



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 03:41 PM UTC

PDB ID : 6ZQ4 / pdb_00006zq4
Title : Crystal structure of Chaetomium thermophilum Glycerol Kinase in complex with substrate in P1 space group
Authors : Wilk, P.; Wator, E.; Grudnik, P.
Deposited on : 2020-07-09
Resolution : 2.02 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

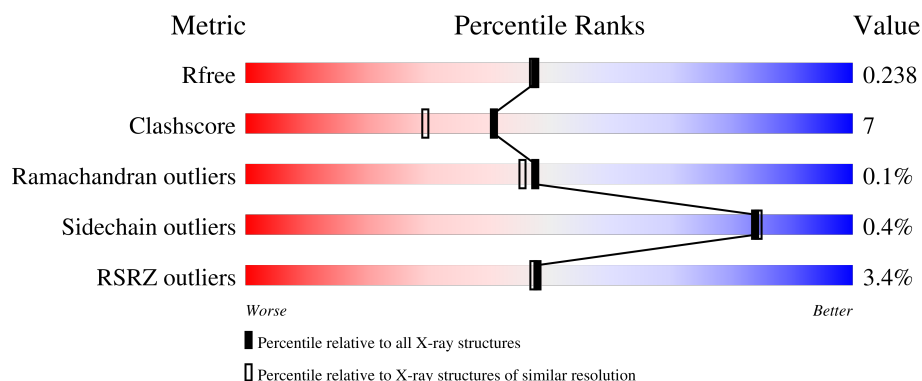
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

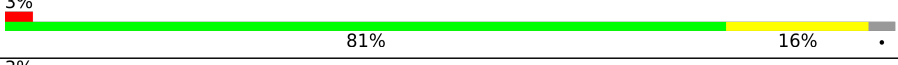
The reported resolution of this entry is 2.02 Å.

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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	526	
1	B	526	
1	C	526	
1	D	526	
1	E	526	

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Mol	Chain	Length	Quality of chain
1	F	526	
1	G	526	
1	H	526	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	601	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 63968 atoms, of which 30941 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 Glycerol kinase-like protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	510	Total	C	H	N	O	S	0	4	0
			7817	2485	3890	681	745	16			
1	B	510	Total	C	H	N	O	S	0	1	0
			7773	2472	3868	677	740	16			
1	C	509	Total	C	H	N	O	S	0	0	0
			7748	2466	3854	673	739	16			
1	D	509	Total	C	H	N	O	S	0	0	0
			7745	2465	3852	673	739	16			
1	E	511	Total	C	H	N	O	S	0	0	0
			7762	2470	3860	675	741	16			
1	F	512	Total	C	H	N	O	S	0	0	0
			7776	2474	3866	677	743	16			
1	G	512	Total	C	H	N	O	S	0	0	0
			7777	2474	3867	677	743	16			
1	H	511	Total	C	H	N	O	S	0	0	0
			7762	2470	3860	675	741	16			

There are 16 discrepancies between the modelled and reference sequences:

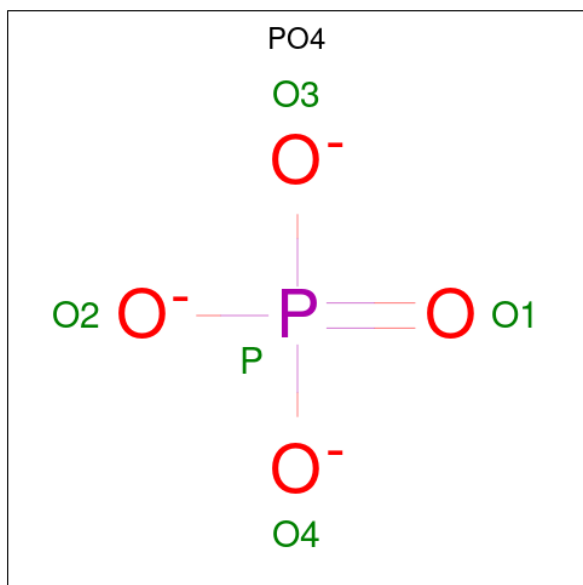
Chain	Residue	Modelled	Actual	Comment	Reference
A	65	GLY	-	expression tag	UNP G0SAG9
A	66	SER	-	expression tag	UNP G0SAG9
B	65	GLY	-	expression tag	UNP G0SAG9
B	66	SER	-	expression tag	UNP G0SAG9
C	65	GLY	-	expression tag	UNP G0SAG9
C	66	SER	-	expression tag	UNP G0SAG9
D	65	GLY	-	expression tag	UNP G0SAG9
D	66	SER	-	expression tag	UNP G0SAG9
E	65	GLY	-	expression tag	UNP G0SAG9
E	66	SER	-	expression tag	UNP G0SAG9
F	65	GLY	-	expression tag	UNP G0SAG9
F	66	SER	-	expression tag	UNP G0SAG9
G	65	GLY	-	expression tag	UNP G0SAG9

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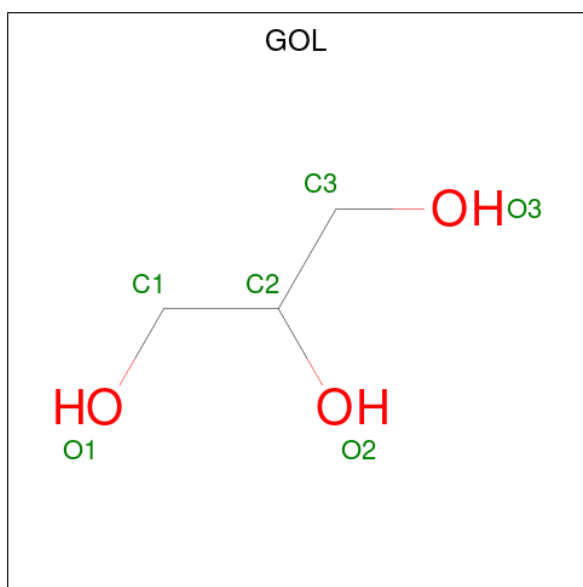
Chain	Residue	Modelled	Actual	Comment	Reference
G	66	SER	-	expression tag	UNP G0SAG9
H	65	GLY	-	expression tag	UNP G0SAG9
H	66	SER	-	expression tag	UNP G0SAG9

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			9	3	3	3		
3	B	1	Total	C	H	O	0	0
			9	3	3	3		
3	C	1	Total	C	H	O	0	0
			9	3	3	3		
3	D	1	Total	C	H	O	0	0
			9	3	3	3		
3	E	1	Total	C	H	O	0	0
			9	3	3	3		
3	F	1	Total	C	H	O	0	0
			9	3	3	3		
3	G	1	Total	C	H	O	0	0
			9	3	3	3		
3	H	1	Total	C	H	O	0	0
			9	3	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	192	Total	O	0	0
			192	192		
4	B	276	Total	O	0	0
			276	276		
4	C	243	Total	O	0	0
			243	243		
4	D	208	Total	O	0	0
			208	208		

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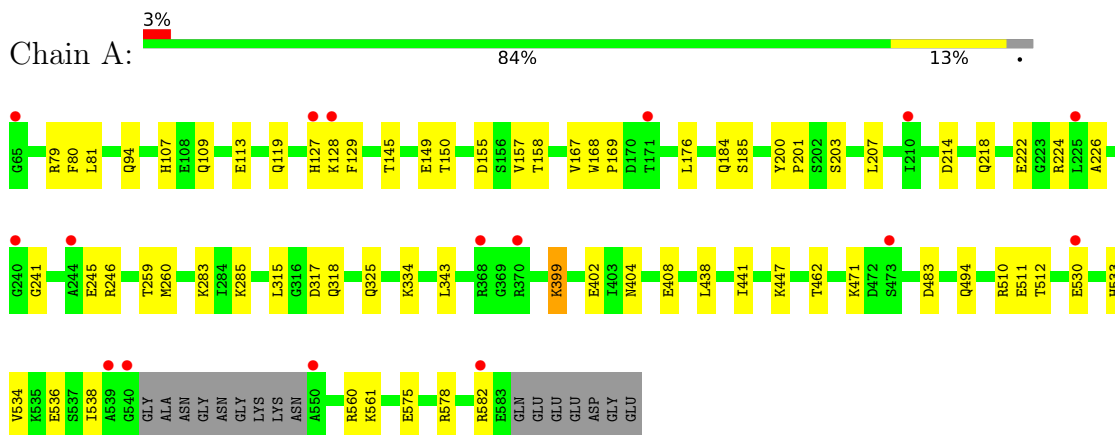
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	220	Total 220	O 220	0	0
4	F	234	Total 234	O 234	0	0
4	G	186	Total 186	O 186	0	0
4	H	147	Total 147	O 147	0	0

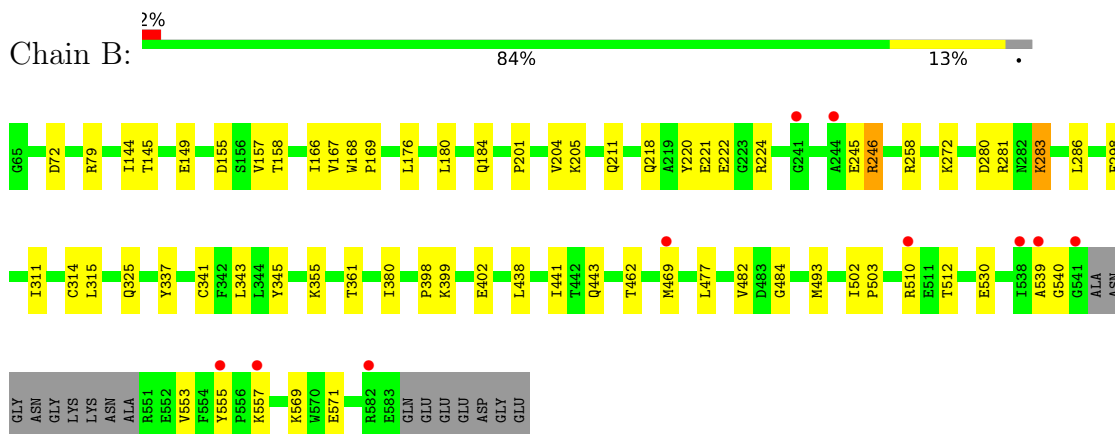
3 Residue-property plots [i](#)

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.

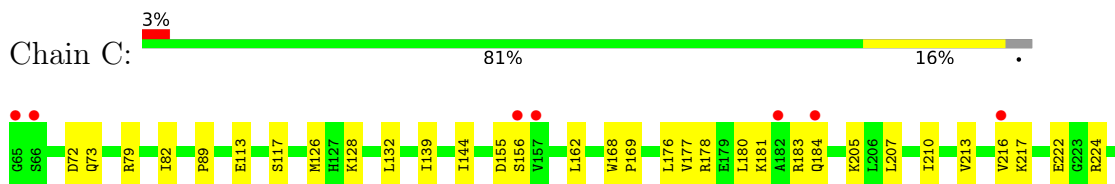
- Molecule 1: Glycerol kinase-like protein

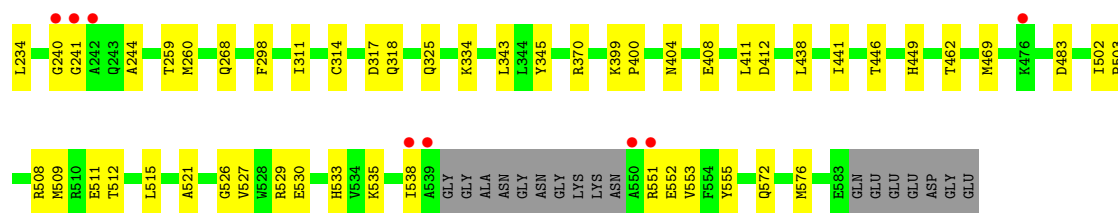


- Molecule 1: Glycerol kinase-like protein

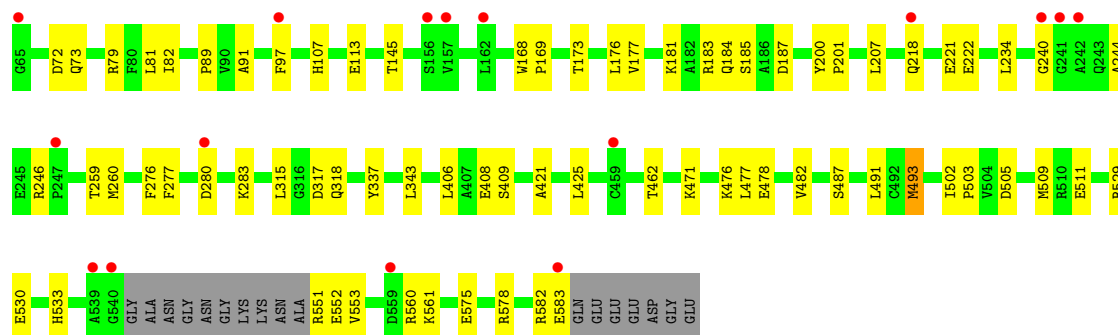
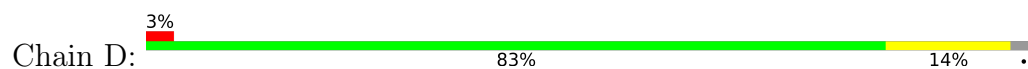


- Molecule 1: Glycerol kinase-like protein

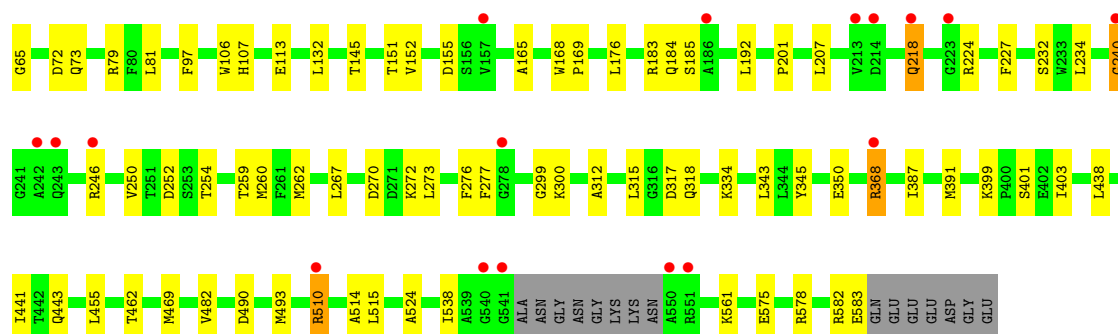
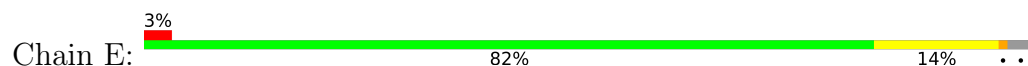




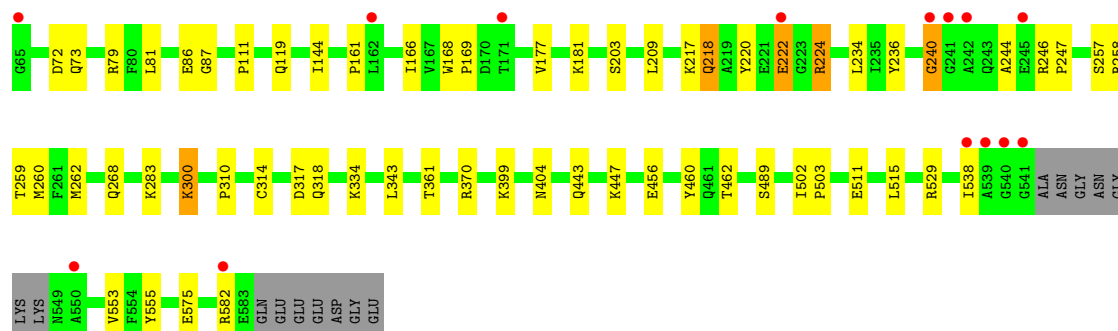
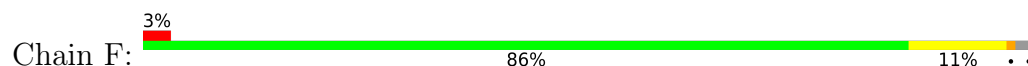
• Molecule 1: Glycerol kinase-like protein



• Molecule 1: Glycerol kinase-like protein



• Molecule 1: Glycerol kinase-like protein



Chain G:

Chain H:

Amino Acid	Type
G65	Red
D72	Yellow
R79	Yellow
F80	Yellow
L81	Yellow
I82	Yellow
F83	Yellow
E86	Yellow
G87	Yellow
R88	Yellow
P89	Yellow
I95	Red
R99	Red
P102	Red
W106	Red
L114	Yellow
S117	Yellow
D123	Yellow
M126	Yellow
H127	Yellow
K128	Red
F129	Yellow
L132	Yellow
I142	Yellow
G143	Yellow
I144	Yellow
T145	Yellow
V153	Yellow
W154	Yellow
D155	Yellow
S156	Yellow
V157	Red
T158	Yellow
G159	Red
L162	Yellow
I166	Yellow
V167	Yellow
W168	Yellow
P169	Yellow
D170	Yellow
T171	Red
L176	Yellow
Q184	Yellow
S185	Yellow
L195	Yellow
S203	Yellow
V204	Yellow
K205	Yellow
L206	Yellow
L207	Yellow
W208	Yellow
L209	Yellow
V216	Yellow
K217	Yellow
Q218	Yellow
A219	Yellow
Y220	Red
E221	Yellow
E222	Yellow
G223	Red
R224	Red
L225	Red
A226	Yellow
W233	Yellow
L234	Yellow
L235	Yellow
Y236	Yellow
K237	Yellow
G240	Red
G241	Red
A242	Red
Q243	Red
A244	Red
R258	Yellow
T259	Yellow
F277	Yellow
K283	Yellow
I284	Yellow
K285	Yellow
A497	Yellow
D498	Yellow
G299	Yellow
I311	Yellow
A312	Yellow
L315	Yellow
G316	Yellow
D317	Yellow
Q318	Yellow
Q325	Yellow
K334	Yellow
L359	Yellow
A360	Yellow
T361	Yellow
G367	Red
R370	Yellow
K371	Yellow
E377	Yellow
F396	Yellow
K399	Yellow
P400	Yellow
S401	Yellow
M404	Yellow
E408	Yellow
A421	Yellow
L425	Yellow
F426	Yellow
K447	Yellow
C459	Yellow
S473	Red
K476	Red
V482	Yellow
D483	Yellow
L486	Yellow
S487	Yellow
M493	Yellow
Q494	Yellow
T495	Yellow
Q496	Yellow
A497	Yellow
D498	Yellow
V504	Yellow
P507	Yellow
R508	Yellow
M509	Red
R510	Yellow
E511	Yellow
T512	Yellow
L515	Yellow
A524	Yellow
E530	Yellow
L531	Yellow
D532	Yellow
K535	Yellow
I538	Red
A539	Yellow
G540	Red
G541	Red
ALA	Yellow
ASN	Yellow
GLY	Yellow
ASN	Yellow
GLY	Yellow
GLY	Yellow
LYS	Yellow
ASN	Yellow
A550	Red
R551	Yellow
E552	Yellow
K557	Red
R560	Yellow
R565	Yellow
E571	Yellow
R582	Red
E583	Yellow
GLN	Yellow
GLU	Yellow
GLU	Yellow
GLU	Yellow
ASP	Yellow
GLY	Yellow
GLU	Yellow

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.38Å 112.82Å 179.54Å 85.77° 90.04° 85.45°	Depositor
Resolution (Å)	23.01 – 2.02 23.01 – 2.02	Depositor EDS
% Data completeness (in resolution range)	97.3 (23.01-2.02) 97.7 (23.01-2.02)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 2.01Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.205 , 0.240 0.206 , 0.238	Depositor DCC
R_{free} test set	3228 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 63.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	63968	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.49	3/4018 (0.1%)	0.71	13/5445 (0.2%)
1	B	0.58	5/3990 (0.1%)	0.67	8/5407 (0.1%)
1	C	0.40	2/3976 (0.1%)	0.61	11/5390 (0.2%)
1	D	0.38	2/3975 (0.1%)	0.53	3/5388 (0.1%)
1	E	0.45	5/3984 (0.1%)	0.61	8/5400 (0.1%)
1	F	0.46	6/3992 (0.2%)	0.61	14/5411 (0.3%)
1	G	0.38	3/3992 (0.1%)	0.60	8/5411 (0.1%)
1	H	0.42	3/3984 (0.1%)	0.61	7/5400 (0.1%)
All	All	0.45	29/31911 (0.1%)	0.62	72/43252 (0.2%)

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	B	0	2
1	E	0	1
All	All	0	3

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	246	ARG	C-N	15.72	1.54	1.33
1	B	246	ARG	C-N	15.08	1.53	1.33
1	F	246	ARG	C-N	14.54	1.53	1.33
1	A	246	ARG	C-N	14.52	1.53	1.33
1	B	286	LEU	C-N	13.83	1.51	1.33

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	285	LYS	CG-CD-CE	11.34	137.39	111.30
1	A	399	LYS	CA-CB-CG	11.25	136.60	114.10
1	A	582	ARG	NE-CZ-NH1	11.15	132.65	121.50
1	A	510	ARG	CA-CB-CG	9.97	134.04	114.10
1	E	510	ARG	CB-CG-CD	9.43	132.98	111.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	539	ALA	Peptide
1	B	540	GLY	Peptide
1	E	510	ARG	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	3927	3890	3881	40	0
1	B	3905	3868	3868	45	1
1	C	3894	3854	3854	57	0
1	D	3893	3852	3852	51	0
1	E	3902	3860	3860	51	0
1	F	3910	3866	3866	44	0
1	G	3910	3867	3866	44	1
1	H	3902	3860	3860	78	0
2	A	5	0	0	2	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	1	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	6	3	8	1	0
3	B	6	3	8	1	0
3	C	6	3	8	0	0
3	D	6	3	8	0	0
3	E	6	3	8	0	0
3	F	6	3	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	6	3	8	0	0
3	H	6	3	8	0	0
4	A	192	0	0	7	0
4	B	276	0	0	6	0
4	C	243	0	0	9	0
4	D	208	0	0	7	0
4	E	220	0	0	9	0
4	F	234	0	0	7	0
4	G	186	0	0	3	0
4	H	147	0	0	7	0
All	All	33027	30941	30971	406	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 7.

The worst 5 of 406 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:GLU:OE1	1:B:283:LYS:NZ	1.94	1.01
1:D:183:ARG:NH2	1:D:276:PHE:O	1.95	0.98
1:B:221:GLU:HA	1:B:283:LYS:HE2	1.49	0.95
1:H:482:VAL:HG11	1:H:493:MET:HE1	1.47	0.94
1:A:119:GLN:OE1	4:A:701:HOH:O	1.86	0.93

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:B:280:ASP:OD2	1:G:184:GLN:NE2[1_455]	2.03	0.17

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	510/526 (97%)	495 (97%)	14 (3%)	1 (0%)	43	40
1	B	507/526 (96%)	493 (97%)	13 (3%)	1 (0%)	43	40
1	C	505/526 (96%)	490 (97%)	15 (3%)	0	100	100
1	D	505/526 (96%)	492 (97%)	13 (3%)	0	100	100
1	E	507/526 (96%)	495 (98%)	12 (2%)	0	100	100
1	F	508/526 (97%)	495 (97%)	13 (3%)	0	100	100
1	G	508/526 (97%)	492 (97%)	15 (3%)	1 (0%)	43	40
1	H	507/526 (96%)	490 (97%)	17 (3%)	0	100	100
All	All	4057/4208 (96%)	3942 (97%)	112 (3%)	3 (0%)	48	45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	GLY
1	G	241	GLY
1	B	245	GLU

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	413/420 (98%)	411 (100%)	2 (0%)	81	81
1	B	410/420 (98%)	409 (100%)	1 (0%)	87	88
1	C	409/420 (97%)	409 (100%)	0	100	100
1	D	409/420 (97%)	408 (100%)	1 (0%)	87	88
1	E	409/420 (97%)	406 (99%)	3 (1%)	76	77
1	F	410/420 (98%)	410 (100%)	0	100	100
1	G	410/420 (98%)	407 (99%)	3 (1%)	76	77
1	H	409/420 (97%)	406 (99%)	3 (1%)	76	77
All	All	3279/3360 (98%)	3266 (100%)	13 (0%)	84	84

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	92	SER
1	G	370	ARG
1	H	551	ARG
1	H	370	ARG
1	H	530	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	212	ASN
1	F	549	ASN
1	H	572	GLN
1	G	212	ASN
1	B	282	ASN

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 ⓘ

14 ligands are 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
3	GOL	H	601	-	5,5,5	0.97	0	5,5,5	1.18	1 (20%)
3	GOL	C	602	-	5,5,5	0.80	0	5,5,5	1.15	1 (20%)
2	PO4	F	601	-	4,4,4	1.94	1 (25%)	6,6,6	0.43	0
3	GOL	F	602	-	5,5,5	0.81	0	5,5,5	1.18	1 (20%)
2	PO4	B	601	-	4,4,4	1.85	1 (25%)	6,6,6	0.71	0
3	GOL	G	601	-	5,5,5	0.93	0	5,5,5	1.12	1 (20%)
3	GOL	A	602	-	5,5,5	0.89	0	5,5,5	1.16	1 (20%)
2	PO4	E	601	-	4,4,4	1.46	1 (25%)	6,6,6	0.79	0
3	GOL	D	602	-	5,5,5	0.66	0	5,5,5	1.15	1 (20%)
2	PO4	C	601	-	4,4,4	0.99	0	6,6,6	0.56	0
2	PO4	A	601	-	4,4,4	1.63	1 (25%)	6,6,6	0.50	0
2	PO4	D	601	-	4,4,4	0.95	0	6,6,6	0.61	0
3	GOL	E	602	-	5,5,5	0.26	0	5,5,5	0.30	0
3	GOL	B	602	-	5,5,5	0.70	0	5,5,5	1.15	1 (20%)

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	GOL	H	601	-	-	3/4/4/4	-
3	GOL	C	602	-	-	0/4/4/4	-
3	GOL	F	602	-	-	0/4/4/4	-
3	GOL	G	601	-	-	0/4/4/4	-
3	GOL	A	602	-	-	0/4/4/4	-
3	GOL	D	602	-	-	1/4/4/4	-
3	GOL	E	602	-	-	0/4/4/4	-
3	GOL	B	602	-	-	0/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	PO4	P-O4	-3.29	1.45	1.54
2	F	601	PO4	P-O3	-2.46	1.47	1.54
2	A	601	PO4	P-O2	-2.11	1.48	1.54
2	E	601	PO4	P-O2	-2.05	1.48	1.54

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	GOL	C3-C2-C1	-2.28	103.42	111.80
3	H	601	GOL	C3-C2-C1	-2.27	103.47	111.80
3	F	602	GOL	C3-C2-C1	-2.24	103.59	111.80
3	B	602	GOL	C3-C2-C1	-2.22	103.67	111.80
3	A	602	GOL	C3-C2-C1	-2.21	103.68	111.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	601	GOL	O1-C1-C2-C3
3	H	601	GOL	O1-C1-C2-O2
3	H	601	GOL	O2-C2-C3-O3
3	D	602	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	GOL	1	0
2	A	601	PO4	2	0
2	D	601	PO4	1	0
3	B	602	GOL	1	0

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](#)

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	510/526 (96%)	0.17	16 (3%) 51 51	19, 51, 88, 119	3 (0%)
1	B	510/526 (96%)	-0.00	10 (1%) 65 65	23, 45, 86, 115	1 (0%)
1	C	509/526 (96%)	0.13	15 (2%) 53 53	30, 50, 89, 155	0
1	D	509/526 (96%)	0.15	16 (3%) 51 51	25, 49, 90, 135	0
1	E	511/526 (97%)	0.17	17 (3%) 49 48	26, 51, 98, 136	0
1	F	512/526 (97%)	0.10	14 (2%) 56 56	29, 49, 89, 168	0
1	G	512/526 (97%)	0.27	20 (3%) 43 43	33, 56, 93, 167	0
1	H	511/526 (97%)	0.42	29 (5%) 29 28	34, 60, 105, 194	0
All	All	4084/4208 (97%)	0.17	137 (3%) 48 47	19, 52, 93, 194	4 (0%)

The worst 5 of 137 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	469	MET	6.0
1	H	550	ALA	5.8
1	G	550	ALA	5.7
1	D	459	CYS	5.2
1	C	242	ALA	5.0

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

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

6.3 Carbohydrates [i](#)

There are no 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	PO4	E	601	5/5	0.79	0.17	56,60,67,67	5
2	PO4	A	601	5/5	0.81	0.18	57,60,66,68	5
2	PO4	C	601	5/5	0.82	0.20	54,59,64,68	5
2	PO4	F	601	5/5	0.83	0.17	47,51,58,58	5
2	PO4	B	601	5/5	0.87	0.16	55,57,65,66	5
2	PO4	D	601	5/5	0.87	0.16	53,56,65,69	5
3	GOL	H	601	6/6	0.95	0.11	32,37,45,45	0
3	GOL	A	602	6/6	0.96	0.06	30,34,41,41	0
3	GOL	E	602	6/6	0.97	0.05	32,33,42,46	0
3	GOL	F	602	6/6	0.97	0.05	30,31,39,39	0
3	GOL	G	601	6/6	0.97	0.05	32,34,40,41	0
3	GOL	C	602	6/6	0.97	0.06	23,26,31,33	0
3	GOL	B	602	6/6	0.98	0.04	22,26,31,31	0
3	GOL	D	602	6/6	0.98	0.04	24,29,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.