



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:39 PM GMT

PDB ID : 1GLF
Title : CRYSTAL STRUCTURES OF ESCHERICHIA COLI GLYCEROL KINASE AND THE MUTANT A65T IN AN INACTIVE TETRAMER: CONFORMATIONAL CHANGES AND IMPLICATIONS FOR ALLOSTERIC REGULATION
Authors : Feese, M.D.; Faber, H.R.; Bystrom, C.E.; Pettigrew, D.W.; Remington, S.J.
Deposited on : 1998-08-30
Resolution : 2.62 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

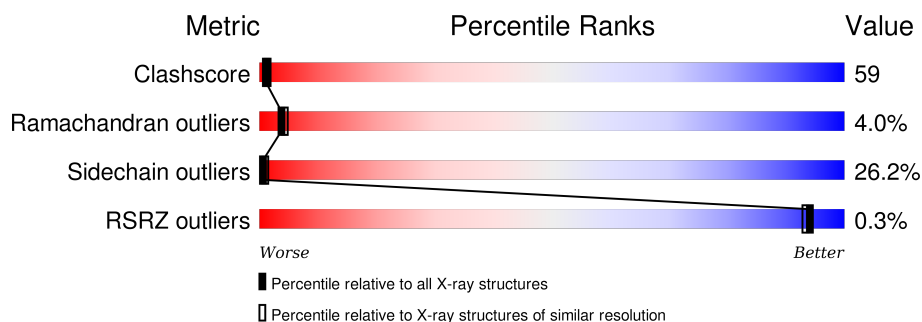
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

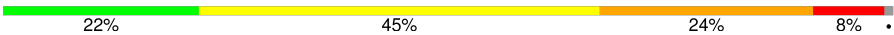
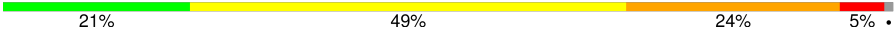
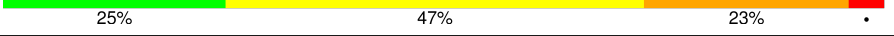
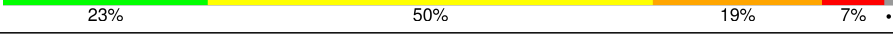
The reported resolution of this entry is 2.62 Å.

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	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	O	501	
1	X	501	
1	Y	501	
1	Z	501	

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	O	601	-	-	X	-
3	ADP	O	607	X	-	-	-
4	GOL	Y	604	-	-	-	X
4	GOL	Z	605	-	-	X	-

2 Entry composition [i](#)

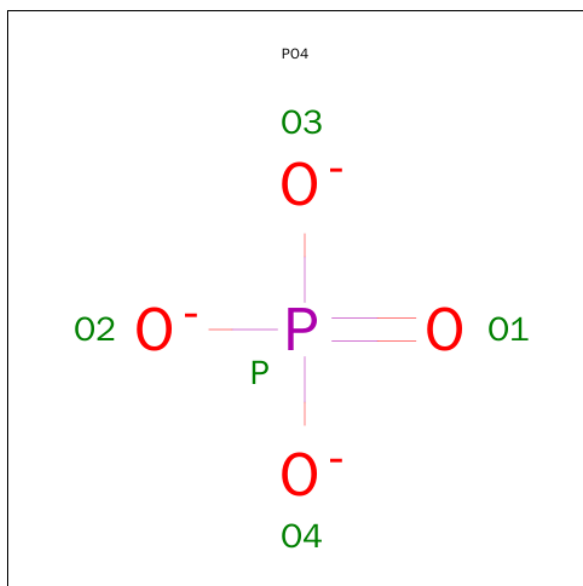
There are 5 unique types of molecules in this entry. The entry contains 15981 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (GLYCEROL KINASE).

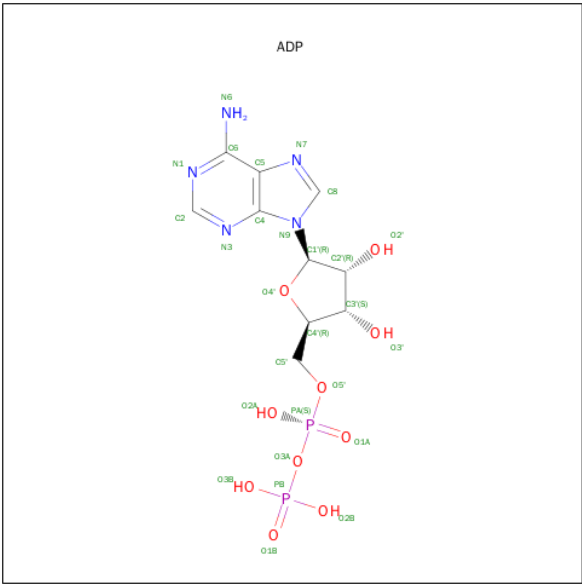
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	498	Total	C	N	O	S	0	0	0
			3913	2467	684	743	19			
1	Y	499	Total	C	N	O	S	0	0	0
			3909	2465	683	742	19			
1	Z	498	Total	C	N	O	S	0	0	0
			3907	2465	682	741	19			
1	X	498	Total	C	N	O	S	0	0	0
			3910	2467	684	740	19			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	O	1	Total	O	P	0	0
			5	4	1		
2	Y	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	O	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	Y	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	Z	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	X	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	O	1	Total	C	O	0	0
			6	3	3		
4	Y	1	Total	C	O	0	0
			6	3	3		
4	Z	1	Total	C	O	0	0
			6	3	3		
4	X	1	Total	C	O	0	0
			6	3	3		

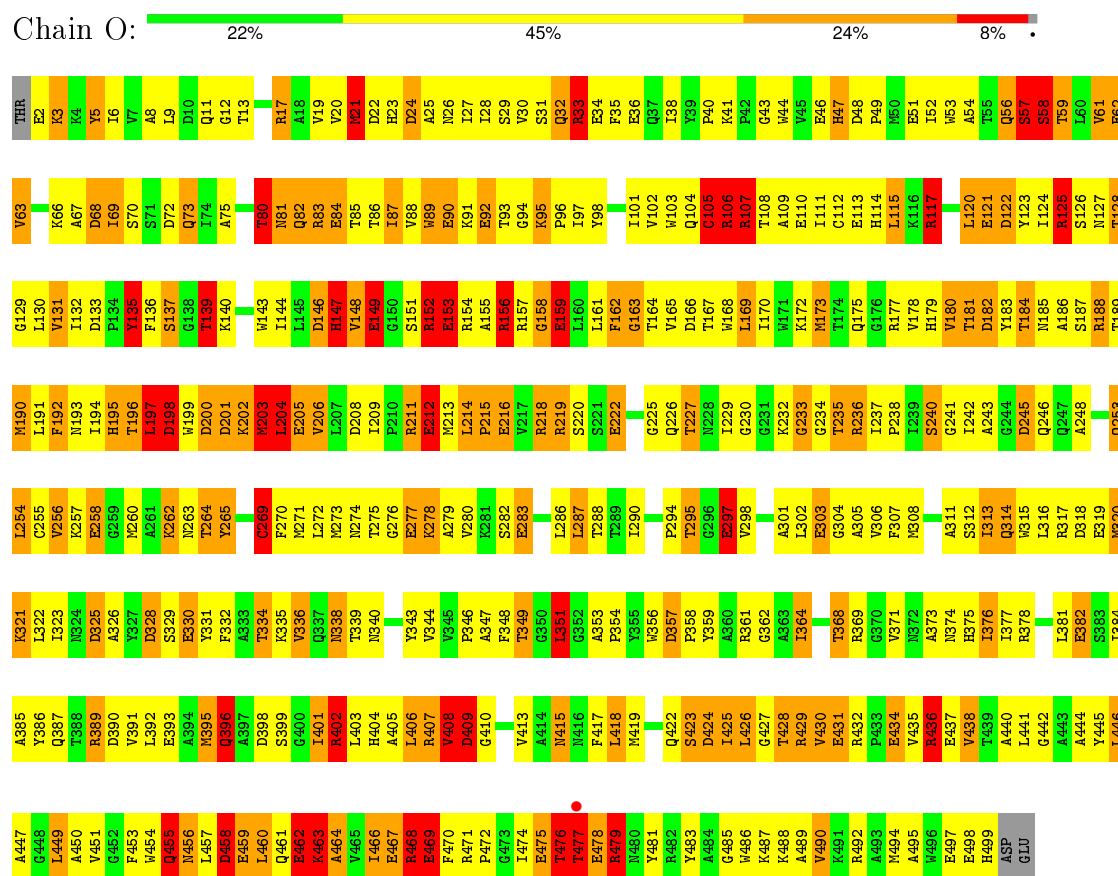
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	O	46	Total	O	0	0
			46	46		
5	X	50	Total	O	0	0
			50	50		
5	Y	51	Total	O	0	0
			51	51		
5	Z	53	Total	O	0	0
			53	53		

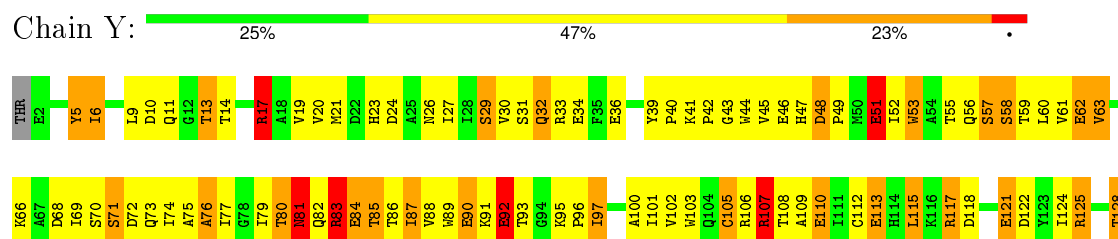
3 Residue-property plots

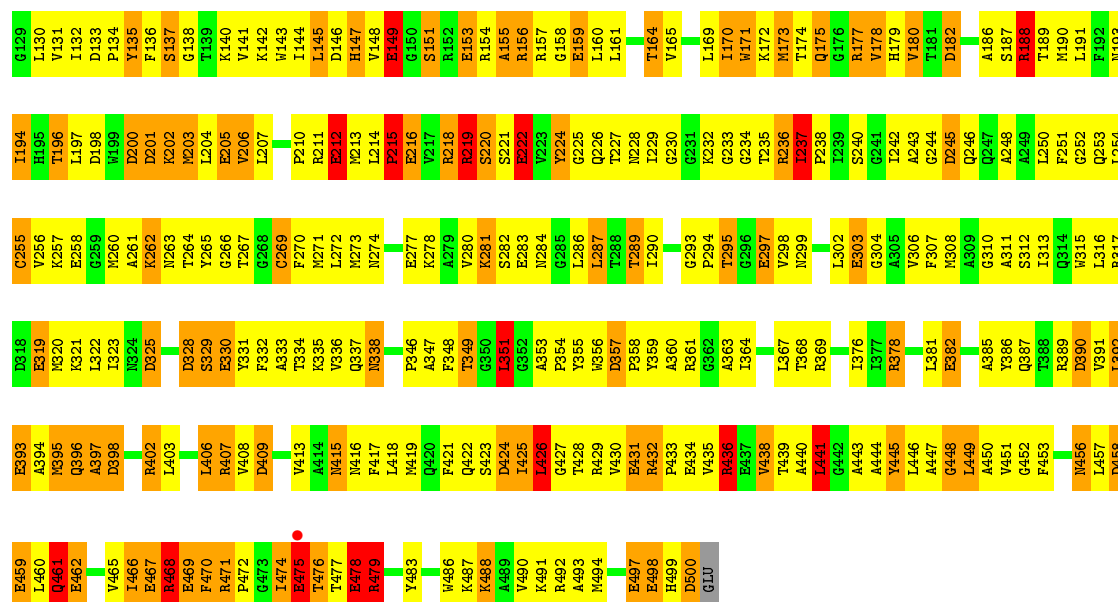
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: PROTEIN (GLYCEROL KINASE)

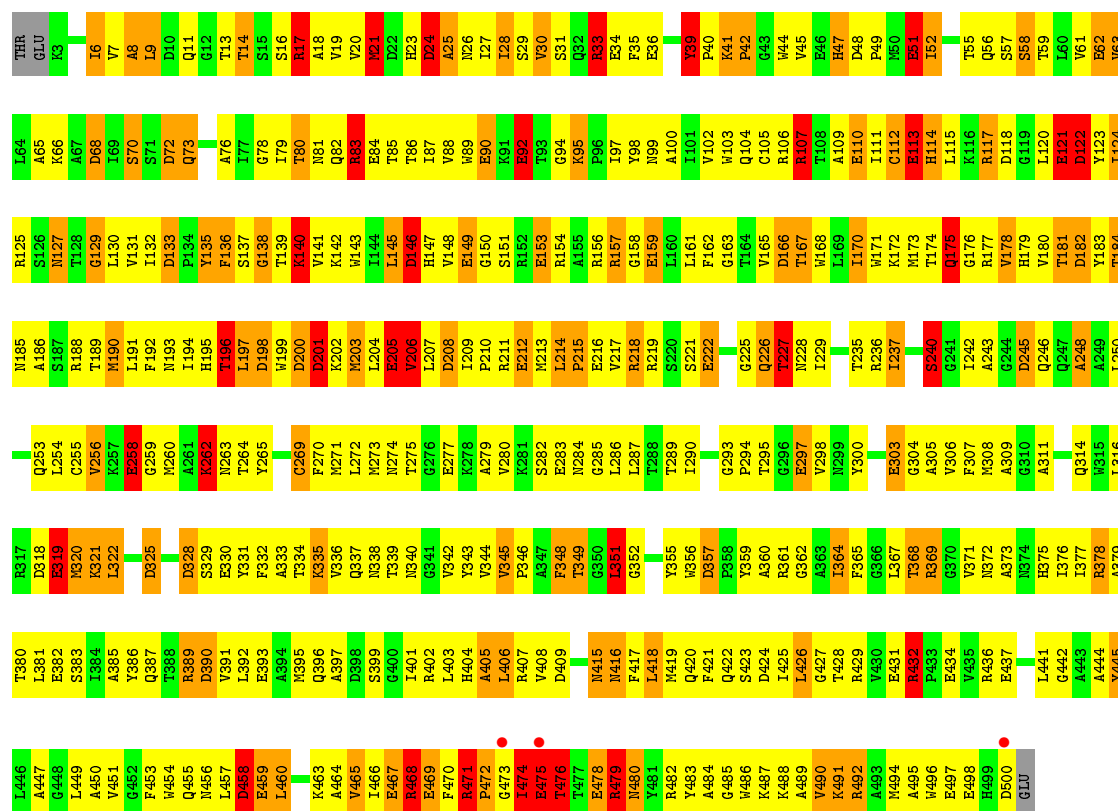


• Molecule 1: PROTEIN (GLYCEROL KINASE)





• Molecule 1: PROTEIN (GLYCEROL KINASE)



• Molecule 1: PROTEIN (GLYCEROL KINASE)



A447	A385	R317	Q253	N193	I132	A67	THR
G448	Y386	D318	L284	I194	D133	D68	GLU
L449	Q387	E319	C255	H195	P134	I69	K3
A450	T388	N320	V256	T196	Y135	S70	K4
V451	R389	K321	K257	L197	F136	S71	Y5
G452	D390	L322	E258	D198	S137	D72	
F453	V391	T323	C259	H199	G138	D73	L9
V454	L392	N324	M260	D200	T139	I74	D10
Q455	E393	D325	A261	D201	K140		
N456	A394	A326	K262	K202	V141	G78	T13
L457	M395	Y327	N263	L203	K142	I79	T14
D458	Q396	K328	T264	L204	H143	T80	S15
E459	A397	S329	Y265	E205	I144	N81	S16
L460	D398	E330		V206	L145	Q82	R17
Q461	S399	Y331	C269	D207		R83	
F462	G400	N338	F270	L208	V148	E84	V20
K463	I401	T339	M271	I209	E149	T85	M21
A464			L272	P210	G150	T86	D22
V465	A405		M273	R211	S151	I87	H23
L466	L406	Y342	N274	E212	R152	V88	D24
E467	R407	Y343	T275	M213	E153	W89	A25
R468	V408	V344	G276	L214	R154	E90	M26
E469	D409	V345	E277	P215	A155	K91	I27
F470	G410	F346	K278	E216	R156		
S471	G411	A347	A279	V217	R157	E92	I28
P472	A412	F348	V280	R218	G158	K95	S29
G473	V413	T349	K281	R219	E159	P96	V30
L474	A414	G350	S282	S220	L160	I97	S31
E475	N415	L351	E283	S221	L161		Q32
T476	N416	G352	N284	E222	F162		R33
T477	F417		G285	V223	G163	I101	E34
E478	L418	Y355	L286	Y224	T164	M103	F35
R479	M419	M356	L287	Q225	V165	Q104	E36
N480	Q420	D357		T227	T167	C105	Q37
R482	Q422	Y359	I290	N228	M168	R107	K41
Y483	S423	R361	C292	G230	L169	T108	P42
	D424	G362	G293	G231	M171	A109	G43
	I425	A363	T294	K232	K172	E110	G44
	L426	G364	T295	G233	M173	C112	V45
	G427	F365	G296	G234	T174	H47	D48
	T428	G366	E297	G235	Q175	P49	
R429	V430	L367	V298	R236	G176	M50	
V431	E431	T368	N299	I237	R177	E51	
R432	R432	R369	Y300	P238	V178	I52	
E497	P433	G370	A301	I239	H179	M53	
E498	E434	V371	L302	S240	G119	A54	
H499	V435	N372	G304	G241	L120	T55	
D500	R436		A305	I242	D121	Q56	
	E437	H375	V306	A243	D122	S57	
	V438	I376	F307	G244	Y123	S58	
	T439	I377	M308	D245	I124	T59	
	A440	R378		Q246	R125	L50	
	L441	A379	A311	Q247	S126	V61	
	G442	T380	S312	A248	M127	B62	
	A443	L381	I313	A249	T128	V63	
	A444	E382	Q314	L250	G129	L64	
	Y445	S383	Y315	F251	L130	A65	
	L446	I384	L316	G252	V131	K66	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.10Å 117.40Å 108.40Å 90.00° 93.10° 90.00°	Depositor
Resolution (Å)	20.00 – 2.62 20.00 – 2.62	Depositor EDS
% Data completeness (in resolution range)	84.0 (20.00-2.62) 84.4 (20.00-2.62)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.63Å)	Xtriage
Refinement program	TNT V. 5-F-6	Depositor
R, R_{free}	0.146 , (Not available) 0.138 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	1.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 117.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	3 of 58961 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15981	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.84 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.4046e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, ADP

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	O	1.34	41/3993 (1.0%)	1.82	99/5416 (1.8%)
1	X	1.34	36/3990 (0.9%)	1.75	79/5411 (1.5%)
1	Y	1.32	38/3989 (1.0%)	1.77	84/5412 (1.6%)
1	Z	1.32	32/3987 (0.8%)	1.79	88/5408 (1.6%)
All	All	1.33	147/15959 (0.9%)	1.78	350/21647 (1.6%)

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	X	1	1
1	Y	1	0
All	All	2	1

The worst 5 of 147 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Z	121	GLU	CD-OE1	10.08	1.36	1.25
1	O	475	GLU	CD-OE1	9.83	1.36	1.25
1	Y	277	GLU	CD-OE1	9.55	1.36	1.25
1	X	478	GLU	CD-OE1	9.33	1.35	1.25
1	Z	149	GLU	CD-OE1	9.21	1.35	1.25

The worst 5 of 350 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	479	ARG	NE-CZ-NH2	-21.02	109.79	120.30
1	O	479	ARG	NE-CZ-NH1	15.27	127.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	200	ASP	CB-CG-OD1	-14.20	105.52	118.30
1	O	245	ASP	CB-CG-OD2	-13.98	105.72	118.30
1	Y	177	ARG	NE-CZ-NH1	12.26	126.43	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	Y	155	ALA	CA
1	X	31	SER	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	478	GLU	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	3913	0	3830	495	0
1	X	3910	0	3833	478	0
1	Y	3909	0	3822	435	0
1	Z	3907	0	3826	459	0
2	O	5	0	0	2	0
2	Y	5	0	0	1	0
3	O	27	0	11	1	0
3	X	27	0	11	1	0
3	Y	27	0	12	0	0
3	Z	27	0	12	0	0
4	O	6	0	8	2	0
4	X	6	0	8	2	0
4	Y	6	0	8	3	0
4	Z	6	0	8	9	0
5	O	46	0	0	9	0
5	X	50	0	0	6	0
5	Y	51	0	0	11	0
5	Z	53	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15981	0	15389	1827	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 59.

The worst 5 of 1827 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:Y:200:ASP:HB3	1:Y:203:MET:HB2	1.14	1.13
1:Y:155:ALA:HB2	1:Y:160:LEU:HB2	1.10	1.08
1:Z:468:ARG:HG3	1:Z:468:ARG:HH11	1.17	1.07
1:O:84:GLU:HB2	1:O:103:TRP:HB3	1.31	1.06
1:X:422:GLN:HE21	1:X:426:LEU:HD22	1.18	1.06

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	O	496/501 (99%)	409 (82%)	65 (13%)	22 (4%)	3	3
1	X	496/501 (99%)	411 (83%)	69 (14%)	16 (3%)	5	7
1	Y	497/501 (99%)	414 (83%)	60 (12%)	23 (5%)	3	3
1	Z	496/501 (99%)	425 (86%)	52 (10%)	19 (4%)	4	5
All	All	1985/2004 (99%)	1659 (84%)	246 (12%)	80 (4%)	4	4

5 of 80 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	149	GLU
1	O	159	GLU

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Mol	Chain	Res	Type
1	O	203	MET
1	O	204	LEU
1	O	233	GLY

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	O	406/412 (98%)	294 (72%)	112 (28%)	0	1
1	X	405/412 (98%)	295 (73%)	110 (27%)	0	1
1	Y	405/412 (98%)	305 (75%)	100 (25%)	1	1
1	Z	405/412 (98%)	303 (75%)	102 (25%)	1	1
All	All	1621/1648 (98%)	1197 (74%)	424 (26%)	0	1

5 of 424 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Y	426	LEU
1	Z	107	ARG
1	X	338	ASN
1	Y	456	ASN
1	Z	17	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
1	Y	387	GLN
1	Z	73	GLN
1	X	415	ASN
1	Y	456	ASN
1	Z	226	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

10 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$
2	PO4	O	601	-	4,4,4	1.46	1 (25%)	6,6,6	0.30	0
4	GOL	O	603	-	5,5,5	0.60	0	5,5,5	0.26	0
3	ADP	O	607	-	22,29,29	1.21	1 (4%)	27,45,45	3.32	5 (18%)
4	GOL	X	606	-	5,5,5	0.57	0	5,5,5	0.74	0
3	ADP	X	610	-	22,29,29	1.33	3 (13%)	27,45,45	4.21	9 (33%)
2	PO4	Y	602	-	4,4,4	2.40	3 (75%)	6,6,6	0.29	0
4	GOL	Y	604	-	5,5,5	0.65	0	5,5,5	0.52	0
3	ADP	Y	608	-	22,29,29	1.21	2 (9%)	27,45,45	3.77	9 (33%)
4	GOL	Z	605	-	5,5,5	0.47	0	5,5,5	0.66	0
3	ADP	Z	609	-	22,29,29	0.84	0	27,45,45	2.42	6 (22%)

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	PO4	O	601	-	-	0/0/0/0	0/0/0/0
4	GOL	O	603	-	-	0/4/4/4	0/0/0/0
3	ADP	O	607	-	1/1/6/6	0/12/32/32	0/3/3/3
4	GOL	X	606	-	-	0/4/4/4	0/0/0/0
3	ADP	X	610	-	-	0/12/32/32	0/3/3/3
2	PO4	Y	602	-	-	0/0/0/0	0/0/0/0
4	GOL	Y	604	-	-	0/4/4/4	0/0/0/0
3	ADP	Y	608	-	-	0/12/32/32	0/3/3/3
4	GOL	Z	605	-	-	0/4/4/4	0/0/0/0
3	ADP	Z	609	-	-	0/12/32/32	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	601	PO4	P-O4	-2.58	1.44	1.53
3	X	610	ADP	PB-O2B	-2.44	1.45	1.54
2	Y	602	PO4	P-O4	-2.21	1.45	1.53
3	Y	608	ADP	C2-N3	2.03	1.35	1.32
3	X	610	ADP	C2-N1	2.87	1.39	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	607	ADP	C1'-N9-C4	-15.21	104.00	126.94
3	X	610	ADP	O3A-PA-O5'	-12.45	69.91	102.94
3	X	610	ADP	C1'-N9-C4	-11.69	109.31	126.94
3	Y	608	ADP	C1'-N9-C4	-11.60	109.44	126.94
3	Y	608	ADP	O3A-PA-O5'	-8.57	80.20	102.94

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	O	607	ADP	C2'

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	601	PO4	2	0
4	O	603	GOL	2	0
3	O	607	ADP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	X	606	GOL	2	0
3	X	610	ADP	1	0
2	Y	602	PO4	1	0
4	Y	604	GOL	3	0
4	Z	605	GOL	9	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	O	498/501 (99%)	-0.88	1 (0%) 95 94	7, 28, 61, 75	0
1	X	498/501 (99%)	-0.90	1 (0%) 95 94	7, 27, 60, 75	0
1	Y	499/501 (99%)	-0.89	1 (0%) 95 94	6, 27, 59, 73	0
1	Z	498/501 (99%)	-0.98	3 (0%) 90 88	6, 24, 58, 75	0
All	All	1993/2004 (99%)	-0.91	6 (0%) 94 93	6, 26, 60, 75	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Z	500	ASP	3.2
1	O	477	THR	3.0
1	Y	475	GLU	2.7
1	Z	473	GLY	2.6
1	X	500	ASP	2.3

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
4	GOL	Y	604	6/6	0.99	0.13	4.14	5,19,42,48	0
4	GOL	O	603	6/6	0.97	0.12	1.90	5,7,49,55	0
4	GOL	X	606	6/6	0.98	0.10	0.87	5,18,38,43	0
3	ADP	X	610	27/27	0.98	0.10	0.13	5,49,75,75	0
2	PO4	Y	602	5/5	0.97	0.12	0.04	29,31,53,75	0
3	ADP	Z	609	27/27	0.98	0.09	-0.32	5,26,57,75	0
3	ADP	O	607	27/27	0.98	0.09	-0.35	5,39,75,75	0
3	ADP	Y	608	27/27	0.98	0.08	-0.39	5,27,75,75	0
4	GOL	Z	605	6/6	0.99	0.08	-0.56	5,10,25,51	0
2	PO4	O	601	5/5	0.99	0.09	-0.99	5,31,56,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.