



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:01 PM UTC

PDB ID : 2J5T / pdb_00002j5t
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

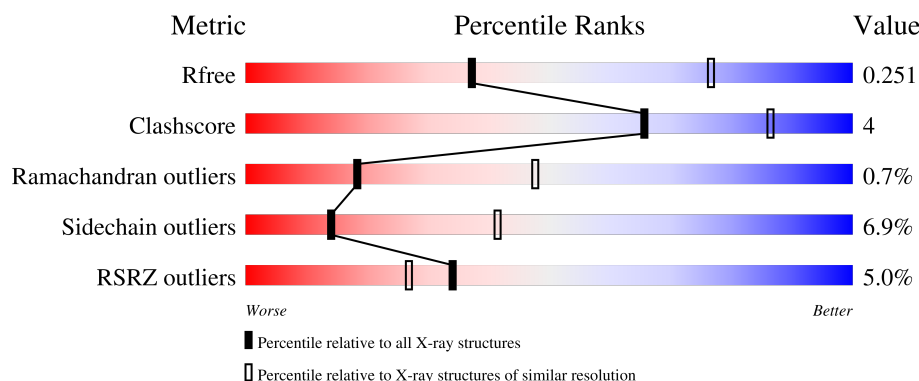
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 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	367	2% 84% 12% ..
1	B	367	8% 83% 13% ..
1	C	367	2% 86% 9% ..
1	D	367	3% 84% 12% ..
1	E	367	2% 85% 11% ..

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Mol	Chain	Length	Quality of chain
1	F	367	
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 (CCD ID: GLU) (formula: C₅H₉NO₄).



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 (CCD ID: SO4) (formula: O₄S).



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 (CCD ID: CL) (formula: Cl).

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

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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Mg 1	0	0
5	B	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	F	1	Total 1	Mg 1	0	0
5	G	1	Total 1	Mg 1	0	0
5	H	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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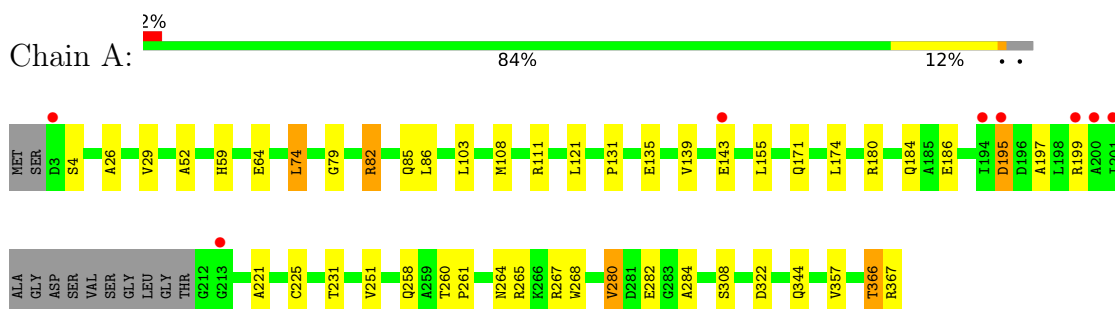
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	13	Total	O	0	0
			13	13		
6	H	15	Total	O	0	0
			15	15		

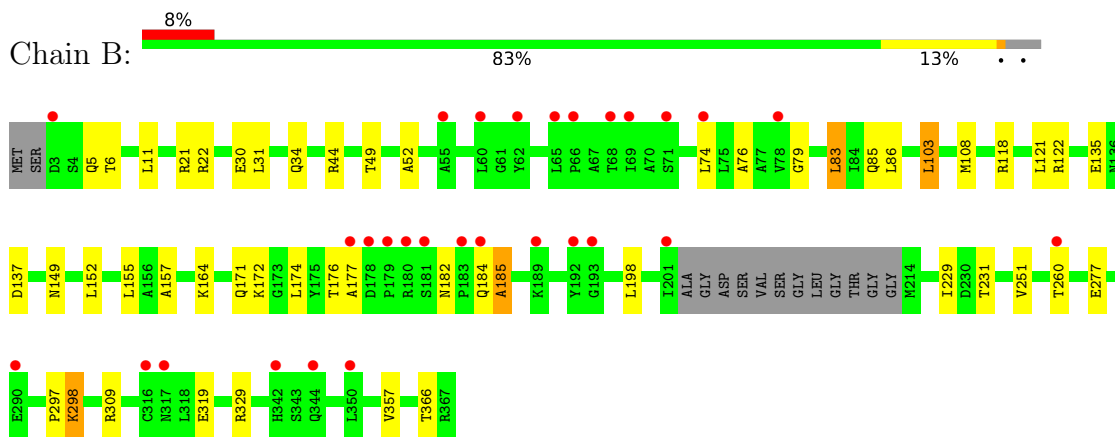
3 Residue-property plots [i](#)

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.

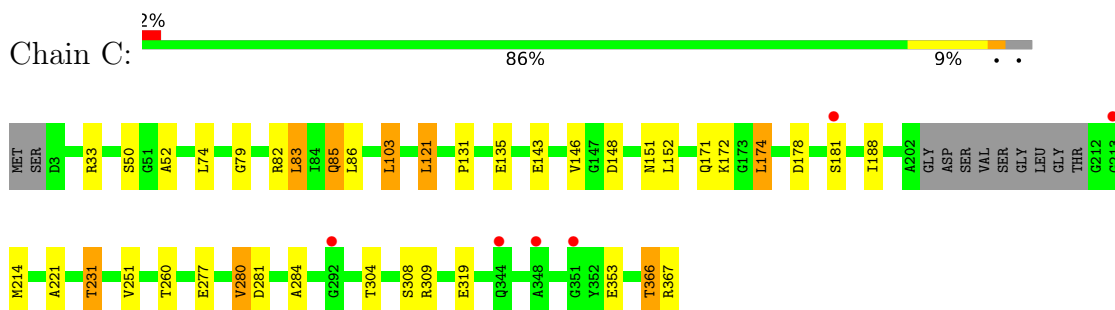
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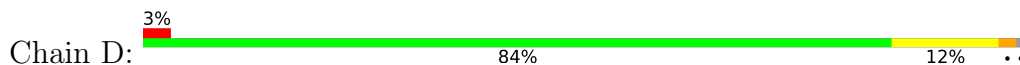
• Molecule 1: GLUTAMATE 5-KINASE

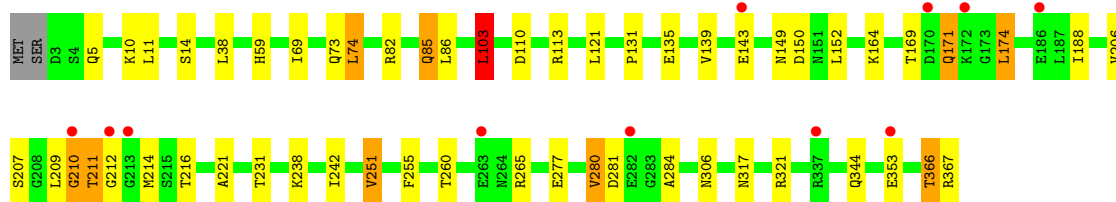


• Molecule 1: GLUTAMATE 5-KINASE

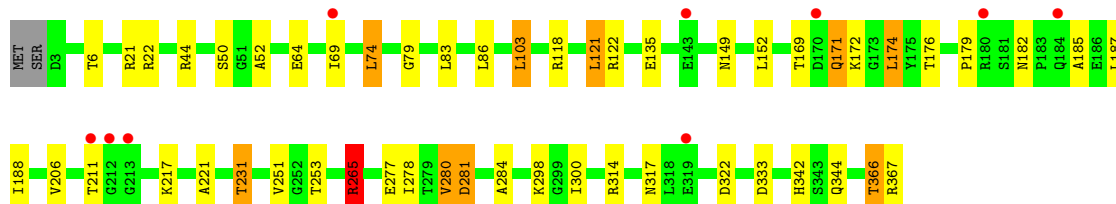
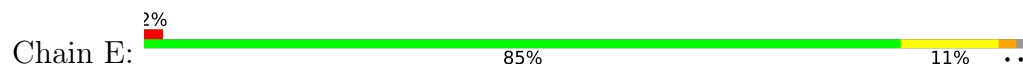


• Molecule 1: GLUTAMATE 5-KINASE

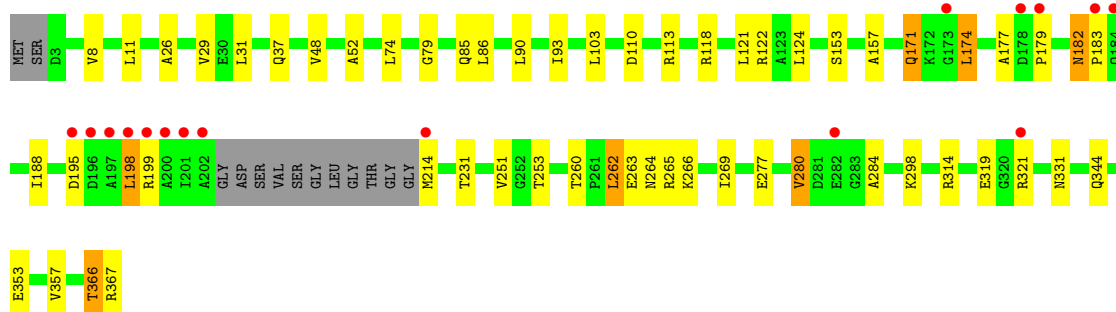
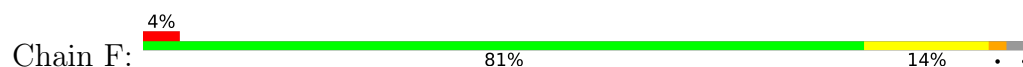




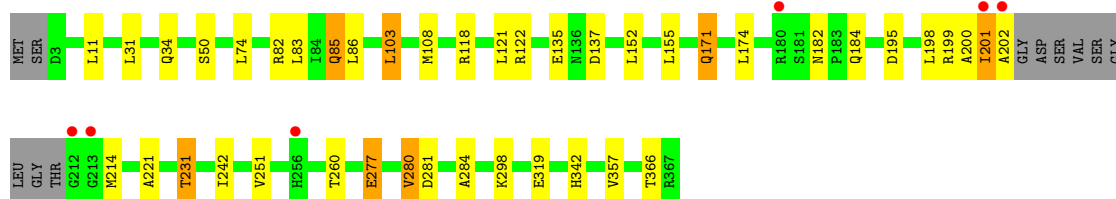
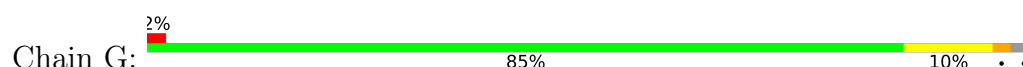
• Molecule 1: GLUTAMATE 5-KINASE



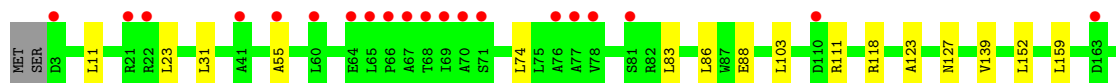
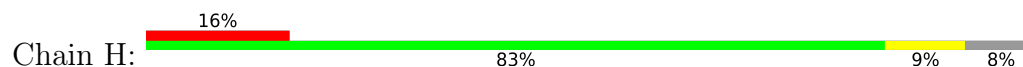
• Molecule 1: GLUTAMATE 5-KINASE

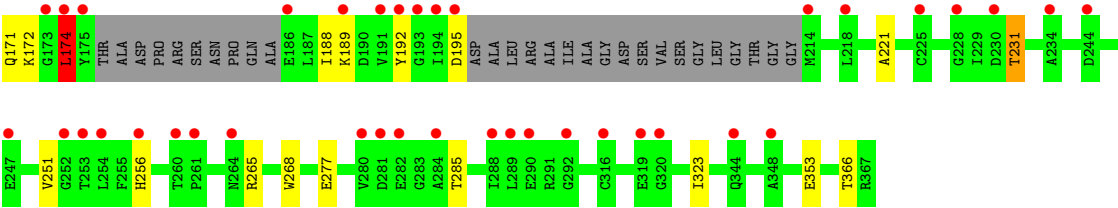


• Molecule 1: GLUTAMATE 5-KINASE



• Molecule 1: GLUTAMATE 5-KINASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.30Å 124.11Å 144.93Å 90.00° 93.96° 90.00°	Depositor
Resolution (Å)	25.00 – 2.90 25.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (25.00-2.90) 99.1 (25.00-2.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.91Å)	Xtrriage
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 ²)	28.2	Xtrriage
Anisotropy	0.841	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	21612	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtrriage'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.*

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: MG, CL, SO4

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	0.63	0/2691	0.83	0/3646
1	B	0.57	0/2696	0.79	0/3653
1	C	0.59	0/2704	0.82	0/3663
1	D	0.61	0/2764	0.82	2/3746 (0.1%)
1	E	0.61	0/2764	0.82	0/3746
1	F	0.63	0/2697	0.83	2/3654 (0.1%)
1	G	0.62	0/2709	0.81	1/3670 (0.0%)
1	H	0.57	0/2575	0.79	0/3485
All	All	0.61	0/21600	0.81	5/29263 (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 (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	182	ASN	CA-C-N	7.42	129.12	119.84
1	F	182	ASN	C-N-CA	7.42	129.12	119.84
1	D	212	GLY	N-CA-C	-6.30	98.24	113.18
1	G	277	GLU	N-CA-C	5.53	117.48	109.07
1	D	103	LEU	N-CA-C	5.16	116.82	109.14

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	20	0
1	B	2661	0	2706	19	0
1	C	2669	0	2710	19	0
1	D	2728	0	2768	30	0
1	E	2728	0	2768	32	0
1	F	2662	0	2708	19	0
1	G	2674	0	2717	22	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

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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	164	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 (164) 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:HE1	1.26	0.98
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:A:108:MET:HE1	1:A:155:LEU:HD13	1.85	0.57
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:195:ASP:C	1:A:197:ALA:H	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:THR:O	1:C:367:ARG:HB2	2.08	0.54
1:H:118:ARG:HG3	1:H:159:LEU:O	2.08	0.53
1:A:322:ASP:OD1	1:A:322:ASP:C	2.51	0.53
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:C:135:GLU:OE1	1:C:146:VAL:N	2.34	0.51
1:E:171:GLN:HE21	1:E:171:GLN:H	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:B:184:GLN:O	1:B:185:ALA:C	2.54	0.50
1:A:197:ALA:C	1:A:199:ARG:H	2.20	0.49
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: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:C:148:ASP:CG	1:C:151:ASN:HD22	2.21	0.48
1:E:265:ARG:CG	1:E:265:ARG:HH11	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:C:171:GLN:HE21	1:C:214:MET:HE3	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:OE1	1:A:143:GLU:N	2.48	0.47
1:D:317:ASN:OD1	1:D:317:ASN:C	2.58	0.46
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:D:74:LEU:C	1:D:74:LEU:HD12	2.40	0.46
1:A:111:ARG:HD2	1:A:268:TRP:CD1	2.51	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: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:F:171:GLN:HE22	1:F:214:MET:HE1	1.82	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:HE21	1:E:171:GLN:N	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:D:231:THR:HG23	1:D:255:PHE:HB2	1.99	0.44
1:E:317:ASN:OD1	1:E:317:ASN:C	2.61	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:A:85:GLN:HG3	1:B:85:GLN:HG3	2.00	0.44
1:B:30:GLU:O	1:B:34:GLN:HG3	2.18	0.44
1:F:188:ILE:O	1:F:253:THR:OG1	2.24	0.44
1:B:49:THR:O	1:B:149:ASN:ND2	2.51	0.43
1:B:157:ALA:HB1	1:B:229:ILE:HD13	2.00	0.43
1:D:103:LEU:CD1	1:D:152:LEU:HD11	2.48	0.43
1:D:14:SER:OG	3:D:1370:SO4:O3	2.26	0.43
1:F:266:LYS:HB2	1:F:269:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:182:ASN:HD22	1:G:182:ASN:C	2.25	0.43
1:G:201:ILE:O	1:G:202:ALA:C	2.61	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
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:F:262:LEU:O	1:F:263:GLU:C	2.63	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:D:143:GLU:N	1:D:143:GLU:CD	2.78	0.42
1:E:69:ILE:HD12	1:E:69:ILE:H	1.84	0.42
1:E:149:ASN:HA	1:E:152:LEU:HB3	2.01	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:74:LEU:HD13	1:F:124:LEU:HD23	2.02	0.42
1:E:103:LEU:CD1	1:E:152:LEU:HD11	2.49	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:C:309:ARG:HG2	1:D:306:ASN:CG	2.45	0.41
1:D:38:LEU:HD11	1:D:242:ILE:HG22	2.02	0.41
1:D:209:LEU:O	1:D:210:GLY:O	2.38	0.41
1:A:221:ALA:O	1:A:225:CYS:SG	2.78	0.41
1:B:108:MET:HE1	1:B:155:LEU:HD13	2.02	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:A:26:ALA:O	1:A:29:VAL:HG12	2.20	0.41
1:A:264:ASN:HA	1:A:267:ARG:CD	2.51	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:A:74:LEU:C	1:A:74:LEU:HD12	2.45	0.41
1:B:149:ASN:HA	1:B:152:LEU:HB3	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:103:LEU:HB3	1:H:139:VAL:HG11	2.02	0.41
1:G:298:LYS:HE3	1:G:342:HIS:HE1	1.86	0.41
1:A:280:VAL:HG13	1:A:284:ALA:CB	2.44	0.41
1:F:90:LEU:O	1:F:93:ILE:HB	2.21	0.41
1:F:277:GLU:HB3	1:F:314:ARG:HB3	2.03	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: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:182:ASN:ND2	1:G:182:ASN:C	2.80	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:C:103:LEU:HB3	1:D:139:VAL:HG11	2.04	0.40
1:D:110:ASP:HB2	1:D:113:ARG:H	1.86	0.40
1:G:85:GLN:NE2	1:H:88:GLU:OE2	2.54	0.40
1:G:108:MET:HE1	1:G:155:LEU:HD13	2.03	0.40
1:B:297:PRO:O	1:B:298:LYS:C	2.65	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%)	36	65
1	B	349/367 (95%)	332 (95%)	14 (4%)	3 (1%)	14	41
1	C	352/367 (96%)	333 (95%)	19 (5%)	0	100	100
1	D	363/367 (99%)	342 (94%)	17 (5%)	4 (1%)	11	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	363/367 (99%)	346 (95%)	15 (4%)	2 (1%)	21	51
1	F	350/367 (95%)	325 (93%)	18 (5%)	7 (2%)	6	22
1	G	352/367 (96%)	333 (95%)	17 (5%)	2 (1%)	21	51
1	H	331/367 (90%)	313 (95%)	16 (5%)	2 (1%)	21	51
All	All	2811/2936 (96%)	2658 (95%)	132 (5%)	21 (1%)	18	48

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%)	253 (92%)	22 (8%)	11	34
1	B	277/285 (97%)	258 (93%)	19 (7%)	14	41
1	C	276/285 (97%)	256 (93%)	20 (7%)	13	39
1	D	283/285 (99%)	265 (94%)	18 (6%)	16	44
1	E	283/285 (99%)	264 (93%)	19 (7%)	15	43
1	F	276/285 (97%)	255 (92%)	21 (8%)	12	36
1	G	277/285 (97%)	259 (94%)	18 (6%)	15	44
1	H	265/285 (93%)	252 (95%)	13 (5%)	22	54
All	All	2212/2280 (97%)	2062 (93%)	150 (7%)	14	42

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	64	GLU
1	A	74	LEU
1	A	82	ARG
1	A	86	LEU
1	A	103	LEU
1	A	135	GLU
1	A	171	GLN
1	A	174	LEU
1	A	180	ARG
1	A	184	GLN
1	A	186	GLU
1	A	195	ASP
1	A	231	THR
1	A	251	VAL
1	A	260	THR
1	A	280	VAL
1	A	282	GLU
1	A	308	SER
1	A	344	GLN
1	A	357	VAL
1	A	366	THR
1	B	21	ARG
1	B	22	ARG
1	B	74	LEU
1	B	83	LEU
1	B	86	LEU

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Mol	Chain	Res	Type
1	B	103	LEU
1	B	121	LEU
1	B	135	GLU
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	277	GLU
1	B	319	GLU
1	B	357	VAL
1	B	366	THR
1	C	33	ARG
1	C	74	LEU
1	C	82	ARG
1	C	83	LEU
1	C	85	GLN
1	C	86	LEU
1	C	103	LEU
1	C	121	LEU
1	C	143	GLU
1	C	172	LYS
1	C	174	LEU
1	C	231	THR
1	C	251	VAL
1	C	260	THR
1	C	280	VAL
1	C	281	ASP
1	C	308	SER
1	C	319	GLU
1	C	353	GLU
1	C	366	THR
1	D	11	LEU
1	D	74	LEU
1	D	85	GLN
1	D	86	LEU
1	D	103	LEU
1	D	135	GLU
1	D	171	GLN
1	D	174	LEU

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Mol	Chain	Res	Type
1	D	207	SER
1	D	216	THR
1	D	251	VAL
1	D	260	THR
1	D	277	GLU
1	D	280	VAL
1	D	321	ARG
1	D	344	GLN
1	D	353	GLU
1	D	366	THR
1	E	64	GLU
1	E	74	LEU
1	E	86	LEU
1	E	103	LEU
1	E	121	LEU
1	E	135	GLU
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	37	GLN
1	F	74	LEU
1	F	85	GLN
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	198	LEU
1	F	231	THR
1	F	251	VAL
1	F	260	THR

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Mol	Chain	Res	Type
1	F	262	LEU
1	F	264	ASN
1	F	280	VAL
1	F	321	ARG
1	F	344	GLN
1	F	353	GLU
1	F	357	VAL
1	F	366	THR
1	G	74	LEU
1	G	82	ARG
1	G	85	GLN
1	G	86	LEU
1	G	103	LEU
1	G	121	LEU
1	G	135	GLU
1	G	171	GLN
1	G	174	LEU
1	G	199	ARG
1	G	231	THR
1	G	251	VAL
1	G	260	THR
1	G	277	GLU
1	G	280	VAL
1	G	319	GLU
1	G	357	VAL
1	G	366	THR
1	H	74	LEU
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	277	GLU
1	H	353	GLU
1	H	366	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	34	GLN
1	A	39	HIS
1	A	85	GLN
1	A	116	ASN
1	A	171	GLN
1	A	219	GLN
1	A	258	GLN
1	A	342	HIS
1	B	5	GLN
1	B	73	GLN
1	B	85	GLN
1	B	182	ASN
1	B	258	GLN
1	C	128	ASN
1	C	171	GLN
1	C	182	ASN
1	C	258	GLN
1	C	331	ASN
1	D	5	GLN
1	D	128	ASN
1	D	171	GLN
1	D	182	ASN
1	D	184	GLN
1	D	331	ASN
1	E	85	GLN
1	E	149	ASN
1	E	171	GLN
1	E	182	ASN
1	E	184	GLN
1	E	219	GLN
1	E	258	GLN
1	E	264	ASN
1	F	5	GLN
1	F	80	GLN
1	F	182	ASN
1	F	331	ASN
1	G	27	HIS
1	G	116	ASN
1	G	127	ASN
1	G	149	ASN
1	G	171	GLN
1	G	182	ASN

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Mol	Chain	Res	Type
1	G	264	ASN
1	G	342	HIS
1	H	73	GLN
1	H	258	GLN
1	H	264	ASN

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 oligosaccharides 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	$\# Z > 2$
2	GLU	B	1371	-	8,9,9	1.07	0	8,11,11	0.90	0
2	GLU	F	1372	-	8,9,9	1.14	0	8,11,11	0.65	0
2	GLU	D	1371	-	8,9,9	1.03	0	8,11,11	1.15	0
3	SO4	C	1370	-	4,4,4	0.25	0	6,6,6	0.31	0
3	SO4	E	1371	-	4,4,4	0.23	0	6,6,6	0.20	0
3	SO4	A	1372	-	4,4,4	0.29	0	6,6,6	0.30	0
3	SO4	B	1370	-	4,4,4	0.26	0	6,6,6	0.23	0
3	SO4	F	1370	-	4,4,4	0.25	0	6,6,6	0.10	0
3	SO4	D	1370	-	4,4,4	0.28	0	6,6,6	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLU	G	1371	-	8,9,9	1.02	0	8,11,11	0.91	0
3	SO4	G	1370	-	4,4,4	0.30	0	6,6,6	0.15	0
2	GLU	E	1373	-	8,9,9	1.07	0	8,11,11	1.13	1 (12%)
2	GLU	E	1372	-	8,9,9	1.03	0	8,11,11	0.84	0
2	GLU	C	1371	-	8,9,9	1.12	0	8,11,11	1.21	1 (12%)
2	GLU	D	1372	-	8,9,9	1.04	0	8,11,11	1.17	1 (12%)
2	GLU	G	1372	-	8,9,9	1.08	0	8,11,11	1.07	0
2	GLU	A	1373	-	8,9,9	1.06	0	8,11,11	1.01	1 (12%)
2	GLU	F	1371	-	8,9,9	1.00	0	8,11,11	0.78	0
3	SO4	H	1369	-	4,4,4	0.25	0	6,6,6	0.09	0
2	GLU	A	1374	-	8,9,9	1.06	0	8,11,11	1.00	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
2	GLU	B	1371	-	-	2/9/9/9	-
2	GLU	D	1372	-	-	0/9/9/9	-
2	GLU	G	1372	-	-	4/9/9/9	-
2	GLU	F	1372	-	-	3/9/9/9	-
2	GLU	D	1371	-	-	3/9/9/9	-
2	GLU	A	1373	-	-	5/9/9/9	-
2	GLU	E	1372	-	-	5/9/9/9	-
2	GLU	F	1371	-	-	4/9/9/9	-
2	GLU	E	1373	-	-	2/9/9/9	-
2	GLU	C	1371	-	-	0/9/9/9	-
2	GLU	A	1374	-	-	5/9/9/9	-
2	GLU	G	1371	-	-	6/9/9/9	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1372	GLU	OE2-CD-CG	2.41	121.60	114.00
2	C	1371	GLU	OE2-CD-CG	2.40	121.58	114.00
2	E	1373	GLU	OE2-CD-CG	2.25	121.11	114.00
2	A	1373	GLU	CB-CA-N	-2.03	104.83	110.12

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1373	GLU	N-CA-CB-CG
2	A	1374	GLU	N-CA-CB-CG
2	E	1372	GLU	C-CA-CB-CG
2	F	1371	GLU	N-CA-CB-CG
2	F	1372	GLU	C-CA-CB-CG
2	G	1371	GLU	N-CA-CB-CG
2	G	1371	GLU	C-CA-CB-CG
2	A	1373	GLU	CA-CB-CG-CD
2	A	1373	GLU	C-CA-CB-CG
2	A	1374	GLU	C-CA-CB-CG
2	F	1371	GLU	C-CA-CB-CG
2	E	1372	GLU	OXT-C-CA-CB
2	E	1372	GLU	N-CA-CB-CG
2	A	1373	GLU	O-C-CA-CB
2	E	1372	GLU	O-C-CA-CB
2	A	1373	GLU	OXT-C-CA-CB
2	D	1371	GLU	O-C-CA-CB
2	D	1371	GLU	OXT-C-CA-CB
2	G	1372	GLU	O-C-CA-N
2	G	1372	GLU	OE2-CD-CG-CB
2	A	1374	GLU	OE1-CD-CG-CB
2	G	1372	GLU	OE1-CD-CG-CB
2	D	1371	GLU	CA-CB-CG-CD
2	A	1374	GLU	OXT-C-CA-N
2	G	1371	GLU	O-C-CA-CB
2	G	1371	GLU	OXT-C-CA-CB
2	F	1371	GLU	OE2-CD-CG-CB
2	A	1374	GLU	OE2-CD-CG-CB
2	B	1371	GLU	OE2-CD-CG-CB
2	F	1372	GLU	OE2-CD-CG-CB
2	F	1371	GLU	OE1-CD-CG-CB
2	E	1373	GLU	OXT-C-CA-N
2	G	1371	GLU	OXT-C-CA-N
2	G	1372	GLU	OXT-C-CA-N
2	F	1372	GLU	OE1-CD-CG-CB
2	B	1371	GLU	OE1-CD-CG-CB
2	E	1372	GLU	OXT-C-CA-N
2	E	1373	GLU	O-C-CA-N
2	G	1371	GLU	O-C-CA-N

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1370	SO4	1	0
2	E	1372	GLU	1	0
2	G	1372	GLU	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 ⓘ

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, 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	355/367 (96%)	0.03	8 (2%) 61 52	19, 25, 32, 54	0
1	B	353/367 (96%)	0.73	29 (8%) 17 14	19, 25, 32, 39	0
1	C	356/367 (97%)	0.29	6 (1%) 69 61	19, 25, 31, 36	0
1	D	365/367 (99%)	0.22	11 (3%) 52 43	17, 25, 31, 36	0
1	E	365/367 (99%)	0.20	9 (2%) 58 48	14, 25, 31, 36	0
1	F	354/367 (96%)	0.33	16 (4%) 38 30	19, 25, 33, 53	0
1	G	356/367 (97%)	0.12	6 (1%) 69 61	8, 25, 33, 57	1 (0%)
1	H	337/367 (91%)	1.15	58 (17%) 4 3	19, 25, 30, 35	0
All	All	2841/2936 (96%)	0.38	143 (5%) 34 27	8, 25, 31, 57	1 (0%)

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	256	HIS	13.2
1	F	197	ALA	6.8
1	H	192	TYR	6.8
1	H	173	GLY	6.1
1	F	202	ALA	5.5
1	B	3	ASP	4.7
1	H	225	CYS	4.6
1	H	69	ILE	4.5
1	B	179	PRO	4.5
1	A	201	ILE	4.4
1	H	194	ILE	4.4
1	H	290	GLU	4.3
1	A	213	GLY	4.2
1	H	244	ASP	4.2
1	B	192	TYR	4.2
1	G	202	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	H	193	GLY	3.8
1	H	175	TYR	3.8
1	H	261	PRO	3.7
1	D	212	GLY	3.7
1	H	64	GLU	3.7
1	E	212	GLY	3.7
1	B	184	GLN	3.7
1	H	3	ASP	3.7
1	G	212	GLY	3.7
1	F	195	ASP	3.6
1	H	282	GLU	3.6
1	F	201	ILE	3.5
1	H	195	ASP	3.4
1	H	174	LEU	3.4
1	F	196	ASP	3.3
1	H	214	MET	3.3
1	F	198	LEU	3.3
1	C	213	GLY	3.3
1	H	320	GLY	3.3
1	B	178	ASP	3.3
1	H	230	ASP	3.3
1	E	211	THR	3.3
1	F	184	GLN	3.2
1	H	260	THR	3.2
1	H	110	ASP	3.2
1	E	213	GLY	3.2
1	H	65	LEU	3.2
1	H	60	LEU	3.1
1	F	200	ALA	3.1
1	C	344	GLN	3.0
1	B	342	HIS	3.0
1	G	213	GLY	2.9
1	H	78	VAL	2.9
1	H	228	GLY	2.9
1	H	191	VAL	2.9
1	H	22	ARG	2.9
1	B	260	THR	2.9
1	C	181	SER	2.8
1	F	178	ASP	2.8
1	C	348	ALA	2.8
1	B	316	CYS	2.8
1	B	290	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	252	GLY	2.7
1	B	183	PRO	2.7
1	D	353	GLU	2.7
1	B	201	ILE	2.6
1	H	55	ALA	2.6
1	F	183	PRO	2.6
1	E	170	ASP	2.6
1	B	177	ALA	2.6
1	H	70	ALA	2.6
1	H	68	THR	2.6
1	C	351	GLY	2.6
1	F	173	GLY	2.6
1	G	201	ILE	2.6
1	B	344	GLN	2.6
1	B	60	LEU	2.6
1	F	214	MET	2.5
1	D	337	ARG	2.5
1	H	344	GLN	2.5
1	H	316	CYS	2.5
1	B	71	SER	2.5
1	B	55	ALA	2.5
1	B	181	SER	2.5
1	H	66	PRO	2.5
1	F	199	ARG	2.5
1	B	74	LEU	2.4
1	A	200	ALA	2.4
1	B	69	ILE	2.4
1	B	180	ARG	2.4
1	D	172	LYS	2.4
1	H	76	ALA	2.4
1	B	350	LEU	2.4
1	D	170	ASP	2.4
1	A	199	ARG	2.4
1	D	143	GLU	2.4
1	H	289	LEU	2.4
1	D	263	GLU	2.4
1	E	319	GLU	2.4
1	H	254	LEU	2.3
1	A	3	ASP	2.3
1	E	143	GLU	2.3
1	H	71	SER	2.3
1	H	256	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	253	THR	2.3
1	G	180	ARG	2.3
1	B	317	ASN	2.3
1	D	282	GLU	2.3
1	B	68	THR	2.3
1	D	213	GLY	2.3
1	H	292	GLY	2.3
1	H	264	ASN	2.2
1	A	194	ILE	2.2
1	H	288	ILE	2.2
1	D	186	GLU	2.2
1	H	281	ASP	2.2
1	B	193	GLY	2.2
1	B	189	LYS	2.2
1	E	69	ILE	2.2
1	E	180	ARG	2.2
1	H	189	LYS	2.2
1	H	77	ALA	2.2
1	B	66	PRO	2.2
1	H	163	ASP	2.2
1	B	62	TYR	2.2
1	B	65	LEU	2.2
1	F	179	PRO	2.1
1	H	284	ALA	2.1
1	H	186	GLU	2.1
1	H	319	GLU	2.1
1	E	184	GLN	2.1
1	A	195	ASP	2.1
1	C	292	GLY	2.1
1	F	321	ARG	2.1
1	H	67	ALA	2.1
1	H	234	ALA	2.1
1	A	143	GLU	2.1
1	H	218	LEU	2.1
1	H	21	ARG	2.1
1	F	282	GLU	2.1
1	H	247	GLU	2.1
1	H	81	SER	2.0
1	H	348	ALA	2.0
1	B	78	VAL	2.0
1	H	280	VAL	2.0
1	D	210	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	41	ALA	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	E	1377	1/1	0.56	0.40	67,67,67,67	0
3	SO4	H	1369	5/5	0.71	0.18	80,80,81,81	0
2	GLU	F	1371	10/10	0.75	0.18	50,50,51,51	0
5	MG	H	1371	1/1	0.75	0.28	57,57,57,57	0
5	MG	F	1375	1/1	0.77	0.27	49,49,49,49	0
5	MG	G	1376	1/1	0.79	0.22	46,46,46,46	0
2	GLU	D	1371	10/10	0.79	0.16	28,29,29,29	0
2	GLU	B	1371	10/10	0.80	0.16	46,46,47,48	0
2	GLU	E	1373	10/10	0.81	0.18	39,39,42,43	0
4	CL	E	1375	1/1	0.81	0.10	50,50,50,50	0
2	GLU	C	1371	10/10	0.81	0.16	33,34,35,35	0
2	GLU	E	1372	10/10	0.83	0.15	29,30,31,32	0
2	GLU	A	1374	10/10	0.86	0.17	39,40,41,41	0
2	GLU	F	1372	10/10	0.87	0.16	35,36,36,36	0
4	CL	F	1373	1/1	0.87	0.10	44,44,44,44	0
4	CL	F	1374	1/1	0.87	0.07	40,40,40,40	0
5	MG	B	1375	1/1	0.87	0.18	43,43,43,43	0
3	SO4	D	1370	5/5	0.87	0.16	55,56,56,57	0
3	SO4	F	1370	5/5	0.87	0.17	59,59,60,60	0
2	GLU	D	1372	10/10	0.87	0.14	34,35,35,35	0
4	CL	B	1374	1/1	0.87	0.11	37,37,37,37	0
2	GLU	G	1372	10/10	0.88	0.14	30,31,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	E	1371	5/5	0.89	0.18	71,72,72,72	0
3	SO4	B	1370	5/5	0.89	0.16	65,66,66,66	0
4	CL	A	1377	1/1	0.90	0.12	34,34,34,34	0
4	CL	E	1374	1/1	0.90	0.15	37,37,37,37	0
2	GLU	G	1371	10/10	0.91	0.13	19,20,22,23	0
4	CL	B	1372	1/1	0.91	0.07	49,49,49,49	0
3	SO4	C	1370	5/5	0.91	0.16	70,70,70,70	0
4	CL	C	1374	1/1	0.91	0.12	36,36,36,36	0
4	CL	H	1370	1/1	0.91	0.17	46,46,46,46	0
4	CL	D	1374	1/1	0.93	0.11	33,33,33,33	0
5	MG	A	1378	1/1	0.93	0.12	26,26,26,26	0
4	CL	E	1376	1/1	0.93	0.07	27,27,27,27	0
5	MG	E	1370	1/1	0.93	0.08	17,17,17,17	0
2	GLU	A	1373	10/10	0.94	0.12	12,13,14,15	0
4	CL	G	1374	1/1	0.94	0.08	35,35,35,35	0
4	CL	A	1376	1/1	0.95	0.11	25,25,25,25	0
4	CL	A	1375	1/1	0.96	0.09	34,34,34,34	0
5	MG	D	1369	1/1	0.96	0.08	18,18,18,18	0
4	CL	G	1373	1/1	0.96	0.07	32,32,32,32	0
4	CL	C	1372	1/1	0.96	0.09	24,24,24,24	0
4	CL	G	1375	1/1	0.96	0.17	39,39,39,39	0
3	SO4	G	1370	5/5	0.96	0.14	36,36,37,37	0
4	CL	B	1373	1/1	0.96	0.10	30,30,30,30	0
3	SO4	A	1372	5/5	0.97	0.12	36,38,38,38	0
4	CL	D	1373	1/1	0.98	0.11	18,18,18,18	0
4	CL	C	1373	1/1	0.99	0.09	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.