



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 11:07 pm BST

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 Full wwPDB X-ray Structure Validation 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11



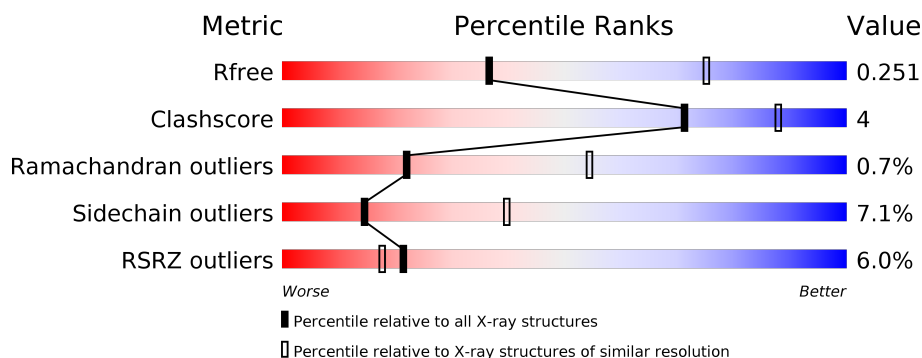
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 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	367	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>85%</span> <span>10%</span> <span>..</span> </div> </div>
1	B	367	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>83%</span> <span>12%</span> <span>..</span> </div> </div>
1	C	367	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>86%</span> <span>9%</span> <span>..</span> </div> </div>
1	D	367	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>84%</span> <span>12%</span> <span>..</span> </div> </div>
1	E	367	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>85%</span> <span>12%</span> <span>..</span> </div> </div>
1	F	367	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>81%</span> <span>14%</span> <span>..</span> </div> </div>

Continued on next page...



*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	G	367	
1	H	367	

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
5	MG	E	1377	-	-	-	X



## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21612 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 GLUTAMATE 5-KINASE.

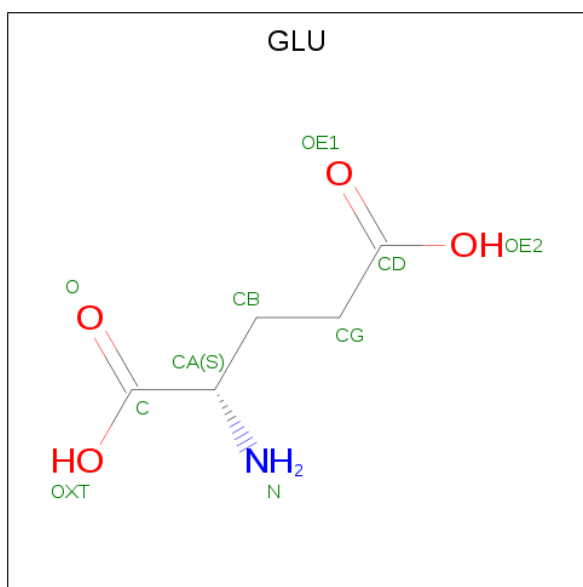
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	0	1
			2656	1653	489	506	8			
1	B	353	Total	C	N	O	S	0	0	0
			2661	1658	490	505	8			
1	C	356	Total	C	N	O	S	0	0	0
			2669	1662	492	507	8			
1	D	365	Total	C	N	O	S	0	0	0
			2728	1696	502	522	8			
1	E	365	Total	C	N	O	S	0	0	0
			2728	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>).

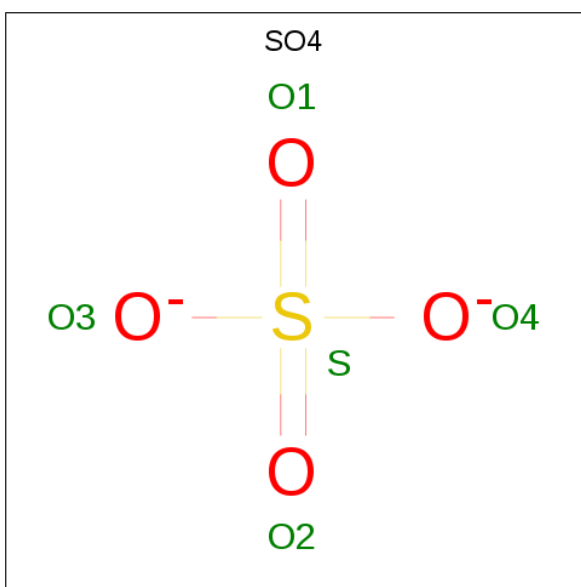




Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		
2	A	1	Total	C	N	O	0	0
			10	5	1	4		
2	B	1	Total	C	N	O	0	0
			10	5	1	4		
2	C	1	Total	C	N	O	0	0
			10	5	1	4		
2	D	1	Total	C	N	O	0	0
			10	5	1	4		
2	D	1	Total	C	N	O	0	0
			10	5	1	4		
2	E	1	Total	C	N	O	0	0
			10	5	1	4		
2	E	1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

*Continued on next page...*



*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

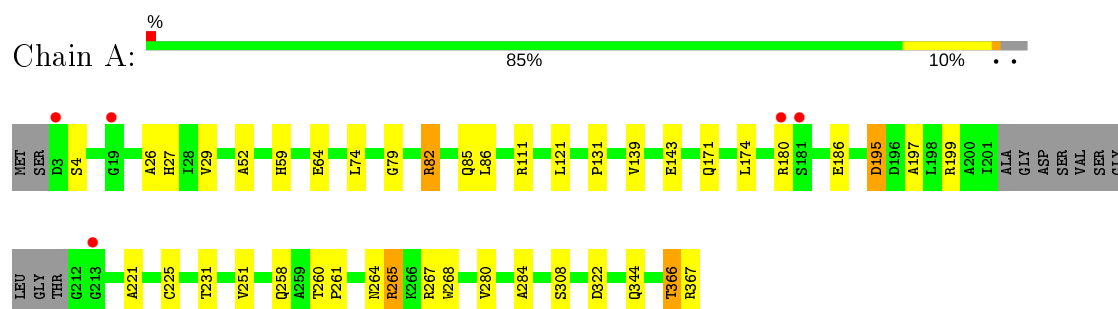
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	13	Total	O	0	0
			13	13		
6	H	15	Total	O	0	0
			15	15		



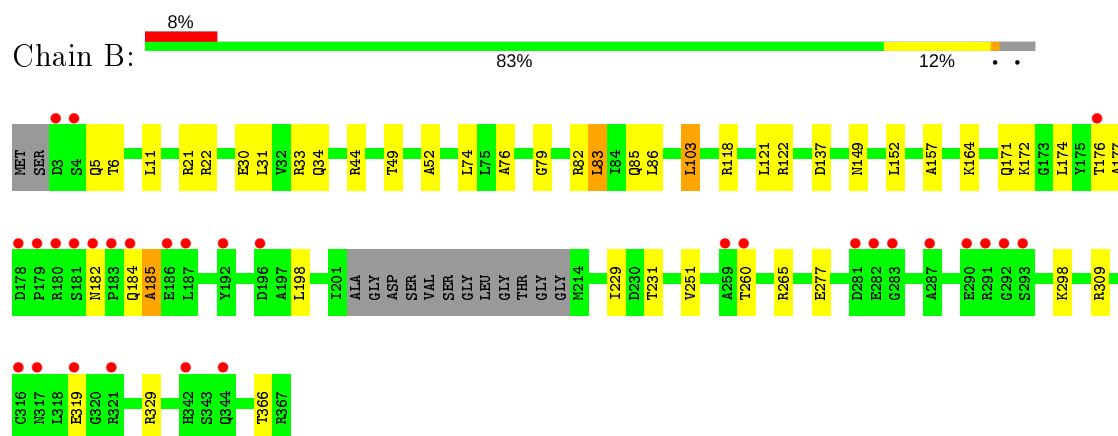
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

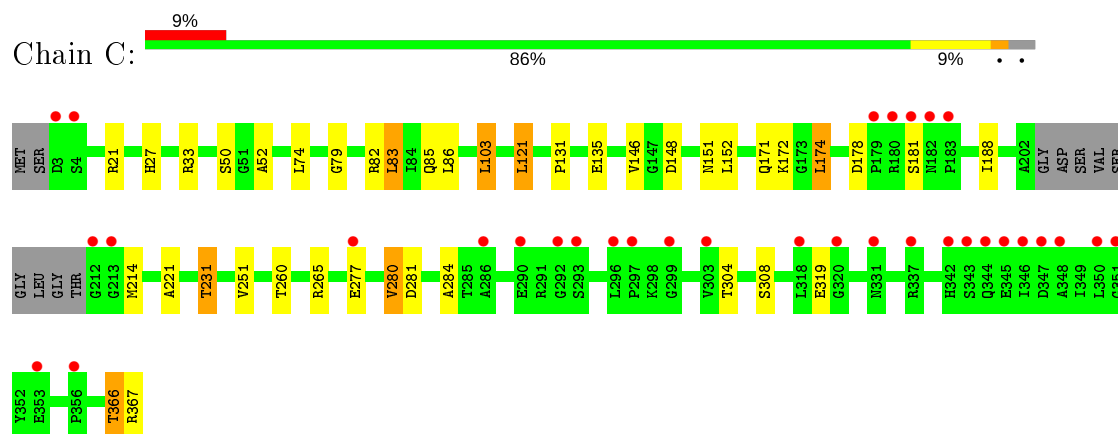
#### • Molecule 1: GLUTAMATE 5-KINASE



#### • Molecule 1: GLUTAMATE 5-KINASE




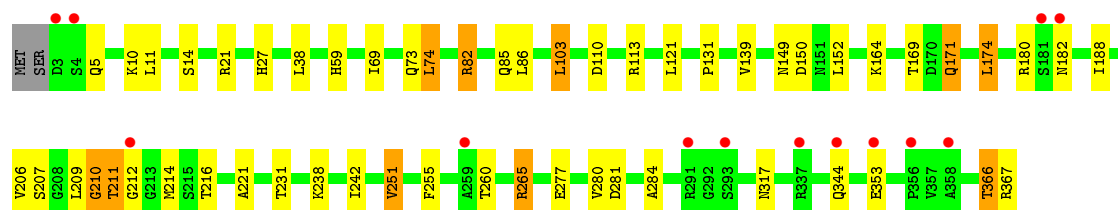
#### • Molecule 1: GLUTAMATE 5-KINASE






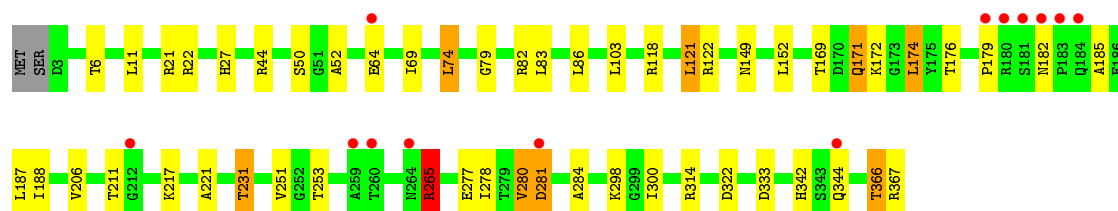
- Molecule 1: GLUTAMATE 5-KINASE

Chain D: 




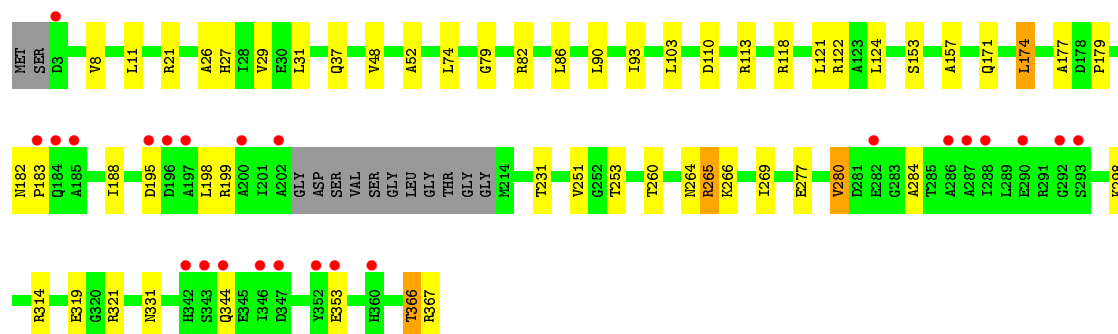
- Molecule 1: GLUTAMATE 5-KINASE

Chain E: 




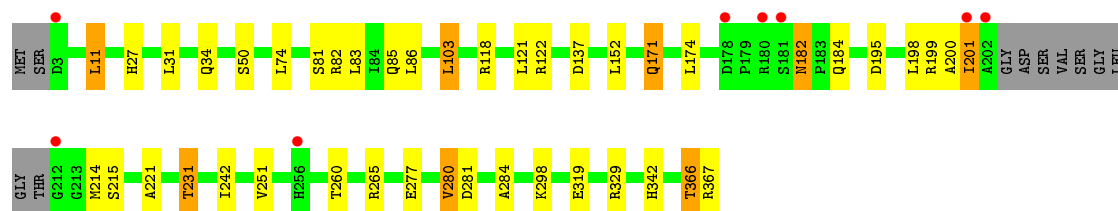
- Molecule 1: GLUTAMATE 5-KINASE

Chain F: 




- Molecule 1: GLUTAMATE 5-KINASE

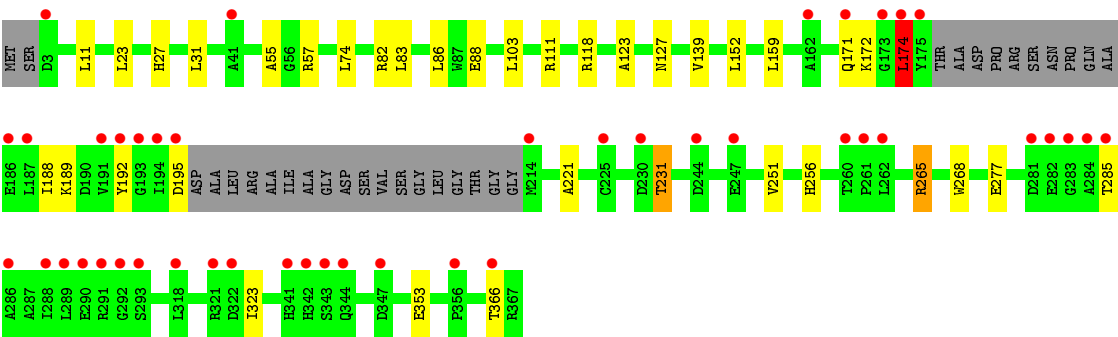
Chain G: 



- 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 (5.04%)	wwPDB-VP
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> )	0.36 , 44.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	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.

<sup>2</sup>Theoretical 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: 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 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	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
5	A	1	0	0	0	0
5	B	1	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 4.

All (153) 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: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
1:D:280:VAL:HG13	1:D:284:ALA:HB3	1.80	0.62
1:G:280:VAL:HG13	1:G:284:ALA:HB3	1.82	0.61
1:A:59:HIS:CG	1:A:82:ARG:HD2	2.37	0.60
1:D:59:HIS:ND1	1:D:82:ARG:HD2	2.20	0.57
1:D:164:LYS:HG2	6:D:2009:HOH:O	2.04	0.56
1:A:139:VAL:HG11	1:B:103:LEU:HB3	1.87	0.56
1:E:284:ALA:HB2	2:E:1372:GLU:HB3	1.88	0.56
1:D:59:HIS:CG	1:D:82:ARG:HD2	2.41	0.55
1:B:177:ALA:CB	1:B:182:ASN:HD22	2.19	0.55
1:D:174:LEU:HD13	1:D:188:ILE:HD12	1.88	0.55
1:D:221:ALA:HA	1:D:231:THR:HG21	1.90	0.54
1:C:221:ALA:HA	1:C:231:THR:HG21	1.88	0.54
1:C:366:THR:O	1:C:367:ARG:HB2	2.08	0.54
1:G:171:GLN:HE22	1:G:214:MET:HE1	1.69	0.54
1:H:118:ARG:HG3	1:H:159:LEU:O	2.08	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:280:VAL:HG13	1:F:284:ALA:HB3	1.90	0.53
1:C:174:LEU:HD13	1:C:188:ILE:HD12	1.90	0.53
1:B:118:ARG:O	1:B:122:ARG:HG2	2.09	0.53
1:C:85:GLN:HG2	1:D:85:GLN:HG2	1.91	0.52
1:D:164:LYS:NZ	6:D:2009:HOH:O	2.42	0.52
1:D:238:LYS:HD3	1:D:251:VAL:HG22	1.91	0.52
1:E:6:THR:OG1	1:E:44:ARG:HD3	2.10	0.52
1:F:195:ASP:OD1	1:F:198:LEU:HD22	2.09	0.52
1:D:14:SER:OG	3:D:1370:SO4:O3	2.26	0.52
1:C:135:GLU:OE1	1:C:146:VAL:N	2.34	0.51
1:E:171:GLN:H	1:E:171:GLN:HE21	1.57	0.51
1:H:11:LEU:CD2	1:H:31:LEU:HD13	2.40	0.51
1:D:82:ARG:O	1:D:85:GLN:HB2	2.11	0.50
1:C:85:GLN:CG	1:D:85:GLN:HG2	2.42	0.50
1:E:366:THR:O	1:E:367:ARG:HB2	2.11	0.50
1:C:103:LEU:CD1	1:C:152:LEU:HD11	2.41	0.50
1:F:319:GLU:N	1:F:319:GLU:OE2	2.43	0.50
1:A:195:ASP:C	1:A:197:ALA:H	2.14	0.50
1:E:188:ILE:O	1:E:253:THR:HG23	2.12	0.49
1:H:221:ALA:HA	1:H:231:THR:HG21	1.94	0.49
1:C:121:LEU:CD1	1:C:131:PRO:HG2	2.42	0.49
1:F:110:ASP:HB2	1:F:113:ARG:H	1.77	0.49
1:G:198:LEU:HD22	1:G:201:ILE:HD11	1.94	0.49
1:F:8:VAL:HG21	1:F:157:ALA:HA	1.94	0.49
1:A:322:ASP:OD1	1:A:322:ASP:C	2.51	0.49
1:A:264:ASN:HA	1:A:267:ARG:HD2	1.94	0.48
1:G:298:LYS:HE3	1:G:342:HIS:CE1	2.48	0.48
1:B:103:LEU:CD1	1:B:152:LEU:HD11	2.43	0.48
1:E:171:GLN:H	1:E:171:GLN:NE2	2.10	0.48
1:D:69:ILE:O	1:D:73:GLN:HG3	2.14	0.48
1:E:277:GLU:HB3	1:E:314:ARG:HB3	1.94	0.48
1:E:265:ARG:HH11	1:E:265:ARG:CG	2.26	0.48
1:H:123:ALA:O	1:H:127:ASN:ND2	2.43	0.48
1:E:333:ASP:OD2	1:F:331:ASN:ND2	2.45	0.48
1:B:52:ALA:O	1:B:79:GLY:HA3	2.13	0.48
1:F:11:LEU:CD2	1:F:31:LEU:HD13	2.44	0.48
1:H:192:TYR:CE1	1:H:256:HIS:CD2	3.02	0.48
1:D:366:THR:O	1:D:367:ARG:HB2	2.14	0.47
1:B:5:GLN:HE22	1:B:164:LYS:NZ	2.12	0.47
1:E:182:ASN:HB3	1:E:185:ALA:HB2	1.96	0.47
1:C:52:ALA:O	1:C:79:GLY:HA3	2.13	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:174:LEU:HD13	1:H:188:ILE:HD12	1.97	0.47
1:B:79:GLY:O	1:B:83:LEU:HB2	2.14	0.47
1:C:50:SER:O	1:C:83:LEU:HD11	2.14	0.47
1:G:200:ALA:O	1:G:201:ILE:HG23	2.15	0.47
1:G:182:ASN:ND2	1:G:184:GLN:H	2.12	0.47
1:E:52:ALA:O	1:E:79:GLY:HA3	2.14	0.47
1:H:23:LEU:HD11	1:H:55:ALA:HB2	1.97	0.47
1:A:143:GLU:N	1:A:143:GLU:OE1	2.48	0.47
1:G:137:ASP:OD2	2:G:1372:GLU:N	2.48	0.46
1:E:21:ARG:HG2	1:E:22:ARG:NH1	2.30	0.46
1:C:366:THR:HG23	1:C:367:ARG:N	2.31	0.46
1:A:111:ARG:HD2	1:A:268:TRP:CD1	2.51	0.45
1:A:197:ALA:C	1:A:199:ARG:H	2.20	0.45
1:D:149:ASN:HA	1:D:152:LEU:HB3	1.99	0.45
1:E:121:LEU:HD12	1:E:121:LEU:O	2.17	0.45
1:B:184:GLN:O	1:B:185:ALA:C	2.54	0.45
1:B:309:ARG:HB2	1:B:329:ARG:O	2.17	0.45
1:B:6:THR:OG1	1:B:44:ARG:HD3	2.16	0.45
1:D:10:LYS:NZ	1:D:150:ASP:OD1	2.43	0.44
1:B:11:LEU:CD2	1:B:31:LEU:HD13	2.47	0.44
1:D:5:GLN:HE22	1:D:164:LYS:NZ	2.14	0.44
1:E:171:GLN:N	1:E:171:GLN:HE21	2.15	0.44
1:D:206:VAL:HG11	1:D:211:THR:HG23	1.99	0.44
1:C:277:GLU:HG2	1:C:304:THR:HB	1.98	0.44
1:C:148:ASP:CG	1:C:151:ASN:HD22	2.21	0.44
1:D:231:THR:HG23	1:D:255:PHE:HB2	1.99	0.44
1:A:52:ALA:O	1:A:79:GLY:HA3	2.17	0.44
1:H:111:ARG:HD2	1:H:268:TRP:CD1	2.53	0.44
1:B:30:GLU:O	1:B:34:GLN:HG3	2.18	0.44
1:A:85:GLN:HG3	1:B:85:GLN:HG3	2.00	0.44
1:F:188:ILE:O	1:F:253:THR:OG1	2.24	0.44
1:B:157:ALA:HB1	1:B:229:ILE:HD13	2.00	0.43
1:B:49:THR:O	1:B:149:ASN:ND2	2.51	0.43
1:D:103:LEU:CD1	1:D:152:LEU:HD11	2.48	0.43
1:F:266:LYS:HB2	1:F:269:ILE:HD12	2.00	0.43
1:E:265:ARG:HH11	1:E:265:ARG:HG3	1.84	0.43
1:E:366:THR:HG23	1:E:367:ARG:N	2.33	0.43
1:G:103:LEU:CD1	1:G:152:LEU:HD11	2.49	0.43
1:H:103:LEU:CD1	1:H:152:LEU:HD11	2.49	0.43
1:H:11:LEU:HD22	1:H:31:LEU:HD13	2.00	0.43
1:C:280:VAL:HG13	1:C:284:ALA:HB3	2.01	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:THR:HG23	1:D:171:GLN:O	2.20	0.42
1:C:171:GLN:HE21	1:C:214:MET:CE	2.32	0.42
1:G:11:LEU:CD2	1:G:31:LEU:HD13	2.49	0.42
1:E:179:PRO:HA	1:E:185:ALA:HB3	2.00	0.42
1:G:34:GLN:HB2	1:G:242:ILE:HD12	2.00	0.42
1:F:48:VAL:HG21	1:F:153:SER:HA	2.01	0.42
1:E:149:ASN:HA	1:E:152:LEU:HB3	2.01	0.42
1:E:69:ILE:H	1:E:69:ILE:HD12	1.84	0.42
1:A:258:GLN:HE21	1:A:261:PRO:HA	1.84	0.42
1:A:366:THR:O	1:A:367:ARG:HB2	2.20	0.42
1:E:103:LEU:CD1	1:E:152:LEU:HD11	2.49	0.42
1:E:74:LEU:HD13	1:F:124:LEU:HD23	2.02	0.42
1:A:121:LEU:CD1	1:A:131:PRO:HG2	2.50	0.42
1:C:178:ASP:HB3	1:C:181:SER:OG	2.20	0.42
1:E:118:ARG:O	1:E:122:ARG:HG2	2.20	0.42
1:G:118:ARG:O	1:G:122:ARG:HG2	2.19	0.42
1:D:209:LEU:O	1:D:210:GLY:O	2.38	0.41
1:D:38:LEU:HD11	1:D:242:ILE:HG22	2.02	0.41
1:D:317:ASN:OD1	1:D:317:ASN:C	2.58	0.41
1:D:74:LEU:HD12	1:D:74:LEU:C	2.40	0.41
1:A:221:ALA:O	1:A:225:CYS:SG	2.78	0.41
1:E:176:THR:HG22	1:E:188:ILE:HG12	2.03	0.41
1:F:26:ALA:O	1:F:29:VAL:HG12	2.21	0.41
1:G:171:GLN:HE22	1:G:214:MET:HE3	1.84	0.41
1:A:264:ASN:HA	1:A:267:ARG:CD	2.51	0.41
1:A:26:ALA:O	1:A:29:VAL:HG12	2.20	0.41
1:E:174:LEU:CD1	1:E:188:ILE:HD12	2.50	0.41
1:F:52:ALA:O	1:F:79:GLY:HA3	2.21	0.41
1:B:149:ASN:HA	1:B:152:LEU:HB3	2.03	0.41
1:C:171:GLN:HE21	1:C:214:MET:HE1	1.85	0.41
1:D:121:LEU:CD1	1:D:131:PRO:HG2	2.50	0.41
1:F:366:THR:HG23	1:F:367:ARG:HG3	2.02	0.41
1:G:298:LYS:HE3	1:G:342:HIS:HE1	1.86	0.41
1:G:103:LEU:HB3	1:H:139:VAL:HG11	2.02	0.41
1:A:280:VAL:HG13	1:A:284:ALA:CB	2.44	0.41
1:F:277:GLU:HB3	1:F:314:ARG:HB3	2.03	0.41
1:F:90:LEU:O	1:F:93:ILE:HB	2.21	0.41
1:E:169:THR:HB	1:E:217:LYS:HE2	2.03	0.40
1:E:281:ASP:HB3	1:E:284:ALA:H	1.85	0.40
1:F:118:ARG:O	1:F:122:ARG:HG2	2.20	0.40
1:G:366:THR:O	1:G:367:ARG:HB2	2.20	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:50:SER:O	1:G:83:LEU:HD11	2.20	0.40
1:B:76:ALA:HB1	1:B:137:ASP:HB2	2.03	0.40
1:G:195:ASP:HA	1:G:198:LEU:HG	2.03	0.40
1:H:285:THR:HG23	1:H:323:ILE:HD13	2.02	0.40
1:E:278:ILE:HG23	1:E:300:ILE:HG23	2.03	0.40
1:G:221:ALA:HA	1:G:231:THR:HG21	2.04	0.40
1:D:110:ASP:HB2	1:D:113:ARG:H	1.86	0.40
1:C:103:LEU:HB3	1:D:139:VAL:HG11	2.04	0.40
1:G:85:GLN:NE2	1:H:88:GLU:OE2	2.54	0.40
1:E:221:ALA:HA	1:E:231:THR:HG21	2.02	0.40

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%)	41	71
1	B	349/367 (95%)	332 (95%)	14 (4%)	3 (1%)	17	48
1	C	352/367 (96%)	333 (95%)	19 (5%)	0	100	100
1	D	363/367 (99%)	342 (94%)	17 (5%)	4 (1%)	14	42
1	E	363/367 (99%)	346 (95%)	15 (4%)	2 (1%)	25	58
1	F	350/367 (95%)	325 (93%)	18 (5%)	7 (2%)	7	27
1	G	352/367 (96%)	333 (95%)	17 (5%)	2 (1%)	25	58
1	H	331/367 (90%)	313 (95%)	16 (5%)	2 (1%)	25	58
All	All	2811/2936 (96%)	2658 (95%)	132 (5%)	21 (1%)	22	54

All (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
1	F	183	PRO
1	F	199	ARG
1	A	265	ARG
1	B	185	ALA
1	D	214	MET
1	G	281	ASP
1	H	265	ARG
1	E	265	ARG
1	E	322	ASP
1	F	265	ARG
1	H	174	LEU
1	B	176	THR
1	F	177	ALA
1	F	298	LYS
1	G	201	ILE
1	F	179	PRO

### 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%)	17	45
1	B	277/285 (97%)	257 (93%)	20 (7%)	14	39
1	C	276/285 (97%)	256 (93%)	20 (7%)	14	39
1	D	283/285 (99%)	263 (93%)	20 (7%)	14	40
1	E	283/285 (99%)	263 (93%)	20 (7%)	14	40
1	F	276/285 (97%)	255 (92%)	21 (8%)	13	36
1	G	277/285 (97%)	255 (92%)	22 (8%)	12	34
1	H	265/285 (93%)	248 (94%)	17 (6%)	17	45

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2212/2280 (97%)	2054 (93%)	158 (7%)	14	40

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	27	HIS
1	A	64	GLU
1	A	74	LEU
1	A	82	ARG
1	A	86	LEU
1	A	171	GLN
1	A	174	LEU
1	A	180	ARG
1	A	186	GLU
1	A	195	ASP
1	A	231	THR
1	A	251	VAL
1	A	260	THR
1	A	265	ARG
1	A	308	SER
1	A	344	GLN
1	A	366	THR
1	B	21	ARG
1	B	22	ARG
1	B	33	ARG
1	B	74	LEU
1	B	82	ARG
1	B	83	LEU
1	B	86	LEU
1	B	103	LEU
1	B	121	LEU
1	B	171	GLN
1	B	172	LYS
1	B	174	LEU
1	B	198	LEU
1	B	231	THR
1	B	251	VAL
1	B	260	THR
1	B	265	ARG
1	B	277	GLU
1	B	319	GLU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	366	THR
1	C	21	ARG
1	C	27	HIS
1	C	33	ARG
1	C	74	LEU
1	C	82	ARG
1	C	83	LEU
1	C	86	LEU
1	C	103	LEU
1	C	121	LEU
1	C	172	LYS
1	C	174	LEU
1	C	231	THR
1	C	251	VAL
1	C	260	THR
1	C	265	ARG
1	C	280	VAL
1	C	281	ASP
1	C	308	SER
1	C	319	GLU
1	C	366	THR
1	D	11	LEU
1	D	21	ARG
1	D	27	HIS
1	D	74	LEU
1	D	82	ARG
1	D	86	LEU
1	D	103	LEU
1	D	171	GLN
1	D	174	LEU
1	D	180	ARG
1	D	182	ASN
1	D	207	SER
1	D	216	THR
1	D	251	VAL
1	D	260	THR
1	D	265	ARG
1	D	277	GLU
1	D	344	GLN
1	D	353	GLU
1	D	366	THR
1	E	11	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	E	27	HIS
1	E	64	GLU
1	E	74	LEU
1	E	82	ARG
1	E	86	LEU
1	E	121	LEU
1	E	171	GLN
1	E	172	LYS
1	E	174	LEU
1	E	187	LEU
1	E	206	VAL
1	E	211	THR
1	E	231	THR
1	E	251	VAL
1	E	265	ARG
1	E	280	VAL
1	E	281	ASP
1	E	344	GLN
1	E	366	THR
1	F	21	ARG
1	F	27	HIS
1	F	37	GLN
1	F	74	LEU
1	F	82	ARG
1	F	86	LEU
1	F	103	LEU
1	F	121	LEU
1	F	171	GLN
1	F	174	LEU
1	F	182	ASN
1	F	231	THR
1	F	251	VAL
1	F	260	THR
1	F	264	ASN
1	F	265	ARG
1	F	280	VAL
1	F	321	ARG
1	F	344	GLN
1	F	353	GLU
1	F	366	THR
1	G	11	LEU
1	G	27	HIS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	G	74	LEU
1	G	81	SER
1	G	82	ARG
1	G	86	LEU
1	G	103	LEU
1	G	121	LEU
1	G	171	GLN
1	G	174	LEU
1	G	182	ASN
1	G	199	ARG
1	G	215	SER
1	G	231	THR
1	G	251	VAL
1	G	260	THR
1	G	265	ARG
1	G	277	GLU
1	G	280	VAL
1	G	319	GLU
1	G	329	ARG
1	G	366	THR
1	H	27	HIS
1	H	57	ARG
1	H	74	LEU
1	H	82	ARG
1	H	83	LEU
1	H	86	LEU
1	H	171	GLN
1	H	172	LYS
1	H	174	LEU
1	H	189	LYS
1	H	195	ASP
1	H	231	THR
1	H	251	VAL
1	H	265	ARG
1	H	277	GLU
1	H	353	GLU
1	H	366	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	85	GLN
1	A	116	ASN
1	A	258	GLN
1	B	5	GLN
1	B	73	GLN
1	B	85	GLN
1	B	182	ASN
1	B	184	GLN
1	C	128	ASN
1	C	171	GLN
1	C	182	ASN
1	C	331	ASN
1	D	5	GLN
1	D	128	ASN
1	D	171	GLN
1	E	85	GLN
1	E	171	GLN
1	E	184	GLN
1	E	344	GLN
1	F	5	GLN
1	F	171	GLN
1	F	182	ASN
1	F	264	ASN
1	F	331	ASN
1	G	116	ASN
1	G	128	ASN
1	G	171	GLN
1	G	182	ASN
1	G	342	HIS
1	H	73	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	0.19	0	6,6,6	0.28	0
3	SO4	F	1370	-	4,4,4	0.15	0	6,6,6	0.14	0
3	SO4	D	1370	-	4,4,4	0.18	0	6,6,6	0.21	0
3	SO4	E	1371	-	4,4,4	0.13	0	6,6,6	0.23	0
3	SO4	C	1370	-	4,4,4	0.15	0	6,6,6	0.29	0
3	SO4	H	1369	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	G	1370	-	4,4,4	0.20	0	6,6,6	0.17	0
3	SO4	B	1370	-	4,4,4	0.15	0	6,6,6	0.20	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1370	SO4	1	0

## 5.7 Other polymers [i](#)

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%)	-0.08	5 (1%) 75 75	19, 25, 32, 54	0
1	B	353/367 (96%)	0.41	30 (8%) 10 8	19, 25, 32, 39	0
1	C	356/367 (97%)	0.44	33 (9%) 8 6	19, 25, 31, 36	0
1	D	365/367 (99%)	0.20	13 (3%) 42 37	17, 25, 31, 36	0
1	E	365/367 (99%)	0.18	13 (3%) 42 37	14, 25, 31, 36	0
1	F	354/367 (96%)	0.31	24 (6%) 17 13	19, 25, 33, 53	0
1	G	356/367 (97%)	0.03	8 (2%) 62 59	19, 25, 33, 57	1 (0%)
1	H	337/367 (91%)	0.77	44 (13%) 3 2	19, 25, 30, 35	0
All	All	2841/2936 (96%)	0.28	170 (5%) 21 18	14, 25, 31, 57	1 (0%)

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	197	ALA	7.4
1	H	192	TYR	6.3
1	C	344	GLN	5.9
1	G	256	HIS	5.8
1	B	3	ASP	5.6
1	B	179	PRO	5.5
1	B	184	GLN	5.4
1	H	173	GLY	5.2
1	C	343	SER	5.0
1	B	183	PRO	4.8
1	G	202	ALA	4.7
1	G	212	GLY	4.6
1	H	175	TYR	4.6
1	H	290	GLU	4.6
1	H	174	LEU	4.5
1	F	184	GLN	4.5

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	345	GLU	4.4
1	H	194	ILE	4.4
1	G	181	SER	4.3
1	C	181	SER	4.2
1	H	3	ASP	4.2
1	C	346	ILE	4.2
1	B	181	SER	4.1
1	D	3	ASP	3.9
1	E	183	PRO	3.9
1	C	213	GLY	3.9
1	B	282	GLU	3.8
1	H	286	ALA	3.7
1	B	180	ARG	3.7
1	H	344	GLN	3.7
1	E	181	SER	3.7
1	F	292	GLY	3.7
1	B	317	ASN	3.6
1	B	283	GLY	3.6
1	H	283	GLY	3.6
1	H	193	GLY	3.6
1	H	261	PRO	3.6
1	F	202	ALA	3.5
1	C	351	GLY	3.5
1	F	343	SER	3.5
1	G	180	ARG	3.5
1	H	214	MET	3.5
1	F	344	GLN	3.5
1	C	348	ALA	3.4
1	C	3	ASP	3.4
1	B	290	GLU	3.3
1	F	183	PRO	3.3
1	B	293	SER	3.3
1	H	293	SER	3.3
1	B	196	ASP	3.2
1	H	289	LEU	3.2
1	H	292	GLY	3.2
1	H	187	LEU	3.2
1	C	347	ASP	3.2
1	B	342	HIS	3.2
1	B	182	ASN	3.1
1	H	288	ILE	3.1
1	C	292	GLY	3.1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	342	HIS	3.1
1	B	186	GLU	3.1
1	H	356	PRO	3.0
1	E	212	GLY	3.0
1	D	293	SER	3.0
1	H	342	HIS	3.0
1	H	260	THR	2.9
1	A	19	GLY	2.9
1	G	201	ILE	2.9
1	H	225	CYS	2.9
1	H	230	ASP	2.9
1	B	260	THR	2.9
1	H	282	GLU	2.9
1	E	180	ARG	2.9
1	F	347	ASP	2.9
1	C	337	ARG	2.9
1	A	3	ASP	2.9
1	F	195	ASP	2.9
1	H	244	ASP	2.8
1	B	344	GLN	2.8
1	H	343	SER	2.8
1	H	195	ASP	2.8
1	H	281	ASP	2.8
1	H	284	ALA	2.8
1	B	187	LEU	2.7
1	F	3	ASP	2.7
1	G	178	ASP	2.7
1	B	281	ASP	2.7
1	F	185	ALA	2.7
1	B	192	TYR	2.7
1	D	337	ARG	2.7
1	B	178	ASP	2.7
1	C	297	PRO	2.7
1	H	291	ARG	2.7
1	H	162	ALA	2.7
1	C	277	GLU	2.7
1	F	196	ASP	2.7
1	E	344	GLN	2.6
1	B	176	THR	2.6
1	C	180	ARG	2.6
1	F	290	GLU	2.6
1	B	316	CYS	2.6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	186	GLU	2.5
1	C	212	GLY	2.5
1	A	180	ARG	2.5
1	E	64	GLU	2.5
1	C	293	SER	2.5
1	F	287	ALA	2.4
1	F	282	GLU	2.4
1	A	181	SER	2.4
1	C	183	PRO	2.4
1	C	320	GLY	2.4
1	D	182	ASN	2.4
1	F	200	ALA	2.4
1	C	290	GLU	2.4
1	D	353	GLU	2.4
1	H	191	VAL	2.4
1	B	291	ARG	2.4
1	E	184	GLN	2.3
1	H	321	ARG	2.3
1	C	286	ALA	2.3
1	C	356	PRO	2.3
1	C	182	ASN	2.3
1	B	321	ARG	2.3
1	F	352	TYR	2.3
1	E	259	ALA	2.3
1	H	318	LEU	2.3
1	H	262	LEU	2.3
1	C	299	GLY	2.3
1	F	353	GLU	2.3
1	A	213	GLY	2.3
1	E	182	ASN	2.2
1	C	4	SER	2.2
1	F	286	ALA	2.2
1	F	288	ILE	2.2
1	C	303	VAL	2.2
1	B	4	SER	2.2
1	E	260	THR	2.2
1	C	179	PRO	2.2
1	F	342	HIS	2.2
1	C	318	LEU	2.2
1	B	259	ALA	2.2
1	H	247	GLU	2.2
1	C	353	GLU	2.2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	366	THR	2.2
1	D	356	PRO	2.2
1	D	291	ARG	2.2
1	D	181	SER	2.2
1	F	360	HIS	2.2
1	E	264	ASN	2.2
1	H	171	GLN	2.2
1	H	341	HIS	2.2
1	H	41	ALA	2.1
1	E	179	PRO	2.1
1	D	4	SER	2.1
1	B	319	GLU	2.1
1	F	346	ILE	2.1
1	G	3	ASP	2.1
1	C	296	LEU	2.1
1	D	259	ALA	2.1
1	C	350	LEU	2.1
1	E	281	ASP	2.1
1	H	285	THR	2.1
1	B	292	GLY	2.1
1	D	344	GLN	2.1
1	F	293	SER	2.1
1	D	358	ALA	2.1
1	B	287	ALA	2.0
1	H	322	ASP	2.0
1	H	347	ASP	2.0
1	C	331	ASN	2.0
1	D	212	GLY	2.0

## 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 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. 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	MG	E	1377	1/1	0.70	0.46	67,67,67,67	0
5	MG	H	1371	1/1	0.76	0.31	57,57,57,57	0
4	CL	F	1374	1/1	0.77	0.10	40,40,40,40	0
5	MG	F	1375	1/1	0.79	0.31	49,49,49,49	0
2	GLU	C	1371	10/10	0.80	0.22	33,34,35,35	0
2	GLU	F	1371	10/10	0.82	0.37	50,50,51,51	0
4	CL	B	1372	1/1	0.82	0.14	49,49,49,49	0
4	CL	E	1375	1/1	0.82	0.25	50,50,50,50	0
4	CL	C	1374	1/1	0.83	0.21	36,36,36,36	0
2	GLU	B	1371	10/10	0.84	0.21	46,46,47,48	0
4	CL	B	1374	1/1	0.85	0.17	37,37,37,37	0
2	GLU	E	1373	10/10	0.86	0.20	39,39,42,43	0
2	GLU	D	1371	10/10	0.86	0.27	28,29,29,29	0
2	GLU	A	1374	10/10	0.86	0.24	39,40,41,41	0
4	CL	H	1370	1/1	0.87	0.27	46,46,46,46	0
3	SO4	H	1369	5/5	0.87	0.28	80,80,81,81	0
5	MG	G	1376	1/1	0.88	0.26	46,46,46,46	0
2	GLU	E	1372	10/10	0.88	0.31	29,30,31,32	0
4	CL	D	1374	1/1	0.89	0.15	33,33,33,33	0
4	CL	E	1374	1/1	0.90	0.16	37,37,37,37	0
3	SO4	E	1371	5/5	0.90	0.24	71,72,72,72	0
2	GLU	F	1372	10/10	0.90	0.21	35,36,36,36	0
4	CL	E	1376	1/1	0.90	0.10	27,27,27,27	0
2	GLU	D	1372	10/10	0.90	0.18	34,35,35,35	0
2	GLU	G	1372	10/10	0.91	0.17	30,31,32,32	0
3	SO4	F	1370	5/5	0.91	0.23	59,59,60,60	0
3	SO4	D	1370	5/5	0.92	0.20	55,56,56,57	0
4	CL	B	1373	1/1	0.92	0.15	30,30,30,30	0
2	GLU	G	1371	10/10	0.93	0.26	19,20,22,23	0
5	MG	B	1375	1/1	0.93	0.22	43,43,43,43	0
3	SO4	C	1370	5/5	0.93	0.22	70,70,70,70	0
4	CL	G	1374	1/1	0.94	0.12	35,35,35,35	0
2	GLU	A	1373	10/10	0.94	0.17	12,13,14,15	0
4	CL	A	1377	1/1	0.94	0.12	34,34,34,34	0
4	CL	A	1375	1/1	0.94	0.15	34,34,34,34	0
4	CL	A	1376	1/1	0.95	0.11	25,25,25,25	0
5	MG	A	1378	1/1	0.95	0.27	26,26,26,26	0
3	SO4	B	1370	5/5	0.95	0.18	65,66,66,66	0
4	CL	F	1373	1/1	0.96	0.15	44,44,44,44	0
4	CL	C	1372	1/1	0.96	0.09	24,24,24,24	0
4	CL	G	1373	1/1	0.96	0.12	32,32,32,32	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	A	1372	5/5	0.96	0.15	36,38,38,38	0
3	SO4	G	1370	5/5	0.97	0.20	36,36,37,37	0
4	CL	G	1375	1/1	0.98	0.20	39,39,39,39	0
5	MG	D	1369	1/1	0.98	0.13	18,18,18,18	0
4	CL	D	1373	1/1	0.98	0.06	18,18,18,18	0
5	MG	E	1370	1/1	0.98	0.09	17,17,17,17	0
4	CL	C	1373	1/1	0.99	0.04	14,14,14,14	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.