



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 02:53 PM GMT

PDB ID : 2J5T  
Title : GLUTAMATE 5-KINASE FROM ESCHERICHIA COLI COMPLEXED  
WITH GLUTAMATE  
Authors : Marco-Marin, C.; Gil-Ortiz, F.; Perez-Arellano, I.; Cervera, J.; Fita, I.; Rubio,  
V.  
Deposited on : 2006-09-19  
Resolution : 2.90 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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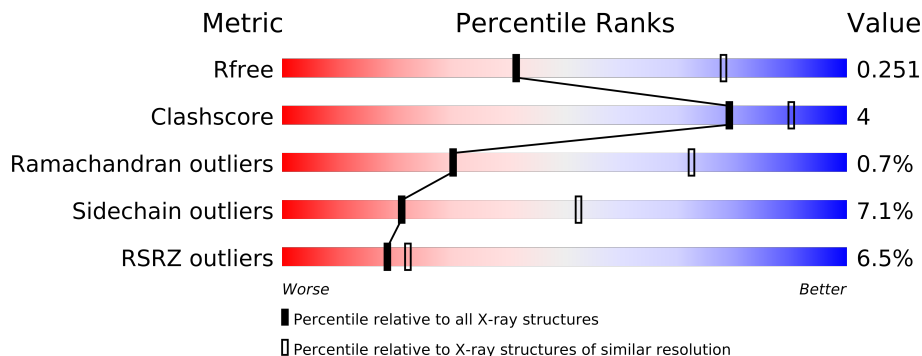
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.90 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))
$R_{free}$	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	367	
1	B	367	
1	C	367	
1	D	367	
1	E	367	
1	F	367	
1	G	367	
1	H	367	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	GLU	B	1371	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	GLU	E	1373	-	X
4	CL	B	1372	-	X
4	CL	G	1375	-	X
5	MG	A	1378	-	X
5	MG	B	1375	-	X
5	MG	E	1377	-	X
5	MG	F	1375	-	X
5	MG	G	1376	-	X
5	MG	H	1371	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21612 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

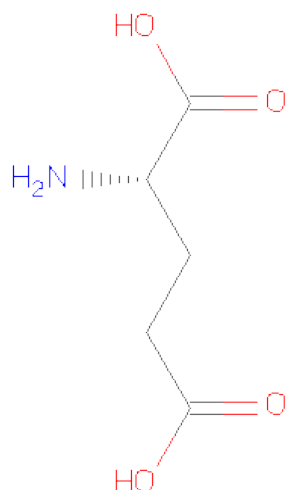
- Molecule 1 is a protein called GLUTAMATE 5-KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	0	1
			2656	1653	489	506	8			
1	B	353	Total	C	N	O	S	0	0	0
			2661	1658	490	505	8			
1	C	356	Total	C	N	O	S	0	0	0
			2669	1662	492	507	8			
1	D	365	Total	C	N	O	S	0	0	0
			2728	1696	502	522	8			
1	E	365	Total	C	N	O	S	0	0	0
			2728	1696	502	522	8			
1	F	354	Total	C	N	O	S	0	0	0
			2662	1659	491	504	8			
1	G	356	Total	C	N	O	S	0	0	0
			2674	1665	493	508	8			
1	H	337	Total	C	N	O	S	0	0	0
			2543	1588	466	481	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	VAL	ILE	ENGINEERED MUTATION	UNP P0A7B5
B	129	VAL	ILE	ENGINEERED MUTATION	UNP P0A7B5
C	129	VAL	ILE	ENGINEERED MUTATION	UNP P0A7B5
D	129	VAL	ILE	ENGINEERED MUTATION	UNP P0A7B5
E	129	VAL	ILE	ENGINEERED MUTATION	UNP P0A7B5
F	129	VAL	ILE	ENGINEERED MUTATION	UNP P0A7B5
G	129	VAL	ILE	ENGINEERED MUTATION	UNP P0A7B5
H	129	VAL	ILE	ENGINEERED MUTATION	UNP P0A7B5

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		
2	A	1	Total	C	N	O	0	0
			10	5	1	4		
2	B	1	Total	C	N	O	0	0
			10	5	1	4		
2	C	1	Total	C	N	O	0	0
			10	5	1	4		
2	D	1	Total	C	N	O	0	0
			10	5	1	4		
2	D	1	Total	C	N	O	0	0
			10	5	1	4		
2	E	1	Total	C	N	O	0	0
			10	5	1	4		
2	E	1	Total	C	N	O	0	0
			10	5	1	4		
2	F	1	Total	C	N	O	0	0
			10	5	1	4		
2	F	1	Total	C	N	O	0	0
			10	5	1	4		
2	G	1	Total	C	N	O	0	0
			10	5	1	4		
2	G	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	3	Total	Cl	0	0
			3	3		
4	D	2	Total	Cl	0	0
			2	2		
4	E	3	Total	Cl	0	0
			3	3		
4	H	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total 3	Cl 3	0	0
4	C	3	Total 3	Cl 3	0	0
4	A	3	Total 3	Cl 3	0	0
4	F	2	Total 2	Cl 2	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total 1	Mg 1	0	0
5	D	1	Total 1	Mg 1	0	0
5	E	2	Total 2	Mg 2	0	0
5	H	1	Total 1	Mg 1	0	0
5	B	1	Total 1	Mg 1	0	0
5	A	1	Total 1	Mg 1	0	0
5	F	1	Total 1	Mg 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	17	Total 17	O 17	0	0
6	B	8	Total 8	O 8	0	0
6	C	10	Total 10	O 10	0	0
6	D	14	Total 14	O 14	0	0
6	E	14	Total 14	O 14	0	0
6	F	12	Total 12	O 12	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	13	Total	O	0	0
			13	13		
6	H	15	Total	O	0	0
			15	15		



### 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.

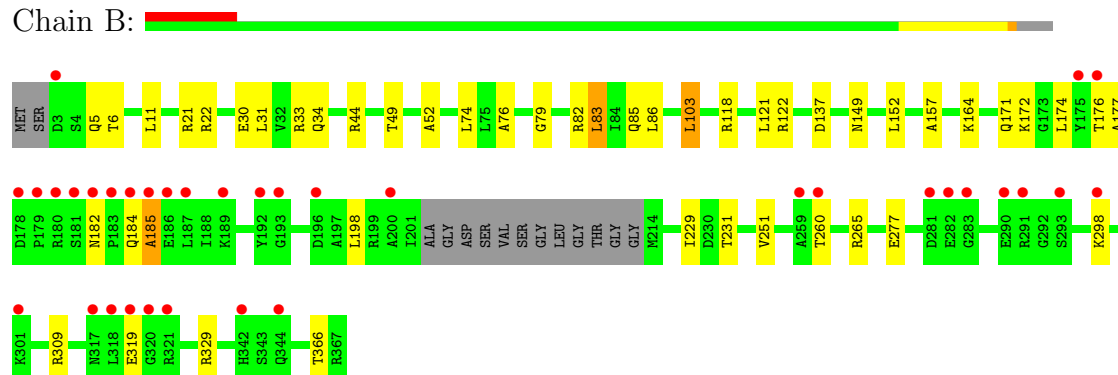
#### • Molecule 1: GLUTAMATE 5-KINASE

Chain A:



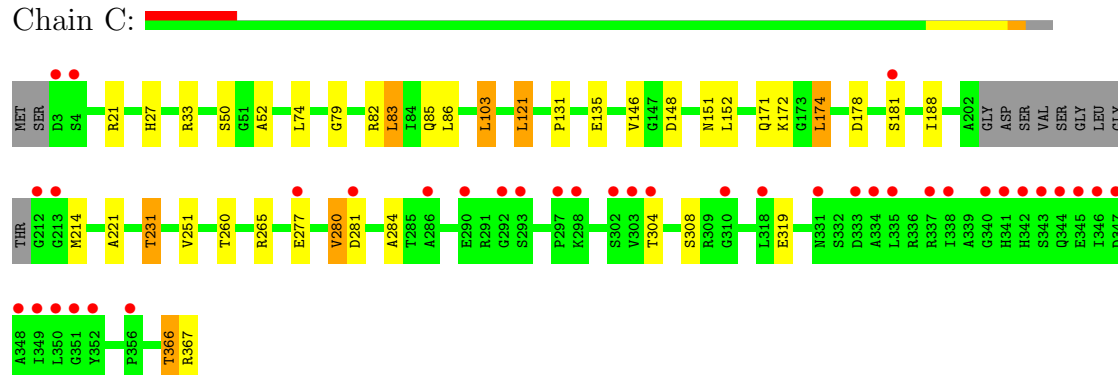
#### • Molecule 1: GLUTAMATE 5-KINASE

Chain B:



#### • Molecule 1: GLUTAMATE 5-KINASE

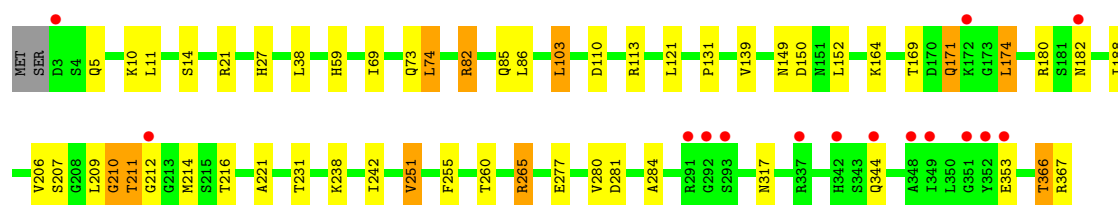
Chain C:



#### • Molecule 1: GLUTAMATE 5-KINASE

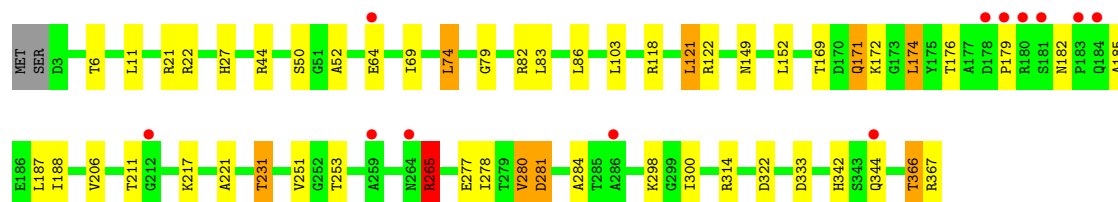
Chain D:





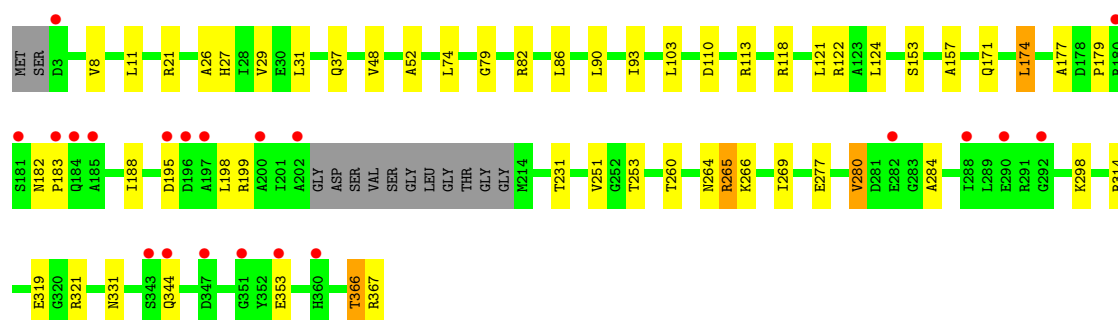
• Molecule 1: GLUTAMATE 5-KINASE

Chain E:



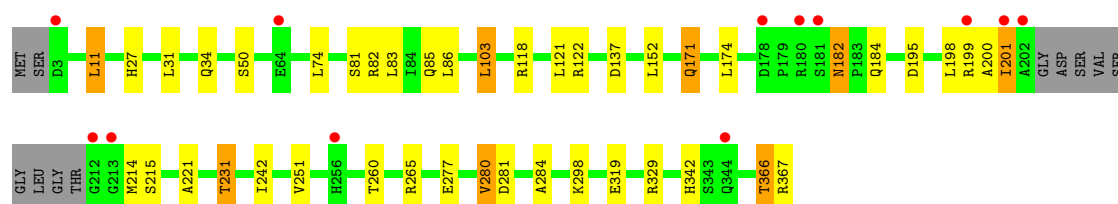
• Molecule 1: GLUTAMATE 5-KINASE

Chain F:



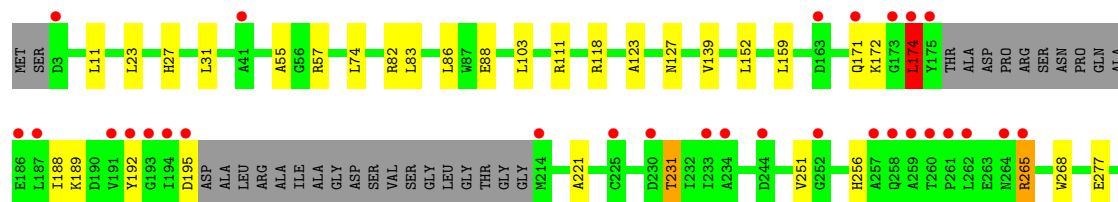
• Molecule 1: GLUTAMATE 5-KINASE

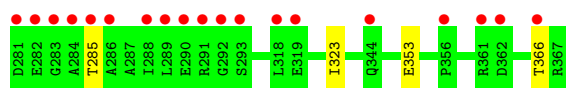
Chain G:



• Molecule 1: GLUTAMATE 5-KINASE

Chain H:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.30Å 124.11Å 144.93Å 90.00° 93.96° 90.00°	Depositor
Resolution (Å)	25.00 – 2.90 49.63 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (25.00-2.90) 99.2 (49.63-2.90)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.68 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.197 , 0.246 0.208 , 0.251	Depositor DCC
$R_{free}$ test set	3774 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.2	Xtriage
Anisotropy	0.841	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 5.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 74871 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	21612	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	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 27.43 % 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 2.2009e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SO4, CL

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	0.47	0/2691	0.63	0/3646
1	B	0.41	0/2696	0.58	0/3653
1	C	0.42	0/2704	0.59	0/3663
1	D	0.44	0/2764	0.61	1/3746 (0.0%)
1	E	0.45	0/2764	0.64	1/3746 (0.0%)
1	F	0.45	0/2697	0.62	0/3654
1	G	0.46	0/2709	0.62	0/3670
1	H	0.41	0/2575	0.58	0/3485
All	All	0.44	0/21600	0.61	2/29263 (0.0%)

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	D	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	265	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	D	212	GLY	N-CA-C	-5.95	98.24	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	211	THR	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2656	0	2690	18	0
1	B	2661	0	2706	17	0
1	C	2669	0	2710	18	0
1	D	2728	0	2768	28	0
1	E	2728	0	2768	31	0
1	F	2662	0	2708	17	0
1	G	2674	0	2717	20	0
1	H	2543	0	2589	13	0
2	A	20	0	10	0	0
2	B	10	0	5	0	0
2	C	10	0	5	0	0
2	D	20	0	10	0	0
2	E	20	0	10	1	0
2	F	20	0	10	0	0
2	G	20	0	10	1	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	1	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	2	0	0	0	0
4	E	3	0	0	0	0
4	F	2	0	0	0	0
4	G	3	0	0	0	0
4	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	E	2	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	17	0	0	0	0
6	B	8	0	0	0	0
6	C	10	0	0	0	0
6	D	14	0	0	2	0
6	E	14	0	0	0	0
6	F	12	0	0	0	0
6	G	13	0	0	0	0
6	H	15	0	0	0	0
All	All	21612	0	21716	153	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

The worst 5 of 153 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:171:GLN:HE22	1:G:214:MET:CE	1.98	0.76
1:A:280:VAL:HG13	1:A:284:ALA:HB3	1.68	0.75
1:E:298:LYS:HE3	1:E:342:HIS:ND1	2.10	0.66
1:E:280:VAL:HG13	1:E:284:ALA:HB3	1.78	0.65
1:E:50:SER:O	1:E:83:LEU:HD11	1.99	0.62

There are no symmetry-related clashes.

## 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	351/367 (96%)	334 (95%)	16 (5%)	1 (0%)	50 85

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	349/367 (95%)	332 (95%)	14 (4%)	3 (1%)	25	66
1	C	352/367 (96%)	333 (95%)	19 (5%)	0	100	100
1	D	363/367 (99%)	342 (94%)	17 (5%)	4 (1%)	21	60
1	E	363/367 (99%)	346 (95%)	15 (4%)	2 (1%)	33	76
1	F	350/367 (95%)	325 (93%)	18 (5%)	7 (2%)	11	40
1	G	352/367 (96%)	333 (95%)	17 (5%)	2 (1%)	33	76
1	H	331/367 (90%)	313 (95%)	16 (5%)	2 (1%)	33	76
All	All	2811/2936 (96%)	2658 (95%)	132 (5%)	21 (1%)	30	72

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	298	LYS
1	D	210	GLY
1	D	265	ARG
1	D	281	ASP
1	F	174	LEU

### 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	275/285 (96%)	257 (94%)	18 (6%)	24	58
1	B	277/285 (97%)	257 (93%)	20 (7%)	21	51
1	C	276/285 (97%)	256 (93%)	20 (7%)	21	51
1	D	283/285 (99%)	263 (93%)	20 (7%)	21	52
1	E	283/285 (99%)	263 (93%)	20 (7%)	21	52
1	F	276/285 (97%)	255 (92%)	21 (8%)	19	48
1	G	277/285 (97%)	255 (92%)	22 (8%)	18	46
1	H	265/285 (93%)	248 (94%)	17 (6%)	25	59
All	All	2212/2280 (97%)	2054 (93%)	158 (7%)	21	52



5 of 158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	251	VAL
1	E	187	LEU
1	H	86	LEU
1	D	265	ARG
1	E	64	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	128	ASN
1	E	171	GLN
1	G	182	ASN
1	D	171	GLN
1	E	184	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 48 ligands modelled in this entry, 28 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	A	1372	-	4,4,4	0.24	0	6,6,6	0.19	0
2	GLU	A	1373	-	9,9,9	0.88	0	11,11,11	0.99	1 (9%)
2	GLU	A	1374	-	9,9,9	0.87	0	11,11,11	0.86	0
3	SO4	B	1370	-	4,4,4	0.13	0	6,6,6	0.20	0
2	GLU	B	1371	-	9,9,9	0.87	0	11,11,11	0.81	0
3	SO4	C	1370	-	4,4,4	0.17	0	6,6,6	0.32	0
2	GLU	C	1371	-	9,9,9	0.90	0	11,11,11	1.05	1 (9%)
3	SO4	D	1370	-	4,4,4	0.16	0	6,6,6	0.16	0
2	GLU	D	1371	-	9,9,9	0.85	0	11,11,11	1.08	0
2	GLU	D	1372	-	9,9,9	0.85	0	11,11,11	0.98	1 (9%)
3	SO4	E	1371	-	4,4,4	0.19	0	6,6,6	0.19	0
2	GLU	E	1372	-	9,9,9	0.82	0	11,11,11	0.77	0
2	GLU	E	1373	-	9,9,9	0.87	0	11,11,11	1.03	0
3	SO4	F	1370	-	4,4,4	0.13	0	6,6,6	0.11	0
2	GLU	F	1371	-	9,9,9	0.83	0	11,11,11	0.70	0
2	GLU	F	1372	-	9,9,9	0.93	0	11,11,11	0.68	0
3	SO4	G	1370	-	4,4,4	0.25	0	6,6,6	0.16	0
2	GLU	G	1371	-	9,9,9	0.81	0	11,11,11	0.96	0
2	GLU	G	1372	-	9,9,9	0.88	0	11,11,11	0.96	0
3	SO4	H	1369	-	4,4,4	0.12	0	6,6,6	0.07	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
3	SO4	A	1372	-	-	0/0/0/0	0/0/0/0
2	GLU	A	1373	-	-	0/9/9/9	0/0/0/0
2	GLU	A	1374	-	-	0/9/9/9	0/0/0/0
3	SO4	B	1370	-	-	0/0/0/0	0/0/0/0
2	GLU	B	1371	-	-	0/9/9/9	0/0/0/0
3	SO4	C	1370	-	-	0/0/0/0	0/0/0/0
2	GLU	C	1371	-	-	0/9/9/9	0/0/0/0
3	SO4	D	1370	-	-	0/0/0/0	0/0/0/0
2	GLU	D	1371	-	-	0/9/9/9	0/0/0/0
2	GLU	D	1372	-	-	0/9/9/9	0/0/0/0
3	SO4	E	1371	-	-	0/0/0/0	0/0/0/0
2	GLU	E	1372	-	-	0/9/9/9	0/0/0/0
2	GLU	E	1373	-	-	0/9/9/9	0/0/0/0
3	SO4	F	1370	-	-	0/0/0/0	0/0/0/0
2	GLU	F	1371	-	-	0/9/9/9	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLU	F	1372	-	-	0/9/9/9	0/0/0/0
3	SO4	G	1370	-	-	0/0/0/0	0/0/0/0
2	GLU	G	1371	-	-	0/9/9/9	0/0/0/0
2	GLU	G	1372	-	-	0/9/9/9	0/0/0/0
3	SO4	H	1369	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1373	GLU	CB-CA-N	-2.17	104.83	110.14
2	D	1372	GLU	OE2-CD-CG	2.09	121.60	114.22
2	C	1371	GLU	OE2-CD-CG	2.08	121.58	114.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	355/367 (96%)	0.13	6 (1%) 67 76	19, 25, 32, 54	0
1	B	353/367 (96%)	0.49	35 (9%) 8 10	19, 25, 32, 39	0
1	C	356/367 (97%)	0.45	38 (10%) 6 8	19, 25, 31, 36	0
1	D	365/367 (99%)	0.22	15 (4%) 35 43	17, 25, 31, 36	0
1	E	365/367 (99%)	0.20	12 (3%) 44 53	14, 25, 31, 36	0
1	F	354/367 (96%)	0.30	21 (5%) 22 25	19, 25, 33, 53	0
1	G	356/367 (97%)	0.17	12 (3%) 43 51	19, 25, 33, 57	1 (0%)
1	H	337/367 (91%)	0.82	48 (14%) 3 5	19, 25, 30, 35	0
All	All	2841/2936 (96%)	0.34	187 (6%) 18 21	14, 25, 31, 57	1 (0%)

The worst 5 of 187 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	179	PRO	6.0
1	G	256	HIS	6.0
1	F	202	ALA	5.9
1	H	192	TYR	5.6
1	C	344	GLN	5.5

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	MG	G	1376	1/1	0.39	25.38	46,46,46,46	0
5	MG	E	1377	1/1	0.52	13.33	67,67,67,67	0
5	MG	A	1378	1/1	0.30	9.67	26,26,26,26	0
5	MG	F	1375	1/1	0.41	5.13	49,49,49,49	0
5	MG	H	1371	1/1	0.43	4.91	57,57,57,57	0
2	GLU	E	1373	10/10	0.28	3.85	39,39,42,43	0
4	CL	G	1375	1/1	0.23	3.71	39,39,39,39	0
5	MG	B	1375	1/1	0.31	2.73	43,43,43,43	0
4	CL	B	1372	1/1	0.20	2.72	49,49,49,49	0
2	GLU	B	1371	10/10	0.24	2.12	46,46,47,48	0
2	GLU	C	1371	10/10	0.22	1.85	33,34,35,35	0
4	CL	C	1374	1/1	0.20	1.27	36,36,36,36	0
2	GLU	F	1371	10/10	0.34	1.24	50,50,51,51	0
5	MG	D	1369	1/1	0.24	1.18	18,18,18,18	0
3	SO4	F	1370	5/5	0.20	0.91	59,59,60,60	0
2	GLU	G	1371	10/10	0.23	0.49	19,20,22,23	0
2	GLU	D	1372	10/10	0.18	0.25	34,35,35,35	0
2	GLU	E	1372	10/10	0.25	0.18	29,30,31,32	0
3	SO4	H	1369	5/5	0.23	0.12	80,80,81,81	0
2	GLU	A	1374	10/10	0.19	0.12	39,40,41,41	0
2	GLU	G	1372	10/10	0.19	0.09	30,31,32,32	0
2	GLU	F	1372	10/10	0.18	0.05	35,36,36,36	0
2	GLU	D	1371	10/10	0.27	-0.13	28,29,29,29	0
3	SO4	C	1370	5/5	0.19	-0.22	70,70,70,70	0
2	GLU	A	1373	10/10	0.18	-0.69	12,13,14,15	0
4	CL	H	1370	1/1	0.16	-0.95	46,46,46,46	0
3	SO4	E	1371	5/5	0.17	-1.27	71,72,72,72	0
3	SO4	D	1370	5/5	0.15	-1.40	55,56,56,57	0
3	SO4	B	1370	5/5	0.11	-1.44	65,66,66,66	0
4	CL	G	1373	1/1	0.09	-1.54	32,32,32,32	0
5	MG	E	1370	1/1	0.12	-1.58	17,17,17,17	0
3	SO4	A	1372	5/5	0.13	-1.70	36,38,38,38	0
4	CL	D	1374	1/1	0.10	-2.39	33,33,33,33	0
3	SO4	G	1370	5/5	0.12	-2.49	36,36,37,37	0
4	CL	C	1373	1/1	0.11	-2.73	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CL	C	1372	1/1	0.05	-3.34	24,24,24,24	0
4	CL	A	1376	1/1	0.08	-3.43	25,25,25,25	0
4	CL	G	1374	1/1	0.12	-3.54	35,35,35,35	0
4	CL	E	1374	1/1	0.15	-3.62	37,37,37,37	0
4	CL	B	1373	1/1	0.10	-4.99	30,30,30,30	0
4	CL	B	1374	1/1	0.11	-5.15	37,37,37,37	0
4	CL	F	1373	1/1	0.12	-5.65	44,44,44,44	0
4	CL	A	1377	1/1	0.12	-6.08	34,34,34,34	0
4	CL	A	1375	1/1	0.14	-6.57	34,34,34,34	0
4	CL	E	1376	1/1	0.09	-7.86	27,27,27,27	0
4	CL	D	1373	1/1	0.05	-18.44	18,18,18,18	0
4	CL	F	1374	1/1	0.12	-55.00	40,40,40,40	0
4	CL	E	1375	1/1	0.17	-	50,50,50,50	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.