



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:47 PM UTC

PDB ID : 7Q5U / pdb_00007q5u
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 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

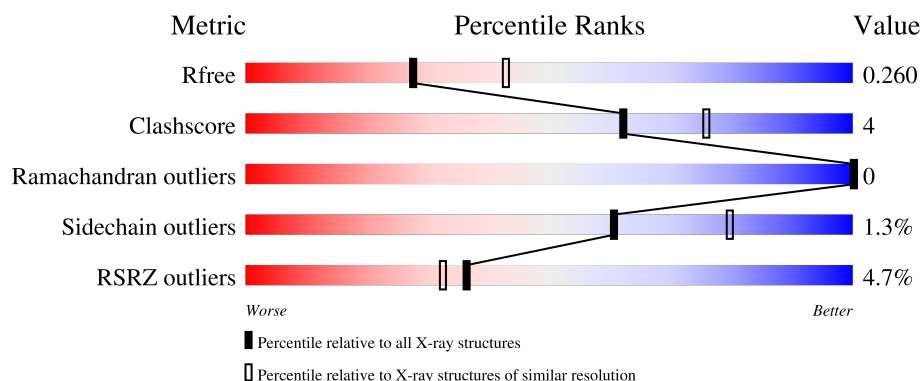
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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	0% 88% 9% .
1	BBB	265	3% 88% 9% .
1	CCC	265	2% 90% 8% .
1	DDD	265	6% 88% 8% ..
1	EEE	265	3% 85% 12% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	FFF	265	8% 88% 9%
2	GGG	20	20% 75% 5% 10% 10%
2	HHH	20	15% 80% 10% 10%
2	III	20	10% 85% 5% 10%
2	JJJ	20	10% 70% 15% 5% 10%
2	KKK	20	15% 85% 5% 10%
2	LLL	20	5% 75% 20% 5%

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.

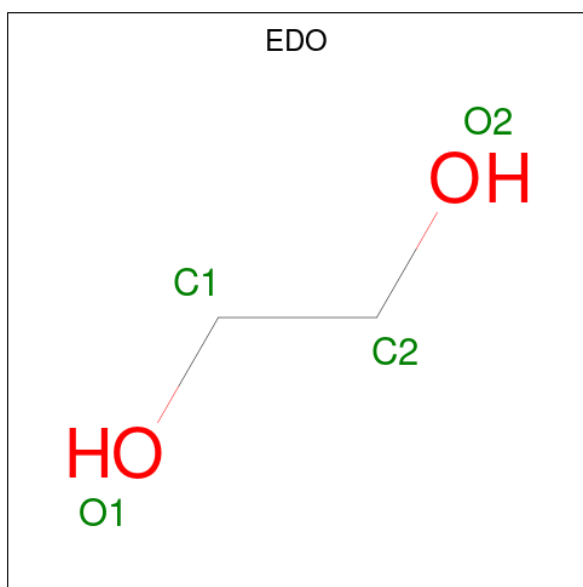
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	GGG	18	Total	C	N	O	P	0	0	0
			168	99	28	39	2			
2	HHH	18	Total	C	N	O	P	0	0	0
			168	99	28	39	2			
2	III	18	Total	C	N	O	P	0	0	0
			168	99	28	39	2			

Continued on next page...

Continued from previous page...

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 (CCD ID: EDO) (formula: $C_2H_6O_2$).



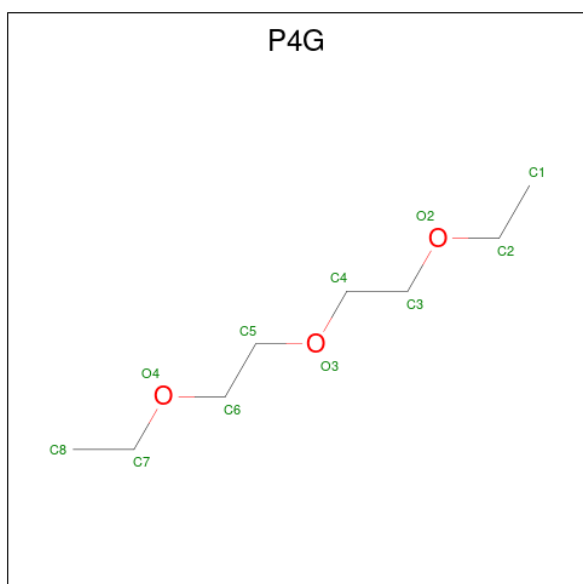
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	CCC	1	Total	C	O	0	0
			4	2	2		
3	CCC	1	Total	C	O	0	0
			4	2	2		
3	DDD	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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 (CCD ID: P4G) (formula: $C_8H_{18}O_3$).



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			

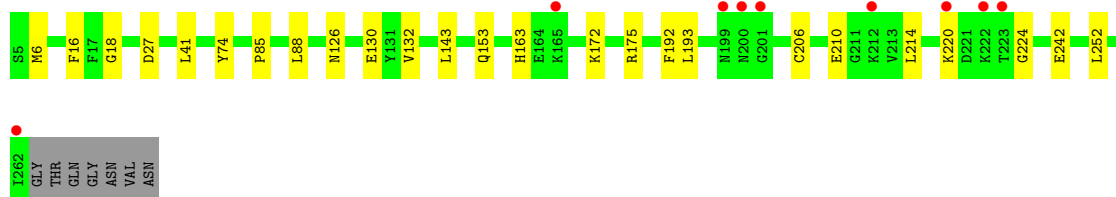
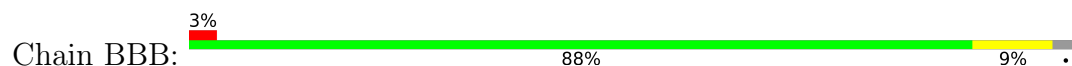
3 Residue-property plots [i](#)

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



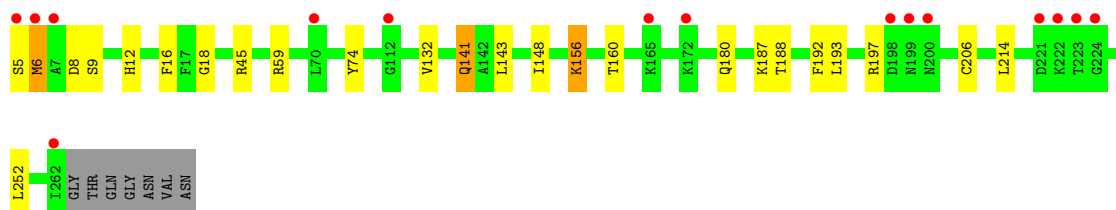
- Molecule 1: Tyrosine-protein kinase SYK



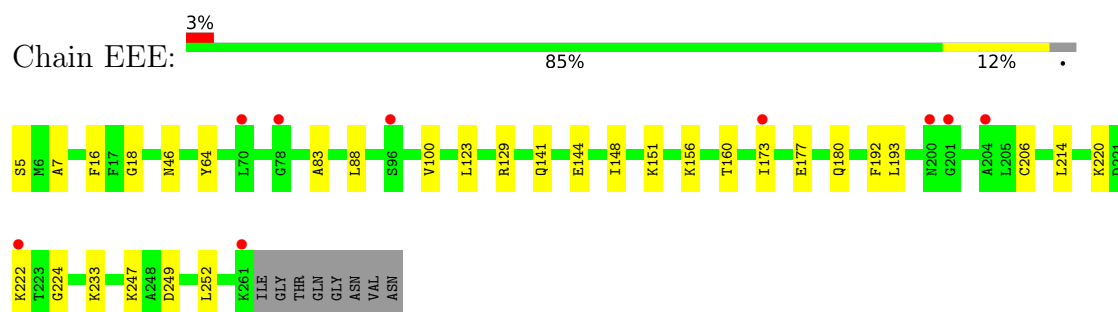
- Molecule 1: Tyrosine-protein kinase SYK



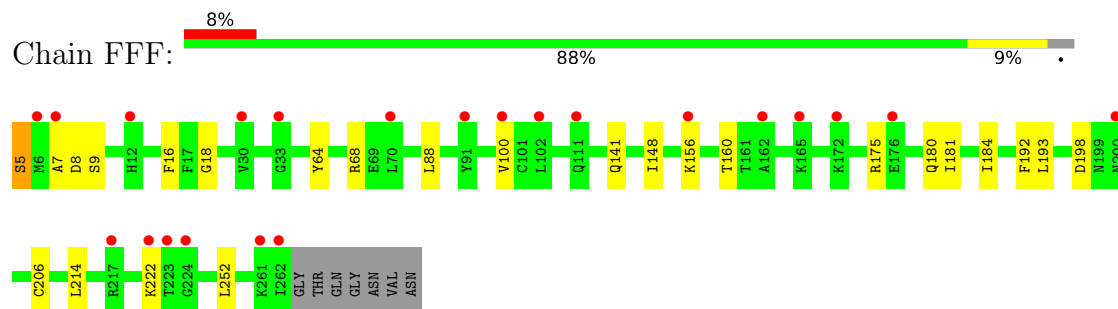
- Molecule 1: Tyrosine-protein kinase SYK



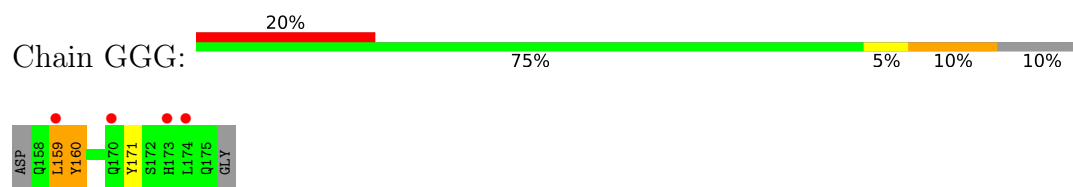
- Molecule 1: Tyrosine-protein kinase SYK



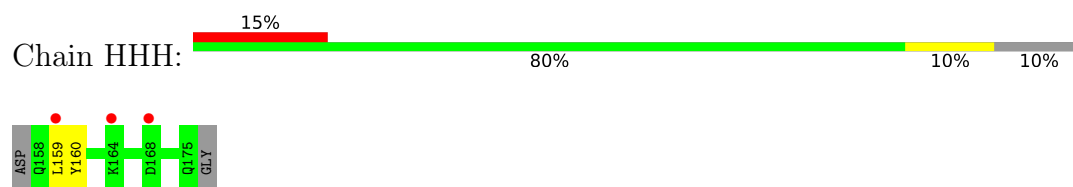
- Molecule 1: Tyrosine-protein kinase SYK



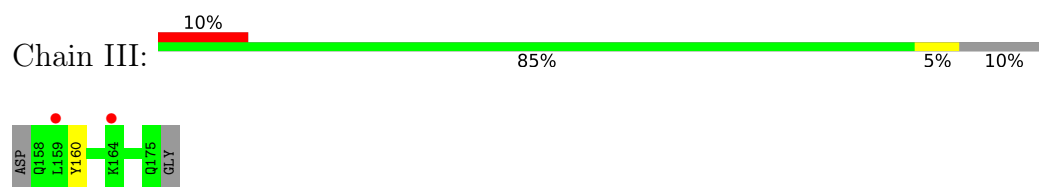
- Molecule 2: T-cell surface glycoprotein CD3 gamma chain



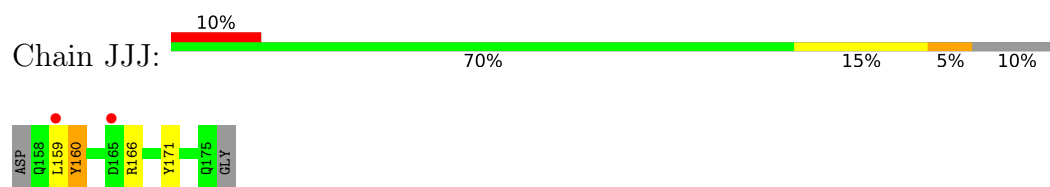
- Molecule 2: T-cell surface glycoprotein CD3 gamma chain



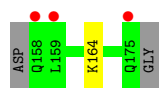
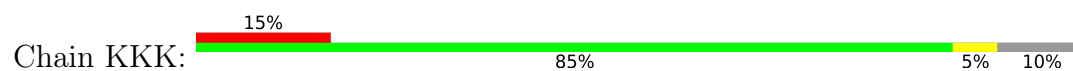
- Molecule 2: T-cell surface glycoprotein CD3 gamma chain



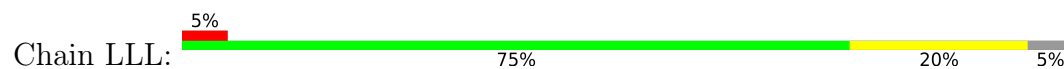
- Molecule 2: T-cell surface glycoprotein CD3 gamma chain



- 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)	0.29 , 33.8	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	0.94	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: EDO, PEG, P4G, 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	1.06	0/2106	1.35	0/2840
1	BBB	1.06	1/2106 (0.0%)	1.34	1/2840 (0.0%)
1	CCC	1.06	1/2118 (0.0%)	1.32	0/2856
1	DDD	1.05	0/2106	1.34	0/2840
1	EEE	1.06	1/2116 (0.0%)	1.34	1/2853 (0.0%)
1	FFF	1.06	0/2106	1.34	5/2840 (0.2%)
2	GGG	1.02	0/135	1.14	0/177
2	HHH	0.96	0/135	1.25	0/177
2	III	1.03	0/135	1.22	0/177
2	JJJ	0.95	0/135	1.20	0/177
2	KKK	1.00	0/135	1.26	0/177
2	LLL	1.05	0/140	1.15	0/182
All	All	1.05	3/13473 (0.0%)	1.33	7/18136 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	EEE	144	GLU	C-O	-6.23	1.16	1.24
1	BBB	163	HIS	CE1-NE2	6.08	1.38	1.32
1	CCC	163	HIS	CE1-NE2	5.03	1.37	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	FFF	198	ASP	CA-CB-CG	7.06	119.66	112.60
1	FFF	7	ALA	CA-C-N	6.35	129.12	120.54
1	FFF	7	ALA	C-N-CA	6.35	129.12	120.54
1	BBB	242	GLU	CB-CG-CD	5.67	122.23	112.60
1	EEE	148	ILE	CA-C-O	-5.60	115.23	121.17
1	FFF	8	ASP	CA-C-N	5.35	127.71	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	FFF	8	ASP	C-N-CA	5.35	127.71	120.38

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	16	0
1	BBB	2059	0	2047	16	0
1	CCC	2068	0	2056	14	0
1	DDD	2059	0	2047	25	0
1	EEE	2063	0	2048	25	0
1	FFF	2059	0	2047	17	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	1	0
6	DDD	86	0	0	6	0
6	EEE	100	0	0	3	0
6	FFF	64	0	0	1	0
6	GGG	6	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	110	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 (110) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:AAA:193:LEU:C	1:AAA:193:LEU:HD12	2.37	0.51
1:BBB:193:LEU:C	1:BBB:193:LEU:HD12	2.36	0.51
1:DDD:193:LEU:C	1:DDD:193:LEU:HD12	2.36	0.50
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:193:LEU:C	1:EEE:193:LEU:HD12	2.36	0.50
1:CCC:193:LEU:HD12	1:CCC:193:LEU:C	2.37	0.50
1:EEE:129:ARG:HD3	6:EEE:486:HOH:O	2.11	0.50
1:FFF:193:LEU:C	1:FFF:193:LEU:HD12	2.36	0.49
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:OE1	1:DDD:141:GLN:HA	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:DDD:6:MET:HE1	6:DDD:444:HOH:O	2.16	0.45
1:EEE:5:SER:CB	1:EEE:83:ALA:O	2.64	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: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
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:BBB:6:MET:O	1:BBB:6:MET:HE3	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:C	1:FFF:9:SER:HB3	2.45	0.41
1:FFF:5:SER:CA	1:FFF:9:SER:HB3	2.50	0.41
1:CCC:88:LEU:C	1:CCC:88:LEU:HD23	2.45	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:AAA:88:LEU:C	1:AAA:88:LEU:HD23	2.46	0.41
1:DDD:197:ARG:NH2	6:DDD:415:HOH:O	2.54	0.41
1:EEE:88:LEU:C	1:EEE:88:LEU:HD23	2.46	0.41
1:FFF:88:LEU:C	1:FFF:88:LEU:HD23	2.46	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:BBB:88:LEU:C	1:BBB:88:LEU:HD23	2.46	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
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 [i](#)

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%)	59	79
1	BBB	219/224 (98%)	218 (100%)	1 (0%)	81	91
1	CCC	220/224 (98%)	218 (99%)	2 (1%)	70	85
1	DDD	219/224 (98%)	215 (98%)	4 (2%)	51	73
1	EEE	220/224 (98%)	218 (99%)	2 (1%)	70	85
1	FFF	219/224 (98%)	216 (99%)	3 (1%)	59	79
2	GGG	16/17 (94%)	15 (94%)	1 (6%)	16	29
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
2	LLL	16/17 (94%)	14 (88%)	2 (12%)	4	6
All	All	1412/1446 (98%)	1394 (99%)	18 (1%)	61	80

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.

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	LLL	171	2	15,16,17	0.47	0	17,22,24	1.11	1 (5%)
2	PTR	JJJ	160	2	15,16,17	0.76	1 (6%)	17,22,24	1.06	3 (17%)
2	PTR	GGG	160	2	15,16,17	0.76	1 (6%)	17,22,24	0.67	0
2	PTR	III	171	2	15,16,17	0.56	0	17,22,24	0.63	0
2	PTR	HHH	160	2	15,16,17	0.40	0	17,22,24	0.77	1 (5%)
2	PTR	GGG	171	2	15,16,17	0.55	0	17,22,24	0.77	1 (5%)
2	PTR	HHH	171	2	15,16,17	0.60	0	17,22,24	0.64	0
2	PTR	III	160	2	15,16,17	0.48	0	17,22,24	0.56	0
2	PTR	KKK	160	2	15,16,17	0.63	0	17,22,24	0.61	0
2	PTR	LLL	160	2	15,16,17	0.90	1 (6%)	17,22,24	1.78	2 (11%)
2	PTR	JJJ	171	2	15,16,17	0.70	1 (6%)	17,22,24	0.66	0
2	PTR	KKK	171	2	15,16,17	0.71	0	17,22,24	0.50	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	LLL	171	2	-	2/10/11/13	0/1/1/1
2	PTR	JJJ	160	2	-	0/10/11/13	0/1/1/1
2	PTR	GGG	160	2	-	0/10/11/13	0/1/1/1
2	PTR	III	171	2	-	0/10/11/13	0/1/1/1
2	PTR	HHH	160	2	-	0/10/11/13	0/1/1/1
2	PTR	GGG	171	2	-	2/10/11/13	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PTR	HHH	171	2	-	2/10/11/13	0/1/1/1
2	PTR	III	160	2	-	0/10/11/13	0/1/1/1
2	PTR	KKK	160	2	-	0/10/11/13	0/1/1/1
2	PTR	LLL	160	2	-	1/10/11/13	0/1/1/1
2	PTR	JJJ	171	2	-	0/10/11/13	0/1/1/1
2	PTR	KKK	171	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	JJJ	171	PTR	P-O3P	-2.13	1.46	1.54
2	GGG	160	PTR	P-OH	-2.13	1.55	1.59
2	JJJ	160	PTR	P-OH	-2.07	1.55	1.59
2	LLL	160	PTR	P-OH	-2.01	1.55	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	LLL	160	PTR	OH-P-O1P	-4.95	92.98	109.48
2	LLL	160	PTR	O2P-P-OH	4.91	119.85	105.32
2	JJJ	160	PTR	OH-P-O1P	-2.43	101.37	109.48
2	GGG	171	PTR	O3P-P-OH	2.15	111.66	105.32
2	JJJ	160	PTR	O3P-P-OH	2.10	111.54	105.32
2	LLL	171	PTR	O2P-P-OH	2.10	111.53	105.32
2	HHH	160	PTR	O3P-P-OH	2.08	111.46	105.32
2	JJJ	160	PTR	O2P-P-OH	2.06	111.40	105.32

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	LLL	160	PTR	CZ-OH-P-O2P
2	HHH	171	PTR	N-CA-CB-CG
2	LLL	171	PTR	N-CA-CB-CG
2	LLL	171	PTR	C-CA-CB-CG
2	GGG	171	PTR	CZ-OH-P-O1P
2	GGG	171	PTR	C-CA-CB-CG
2	HHH	171	PTR	C-CA-CB-CG
2	KKK	171	PTR	C-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	JJJ	160	PTR	1	0
2	GGG	160	PTR	1	0
2	III	160	PTR	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 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	EDO	AAA	302	-	3,3,3	0.56	0	2,2,2	0.80	0
3	EDO	CCC	301	-	3,3,3	0.37	0	2,2,2	0.47	0
5	P4G	EEE	302	-	10,10,10	0.41	0	9,9,9	0.22	0
3	EDO	CCC	302	-	3,3,3	0.28	0	2,2,2	0.21	0
3	EDO	DDD	301	-	3,3,3	0.34	0	2,2,2	0.46	0
3	EDO	AAA	301	-	3,3,3	0.26	0	2,2,2	0.50	0
4	PEG	EEE	301	-	6,6,6	0.22	0	5,5,5	0.30	0
4	PEG	AAA	303	-	6,6,6	0.15	0	5,5,5	0.20	0
5	P4G	AAA	304	-	10,10,10	0.44	0	9,9,9	0.36	0
4	PEG	FFF	301	-	6,6,6	0.18	0	5,5,5	0.14	0
4	PEG	BBB	301	-	6,6,6	0.36	0	5,5,5	0.25	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
3	EDO	AAA	302	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	CCC	301	-	-	1/1/1/1	-
5	P4G	EEE	302	-	-	4/8/8/8	-
3	EDO	CCC	302	-	-	1/1/1/1	-
3	EDO	DDD	301	-	-	1/1/1/1	-
3	EDO	AAA	301	-	-	0/1/1/1	-
4	PEG	EEE	301	-	-	1/4/4/4	-
4	PEG	AAA	303	-	-	1/4/4/4	-
5	P4G	AAA	304	-	-	5/8/8/8	-
4	PEG	FFF	301	-	-	3/4/4/4	-
4	PEG	BBB	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	AAA	304	P4G	O2-C3-C4-O3
4	AAA	303	PEG	O2-C3-C4-O4
5	EEE	302	P4G	O2-C3-C4-O3
3	DDD	301	EDO	O1-C1-C2-O2
5	EEE	302	P4G	C3-C4-O3-C5
4	BBB	301	PEG	O1-C1-C2-O2
4	BBB	301	PEG	C4-C3-O2-C2
4	FFF	301	PEG	C4-C3-O2-C2
5	EEE	302	P4G	C6-C5-O3-C4
5	AAA	304	P4G	C6-C5-O3-C4
4	EEE	301	PEG	C4-C3-O2-C2
4	FFF	301	PEG	O1-C1-C2-O2
5	AAA	304	P4G	C5-C6-O4-C7
5	AAA	304	P4G	C1-C2-O2-C3
3	AAA	302	EDO	O1-C1-C2-O2
3	CCC	302	EDO	O1-C1-C2-O2
4	FFF	301	PEG	C1-C2-O2-C3
5	EEE	302	P4G	O3-C5-C6-O4
5	AAA	304	P4G	O3-C5-C6-O4
3	CCC	301	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	302	EDO	3	0
5	AAA	304	P4G	2	0
4	BBB	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 ⓘ

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%)	-0.14	2 (0%) 82 80	23, 36, 61, 87	0
1	BBB	258/265 (97%)	0.06	9 (3%) 47 43	24, 39, 67, 114	0
1	CCC	259/265 (97%)	0.06	5 (1%) 66 62	24, 41, 70, 110	1 (0%)
1	DDD	258/265 (97%)	0.37	15 (5%) 29 25	29, 47, 80, 151	0
1	EEE	257/265 (96%)	0.25	9 (3%) 47 43	29, 45, 77, 116	2 (0%)
1	FFF	258/265 (97%)	0.68	22 (8%) 16 13	33, 53, 86, 144	0
2	GGG	16/20 (80%)	1.50	4 (25%) 2 1	60, 78, 96, 100	0
2	HHH	16/20 (80%)	1.18	3 (18%) 3 3	38, 60, 93, 96	0
2	III	16/20 (80%)	0.64	2 (12%) 8 6	28, 53, 79, 86	0
2	JJJ	16/20 (80%)	0.75	2 (12%) 8 6	38, 59, 83, 94	0
2	KKK	16/20 (80%)	1.10	3 (18%) 3 3	43, 64, 86, 90	0
2	LLL	17/20 (85%)	0.48	1 (5%) 28 24	31, 52, 84, 95	0
All	All	1645/1710 (96%)	0.26	77 (4%) 36 32	23, 44, 80, 151	3 (0%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	EEE	201	GLY	4.4
1	FFF	7	ALA	4.4
1	EEE	200	ASN	4.3
1	FFF	200	ASN	4.1
1	DDD	7	ALA	4.1
1	FFF	262	ILE	4.1
2	HHH	159	LEU	4.0
1	DDD	224	GLY	3.9
1	BBB	222	LYS	3.8
1	DDD	262	ILE	3.8
1	DDD	199	ASN	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	DDD	112	GLY	3.6
1	CCC	199	ASN	3.6
1	BBB	201	GLY	3.5
1	AAA	262	ILE	3.5
1	FFF	6	MET	3.4
1	CCC	263	GLY	3.4
2	LLL	176	GLY	3.3
1	BBB	199	ASN	3.3
1	BBB	220	LYS	3.1
2	III	164	LYS	3.0
2	GGG	159	LEU	3.0
1	EEE	261	LYS	3.0
1	FFF	223	THR	3.0
1	BBB	165	LYS	3.0
1	FFF	100	VAL	2.9
1	DDD	200	ASN	2.8
2	KKK	159	LEU	2.8
1	DDD	165	LYS	2.8
1	BBB	262	ILE	2.8
1	DDD	5	SER	2.7
2	HHH	168	ASP	2.7
1	DDD	70	LEU	2.7
1	DDD	172	LYS	2.6
1	FFF	30	VAL	2.6
1	DDD	221	ASP	2.5
1	CCC	262	ILE	2.5
1	EEE	70	LEU	2.5
1	CCC	260	GLN	2.5
1	EEE	173	ILE	2.5
1	FFF	176	GLU	2.5
1	FFF	102	LEU	2.5
1	BBB	212	LYS	2.5
2	KKK	175	GLN	2.5
1	BBB	223	THR	2.5
1	DDD	6	MET	2.5
1	FFF	33	GLY	2.4
1	FFF	222	LYS	2.4
1	EEE	222	LYS	2.4
2	JJJ	165	ASP	2.3
1	DDD	222	LYS	2.3
1	DDD	198	ASP	2.3
1	FFF	261	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	EEE	78	GLY	2.3
1	EEE	96	SER	2.3
1	FFF	165	LYS	2.3
1	FFF	162	ALA	2.3
1	FFF	217	ARG	2.3
1	FFF	224	GLY	2.2
1	DDD	223	THR	2.2
1	AAA	260	GLN	2.2
2	KKK	158	GLN	2.2
2	JJJ	159	LEU	2.1
2	GGG	170	GLN	2.1
1	EEE	204	ALA	2.1
1	FFF	91	TYR	2.1
2	GGG	173	HIS	2.1
1	BBB	200	ASN	2.1
1	CCC	200	ASN	2.1
2	GGG	174	LEU	2.1
2	HHH	164	LYS	2.1
1	FFF	70	LEU	2.1
2	III	159	LEU	2.1
1	FFF	156	LYS	2.1
1	FFF	111	GLN	2.0
1	FFF	172	LYS	2.0
1	FFF	12	HIS	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	0.91	0.09	45,53,68,72	0
2	PTR	HHH	160	16/17	0.93	0.09	50,56,64,66	0
2	PTR	KKK	160	16/17	0.93	0.11	49,58,66,67	0
2	PTR	JJJ	160	16/17	0.95	0.09	38,55,58,59	0
2	PTR	III	160	16/17	0.95	0.10	35,52,58,62	0
2	PTR	GGG	171	16/17	0.96	0.11	39,57,64,64	0
2	PTR	LLL	160	16/17	0.96	0.07	32,33,38,39	0
2	PTR	III	171	16/17	0.97	0.09	24,31,33,37	0
2	PTR	JJJ	171	16/17	0.97	0.07	26,38,41,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PTR	KKK	171	16/17	0.98	0.07	29,41,44,44	0
2	PTR	HHH	171	16/17	0.98	0.08	25,37,41,42	0
2	PTR	LLL	171	16/17	0.98	0.06	20,30,38,41	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	CCC	302	4/4	0.55	0.27	66,73,73,75	0
3	EDO	CCC	301	4/4	0.66	0.27	69,70,83,87	0
3	EDO	AAA	301	4/4	0.78	0.17	60,61,64,64	0
5	P4G	AAA	304	11/11	0.78	0.24	66,79,88,89	0
3	EDO	AAA	302	4/4	0.79	0.18	58,61,63,66	0
5	P4G	EEE	302	11/11	0.81	0.26	70,86,100,103	0
4	PEG	BBB	301	7/7	0.86	0.16	57,67,76,76	0
4	PEG	AAA	303	7/7	0.87	0.12	53,58,63,63	0
3	EDO	DDD	301	4/4	0.89	0.14	52,52,54,55	0
4	PEG	FFF	301	7/7	0.90	0.12	58,69,73,75	0
4	PEG	EEE	301	7/7	0.92	0.11	50,53,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.