



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 20, 2024 – 05:25 pm GMT

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

This is a wwPDB X-ray Structure Validation Summary 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

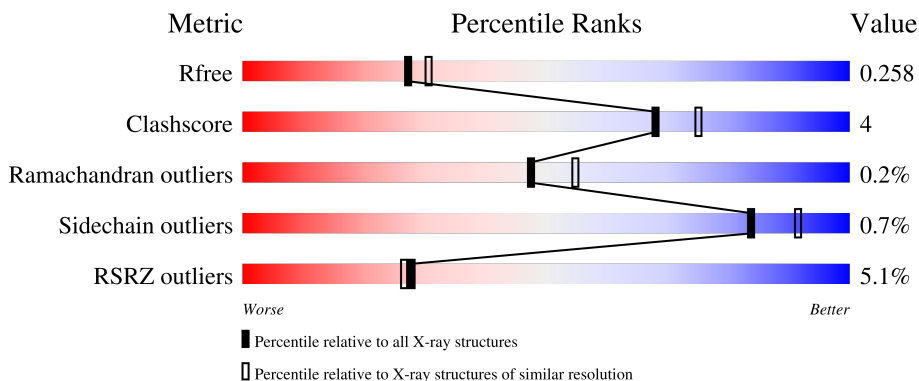
1 Overall quality at a glance

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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	<p>18% 83% 11% 7%</p>
2	GGG	20	<p>5% 80% 10% 10%</p>
2	HHH	20	<p>5% 85% 5% 10%</p>
2	III	20	<p>90% 5% 5%</p>
2	JJJ	20	<p>65% 20% 15%</p>
2	KKK	20	<p>85% 10% 5%</p>
2	LLL	20	<p>15% 55% 20% 25%</p>

2 Entry composition [i](#)

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

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.

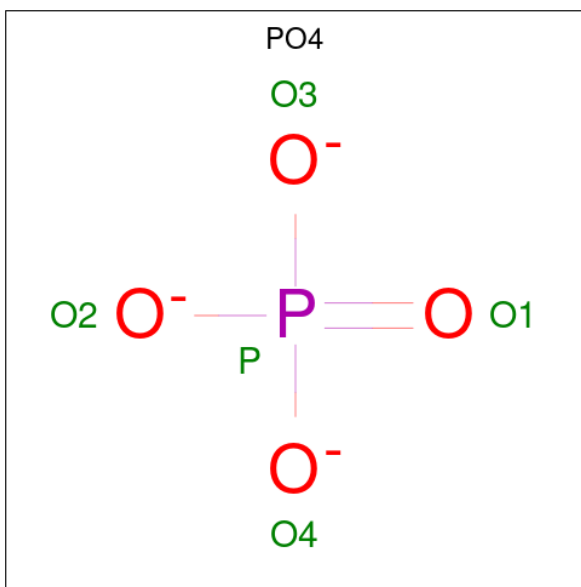
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	GGG	18	Total 152	C 89	N 24	O 37	P 2	0	0	0
2	HHH	18	Total 152	C 89	N 24	O 37	P 2	0	0	0
2	III	19	Total 163	C 95	N 27	O 39	P 2	0	0	0

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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: 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 5 4 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 6 is water.

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

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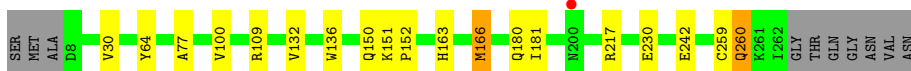
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	KKK	10	Total O 10 10	0	0
6	LLL	1	Total O 1 1	0	0

3 Residue-property plots [i](#)

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

- Molecule 1: Tyrosine-protein kinase SYK

Chain AAA:  89% 6% . .



- Molecule 1: Tyrosine-protein kinase SYK

Chain BBB:  91% 6% .




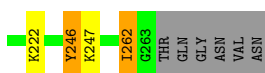
- Molecule 1: Tyrosine-protein kinase SYK

Chain CCC:  90% 9% .



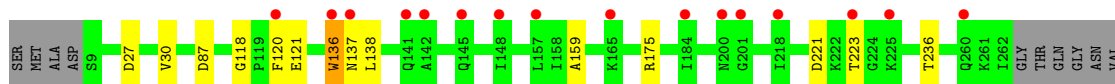
- Molecule 1: Tyrosine-protein kinase SYK

Chain DDD:  85% 9% . 6% 4%



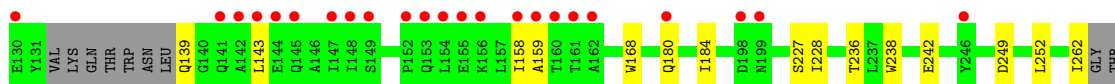
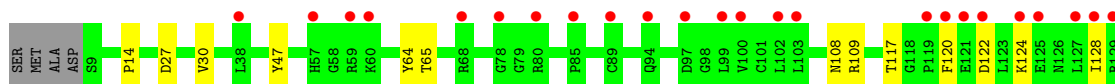
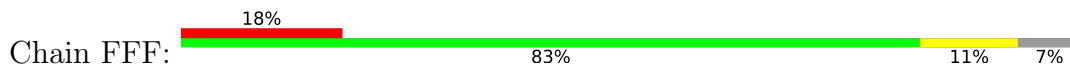
- Molecule 1: Tyrosine-protein kinase SYK

Chain EEE:  91% 5% . 6%



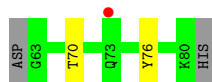
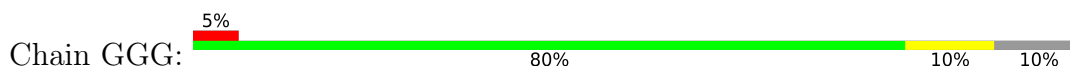
ASN

- Molecule 1: Tyrosine-protein kinase SYK

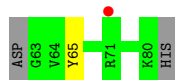
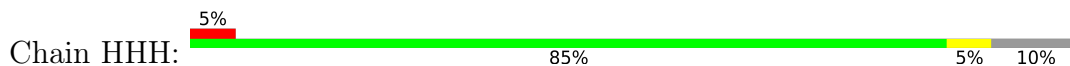


GLN, GLY, ASN, VAL, ASN

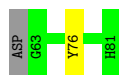
- Molecule 2: High affinity immunoglobulin epsilon receptor subunit gamma



- Molecule 2: High affinity immunoglobulin epsilon receptor subunit gamma




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- Molecule 2: High affinity immunoglobulin epsilon receptor subunit gamma



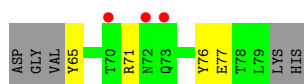
- Molecule 2: High affinity immunoglobulin epsilon receptor subunit gamma

Chain KKK:  85% 10% 5%



- Molecule 2: High affinity immunoglobulin epsilon receptor subunit gamma

Chain LLL:  15% 55% 20% 25%



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)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.207 , 0.255 0.212 , 0.258	Depositor DCC
R_{free} test set	1981 reflections (2.18%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtrriage
Anisotropy	0.465	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13506	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

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

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, PO4, PTR, PEG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AAA	0.72	1/2087 (0.0%)	0.84	1/2815 (0.0%)
1	BBB	0.70	0/2098	0.82	0/2830
1	CCC	0.69	0/2155	0.81	0/2906
1	DDD	0.67	0/2046	0.82	0/2758
1	EEE	0.67	0/2079	0.81	1/2804 (0.0%)
1	FFF	0.65	0/2014	0.79	1/2713 (0.0%)
2	GGG	0.75	0/117	0.83	0/153
2	HHH	0.81	0/117	0.95	0/153
2	III	0.75	0/129	0.78	0/168
2	JJJ	0.72	0/113	0.79	0/148
2	KKK	0.83	0/129	1.00	0/168
2	LLL	0.62	0/98	0.86	0/130
All	All	0.69	1/13182 (0.0%)	0.82	3/17746 (0.0%)

All (1) bond length outliers are listed below:

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

All (3) bond angle outliers are listed below:

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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	2040	0	2028	12	0
1	BBB	2051	0	2038	12	0
1	CCC	2098	0	2085	18	0
1	DDD	2000	0	1991	26	0
1	EEE	2032	0	2024	12	0
1	FFF	1970	0	1959	21	0
2	GGG	152	0	135	2	0
2	HHH	152	0	135	0	0
2	III	163	0	142	0	0
2	JJJ	148	0	132	1	0
2	KKK	163	0	142	0	0
2	LLL	132	0	113	3	0
3	AAA	10	0	0	0	0
3	BBB	10	0	0	0	0
3	CCC	10	0	0	0	0
3	DDD	15	0	0	0	0
4	AAA	4	0	6	0	0
4	CCC	8	0	12	0	0
5	BBB	7	0	10	2	0
5	EEE	7	0	10	1	0
6	AAA	96	0	0	1	0
6	BBB	101	0	0	1	0
6	CCC	59	0	0	1	0
6	DDD	24	0	0	1	0
6	EEE	10	0	0	0	0
6	FFF	4	0	0	0	0
6	GGG	5	0	0	0	0
6	HHH	7	0	0	1	0
6	III	5	0	0	0	0
6	JJJ	12	0	0	0	0
6	KKK	10	0	0	0	0
6	LLL	1	0	0	0	0
All	All	13506	0	12962	98	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 98 close contacts within the same asymmetric unit are listed below, sorted by their

clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FFF:64:TYR:CE1	2:LLL:77:GLU:HB3	2.18	0.78
1:DDD:117:THR:HG23	1:DDD:121:GLU:HB3	1.69	0.75
1:DDD:184:ILE:HD12	1:EEE:30:VAL:CG1	2.17	0.75
1:AAA:260:GLN:OE1	1:AAA:260:GLN:HA	1.88	0.74
1:EEE:120:PHE:CD1	1:EEE:121:GLU:N	2.57	0.73

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	253/265 (96%)	250 (99%)	3 (1%)	0	100	100
1	BBB	255/265 (96%)	252 (99%)	2 (1%)	1 (0%)	34	37
1	CCC	262/265 (99%)	259 (99%)	3 (1%)	0	100	100
1	DDD	246/265 (93%)	243 (99%)	2 (1%)	1 (0%)	34	37
1	EEE	252/265 (95%)	248 (98%)	3 (1%)	1 (0%)	34	37
1	FFF	243/265 (92%)	241 (99%)	2 (1%)	0	100	100
2	GGG	14/20 (70%)	12 (86%)	2 (14%)	0	100	100
2	HHH	14/20 (70%)	14 (100%)	0	0	100	100
2	III	15/20 (75%)	13 (87%)	2 (13%)	0	100	100
2	JJJ	13/20 (65%)	13 (100%)	0	0	100	100
2	KKK	15/20 (75%)	14 (93%)	1 (7%)	0	100	100
2	LLL	12/20 (60%)	11 (92%)	1 (8%)	0	100	100
All	All	1594/1710 (93%)	1570 (98%)	21 (1%)	3 (0%)	47	55

All (3) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [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	217/224 (97%)	213 (98%)	4 (2%)	59	72
1	BBB	218/224 (97%)	218 (100%)	0	100	100
1	CCC	224/224 (100%)	224 (100%)	0	100	100
1	DDD	212/224 (95%)	208 (98%)	4 (2%)	57	71
1	EEE	216/224 (96%)	215 (100%)	1 (0%)	88	94
1	FFF	209/224 (93%)	208 (100%)	1 (0%)	88	94
2	GGG	14/16 (88%)	14 (100%)	0	100	100
2	HHH	14/16 (88%)	14 (100%)	0	100	100
2	III	15/16 (94%)	15 (100%)	0	100	100
2	JJJ	14/16 (88%)	14 (100%)	0	100	100
2	KKK	15/16 (94%)	15 (100%)	0	100	100
2	LLL	12/16 (75%)	12 (100%)	0	100	100
All	All	1380/1440 (96%)	1370 (99%)	10 (1%)	84	91

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DDD	246	TYR
1	EEE	136	TRP
1	FFF	262	ILE
1	AAA	260	GLN
1	DDD	104	LYS

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	GGG	76	2	15,16,17	0.71	0	19,22,24	0.94	1 (5%)
2	PTR	III	65	2	15,16,17	0.68	0	19,22,24	0.69	0
2	PTR	III	76	2	15,16,17	0.58	0	19,22,24	0.95	1 (5%)
2	PTR	HHH	76	2	15,16,17	0.52	0	19,22,24	0.48	0
2	PTR	KKK	65	2	15,16,17	1.25	1 (6%)	19,22,24	1.01	0
2	PTR	GGG	65	2	15,16,17	0.54	0	19,22,24	0.85	0
2	PTR	HHH	65	2	15,16,17	0.55	0	19,22,24	0.78	1 (5%)
2	PTR	LLL	76	2	15,16,17	0.57	0	19,22,24	0.82	1 (5%)
2	PTR	KKK	76	2	15,16,17	0.89	2 (13%)	19,22,24	0.73	0
2	PTR	JJJ	65	2	15,16,17	0.83	1 (6%)	19,22,24	0.83	1 (5%)
2	PTR	LLL	65	2	15,16,17	0.52	0	19,22,24	0.87	1 (5%)
2	PTR	JJJ	76	2	15,16,17	0.75	1 (6%)	19,22,24	0.90	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	GGG	76	2	-	1/10/11/13	0/1/1/1
2	PTR	III	65	2	-	0/10/11/13	0/1/1/1
2	PTR	III	76	2	-	1/10/11/13	0/1/1/1
2	PTR	HHH	76	2	-	0/10/11/13	0/1/1/1
2	PTR	KKK	65	2	-	2/10/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PTR	GGG	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	KKK	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	LLL	65	2	-	0/10/11/13	0/1/1/1
2	PTR	JJJ	76	2	-	0/10/11/13	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	KKK	65	PTR	P-OH	-3.88	1.53	1.59
2	JJJ	65	PTR	P-OH	-2.37	1.55	1.59
2	KKK	76	PTR	P-O2P	-2.25	1.46	1.54
2	JJJ	76	PTR	P-O3P	-2.01	1.47	1.54
2	KKK	76	PTR	P-OH	-2.00	1.56	1.59

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	III	76	PTR	O2P-P-OH	3.04	114.74	105.24
2	HHH	65	PTR	O3P-P-OH	2.81	114.03	105.24
2	GGG	76	PTR	O2P-P-OH	2.77	113.91	105.24
2	LLL	65	PTR	O2P-P-OH	2.16	111.99	105.24
2	JJJ	65	PTR	O3P-P-OH	2.14	111.94	105.24

There are no chirality outliers.

All (5) 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	KKK	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 monosaccharides 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	303	-	4,4,4	0.82	0	6,6,6	0.38	0
4	EDO	AAA	303	-	3,3,3	0.30	0	2,2,2	0.45	0
4	EDO	CCC	303	-	3,3,3	0.07	0	2,2,2	0.29	0
5	PEG	EEE	301	-	6,6,6	0.25	0	5,5,5	0.16	0
4	EDO	CCC	304	-	3,3,3	0.33	0	2,2,2	0.67	0
3	PO4	CCC	301	-	4,4,4	0.35	0	6,6,6	0.71	0
3	PO4	AAA	301	-	4,4,4	0.73	0	6,6,6	0.47	0
3	PO4	AAA	302	-	4,4,4	0.72	0	6,6,6	0.45	0
3	PO4	DDD	301	-	4,4,4	0.86	0	6,6,6	0.45	0
3	PO4	DDD	302	-	4,4,4	0.70	0	6,6,6	0.45	0
5	PEG	BBB	303	-	6,6,6	0.29	0	5,5,5	0.29	0
3	PO4	BBB	301	-	4,4,4	0.82	0	6,6,6	0.54	0
3	PO4	BBB	302	-	4,4,4	1.34	1 (25%)	6,6,6	0.28	0
3	PO4	CCC	302	-	4,4,4	0.63	0	6,6,6	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
5	PEG	EEE	301	-	-	3/4/4/4	-
4	EDO	CCC	303	-	-	0/1/1/1	-
4	EDO	AAA	303	-	-	1/1/1/1	-
4	EDO	CCC	304	-	-	1/1/1/1	-
5	PEG	BBB	303	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BBB	302	PO4	P-O1	2.44	1.56	1.50

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	EEE	301	PEG	1	0
5	BBB	303	PEG	2	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	1 (0%) 92 91	33, 45, 71, 105	0
1	BBB	257/265 (96%)	-0.23	1 (0%) 92 91	33, 46, 76, 129	0
1	CCC	261/265 (98%)	-0.18	2 (0%) 86 85	35, 52, 76, 122	0
1	DDD	250/265 (94%)	0.20	11 (4%) 34 32	42, 64, 118, 157	0
1	EEE	254/265 (95%)	0.37	16 (6%) 20 19	45, 75, 123, 156	0
1	FFF	247/265 (93%)	0.86	47 (19%) 1 1	50, 89, 152, 185	0
2	GGG	16/20 (80%)	0.62	1 (6%) 20 19	66, 84, 116, 126	0
2	HHH	16/20 (80%)	0.17	1 (6%) 20 19	45, 74, 106, 129	0
2	III	17/20 (85%)	-0.10	0 100 100	49, 70, 98, 118	0
2	JJJ	15/20 (75%)	0.04	0 100 100	43, 60, 115, 123	0
2	KKK	17/20 (85%)	-0.08	0 100 100	41, 64, 99, 127	0
2	LLL	13/20 (65%)	1.01	3 (23%) 0 0	60, 103, 132, 134	0
All	All	1618/1710 (94%)	0.14	83 (5%) 28 26	33, 59, 123, 185	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	FFF	143	LEU	7.6
1	EEE	136	TRP	7.3
1	FFF	158	ILE	6.7
1	EEE	223	THR	5.4
1	FFF	129	ARG	5.3

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	LLL	65	16/17	0.92	0.13	76,88,105,113	0
2	PTR	GGG	65	16/17	0.96	0.11	70,81,90,92	0
2	PTR	III	65	16/17	0.97	0.11	50,56,62,64	0
2	PTR	JJJ	65	16/17	0.97	0.11	35,46,50,52	0
2	PTR	GGG	76	16/17	0.97	0.11	45,60,74,78	0
2	PTR	III	76	16/17	0.98	0.10	49,52,59,64	0
2	PTR	HHH	76	16/17	0.98	0.11	33,40,48,49	0
2	PTR	KKK	65	16/17	0.98	0.12	37,46,51,53	0
2	PTR	HHH	65	16/17	0.98	0.12	52,61,66,68	0
2	PTR	LLL	76	16/17	0.98	0.10	59,72,79,80	0
2	PTR	JJJ	76	16/17	0.99	0.12	33,38,45,46	0
2	PTR	KKK	76	16/17	0.99	0.10	34,41,51,52	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(Å ²)	Q<0.9
5	PEG	EEE	301	7/7	0.69	0.27	82,92,110,115	0
3	PO4	AAA	302	5/5	0.74	0.20	112,132,135,140	0
4	EDO	AAA	303	4/4	0.78	0.19	67,72,74,75	0
3	PO4	DDD	303	5/5	0.79	0.31	110,122,129,149	0
5	PEG	BBB	303	7/7	0.84	0.20	63,68,70,71	0
4	EDO	CCC	304	4/4	0.85	0.15	61,68,69,71	0
3	PO4	BBB	302	5/5	0.86	0.14	81,84,96,98	0
3	PO4	CCC	302	5/5	0.88	0.14	82,90,114,115	0
4	EDO	CCC	303	4/4	0.89	0.14	63,63,67,71	0
3	PO4	CCC	301	5/5	0.89	0.13	73,83,90,95	0
3	PO4	DDD	302	5/5	0.90	0.11	87,89,103,104	0
3	PO4	BBB	301	5/5	0.92	0.09	63,80,92,94	0
3	PO4	AAA	301	5/5	0.93	0.08	81,90,102,103	0
3	PO4	DDD	301	5/5	0.94	0.08	72,79,89,93	0

6.5 Other polymers [i](#)

There are no such residues in this entry.