



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 17, 2021 – 04:06 pm GMT

PDB ID : 7Q5U
Title : The tandem SH2 domains of SYK with a bound CD3G 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 : 2.40 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 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

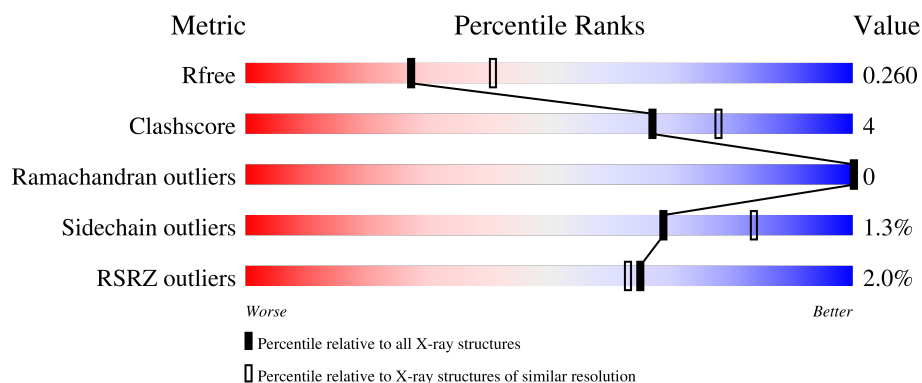
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	AAA	265	
1	BBB	265	
1	CCC	265	
1	DDD	265	
1	EEE	265	

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Mol	Chain	Length	Quality of chain
1	FFF	265	<div><div></div><div>4%</div><div>89%</div><div>8%</div><div></div></div>
2	GGG	20	<div><div></div><div>80%</div><div>5%</div><div>5%</div><div>10%</div></div>
2	HHH	20	<div><div></div><div>5%</div><div>85%</div><div>5%</div><div>10%</div></div>
2	III	20	<div><div></div><div>85%</div><div>5%</div><div>10%</div></div>
2	JJJ	20	<div><div></div><div>75%</div><div>15%</div><div>10%</div></div>
2	KKK	20	<div><div></div><div>85%</div><div>5%</div><div>10%</div></div>
2	LLL	20	<div><div></div><div>5%</div><div>85%</div><div>10%</div><div>5%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14063 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	258	Total	C	N	O	S	0	0	0
			2059	1306	368	378	7			
1	BBB	258	Total	C	N	O	S	0	0	0
			2059	1306	368	378	7			
1	CCC	259	Total	C	N	O	S	0	1	0
			2068	1311	370	380	7			
1	DDD	258	Total	C	N	O	S	0	0	0
			2059	1306	368	378	7			
1	EEE	257	Total	C	N	O	S	0	2	0
			2063	1308	367	381	7			
1	FFF	258	Total	C	N	O	S	0	0	0
			2059	1306	368	378	7			

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 T-cell surface glycoprotein CD3 gamma chain.

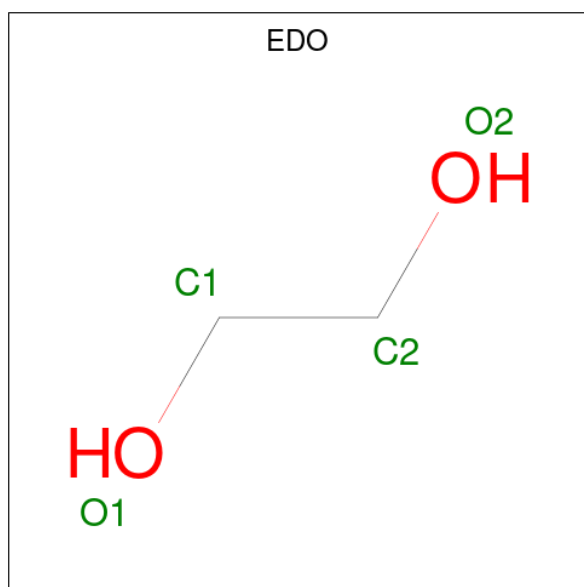
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	GGG	18	Total	C	N	O	P	0	0	0
			168	99	28	39	2			
2	HHH	18	Total	C	N	O	P	0	0	0
			168	99	28	39	2			
2	III	18	Total	C	N	O	P	0	0	0
			168	99	28	39	2			

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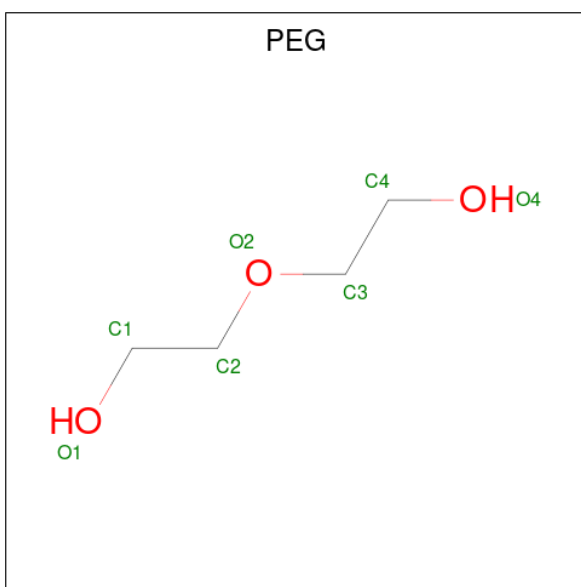
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	JJJ	18	Total	C	N	O	P	0	0	0
			168	99	28	39	2			
2	KKK	18	Total	C	N	O	P	0	0	0
			168	99	28	39	2			
2	LLL	19	Total	C	N	O	P	0	0	0
			173	101	29	41	2			

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



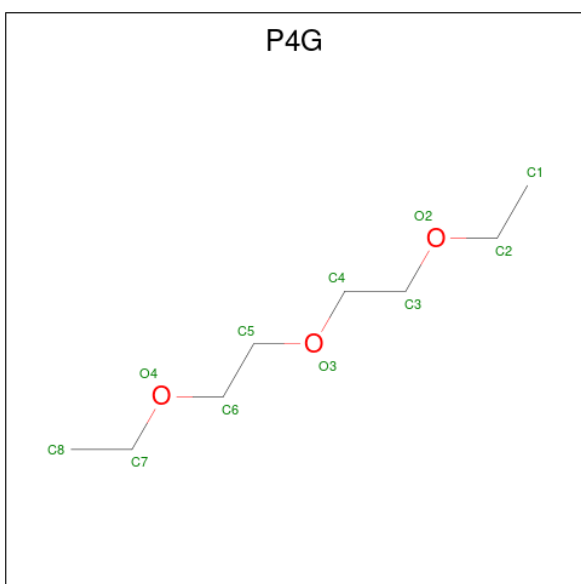
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	CCC	1	Total	C	O	0	0
			4	2	2		
3	CCC	1	Total	C	O	0	0
			4	2	2		
3	DDD	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 5 is 1-ETHOXY-2-(2-ETHOXYETHOXY)ETHANE (three-letter code: P4G) (formula: C₈H₁₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AAA	1	Total	C	O	0	0
			11	8	3		
5	EEE	1	Total	C	O	0	0
			11	8	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	AAA	127	Total	O		0	0
			127	127			
6	BBB	86	Total	O		0	0
			86	86			
6	CCC	83	Total	O		0	0
			83	83			
6	DDD	86	Total	O		0	0
			86	86			
6	EEE	100	Total	O		0	0
			100	100			
6	FFF	64	Total	O		0	0
			64	64			
6	GGG	6	Total	O		0	0
			6	6			
6	HHH	12	Total	O		0	0
			12	12			
6	III	13	Total	O		0	0
			13	13			
6	JJJ	9	Total	O		0	0
			9	9			
6	KKK	11	Total	O		0	0
			11	11			
6	LLL	16	Total	O		0	0
			16	16			

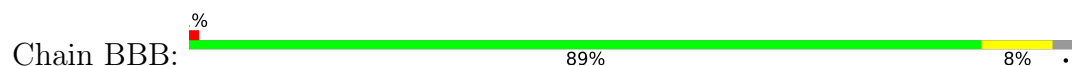
3 Residue-property plots [i](#)

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



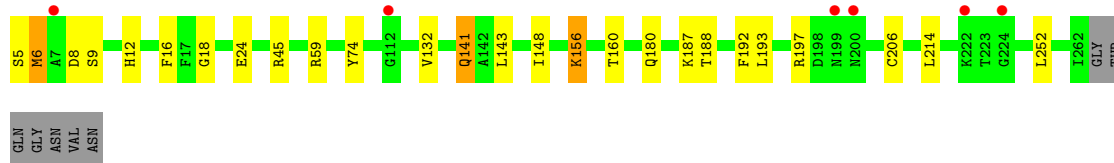
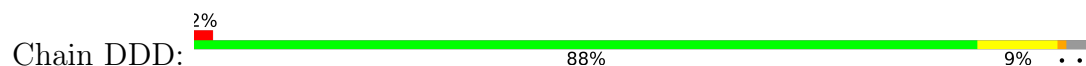
- Molecule 1: Tyrosine-protein kinase SYK



- Molecule 1: Tyrosine-protein kinase SYK

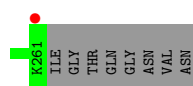


- Molecule 1: Tyrosine-protein kinase SYK

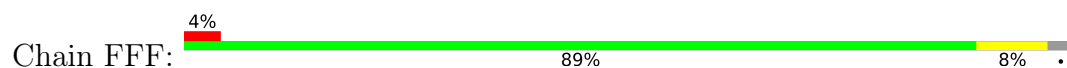


- Molecule 1: Tyrosine-protein kinase SYK

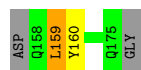
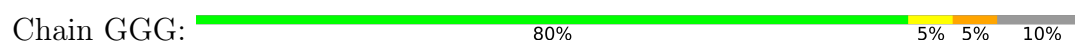




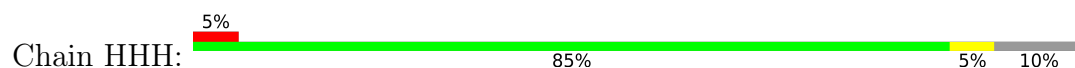
- Molecule 1: Tyrosine-protein kinase SYK



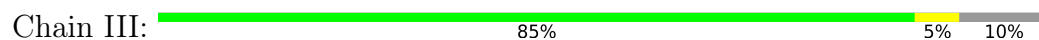
- Molecule 2: T-cell surface glycoprotein CD3 gamma chain



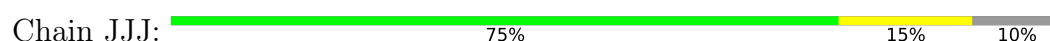
- Molecule 2: T-cell surface glycoprotein CD3 gamma chain



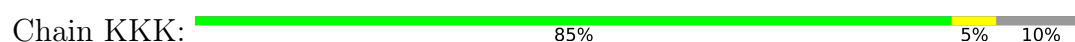
- Molecule 2: T-cell surface glycoprotein CD3 gamma chain



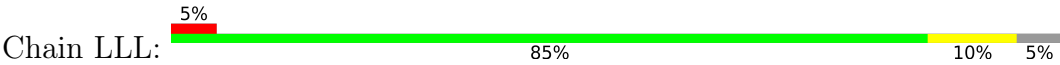
- Molecule 2: T-cell surface glycoprotein CD3 gamma chain



- Molecule 2: T-cell surface glycoprotein CD3 gamma chain



- Molecule 2: T-cell surface glycoprotein CD3 gamma chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.32Å 129.31Å 95.35Å 90.00° 100.23° 90.00°	Depositor
Resolution (Å)	93.83 – 2.40 93.83 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (93.83-2.40) 99.9 (93.83-2.40)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.216 , 0.259 0.220 , 0.260	Depositor DCC
R_{free} test set	1977 reflections (2.30%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.068 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14063	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PTR, PEG, P4G, EDO

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	0.71	0/2106	0.83	1/2840 (0.0%)
1	BBB	0.73	0/2106	0.83	0/2840
1	CCC	0.72	0/2118	0.80	0/2856
1	DDD	0.71	1/2106 (0.0%)	0.81	0/2840
1	EEE	0.71	0/2116	0.81	0/2853
1	FFF	0.71	0/2106	0.79	0/2840
2	GGG	0.69	0/135	0.76	0/177
2	HHH	0.66	0/135	0.92	0/177
2	III	0.68	0/135	0.82	0/177
2	JJJ	0.70	0/135	0.81	0/177
2	KKK	0.69	0/135	0.89	0/177
2	LLL	0.73	0/140	0.79	0/182
All	All	0.71	1/13473 (0.0%)	0.81	1/18136 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	DDD	24	GLU	CD-OE2	-5.19	1.20	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	175	ARG	NE-CZ-NH2	-5.64	117.48	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	2059	0	2047	15	0
1	BBB	2059	0	2047	14	0
1	CCC	2068	0	2056	14	0
1	DDD	2059	0	2047	25	0
1	EEE	2063	0	2048	24	0
1	FFF	2059	0	2047	15	0
2	GGG	168	0	141	2	0
2	HHH	168	0	141	1	0
2	III	168	0	141	1	0
2	JJJ	168	0	141	3	0
2	KKK	168	0	141	1	0
2	LLL	173	0	144	0	0
3	AAA	8	0	12	3	0
3	CCC	8	0	12	0	0
3	DDD	4	0	6	0	0
4	AAA	7	0	10	0	0
4	BBB	7	0	10	1	0
4	EEE	7	0	10	0	0
4	FFF	7	0	10	0	0
5	AAA	11	0	18	2	0
5	EEE	11	0	18	0	0
6	AAA	127	0	0	4	0
6	BBB	86	0	0	1	0
6	CCC	83	0	0	2	0
6	DDD	86	0	0	5	0
6	EEE	100	0	0	3	0
6	FFF	64	0	0	1	0
6	GGG	6	0	0	0	0
6	HHH	12	0	0	1	0
6	III	13	0	0	0	0
6	JJJ	9	0	0	0	0
6	KKK	11	0	0	0	0
6	LLL	16	0	0	0	0
All	All	14063	0	13247	104	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 (104) 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:DDD:6:MET:HB3	1:DDD:74:TYR:OH	1.61	1.00
1:DDD:5:SER:HB2	1:DDD:8:ASP:HB2	1.50	0.91
1:DDD:132:VAL:HG11	1:DDD:143:LEU:HD11	1.59	0.84
1:DDD:187:LYS:HE2	6:DDD:406:HOH:O	1.78	0.83
1:EEE:141:GLN:HG3	6:EEE:492:HOH:O	1.80	0.82
1:DDD:148:ILE:HD12	1:EEE:7:ALA:HB1	1.62	0.80
1:FFF:68:ARG:HD2	6:FFF:453:HOH:O	1.86	0.76
1:FFF:181:ILE:O	1:FFF:184:ILE:HG22	1.88	0.74
1:BBB:132:VAL:HG12	1:BBB:143:LEU:HD12	1.75	0.69
1:DDD:148:ILE:HD12	1:EEE:7:ALA:CB	2.25	0.67
1:CCC:132:VAL:HG12	1:CCC:143:LEU:HD12	1.76	0.66
1:DDD:132:VAL:CG1	1:DDD:143:LEU:HD11	2.25	0.65
1:DDD:188:THR:OG1	6:DDD:401:HOH:O	2.16	0.63
1:BBB:27:ASP:HB3	4:BBB:301:PEG:H41	1.82	0.62
1:EEE:173:ILE:HG23	1:EEE:177[A]:GLU:HB2	1.82	0.61
1:FFF:175:ARG:NH2	2:GGG:159:LEU:O	2.32	0.60
1:DDD:148:ILE:CD1	1:EEE:7:ALA:HB1	2.31	0.59
1:EEE:64:TYR:OH	1:EEE:100:VAL:HG13	2.02	0.59
1:BBB:210:GLU:OE2	6:BBB:401:HOH:O	2.17	0.59
1:EEE:5:SER:HB3	1:EEE:83:ALA:O	2.04	0.58
1:DDD:132:VAL:HG11	1:DDD:143:LEU:CD1	2.33	0.58
1:DDD:6:MET:HA	6:DDD:469:HOH:O	2.04	0.58
1:EEE:220:LYS:HE2	1:EEE:224:GLY:HA2	1.86	0.57
1:EEE:173:ILE:HG23	1:EEE:177[B]:GLU:HB3	1.86	0.57
1:EEE:173:ILE:HG23	1:EEE:177[A]:GLU:CB	2.34	0.57
1:DDD:45:ARG:NH1	6:DDD:404:HOH:O	2.39	0.55
1:BBB:220:LYS:HE3	1:BBB:224:GLY:HA2	1.90	0.54
3:AAA:302:EDO:H11	1:FFF:148:ILE:HD11	1.89	0.54
1:BBB:132:VAL:CG1	1:BBB:143:LEU:HD12	2.38	0.53
1:BBB:16:PHE:CZ	1:BBB:18:GLY:HA2	2.44	0.53
1:FFF:5:SER:HA	1:FFF:9:SER:HB3	1.90	0.53
1:BBB:126:ASN:ND2	1:BBB:130:GLU:OE2	2.41	0.53
1:AAA:16:PHE:CZ	1:AAA:18:GLY:HA2	2.44	0.53
1:AAA:262:ILE:HG22	1:DDD:59:ARG:HD2	1.91	0.53
1:EEE:156:LYS:O	1:EEE:160:THR:HG23	2.09	0.52
1:CCC:132:VAL:CG1	1:CCC:143:LEU:HD12	2.39	0.52
1:DDD:16:PHE:CZ	1:DDD:18:GLY:HA2	2.44	0.52
1:FFF:16:PHE:CZ	1:FFF:18:GLY:HA2	2.45	0.52
1:AAA:45:ARG:NH1	6:AAA:404:HOH:O	2.42	0.51
1:EEE:16:PHE:CZ	1:EEE:18:GLY:HA2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:148:ILE:CD1	1:EEE:7:ALA:CB	2.88	0.51
1:AAA:27:ASP:HB3	5:AAA:304:P4G:H52	1.91	0.51
5:AAA:304:P4G:H12	6:AAA:502:HOH:O	2.10	0.51
1:CCC:247:LYS:NZ	6:CCC:405:HOH:O	2.44	0.51
1:EEE:173:ILE:CG2	1:EEE:177[A]:GLU:HB2	2.41	0.50
1:DDD:156:LYS:O	1:DDD:160:THR:HG23	2.12	0.50
1:CCC:16:PHE:CZ	1:CCC:18:GLY:HA2	2.45	0.50
1:AAA:177:GLU:HG2	6:AAA:464:HOH:O	2.11	0.50
1:EEE:129:ARG:HD3	6:EEE:486:HOH:O	2.11	0.50
3:AAA:302:EDO:H11	1:FFF:148:ILE:CD1	2.42	0.49
1:CCC:41:LEU:HD21	1:CCC:85:PRO:HB2	1.95	0.48
1:CCC:175:ARG:NH2	2:JJJ:159:LEU:O	2.41	0.48
1:CCC:153:GLN:HA	1:CCC:153:GLN:OE1	2.14	0.48
1:DDD:141:GLN:HA	1:DDD:141:GLN:OE1	2.13	0.47
1:FFF:156:LYS:O	1:FFF:160:THR:HG23	2.15	0.47
1:AAA:27:ASP:O	1:AAA:30:VAL:HG22	2.15	0.47
1:BBB:175:ARG:NH1	2:III:160:PTR:O3P	2.45	0.47
1:AAA:27:ASP:HA	1:AAA:30:VAL:HG22	1.97	0.47
1:AAA:217:ARG:HG2	6:AAA:488:HOH:O	2.15	0.47
1:CCC:175:ARG:NH1	2:JJJ:160:PTR:O3P	2.44	0.46
1:EEE:151:LYS:HD3	6:EEE:483:HOH:O	2.14	0.46
1:AAA:193:LEU:C	1:AAA:193:LEU:HD12	2.37	0.46
1:BBB:193:LEU:C	1:BBB:193:LEU:HD12	2.36	0.46
1:DDD:193:LEU:C	1:DDD:193:LEU:HD12	2.36	0.46
1:EEE:252:LEU:HD23	2:KKK:164:LYS:HD3	1.98	0.46
1:FFF:175:ARG:NH1	2:GGG:160:PTR:O3P	2.40	0.46
1:BBB:41:LEU:HD21	1:BBB:85:PRO:HB2	1.97	0.46
1:BBB:153:GLN:HA	1:BBB:153:GLN:OE1	2.16	0.46
1:CCC:62:HIS:ND1	6:CCC:402:HOH:O	2.35	0.45
1:EEE:5:SER:CB	1:EEE:83:ALA:O	2.64	0.45
1:EEE:193:LEU:C	1:EEE:193:LEU:HD12	2.36	0.45
1:CCC:193:LEU:HD12	1:CCC:193:LEU:C	2.37	0.45
1:EEE:214:LEU:HD11	1:EEE:252:LEU:HD12	1.99	0.45
1:EEE:222:LYS:HD3	1:EEE:222:LYS:HA	1.82	0.45
1:AAA:12:HIS:ND1	3:AAA:302:EDO:H12	2.31	0.45
1:FFF:193:LEU:C	1:FFF:193:LEU:HD12	2.36	0.45
1:EEE:247:LYS:HG3	1:EEE:249:ASP:HB2	1.98	0.45
1:FFF:214:LEU:HD11	1:FFF:252:LEU:HD12	1.98	0.44
1:DDD:214:LEU:HD11	1:DDD:252:LEU:HD12	1.98	0.44
1:FFF:192:PHE:HA	1:FFF:206:CYS:O	2.18	0.44
1:AAA:214:LEU:HD11	1:AAA:252:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:6:MET:HG2	1:BBB:74:TYR:OH	2.17	0.44
1:BBB:214:LEU:HD11	1:BBB:252:LEU:HD12	2.00	0.44
1:FFF:141:GLN:OE1	1:FFF:141:GLN:HA	2.18	0.43
1:FFF:64:TYR:OH	1:FFF:100:VAL:HG23	2.18	0.43
1:DDD:9:SER:HA	1:DDD:12:HIS:CD2	2.54	0.43
1:DDD:6:MET:CB	1:DDD:74:TYR:OH	2.50	0.43
1:DDD:192:PHE:HA	1:DDD:206:CYS:O	2.19	0.43
1:CCC:192:PHE:HA	1:CCC:206:CYS:O	2.19	0.42
1:EEE:192:PHE:HA	1:EEE:206:CYS:O	2.19	0.42
2:HHH:159:LEU:HD13	6:HHH:208:HOH:O	2.18	0.42
1:AAA:247:LYS:HG3	1:AAA:249:ASP:HB2	2.02	0.42
1:CCC:231:GLY:HA2	2:JJJ:166:ARG:HD2	2.02	0.42
1:AAA:192:PHE:HA	1:AAA:206:CYS:O	2.20	0.41
1:FFF:5:SER:CA	1:FFF:9:SER:HB3	2.50	0.41
1:CCC:214:LEU:HD11	1:CCC:252:LEU:HD12	2.01	0.41
1:BBB:192:PHE:HA	1:BBB:206:CYS:O	2.20	0.41
1:DDD:197:ARG:NH2	6:DDD:415:HOH:O	2.54	0.41
1:AAA:150:GLN:OE1	1:AAA:153:GLN:NE2	2.54	0.41
1:AAA:151:LYS:HB3	1:AAA:152:PRO:HD3	2.03	0.40
1:DDD:6:MET:HB3	1:DDD:74:TYR:HH	1.75	0.40
1:EEE:46:ASN:HB2	1:EEE:233:LYS:O	2.21	0.40
1:CCC:6:MET:HG2	1:CCC:74:TYR:OH	2.22	0.40
1:DDD:132:VAL:CG1	1:DDD:143:LEU:CD1	2.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	256/265 (97%)	252 (98%)	4 (2%)	0	100	100
1	BBB	256/265 (97%)	253 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CCC	258/265 (97%)	252 (98%)	6 (2%)	0	100	100
1	DDD	256/265 (97%)	254 (99%)	2 (1%)	0	100	100
1	EEE	257/265 (97%)	251 (98%)	6 (2%)	0	100	100
1	FFF	256/265 (97%)	253 (99%)	3 (1%)	0	100	100
2	GGG	14/20 (70%)	11 (79%)	3 (21%)	0	100	100
2	HHH	14/20 (70%)	11 (79%)	3 (21%)	0	100	100
2	III	14/20 (70%)	11 (79%)	3 (21%)	0	100	100
2	JJJ	14/20 (70%)	11 (79%)	3 (21%)	0	100	100
2	KKK	14/20 (70%)	11 (79%)	3 (21%)	0	100	100
2	LLL	15/20 (75%)	12 (80%)	3 (20%)	0	100	100
All	All	1624/1710 (95%)	1582 (97%)	42 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	219/224 (98%)	216 (99%)	3 (1%)	67	82
1	BBB	219/224 (98%)	218 (100%)	1 (0%)	88	95
1	CCC	220/224 (98%)	218 (99%)	2 (1%)	78	90
1	DDD	219/224 (98%)	215 (98%)	4 (2%)	59	76
1	EEE	220/224 (98%)	218 (99%)	2 (1%)	78	90
1	FFF	219/224 (98%)	216 (99%)	3 (1%)	67	82
2	GGG	16/17 (94%)	15 (94%)	1 (6%)	18	28
2	HHH	16/17 (94%)	16 (100%)	0	100	100
2	III	16/17 (94%)	16 (100%)	0	100	100
2	JJJ	16/17 (94%)	16 (100%)	0	100	100
2	KKK	16/17 (94%)	16 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	LLL	16/17 (94%)	14 (88%)	2 (12%)	4 5
All	All	1412/1446 (98%)	1394 (99%)	18 (1%)	69 84

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	141	GLN
1	AAA	149	SER
1	AAA	156	LYS
1	BBB	172	LYS
1	CCC	156	LYS
1	CCC	180	GLN
1	DDD	6	MET
1	DDD	141	GLN
1	DDD	156	LYS
1	DDD	180	GLN
1	EEE	123	LEU
1	EEE	180	GLN
1	FFF	5	SER
1	FFF	180	GLN
1	FFF	222	LYS
2	GGG	159	LEU
2	LLL	166	ARG
2	LLL	170	GLN

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 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 [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	AAA	258/265 (97%)	-0.01	3 (1%) 79 77	23, 36, 61, 87	0
1	BBB	258/265 (97%)	0.02	3 (1%) 79 77	24, 39, 67, 114	0
1	CCC	259/265 (97%)	-0.07	2 (0%) 86 84	26, 41, 70, 110	0
1	DDD	258/265 (97%)	0.10	6 (2%) 60 58	29, 47, 80, 151	0
1	EEE	257/265 (96%)	-0.06	6 (2%) 60 58	29, 46, 77, 116	0
1	FFF	258/265 (97%)	0.16	11 (4%) 35 33	33, 53, 86, 144	0
2	GGG	16/20 (80%)	0.27	0 100 100	60, 78, 96, 100	0
2	HHH	16/20 (80%)	0.58	1 (6%) 20 18	38, 60, 93, 96	0
2	III	16/20 (80%)	-0.25	0 100 100	28, 53, 79, 86	0
2	JJJ	16/20 (80%)	-0.25	0 100 100	38, 59, 83, 94	0
2	KKK	16/20 (80%)	0.27	0 100 100	43, 64, 86, 90	0
2	LLL	17/20 (85%)	0.67	1 (5%) 22 21	31, 52, 84, 95	0
All	All	1645/1710 (96%)	0.03	33 (2%) 65 63	23, 44, 80, 151	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	199	ASN	7.8
1	BBB	199	ASN	6.9
2	LLL	176	GLY	5.9
1	CCC	199	ASN	5.8
1	EEE	200	ASN	5.3
1	FFF	222	LYS	4.9
1	DDD	200	ASN	4.4
1	BBB	200	ASN	4.0
1	FFF	200	ASN	3.9
1	FFF	111	GLN	3.7
1	EEE	201	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	EEE	261	LYS	3.6
1	EEE	199	ASN	3.5
1	DDD	7	ALA	3.3
1	FFF	6	MET	3.2
1	AAA	262	ILE	3.1
1	DDD	224	GLY	3.1
1	DDD	112	GLY	2.9
1	BBB	222	LYS	2.8
1	FFF	223	THR	2.8
1	FFF	7	ALA	2.7
1	EEE	96	SER	2.7
1	CCC	200	ASN	2.7
1	FFF	17	PHE	2.7
1	FFF	59	ARG	2.7
1	FFF	224	GLY	2.3
1	AAA	170	HIS	2.3
1	FFF	176	GLU	2.2
1	DDD	222	LYS	2.1
1	EEE	173	ILE	2.1
2	HHH	165	ASP	2.1
1	AAA	199	ASN	2.0
1	FFF	107	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	PTR	GGG	160	16/17	0.93	0.13	45,53,68,72	0
2	PTR	HHH	160	16/17	0.93	0.12	50,56,64,66	0
2	PTR	KKK	160	16/17	0.93	0.15	49,58,66,67	0
2	PTR	III	160	16/17	0.94	0.15	35,52,58,62	0
2	PTR	JJJ	160	16/17	0.95	0.11	38,55,58,59	0
2	PTR	III	171	16/17	0.95	0.17	24,31,33,37	0
2	PTR	LLL	171	16/17	0.95	0.15	20,30,38,41	0
2	PTR	JJJ	171	16/17	0.96	0.12	26,38,41,46	0
2	PTR	HHH	171	16/17	0.96	0.14	25,37,41,42	0
2	PTR	LLL	160	16/17	0.96	0.12	32,33,38,39	0
2	PTR	GGG	171	16/17	0.96	0.14	39,57,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PTR	KKK	171	16/17	0.97	0.14	29,41,44,44	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, 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(\AA^2)	Q<0.9
5	P4G	AAA	304	11/11	0.57	0.26	66,79,88,89	0
3	EDO	CCC	302	4/4	0.60	0.17	66,73,73,75	0
3	EDO	CCC	301	4/4	0.64	0.36	69,70,83,87	0
3	EDO	AAA	302	4/4	0.70	0.22	58,61,63,66	0
5	P4G	EEE	302	11/11	0.71	0.19	70,86,100,103	0
3	EDO	AAA	301	4/4	0.76	0.21	60,61,64,64	0
4	PEG	BBB	301	7/7	0.79	0.20	57,67,76,76	0
3	EDO	DDD	301	4/4	0.85	0.13	52,52,54,55	0
4	PEG	FFF	301	7/7	0.85	0.16	58,69,73,75	0
4	PEG	AAA	303	7/7	0.86	0.15	53,58,63,63	0
4	PEG	EEE	301	7/7	0.94	0.12	50,53,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.