



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 17, 2021 – 04:06 pm GMT

PDB ID : 7Q5T  
Title : The tandem SH2 domains of SYK with a bound FCER1G diphospho-ITAM peptide  
Authors : Bradshaw, W.J.; Katis, V.L.; Chen, Z.; Bountra, C.; von Delft, F.; Gileadi, O.; Brennan, P.E.  
Deposited on : 2021-11-04  
Resolution : 2.20 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.

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

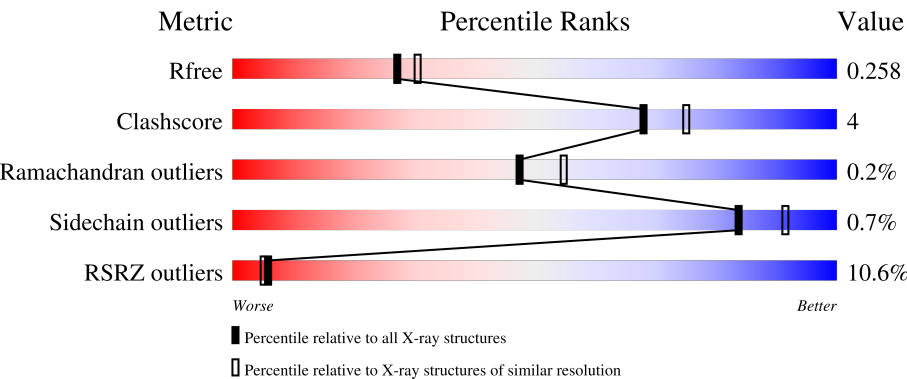
MolProbity : 4.02b-467  
Mogul : 1.8.4 (270009), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 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	AAA	265	<div><div>2%</div><div>89%</div><div>6%</div><div>.</div><div>.</div></div>
1	BBB	265	<div><div>%</div><div>91%</div><div>6%</div><div>.</div></div>
1	CCC	265	<div><div>3%</div><div>90%</div><div>9%</div><div>.</div></div>
1	DDD	265	<div><div>10%</div><div>85%</div><div>9%</div><div>6%</div></div>
1	EEE	265	<div><div>16%</div><div>91%</div><div>5%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
1	FFF	265	
2	GGG	20	
2	HHH	20	
2	III	20	
2	JJJ	20	
2	KKK	20	
2	LLL	20	

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
3	PO4	DDD	303	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13506 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 Tyrosine-protein kinase SYK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	255	Total	C	N	O	S	0	0	0
			2040	1295	365	374	6			
1	BBB	257	Total	C	N	O	S	0	0	0
			2051	1301	367	377	6			
1	CCC	261	Total	C	N	O	S	0	3	0
			2098	1329	377	386	6			
1	DDD	250	Total	C	N	O	S	0	0	0
			2000	1272	358	364	6			
1	EEE	254	Total	C	N	O	S	0	0	0
			2032	1291	364	371	6			
1	FFF	247	Total	C	N	O	S	0	0	0
			1970	1250	353	361	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	5	SER	-	expression tag	UNP P43405
BBB	5	SER	-	expression tag	UNP P43405
CCC	5	SER	-	expression tag	UNP P43405
DDD	5	SER	-	expression tag	UNP P43405
EEE	5	SER	-	expression tag	UNP P43405
FFF	5	SER	-	expression tag	UNP P43405

- Molecule 2 is a protein called High affinity immunoglobulin epsilon receptor subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	GGG	18	Total	C	N	O	P	0	0	0
			152	89	24	37	2			
2	HHH	18	Total	C	N	O	P	0	0	0
			152	89	24	37	2			
2	III	19	Total	C	N	O	P	0	0	0
			163	95	27	39	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	JJJ	17	Total	C	N	O	P	0	0	0
			148	87	23	36	2			
2	KKK	19	Total	C	N	O	P	0	0	0
			163	95	27	39	2			
2	LLL	15	Total	C	N	O	P	0	0	0
			132	76	20	34	2			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	O	P	0	0
			5	4	1		
3	AAA	1	Total	O	P	0	0
			5	4	1		
3	BBB	1	Total	O	P	0	0
			5	4	1		
3	BBB	1	Total	O	P	0	0
			5	4	1		
3	CCC	1	Total	O	P	0	0
			5	4	1		
3	CCC	1	Total	O	P	0	0
			5	4	1		
3	DDD	1	Total	O	P	0	0
			5	4	1		
3	DDD	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	DDD	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			4	2	2		
4	CCC	1	Total	C	O	0	0
			4	2	2		
4	CCC	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	BBB	1	Total	C	O	0	0
			7	4	3		
5	EEE	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	96	Total	O	0	0
			96	96		
6	BBB	101	Total	O	0	0
			101	101		
6	CCC	59	Total	O	0	0
			59	59		
6	DDD	24	Total	O	0	0
			24	24		
6	EEE	10	Total	O	0	0
			10	10		
6	FFF	4	Total	O	0	0
			4	4		
6	GGG	5	Total	O	0	0
			5	5		
6	HHH	7	Total	O	0	0
			7	7		
6	III	5	Total	O	0	0
			5	5		
6	JJJ	12	Total	O	0	0
			12	12		

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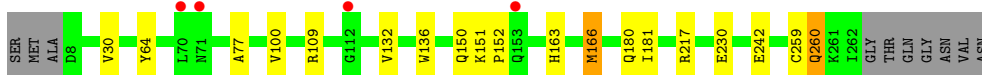
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	KKK	10	Total 10	O 10	0	0
6	LLL	1	Total 1	O 1	0	0



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

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Tyrosine-protein kinase SYK



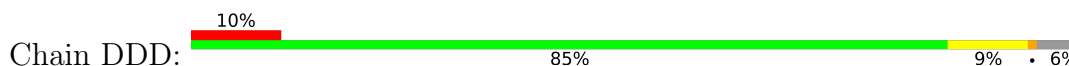
- Molecule 1: Tyrosine-protein kinase SYK



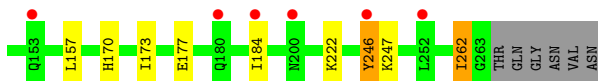
- Molecule 1: Tyrosine-protein kinase SYK

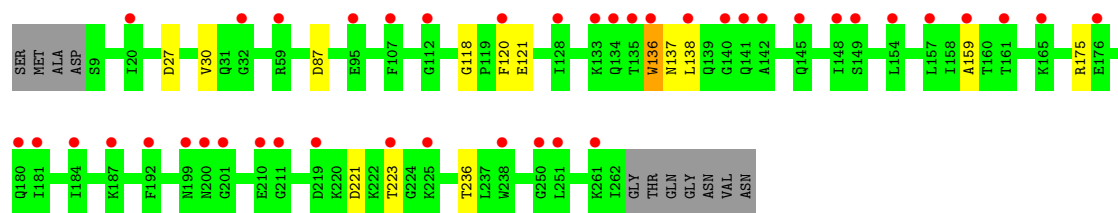


- Molecule 1: Tyrosine-protein kinase SYK

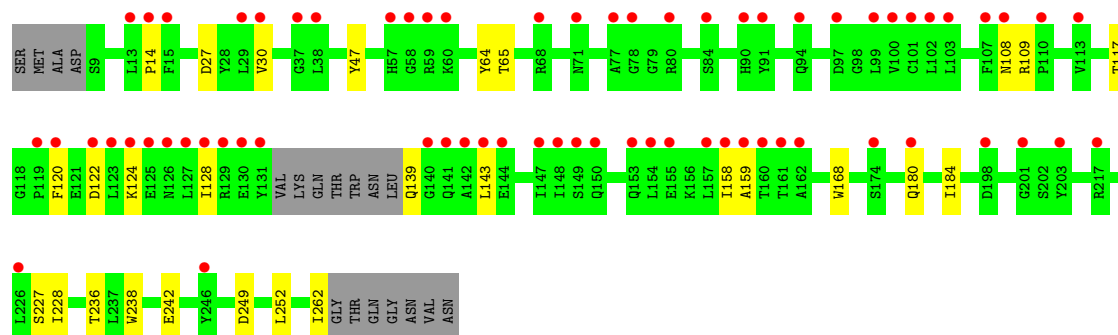
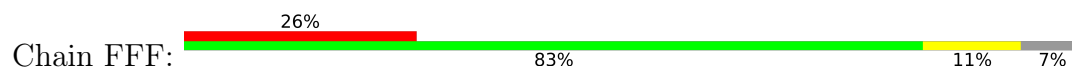


- Molecule 1: Tyrosine-protein kinase SYK

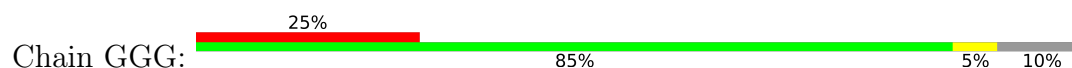




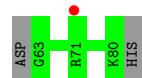
• Molecule 1: Tyrosine-protein kinase SYK



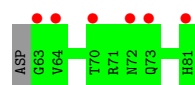
• Molecule 2: High affinity immunoglobulin epsilon receptor subunit gamma



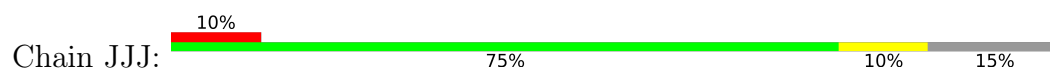
• Molecule 2: High affinity immunoglobulin epsilon receptor subunit gamma



• Molecule 2: High affinity immunoglobulin epsilon receptor subunit gamma

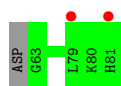


• Molecule 2: High affinity immunoglobulin epsilon receptor subunit gamma



- Molecule 2: High affinity immunoglobulin epsilon receptor subunit gamma

Chain KKK: 



- Molecule 2: High affinity immunoglobulin epsilon receptor subunit gamma

Chain LLL: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.14Å 88.03Å 158.49Å 90.00° 113.58° 90.00°	Depositor
Resolution (Å)	73.26 – 2.20 73.26 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.3 (73.26-2.20) 98.3 (73.26-2.20)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.207 , 0.255 0.212 , 0.258	Depositor DCC
$R_{free}$ test set	1981 reflections (2.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.6	Xtrriage
Anisotropy	0.465	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13506	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, PEG, PO4, PTR

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	AAA	0.72	1/2087 (0.0%)	0.84	1/2815 (0.0%)
1	BBB	0.70	0/2098	0.82	0/2830
1	CCC	0.69	0/2155	0.81	0/2906
1	DDD	0.67	0/2046	0.82	0/2758
1	EEE	0.67	0/2079	0.81	1/2804 (0.0%)
1	FFF	0.65	0/2014	0.79	1/2713 (0.0%)
2	GGG	0.75	0/117	0.83	0/153
2	HHH	0.81	0/117	0.95	0/153
2	III	0.75	0/129	0.78	0/168
2	JJJ	0.72	0/113	0.79	0/148
2	KKK	0.83	0/129	1.00	0/168
2	LLL	0.62	0/98	0.86	0/130
All	All	0.69	1/13182 (0.0%)	0.82	3/17746 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	242	GLU	CD-OE1	5.67	1.31	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	109	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	EEE	175	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	FFF	109	ARG	NE-CZ-NH2	-5.24	117.68	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	AAA	2040	0	2028	12	0
1	BBB	2051	0	2038	12	0
1	CCC	2098	0	2085	18	0
1	DDD	2000	0	1991	26	0
1	EEE	2032	0	2024	12	0
1	FFF	1970	0	1959	21	0
2	GGG	152	0	135	2	0
2	HHH	152	0	135	0	0
2	III	163	0	142	0	0
2	JJJ	148	0	132	1	0
2	KKK	163	0	142	0	0
2	LLL	132	0	113	3	0
3	AAA	10	0	0	0	0
3	BBB	10	0	0	0	0
3	CCC	10	0	0	0	0
3	DDD	15	0	0	0	0
4	AAA	4	0	6	0	0
4	CCC	8	0	12	0	0
5	BBB	7	0	10	2	0
5	EEE	7	0	10	1	0
6	AAA	96	0	0	1	0
6	BBB	101	0	0	1	0
6	CCC	59	0	0	1	0
6	DDD	24	0	0	1	0
6	EEE	10	0	0	0	0
6	FFF	4	0	0	0	0
6	GGG	5	0	0	0	0
6	HHH	7	0	0	1	0
6	III	5	0	0	0	0
6	JJJ	12	0	0	0	0
6	KKK	10	0	0	0	0
6	LLL	1	0	0	0	0
All	All	13506	0	12962	98	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 (98) 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:FFF:64:TYR:CE1	2:LLL:77:GLU:HB3	2.18	0.78
1:DDD:117:THR:HG23	1:DDD:121:GLU:HB3	1.69	0.75
1:DDD:184:ILE:HD12	1:EEE:30:VAL:CG1	2.17	0.75
1:AAA:260:GLN:OE1	1:AAA:260:GLN:HA	1.88	0.74
1:EEE:120:PHE:CD1	1:EEE:121:GLU:N	2.57	0.73
1:FFF:159:ALA:HB1	1:FFF:236:THR:HG21	1.75	0.68
1:BBB:126:ASN:HB2	6:BBB:482:HOH:O	1.94	0.67
1:EEE:136:TRP:O	1:EEE:138:LEU:N	2.28	0.66
1:BBB:181:ILE:HG22	1:BBB:259:CYS:SG	2.37	0.65
1:AAA:64:TYR:OH	1:AAA:100:VAL:HG13	1.98	0.64
1:AAA:181:ILE:HG22	1:AAA:259:CYS:SG	2.38	0.64
1:DDD:82:HIS:CE1	1:DDD:88:LEU:CD2	2.81	0.63
1:FFF:249:ASP:OD1	2:LLL:71:ARG:HB2	1.99	0.62
1:DDD:117:THR:HG23	1:DDD:121:GLU:CB	2.30	0.61
1:EEE:120:PHE:CG	1:EEE:121:GLU:N	2.68	0.61
1:EEE:159:ALA:HB1	1:EEE:236:THR:HG21	1.81	0.60
1:DDD:53:LEU:CD1	1:DDD:55:VAL:CG2	2.80	0.60
1:DDD:134:GLN:OE1	1:DDD:134:GLN:HA	2.03	0.59
1:DDD:82:HIS:CE1	1:DDD:88:LEU:HD22	2.38	0.59
1:DDD:184:ILE:HD12	1:EEE:30:VAL:HG12	1.84	0.58
1:CCC:216:TYR:OH	1:CCC:252:LEU:HD13	2.04	0.57
1:DDD:53:LEU:HD13	1:DDD:55:VAL:CG2	2.35	0.56
1:BBB:68:ARG:NH1	1:BBB:72:GLY:O	2.39	0.56
1:FFF:159:ALA:HB1	1:FFF:236:THR:CG2	2.36	0.55
1:DDD:143:LEU:O	1:DDD:147:ILE:HG12	2.05	0.55
1:FFF:139:GLN:HB2	1:FFF:143:LEU:HG	1.88	0.55
1:FFF:128:ILE:HG12	1:FFF:158:ILE:HD13	1.89	0.55
1:DDD:82:HIS:ND1	1:DDD:88:LEU:HD23	2.22	0.54
1:DDD:173:ILE:HG23	1:DDD:177:GLU:HB2	1.89	0.54
1:BBB:68:ARG:HG3	1:BBB:68:ARG:HH11	1.72	0.54
1:FFF:14:PRO:HB2	1:FFF:108:ASN:ND2	2.23	0.53
1:DDD:82:HIS:CE1	1:DDD:88:LEU:HD23	2.44	0.53
1:FFF:117:THR:HG21	1:FFF:122:ASP:OD1	2.09	0.53
1:AAA:77:ALA:HA	1:CCC:268:VAL:HB	1.90	0.52
1:DDD:170:HIS:O	1:DDD:173:ILE:HD13	2.10	0.52
1:EEE:118:GLY:HA3	1:EEE:120:PHE:CE2	2.45	0.52
1:FFF:27:ASP:O	1:FFF:30:VAL:HG12	2.11	0.51
1:CCC:172:LYS:O	1:CCC:265:GLN:HG2	2.11	0.51
1:FFF:120:PHE:CD1	1:FFF:242:GLU:HG3	2.46	0.50
1:AAA:132:VAL:O	1:AAA:136:TRP:HB2	2.12	0.50
1:AAA:181:ILE:CG2	1:AAA:259:CYS:SG	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EEE:87:ASP:HB3	5:EEE:301:PEG:H11	1.93	0.50
1:CCC:261:LYS:HB2	1:CCC:263:GLY:O	2.13	0.49
1:CCC:128:ILE:CG1	1:CCC:158:ILE:HD13	2.43	0.48
1:CCC:252:LEU:CD1	6:HHH:101:HOH:O	2.60	0.48
1:FFF:120:PHE:CD1	1:FFF:242:GLU:CG	2.96	0.48
1:BBB:219:ASP:OD2	1:DDD:222:LYS:HG3	2.14	0.48
1:BBB:27:ASP:HB3	5:BBB:303:PEG:H22	1.95	0.47
1:EEE:120:PHE:CE1	1:EEE:121:GLU:HB2	2.48	0.47
1:AAA:230:GLU:HB2	2:GGG:70:THR:HG21	1.97	0.47
1:FFF:139:GLN:CB	1:FFF:143:LEU:HG	2.45	0.47
1:DDD:45:ARG:HD2	6:DDD:405:HOH:O	2.15	0.47
1:FFF:117:THR:CG2	1:FFF:122:ASP:OD1	2.63	0.47
1:AAA:230:GLU:HG3	2:GGG:70:THR:HB	1.97	0.46
1:DDD:133:LYS:O	1:DDD:137:ASN:HA	2.16	0.46
1:FFF:180:GLN:O	1:FFF:184:ILE:HG12	2.15	0.46
1:CCC:170:HIS:CE1	1:CCC:261:LYS:HA	2.50	0.46
1:DDD:117:THR:CG2	1:DDD:122:ASP:OD1	2.64	0.46
1:AAA:163:HIS:HA	1:AAA:166:MET:HG3	1.96	0.46
1:CCC:180:GLN:O	1:CCC:184:ILE:HG12	2.16	0.46
1:CCC:214:LEU:HD13	1:CCC:252:LEU:HD22	1.97	0.46
1:BBB:132:VAL:CG1	1:BBB:143:LEU:HD12	2.46	0.45
1:DDD:246:TYR:CZ	1:DDD:247:LYS:HD2	2.51	0.45
1:DDD:53:LEU:HD13	1:DDD:55:VAL:HG23	1.97	0.45
1:CCC:128:ILE:HG12	1:CCC:158:ILE:HD13	1.99	0.45
1:AAA:30:VAL:HG23	6:AAA:425:HOH:O	2.17	0.45
1:DDD:88:LEU:C	1:DDD:88:LEU:HD13	2.38	0.44
2:JJJ:70:THR:HG22	2:JJJ:71:ARG:O	2.17	0.44
1:CCC:214:LEU:CD1	1:CCC:252:LEU:HD22	2.47	0.44
1:CCC:221:ASP:OD2	1:CCC:233:LYS:HE3	2.17	0.44
1:CCC:82:HIS:HE1	6:CCC:409:HOH:O	2.01	0.44
1:BBB:222:LYS:HA	1:BBB:222:LYS:HD3	1.78	0.44
1:CCC:182:VAL:O	1:CCC:191:LYS:HE2	2.18	0.44
1:FFF:124:LYS:CE	1:FFF:158:ILE:HG22	2.48	0.43
1:BBB:180:GLN:O	1:BBB:184:ILE:HG12	2.18	0.43
1:EEE:159:ALA:HB1	1:EEE:236:THR:CG2	2.47	0.43
1:FFF:120:PHE:HE2	1:FFF:168:TRP:HE1	1.66	0.43
1:FFF:227:SER:OG	1:FFF:228:ILE:O	2.34	0.43
1:FFF:64:TYR:CD1	2:LLL:77:GLU:HB3	2.53	0.42
1:CCC:151:LYS:O	1:CCC:155:GLU:HG2	2.18	0.42
1:DDD:53:LEU:CD1	1:DDD:55:VAL:HG22	2.49	0.42
1:FFF:120:PHE:CD2	1:FFF:238:TRP:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:181:ILE:CG2	1:BBB:259:CYS:SG	3.08	0.41
1:CCC:154:LEU:HB3	1:CCC:158:ILE:HD12	2.02	0.41
1:CCC:151:LYS:HB3	1:CCC:152:PRO:HD3	2.02	0.41
1:FFF:252:LEU:HD23	1:FFF:252:LEU:HA	1.96	0.41
1:AAA:136:TRP:CZ2	1:AAA:150:GLN:HG3	2.56	0.41
1:FFF:47:TYR:CD1	1:FFF:65:THR:HG21	2.56	0.41
1:EEE:27:ASP:O	1:EEE:30:VAL:HG22	2.21	0.41
1:CCC:268:VAL:O	1:CCC:269:ASN:HB2	2.21	0.41
1:EEE:221:ASP:OD1	1:EEE:223:THR:OG1	2.31	0.41
1:DDD:134:GLN:OE1	1:DDD:134:GLN:CA	2.68	0.41
1:BBB:151:LYS:HB3	1:BBB:152:PRO:HD3	2.03	0.40
1:BBB:28:TYR:CZ	5:BBB:303:PEG:H32	2.56	0.40
1:DDD:27:ASP:O	1:DDD:30:VAL:HG22	2.21	0.40
1:DDD:130:GLU:OE2	1:DDD:134:GLN:NE2	2.54	0.40
1:AAA:151:LYS:N	1:AAA:152:PRO:HD2	2.37	0.40
1:DDD:262:ILE:O	1:DDD:262:ILE:CG2	2.69	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	AAA	253/265 (96%)	250 (99%)	3 (1%)	0	100	100
1	BBB	255/265 (96%)	252 (99%)	2 (1%)	1 (0%)	34	37
1	CCC	262/265 (99%)	259 (99%)	3 (1%)	0	100	100
1	DDD	246/265 (93%)	243 (99%)	2 (1%)	1 (0%)	34	37
1	EEE	252/265 (95%)	248 (98%)	3 (1%)	1 (0%)	34	37
1	FFF	243/265 (92%)	241 (99%)	2 (1%)	0	100	100
2	GGG	14/20 (70%)	12 (86%)	2 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	HHH	14/20 (70%)	14 (100%)	0	0	100	100
2	III	15/20 (75%)	13 (87%)	2 (13%)	0	100	100
2	JJJ	13/20 (65%)	13 (100%)	0	0	100	100
2	KKK	15/20 (75%)	14 (93%)	1 (7%)	0	100	100
2	LLL	12/20 (60%)	11 (92%)	1 (8%)	0	100	100
All	All	1594/1710 (93%)	1570 (98%)	21 (1%)	3 (0%)	47	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	9	SER
1	EEE	137	ASN
1	DDD	262	ILE

### 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	AAA	217/224 (97%)	213 (98%)	4 (2%)	59	72
1	BBB	218/224 (97%)	218 (100%)	0	100	100
1	CCC	224/224 (100%)	224 (100%)	0	100	100
1	DDD	212/224 (95%)	208 (98%)	4 (2%)	57	71
1	EEE	216/224 (96%)	215 (100%)	1 (0%)	88	94
1	FFF	209/224 (93%)	208 (100%)	1 (0%)	88	94
2	GGG	14/16 (88%)	14 (100%)	0	100	100
2	HHH	14/16 (88%)	14 (100%)	0	100	100
2	III	15/16 (94%)	15 (100%)	0	100	100
2	JJJ	14/16 (88%)	14 (100%)	0	100	100
2	KKK	15/16 (94%)	15 (100%)	0	100	100
2	LLL	12/16 (75%)	12 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1380/1440 (96%)	1370 (99%)	10 (1%)	84	91

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	166	MET
1	AAA	180	GLN
1	AAA	217	ARG
1	AAA	260	GLN
1	DDD	104	LYS
1	DDD	134	GLN
1	DDD	157	LEU
1	DDD	246	TYR
1	EEE	136	TRP
1	FFF	262	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

14 ligands are modelled in this entry.

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.

No monomer is involved in short contacts.

## 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	AAA	255/265 (96%)	0.37	4 (1%) 72 70	33, 45, 71, 105	0
1	BBB	257/265 (96%)	0.32	3 (1%) 79 77	33, 46, 76, 129	0
1	CCC	261/265 (98%)	0.39	7 (2%) 54 52	35, 52, 76, 122	0
1	DDD	250/265 (94%)	0.80	27 (10%) 5 5	42, 64, 118, 157	0
1	EEE	254/265 (95%)	1.11	42 (16%) 1 1	45, 75, 123, 156	0
1	FFF	247/265 (93%)	1.59	68 (27%) 0 0	50, 89, 152, 185	0
2	GGG	16/20 (80%)	1.63	5 (31%) 0 0	66, 84, 116, 126	0
2	HHH	16/20 (80%)	0.67	1 (6%) 20 19	45, 74, 106, 129	0
2	III	17/20 (85%)	1.17	6 (35%) 0 0	49, 70, 98, 118	0
2	JJJ	15/20 (75%)	0.84	2 (13%) 3 3	43, 60, 115, 123	0
2	KKK	17/20 (85%)	0.72	2 (11%) 4 4	41, 64, 99, 127	0
2	LLL	13/20 (65%)	1.49	4 (30%) 0 0	60, 103, 132, 134	0
All	All	1618/1710 (94%)	0.77	171 (10%) 6 5	33, 59, 123, 185	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	FFF	153	GLN	11.1
1	DDD	147	ILE	10.8
1	DDD	143	LEU	9.6
1	FFF	154	LEU	8.4
1	FFF	140	GLY	8.3
1	FFF	143	LEU	7.9
1	FFF	142	ALA	7.5
1	FFF	100	VAL	7.4
1	DDD	142	ALA	7.3
1	FFF	120	PHE	7.3
1	EEE	141	GLN	7.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	III	63	GLY	7.1
1	FFF	58	GLY	7.0
1	FFF	103	LEU	7.0
1	DDD	153	GLN	6.8
1	FFF	38	LEU	6.7
1	FFF	127	LEU	6.7
1	EEE	200	ASN	6.7
1	DDD	148	ILE	6.0
1	EEE	142	ALA	5.9
1	CCC	268	VAL	5.5
1	FFF	129	ARG	5.5
1	FFF	78	GLY	5.4
1	DDD	134	GLN	5.3
1	FFF	162	ALA	5.3
1	EEE	148	ILE	5.3
1	EEE	145	GLN	5.2
1	EEE	201	GLY	5.1
1	EEE	187	LYS	5.1
1	EEE	140	GLY	5.0
1	FFF	102	LEU	4.9
1	FFF	59	ARG	4.9
1	FFF	158	ILE	4.9
2	GGG	73	GLN	4.8
1	EEE	136	TRP	4.8
1	FFF	131	TYR	4.8
1	FFF	107	PHE	4.7
1	FFF	99	LEU	4.7
1	FFF	141	GLN	4.5
2	JJJ	72	ASN	4.5
1	EEE	165	LYS	4.5
2	HHH	71	ARG	4.4
1	DDD	184	ILE	4.3
1	FFF	148	ILE	4.3
1	EEE	180	GLN	4.2
1	FFF	97	ASP	4.2
2	LLL	72	ASN	4.2
2	LLL	70	THR	4.2
2	KKK	81	HIS	4.2
1	FFF	37	GLY	4.1
1	FFF	124	LYS	4.1
1	FFF	198	ASP	4.1
1	EEE	112	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	FFF	60	LYS	4.1
2	JJJ	73	GLN	4.1
1	FFF	149	SER	4.1
1	DDD	135	THR	4.0
2	GGG	67	GLY	4.0
1	FFF	119	PRO	4.0
1	EEE	211	GLY	4.0
1	FFF	160	THR	4.0
1	FFF	101	CYS	3.9
2	LLL	71	ARG	3.9
1	FFF	125	GLU	3.9
1	FFF	84	SER	3.9
1	CCC	198	ASP	3.9
1	DDD	146	ALA	3.9
1	BBB	199	ASN	3.8
1	FFF	147	ILE	3.8
1	EEE	107	PHE	3.7
1	EEE	128	ILE	3.7
1	EEE	199	ASN	3.7
1	EEE	138	LEU	3.7
1	FFF	159	ALA	3.7
1	DDD	200	ASN	3.7
1	EEE	210	GLU	3.6
1	FFF	150	GLN	3.6
1	FFF	123	LEU	3.6
1	EEE	159	ALA	3.5
1	DDD	127	LEU	3.5
1	EEE	157	LEU	3.5
1	EEE	219	ASP	3.5
1	BBB	8	ASP	3.4
1	BBB	78	GLY	3.4
1	FFF	77	ALA	3.4
1	FFF	126	ASN	3.3
1	DDD	149	SER	3.3
1	DDD	124	LYS	3.3
1	DDD	132	VAL	3.3
1	FFF	71	ASN	3.2
1	EEE	184	ILE	3.2
1	DDD	10	ALA	3.2
2	III	73	GLN	3.2
1	FFF	80	ARG	3.2
1	EEE	223	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	EEE	225	LYS	3.1
1	FFF	128	ILE	3.1
1	FFF	155	GLU	3.1
1	EEE	238	TRP	3.0
1	EEE	250	GLY	3.0
1	FFF	217	ARG	2.9
1	DDD	102	LEU	2.9
1	FFF	226	LEU	2.9
1	FFF	203	TYR	2.9
1	FFF	91	TYR	2.9
1	DDD	123	LEU	2.8
1	DDD	136	TRP	2.8
1	DDD	246	TYR	2.8
1	FFF	130	GLU	2.8
1	EEE	135	THR	2.8
1	FFF	57	HIS	2.8
1	FFF	122	ASP	2.8
1	FFF	94	GLN	2.7
2	GGG	63	GLY	2.7
1	DDD	104	LYS	2.7
1	EEE	133	LYS	2.7
1	FFF	30	VAL	2.7
1	FFF	108	ASN	2.7
1	FFF	68	ARG	2.7
1	FFF	180	GLN	2.7
1	EEE	120	PHE	2.6
2	KKK	79	LEU	2.6
1	DDD	59	ARG	2.5
1	DDD	252	LEU	2.5
1	EEE	32	GLY	2.5
1	CCC	128	ILE	2.5
1	DDD	126	ASN	2.5
1	EEE	149	SER	2.5
1	FFF	13	LEU	2.5
1	CCC	269	ASN	2.5
1	EEE	161	THR	2.5
1	AAA	112	GLY	2.5
1	EEE	176	GLU	2.4
1	EEE	154	LEU	2.4
1	FFF	110	PRO	2.4
1	EEE	134	GLN	2.4
1	FFF	157	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	III	64	VAL	2.4
1	FFF	161	THR	2.3
1	EEE	192	PHE	2.3
2	GGG	71	ARG	2.3
2	III	72	ASN	2.3
2	III	70	THR	2.3
1	AAA	70	LEU	2.2
1	DDD	144	GLU	2.2
1	AAA	153	GLN	2.2
1	FFF	113	VAL	2.2
2	III	81	HIS	2.2
1	EEE	59	ARG	2.2
1	FFF	174	SER	2.2
1	EEE	95	GLU	2.2
1	FFF	90	HIS	2.2
1	CCC	70	LEU	2.2
1	FFF	14	PRO	2.2
2	GGG	80	LYS	2.1
1	DDD	129	ARG	2.1
2	LLL	73	GLN	2.1
1	AAA	71	ASN	2.1
1	EEE	251	LEU	2.1
1	FFF	246	TYR	2.1
1	CCC	267	ASN	2.1
1	FFF	201	GLY	2.1
1	CCC	9	SER	2.1
1	EEE	261	LYS	2.1
1	FFF	15	PHE	2.1
1	DDD	180	GLN	2.1
1	FFF	144	GLU	2.1
1	EEE	20	ILE	2.0
1	EEE	181	ILE	2.0
1	FFF	29	LEU	2.0
1	DDD	35	SER	2.0

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

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( $\text{\AA}^2$ )	Q<0.9
2	PTR	LLL	65	16/17	0.88	0.15	76,88,105,113	0
2	PTR	GGG	65	16/17	0.89	0.13	70,81,90,92	0
2	PTR	LLL	76	16/17	0.91	0.17	59,72,79,80	0
2	PTR	GGG	76	16/17	0.93	0.13	45,60,74,78	0
2	PTR	III	65	16/17	0.93	0.14	50,56,62,64	0
2	PTR	JJJ	65	16/17	0.94	0.13	35,46,50,52	0
2	PTR	III	76	16/17	0.95	0.11	49,52,59,64	0
2	PTR	HHH	65	16/17	0.95	0.16	52,61,66,68	0
2	PTR	KKK	76	16/17	0.96	0.13	34,41,51,52	0
2	PTR	HHH	76	16/17	0.96	0.14	33,40,48,49	0
2	PTR	JJJ	76	16/17	0.96	0.15	33,38,45,46	0
2	PTR	KKK	65	16/17	0.97	0.15	37,46,51,53	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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( $\text{\AA}^2$ )	Q<0.9
5	PEG	EEE	301	7/7	0.46	0.36	82,92,110,115	0
3	PO4	DDD	303	5/5	0.64	0.43	110,122,129,149	0
3	PO4	AAA	302	5/5	0.68	0.21	112,132,135,140	0
4	EDO	CCC	304	4/4	0.71	0.24	61,68,69,71	0
4	EDO	AAA	303	4/4	0.75	0.30	67,72,74,75	0
4	EDO	CCC	303	4/4	0.76	0.22	63,63,67,71	0
5	PEG	BBB	303	7/7	0.77	0.23	63,68,70,71	0
3	PO4	CCC	301	5/5	0.77	0.22	73,83,90,95	0
3	PO4	CCC	302	5/5	0.78	0.36	82,90,114,115	0
3	PO4	BBB	302	5/5	0.80	0.19	81,84,96,98	0
3	PO4	DDD	302	5/5	0.87	0.16	87,89,103,104	0
3	PO4	BBB	301	5/5	0.88	0.13	63,80,92,94	0
3	PO4	DDD	301	5/5	0.89	0.12	72,79,89,93	0
3	PO4	AAA	301	5/5	0.92	0.10	81,90,102,103	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.