



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 19, 2019 – 01:14 PM EDT

PDB ID : 2Q7X  
Title : Crystal structure of a putative phospho transferase (sp\_1565) from streptococcus pneumoniae tigr4 at 2.00 Å resolution  
Authors : Joint Center for Structural Genomics (JCSG)  
Deposited on : 2007-06-07  
Resolution : 2.00 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : 2.3.2  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.3.2

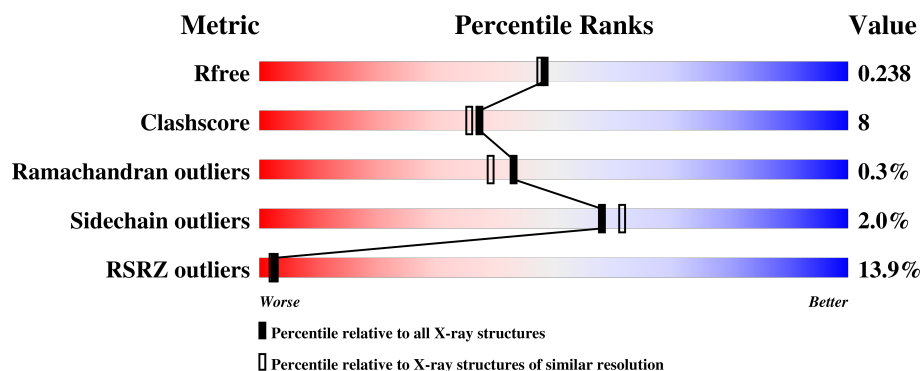
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	111664	7193 (2.00-2.00)
Clashscore	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)
RSRZ outliers	108989	7011 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	A	326	<div> <div>13%</div> <div>79%</div> <div>17%</div> <div>• •</div> </div>
1	B	326	<div> <div>12%</div> <div>81%</div> <div>12%</div> <div>• 6%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5147 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 UPF0052 protein SP\_1565.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	Se	0	5	0
			2465	1560	419	474	2	10			
1	B	305	Total	C	N	O	S	Se	0	7	0
			2385	1516	408	451	2	8			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	LEADER SEQUENCE	UNP Q97PN8
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
A	3	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
A	5	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
A	20	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
A	25	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
A	47	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
A	49	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
A	65	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
A	68	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
A	70	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
A	74	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
A	103	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
A	111	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
A	116	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
A	123	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
A	186	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
A	205	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
A	215	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
A	225	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
A	261	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
A	267	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
A	288	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
A	318	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
A	324	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8

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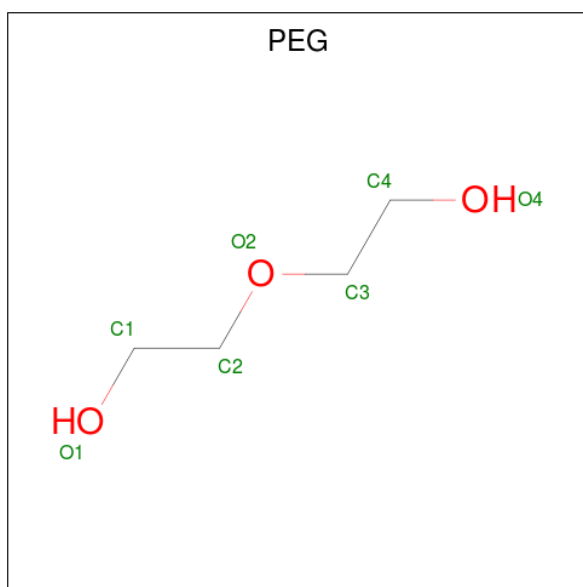
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Chain	Residue	Modelled	Actual	Comment	Reference
A	325	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
B	0	GLY	-	LEADER SEQUENCE	UNP Q97PN8
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
B	3	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
B	5	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
B	20	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
B	25	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
B	47	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
B	49	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
B	65	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
B	68	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
B	70	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
B	74	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
B	103	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
B	111	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
B	116	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
B	123	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
B	186	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
B	205	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
B	215	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
B	225	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
B	261	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
B	267	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
B	288	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
B	318	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
B	324	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
B	325	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

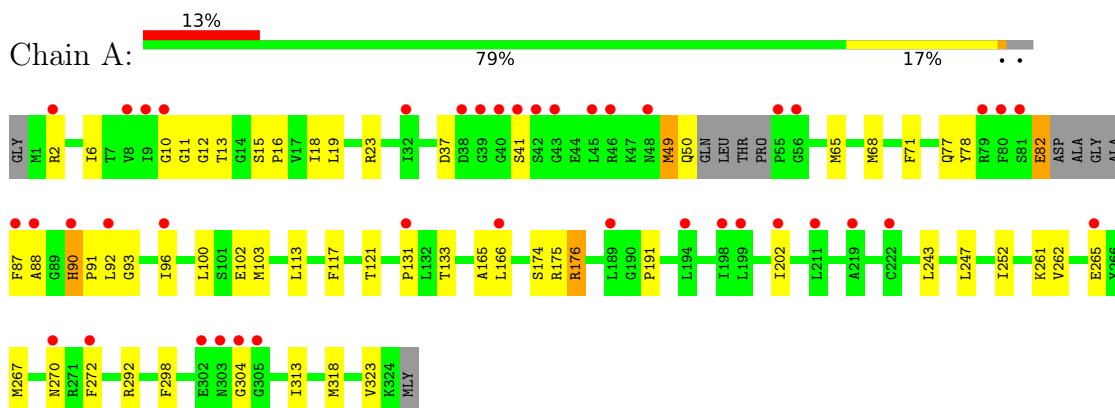
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	163	Total	O	0	0
			163	163		
4	B	119	Total	O	0	0
			119	119		

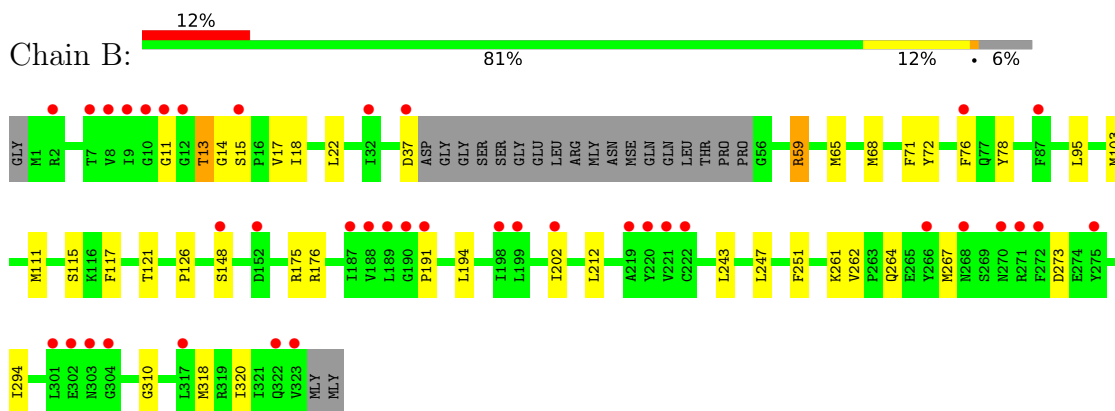
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: UPF0052 protein SP\_1565



#### • Molecule 1: UPF0052 protein SP\_1565



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.52Å 69.35Å 169.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.55 – 2.00 29.55 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.55-2.00) 99.7 (29.55-2.00)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019, PHENIX	Depositor
R, $R_{free}$	0.195 , 0.236 0.197 , 0.238	Depositor DCC
$R_{free}$ test set	2656 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.1	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 54.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5147	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PEG, MLY, CL

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	A	0.83	0/2380	0.84	2/3221 (0.1%)
1	B	0.70	0/2310	0.75	0/3132
All	All	0.77	0/4690	0.80	2/6353 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	ARG	NE-CZ-NH1	9.51	125.05	120.30
1	A	292	ARG	NE-CZ-NH2	-8.09	116.25	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	175	ARG	Peptide
1	B	13	THR	Peptide



## 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	A	2465	0	2395	46	0
1	B	2385	0	2330	44	0
2	A	1	0	0	0	0
3	A	14	0	20	0	0
4	A	163	0	0	1	0
4	B	119	0	0	0	0
All	All	5147	0	4745	81	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 8.

All (81) 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:B:212:LEU:HD21	1:B:247[A]:LEU:CD2	1.98	0.93
1:B:11[B]:GLY:HA2	1:B:191:PRO:O	1.71	0.88
1:A:261:MLY:HH13	1:A:267:MSE:HE1	1.55	0.87
1:A:103:MSE:HE2	1:B:78:TYR:HB2	1.67	0.74
1:A:90:HIS:ND1	1:A:91:PRO:HD2	2.02	0.74
1:A:18:ILE:HD12	1:A:191:PRO:HD3	1.70	0.73
1:B:175:ARG:O	1:B:176:ARG:HB2	1.89	0.73
1:A:261:MLY:HH12	1:A:262:VAL:O	1.89	0.72
1:A:270:ASN:OD1	1:A:304:GLY:HA2	1.91	0.71
1:B:261:MLY:HH12	1:B:267:MSE:HE1	1.74	0.70
1:B:212:LEU:CD2	1:B:247[A]:LEU:HD21	2.22	0.69
1:B:262:VAL:O	1:B:267:MSE:HE2	1.92	0.69
1:B:212:LEU:CG	1:B:247[A]:LEU:HD21	2.23	0.68
1:B:212:LEU:HD21	1:B:247[A]:LEU:HD21	1.75	0.68
1:A:92:LEU:HD23	1:A:93:GLY:N	2.10	0.67
1:A:82:GLU:OE2	1:A:87:PHE:N	2.28	0.67
1:A:68:MSE:HE3	1:A:71:PHE:CD2	2.30	0.67
1:B:212:LEU:HG	1:B:247[A]:LEU:HD21	1.77	0.66
1:A:37:ASP:OD1	1:A:133:THR:HG23	1.96	0.66
1:B:212:LEU:HD21	1:B:247[A]:LEU:HD22	1.76	0.66
1:A:18:ILE:HD12	1:A:191:PRO:CD	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:MLY:CH1	1:A:267:MSE:HE1	2.25	0.65
1:A:243:LEU:HD13	1:A:252:ILE:HD11	1.78	0.63
1:B:68:MSE:HE3	1:B:71:PHE:CD2	2.35	0.61
1:A:298:PHE:CD1	1:A:313:ILE:HD13	2.35	0.61
1:A:87:PHE:HB3	1:A:88:ALA:HA	1.82	0.60
1:B:22:LEU:HD23	1:B:318:MSE:CE	2.32	0.60
1:A:2:ARG:NH2	1:A:323:VAL:HG13	2.17	0.59
1:A:96:ILE:O	1:A:100:LEU:HD13	2.05	0.57
1:A:41:SER:OG	1:A:166:LEU:HD21	2.06	0.55
1:B:13:THR:N	1:B:14:GLY:HA3	2.22	0.55
1:B:294:ILE:HD11	1:B:320:ILE:HD11	1.88	0.55
1:B:212:LEU:CD2	1:B:247[A]:LEU:CD2	2.75	0.54
1:A:267:MSE:HG2	1:A:272:PHE:CD2	2.44	0.52
1:A:18:ILE:CD1	1:A:191:PRO:HD3	2.40	0.52
1:B:72:TYR:O	1:B:76:PHE:HB2	2.10	0.51
1:A:113:LEU:HD22	1:B:71:PHE:HE1	1.75	0.50
1:B:202:ILE:O	1:B:247[B]:LEU:HD21	2.11	0.50
1:B:247[A]:LEU:HD23	1:B:247[A]:LEU:O	2.11	0.50
1:B:17:VAL:HG12	1:B:310:GLY:HA3	1.93	0.49
1:B:294:ILE:CD1	1:B:320:ILE:HD11	2.43	0.49
1:A:131:PRO:HB2	1:A:165:ALA:HB3	1.96	0.48
1:A:102:GLU:OE1	1:B:78:TYR:OH	2.21	0.48
1:A:78:TYR:CB	1:B:103:MSE:HE2	2.44	0.48
1:A:6:ILE:HD11	1:A:318:MSE:HE1	1.95	0.48
1:B:11[B]:GLY:HA3	1:B:15[B]:SER:OG	2.13	0.48
1:B:264:GLN:HA	1:B:267:MSE:HE3	1.96	0.48
1:A:78:TYR:HB3	1:B:103:MSE:HE2	1.95	0.47
1:A:174:SER:O	1:A:176:ARG:HG2	2.15	0.47
1:A:49:MSE:O	1:A:49:MSE:HG3	2.14	0.46
1:B:22:LEU:HD23	1:B:318:MSE:HE2	1.97	0.45
1:A:113:LEU:HD22	1:B:71:PHE:CE1	2.51	0.45
1:B:202:ILE:HD12	1:B:247[B]:LEU:HG	1.98	0.45
1:B:22:LEU:CD2	1:B:318:MSE:CE	2.95	0.45
1:A:261:MLY:HH13	1:A:267:MSE:CE	2.38	0.45
1:B:111:MSE:CE	1:B:126:PRO:HD3	2.47	0.44
1:A:19:LEU:O	1:A:23:ARG:HG3	2.17	0.44
1:A:10[B]:GLY:O	1:A:12:GLY:N	2.50	0.44
1:A:96:ILE:HD13	1:A:117:PHE:CZ	2.52	0.44
1:B:111:MSE:HE2	1:B:126:PRO:CD	2.48	0.44
1:B:194:LEU:HD11	1:B:243:LEU:HG	2.00	0.43
1:A:65[A]:MSE:HE3	1:A:121:THR:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:PHE:CE2	1:B:95:LEU:HD21	2.53	0.43
1:A:13:THR:CG2	4:A:377:HOH:O	2.66	0.43
1:A:49:MSE:O	1:A:50:GLN:HB2	2.18	0.43
1:A:261:MLY:CH1	1:A:262:VAL:O	2.61	0.42
1:B:111:MSE:HE2	1:B:126:PRO:CG	2.49	0.42
1:B:11[A]:GLY:HA3	1:B:15[A]:SER:HB3	1.99	0.42
1:A:202:ILE:HD12	1:A:247:LEU:HB2	2.02	0.42
1:A:65[A]:MSE:O	1:A:121:THR:HG22	2.20	0.42
1:B:273:ASP:C	1:B:273:ASP:OD1	2.58	0.42
1:A:103:MSE:HE2	1:B:78:TYR:CB	2.43	0.41
1:A:15[B]:SER:N	1:A:16:PRO:CD	2.83	0.41
1:A:6:ILE:CD1	1:A:318:MSE:HE1	2.49	0.41
1:A:267:MSE:HG2	1:A:272:PHE:CE2	2.54	0.41
1:B:11[A]:GLY:CA	1:B:15[A]:SER:HB3	2.50	0.41
1:B:65:MSE:HE3	1:B:121:THR:O	2.21	0.41
1:A:15[A]:SER:N	1:A:16:PRO:CD	2.84	0.41
1:B:247[A]:LEU:HD13	1:B:251:PHE:CE1	2.56	0.41
1:A:117:PHE:CZ	1:B:117:PHE:HZ	2.39	0.40
1:B:59[B]:ARG:HG2	1:B:76:PHE:CZ	2.56	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	A	302/326 (93%)	292 (97%)	8 (3%)	2 (1%)	24	17
1	B	296/326 (91%)	287 (97%)	9 (3%)	0	100	100
All	All	598/652 (92%)	579 (97%)	17 (3%)	2 (0%)	43	39

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	GLY
1	A	77	GLN

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	258/257 (100%)	252 (98%)	6 (2%)	53	56
1	B	246/257 (96%)	240 (98%)	6 (2%)	52	54
All	All	504/514 (98%)	492 (98%)	12 (2%)	58	54

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	MSE
1	A	82	GLU
1	A	90	HIS
1	A	176	ARG
1	A	265[A]	GLU
1	A	265[B]	GLU
1	B	18	ILE
1	B	37	ASP
1	B	59[A]	ARG
1	B	59[B]	ARG
1	B	115	SER
1	B	148	SER

Some 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 ⓘ

26 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	$\# Z  > 2$
1	MLY	A	116	1	8,8,11	0.76	0	4,8,13	1.04	0
1	MLY	A	123	1	5,5,11	0.71	0	2,5,13	1.75	0
1	MLY	A	20	1	5,5,11	0.82	0	2,5,13	1.45	0
1	MLY	A	205	1	10,10,11	0.49	0	7,11,13	2.06	3 (42%)
1	MLY	A	215	1	8,8,11	0.58	0	4,8,13	1.27	1 (25%)
1	MLY	A	25	1	10,10,11	0.47	0	7,11,13	2.26	2 (28%)
1	MLY	A	261	1	10,10,11	0.83	0	7,11,13	2.12	3 (42%)
1	MLY	A	288	1	8,8,11	0.79	0	4,8,13	0.98	0
1	MLY	A	3	1	8,8,11	0.69	0	4,8,13	1.05	0
1	MLY	A	324	1	10,10,11	0.73	0	7,11,13	2.13	2 (28%)
1	MLY	A	47	1	4,4,11	0.98	0	1,4,13	0.69	0
1	MLY	A	5	1	10,10,11	0.65	0	7,11,13	2.17	4 (57%)
1	MLY	A	70	1	5,5,11	0.76	0	2,5,13	1.38	0
1	MLY	A	74	1	4,4,11	0.56	0	1,4,13	1.07	0
1	MLY	B	116	1	8,8,11	0.61	0	4,8,13	0.96	0
1	MLY	B	123	1	10,10,11	0.57	0	7,11,13	2.02	3 (42%)
1	MLY	B	20	1	8,8,11	0.53	0	4,8,13	0.91	0
1	MLY	B	205	1	6,6,11	0.65	0	3,6,13	1.28	0
1	MLY	B	215	1	5,5,11	0.81	0	2,5,13	1.64	1 (50%)
1	MLY	B	25	1	10,10,11	0.54	0	7,11,13	2.18	2 (28%)
1	MLY	B	261	1	10,10,11	0.51	0	7,11,13	2.03	2 (28%)
1	MLY	B	288	1	5,5,11	1.05	0	2,5,13	1.00	0
1	MLY	B	3	1	8,8,11	0.45	0	4,8,13	0.89	0
1	MLY	B	5	1	8,8,11	0.82	0	4,8,13	0.92	0
1	MLY	B	70	1	10,10,11	0.66	0	7,11,13	2.03	3 (42%)
1	MLY	B	74	1	8,8,11	0.63	0	4,8,13	0.74	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
1	MLY	A	116	1	-	1/5/7/11	-
1	MLY	A	123	1	-	0/2/4/11	-
1	MLY	A	20	1	-	0/2/4/11	-
1	MLY	A	205	1	-	1/7/9/11	-
1	MLY	A	215	1	-	0/5/7/11	-
1	MLY	A	25	1	-	3/7/9/11	-
1	MLY	A	261	1	-	5/7/9/11	-
1	MLY	A	288	1	-	0/5/7/11	-
1	MLY	A	3	1	-	0/5/7/11	-
1	MLY	A	324	1	-	1/7/9/11	-
1	MLY	A	47	1	-	0/0/2/11	-
1	MLY	A	5	1	-	2/7/9/11	-
1	MLY	A	70	1	-	1/2/4/11	-
1	MLY	A	74	1	-	0/0/2/11	-
1	MLY	B	116	1	-	1/5/7/11	-
1	MLY	B	123	1	-	1/7/9/11	-
1	MLY	B	20	1	-	0/5/7/11	-
1	MLY	B	205	1	-	1/3/5/11	-
1	MLY	B	215	1	-	0/2/4/11	-
1	MLY	B	25	1	-	2/7/9/11	-
1	MLY	B	261	1	-	2/7/9/11	-
1	MLY	B	288	1	-	1/2/4/11	-
1	MLY	B	3	1	-	2/5/7/11	-
1	MLY	B	5	1	-	0/5/7/11	-
1	MLY	B	70	1	-	2/7/9/11	-
1	MLY	B	74	1	-	0/5/7/11	-

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	MLY	CH2-NZ-CH1	4.52	121.62	109.72
1	A	324	MLY	CH2-NZ-CH1	4.22	120.82	109.72
1	B	25	MLY	CH2-NZ-CH1	4.07	120.43	109.72
1	A	5	MLY	CH2-NZ-CH1	3.91	120.00	109.72
1	B	123	MLY	CH2-NZ-CH1	3.64	119.31	109.72
1	B	261	MLY	CH2-NZ-CH1	3.62	119.25	109.72
1	A	205	MLY	CH2-NZ-CH1	3.49	118.92	109.72
1	A	261	MLY	CH2-NZ-CH1	3.47	118.86	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	70	MLY	CH2-NZ-CH1	3.42	118.72	109.72
1	A	205	MLY	CH2-NZ-CE	2.83	122.13	110.73
1	B	261	MLY	CH2-NZ-CE	2.83	122.11	110.73
1	A	25	MLY	CH2-NZ-CE	2.76	121.83	110.73
1	A	324	MLY	CH1-NZ-CE	2.71	121.63	110.73
1	B	70	MLY	CH2-NZ-CE	2.61	121.22	110.73
1	B	25	MLY	CH1-NZ-CE	2.60	121.20	110.73
1	A	261	MLY	CH1-NZ-CE	2.56	121.02	110.73
1	A	5	MLY	CH1-NZ-CE	2.50	120.81	110.73
1	B	123	MLY	CH2-NZ-CE	2.48	120.70	110.73
1	A	215	MLY	O-C-CA	-2.36	118.64	124.98
1	A	261	MLY	CH2-NZ-CE	2.33	120.10	110.73
1	B	70	MLY	CH1-NZ-CE	2.32	120.06	110.73
1	B	123	MLY	CH1-NZ-CE	2.29	119.97	110.73
1	A	5	MLY	CH2-NZ-CE	2.10	119.18	110.73
1	B	215	MLY	O-C-CA	-2.07	119.42	124.98
1	A	205	MLY	CH1-NZ-CE	2.04	118.96	110.73
1	A	5	MLY	CD-CE-NZ	-2.04	108.17	113.78

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	116	MLY	C-CA-CB-CG
1	A	70	MLY	N-CA-CB-CG
1	A	261	MLY	N-CA-CB-CG
1	A	261	MLY	C-CA-CB-CG
1	B	261	MLY	CD-CE-NZ-CH1
1	B	123	MLY	CD-CE-NZ-CH2
1	A	261	MLY	CD-CE-NZ-CH2
1	A	5	MLY	CD-CE-NZ-CH2
1	A	5	MLY	CG-CD-CE-NZ
1	B	70	MLY	CD-CE-NZ-CH2
1	A	25	MLY	CD-CE-NZ-CH2
1	B	25	MLY	CA-CB-CG-CD
1	A	205	MLY	CD-CE-NZ-CH2
1	A	324	MLY	CD-CE-NZ-CH1
1	B	205	MLY	CA-CB-CG-CD
1	B	25	MLY	CD-CE-NZ-CH1
1	A	261	MLY	CG-CD-CE-NZ
1	A	25	MLY	CE-CD-CG-CB
1	A	25	MLY	CA-CB-CG-CD

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Mol	Chain	Res	Type	Atoms
1	B	70	MLY	CE-CD-CG-CB
1	B	261	MLY	CD-CE-NZ-CH2
1	A	261	MLY	CA-CB-CG-CD
1	B	288	MLY	C-CA-CB-CG
1	B	116	MLY	CG-CD-CE-NZ
1	B	3	MLY	CA-CB-CG-CD
1	B	3	MLY	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	261	MLY	5	0
1	B	261	MLY	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	PEG	A	327	-	6,6,6	0.84	0	5,5,5	0.75	0
3	PEG	A	328	-	6,6,6	0.69	0	5,5,5	0.64	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	PEG	A	327	-	-	1/4/4/4	-
3	PEG	A	328	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	327	PEG	O2-C3-C4-O4
3	A	328	PEG	O1-C1-C2-O2
3	A	328	PEG	O2-C3-C4-O4
3	A	328	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	292/326 (89%)	0.62	41 (14%) <b>2</b> <b>2</b>	24, 36, 63, 86	0
1	B	284/326 (87%)	0.61	39 (13%) <b>3</b> <b>2</b>	26, 43, 69, 88	0
All	All	576/652 (88%)	0.61	80 (13%) <b>2</b> <b>2</b>	24, 40, 68, 88	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	323	VAL	7.4
1	A	41	SER	6.9
1	B	10[A]	GLY	6.5
1	A	55	PRO	5.4
1	B	304	GLY	5.3
1	B	9	ILE	5.2
1	B	189	LEU	4.9
1	A	40	GLY	4.6
1	B	188	VAL	4.6
1	B	275	TYR	4.5
1	A	48	ASN	4.4
1	A	9	ILE	4.3
1	B	8	VAL	4.3
1	B	272	PHE	4.1
1	A	42	SER	4.0
1	B	37	ASP	3.9
1	B	270	ASN	3.8
1	B	301	LEU	3.7
1	A	92	LEU	3.7
1	A	198	ILE	3.6
1	B	187	ILE	3.6
1	A	303	ASN	3.6
1	A	88	ALA	3.6
1	B	266	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	270	ASN	3.6
1	A	43	GLY	3.6
1	A	81	SER	3.5
1	A	202	ILE	3.5
1	A	79	ARG	3.5
1	A	87	PHE	3.5
1	B	87	PHE	3.3
1	B	198	ILE	3.2
1	A	166	LEU	3.2
1	B	221	VAL	3.2
1	B	220	TYR	3.2
1	B	11[A]	GLY	3.2
1	A	199	LEU	3.2
1	B	219	ALA	3.1
1	B	12	GLY	3.1
1	A	302	GLU	3.0
1	B	303	ASN	2.9
1	B	191	PRO	2.9
1	B	190	GLY	2.9
1	A	189	LEU	2.8
1	B	76	PHE	2.7
1	B	302	GLU	2.7
1	A	10[A]	GLY	2.7
1	A	45	LEU	2.6
1	A	8	VAL	2.6
1	A	38	ASP	2.5
1	B	7	THR	2.5
1	B	271	ARG	2.5
1	A	194	LEU	2.4
1	B	152	ASP	2.4
1	A	305	GLY	2.4
1	A	272	PHE	2.4
1	A	80	PHE	2.4
1	A	46	ARG	2.4
1	B	202	ILE	2.4
1	A	304	GLY	2.3
1	B	32	ILE	2.3
1	A	265[A]	GLU	2.3
1	A	219	ALA	2.2
1	B	222	CYS	2.2
1	B	322	GLN	2.2
1	A	39	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	222	CYS	2.1
1	A	2	ARG	2.1
1	B	15[A]	SER	2.1
1	A	32	ILE	2.1
1	A	96	ILE	2.1
1	A	90	HIS	2.1
1	B	317	LEU	2.1
1	B	268	ASN	2.1
1	B	2	ARG	2.1
1	A	211	LEU	2.1
1	A	131	PRO	2.0
1	A	56	GLY	2.0
1	B	199	LEU	2.0
1	B	148	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	MLY	A	74	5/12	0.79	0.18	44,46,50,53	0
1	MLY	A	47	5/12	0.87	0.14	66,69,73,74	0
1	MLY	A	261	11/12	0.88	0.16	28,35,58,64	0
1	MLY	A	3	9/12	0.90	0.35	41,51,65,68	0
1	MLY	B	116	9/12	0.92	0.14	35,42,51,57	0
1	MLY	A	20	6/12	0.92	0.11	37,39,41,43	0
1	MLY	B	74	9/12	0.92	0.11	44,46,50,53	0
1	MLY	B	123	11/12	0.93	0.17	38,46,76,81	0
1	MLY	A	288	9/12	0.93	0.17	29,31,49,60	0
1	MLY	A	324	11/12	0.93	0.16	34,40,48,51	0
1	MLY	B	288	6/12	0.93	0.24	41,43,43,43	0
1	MLY	B	70	11/12	0.93	0.27	32,38,75,77	0
1	MLY	B	20	9/12	0.93	0.19	38,41,59,62	0
1	MLY	B	25	11/12	0.94	0.18	39,43,64,69	0
1	MLY	B	3	9/12	0.94	0.16	45,54,65,68	0
1	MLY	B	215	6/12	0.95	0.11	35,35,36,39	0
1	MLY	A	205	11/12	0.95	0.16	27,32,72,73	0
1	MLY	A	70	6/12	0.95	0.08	40,40,42,49	0
1	MLY	A	25	11/12	0.95	0.10	39,41,67,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MLY	A	116	9/12	0.96	0.10	33,34,42,43	0
1	MLY	B	261	11/12	0.96	0.20	41,43,58,61	0
1	MLY	A	215	9/12	0.96	0.10	25,27,40,51	0
1	MLY	A	123	6/12	0.96	0.07	36,39,44,46	0
1	MLY	B	5	9/12	0.97	0.10	37,39,47,53	0
1	MLY	A	5	11/12	0.97	0.10	29,38,66,69	0
1	MLY	B	205	7/12	0.98	0.11	32,34,42,54	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 95<sup>th</sup> 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	PEG	A	328	7/7	0.65	0.21	52,60,69,73	0
3	PEG	A	327	7/7	0.89	0.18	29,57,63,66	0
2	CL	A	326	1/1	0.99	0.04	38,38,38,38	0

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

There are no such residues in this entry.