



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:47 AM UTC

PDB ID : 1C47 / pdb_00001c47
Title : BINDING DRIVEN STRUCTURAL CHANGES IN CRYSTALLINE 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 ⓘ 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)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

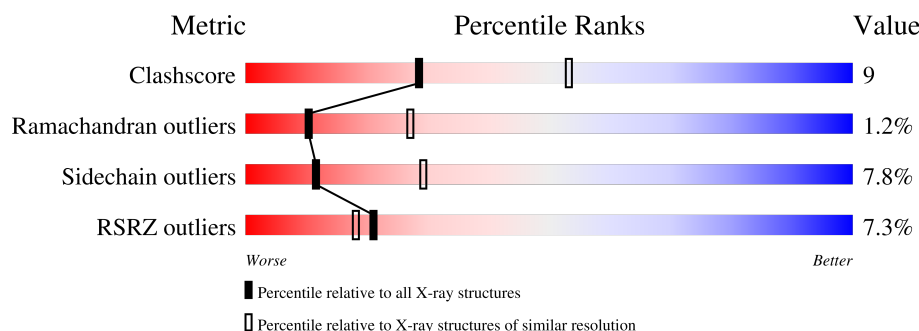
1 Overall quality at a glance

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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 $\leq 5\%$. 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	561	12% 60% 31% 8%
1	B	561	3% 58% 32% 8%

2 Entry composition [i](#)

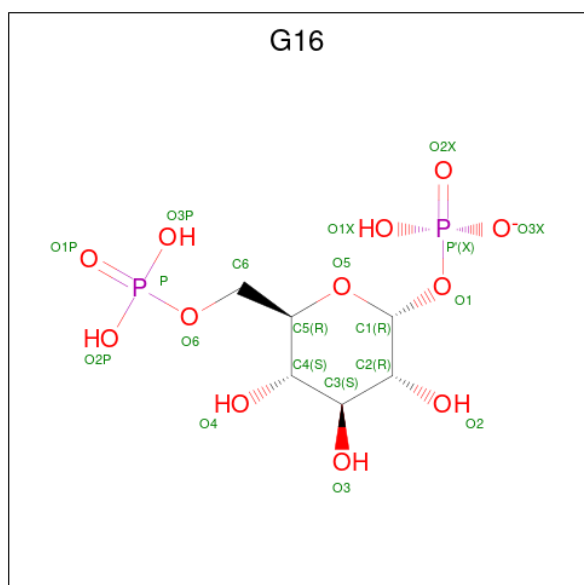
There are 4 unique types of molecules in this entry. The entry contains 8828 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
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 1,6-di-O-phosphono-alpha-D-glucopyranose (CCD ID: G16) (formula: $C_6H_{13}O_{12}P_2$).



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

- Molecule 3 is CADMIUM ION (CCD ID: CD) (formula: Cd).

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

- Molecule 4 is water.

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

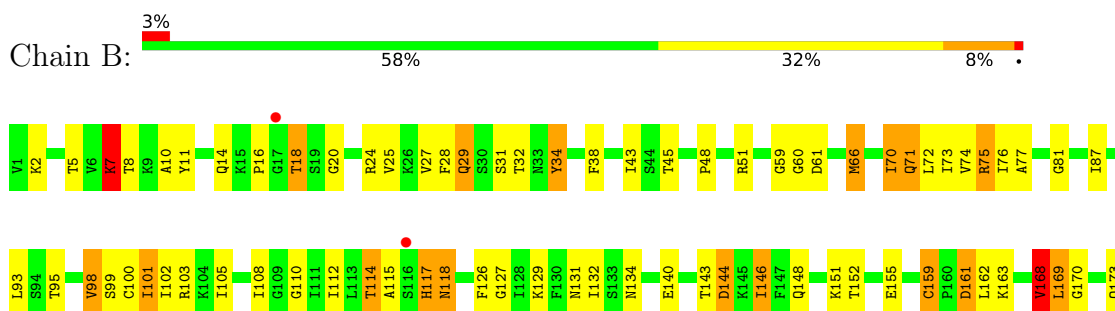
3 Residue-property plots [i](#)

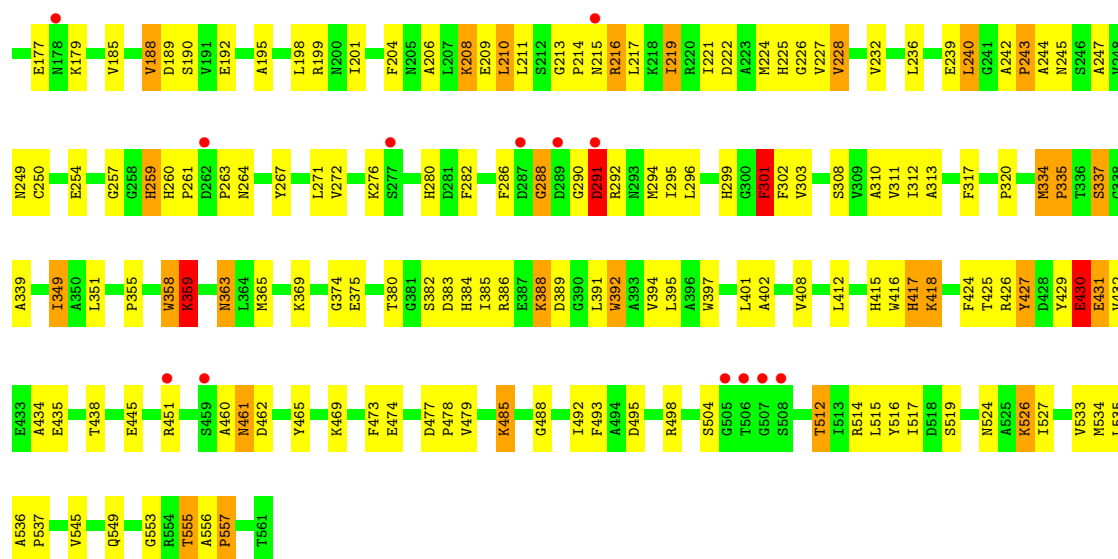
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ALPHA-D-GLUCOSE 1,6-BISPHOSPHATE PHOSPHOTRANSFERASE



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





4 Data and refinement statistics

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 6.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.5 (6.00-2.70) 86.7 (6.00-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.58Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.183 , 0.248 0.257 , (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 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	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.*

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: 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	2.04	119/4416 (2.7%)	1.26	17/5969 (0.3%)
1	B	2.16	154/4416 (3.5%)	1.26	22/5969 (0.4%)
All	All	2.10	273/8832 (3.1%)	1.26	39/11938 (0.3%)

All (273) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	385	ILE	CA-C	15.78	1.67	1.52
1	B	312	ILE	C-O	-12.84	1.09	1.24
1	B	555	THR	CA-C	12.12	1.69	1.52
1	A	432	VAL	CA-C	12.07	1.63	1.52
1	B	351	LEU	C-O	-10.98	1.10	1.24
1	B	95	THR	CA-C	10.31	1.64	1.52
1	B	384	HIS	CG-ND1	-9.92	1.27	1.38
1	B	87	ILE	C-O	-9.52	1.12	1.24
1	A	192	GLU	N-CA	9.38	1.58	1.46
1	B	117	HIS	CD2-NE2	-8.63	1.28	1.37
1	A	280	HIS	CG-ND1	-8.51	1.28	1.38
1	A	110	GLY	C-O	-8.48	1.15	1.24
1	B	110	GLY	CA-C	8.33	1.59	1.51
1	A	432	VAL	C-O	7.97	1.31	1.23
1	A	415	HIS	CG-ND1	-7.96	1.29	1.38
1	A	87	ILE	C-O	-7.95	1.16	1.24
1	A	359	LYS	N-CA	7.88	1.56	1.46
1	B	201	ILE	C-O	7.86	1.33	1.24
1	B	132	ILE	CA-C	7.74	1.62	1.52
1	B	102	ILE	CA-CB	7.72	1.63	1.54
1	B	192	GLU	N-CA	7.59	1.55	1.46
1	B	188	VAL	CA-C	7.58	1.62	1.52
1	A	395	LEU	CA-C	7.58	1.63	1.52
1	A	421	ARG	C-O	-7.54	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	415	HIS	CG-ND1	-7.51	1.29	1.38
1	A	334	MET	CA-C	7.44	1.60	1.52
1	B	375	GLU	CA-C	7.38	1.61	1.52
1	A	384	HIS	CD2-NE2	-7.36	1.29	1.37
1	A	435	GLU	CA-C	7.17	1.61	1.52
1	A	129	LYS	CA-C	7.14	1.61	1.52
1	B	311	VAL	CA-C	7.13	1.61	1.52
1	A	130	PHE	C-O	-7.09	1.15	1.24
1	A	362	GLY	CA-C	-7.08	1.43	1.52
1	A	359	LYS	CA-C	7.04	1.62	1.52
1	B	415	HIS	CD2-NE2	-6.99	1.30	1.37
1	A	480	ASP	CA-C	6.92	1.62	1.52
1	B	254	GLU	N-CA	6.86	1.55	1.46
1	A	79	ALA	CA-CB	-6.79	1.42	1.53
1	A	532	GLN	N-CA	6.78	1.54	1.46
1	B	110	GLY	C-O	-6.74	1.17	1.24
1	B	70	ILE	N-CA	6.74	1.54	1.46
1	B	431	GLU	CA-C	6.70	1.61	1.52
1	B	243	PRO	CA-CB	-6.67	1.44	1.53
1	A	384	HIS	CA-C	6.66	1.62	1.52
1	B	32	THR	C-O	-6.65	1.15	1.23
1	A	225	HIS	CG-ND1	-6.62	1.30	1.38
1	A	319	ILE	CA-C	6.62	1.58	1.53
1	B	557	PRO	CA-CB	-6.60	1.44	1.53
1	A	434	ALA	N-CA	6.58	1.53	1.46
1	B	48	PRO	CA-C	6.56	1.61	1.52
1	A	374	GLY	CA-C	6.52	1.58	1.51
1	A	161	ASP	CA-C	6.51	1.61	1.52
1	B	337	SER	C-O	-6.49	1.16	1.23
1	B	427	TYR	CA-CB	-6.48	1.44	1.53
1	B	66	MET	CA-C	6.47	1.61	1.52
1	B	219	ILE	C-O	-6.47	1.16	1.23
1	B	485	LYS	N-CA	6.47	1.53	1.45
1	B	358	TRP	CG-CD2	-6.45	1.32	1.43
1	A	187	ILE	CA-C	6.45	1.59	1.52
1	A	543	LEU	CA-C	6.45	1.60	1.52
1	A	316	ILE	CA-C	6.44	1.61	1.52
1	A	339	ALA	N-CA	6.44	1.54	1.46
1	B	349	ILE	CA-C	6.43	1.60	1.52
1	B	170	GLY	C-O	-6.41	1.17	1.23
1	B	87	ILE	CA-C	6.39	1.60	1.52
1	A	154	GLU	CA-C	6.39	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	533	VAL	CA-C	6.38	1.61	1.52
1	B	392	TRP	CA-C	6.38	1.61	1.52
1	A	536	ALA	N-CA	6.38	1.55	1.46
1	B	384	HIS	CD2-NE2	-6.35	1.30	1.37
1	A	462	ASP	CA-C	6.30	1.59	1.52
1	B	208	LYS	N-CA	6.28	1.53	1.46
1	A	22	ARG	N-CA	6.27	1.53	1.46
1	B	195	ALA	CA-CB	-6.25	1.43	1.53
1	A	213	GLY	N-CA	6.23	1.51	1.43
1	B	429	TYR	C-O	-6.23	1.16	1.23
1	B	335	PRO	CA-CB	-6.20	1.44	1.53
1	B	242	ALA	CA-C	6.16	1.59	1.53
1	B	118	ASN	CA-C	6.14	1.59	1.52
1	B	259	HIS	CG-ND1	-6.13	1.31	1.38
1	A	158	ILE	CA-C	6.13	1.60	1.52
1	B	28	PHE	N-CA	6.12	1.53	1.46
1	B	320	PRO	CA-CB	-6.10	1.45	1.53
1	A	305	PRO	CA-CB	-6.07	1.45	1.53
1	B	417	HIS	CG-ND1	-6.05	1.31	1.38
1	B	473	PHE	N-CA	6.03	1.54	1.46
1	A	415	HIS	CD2-NE2	-6.01	1.31	1.37
1	A	321	TYR	N-CA	6.01	1.53	1.46
1	B	498	ARG	CZ-NH2	-6.00	1.25	1.33
1	B	351	LEU	C-N	-5.97	1.25	1.33
1	B	260	HIS	CG-ND1	-5.96	1.31	1.38
1	A	552	THR	N-CA	5.95	1.53	1.45
1	B	397	TRP	CG-CD2	-5.94	1.33	1.43
1	A	524	ASN	CA-C	5.93	1.60	1.52
1	B	11	TYR	CA-C	5.92	1.59	1.52
1	B	299	HIS	CD2-NE2	-5.91	1.31	1.37
1	B	2	LYS	CA-C	5.90	1.60	1.52
1	A	197	MET	N-CA	5.90	1.53	1.46
1	A	494	ALA	CA-C	5.88	1.60	1.52
1	B	317	PHE	CA-C	5.88	1.61	1.52
1	A	117	HIS	CA-C	5.87	1.61	1.52
1	B	408	VAL	N-CA	5.85	1.53	1.46
1	B	72	LEU	C-O	5.84	1.30	1.24
1	B	222	ASP	C-O	-5.84	1.17	1.24
1	A	498	ARG	CD-NE	5.83	1.54	1.46
1	A	194	TYR	CA-C	5.82	1.60	1.52
1	A	334	MET	CA-CB	5.82	1.59	1.54
1	A	511	ALA	CA-C	5.81	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	159	CYS	C-O	-5.80	1.17	1.24
1	B	81	GLY	CA-C	5.79	1.59	1.51
1	A	555	THR	N-CA	5.78	1.53	1.46
1	B	117	HIS	CG-ND1	-5.77	1.31	1.38
1	B	209	GLU	CA-C	5.77	1.60	1.52
1	A	139	PRO	CA-C	5.76	1.59	1.52
1	B	355	PRO	C-O	-5.75	1.17	1.23
1	B	308	SER	C-O	-5.75	1.17	1.24
1	A	494	ALA	N-CA	5.74	1.53	1.46
1	B	146	ILE	N-CA	5.73	1.53	1.46
1	B	556	ALA	CA-CB	-5.73	1.45	1.54
1	B	29	GLN	N-CA	5.73	1.53	1.46
1	B	127	GLY	CA-C	5.72	1.57	1.51
1	B	213	GLY	CA-C	5.71	1.60	1.51
1	B	280	HIS	CG-ND1	-5.69	1.31	1.38
1	B	519	SER	CA-C	5.68	1.60	1.52
1	A	526	LYS	CA-C	5.68	1.60	1.52
1	B	526	LYS	CA-C	5.67	1.60	1.52
1	B	102	ILE	N-CA	5.67	1.53	1.46
1	A	467	VAL	N-CA	5.67	1.52	1.46
1	A	160	PRO	N-CA	5.66	1.55	1.47
1	A	497	SER	N-CA	5.66	1.52	1.45
1	A	372	LEU	CA-C	5.66	1.59	1.52
1	B	299	HIS	N-CA	5.65	1.52	1.46
1	B	295	ILE	CA-C	5.64	1.59	1.52
1	B	417	HIS	CD2-NE2	-5.64	1.31	1.37
1	A	294	MET	CA-C	5.63	1.59	1.52
1	A	443	ASP	C-O	5.63	1.30	1.24
1	A	335	PRO	C-N	5.63	1.41	1.33
1	A	304	ASN	CA-C	5.62	1.59	1.53
1	A	526	LYS	N-CA	5.61	1.53	1.46
1	B	288	GLY	N-CA	5.61	1.53	1.45
1	A	124	GLY	CA-C	5.61	1.59	1.51
1	A	239	GLU	CA-C	-5.60	1.45	1.52
1	B	310	ALA	CA-C	-5.60	1.45	1.52
1	A	280	HIS	CD2-NE2	-5.58	1.31	1.37
1	A	489	LEU	CA-CB	5.57	1.59	1.53
1	B	100	CYS	N-CA	5.56	1.53	1.46
1	A	22	ARG	CA-C	5.53	1.60	1.52
1	B	103	ARG	CA-C	5.53	1.60	1.52
1	B	98	VAL	C-O	-5.52	1.17	1.24
1	A	420	GLY	C-O	5.51	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	177	GLU	CA-C	5.51	1.59	1.52
1	B	416	TRP	CG-CD2	-5.51	1.33	1.43
1	B	152	THR	N-CA	5.50	1.53	1.46
1	A	416	TRP	N-CA	5.50	1.53	1.46
1	B	526	LYS	C-N	5.50	1.40	1.34
1	A	428	ASP	CA-C	5.49	1.59	1.52
1	B	219	ILE	CA-C	-5.49	1.48	1.52
1	B	365	MET	N-CA	5.49	1.52	1.46
1	B	43	ILE	N-CA	5.48	1.53	1.46
1	B	185	VAL	C-O	-5.48	1.18	1.24
1	B	383	ASP	CA-C	5.48	1.60	1.52
1	A	416	TRP	CG-CD2	-5.47	1.33	1.43
1	B	7	LYS	CA-C	5.46	1.59	1.52
1	A	133	SER	N-CA	5.46	1.53	1.46
1	B	380	THR	CA-C	-5.45	1.45	1.52
1	A	20	GLY	C-O	-5.44	1.16	1.23
1	A	385	ILE	CA-CB	5.44	1.61	1.54
1	B	168	VAL	CA-C	5.43	1.59	1.52
1	B	34	TYR	N-CA	5.43	1.53	1.46
1	B	313	ALA	C-O	-5.43	1.17	1.24
1	B	240	LEU	C-O	5.42	1.31	1.24
1	B	45	THR	N-CA	5.42	1.53	1.46
1	A	191	VAL	N-CA	5.41	1.53	1.46
1	B	114	THR	N-CA	5.41	1.52	1.46
1	B	169	LEU	N-CA	5.41	1.52	1.45
1	B	225	HIS	CG-ND1	-5.41	1.32	1.38
1	A	261	PRO	CA-CB	-5.41	1.47	1.53
1	A	211	LEU	CA-C	5.39	1.60	1.52
1	B	161	ASP	N-CA	5.38	1.53	1.46
1	A	96	PRO	CA-C	5.37	1.60	1.52
1	B	374	GLY	CA-C	5.37	1.57	1.51
1	B	308	SER	N-CA	5.36	1.52	1.46
1	A	550	GLU	CA-C	5.36	1.59	1.52
1	B	77	ALA	N-CA	5.36	1.52	1.46
1	B	226	GLY	C-O	-5.34	1.18	1.23
1	B	418	LYS	C-O	-5.34	1.17	1.23
1	B	311	VAL	C-O	-5.33	1.18	1.24
1	B	38	PHE	C-N	5.33	1.40	1.33
1	A	260	HIS	CD2-NE2	-5.31	1.32	1.37
1	A	444	LEU	C-N	5.30	1.40	1.33
1	B	189	ASP	CA-C	5.30	1.60	1.52
1	A	51	ARG	CA-C	5.30	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	131	ASN	C-O	-5.30	1.17	1.23
1	B	553	GLY	CA-C	5.30	1.59	1.51
1	A	220	ARG	CZ-NH1	5.29	1.40	1.32
1	B	95	THR	N-CA	5.29	1.51	1.46
1	A	397	TRP	CG-CD2	-5.28	1.34	1.43
1	B	206	ALA	N-CA	5.26	1.52	1.46
1	B	308	SER	CB-OG	-5.26	1.31	1.42
1	A	24	ARG	N-CA	5.26	1.52	1.46
1	A	74	VAL	CA-C	5.25	1.59	1.52
1	A	64	PHE	CA-C	5.25	1.59	1.52
1	A	262	ASP	CA-C	5.25	1.57	1.52
1	B	488	GLY	CA-C	-5.23	1.44	1.51
1	B	384	HIS	ND1-CE1	5.23	1.37	1.32
1	A	202	PHE	CA-C	5.22	1.58	1.52
1	A	456	LYS	CA-C	5.22	1.59	1.52
1	A	182	PRO	CA-C	5.21	1.58	1.52
1	B	8	THR	CA-C	5.21	1.59	1.52
1	A	558	THR	N-CA	5.20	1.52	1.46
1	B	334	MET	CA-C	5.20	1.58	1.52
1	B	424	PHE	C-N	5.19	1.40	1.33
1	A	325	THR	CA-C	5.18	1.59	1.52
1	B	301	PHE	C-O	-5.18	1.17	1.24
1	A	402	ALA	N-CA	5.17	1.52	1.46
1	A	433	GLU	C-O	5.16	1.30	1.24
1	B	382	SER	CA-C	-5.16	1.46	1.52
1	B	296	LEU	C-N	-5.15	1.28	1.33
1	A	130	PHE	CA-CB	-5.14	1.46	1.53
1	B	18	THR	N-CA	5.14	1.53	1.46
1	B	159	CYS	CA-C	5.14	1.59	1.52
1	B	302	PHE	N-CA	5.14	1.52	1.46
1	A	141	ALA	N-CA	5.13	1.52	1.46
1	B	101	ILE	C-O	-5.12	1.18	1.24
1	B	545	VAL	N-CA	5.12	1.52	1.46
1	B	72	LEU	CA-CB	-5.12	1.45	1.53
1	B	76	ILE	C-O	5.11	1.30	1.24
1	B	363	ASN	N-CA	5.11	1.52	1.46
1	A	451	ARG	CA-C	5.11	1.59	1.52
1	B	498	ARG	NE-CZ	-5.10	1.27	1.33
1	A	423	PHE	N-CA	5.10	1.52	1.46
1	A	492	ILE	CA-C	5.09	1.58	1.52
1	B	73	ILE	N-CA	5.09	1.52	1.46
1	B	291	ASP	CA-C	5.09	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	311	VAL	N-CA	5.09	1.52	1.46
1	A	416	TRP	C-O	-5.08	1.17	1.24
1	A	485	LYS	CA-C	5.08	1.60	1.53
1	B	259	HIS	C-O	5.08	1.30	1.23
1	A	191	VAL	C-N	5.08	1.40	1.33
1	A	464	VAL	CA-C	5.08	1.58	1.52
1	B	144	ASP	N-CA	5.08	1.52	1.46
1	A	131	ASN	C-O	5.08	1.29	1.23
1	B	514	ARG	N-CA	-5.08	1.40	1.46
1	A	253	LEU	CA-C	5.07	1.58	1.52
1	A	532	GLN	CA-C	5.07	1.59	1.52
1	B	294	MET	N-CA	5.06	1.52	1.46
1	B	369	LYS	N-CA	5.06	1.53	1.45
1	B	391	LEU	N-CA	5.06	1.52	1.46
1	A	270	ASP	N-CA	5.06	1.52	1.46
1	A	313	ALA	N-CA	5.05	1.52	1.46
1	A	549	GLN	N-CA	5.05	1.52	1.46
1	A	100	CYS	C-N	5.05	1.40	1.33
1	B	99	SER	N-CA	5.05	1.52	1.46
1	B	359	LYS	N-CA	5.05	1.52	1.46
1	A	294	MET	N-CA	5.04	1.52	1.46
1	B	244	ALA	C-O	-5.04	1.17	1.24
1	A	476	HIS	CD2-NE2	-5.04	1.32	1.37
1	A	199	ARG	NE-CZ	-5.04	1.27	1.33
1	A	474	GLU	C-O	5.04	1.30	1.23
1	A	82	ILE	CA-C	5.03	1.58	1.52
1	B	71	GLN	CA-C	5.03	1.59	1.52
1	B	151	LYS	CA-C	5.03	1.59	1.52
1	A	44	SER	N-CA	5.02	1.52	1.46
1	B	249	ASN	CA-C	5.01	1.60	1.52
1	B	495	ASP	CA-C	5.01	1.59	1.52
1	B	117	HIS	CB-CG	5.01	1.57	1.50
1	B	445	GLU	C-N	5.01	1.40	1.33
1	A	204	PHE	CA-C	5.01	1.59	1.52
1	B	339	ALA	N-CA	5.01	1.52	1.46
1	B	351	LEU	N-CA	5.00	1.52	1.46
1	A	549	GLN	CA-C	5.00	1.59	1.52
1	B	38	PHE	CA-C	5.00	1.59	1.52
1	B	435	GLU	N-CA	5.00	1.52	1.46

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	392	TRP	CD1-CG-CD2	7.28	117.95	106.30
1	B	416	TRP	CD1-CG-CD2	7.08	117.62	106.30
1	B	397	TRP	CD1-CG-CD2	6.87	117.29	106.30
1	B	358	TRP	CD1-CG-CD2	6.82	117.21	106.30
1	A	416	TRP	CD1-CG-CD2	6.78	117.15	106.30
1	A	397	TRP	CD1-CG-CD2	6.69	117.00	106.30
1	B	392	TRP	CB-CG-CD1	-6.67	116.89	126.90
1	A	392	TRP	CD1-CG-CD2	6.60	116.87	106.30
1	B	358	TRP	CE2-CD2-CG	-6.57	99.32	107.20
1	B	10	ALA	N-CA-C	6.41	118.60	110.33
1	B	216	ARG	N-CA-C	6.17	118.49	110.53
1	A	116	SER	CB-CA-C	-6.13	109.52	116.63
1	B	416	TRP	CE2-CD2-CG	-5.85	100.18	107.20
1	B	337	SER	N-CA-C	5.84	117.83	110.24
1	B	392	TRP	CG-CD2-CE3	5.74	139.64	133.90
1	B	392	TRP	CE2-CD2-CG	-5.67	100.39	107.20
1	A	10	ALA	N-CA-C	5.62	117.95	110.53
1	B	51	ARG	N-CA-C	5.60	117.06	111.07
1	A	392	TRP	CE2-CD2-CG	-5.60	100.48	107.20
1	A	384	HIS	CB-CG-CD2	-5.58	123.94	131.20
1	A	397	TRP	CE2-CD2-CG	-5.57	100.51	107.20
1	A	530	ASP	N-CA-C	5.51	116.35	109.57
1	A	397	TRP	CB-CG-CD1	-5.51	118.64	126.90
1	B	416	TRP	CB-CG-CD1	-5.49	118.66	126.90
1	B	434	ALA	N-CA-C	5.43	117.63	111.11
1	A	392	TRP	CB-CG-CD1	-5.37	118.84	126.90
1	A	291	ASP	CA-CB-CG	5.35	117.95	112.60
1	B	397	TRP	CB-CG-CD1	-5.28	118.98	126.90
1	A	116	SER	N-CA-C	5.21	116.88	108.08
1	B	473	PHE	N-CA-C	5.20	118.00	110.42
1	A	416	TRP	CE2-CD2-CG	-5.18	100.98	107.20
1	B	397	TRP	CG-CD1-NE1	-5.13	103.53	110.20
1	B	221	ILE	N-CA-C	5.08	115.17	107.80
1	B	416	TRP	CG-CD1-NE1	-5.07	103.61	110.20
1	B	397	TRP	CE2-CD2-CG	-5.06	101.12	107.20
1	A	430	GLU	N-CA-C	5.05	117.75	110.28
1	A	500	ILE	N-CA-C	5.04	115.17	108.11
1	B	358	TRP	CB-CG-CD1	-5.02	119.37	126.90
1	A	473	PHE	N-CA-C	5.00	117.80	110.30

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	4329	0	4332	74	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	3	1
4	B	89	0	0	7	0
All	All	8828	0	8673	153	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 (153) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:440:MET:HE1	1:A:513:ILE:HD13	1.96	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:A:441:MET:HE3	4:A:596:HOH:O	2.15	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:B:526:LYS:HD3	1:B:534:MET:HE1	1.97	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:526:LYS:HD2	1:A:534:MET:HE1	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:A:334:MET:HE3	1:A:334:MET:HB3	1.88	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
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:B:208:LYS:HB3	1:B:208:LYS:HE3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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%)	517 (92%)	34 (6%)	8 (1%)	9	23
1	B	559/561 (100%)	517 (92%)	37 (7%)	5 (1%)	14	35
All	All	1118/1122 (100%)	1034 (92%)	71 (6%)	13 (1%)	10	27

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	430	GLU
1	B	461	ASN
1	A	358	TRP

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Mol	Chain	Res	Type
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%)	417 (90%)	45 (10%)	8	20
1	B	462/462 (100%)	435 (94%)	27 (6%)	18	42
All	All	924/924 (100%)	852 (92%)	72 (8%)	11	29

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	22	ARG
1	A	116	SER
1	A	123	ASN
1	A	125	ASP
1	A	132	ILE
1	A	133	SER
1	A	148	GLN
1	A	151	LYS
1	A	154	GLU
1	A	161	ASP
1	A	163	LYS
1	A	166	LEU

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Mol	Chain	Res	Type
1	A	168	VAL
1	A	210	LEU
1	A	212	SER
1	A	218	LYS
1	A	276	LYS
1	A	281	ASP
1	A	309	VAL
1	A	324	GLN
1	A	325	THR
1	A	328	ARG
1	A	337	SER
1	A	356	THR
1	A	359	LYS
1	A	417	HIS
1	A	418	LYS
1	A	426	ARG
1	A	428	ASP
1	A	431	GLU
1	A	435	GLU
1	A	439	LYS
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	561	THR
1	B	5	THR
1	B	7	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
1	B	169	LEU

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Mol	Chain	Res	Type
1	B	173	GLN
1	B	188	VAL
1	B	190	SER
1	B	210	LEU
1	B	215	ASN
1	B	228	VAL
1	B	271	LEU
1	B	291	ASP
1	B	337	SER
1	B	349	ILE
1	B	359	LYS
1	B	388	LYS
1	B	418	LYS
1	B	430	GLU
1	B	432	VAL
1	B	462	ASP
1	B	512	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	50	GLN
1	A	131	ASN
1	A	173	GLN
1	A	215	ASN
1	A	299	HIS
1	A	345	ASN
1	A	422	ASN
1	A	486	ASN
1	A	529	GLN
1	A	532	GLN
1	A	547	GLN
1	B	14	GLN
1	B	29	GLN
1	B	37	ASN
1	B	89	GLN
1	B	117	HIS
1	B	205	ASN
1	B	476	HIS
1	B	532	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	2.02	4 (21%)	30,31,31	1.47	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	-	1/11/31/31	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	-5.96	1.49	1.59
2	A	563	G16	O4-C4	-3.55	1.34	1.43
2	A	563	G16	O6-C6	-2.93	1.33	1.44
2	A	563	G16	C4-C5	2.19	1.57	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	563	G16	O5-C5-C6	3.44	113.51	106.69
2	A	563	G16	O3-C3-C2	-3.10	103.06	110.38
2	A	563	G16	O1-C1-C2	-2.90	103.07	108.38
2	A	563	G16	C1-O5-C5	2.66	118.91	113.72

There are no chirality outliers.

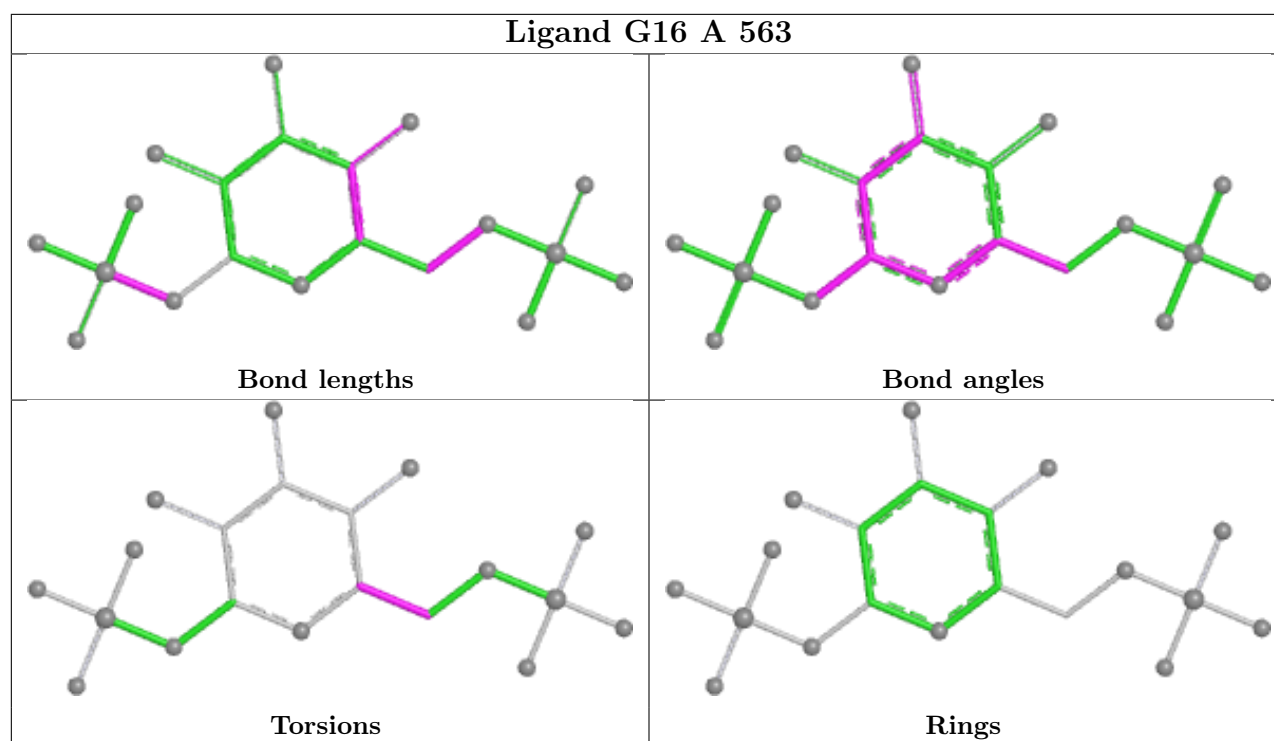
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	563	G16	C4-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 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	561/561 (100%)	0.45	67 (11%) 9 7	2, 25, 55, 67	0
1	B	561/561 (100%)	-0.12	15 (2%) 56 53	2, 13, 39, 58	0
All	All	1122/1122 (100%)	0.17	82 (7%) 21 18	2, 18, 51, 67	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	508	SER	6.3
1	A	17	GLY	5.5
1	A	559	VAL	5.4
1	A	446	ALA	4.7
1	A	539	ILE	4.6
1	B	507	GLY	4.5
1	B	289	ASP	4.3
1	B	17	GLY	4.1
1	A	461	ASN	4.0
1	A	552	THR	4.0
1	B	451	ARG	3.9
1	B	291	ASP	3.8
1	A	542	ALA	3.8
1	A	432	VAL	3.8
1	A	509	ALA	3.7
1	A	452	SER	3.7
1	B	506	THR	3.7
1	A	462	ASP	3.5
1	A	427	TYR	3.5
1	A	441	MET	3.4
1	A	555	THR	3.4
1	A	450	ASP	3.4
1	A	435	GLU	3.3
1	A	547	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	540	SER	3.3
1	A	503	LEU	3.2
1	B	505	GLY	3.2
1	A	536	ALA	3.2
1	A	496	GLY	3.2
1	A	453	PHE	3.1
1	B	116	SER	3.1
1	B	215	ASN	3.1
1	A	506	THR	3.0
1	A	557	PRO	3.0
1	A	466	THR	3.0
1	A	553	GLY	3.0
1	A	436	GLY	2.9
1	A	546	SER	2.9
1	A	18	THR	2.9
1	A	511	ALA	2.9
1	A	471	ASP	2.8
1	A	437	ALA	2.8
1	A	494	ALA	2.8
1	A	448	MET	2.7
1	A	428	ASP	2.7
1	A	549	GLN	2.7
1	A	459	SER	2.7
1	A	458	PHE	2.7
1	A	513	ILE	2.6
1	A	545	VAL	2.6
1	A	489	LEU	2.6
1	A	443	ASP	2.6
1	A	482	SER	2.5
1	A	434	ALA	2.5
1	A	447	LEU	2.5
1	A	460	ALA	2.5
1	A	532	GLN	2.5
1	A	537	PRO	2.5
1	A	438	THR	2.4
1	A	465	TYR	2.4
1	A	508	SER	2.4
1	A	464	VAL	2.4
1	A	19	SER	2.3
1	B	287	ASP	2.3
1	A	178	ASN	2.3
1	A	444	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	214	PRO	2.3
1	B	178	ASN	2.2
1	A	479	VAL	2.2
1	A	431	GLU	2.2
1	B	262	ASP	2.2
1	A	463	LYS	2.2
1	B	277	SER	2.2
1	A	445	GLU	2.2
1	A	515	LEU	2.1
1	A	455	GLY	2.1
1	A	488	GLY	2.1
1	A	483	VAL	2.1
1	B	459	SER	2.1
1	A	478	PRO	2.1
1	A	123	ASN	2.1
1	A	510	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

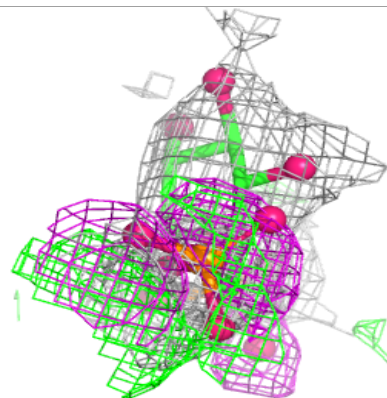
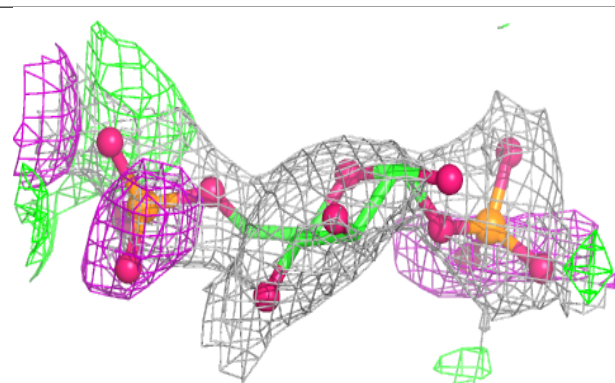
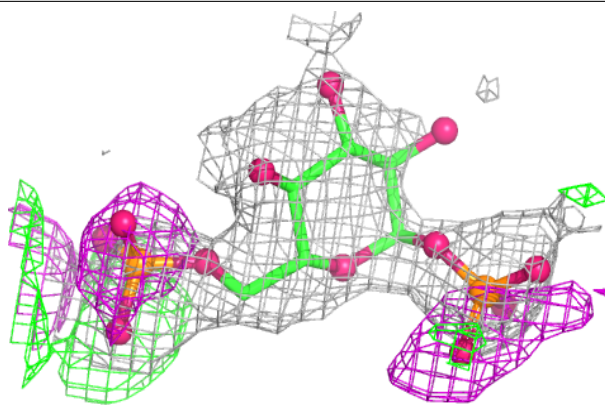
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	G16	A	563	20/20	0.67	0.23	19,26,32,33	0
3	CD	B	562	1/1	0.83	0.42	2,2,2,2	0
3	CD	A	562	1/1	0.85	0.36	3,3,3,3	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 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](#)

There are no such residues in this entry.