



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 20, 2024 – 11:43 pm GMT

PDB ID : 7Q5W
Title : The tandem SH2 domains of SYK with a bound TYROBP 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 : 4.02b-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

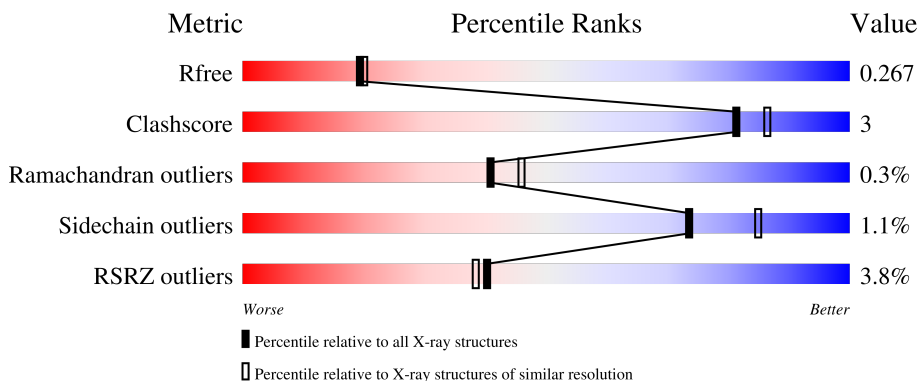
1 Overall quality at a glance

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	 2% 91% 5%
1	BBB	265	 2% 89% 6%
1	CCC	265	 % 91% 5%
1	DDD	265	 2% 89% 8%
1	EEE	265	 8% 88% 8%

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Mol	Chain	Length	Quality of chain
1	FFF	265	<p>6% 90% 6%</p>
2	GGG	20	<p>65% 25% 10%</p>
2	HHH	20	<p>10% 60% 25% 15%</p>
2	III	20	<p>20% 85% 15%</p>
2	JJJ	20	<p>75% 15% 10%</p>
2	KKK	20	<p>80% 5% 15%</p>
2	LLL	20	<p>5% 85% 15%</p>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13517 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	254	2032	1291	364	371	6	0	0	0
1	BBB	254	2032	1291	364	371	6	0	0	0
1	CCC	254	2032	1289	364	373	6	0	0	0
1	DDD	257	2049	1300	367	376	6	0	0	0
1	EEE	254	2038	1295	364	373	6	0	1	0
1	FFF	255	2040	1295	365	374	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 TYRO protein tyrosine kinase-binding protein.

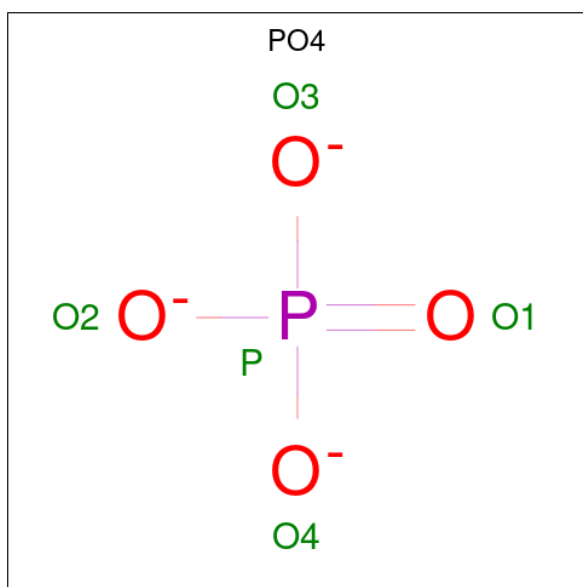
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	GGG	18	157	90	25	40	2	0	0	0
2	HHH	17	149	86	24	37	2	0	0	0
2	III	17	149	86	24	37	2	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	JJJ	18	Total	C	N	O	P	0	0	0
			155	89	25	39	2			
2	KKK	17	Total	C	N	O	P	0	0	0
			149	86	24	37	2			
2	LLL	20	Total	C	N	O	P	0	0	0
			172	98	27	45	2			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



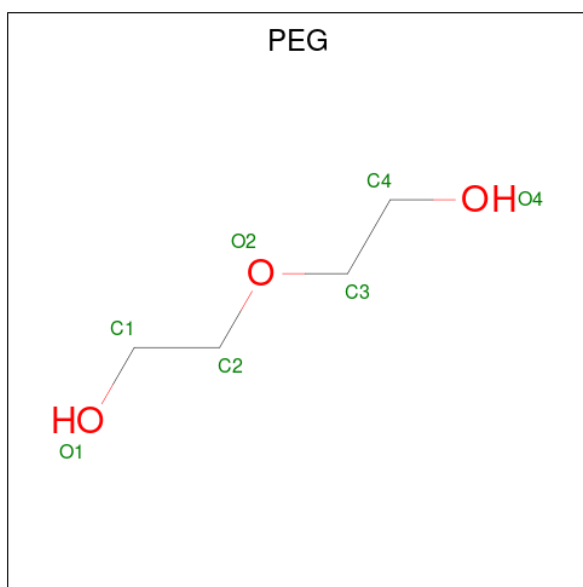
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	1	Total	O P	0	0
			5	4 1		
3	BBB	1	Total	O P	0	0
			5	4 1		
3	CCC	1	Total	O P	0	0
			5	4 1		
3	DDD	1	Total	O P	0	0
			5	4 1		
3	EEE	1	Total	O P	0	0
			5	4 1		
3	FFF	1	Total	O P	0	0
			5	4 1		

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



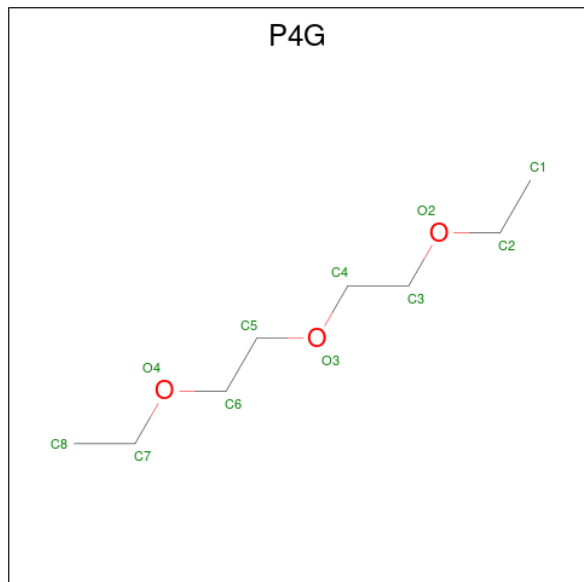
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C O 4 2 2	0	0
4	BBB	1	Total C O 4 2 2	0	0
4	DDD	1	Total C O 4 2 2	0	0

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



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

- Molecule 6 is 1-ETHOXY-2-(2-ETHOXYETHOXY)ETHANE (three-letter code: P4G) (formula: C₈H₁₈O₃).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	51	Total	O	0	0
			51	51		
7	BBB	56	Total	O	0	0
			56	56		
7	CCC	40	Total	O	0	0
			40	40		
7	DDD	61	Total	O	0	0
			61	61		
7	EEE	33	Total	O	0	0
			33	33		
7	FFF	32	Total	O	0	0
			32	32		
7	GGG	9	Total	O	0	0
			9	9		
7	HHH	1	Total	O	0	0
			1	1		
7	III	3	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	JJJ	4	Total O 4 4	0	0
7	KKK	3	Total O 3 3	0	0
7	LLL	10	Total O 10 10	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: 



- Molecule 1: Tyrosine-protein kinase SYK

Chain BBB: 



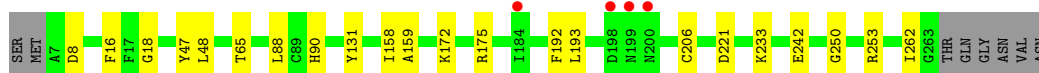
- Molecule 1: Tyrosine-protein kinase SYK

Chain CCC: 




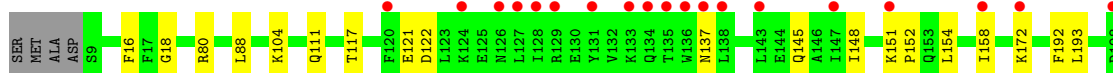
- Molecule 1: Tyrosine-protein kinase SYK

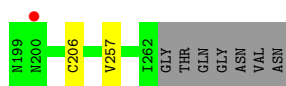
Chain DDD: 



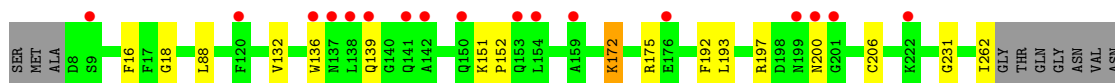
- Molecule 1: Tyrosine-protein kinase SYK

Chain EEE: 

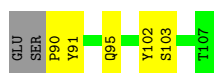




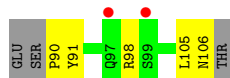
- Molecule 1: Tyrosine-protein kinase SYK



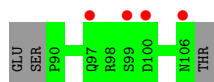
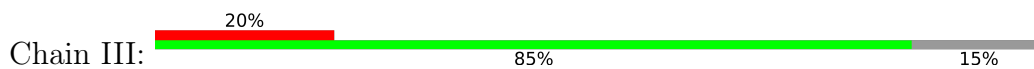
- Molecule 2: TYRO protein tyrosine kinase-binding protein



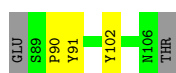
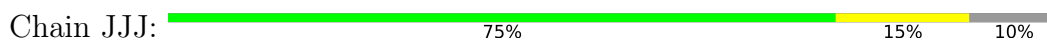
- Molecule 2: TYRO protein tyrosine kinase-binding protein



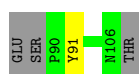
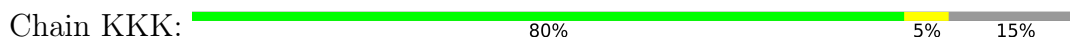
- Molecule 2: TYRO protein tyrosine kinase-binding protein



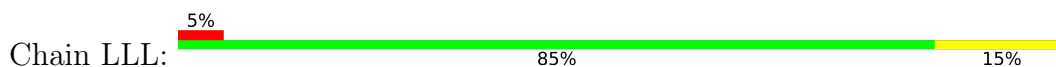
- Molecule 2: TYRO protein tyrosine kinase-binding protein

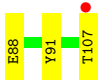


- Molecule 2: TYRO protein tyrosine kinase-binding protein



- Molecule 2: TYRO protein tyrosine kinase-binding protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.95Å 131.93Å 141.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.96 – 2.20 65.96 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (65.96-2.20) 100.0 (65.96-2.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.234 , 0.266 0.237 , 0.267	Depositor DCC
R_{free} test set	2018 reflections (1.80%)	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtrriage
Anisotropy	0.379	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13517	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.64 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.7429e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PTR, PO4, EDO, PEG, P4G

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	0.66	0/2079	0.80	0/2804
1	BBB	0.67	0/2079	0.79	0/2804
1	CCC	0.66	0/2079	0.77	0/2804
1	DDD	0.67	0/2096	0.77	0/2827
1	EEE	0.66	0/2088	0.79	1/2816 (0.0%)
1	FFF	0.66	0/2087	0.76	0/2815
2	GGG	0.67	0/123	0.90	0/160
2	HHH	0.63	0/115	1.02	0/150
2	III	0.70	0/115	0.87	0/150
2	JJJ	0.70	0/121	0.84	0/159
2	KKK	0.61	0/115	0.85	0/150
2	LLL	0.83	0/138	0.95	0/181
All	All	0.66	0/13235	0.79	1/17820 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	EEE	80	ARG	NE-CZ-NH2	-5.68	117.46	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2032	0	2024	8	0
1	BBB	2032	0	2024	10	0
1	CCC	2032	0	2017	8	0
1	DDD	2049	0	2036	15	0
1	EEE	2038	0	2030	15	0
1	FFF	2040	0	2028	11	0
2	GGG	157	0	129	3	0
2	HHH	149	0	122	3	0
2	III	149	0	122	0	0
2	JJJ	155	0	126	1	0
2	KKK	149	0	122	0	0
2	LLL	172	0	139	2	0
3	AAA	5	0	0	0	0
3	BBB	5	0	0	0	0
3	CCC	5	0	0	0	0
3	DDD	5	0	0	0	0
3	EEE	5	0	0	0	0
3	FFF	5	0	0	0	0
4	AAA	4	0	6	0	0
4	BBB	4	0	6	0	0
4	DDD	4	0	6	0	0
5	CCC	7	0	10	0	0
6	EEE	11	0	18	0	0
7	AAA	51	0	0	2	0
7	BBB	56	0	0	1	0
7	CCC	40	0	0	0	0
7	DDD	61	0	0	2	0
7	EEE	33	0	0	1	0
7	FFF	32	0	0	1	0
7	GGG	9	0	0	0	0
7	HHH	1	0	0	0	0
7	III	3	0	0	0	0
7	JJJ	4	0	0	0	0
7	KKK	3	0	0	0	0
7	LLL	10	0	0	0	0
All	All	13517	0	12965	68	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 3.

All (68) 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:CCC:150:GLN:O	1:CCC:154:LEU:HD23	1.74	0.86
1:AAA:35:SER:OG	7:AAA:401:HOH:O	2.11	0.68
1:EEE:117:THR:HG23	1:EEE:121[A]:GLU:HB3	1.78	0.66
1:CCC:150:GLN:O	1:CCC:154:LEU:CD2	2.48	0.61
1:DDD:131:TYR:CB	1:DDD:158:ILE:HD11	2.30	0.60
2:GGG:103:SER:HG	2:LLL:88:GLU:N	1.99	0.59
1:EEE:145:GLN:O	1:EEE:148:ILE:HG12	2.03	0.58
1:CCC:59:ARG:HH12	1:FFF:262:ILE:HB	1.70	0.56
1:EEE:117:THR:HG21	1:EEE:122:ASP:OD1	2.07	0.55
1:DDD:131:TYR:CG	1:DDD:158:ILE:HD11	2.42	0.54
1:BBB:170:HIS:CE1	1:BBB:259:CYS:O	2.62	0.53
1:AAA:193:LEU:C	1:AAA:193:LEU:HD12	2.30	0.52
1:FFF:172:LYS:HE2	1:FFF:197:ARG:O	2.09	0.52
1:BBB:193:LEU:C	1:BBB:193:LEU:HD12	2.30	0.52
1:EEE:193:LEU:C	1:EEE:193:LEU:HD12	2.30	0.52
1:CCC:193:LEU:HD12	1:CCC:193:LEU:C	2.31	0.51
1:FFF:193:LEU:C	1:FFF:193:LEU:HD12	2.31	0.51
1:DDD:193:LEU:C	1:DDD:193:LEU:HD12	2.31	0.51
2:HHH:105:LEU:O	2:HHH:106:ASN:HB2	2.10	0.51
1:FFF:175:ARG:NH2	2:HHH:90:PRO:O	2.29	0.50
1:BBB:129:ARG:NH1	7:BBB:401:HOH:O	2.43	0.50
1:BBB:230:GLU:OE2	1:FFF:200:ASN:HB2	2.12	0.49
1:EEE:145:GLN:HA	1:EEE:148:ILE:HD11	1.95	0.49
1:EEE:117:THR:CG2	1:EEE:122:ASP:OD1	2.61	0.49
1:AAA:180:GLN:O	1:AAA:184:ILE:HG12	2.14	0.48
1:EEE:145:GLN:HA	1:EEE:148:ILE:CD1	2.43	0.48
1:DDD:48:LEU:HD21	1:DDD:159:ALA:HB3	1.98	0.46
1:DDD:250:GLY:HA2	2:GGG:95:GLN:O	2.16	0.46
2:LLL:107:THR:HG22	2:LLL:107:THR:O	2.15	0.46
1:DDD:221:ASP:OD2	1:DDD:233:LYS:HE3	2.16	0.45
1:CCC:150:GLN:C	1:CCC:154:LEU:HD23	2.33	0.45
1:DDD:242:GLU:HG3	7:DDD:425:HOH:O	2.16	0.45
1:DDD:175:ARG:NH2	2:GGG:90:PRO:O	2.43	0.45
1:FFF:16:PHE:CZ	1:FFF:18:GLY:HA2	2.52	0.45
1:EEE:154:LEU:O	1:EEE:158:ILE:HG23	2.16	0.44
1:AAA:175:ARG:NH2	2:JJJ:90:PRO:O	2.29	0.44
1:AAA:109:ARG:NH2	7:AAA:403:HOH:O	2.41	0.44
1:CCC:16:PHE:CZ	1:CCC:18:GLY:HA2	2.53	0.44
1:FFF:151:LYS:N	1:FFF:152:PRO:HD2	2.33	0.44
1:CCC:221:ASP:OD2	1:CCC:233:LYS:HE3	2.16	0.44
1:EEE:16:PHE:CZ	1:EEE:18:GLY:HA2	2.53	0.43
1:EEE:151:LYS:N	1:EEE:152:PRO:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:88:LEU:C	1:BBB:88:LEU:HD23	2.38	0.43
1:BBB:170:HIS:HE1	1:BBB:259:CYS:O	1.99	0.43
1:CCC:88:LEU:C	1:CCC:88:LEU:HD23	2.39	0.43
1:DDD:16:PHE:CZ	1:DDD:18:GLY:HA2	2.53	0.43
1:EEE:137:ASN:O	1:EEE:137:ASN:OD1	2.37	0.43
1:AAA:16:PHE:CZ	1:AAA:18:GLY:HA2	2.53	0.43
1:BBB:16:PHE:CZ	1:BBB:18:GLY:HA2	2.54	0.43
1:AAA:88:LEU:C	1:AAA:88:LEU:HD23	2.38	0.43
1:FFF:88:LEU:HD23	1:FFF:88:LEU:C	2.39	0.42
1:DDD:90:HIS:HB3	7:FFF:413:HOH:O	2.19	0.42
1:FFF:132:VAL:HG12	1:FFF:136:TRP:CZ3	2.53	0.42
1:DDD:131:TYR:HB2	1:DDD:158:ILE:HD11	2.02	0.42
1:EEE:88:LEU:C	1:EEE:88:LEU:HD23	2.39	0.42
1:BBB:68:ARG:HH21	1:BBB:152:PRO:HG3	1.83	0.42
1:DDD:47:TYR:CD1	1:DDD:65:THR:HG21	2.55	0.42
1:DDD:88:LEU:C	1:DDD:88:LEU:HD23	2.40	0.42
1:BBB:151:LYS:N	1:BBB:152:PRO:HD2	2.36	0.41
1:EEE:117:THR:HG23	1:EEE:121[A]:GLU:CB	2.49	0.41
1:FFF:192:PHE:HA	1:FFF:206:CYS:O	2.20	0.41
1:EEE:257:VAL:HG21	7:EEE:433:HOH:O	2.20	0.41
1:BBB:192:PHE:HA	1:BBB:206:CYS:O	2.21	0.41
1:DDD:192:PHE:HA	1:DDD:206:CYS:O	2.21	0.41
1:EEE:192:PHE:HA	1:EEE:206:CYS:O	2.21	0.41
1:AAA:39:TYR:CE2	1:AAA:103:LEU:HB3	2.56	0.40
1:DDD:253:ARG:HD3	7:DDD:422:HOH:O	2.20	0.40
1:FFF:231:GLY:HA2	2:HHH:98:ARG:HD2	2.04	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	252/265 (95%)	247 (98%)	5 (2%)	0	100	100
1	BBB	252/265 (95%)	245 (97%)	6 (2%)	1 (0%)	34	37
1	CCC	252/265 (95%)	244 (97%)	6 (2%)	2 (1%)	19	19
1	DDD	255/265 (96%)	247 (97%)	7 (3%)	1 (0%)	34	37
1	EEE	253/265 (96%)	246 (97%)	7 (3%)	0	100	100
1	FFF	253/265 (96%)	244 (96%)	9 (4%)	0	100	100
2	GGG	14/20 (70%)	13 (93%)	1 (7%)	0	100	100
2	HHH	13/20 (65%)	12 (92%)	1 (8%)	0	100	100
2	III	13/20 (65%)	12 (92%)	1 (8%)	0	100	100
2	JJJ	14/20 (70%)	13 (93%)	1 (7%)	0	100	100
2	KKK	13/20 (65%)	12 (92%)	1 (8%)	0	100	100
2	LLL	16/20 (80%)	14 (88%)	2 (12%)	0	100	100
All	All	1600/1710 (94%)	1549 (97%)	47 (3%)	4 (0%)	41	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	10	ALA
1	CCC	10	ALA
1	CCC	198	ASP
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	216/224 (96%)	213 (99%)	3 (1%)	67	80
1	BBB	216/224 (96%)	213 (99%)	3 (1%)	67	80
1	CCC	216/224 (96%)	214 (99%)	2 (1%)	78	88
1	DDD	217/224 (97%)	215 (99%)	2 (1%)	78	88
1	EEE	217/224 (97%)	214 (99%)	3 (1%)	67	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	FFF	217/224 (97%)	215 (99%)	2 (1%)	78	88
2	GGG	15/17 (88%)	15 (100%)	0	100	100
2	HHH	14/17 (82%)	14 (100%)	0	100	100
2	III	14/17 (82%)	14 (100%)	0	100	100
2	JJJ	15/17 (88%)	15 (100%)	0	100	100
2	KKK	14/17 (82%)	14 (100%)	0	100	100
2	LLL	17/17 (100%)	17 (100%)	0	100	100
All	All	1388/1446 (96%)	1373 (99%)	15 (1%)	73	85

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	111	GLN
1	AAA	156	LYS
1	AAA	172	LYS
1	BBB	111	GLN
1	BBB	165	LYS
1	BBB	172	LYS
1	CCC	102	LEU
1	CCC	172	LYS
1	DDD	8	ASP
1	DDD	172	LYS
1	EEE	104	LYS
1	EEE	111	GLN
1	EEE	172	LYS
1	FFF	139	GLN
1	FFF	172	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	KKK	91	2	15,16,17	0.59	0	19,22,24	0.93	1 (5%)
2	PTR	KKK	102	2	15,16,17	0.48	0	19,22,24	0.56	0
2	PTR	GGG	91	2	15,16,17	0.45	0	19,22,24	0.91	1 (5%)
2	PTR	GGG	102	2	15,16,17	0.69	0	19,22,24	0.73	1 (5%)
2	PTR	III	91	2	15,16,17	0.59	0	19,22,24	0.47	0
2	PTR	III	102	2	15,16,17	0.67	0	19,22,24	0.52	0
2	PTR	HHH	102	2	15,16,17	0.57	0	19,22,24	0.69	0
2	PTR	JJJ	91	2	15,16,17	0.59	0	19,22,24	1.20	2 (10%)
2	PTR	LLL	91	2	15,16,17	0.52	0	19,22,24	0.88	2 (10%)
2	PTR	HHH	91	2	15,16,17	0.61	0	19,22,24	0.75	1 (5%)
2	PTR	JJJ	102	2	15,16,17	0.54	0	19,22,24	0.79	1 (5%)
2	PTR	LLL	102	2	15,16,17	0.59	0	19,22,24	0.79	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	KKK	91	2	-	0/10/11/13	0/1/1/1
2	PTR	KKK	102	2	-	0/10/11/13	0/1/1/1
2	PTR	GGG	91	2	-	0/10/11/13	0/1/1/1
2	PTR	GGG	102	2	-	0/10/11/13	0/1/1/1
2	PTR	III	91	2	-	0/10/11/13	0/1/1/1
2	PTR	III	102	2	-	0/10/11/13	0/1/1/1
2	PTR	HHH	102	2	-	0/10/11/13	0/1/1/1
2	PTR	JJJ	91	2	-	0/10/11/13	0/1/1/1
2	PTR	LLL	91	2	-	0/10/11/13	0/1/1/1
2	PTR	HHH	91	2	-	0/10/11/13	0/1/1/1
2	PTR	JJJ	102	2	-	0/10/11/13	0/1/1/1
2	PTR	LLL	102	2	-	0/10/11/13	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	JJJ	91	PTR	O2P-P-OH	3.94	117.56	105.24
2	GGG	91	PTR	O3P-P-OH	3.35	115.71	105.24
2	KKK	91	PTR	O3P-P-OH	3.19	115.22	105.24
2	JJJ	91	PTR	OH-P-O1P	-2.81	98.72	109.31
2	JJJ	102	PTR	O3P-P-OH	2.37	112.64	105.24
2	GGG	102	PTR	O2P-P-OH	2.26	112.31	105.24
2	HHH	91	PTR	O3P-P-OH	2.21	112.14	105.24
2	LLL	91	PTR	O3P-P-OH	2.14	111.92	105.24
2	LLL	91	PTR	OH-P-O1P	-2.01	101.73	109.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 ligands are modelled in this entry.

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	$\# Z > 2$
4	EDO	AAA	302	-	3,3,3	0.13	0	2,2,2	0.07	0
4	EDO	BBB	302	-	3,3,3	0.18	0	2,2,2	0.36	0
4	EDO	DDD	302	-	3,3,3	0.28	0	2,2,2	0.33	0
3	PO4	DDD	301	-	4,4,4	0.63	0	6,6,6	0.45	0
5	PEG	CCC	302	-	6,6,6	0.15	0	5,5,5	0.07	0
3	PO4	CCC	301	-	4,4,4	0.61	0	6,6,6	0.49	0
3	PO4	EEE	301	-	4,4,4	0.73	0	6,6,6	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	BBB	301	-	4,4,4	0.70	0	6,6,6	0.40	0
3	PO4	AAA	301	-	4,4,4	0.97	0	6,6,6	0.37	0
6	P4G	EEE	302	-	10,10,10	0.43	0	9,9,9	0.32	0
3	PO4	FFF	301	-	4,4,4	0.65	0	6,6,6	0.45	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	AAA	302	-	-	1/1/1/1	-
4	EDO	BBB	302	-	-	0/1/1/1	-
4	EDO	DDD	302	-	-	0/1/1/1	-
5	PEG	CCC	302	-	-	2/4/4/4	-
6	P4G	EEE	302	-	-	3/8/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	EEE	302	P4G	O2-C3-C4-O3
5	CCC	302	PEG	O2-C3-C4-O4
4	AAA	302	EDO	O1-C1-C2-O2
6	EEE	302	P4G	C1-C2-O2-C3
6	EEE	302	P4G	C8-C7-O4-C6
5	CCC	302	PEG	C1-C2-O2-C3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	254/265 (95%)	-0.11	5 (1%) 65 63	36, 54, 86, 143	0
1	BBB	254/265 (95%)	0.05	5 (1%) 65 63	31, 57, 89, 133	0
1	CCC	254/265 (95%)	0.05	3 (1%) 79 77	38, 61, 93, 156	0
1	DDD	257/265 (96%)	0.08	4 (1%) 72 70	32, 55, 90, 133	0
1	EEE	254/265 (95%)	0.27	20 (7%) 12 11	38, 64, 126, 151	0
1	FFF	255/265 (96%)	0.28	17 (6%) 17 16	42, 62, 124, 158	0
2	GGG	16/20 (80%)	0.28	0 100 100	40, 79, 110, 122	0
2	HHH	15/20 (75%)	0.40	2 (13%) 3 3	57, 84, 109, 115	0
2	III	15/20 (75%)	1.10	4 (26%) 0 0	62, 83, 114, 121	0
2	JJJ	16/20 (80%)	0.43	0 100 100	59, 80, 108, 112	0
2	KKK	15/20 (75%)	0.11	0 100 100	62, 86, 103, 104	0
2	LLL	18/20 (90%)	0.46	1 (5%) 24 23	39, 69, 108, 117	0
All	All	1623/1710 (94%)	0.12	61 (3%) 40 38	31, 59, 108, 158	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	200	ASN	7.1
1	FFF	137	ASN	6.1
1	CCC	199	ASN	5.4
1	BBB	201	GLY	5.4
1	FFF	142	ALA	5.2
2	LLL	107	THR	4.8
1	AAA	200	ASN	4.5
1	DDD	198	ASP	4.4
1	CCC	198	ASP	4.3
2	III	97	GLN	4.0
1	BBB	199	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	EEE	137	ASN	4.0
1	EEE	129	ARG	3.9
1	EEE	134	GLN	3.7
1	AAA	198	ASP	3.7
1	DDD	199	ASN	3.7
1	FFF	199	ASN	3.6
2	III	106	ASN	3.6
1	CCC	200	ASN	3.5
1	AAA	199	ASN	3.5
1	FFF	222	LYS	3.5
1	EEE	135	THR	3.4
2	III	100	ASP	3.3
1	EEE	200	ASN	3.2
2	III	99	SER	3.2
1	FFF	159	ALA	3.2
1	AAA	201	GLY	3.1
1	FFF	201	GLY	3.1
1	EEE	198	ASP	3.0
1	FFF	120	PHE	2.9
1	FFF	200	ASN	2.8
1	EEE	131	TYR	2.7
1	EEE	158	ILE	2.7
1	EEE	120	PHE	2.6
1	DDD	200	ASN	2.6
1	EEE	136	TRP	2.6
1	EEE	124	LYS	2.6
1	FFF	176	GLU	2.6
1	EEE	147	ILE	2.6
1	EEE	172	LYS	2.5
1	FFF	153	GLN	2.5
1	FFF	9	SER	2.5
1	EEE	127	LEU	2.3
1	EEE	143	LEU	2.3
1	FFF	136	TRP	2.3
1	FFF	154	LEU	2.3
1	EEE	133	LYS	2.3
1	FFF	150	GLN	2.3
1	FFF	139	GLN	2.2
1	AAA	222	LYS	2.2
1	FFF	141	GLN	2.2
1	EEE	128	ILE	2.2
1	EEE	151	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	BBB	70	LEU	2.2
1	EEE	138	LEU	2.2
1	FFF	138	LEU	2.1
1	DDD	184	ILE	2.1
1	EEE	126	ASN	2.1
2	HHH	99	SER	2.0
2	HHH	97	GLN	2.0
1	BBB	198	ASP	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	HHH	91	16/17	0.93	0.10	61,70,89,98	0
2	PTR	GGG	91	16/17	0.94	0.14	52,67,86,91	0
2	PTR	III	91	16/17	0.94	0.15	76,80,92,94	0
2	PTR	JJJ	91	16/17	0.96	0.10	49,57,74,77	0
2	PTR	KKK	91	16/17	0.96	0.15	50,62,79,82	0
2	PTR	HHH	102	16/17	0.97	0.13	39,63,67,69	0
2	PTR	III	102	16/17	0.97	0.12	40,55,62,71	0
2	PTR	LLL	102	16/17	0.97	0.14	40,54,68,68	0
2	PTR	KKK	102	16/17	0.98	0.13	42,57,69,73	0
2	PTR	LLL	91	16/17	0.98	0.13	35,40,52,52	0
2	PTR	JJJ	102	16/17	0.98	0.11	40,59,66,67	0
2	PTR	GGG	102	16/17	0.99	0.14	37,43,54,58	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	P4G	EEE	302	11/11	0.34	0.28	87,101,105,108	0
4	EDO	DDD	302	4/4	0.68	0.17	63,66,67,72	0
3	PO4	DDD	301	5/5	0.78	0.15	110,112,123,125	0
5	PEG	CCC	302	7/7	0.82	0.13	96,98,105,109	0
4	EDO	BBB	302	4/4	0.88	0.13	54,56,59,62	0
3	PO4	CCC	301	5/5	0.89	0.11	89,103,108,110	0
3	PO4	FFF	301	5/5	0.93	0.10	87,91,98,100	0
4	EDO	AAA	302	4/4	0.93	0.11	58,61,61,62	0
3	PO4	AAA	301	5/5	0.93	0.08	92,95,103,106	0
3	PO4	BBB	301	5/5	0.95	0.08	76,80,91,104	0
3	PO4	EEE	301	5/5	0.96	0.08	89,98,100,106	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.