TRP	CE2-CD2-CG	-9.97	99.32	107.30
1	B	416	TRP	CE2-CD2-CG	-8.90	100.18	107.30
1	B	392	TRP	CE2-CD2-CG	-8.64	100.39	107.30
1	A	392	TRP	CE2-CD2-CG	-8.52	100.48	107.30
1	A	397	TRP	CE2-CD2-CG	-8.49	100.51	107.30
1	A	416	TRP	CE2-CD2-CG	-7.90	100.98	107.30
1	B	392	TRP	CB-CG-CD1	-7.78	116.89	127.00
1	B	397	TRP	CE2-CD2-CG	-7.72	101.12	107.30
1	B	397	TRP	CG-CD1-NE1	-6.58	103.53	110.10
1	B	416	TRP	CG-CD1-NE1	-6.49	103.61	110.10
1	A	397	TRP	CB-CG-CD1	-6.43	118.64	127.00
1	B	416	TRP	CB-CG-CD1	-6.41	118.66	127.00
1	B	392	TRP	CG-CD2-CE3	6.38	139.64	133.90
1	A	392	TRP	CB-CG-CD1	-6.28	118.84	127.00
1	B	397	TRP	CB-CG-CD1	-6.17	118.98	127.00
1	A	416	TRP	CG-CD1-NE1	-5.98	104.12	110.10
1	A	392	TRP	CG-CD1-NE1	-5.95	104.16	110.10
1	B	358	TRP	CG-CD1-NE1	-5.95	104.16	110.10
1	B	392	TRP	CG-CD1-NE1	-5.93	104.17	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	358	TRP	CB-CG-CD1	-5.87	119.37	127.00
1	A	397	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	A	416	TRP	CB-CG-CD1	-5.54	119.79	127.00

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	4329	0	4332	71	1
1	B	4329	0	4332	80	0
2	A	20	0	9	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	59	0	0	2	1
4	B	89	0	0	7	0
All	All	8828	0	8673	150	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (150) 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:428:ASP:HB2	1:A:559:VAL:HB	1.51	0.92
1:B:224:MET:SD	1:B:286:PHE:O	2.44	0.76
1:A:17:GLY:HA3	4:A:616:HOH:O	1.87	0.75
1:B:31:SER:HB2	1:B:34:TYR:HB2	1.71	0.72
1:A:547:GLN:HE21	1:A:547:GLN:HA	1.54	0.72
1:A:22:ARG:HD2	1:A:115:ALA:HA	1.75	0.69
1:A:79:ALA:HB2	1:A:159:CYS:SG	2.34	0.67
1:B:71:GLN:HG3	1:B:75:ARG:NH1	2.12	0.65
1:B:168:VAL:HG22	4:B:585:HOH:O	1.98	0.63
1:B:7:LYS:HA	1:B:155:GLU:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:GLN:HE21	1:A:150:SER:HB2	1.65	0.61
1:A:303:VAL:HG13	1:A:412:LEU:HD11	1.82	0.60
1:B:144:ASP:O	1:B:148:GLN:HG2	2.01	0.60
1:B:247:ALA:HB1	1:B:250:CYS:SG	2.42	0.60
1:B:469:LYS:NZ	4:B:628:HOH:O	2.34	0.60
1:A:24:ARG:HG3	1:A:27:VAL:HG23	1.85	0.59
1:A:61:ASP:HA	1:A:227:VAL:HB	1.86	0.58
1:A:210:LEU:HD22	1:A:217:LEU:HB2	1.84	0.58
1:B:261:PRO:HB2	1:B:288:GLY:N	2.19	0.57
1:A:333:SER:HA	1:A:354:THR:O	2.05	0.57
1:B:60:GLY:HA3	1:B:66:MET:SD	2.45	0.57
1:A:427:TYR:HB2	1:A:515:LEU:HB3	1.85	0.56
1:B:117:HIS:HB3	1:B:292:ARG:HH22	1.69	0.56
1:A:358:TRP:CD1	1:A:388:LYS:HG3	2.39	0.56
1:A:25:VAL:HG22	1:A:126:PHE:HB2	1.87	0.56
1:A:92:ILE:HG23	1:A:227:VAL:HG23	1.88	0.56
1:B:264:ASN:HD21	1:B:267:TYR:HD2	1.52	0.56
1:A:268:ALA:O	1:A:272:VAL:HG23	2.06	0.56
1:B:117:HIS:HB3	1:B:292:ARG:NH2	2.21	0.55
1:B:536:ALA:HB3	1:B:537:PRO:HD3	1.89	0.55
1:B:504:SER:OG	1:B:512:THR:HB	2.07	0.55
1:A:218:LYS:HB2	1:A:218:LYS:NZ	2.21	0.55
1:A:423:PHE:HB2	1:A:519:SER:HB2	1.88	0.55
1:A:164:VAL:HG21	1:A:185:VAL:HG11	1.89	0.55
1:A:432:VAL:HG22	1:A:511:ALA:O	2.06	0.55
1:B:291:ASP:HB2	1:B:388:LYS:O	2.07	0.55
1:A:489:LEU:HB2	1:A:501:PHE:HB2	1.89	0.54
1:B:18:THR:HG21	1:B:359:LYS:HD2	1.88	0.54
1:B:526:LYS:HD3	1:B:534:MET:HE1	1.90	0.53
1:B:210:LEU:HG	1:B:402:ALA:HB2	1.89	0.53
1:B:211:LEU:HD12	1:B:240:LEU:HB3	1.91	0.53
1:B:272:VAL:O	1:B:276:LYS:HG2	2.07	0.53
1:A:247:ALA:HB1	1:A:250:CYS:SG	2.49	0.53
1:A:291:ASP:HB2	1:A:388:LYS:HB2	1.90	0.52
1:A:536:ALA:HB3	1:A:537:PRO:HD3	1.90	0.52
1:A:236:LEU:HD23	1:A:240:LEU:HD12	1.92	0.52
1:B:98:VAL:HG11	1:B:112:ILE:HG12	1.92	0.52
1:A:15:LYS:HD2	1:A:147:PHE:CE1	2.45	0.52
1:B:425:THR:HG22	1:B:517:ILE:HB	1.91	0.52
1:B:70:ILE:O	1:B:74:VAL:HG23	2.09	0.52
1:A:519:SER:OG	1:A:535:LEU:HD23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:PHE:HE2	1:B:412:LEU:HD12	1.75	0.51
1:B:71:GLN:HG3	1:B:75:ARG:HH12	1.73	0.51
1:A:301:PHE:HE2	1:A:412:LEU:HD12	1.74	0.50
1:B:25:VAL:HG22	1:B:126:PHE:HB2	1.92	0.50
1:A:228:VAL:HG12	1:A:232:VAL:HG23	1.92	0.50
1:A:284:ALA:HA	1:A:294:MET:O	2.11	0.50
1:B:426:ARG:HG3	1:B:516:TYR:CD1	2.45	0.50
1:B:75:ARG:HD2	1:B:159:CYS:O	2.12	0.50
1:B:291:ASP:O	1:B:388:LYS:HB3	2.12	0.50
1:B:117:HIS:H	1:B:117:HIS:CD2	2.30	0.49
1:B:358:TRP:CD1	1:B:388:LYS:HG3	2.47	0.49
1:B:417:HIS:ND1	1:B:524:ASN:OD1	2.45	0.49
1:A:428:ASP:CB	1:A:559:VAL:HB	2.34	0.49
1:A:477:ASP:HB3	1:A:480:ASP:OD2	2.12	0.49
1:B:427:TYR:CD1	1:B:557:PRO:HG3	2.48	0.48
1:A:264:ASN:HD21	1:A:267:TYR:HD2	1.59	0.48
1:A:500:ILE:HB	1:A:516:TYR:HB2	1.94	0.48
1:B:243:PRO:HB2	1:B:245:ASN:OD1	2.14	0.48
1:A:263:PRO:HB2	1:A:294:MET:HB2	1.95	0.48
1:B:334:MET:HB3	1:B:335:PRO:HD3	1.95	0.48
1:A:312:ILE:HA	1:A:400:ILE:HD11	1.96	0.47
1:A:547:GLN:O	1:A:550:GLU:HB2	2.14	0.47
1:B:204:PHE:O	1:B:208:LYS:HG3	2.14	0.47
1:B:460:ALA:O	1:B:461:ASN:HB2	2.15	0.47
1:A:384:HIS:CE1	1:A:385:ILE:HG12	2.50	0.47
1:A:389:ASP:HB3	1:A:392:TRP:HB3	1.97	0.47
1:A:431:GLU:HG3	1:A:510:GLY:HA3	1.97	0.47
1:B:75:ARG:HD3	1:B:162:LEU:O	2.14	0.47
1:B:134:ASN:O	1:B:386:ARG:HG3	2.15	0.47
1:A:358:TRP:CH2	1:A:365:MET:SD	3.08	0.46
1:B:101:ILE:O	1:B:105:ILE:HG12	2.15	0.46
1:B:115:ALA:HB1	1:B:118:ASN:HB2	1.96	0.46
1:B:389:ASP:HB3	1:B:392:TRP:HB3	1.96	0.46
1:A:418:LYS:NZ	1:A:418:LYS:HB2	2.31	0.46
1:B:217:LEU:HD21	1:B:401:LEU:HD13	1.97	0.46
1:B:179:LYS:HB2	4:B:645:HOH:O	2.15	0.46
1:A:356:THR:HB	4:A:584:HOH:O	2.15	0.45
1:B:363:ASN:O	1:B:479:VAL:HG21	2.16	0.45
1:B:129:LYS:HD2	4:B:639:HOH:O	2.15	0.45
1:B:451:ARG:N	1:B:451:ARG:HD3	2.31	0.45
1:B:427:TYR:HB2	1:B:515:LEU:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:MET:HG3	1:A:473:PHE:CG	2.52	0.45
1:B:14:GLN:O	1:B:16:PRO:HD3	2.17	0.45
1:B:474:GLU:HG3	1:B:485:LYS:HG2	1.98	0.45
1:A:291:ASP:O	1:A:388:LYS:HB3	2.17	0.45
1:B:465:TYR:HB3	1:B:493:PHE:CD1	2.52	0.45
1:B:477:ASP:HA	1:B:478:PRO:HD3	1.86	0.44
1:B:257:GLY:O	1:B:259:HIS:ND1	2.51	0.44
1:A:441:MET:O	1:A:445:GLU:HB2	2.18	0.44
1:B:61:ASP:HA	1:B:227:VAL:HB	1.99	0.44
1:A:116:SER:HB3	1:A:117:HIS:H	1.59	0.44
1:A:218:LYS:HB2	1:A:218:LYS:HZ3	1.83	0.44
1:A:228:VAL:HG11	1:A:286:PHE:CD1	2.53	0.44
1:A:480:ASP:OD1	1:A:482:SER:HB3	2.18	0.44
1:A:286:PHE:CZ	1:A:394:VAL:HG21	2.53	0.43
1:A:23:LYS:HB3	1:A:28:PHE:CE1	2.53	0.43
1:B:146:ILE:HD12	4:B:595:HOH:O	2.18	0.43
1:B:228:VAL:HG23	1:B:290:GLY:HA3	2.01	0.43
1:A:168:VAL:HG21	1:B:239:GLU:HB2	2.00	0.43
1:B:438:THR:HG23	4:B:630:HOH:O	2.19	0.43
1:A:444:LEU:HD22	1:A:546:SER:HB3	2.00	0.43
1:A:142:ILE:O	1:A:146:ILE:HG13	2.19	0.43
1:B:25:VAL:HG12	1:B:29:GLN:NE2	2.34	0.43
1:A:424:PHE:HA	1:A:517:ILE:O	2.19	0.42
1:A:440:MET:SD	1:A:548:LEU:HA	2.59	0.42
1:A:503:LEU:HD13	1:A:513:ILE:HG12	2.00	0.42
1:B:303:VAL:HG13	1:B:412:LEU:HD11	2.02	0.42
1:B:549:GLN:OE1	1:B:555:THR:HG22	2.19	0.42
1:B:264:ASN:ND2	1:B:267:TYR:HD2	2.17	0.42
1:A:304:ASN:HD21	1:A:424:PHE:HD1	1.67	0.42
1:B:24:ARG:HB2	1:B:27:VAL:HG23	2.01	0.42
1:A:338:GLY:HA2	1:A:341:ASP:OD2	2.19	0.42
1:B:469:LYS:HB3	1:B:492:ILE:HB	2.01	0.42
1:A:55:THR:O	1:A:108:ILE:HG22	2.19	0.42
1:A:219:ILE:HG22	1:A:282:PHE:HB3	2.02	0.42
1:A:388:LYS:HB2	1:A:388:LYS:HE2	1.66	0.42
1:B:286:PHE:CZ	1:B:394:VAL:HG21	2.53	0.42
1:B:219:ILE:HG22	1:B:282:PHE:HB3	2.02	0.42
1:B:59:GLY:HA3	1:B:93:LEU:HB3	2.02	0.41
1:B:199:ARG:HH11	1:B:199:ARG:HD3	1.65	0.41
1:B:425:THR:HB	1:B:535:LEU:HD13	2.02	0.41
1:A:216:ARG:HH11	1:A:216:ARG:HD3	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LYS:HB3	1:B:7:LYS:HE3	1.82	0.41
1:A:7:LYS:HD3	1:A:155:GLU:HB3	2.02	0.41
1:B:198:LEU:HD13	1:B:395:LEU:HD12	2.01	0.41
1:B:20:GLY:HA3	1:B:129:LYS:HA	2.02	0.41
1:B:211:LEU:O	1:B:216:ARG:HD2	2.21	0.41
1:A:526:LYS:HD2	1:A:534:MET:HE1	2.02	0.41
1:B:208:LYS:HB3	1:B:208:LYS:HE3	1.88	0.41
1:B:430:GLU:HB3	1:B:431:GLU:H	1.78	0.41
1:B:524:ASN:O	1:B:527:ILE:HG12	2.20	0.41
1:A:47:GLU:HB3	1:A:50:GLN:HE21	1.86	0.41
1:A:95:THR:HB	1:A:96:PRO:HD3	2.02	0.41
1:A:429:TYR:HB2	1:A:513:ILE:HB	2.03	0.41
1:B:93:LEU:HD23	1:B:98:VAL:HG22	2.03	0.41
1:B:114:THR:HG23	4:B:644:HOH:O	2.20	0.41
1:B:232:VAL:HG13	1:B:236:LEU:HD12	2.03	0.41
1:A:404:ARG:O	1:A:405:LYS:HB2	2.21	0.40
1:A:101:ILE:O	1:A:105:ILE:HG12	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ASN:ND2	4:A:569:HOH:O[3_555]	2.19	0.01

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	559/561 (100%)	517 (92%)	34 (6%)	8 (1%)	11	28
1	B	559/561 (100%)	517 (92%)	37 (7%)	5 (1%)	17	40
All	All	1118/1122 (100%)	1034 (92%)	71 (6%)	13 (1%)	13	32

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	430	GLU
1	B	461	ASN
1	A	358	TRP
1	B	301	PHE
1	A	192	GLU
1	A	216	ARG
1	A	301	PHE
1	A	461	ASN
1	A	548	LEU
1	A	431	GLU
1	B	263	PRO
1	A	288	GLY
1	B	214	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	462/462 (100%)	420 (91%)	42 (9%)	9 21
1	B	462/462 (100%)	435 (94%)	27 (6%)	20 43
All	All	924/924 (100%)	855 (92%)	69 (8%)	13 31

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	22	ARG
1	A	23	LYS
1	A	116	SER
1	A	123	ASN
1	A	125	ASP
1	A	133	SER
1	A	151	LYS
1	A	154	GLU
1	A	161	ASP

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Mol	Chain	Res	Type
1	A	163	LYS
1	A	166	LEU
1	A	168	VAL
1	A	210	LEU
1	A	212	SER
1	A	220	ARG
1	A	281	ASP
1	A	309	VAL
1	A	325	THR
1	A	328	ARG
1	A	337	SER
1	A	356	THR
1	A	358	TRP
1	A	359	LYS
1	A	417	HIS
1	A	426	ARG
1	A	428	ASP
1	A	431	GLU
1	A	435	GLU
1	A	442	LYS
1	A	450	ASP
1	A	459	SER
1	A	462	ASP
1	A	480	ASP
1	A	497	SER
1	A	504	SER
1	A	530	ASP
1	A	543	LEU
1	A	547	GLN
1	A	548	LEU
1	A	551	ARG
1	A	561	THR
1	B	5	THR
1	B	7	LYS
1	B	67	LYS
1	B	75	ARG
1	B	108	ILE
1	B	140	GLU
1	B	143	THR
1	B	161	ASP
1	B	163	LYS
1	B	168	VAL

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Mol	Chain	Res	Type
1	B	169	LEU
1	B	190	SER
1	B	210	LEU
1	B	228	VAL
1	B	270	ASP
1	B	271	LEU
1	B	291	ASP
1	B	328	ARG
1	B	337	SER
1	B	349	ILE
1	B	359	LYS
1	B	418	LYS
1	B	430	GLU
1	B	433	GLU
1	B	451	ARG
1	B	462	ASP
1	B	512	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	50	GLN
1	A	71	GLN
1	A	280	HIS
1	A	345	ASN
1	A	422	ASN
1	A	547	GLN
1	B	14	GLN
1	B	29	GLN
1	B	37	ASN
1	B	117	HIS
1	B	476	HIS

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 3 ligands modelled in this entry, 2 are 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	$\#\|Z\| > 2$
2	G16	A	563	3	19,20,20	1.96	4 (21%)	30,31,31	1.46	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	G16	A	563	3	-	3/11/31/31	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	563	G16	P'-O1	-5.41	1.49	1.59
2	A	563	G16	O4-C4	-3.74	1.34	1.43
2	A	563	G16	O6-C6	-2.93	1.33	1.44
2	A	563	G16	C4-C5	2.21	1.57	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	563	G16	O5-C5-C6	3.39	113.51	106.67
2	A	563	G16	O3-C3-C2	-3.15	103.06	110.35
2	A	563	G16	O1-C1-C2	-2.90	103.07	108.38
2	A	563	G16	C1-O5-C5	2.66	118.91	113.69

There are no chirality outliers.

All (3) torsion outliers are listed below:

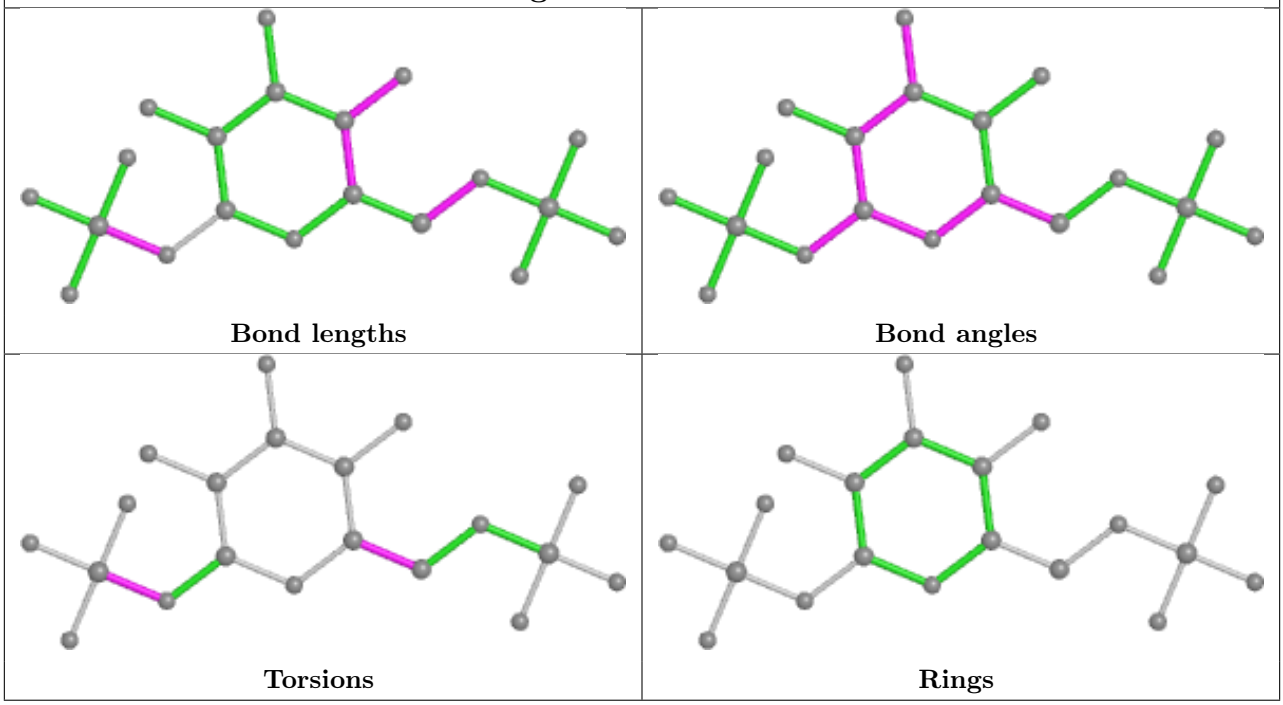
Mol	Chain	Res	Type	Atoms
2	A	563	G16	C4-C5-C6-O6
2	A	563	G16	C1-O1-P'-O2X
2	A	563	G16	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 G16 A 563



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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

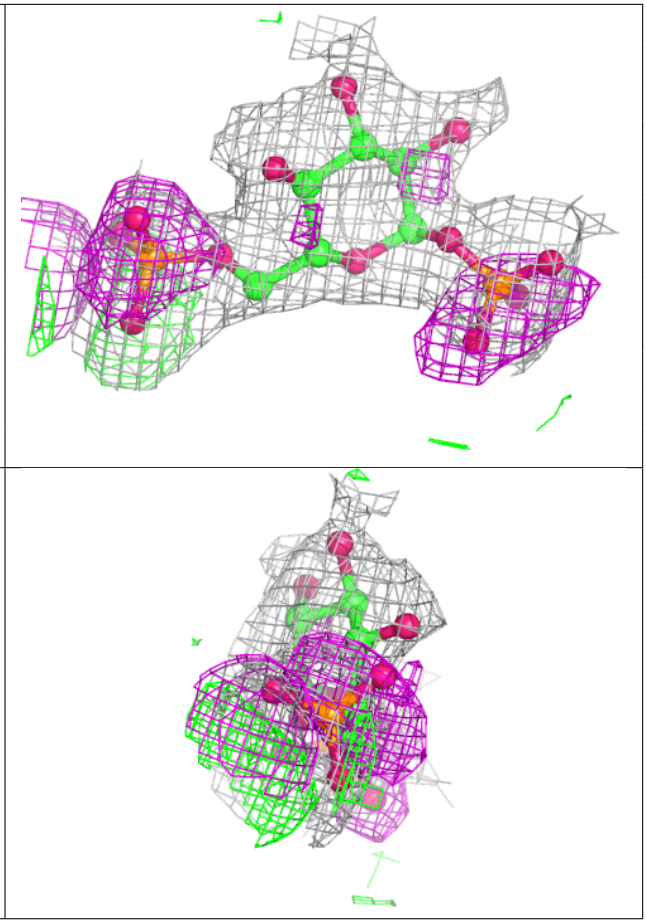
6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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 G16 A 563:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.