Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 09:48 pm GMT

PDB ID	:	6Q36
Title	:	TEAD4(216-434) complexed with optimized peptide 9 and myristoate (covalently bound) at 2.01A resolution: Structure-based design of potent linear peptide inhibitors of the YAP-TEAD protein-protein interaction derived from the YAP omega-loop sequence
Authors	:	Kallen, J.
Deposited on	:	2018-12-03
Resolution	:	2.01 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:

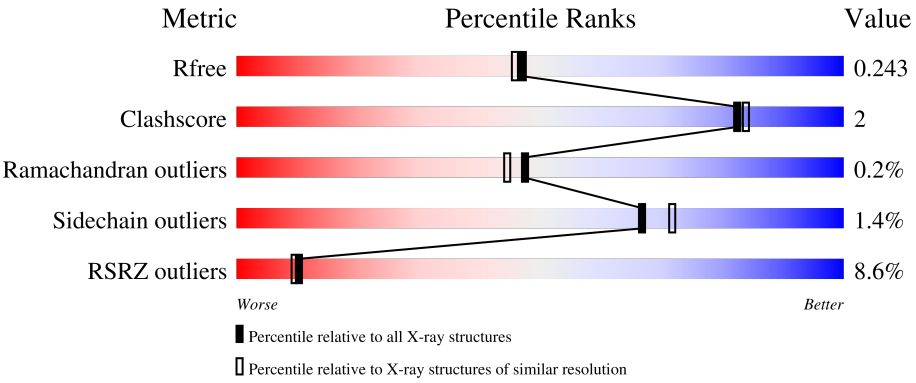
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 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 <=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	220	8% 89% 9% .
1	B	220	9% 90% 8% .
2	C	17	59% 35% 6%
2	D	17	6% 59% 29% 12%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4164 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 Transcriptional enhancer factor TEF-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	7	0
			1795	1151	294	340	10			
1	B	214	Total	C	N	O	S	0	6	0
			1782	1145	292	335	10			

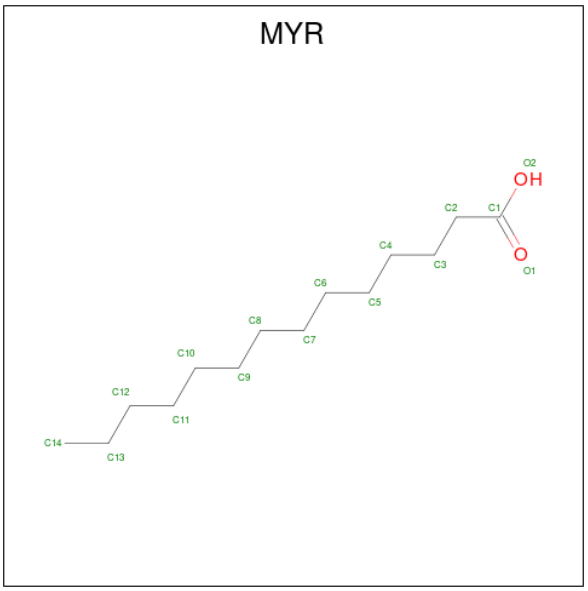
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	215	GLY	-	expression tag	UNP Q15561
A	216	PRO	-	expression tag	UNP Q15561
B	215	GLY	-	expression tag	UNP Q15561
B	216	PRO	-	expression tag	UNP Q15561

- Molecule 2 is a protein called ACE-PRO-6CW-ARG-LEU-ARG-LYS-2JH-HYP-ASP-SER-PHE-ALN-LYS-GLU-PRO-NH2.

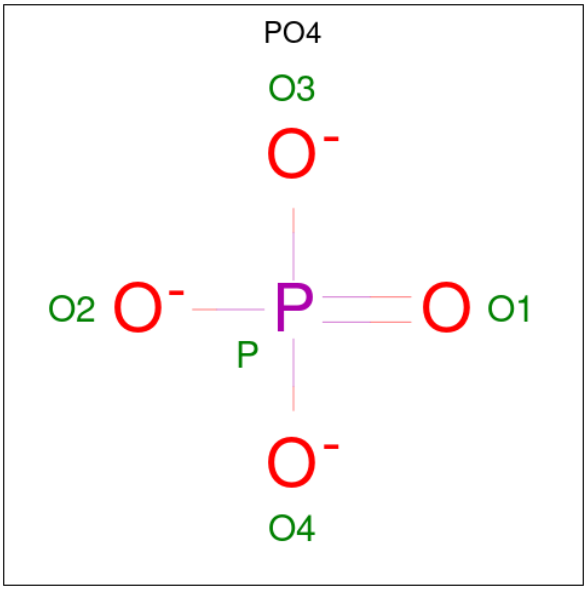
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	17	Total	C	Cl	N	O	0	0	1
			147	99	1	25	22			
2	D	17	Total	C	Cl	N	O	0	0	1
			147	99	1	25	22			

- Molecule 3 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 15 14 1	0	0
3	B	1	Total C O 15 14 1	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0

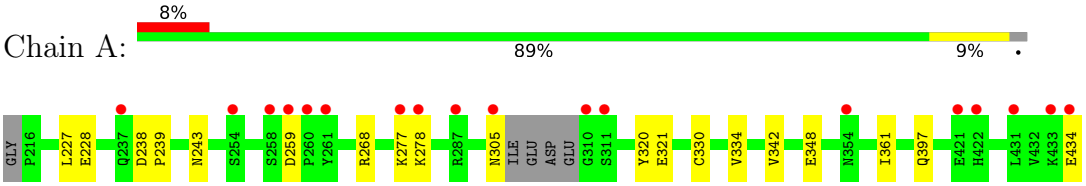
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	117	Total O 117 117	0	0
5	B	105	Total O 105 105	0	0
5	C	14	Total O 14 14	0	0
5	D	7	Total O 7 7	0	0

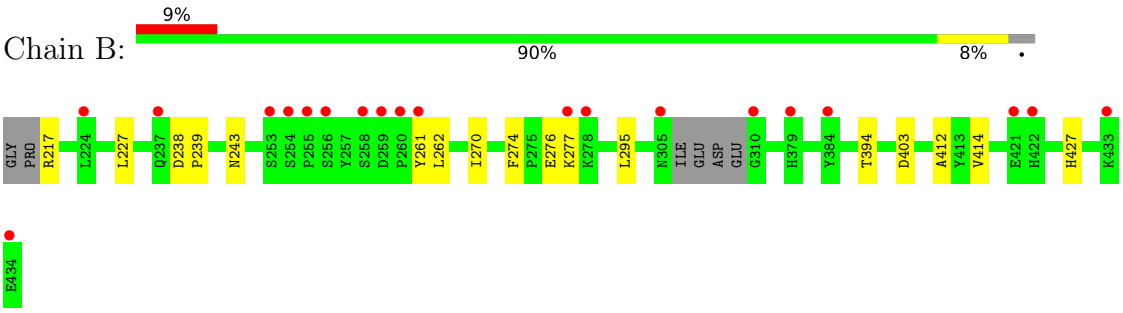
3 Residue-property plots (i)

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: Transcriptional enhancer factor TEF-3

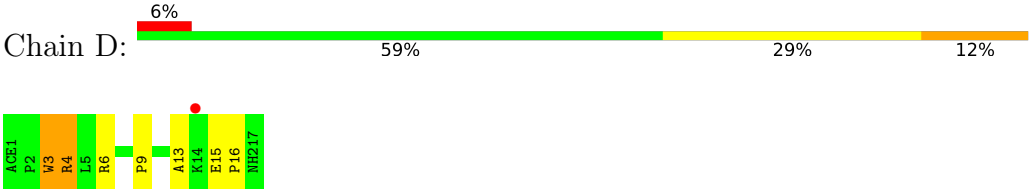


• Molecule 1: Transcriptional enhancer factor TEF-3



• Molecule 2: ACE-PRO-6CW-ARG-LEU-ARG-LYS-2JH-HYP-ASP-SER-PHE-ALN-LYS-GLU-PRO-NH2

• Molecule 2: ACE-PRO-6CW-ARG-LEU-ARG-LYS-2JH-HYP-ASP-SER-PHE-ALN-LYS-GLU-PRO-NH2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	172.87Å 40.44Å 98.03Å 90.00° 93.44° 90.00°	Depositor
Resolution (Å)	19.80 – 2.01 19.80 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.80-2.01) 99.1 (19.80-2.01)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 2.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.217 , 0.244 0.215 , 0.243	Depositor DCC
R_{free} test set	2265 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	38.8	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 41.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4164	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ALN, NH2, MYR, PO4, HYP, 6CW, ACE, 2JH

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	0.41	0/1863	0.53	0/2517
1	B	0.44	0/1846	0.53	0/2494
2	C	1.42	1/96 (1.0%)	1.11	0/122
2	D	1.48	1/96 (1.0%)	1.08	0/122
All	All	0.52	2/3901 (0.1%)	0.57	0/5255

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
2	C	0	2
2	D	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	15	GLU	CD-OE2	7.99	1.34	1.25
2	C	15	GLU	CD-OE1	7.62	1.34	1.25

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	4	ARG	Sidechain
2	C	6	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	D	4	ARG	Sidechain
2	D	6	ARG	Sidechain

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	A	1795	0	1736	10	0
1	B	1782	0	1732	10	0
2	C	147	0	139	0	0
2	D	147	0	139	2	0
3	A	15	0	27	0	0
3	B	15	0	27	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
5	A	117	0	0	0	0
5	B	105	0	0	1	0
5	C	14	0	0	0	0
5	D	7	0	0	0	0
All	All	4164	0	3800	19	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 2.

All (19) 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:A:330[B]:CYS:SG	1:A:348[B]:GLU:OE2	2.21	0.98
1:A:243:ASN:OD1	1:B:243:ASN:ND2	2.16	0.78
1:A:277:LYS:HG2	1:A:278:LYS:H	1.57	0.70
1:B:414:VAL:HG11	2:D:3:6CW:CLL	2.39	0.59
1:A:320:TYR:OH	1:A:397:GLN:NE2	2.41	0.53
1:B:274:PHE:CZ	1:B:412:ALA:HB1	2.45	0.52
1:B:403:ASP:OD1	5:B:601:HOH:O	2.20	0.49
1:B:238:ASP:HB2	1:B:239:PRO:CD	2.43	0.49
1:A:277:LYS:HG2	1:A:278:LYS:N	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ARG:HB3	1:B:262:LEU:HG	1.96	0.48
1:B:270:ILE:HD13	1:B:295[B]:LEU:HD12	1.95	0.47
1:B:276:GLU:O	1:B:277:LYS:HB2	2.16	0.45
1:A:268:ARG:HH21	1:A:434:GLU:HB3	1.82	0.44
1:A:227:LEU:HD11	1:A:321:GLU:HB2	2.00	0.44
1:A:334:VAL:HB	1:A:342:VAL:HG12	2.00	0.44
1:A:238:ASP:HB2	1:A:239:PRO:HD2	2.01	0.43
1:B:427:HIS:CE1	2:D:16:PRO:HG3	2.54	0.42
1:A:348[B]:GLU:OE2	1:A:361:ILE:HD11	2.20	0.42
1:B:274:PHE:CE1	1:B:394:THR:HB	2.56	0.41

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	218/220 (99%)	211 (97%)	6 (3%)	1 (0%)	29	23
1	B	216/220 (98%)	210 (97%)	6 (3%)	0	100	100
2	C	11/17 (65%)	11 (100%)	0	0	100	100
2	D	11/17 (65%)	11 (100%)	0	0	100	100
All	All	456/474 (96%)	443 (97%)	12 (3%)	1 (0%)	47	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	259	ASP

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	A	204/201 (102%)	202 (99%)	2 (1%)	76 81
1	B	202/201 (100%)	200 (99%)	2 (1%)	76 81
2	C	11/11 (100%)	10 (91%)	1 (9%)	9 5
2	D	11/11 (100%)	10 (91%)	1 (9%)	9 5
All	All	428/424 (101%)	422 (99%)	6 (1%)	67 72

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	GLU
1	A	305	ASN
1	B	227	LEU
1	B	261	TYR
2	C	4	ARG
2	D	4	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	303	ASN
1	A	305	ASN
1	A	362	HIS
1	A	397	GLN
1	B	305	ASN
1	B	426	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

8 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	ALN	D	13	2	15,16,17	1.17	1 (6%)	18,21,23	1.10	1 (5%)
2	ALN	C	13	2	15,16,17	1.09	1 (6%)	18,21,23	1.29	1 (5%)
2	HYP	D	9	2	6,8,9	0.59	0	5,10,12	1.10	1 (20%)
2	6CW	D	3	2	14,16,17	1.34	3 (21%)	15,22,24	1.54	4 (26%)
2	6CW	C	3	2	14,16,17	1.33	2 (14%)	15,22,24	1.73	4 (26%)
2	2JH	D	8	2	7,9,10	0.80	0	6,11,13	0.18	0
2	2JH	C	8	2	7,9,10	0.87	1 (14%)	6,11,13	0.50	0
2	HYP	C	9	2	6,8,9	0.69	0	5,10,12	1.18	1 (20%)

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	ALN	D	13	2	-	1/5/6/8	0/2/2/2
2	ALN	C	13	2	-	1/5/6/8	0/2/2/2
2	HYP	D	9	2	-	0/0/11/13	0/1/1/1
2	6CW	D	3	2	-	2/4/6/8	0/2/2/2
2	6CW	C	3	2	-	0/4/6/8	0/2/2/2
2	2JH	D	8	2	-	1/5/12/14	0/1/1/1
2	2JH	C	8	2	-	0/5/12/14	0/1/1/1
2	HYP	C	9	2	-	0/0/11/13	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	6CW	CZ2-CH2	2.63	1.41	1.36
2	D	3	6CW	CD1-NE1	-2.56	1.31	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	6CW	CD1-NE1	-2.40	1.31	1.36
2	D	13	ALN	CD1-CG1	2.19	1.41	1.37
2	D	3	6CW	CZ2-CH2	2.17	1.40	1.36
2	D	3	6CW	CE3-CZ3	2.08	1.41	1.36
2	C	8	2JH	CB-CG	2.08	1.56	1.53
2	C	13	ALN	CD1-CG1	2.02	1.41	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	13	ALN	CG1-CB-CA	-4.06	108.25	114.53
2	C	3	6CW	CH2-CZ2-CE2	-3.44	116.60	119.50
2	C	3	6CW	CE3-CD2-CE2	3.34	122.60	118.17
2	C	3	6CW	CZ3-CE3-CD2	-3.32	116.51	121.13
2	D	13	ALN	CG1-CB-CA	-3.22	109.55	114.53
2	D	3	6CW	CZ3-CE3-CD2	-2.79	117.25	121.13
2	D	3	6CW	CE3-CD2-CE2	2.52	121.51	118.17
2	D	3	6CW	CH2-CZ2-CE2	-2.32	117.54	119.50
2	D	9	HYP	O-C-CA	-2.26	118.85	124.78
2	C	9	HYP	O-C-CA	-2.26	118.87	124.78
2	D	3	6CW	CB-CA-C	-2.21	107.32	111.47
2	C	3	6CW	CB-CA-C	-2.10	107.54	111.47

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3	6CW	C-CA-CB-CG
2	D	8	2JH	CA-CB-CG-CD2
2	C	13	ALN	O-C-CA-CB
2	D	13	ALN	O-C-CA-CB
2	D	3	6CW	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	6CW	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	PO4	B	503	-	4,4,4	0.86	0	6,6,6	0.45	0
3	MYR	B	501	1	14,14,15	0.34	0	13,13,15	0.92	0
3	MYR	A	501	1	14,14,15	0.33	0	13,13,15	1.00	0
4	PO4	A	502	-	4,4,4	0.90	0	6,6,6	0.47	0
4	PO4	A	503	-	4,4,4	0.93	0	6,6,6	0.36	0
4	PO4	B	502	-	4,4,4	0.97	0	6,6,6	0.58	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	MYR	B	501	1	-	5/11/12/13	-
3	MYR	A	501	1	-	8/11/12/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501	MYR	C1-C2-C3-C4
3	B	501	MYR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
3	A	501	MYR	C4-C5-C6-C7
3	B	501	MYR	C4-C5-C6-C7
3	B	501	MYR	C2-C3-C4-C5
3	A	501	MYR	C6-C7-C8-C9
3	A	501	MYR	C1-C2-C3-C4
3	A	501	MYR	C7-C8-C9-C10
3	B	501	MYR	C6-C7-C8-C9
3	A	501	MYR	C10-C11-C12-C13
3	A	501	MYR	C2-C3-C4-C5
3	A	501	MYR	C9-C10-C11-C12
3	A	501	MYR	C3-C4-C5-C6

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^{th} 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	A	215/220 (97%)	0.39	18 (8%) 11 10	25, 38, 60, 72	0
1	B	214/220 (97%)	0.36	20 (9%) 8 8	23, 37, 62, 79	0
2	C	11/17 (64%)	0.40	0 100 100	37, 43, 51, 59	0
2	D	11/17 (64%)	0.03	1 (9%) 9 8	33, 40, 45, 48	0
All	All	451/474 (95%)	0.36	39 (8%) 10 9	23, 38, 61, 79	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	310	GLY	5.2
1	B	379	HIS	4.3
1	A	261	TYR	4.3
1	B	254	SER	4.2
1	B	256	SER	4.0
1	A	311	SER	3.7
1	A	277	LYS	3.6
1	A	254	SER	3.6
1	B	310	GLY	3.5
1	B	422	HIS	3.2
1	B	278	LYS	3.1
1	A	237	GLN	3.1
1	B	384	TYR	3.0
1	A	422	HIS	2.9
1	A	421	GLU	2.9
1	B	253	SER	2.9
1	B	258	SER	2.9
1	B	255	PRO	2.9
1	A	434	GLU	2.8
1	B	261	TYR	2.8
1	B	421	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	237	GLN	2.7
1	A	259	ASP	2.7
1	A	305	ASN	2.6
1	A	278	LYS	2.6
1	B	277	LYS	2.6
1	A	260	PRO	2.6
1	B	433	LYS	2.4
1	B	434	GLU	2.3
1	A	258	SER	2.3
1	B	305	ASN	2.2
1	B	260	PRO	2.2
1	A	287	ARG	2.2
1	A	433	LYS	2.1
1	B	259	ASP	2.1
1	A	431	LEU	2.1
2	D	14	LYS	2.1
1	A	354	ASN	2.0
1	B	224	LEU	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, 95^{th} 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	ALN	D	13	15/16	0.89	0.16	35,37,39,39	0
2	6CW	D	3	15/16	0.91	0.15	41,47,49,49	0
2	6CW	C	3	15/16	0.92	0.10	44,45,50,51	0
2	ALN	C	13	15/16	0.93	0.11	39,39,42,42	0
2	2JH	C	8	9/10	0.94	0.11	34,35,39,39	0
2	2JH	D	8	9/10	0.94	0.12	36,37,37,38	0
2	HYP	C	9	8/9	0.95	0.09	38,39,41,41	0
2	HYP	D	9	8/9	0.96	0.10	36,37,38,38	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MYR	A	501	15/16	0.80	0.26	36,39,50,53	0
3	MYR	B	501	15/16	0.84	0.24	42,44,58,61	0
4	PO4	B	503	5/5	0.87	0.15	80,81,82,83	0
4	PO4	A	502	5/5	0.90	0.16	57,59,63,63	0
4	PO4	A	503	5/5	0.95	0.21	65,67,69,71	0
4	PO4	B	502	5/5	0.98	0.09	35,37,39,40	0

6.5 Other polymers (i)

There are no such residues in this entry.