



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:32 AM UTC

PDB ID : 2XE6 / pdb_00002xe6
Title : The complete reaction cycle of human phosphoglycerate kinase: The open binary complex with 3PG
Authors : Cliff, M.J.; Baxter, N.J.; Blackburn, G.M.; Merli, A.; Vas, M.; Waltho, J.P.; Bowler, M.W.
Deposited on : 2010-05-11
Resolution : 1.74 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
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

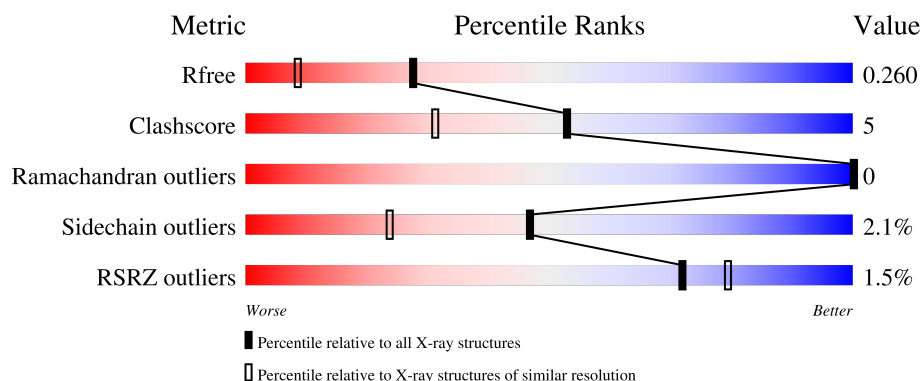
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	417	49% 47% ...

2 Entry composition [i](#)

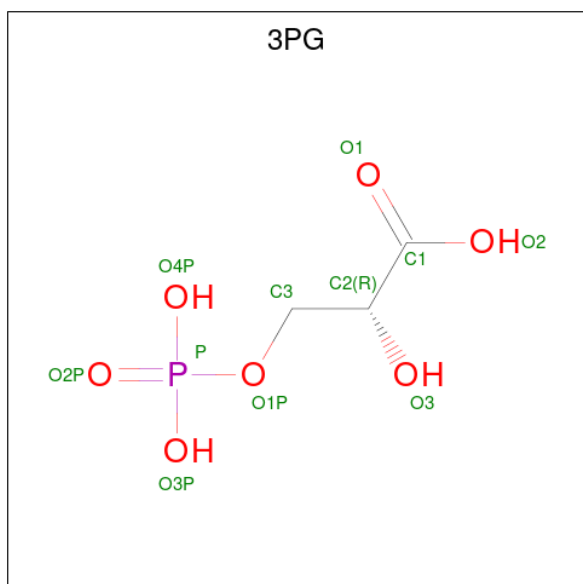
There are 3 unique types of molecules in this entry. The entry contains 3498 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PHOSPHOGLYCERATE KINASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	413	3127	1985	532	590	20	0	6	0

- Molecule 2 is 3-PHOSPHOGLYCERIC ACID (CCD ID: 3PG) (formula: $C_3H_7O_7P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	11	3	7	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	360	Total 360 O 360	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: PHOSPHOGLYCERATE KINASE 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	61.57Å 73.01Å 93.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.74 20.00 – 1.74	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.00-1.74) 98.5 (20.00-1.74)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.206 , 0.253 0.219 , 0.260	Depositor DCC
R_{free} test set	2180 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3498	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 6.59% 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: 3PG

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	2.29	188/3194 (5.9%)	1.12	13/4306 (0.3%)

All (188) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	GLY	C-O	-9.11	1.15	1.24
1	A	399[A]	LEU	N-CA	9.01	1.57	1.46
1	A	399[B]	LEU	N-CA	9.01	1.57	1.46
1	A	45	SER	C-O	-8.20	1.14	1.24
1	A	78[A]	GLU	C-O	-8.05	1.16	1.24
1	A	78[B]	GLU	C-O	-8.05	1.16	1.24
1	A	226	MET	SD-CE	-7.95	1.59	1.79
1	A	43	VAL	C-O	-7.94	1.14	1.24
1	A	180	LEU	C-O	-7.92	1.16	1.24
1	A	320	SER	C-O	-7.76	1.14	1.24
1	A	340	GLY	C-O	-7.65	1.16	1.23
1	A	211	LEU	C-O	-7.60	1.14	1.24
1	A	281	LEU	C-O	-7.54	1.16	1.24
1	A	333	ILE	C-O	-7.52	1.16	1.24
1	A	277	VAL	C-O	-7.51	1.15	1.24
1	A	369	ILE	C-O	-7.50	1.16	1.24
1	A	161	VAL	C-O	-7.45	1.16	1.24
1	A	14	LYS	C-O	-7.44	1.15	1.24
1	A	33	ILE	C-O	-7.39	1.16	1.24
1	A	272	ALA	C-O	-7.30	1.15	1.24
1	A	116	ILE	C-O	-7.28	1.16	1.24
1	A	58	VAL	C-O	-7.22	1.16	1.24
1	A	176	VAL	C-O	-7.22	1.15	1.24
1	A	83	GLU	C-O	-7.21	1.15	1.24
1	A	92	VAL	C-O	-7.20	1.16	1.24
1	A	177	GLY	C-O	-7.04	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208[A]	LEU	N-CA	-7.04	1.37	1.46
1	A	208[B]	LEU	N-CA	-7.04	1.37	1.46
1	A	52	ASN	C-O	-6.97	1.15	1.24
1	A	59	LEU	C-O	-6.92	1.15	1.24
1	A	392	SER	C-O	-6.88	1.15	1.23
1	A	225	ASN	C-O	-6.87	1.16	1.24
1	A	346	ALA	CA-CB	-6.87	1.41	1.53
1	A	300	ALA	C-O	-6.86	1.15	1.23
1	A	147[A]	GLU	C-O	-6.85	1.16	1.24
1	A	147[B]	GLU	C-O	-6.85	1.16	1.24
1	A	288	ALA	C-O	-6.82	1.15	1.23
1	A	243	PHE	C-O	-6.81	1.16	1.24
1	A	80	VAL	C-O	-6.80	1.16	1.24
1	A	17	ARG	C-O	-6.79	1.15	1.24
1	A	224	ASN	C-O	-6.78	1.16	1.24
1	A	18	VAL	C-O	-6.69	1.16	1.24
1	A	192	GLU	C-O	-6.64	1.16	1.24
1	A	388	VAL	C-O	-6.63	1.16	1.23
1	A	122	ARG	C-O	-6.61	1.15	1.24
1	A	140	LYS	C-O	-6.61	1.15	1.24
1	A	55	LYS	C-O	-6.56	1.16	1.24
1	A	223	ILE	C-O	-6.53	1.16	1.24
1	A	298	GLY	C-O	-6.51	1.16	1.23
1	A	314	ASP	C-O	-6.49	1.16	1.23
1	A	354	LEU	C-O	-6.46	1.16	1.24
1	A	410	VAL	C-O	-6.46	1.16	1.24
1	A	11	LEU	C-O	-6.45	1.16	1.23
1	A	86	SER	C-O	-6.44	1.16	1.24
1	A	168	ALA	C-O	-6.42	1.16	1.24
1	A	390	HIS	C-O	-6.35	1.16	1.23
1	A	147[A]	GLU	N-CA	6.34	1.54	1.46
1	A	147[B]	GLU	N-CA	6.34	1.54	1.46
1	A	262	ALA	CA-CB	-6.32	1.43	1.53
1	A	407	LEU	C-O	-6.25	1.17	1.24
1	A	217	ALA	C-O	-6.21	1.16	1.24
1	A	54	ALA	C-O	-6.21	1.16	1.23
1	A	391	VAL	C-O	-6.19	1.17	1.24
1	A	134	ALA	CA-CB	-6.19	1.42	1.53
1	A	302	VAL	C-O	-6.18	1.17	1.24
1	A	245	LYS	C-O	-6.16	1.17	1.24
1	A	28	MET	C-O	-6.14	1.16	1.23
1	A	111	ALA	CA-CB	-6.13	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	372	GLY	C-O	-6.12	1.17	1.23
1	A	379	CYS	C-O	-6.12	1.17	1.24
1	A	23	ASP	C-O	-6.09	1.16	1.23
1	A	209	ALA	C-O	-6.09	1.16	1.24
1	A	212	GLY	C-O	-6.09	1.16	1.23
1	A	77	LEU	C-O	-6.07	1.16	1.24
1	A	321	LYS	C-O	-6.05	1.17	1.24
1	A	377	THR	C-O	-6.05	1.17	1.24
1	A	71	MET	C-O	-6.04	1.17	1.23
1	A	144	ALA	CA-CB	-6.03	1.43	1.53
1	A	41	ALA	CA-CB	-6.03	1.43	1.53
1	A	178	VAL	C-O	-6.02	1.17	1.24
1	A	175	MET	C-O	-6.01	1.16	1.24
1	A	385	GLU	C-O	-5.98	1.17	1.24
1	A	299	GLN	C-O	-5.98	1.16	1.23
1	A	46	ILE	C-O	-5.97	1.17	1.24
1	A	398	SER	C-O	-5.96	1.17	1.24
1	A	202[A]	SER	N-CA	-5.95	1.37	1.46
1	A	202[B]	SER	N-CA	-5.95	1.37	1.46
1	A	103	VAL	C-O	-5.94	1.17	1.24
1	A	336	ASN	C-O	-5.93	1.16	1.23
1	A	145	LYS	C-O	-5.92	1.17	1.24
1	A	22	VAL	C-O	-5.91	1.17	1.23
1	A	60	MET	C-O	-5.91	1.17	1.23
1	A	84	LEU	C-O	-5.88	1.17	1.24
1	A	257	PHE	C-O	-5.87	1.17	1.24
1	A	301	THR	C-O	-5.86	1.16	1.23
1	A	399[A]	LEU	CA-C	-5.85	1.45	1.52
1	A	399[B]	LEU	CA-C	-5.85	1.45	1.52
1	A	337	GLY	C-O	-5.84	1.16	1.24
1	A	344	TRP	C-O	-5.83	1.17	1.24
1	A	323	TYR	C-O	-5.81	1.17	1.24
1	A	334	VAL	C-O	-5.78	1.17	1.24
1	A	400	GLU	C-O	-5.76	1.17	1.24
1	A	139	VAL	C-O	-5.75	1.17	1.23
1	A	295	ALA	C-O	-5.74	1.16	1.23
1	A	315	CYS	C-O	-5.74	1.16	1.23
1	A	153	LEU	C-O	-5.74	1.17	1.24
1	A	127	GLU	C-O	-5.73	1.17	1.24
1	A	236	GLY	C-O	-5.73	1.17	1.23
1	A	184	ALA	C-O	-5.71	1.17	1.24
1	A	292	ASP	C-O	-5.71	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	278	LYS	C-O	-5.68	1.17	1.24
1	A	210	ILE	C-O	-5.68	1.18	1.24
1	A	397	ALA	C-O	-5.68	1.17	1.24
1	A	346	ALA	C-O	-5.67	1.16	1.24
1	A	104	GLU	C-O	-5.67	1.17	1.24
1	A	163	ASP	C-O	-5.66	1.16	1.24
1	A	308	ALA	C-O	-5.65	1.17	1.23
1	A	367	ILE	C-O	-5.65	1.17	1.23
1	A	358	VAL	C-O	-5.64	1.17	1.24
1	A	156	LEU	C-O	-5.63	1.16	1.24
1	A	352	LYS	C-O	-5.63	1.17	1.24
1	A	112	ALA	CA-CB	-5.62	1.43	1.53
1	A	238	GLY	C-O	-5.61	1.16	1.23
1	A	137	ASN	C-O	-5.60	1.17	1.23
1	A	351	THR	C-O	-5.60	1.17	1.24
1	A	300	ALA	CA-CB	-5.59	1.43	1.53
1	A	285	PHE	C-O	-5.58	1.17	1.23
1	A	38	ARG	C-O	-5.57	1.17	1.24
1	A	183	LYS	C-O	-5.56	1.17	1.24
1	A	406	VAL	C-O	-5.56	1.15	1.23
1	A	121	LEU	C-O	-5.55	1.17	1.24
1	A	115	VAL	C-O	-5.55	1.18	1.24
1	A	107	CYS	C-O	-5.55	1.16	1.24
1	A	247	LEU	C-O	-5.55	1.17	1.24
1	A	191	LYS	C-O	-5.54	1.17	1.24
1	A	287	THR	C-O	-5.54	1.16	1.23
1	A	304	SER	C-O	-5.54	1.17	1.24
1	A	167	THR	C-O	-5.54	1.16	1.24
1	A	316	GLY	C-O	-5.52	1.16	1.24
1	A	40	LYS	C-O	-5.52	1.17	1.24
1	A	41	ALA	C-O	-5.50	1.17	1.24
1	A	374	ASP	C-O	-5.49	1.17	1.24
1	A	396	GLY	C-O	-5.48	1.17	1.23
1	A	19	VAL	C-O	-5.48	1.18	1.24
1	A	209	ALA	CA-CB	-5.45	1.45	1.53
1	A	6	LEU	C-O	-5.41	1.17	1.23
1	A	57	VAL	C-O	-5.40	1.18	1.24
1	A	25	ASN	C-O	-5.40	1.17	1.23
1	A	366	CYS	C-O	-5.39	1.17	1.23
1	A	165	PHE	C-O	-5.37	1.17	1.24
1	A	293	GLU	C-O	-5.37	1.17	1.24
1	A	49	CYS	C-O	-5.36	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	LYS	C-O	-5.34	1.18	1.24
1	A	387	LYS	CB-CG	-5.33	1.36	1.52
1	A	93	LEU	C-O	-5.32	1.17	1.24
1	A	114	SER	C-O	-5.32	1.17	1.23
1	A	359	VAL	C-O	-5.31	1.18	1.24
1	A	258	ASP	C-O	-5.30	1.17	1.23
1	A	160	TYR	C-O	-5.29	1.17	1.24
1	A	241	PHE	C-O	-5.28	1.17	1.24
1	A	342	PHE	C-O	-5.26	1.17	1.24
1	A	34	THR	C-O	-5.25	1.17	1.24
1	A	332	GLN	C-O	-5.24	1.17	1.23
1	A	234	ILE	C-O	-5.24	1.18	1.24
1	A	130	LYS	C-O	-5.23	1.17	1.23
1	A	158	ASP	C-O	-5.23	1.17	1.24
1	A	249	ASN	C-O	-5.23	1.16	1.23
1	A	20	MET	C-O	-5.23	1.18	1.24
1	A	164	ALA	C-O	-5.21	1.16	1.23
1	A	170	ARG	C-O	-5.20	1.17	1.24
1	A	149	PHE	C-O	-5.20	1.18	1.24
1	A	284	ASP	C-O	-5.20	1.17	1.23
1	A	96	LYS	C-O	-5.18	1.17	1.24
1	A	296	LYS	C-O	-5.16	1.17	1.23
1	A	318	GLU	C-O	-5.15	1.18	1.24
1	A	69	VAL	C-O	-5.14	1.18	1.24
1	A	150	ARG	C-O	-5.14	1.18	1.24
1	A	148	ALA	C-O	-5.13	1.18	1.24
1	A	195	TYR	C-O	-5.13	1.18	1.24
1	A	39	ILE	C-O	-5.12	1.18	1.24
1	A	133	ASP	C-O	-5.12	1.17	1.23
1	A	345	GLU	C-O	-5.10	1.18	1.24
1	A	208[A]	LEU	CA-C	5.09	1.58	1.52
1	A	208[B]	LEU	CA-C	5.09	1.58	1.52
1	A	383	ASN	C-O	-5.09	1.17	1.23
1	A	233	MET	C-O	-5.06	1.18	1.23
1	A	62	HIS	C-O	-5.03	1.17	1.23
1	A	357	GLU	C-O	-5.02	1.18	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	VAL	CB-CA-C	-7.52	100.68	110.98
1	A	214	ALA	N-CA-C	7.49	119.23	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	VAL	N-CA-C	7.25	117.96	110.05
1	A	303	ALA	N-CA-C	7.16	119.17	111.36
1	A	247	LEU	N-CA-C	6.60	118.55	111.36
1	A	329	ARG	N-CA-C	6.49	119.34	111.82
1	A	365	GLY	N-CA-C	6.34	124.07	115.32
1	A	19	VAL	N-CA-CB	6.33	118.61	111.21
1	A	196	PHE	N-CA-C	5.89	117.78	111.36
1	A	53	GLY	N-CA-C	5.44	123.09	115.43
1	A	87	LEU	N-CA-C	5.40	117.17	111.28
1	A	244	LEU	N-CA-C	5.21	117.03	111.36
1	A	264	ILE	N-CA-C	5.17	117.08	112.17

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	3127	0	3227	32	0
2	A	11	0	4	0	0
3	A	360	0	0	11	0
All	All	3498	0	3231	32	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 5.

All (32) 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:71:MET:HE1	3:A:2091:HOH:O	1.57	1.02
1:A:338:PRO:HD3	3:A:2336:HOH:O	1.63	0.96
1:A:207:PHE:H	1:A:231:ASN:HD22	1.21	0.86
1:A:375:THR:N	3:A:2336:HOH:O	2.09	0.83
1:A:406:VAL:HG21	1:A:411:ASP:OD2	1.82	0.78
1:A:205:ARG:HH21	1:A:231:ASN:HD21	1.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:LYS:HE3	3:A:2301:HOH:O	1.86	0.75
1:A:406:VAL:CG2	1:A:411:ASP:OD2	2.38	0.71
1:A:19:VAL:HG22	1:A:157:GLY:HA3	1.75	0.69
1:A:375:THR:OG1	3:A:2336:HOH:O	2.12	0.66
1:A:205:ARG:HH21	1:A:231:ASN:ND2	1.98	0.60
1:A:384:THR:HA	1:A:387:LYS:HD3	1.82	0.60
1:A:37:GLN:NE2	3:A:2044:HOH:O	2.36	0.59
1:A:226:MET:HE3	1:A:402:LEU:O	2.02	0.59
1:A:205:ARG:HA	1:A:206:PRO:C	2.31	0.55
1:A:5:LYS:HZ3	1:A:415:ASN:HD21	1.55	0.53
1:A:97:ASP:OD1	1:A:124:HIS:HE1	1.91	0.53
1:A:124:HIS:HD2	3:A:2145:HOH:O	1.92	0.53
1:A:78[B]:GLU:HB3	1:A:79:PRO:HD3	1.91	0.52
1:A:167:THR:O	1:A:167:THR:HG22	2.09	0.52
1:A:375:THR:CA	3:A:2336:HOH:O	2.58	0.51
1:A:200:LEU:HD21	1:A:226:MET:HE1	1.93	0.50
1:A:5:LYS:NZ	1:A:415:ASN:ND2	2.60	0.49
1:A:5:LYS:NZ	1:A:415:ASN:HD21	2.12	0.48
1:A:204:GLU:H	1:A:332:GLN:HE21	1.63	0.47
1:A:183:LYS:HE3	1:A:412:ALA:O	2.15	0.47
1:A:226:MET:HA	1:A:226:MET:HE2	1.99	0.43
1:A:361:ALA:O	1:A:364:ARG:HG3	2.18	0.43
1:A:124:HIS:CD2	3:A:2145:HOH:O	2.67	0.42
1:A:207:PHE:N	1:A:231:ASN:HD22	2.03	0.42
1:A:147[A]:GLU:HG3	3:A:2171:HOH:O	2.19	0.42
1:A:101:PRO:O	3:A:2112:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	417/417 (100%)	414 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	338/336 (101%)	330 (98%)	8 (2%)	43	19

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	19	VAL
1	A	198	LYS
1	A	208[A]	LEU
1	A	208[B]	LEU
1	A	274	LYS
1	A	332	GLN
1	A	387	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	37	GLN
1	A	124	HIS
1	A	137	ASN
1	A	224	ASN
1	A	225	ASN
1	A	231	ASN
1	A	332	GLN
1	A	415	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](#)

1 ligand is modelled in this entry.

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	3PG	A	1417	-	9,10,10	1.37	1 (11%)	11,14,14	1.23	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	3PG	A	1417	-	-	0/10/10/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1417	3PG	O1P-C3	-2.04	1.36	1.44

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	413/417 (99%)	0.13	6 (1%) 72 79	11, 21, 32, 36	6 (1%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	ASN	2.9
1	A	416	ILE	2.7
1	A	383	ASN	2.6
1	A	372	GLY	2.2
1	A	371	GLY	2.1
1	A	73	ASP	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(Å ²)	Q<0.9
2	3PG	A	1417	11/11	0.98	0.05	13,16,18,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.