



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 25, 2024 – 01:11 AM EDT

PDB ID : 6ZQ4
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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

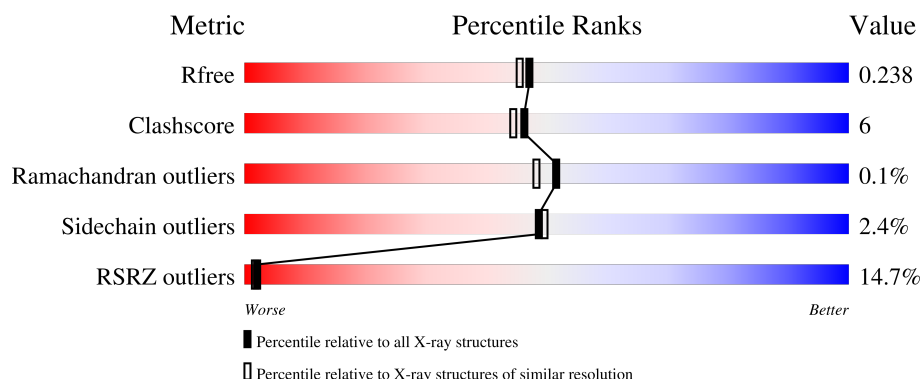
1 Overall quality at a glance ⓘ

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}	130704	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (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	<div> <div>17%</div> <div>83%</div> <div>13%</div> <div>..</div> </div>
1	B	526	<div> <div>10%</div> <div>83%</div> <div>13%</div> <div>..</div> </div>
1	C	526	<div> <div>12%</div> <div>81%</div> <div>14%</div> <div>..</div> </div>
1	D	526	<div> <div>13%</div> <div>82%</div> <div>13%</div> <div>..</div> </div>
1	E	526	<div> <div>14%</div> <div>83%</div> <div>13%</div> <div>..</div> </div>

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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 (three-letter code: 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 (three-letter code: 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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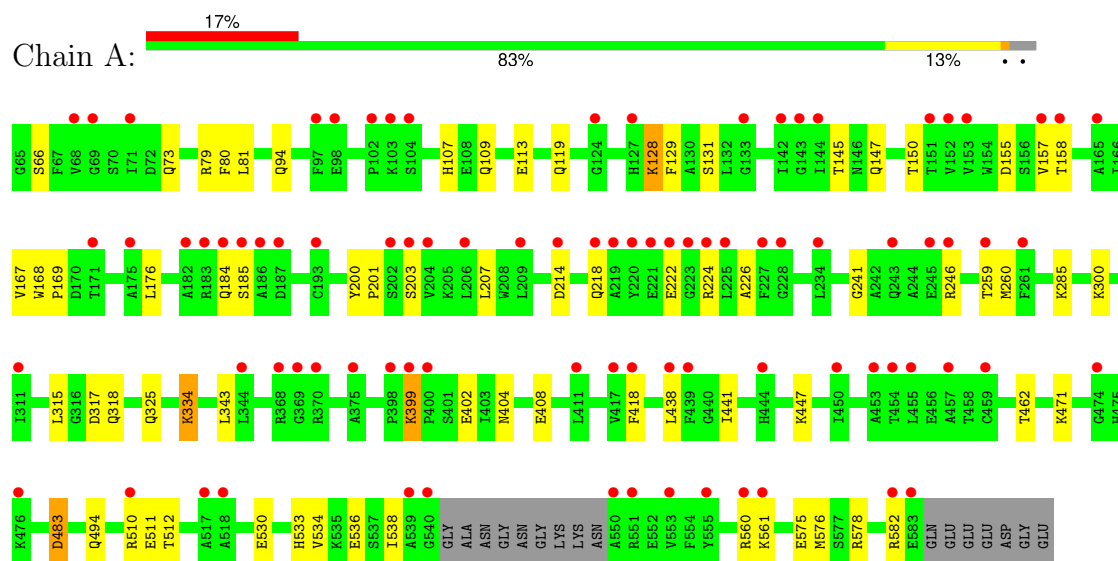
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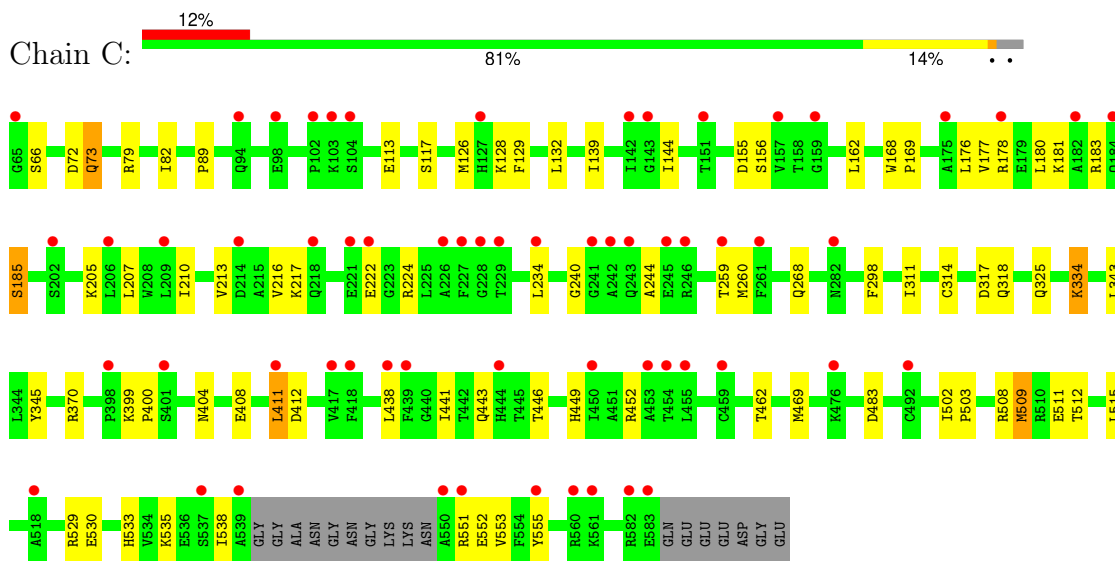
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	220	Total 220	O 220	0	0
4	F	234	Total 234	O 234	0	0
4	G	186	Total 186	O 186	0	0
4	H	147	Total 147	O 147	0	0

3 Residue-property plots [i](#)

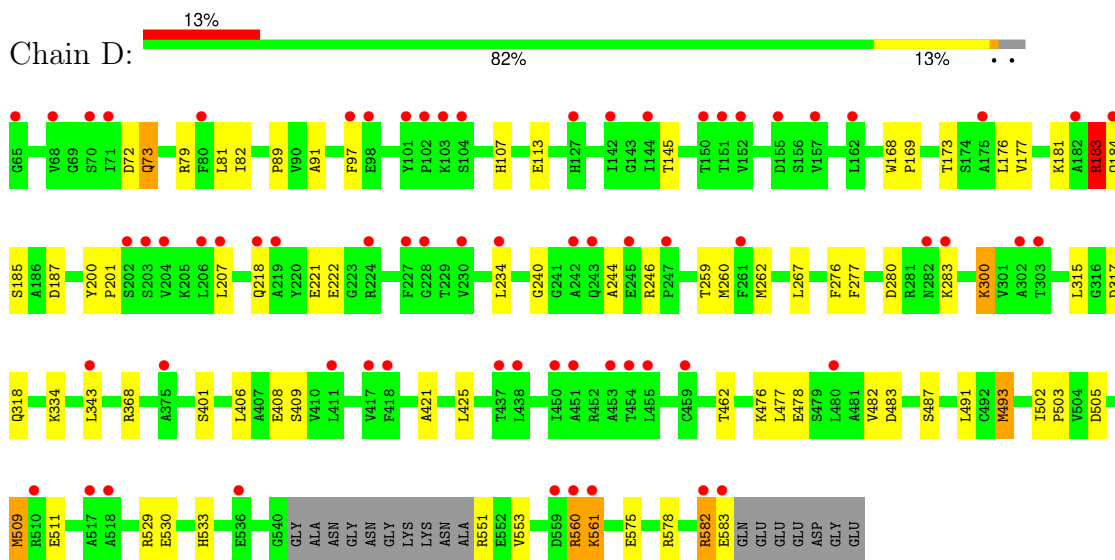
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

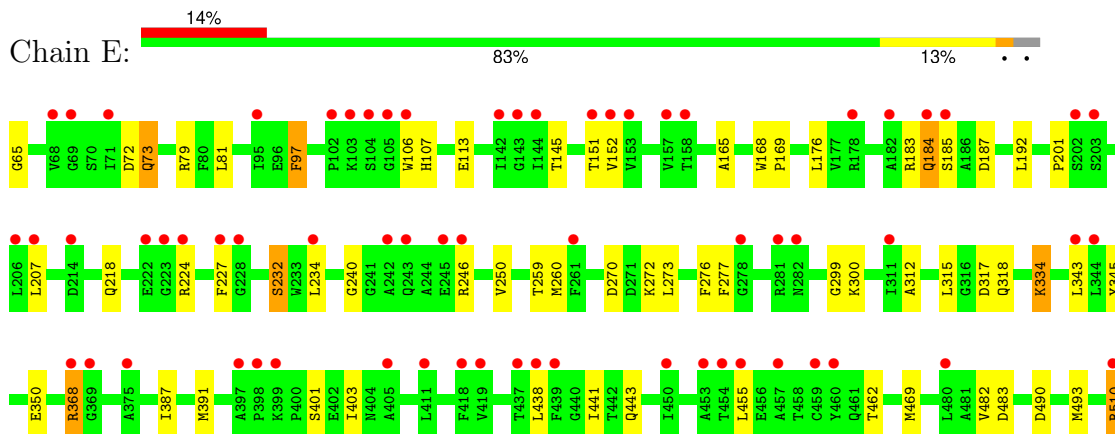


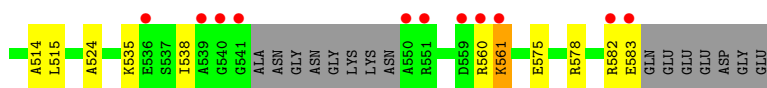


- Molecule 1: Glycerol kinase-like protein

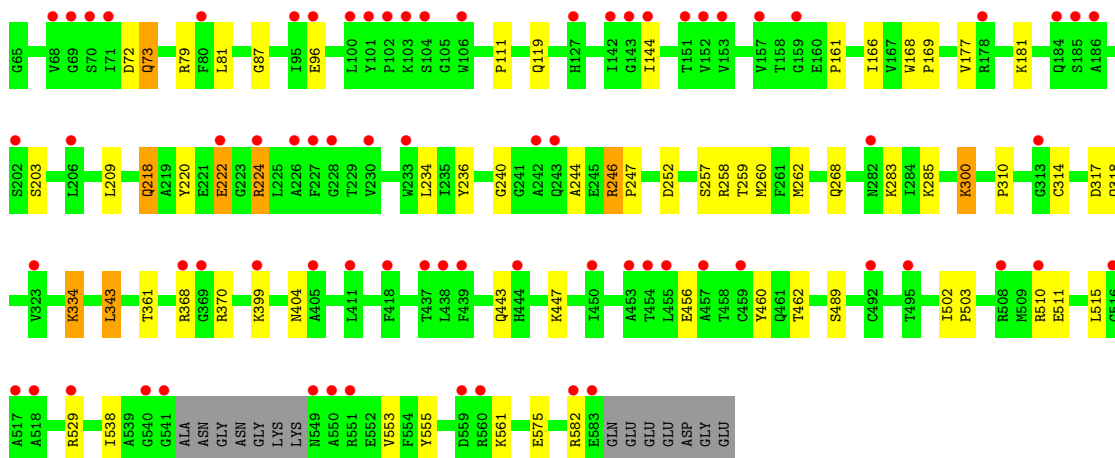
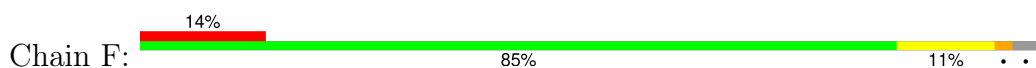


- Molecule 1: Glycerol kinase-like protein

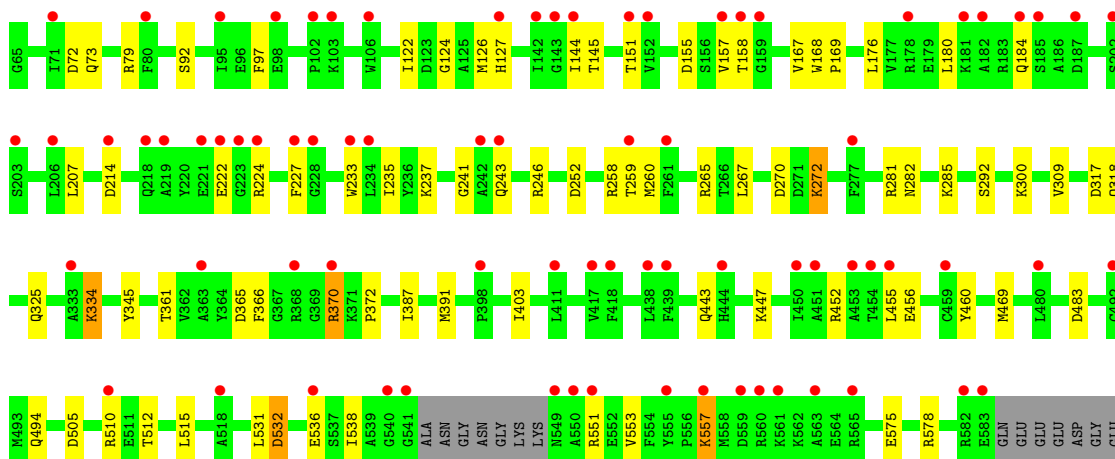
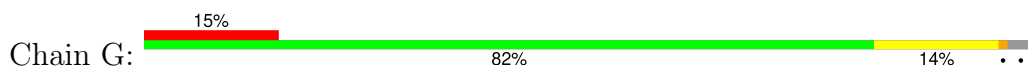




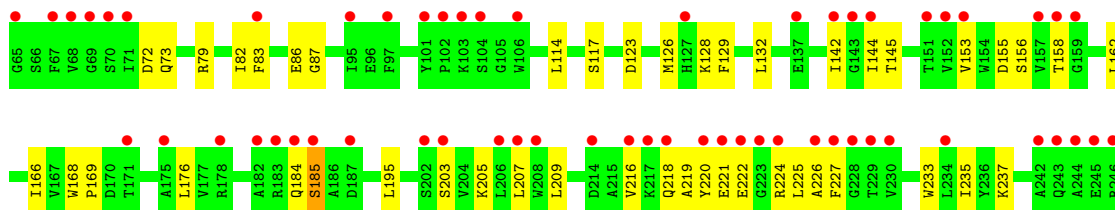
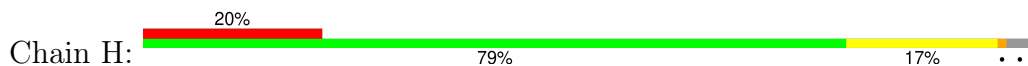
• Molecule 1: Glycerol kinase-like protein

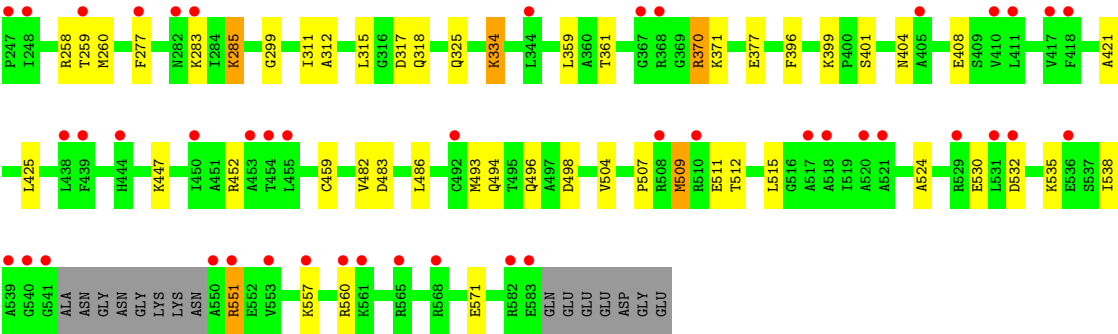


• Molecule 1: Glycerol kinase-like protein



• Molecule 1: Glycerol kinase-like protein





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) 97.4 (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)	0.42 , 55.2	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: GOL, PO4

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%)	0.76	7/5445 (0.1%)
1	B	0.56	10/3990 (0.3%)	0.61	3/5407 (0.1%)
1	C	0.41	2/3976 (0.1%)	0.63	6/5390 (0.1%)
1	D	0.38	2/3975 (0.1%)	0.56	5/5388 (0.1%)
1	E	0.48	4/3984 (0.1%)	0.62	9/5400 (0.2%)
1	F	0.51	5/3992 (0.1%)	0.65	12/5411 (0.2%)
1	G	0.40	2/3992 (0.1%)	0.60	3/5411 (0.1%)
1	H	0.40	2/3984 (0.1%)	0.59	5/5400 (0.1%)
All	All	0.46	30/31911 (0.1%)	0.63	50/43252 (0.1%)

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 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	399	LYS	CE-NZ	-14.32	1.13	1.49
1	A	399	LYS	CE-NZ	-11.96	1.19	1.49
1	E	300	LYS	CD-CE	-11.53	1.22	1.51
1	D	246	ARG	C-N	10.58	1.54	1.34
1	A	582	ARG	CZ-NH1	10.35	1.46	1.33

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	582	ARG	NE-CZ-NH1	24.70	132.65	120.30
1	A	582	ARG	NE-CZ-NH2	-18.43	111.09	120.30
1	C	411	LEU	CB-CG-CD1	13.55	134.04	111.00
1	C	411	LEU	CB-CG-CD2	-10.97	92.36	111.00
1	A	399	LYS	CA-CB-CG	10.54	136.60	113.40

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	42	1
1	C	3894	3854	3854	55	0
1	D	3893	3852	3852	51	0
1	E	3902	3860	3860	49	0
1	F	3910	3866	3866	43	0
1	G	3910	3867	3866	45	1
1	H	3902	3860	3860	74	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	0	0
3	B	6	3	8	0	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	6	0
4	E	220	0	0	10	0
4	F	234	0	0	7	0
4	G	186	0	0	4	0
4	H	147	0	0	7	0
All	All	33027	30941	30971	395	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 6.

The worst 5 of 395 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:H:482:VAL:HG11	1:H:493:MET:HE1	1.27	1.12
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: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 ⓘ

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	510/526 (97%)	495 (97%)	14 (3%)	1 (0%)	47	43
1	B	507/526 (96%)	493 (97%)	13 (3%)	1 (0%)	47	43
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%)	47	43
1	H	507/526 (96%)	490 (97%)	17 (3%)	0	100	100
All	All	4057/4208 (96%)	3942 (97%)	112 (3%)	3 (0%)	51	48

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%)	403 (98%)	10 (2%)	49	49
1	B	410/420 (98%)	402 (98%)	8 (2%)	55	57
1	C	409/420 (97%)	401 (98%)	8 (2%)	55	57
1	D	409/420 (97%)	397 (97%)	12 (3%)	42	41
1	E	409/420 (97%)	398 (97%)	11 (3%)	44	44
1	F	410/420 (98%)	403 (98%)	7 (2%)	60	63
1	G	410/420 (98%)	397 (97%)	13 (3%)	39	37
1	H	409/420 (97%)	401 (98%)	8 (2%)	55	57
All	All	3279/3360 (98%)	3202 (98%)	77 (2%)	49	51

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	92	SER
1	H	227	PHE
1	G	252	ASP
1	G	510	ARG
1	H	530	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	461	GLN

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](#)

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	E	602	-	5,5,5	0.26	0	5,5,5	0.30	0
2	PO4	B	601	-	4,4,4	1.85	1 (25%)	6,6,6	0.71	0

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

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	PO4	2	0
2	D	601	PO4	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%)	0.74	87 (17%) 1 1	27, 46, 79, 110	0
1	B	510/526 (96%)	0.49	55 (10%) 5 5	23, 41, 77, 103	0
1	C	509/526 (96%)	0.64	61 (11%) 4 4	27, 46, 79, 138	0
1	D	509/526 (96%)	0.65	67 (13%) 3 2	23, 45, 82, 122	0
1	E	511/526 (97%)	0.70	76 (14%) 2 2	24, 46, 87, 121	0
1	F	512/526 (97%)	0.67	73 (14%) 2 2	26, 44, 81, 155	0
1	G	512/526 (97%)	0.80	77 (15%) 2 2	29, 51, 85, 149	0
1	H	511/526 (97%)	0.95	103 (20%) 1 0	30, 54, 95, 174	0
All	All	4084/4208 (97%)	0.71	599 (14%) 2 2	23, 47, 84, 174	0

The worst 5 of 599 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	541	GLY	12.9
1	H	184	GLN	9.7
1	F	549	ASN	8.3
1	E	550	ALA	8.3
1	A	550	ALA	8.2

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	0.76	0.22	56,60,67,67	5
2	PO4	A	601	5/5	0.79	0.23	57,60,66,68	5
2	PO4	B	601	5/5	0.80	0.27	55,57,65,66	5
2	PO4	D	601	5/5	0.82	0.24	53,56,65,69	5
2	PO4	C	601	5/5	0.82	0.29	54,59,64,68	5
2	PO4	F	601	5/5	0.85	0.21	47,51,58,58	5
3	GOL	H	601	6/6	0.95	0.13	32,37,45,45	0
3	GOL	G	601	6/6	0.96	0.10	32,34,40,41	0
3	GOL	A	602	6/6	0.96	0.11	30,34,41,41	0
3	GOL	D	602	6/6	0.97	0.09	24,29,34,34	0
3	GOL	B	602	6/6	0.97	0.08	22,26,31,31	0
3	GOL	C	602	6/6	0.97	0.10	23,26,31,33	0
3	GOL	E	602	6/6	0.98	0.09	32,33,42,46	0
3	GOL	F	602	6/6	0.98	0.07	30,31,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.