



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:59 AM UTC

PDB ID : 7Q5T / pdb_00007q5t
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

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

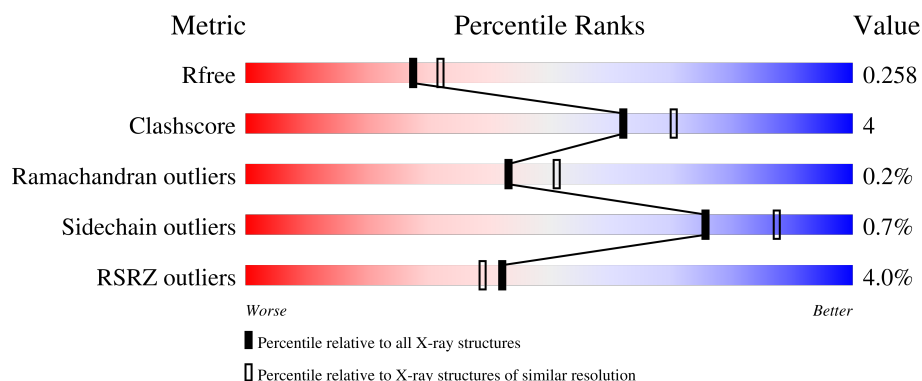
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 ≥ 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	0.2% 88% 7%
1	BBB	265	0.2% 89% 8%
1	CCC	265	2% 89% 9%
1	DDD	265	4% 84% 9% 6%
1	EEE	265	6% 89% 6%

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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	

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 (CCD ID: PO4) (formula: O₄P).



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 (CCD ID: 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 (CCD ID: 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	O	0	0
			10	10		
6	LLL	1	Total	O	0	0
			1	1		

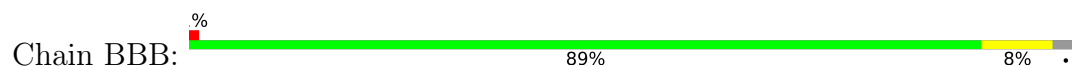
3 Residue-property plots [i](#)

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



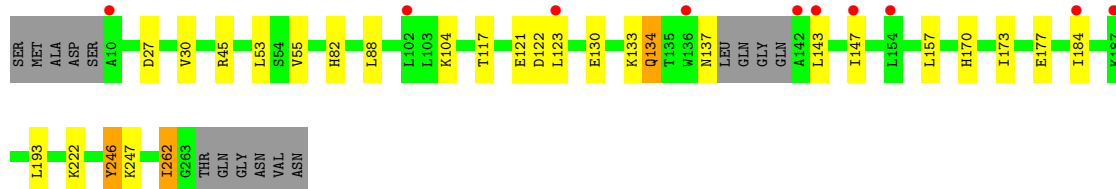
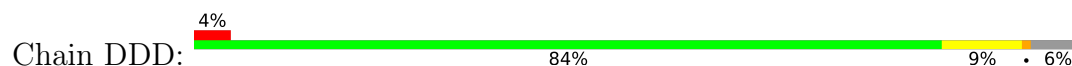
- Molecule 1: Tyrosine-protein kinase SYK



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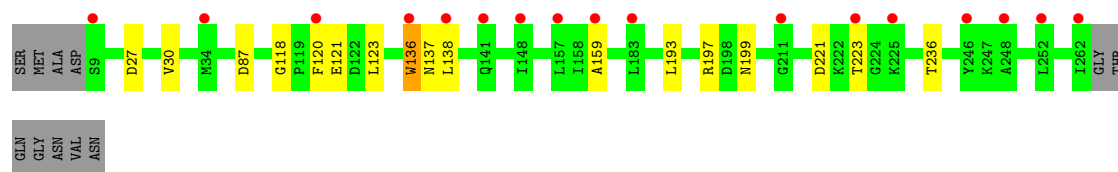


- Molecule 1: Tyrosine-protein kinase SYK

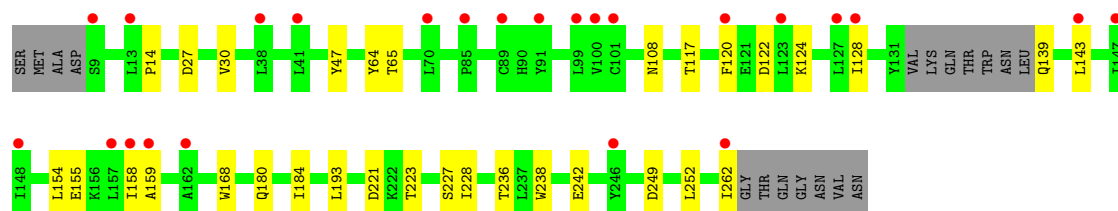
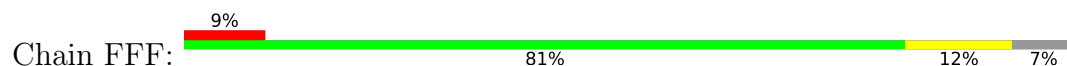


- Molecule 1: Tyrosine-protein kinase SYK

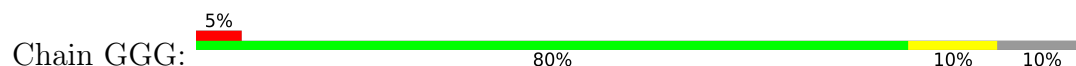




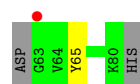
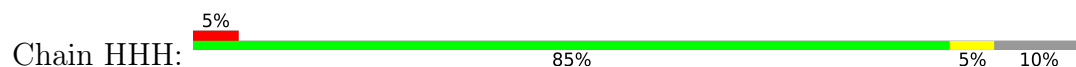
- Molecule 1: Tyrosine-protein kinase SYK



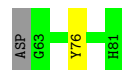
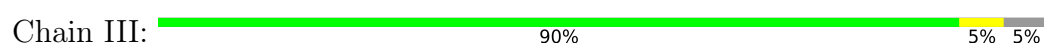
- Molecule 2: High affinity immunoglobulin epsilon receptor subunit gamma



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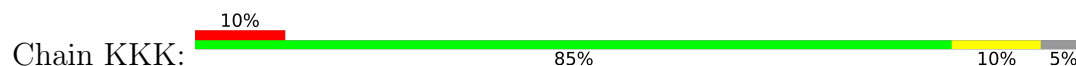
- Molecule 2: High affinity immunoglobulin epsilon receptor subunit gamma

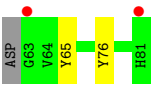


- Molecule 2: High affinity immunoglobulin epsilon receptor subunit gamma



- Molecule 2: High affinity immunoglobulin epsilon receptor subunit gamma





- Molecule 2: High affinity immunoglobulin epsilon receptor subunit gamma



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.20Å)	Xtriage
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 (2.14%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13506	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage'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.*

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: PO4, PEG, PTR, 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	1.05	1/2087 (0.0%)	1.31	1/2815 (0.0%)
1	BBB	1.04	0/2098	1.30	2/2830 (0.1%)
1	CCC	1.02	0/2155	1.29	1/2906 (0.0%)
1	DDD	1.00	0/2046	1.32	2/2758 (0.1%)
1	EEE	1.00	0/2079	1.30	4/2804 (0.1%)
1	FFF	0.98	1/2014 (0.0%)	1.29	1/2713 (0.0%)
2	GGG	0.95	0/117	1.35	0/153
2	HHH	1.06	0/117	1.40	0/153
2	III	1.03	0/129	1.34	0/168
2	JJJ	1.00	0/113	1.26	0/148
2	KKK	1.04	0/129	1.42	0/168
2	LLL	0.89	0/98	1.36	0/130
All	All	1.01	2/13182 (0.0%)	1.30	11/17746 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	FFF	154	LEU	C-O	7.36	1.32	1.24
1	AAA	258	PRO	C-O	-5.53	1.17	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	EEE	199	ASN	CA-C-O	-5.70	114.83	120.82
1	AAA	198	ASP	N-CA-C	-5.56	106.85	113.97
1	CCC	164	GLU	CB-CG-CD	5.48	121.91	112.60
1	EEE	197	ARG	N-CA-C	-5.38	107.08	113.97
1	FFF	155	GLU	CA-C-O	-5.28	115.28	120.82
1	DDD	123	LEU	CA-C-N	5.11	127.39	120.65
1	DDD	123	LEU	C-N-CA	5.11	127.39	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	EEE	123	LEU	CA-C-N	5.10	127.43	120.54
1	EEE	123	LEU	C-N-CA	5.10	127.43	120.54
1	BBB	242	GLU	CB-CG-CD	-5.07	103.99	112.60
1	BBB	154	LEU	CA-C-O	-5.04	114.64	120.24

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	14	0
1	BBB	2051	0	2038	14	0
1	CCC	2098	0	2085	20	0
1	DDD	2000	0	1991	27	0
1	EEE	2032	0	2024	13	0
1	FFF	1970	0	1959	23	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	107	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 (107) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:EEE:87:ASP:HB3	5:EEE:301:PEG:H11	1.93	0.50
1:DDD:88:LEU:C	1:DDD:88:LEU:HD13	2.38	0.49
1:FFF:221:ASP:OD1	1:FFF:223:THR:OG1	2.30	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:30:VAL:HG23	6:AAA:425:HOH:O	2.17	0.45
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:AAA:193:LEU:C	1:AAA:193:LEU:HD12	2.43	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:BBB:193:LEU:C	1:BBB:193:LEU:HD12	2.43	0.43
1:FFF:124:LYS:CE	1:FFF:158:ILE:HG22	2.48	0.43
1:AAA:71:ASN:HD22	1:CCC:164:GLU:CD	2.26	0.43
1:BBB:180:GLN:O	1:BBB:184:ILE:HG12	2.18	0.43
1:FFF:193:LEU:C	1:FFF:193:LEU:HD12	2.43	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:CCC:193:LEU:HD12	1:CCC:193:LEU:C	2.44	0.42
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:DDD:193:LEU:C	1:DDD:193:LEU:HD12	2.45	0.42
1:FFF:120:PHE:CD2	1:FFF:238:TRP:HB2	2.55	0.42
1:BBB:221:ASP:OD1	1:BBB:223:THR:OG1	2.32	0.41
1:BBB:181:ILE:CG2	1:BBB:259:CYS:SG	3.08	0.41
1:EEE:193:LEU:C	1:EEE:193:LEU:HD12	2.44	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%)	30	34
1	CCC	262/265 (99%)	259 (99%)	3 (1%)	0	100	100
1	DDD	246/265 (93%)	243 (99%)	2 (1%)	1 (0%)	30	34
1	EEE	252/265 (95%)	248 (98%)	3 (1%)	1 (0%)	30	34
1	FFF	243/265 (92%)	241 (99%)	2 (1%)	0	100	100
2	GGG	14/20 (70%)	12 (86%)	2 (14%)	0	100	100
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%)	43	51

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%)	51	68
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%)	50	66
1	EEE	216/224 (96%)	215 (100%)	1 (0%)	81	90
1	FFF	209/224 (93%)	208 (100%)	1 (0%)	81	90
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
All	All	1380/1440 (96%)	1370 (99%)	10 (1%)	76	87

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.

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	PTR	HHH	76	2	15,16,17	0.56	0	17,22,24	0.51	0
2	PTR	III	65	2	15,16,17	0.70	0	17,22,24	0.66	0
2	PTR	LLL	65	2	15,16,17	0.54	0	17,22,24	0.95	1 (5%)
2	PTR	KKK	76	2	15,16,17	0.91	1 (6%)	17,22,24	0.63	0
2	PTR	III	76	2	15,16,17	0.55	0	17,22,24	0.94	1 (5%)
2	PTR	KKK	65	2	15,16,17	1.19	1 (6%)	17,22,24	1.07	1 (5%)
2	PTR	GGG	76	2	15,16,17	0.73	0	17,22,24	0.94	1 (5%)
2	PTR	JJJ	65	2	15,16,17	0.82	1 (6%)	17,22,24	0.88	1 (5%)
2	PTR	HHH	65	2	15,16,17	0.57	0	17,22,24	0.87	1 (5%)
2	PTR	LLL	76	2	15,16,17	0.59	0	17,22,24	0.84	2 (11%)
2	PTR	JJJ	76	2	15,16,17	0.78	1 (6%)	17,22,24	0.94	1 (5%)
2	PTR	GGG	65	2	15,16,17	0.48	0	17,22,24	0.85	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	PTR	HHH	76	2	-	0/10/11/13	0/1/1/1
2	PTR	III	65	2	-	0/10/11/13	0/1/1/1
2	PTR	LLL	65	2	-	1/10/11/13	0/1/1/1
2	PTR	KKK	76	2	-	1/10/11/13	0/1/1/1
2	PTR	III	76	2	-	1/10/11/13	0/1/1/1
2	PTR	KKK	65	2	-	2/10/11/13	0/1/1/1
2	PTR	GGG	76	2	-	1/10/11/13	0/1/1/1
2	PTR	JJJ	65	2	-	0/10/11/13	0/1/1/1
2	PTR	HHH	65	2	-	0/10/11/13	0/1/1/1
2	PTR	LLL	76	2	-	0/10/11/13	0/1/1/1
2	PTR	JJJ	76	2	-	0/10/11/13	0/1/1/1
2	PTR	GGG	65	2	-	1/10/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	KKK	65	PTR	P-OH	-3.53	1.53	1.59
2	KKK	76	PTR	P-O2P	-2.32	1.46	1.54
2	JJJ	65	PTR	P-OH	-2.26	1.55	1.59
2	JJJ	76	PTR	P-O3P	-2.07	1.47	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	III	76	PTR	O2P-P-OH	3.19	114.74	105.32
2	HHH	65	PTR	O3P-P-OH	2.95	114.03	105.32
2	GGG	76	PTR	O2P-P-OH	2.91	113.91	105.32
2	LLL	65	PTR	O2P-P-OH	2.26	111.99	105.32
2	JJJ	65	PTR	O3P-P-OH	2.24	111.94	105.32
2	LLL	76	PTR	O3P-P-OH	2.16	111.70	105.32
2	LLL	76	PTR	OH-P-O1P	-2.04	102.66	109.48
2	JJJ	76	PTR	O3P-P-OH	-2.04	99.28	105.32
2	KKK	65	PTR	OH-P-O1P	-2.04	102.67	109.48

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	GGG	76	PTR	O-C-CA-CB
2	III	76	PTR	O-C-CA-CB
2	KKK	65	PTR	CZ-OH-P-O1P
2	KKK	76	PTR	O-C-CA-CB
2	GGG	65	PTR	CZ-OH-P-O2P
2	KKK	65	PTR	CZ-OH-P-O3P
2	LLL	65	PTR	CZ-OH-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	DDD	302	-	4,4,4	0.75	0	6,6,6	0.48	0
3	PO4	DDD	303	-	4,4,4	0.87	0	6,6,6	0.41	0
3	PO4	DDD	301	-	4,4,4	0.91	0	6,6,6	0.48	0
3	PO4	BBB	302	-	4,4,4	1.40	1 (25%)	6,6,6	0.31	0
3	PO4	BBB	301	-	4,4,4	0.87	0	6,6,6	0.57	0
3	PO4	AAA	301	-	4,4,4	0.78	0	6,6,6	0.50	0
4	EDO	CCC	303	-	3,3,3	0.07	0	2,2,2	0.22	0
5	PEG	BBB	303	-	6,6,6	0.29	0	5,5,5	0.29	0
5	PEG	EEE	301	-	6,6,6	0.26	0	5,5,5	0.16	0
4	EDO	CCC	304	-	3,3,3	0.32	0	2,2,2	0.57	0
3	PO4	AAA	302	-	4,4,4	0.77	0	6,6,6	0.48	0
3	PO4	CCC	302	-	4,4,4	0.68	0	6,6,6	0.53	0
3	PO4	CCC	301	-	4,4,4	0.39	0	6,6,6	0.74	0
4	EDO	AAA	303	-	3,3,3	0.29	0	2,2,2	0.37	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
4	EDO	CCC	303	-	-	0/1/1/1	-
5	PEG	EEE	301	-	-	3/4/4/4	-
5	PEG	BBB	303	-	-	2/4/4/4	-
4	EDO	CCC	304	-	-	1/1/1/1	-
4	EDO	AAA	303	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BBB	302	PO4	P-O1	2.56	1.56	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	BBB	303	PEG	O2-C3-C4-O4
5	BBB	303	PEG	O1-C1-C2-O2
5	EEE	301	PEG	O1-C1-C2-O2
4	AAA	303	EDO	O1-C1-C2-O2
5	EEE	301	PEG	C4-C3-O2-C2
4	CCC	304	EDO	O1-C1-C2-O2
5	EEE	301	PEG	O2-C3-C4-O4

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	BBB	303	PEG	2	0
5	EEE	301	PEG	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	255/265 (96%)	-0.20	2 (0%) 82 80	33, 45, 71, 105	0
1	BBB	257/265 (96%)	-0.25	2 (0%) 82 80	33, 46, 76, 129	0
1	CCC	261/265 (98%)	-0.04	4 (1%) 72 69	32, 51, 76, 122	3 (1%)
1	DDD	250/265 (94%)	0.34	10 (4%) 42 39	42, 64, 118, 157	0
1	EEE	254/265 (95%)	0.71	17 (6%) 24 21	45, 75, 123, 156	0
1	FFF	247/265 (93%)	0.80	24 (9%) 13 10	50, 89, 152, 185	0
2	GGG	16/20 (80%)	0.94	1 (6%) 26 23	66, 84, 116, 126	0
2	HHH	16/20 (80%)	0.73	1 (6%) 26 23	45, 74, 106, 129	0
2	III	17/20 (85%)	0.31	0 100 100	49, 70, 98, 118	0
2	JJJ	15/20 (75%)	0.46	2 (13%) 7 5	43, 60, 115, 123	0
2	KKK	17/20 (85%)	0.48	2 (11%) 9 7	41, 64, 99, 127	0
2	LLL	13/20 (65%)	0.77	0 100 100	60, 103, 132, 134	0
All	All	1618/1710 (94%)	0.24	65 (4%) 42 39	32, 59, 123, 185	3 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	268	VAL	3.5
1	FFF	85	PRO	3.5
1	FFF	89	CYS	3.4
1	FFF	162	ALA	3.3
1	EEE	136	TRP	3.3
1	DDD	10	ALA	3.2
1	DDD	184	ILE	3.2
1	EEE	9	SER	3.2
1	EEE	157	LEU	3.1
1	FFF	148	ILE	3.1
1	EEE	211	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	FFF	70	LEU	3.0
1	AAA	201	GLY	3.0
1	FFF	100	VAL	2.9
1	DDD	143	LEU	2.9
1	CCC	9	SER	2.8
1	FFF	127	LEU	2.8
1	AAA	200	ASN	2.8
2	KKK	63	GLY	2.8
1	EEE	223	THR	2.7
1	EEE	262	ILE	2.7
1	EEE	252	LEU	2.7
1	EEE	246	TYR	2.7
1	DDD	142	ALA	2.6
1	FFF	158	ILE	2.6
1	FFF	147	ILE	2.6
1	FFF	157	LEU	2.5
2	HHH	63	GLY	2.5
1	DDD	147	ILE	2.5
2	GGG	64	VAL	2.5
1	DDD	123	LEU	2.5
1	DDD	154	LEU	2.5
1	BBB	8	ASP	2.5
1	FFF	9	SER	2.5
1	FFF	38	LEU	2.5
2	JJJ	64	VAL	2.4
1	FFF	41	LEU	2.4
1	FFF	143	LEU	2.4
1	EEE	141	GLN	2.4
1	BBB	264	THR	2.4
1	FFF	246	TYR	2.3
1	CCC	70	LEU	2.3
1	DDD	136	TRP	2.3
1	EEE	248	ALA	2.3
1	EEE	120	PHE	2.3
1	FFF	99	LEU	2.3
1	FFF	128	ILE	2.2
1	FFF	13	LEU	2.2
2	JJJ	72	ASN	2.2
1	FFF	91	TYR	2.2
1	EEE	138	LEU	2.2
1	DDD	102	LEU	2.2
1	EEE	183	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	FFF	123	LEU	2.2
1	CCC	200	ASN	2.2
1	EEE	34	MET	2.1
2	KKK	81	HIS	2.1
1	EEE	148	ILE	2.1
1	FFF	262	ILE	2.1
1	FFF	120	PHE	2.1
1	FFF	101	CYS	2.1
1	DDD	187	LYS	2.1
1	EEE	159	ALA	2.0
1	EEE	225	LYS	2.0
1	FFF	159	ALA	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, 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	LLL	65	16/17	0.87	0.11	76,88,105,113	0
2	PTR	GGG	65	16/17	0.93	0.08	70,81,90,92	0
2	PTR	LLL	76	16/17	0.95	0.07	59,72,79,80	0
2	PTR	GGG	76	16/17	0.96	0.07	45,60,74,78	0
2	PTR	HHH	65	16/17	0.96	0.08	52,61,66,68	0
2	PTR	JJJ	65	16/17	0.97	0.06	35,46,50,52	0
2	PTR	KKK	65	16/17	0.97	0.06	37,46,51,53	0
2	PTR	III	65	16/17	0.97	0.06	50,56,62,64	0
2	PTR	III	76	16/17	0.97	0.05	49,52,59,64	0
2	PTR	JJJ	76	16/17	0.98	0.05	33,38,45,46	0
2	PTR	HHH	76	16/17	0.98	0.06	33,40,48,49	0
2	PTR	KKK	76	16/17	0.99	0.05	34,41,51,52	0

6.3 Carbohydrates ⓘ

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(Å ²)	Q<0.9
3	PO4	DDD	303	5/5	0.64	0.11	110,122,129,149	0
3	PO4	CCC	302	5/5	0.67	0.08	82,90,114,115	0
3	PO4	AAA	302	5/5	0.67	0.12	112,132,135,140	0
3	PO4	DDD	302	5/5	0.68	0.09	87,89,103,104	0
3	PO4	CCC	301	5/5	0.71	0.09	73,83,90,95	0
3	PO4	BBB	302	5/5	0.71	0.09	81,84,96,98	0
5	PEG	EEE	301	7/7	0.77	0.17	82,92,110,115	0
3	PO4	DDD	301	5/5	0.81	0.08	72,79,89,93	0
3	PO4	AAA	301	5/5	0.81	0.06	81,90,102,103	0
3	PO4	BBB	301	5/5	0.82	0.08	63,80,92,94	0
4	EDO	AAA	303	4/4	0.90	0.14	67,72,74,75	0
4	EDO	CCC	304	4/4	0.92	0.11	61,68,69,71	0
4	EDO	CCC	303	4/4	0.92	0.10	63,63,67,71	0
5	PEG	BBB	303	7/7	0.94	0.10	63,68,70,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.