



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 9, 2026 – 09:51 PM UTC

PDB ID : 9QKQ / pdb_00009qkq
Title : Crystal structure of hTEAD4 YAP binding domain (hTEAD4-YBD) in complex with peptide 6
Authors : Pozzi, C.
Deposited on : 2025-03-20
Resolution : 1.74 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

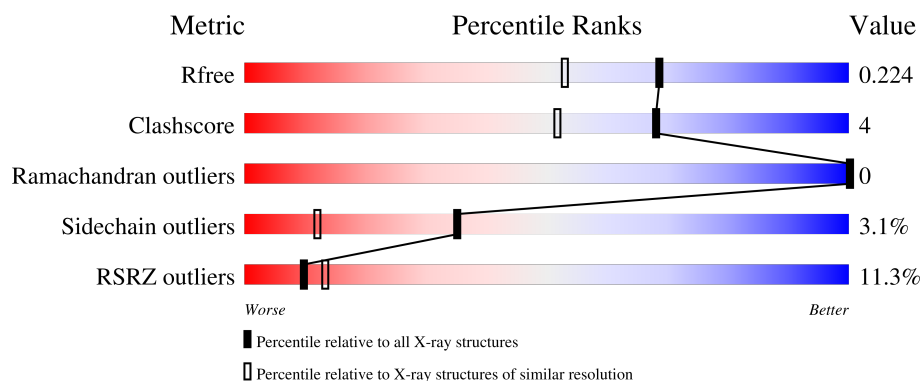
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	A	222	 10% 82% 13% . .
1	B	222	 10% 81% 11% . 7%
2	C	17	 6% 65% 24% 12%
2	D	17	 18% 65% 18% 18%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4388 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	213	Total	C	N	O	S	0	19	0
			1803	1167	293	333	10			
1	B	207	Total	C	N	O	S	0	25	0
			1793	1157	292	334	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	213	GLY	-	expression tag	UNP Q15561
A	214	SER	-	expression tag	UNP Q15561
A	215	HIS	-	expression tag	UNP Q15561
A	216	MET	-	expression tag	UNP Q15561
B	213	GLY	-	expression tag	UNP Q15561
B	214	SER	-	expression tag	UNP Q15561
B	215	HIS	-	expression tag	UNP Q15561
B	216	MET	-	expression tag	UNP Q15561

- Molecule 2 is a protein called peptide 6.

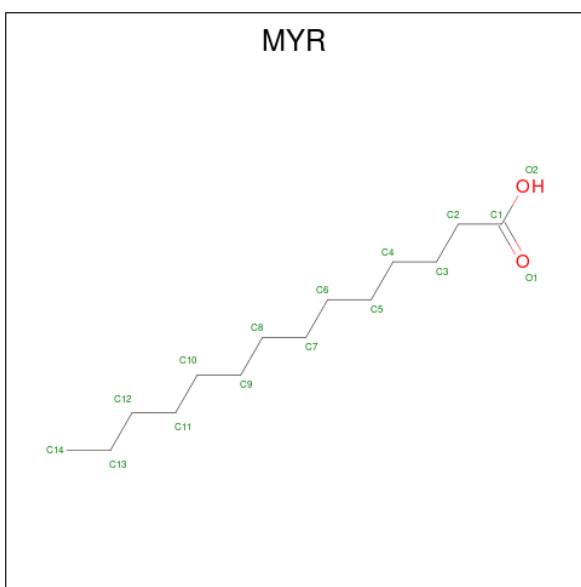
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	17	Total	C	Cl	N	O	0	1	1
			149	103	1	26	19			
2	D	17	Total	C	Cl	N	O	0	1	1
			149	103	1	26	19			

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



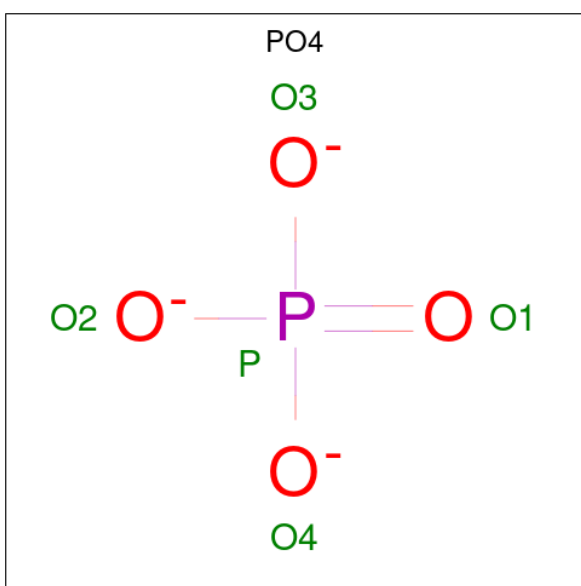
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			16	14	2		
4	B	1	Total	C	O	0	0
			16	14	2		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

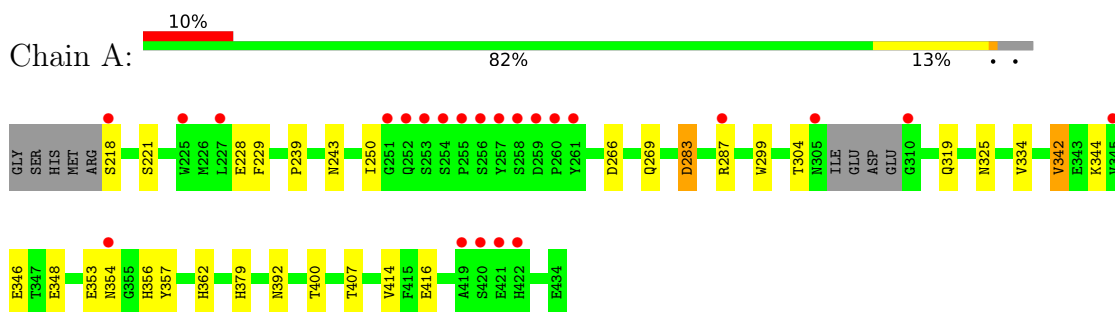
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	199	Total 207	O 207	0	12
6	B	180	Total 186	O 186	0	13
6	C	13	Total 13	O 13	0	0
6	D	11	Total 11	O 11	0	1

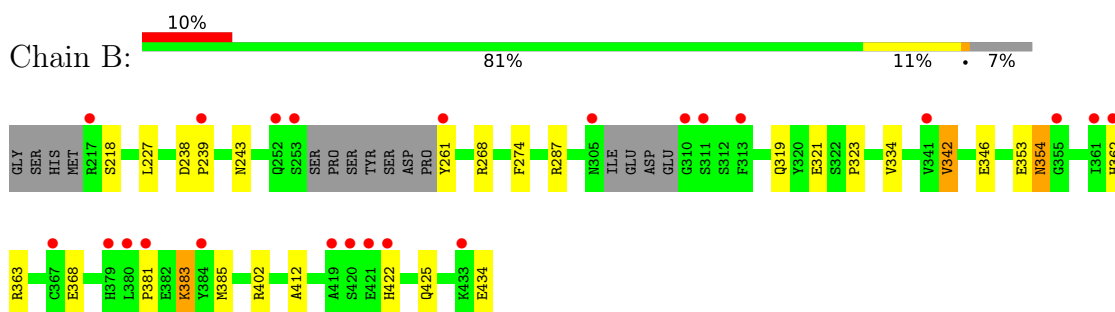
3 Residue-property plots [i](#)

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.

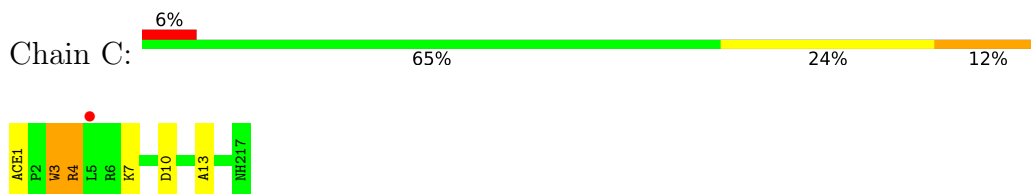
- Molecule 1: Transcriptional enhancer factor TEF-3



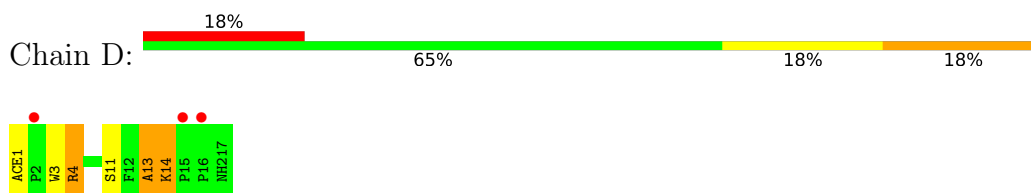
- Molecule 1: Transcriptional enhancer factor TEF-3



- Molecule 2: peptide 6



- Molecule 2: peptide 6



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	171.54Å 40.24Å 97.89Å 90.00° 92.77° 90.00°	Depositor
Resolution (Å)	97.78 – 1.74 97.78 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.0 (97.78-1.74) 99.0 (97.78-1.74)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.183 , 0.221 0.188 , 0.224	Depositor DCC
R_{free} test set	3407 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4388	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.49% 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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.99	2/1893 (0.1%)	1.56	19/2563 (0.7%)
1	B	0.99	2/1878 (0.1%)	1.42	11/2539 (0.4%)
2	C	1.48	1/111 (0.9%)	1.45	1/141 (0.7%)
2	D	1.38	1/112 (0.9%)	1.34	1/145 (0.7%)
All	All	1.02	6/3994 (0.2%)	1.49	32/5388 (0.6%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	ACE	C-N	-10.75	1.32	1.43
2	D	1	ACE	C-N	-9.68	1.33	1.43
1	B	353[A]	GLU	C-O	7.07	1.32	1.23
1	B	353[B]	GLU	C-O	7.07	1.32	1.23
1	A	218	SER	N-CA	5.28	1.56	1.46
1	A	356	HIS	CE1-NE2	5.26	1.37	1.32

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	PRO	CA-C-N	-7.83	110.31	122.37
1	A	239	PRO	C-N-CA	-7.83	110.31	122.37
2	C	10	ASP	CA-CB-CG	6.66	119.26	112.60
1	A	379[A]	HIS	CA-CB-CG	-6.59	107.20	113.80
1	A	250	ILE	CA-C-N	-6.48	116.00	121.58
1	A	250	ILE	C-N-CA	-6.48	116.00	121.58
1	A	354	ASN	CB-CA-C	-6.45	102.28	111.95
1	A	344	LYS	CA-C-N	-6.25	113.71	122.71
1	A	344	LYS	C-N-CA	-6.25	113.71	122.71
1	A	392	ASN	CA-CB-CG	-6.13	106.47	112.60
1	A	362	HIS	CA-CB-CG	-6.04	107.76	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	ASP	CA-CB-CG	5.97	118.57	112.60
1	B	353[A]	GLU	CA-C-O	5.87	127.55	120.27
1	B	353[B]	GLU	CA-C-O	5.87	127.55	120.27
1	A	353	GLU	CB-CA-C	-5.70	102.36	110.34
1	B	323	PRO	N-CA-C	-5.69	106.75	113.86
1	B	402[A]	ARG	CA-C-O	5.56	126.43	120.20
1	B	402[B]	ARG	CA-C-O	5.56	126.43	120.20
1	A	304	THR	CA-CB-OG1	-5.54	101.29	109.60
1	B	353[A]	GLU	O-C-N	-5.45	117.25	123.40
1	B	353[B]	GLU	O-C-N	-5.45	117.25	123.40
2	D	4	ARG	CB-CG-CD	5.40	123.72	111.30
1	A	221	SER	CA-C-N	-5.30	112.19	122.06
1	A	221	SER	C-N-CA	-5.30	112.19	122.06
1	A	348[A]	GLU	CA-C-O	5.14	126.25	120.70
1	A	348[B]	GLU	CA-C-O	5.14	126.25	120.70
1	B	368[A]	GLU	CB-CG-CD	5.14	121.33	112.60
1	B	354	ASN	CA-C-N	-5.11	114.99	122.46
1	B	354	ASN	C-N-CA	-5.11	114.99	122.46
1	A	304	THR	CB-CA-C	-5.08	101.79	111.48
1	A	283	ASP	CB-CA-C	-5.04	102.42	110.79
1	B	287	ARG	CB-CG-CD	5.03	122.87	111.30

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	A	1803	0	1714	8	0
1	B	1793	0	1704	17	0
2	C	149	0	154	3	0
2	D	149	0	155	3	0
3	A	36	0	54	0	0
3	B	4	0	6	1	0
4	A	16	0	27	0	0
4	B	16	0	27	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	5	0	0	0	0
6	A	207	0	0	0	0
6	B	186	0	0	0	0
6	C	13	0	0	0	0
6	D	11	0	0	1	0
All	All	4388	0	3841	28	0

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

All (28) 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:334:VAL:HB	1:B:342:VAL:HG13	1.65	0.78
1:B:227[B]:LEU:HD21	1:B:319[B]:GLN:HG2	1.66	0.76
1:B:268:ARG:HH21	1:B:434:GLU:HA	1.51	0.75
1:B:381:PRO:HD2	1:B:385:MET:SD	2.30	0.71
1:A:334:VAL:HB	1:A:342:VAL:HG13	1.75	0.67
2:D:11:SER:HA	2:D:14[B]:LYS:HG2	1.76	0.66
1:A:299:TRP:HA	1:A:416[B]:GLU:O	1.97	0.64
1:A:414[B]:VAL:HG11	2:C:3:6CW:CLL	2.43	0.55
1:B:268:ARG:NH2	1:B:434:GLU:HA	2.21	0.55
2:C:4:ARG:HB3	2:C:4:ARG:HH11	1.75	0.50
1:A:243[A]:ASN:ND2	1:B:243[A]:ASN:OD1	2.45	0.49
1:B:227[A]:LEU:HD11	1:B:321:GLU:HG3	1.96	0.48
1:A:325:ASN:HB2	1:A:357:TYR:CZ	2.48	0.48
1:B:238:ASP:HB2	1:B:239:PRO:HD3	1.96	0.48
1:A:269:GLN:NE2	2:C:7[B]:LYS:HD3	2.29	0.47
1:B:422[A]:HIS:HB2	1:B:425:GLN:NE2	2.29	0.47
1:B:227[B]:LEU:HD22	1:B:321:GLU:HG3	1.97	0.47
1:A:400[B]:THR:HG22	1:A:407:THR:HA	1.96	0.46
1:B:274:PHE:CZ	1:B:412:ALA:HB1	2.51	0.46
1:B:238:ASP:HB2	1:B:239:PRO:CD	2.47	0.45
1:B:227[A]:LEU:CD1	1:B:321:GLU:HG3	2.47	0.44
2:D:4:ARG:HD3	6:D:110:HOH:O	2.17	0.43
1:A:228[A]:GLU:HG2	1:A:229:PHE:N	2.33	0.42
2:D:13:ALN:HG2	2:D:13:ALN:HB3	1.60	0.41
1:B:383[B]:LYS:HE3	1:B:383[B]:LYS:HB3	1.91	0.41
1:B:362:HIS:CE1	1:B:363:ARG:HG3	2.55	0.40
1:B:227[B]:LEU:HA	3:B:502:EDO:H11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	224/222 (101%)	219 (98%)	5 (2%)	0	100	100
1	B	223/222 (100%)	215 (96%)	8 (4%)	0	100	100
2	C	13/17 (76%)	12 (92%)	1 (8%)	0	100	100
2	D	13/17 (76%)	12 (92%)	1 (8%)	0	100	100
All	All	473/478 (99%)	458 (97%)	15 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	196/203 (97%)	190 (97%)	6 (3%)	35	12
1	B	194/203 (96%)	188 (97%)	6 (3%)	35	12
2	C	13/12 (108%)	12 (92%)	1 (8%)	12	1
2	D	13/12 (108%)	11 (85%)	2 (15%)	2	0
All	All	416/430 (97%)	401 (96%)	15 (4%)	35	9

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

Mol	Chain	Res	Type
1	A	283	ASP
1	A	287[A]	ARG
1	A	287[B]	ARG
1	A	319	GLN
1	A	342	VAL
1	A	346	GLU
1	B	218	SER
1	B	261	TYR
1	B	342	VAL
1	B	346	GLU
1	B	383[A]	LYS
1	B	383[B]	LYS
2	C	4	ARG
2	D	14[A]	LYS
2	D	14[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	236	GLN
1	B	362	HIS
1	B	397	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	1.49	2 (13%)	16,21,23	2.00	5 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	6CW	C	3	2	15,16,17	1.23	2 (13%)	17,22,24	0.87	0
2	6CW	D	3	2	15,16,17	1.28	0	17,22,24	1.12	1 (5%)
2	ALN	C	13	2	15,16,17	1.23	1 (6%)	16,21,23	1.48	2 (12%)
2	NLE	D	8	2	6,7,8	0.61	0	2,7,9	0.94	0
2	NLE	C	8	2	6,7,8	0.64	0	2,7,9	0.97	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	ALN	D	13	2	-	3/5/6/8	0/2/2/2
2	6CW	C	3	2	-	0/5/6/8	0/2/2/2
2	6CW	D	3	2	-	0/5/6/8	0/2/2/2
2	ALN	C	13	2	-	0/5/6/8	0/2/2/2
2	NLE	D	8	2	-	1/5/6/8	-
2	NLE	C	8	2	-	0/5/6/8	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	13	ALN	CE1-CD1	4.03	1.45	1.38
2	C	13	ALN	CE1-CD1	3.49	1.44	1.38
2	C	3	6CW	CH2-CLL	-3.11	1.67	1.74
2	D	13	ALN	CD1-CG1	2.04	1.41	1.37
2	C	3	6CW	CE2-NE1	2.02	1.41	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	13	ALN	CB-CG1-CD2	-4.54	114.29	120.89
2	D	13	ALN	CB-CG1-CD1	3.55	125.55	119.92
2	C	13	ALN	CB-CG1-CD1	3.25	125.07	119.92
2	D	13	ALN	CG2-CD2-CE2	3.05	121.87	117.92
2	C	13	ALN	CB-CG1-CD2	-2.72	116.94	120.89
2	D	13	ALN	CZ2-CE2-CD2	-2.58	115.79	119.12
2	D	3	6CW	CE2-CD2-CG	-2.01	105.13	107.17
2	D	13	ALN	CG2-CD2-CG1	-2.01	119.19	122.55

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	13	ALN	O-C-CA-CB
2	D	8	NLE	CA-CB-CG-CD
2	D	13	ALN	C-CA-CB-CG1
2	D	13	ALN	CA-CB-CG1-CD2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	13	ALN	1	0
2	C	3	6CW	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EDO	A	507	-	3,3,3	0.24	0	2,2,2	0.07	0
5	PO4	B	503	-	4,4,4	0.88	0	6,6,6	0.72	0
3	EDO	A	501	-	3,3,3	0.07	0	2,2,2	0.13	0
3	EDO	A	508	-	3,3,3	0.09	0	2,2,2	0.11	0
4	MYR	B	501	-	15,15,15	0.59	0	15,15,15	0.52	0
3	EDO	A	510	-	3,3,3	0.14	0	2,2,2	0.05	0
3	EDO	B	502	-	3,3,3	0.10	0	2,2,2	0.17	0
3	EDO	A	506	-	3,3,3	0.38	0	2,2,2	0.63	0
3	EDO	A	504	-	3,3,3	0.13	0	2,2,2	0.02	0
3	EDO	A	503	-	3,3,3	0.08	0	2,2,2	0.14	0
4	MYR	A	502	-	15,15,15	0.58	0	15,15,15	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	A	509	-	3,3,3	0.21	0	2,2,2	0.18	0
3	EDO	A	505	-	3,3,3	0.15	0	2,2,2	0.14	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	507	-	-	0/1/1/1	-
3	EDO	A	501	-	-	0/1/1/1	-
3	EDO	A	508	-	-	1/1/1/1	-
4	MYR	B	501	-	-	8/13/13/13	-
3	EDO	A	510	-	-	0/1/1/1	-
3	EDO	B	502	-	-	1/1/1/1	-
3	EDO	A	506	-	-	1/1/1/1	-
3	EDO	A	504	-	-	0/1/1/1	-
3	EDO	A	503	-	-	0/1/1/1	-
4	MYR	A	502	-	-	9/13/13/13	-
3	EDO	A	509	-	-	1/1/1/1	-
3	EDO	A	505	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	MYR	C5-C6-C7-C8
4	A	502	MYR	C2-C3-C4-C5
4	A	502	MYR	C7-C8-C9-C10
3	A	508	EDO	O1-C1-C2-O2
4	A	502	MYR	C10-C11-C12-C13
4	B	501	MYR	C10-C11-C12-C13
3	A	506	EDO	O1-C1-C2-O2
4	A	502	MYR	C11-C12-C13-C14
4	B	501	MYR	C9-C10-C11-C12
3	A	509	EDO	O1-C1-C2-O2
4	A	502	MYR	C3-C4-C5-C6
4	B	501	MYR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
4	B	501	MYR	C4-C5-C6-C7
4	A	502	MYR	C9-C10-C11-C12
4	B	501	MYR	C11-C10-C9-C8
4	A	502	MYR	O1-C1-C2-C3
4	A	502	MYR	C6-C7-C8-C9
4	A	502	MYR	O2-C1-C2-C3
4	B	501	MYR	C3-C4-C5-C6
3	B	502	EDO	O1-C1-C2-O2
4	B	501	MYR	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	A	213/222 (95%)	0.52	23 (10%)	11 14	18, 36, 57, 74	42 (19%)
1	B	207/222 (93%)	0.62	23 (11%)	10 14	16, 37, 58, 76	39 (18%)
2	C	12/17 (70%)	0.83	1 (8%)	17 22	29, 46, 62, 67	3 (25%)
2	D	12/17 (70%)	1.47	3 (25%)	2 2	31, 42, 49, 49	4 (33%)
All	All	444/478 (92%)	0.60	50 (11%)	10 13	16, 37, 59, 76	88 (19%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	253	SER	9.1
2	D	16	PRO	6.9
1	B	421[A]	GLU	5.8
1	A	305	ASN	5.7
1	B	422[A]	HIS	5.2
1	B	420[A]	SER	4.8
1	A	259	ASP	4.6
1	B	261	TYR	4.6
1	A	257	TYR	4.2
1	B	419[A]	ALA	4.1
2	D	15	PRO	4.0
1	A	258	SER	4.0
1	A	255	PRO	3.9
1	B	310	GLY	3.9
1	A	253	SER	3.9
1	A	420	SER	3.9
1	B	379	HIS	3.9
2	D	2	PRO	3.7
1	A	422[A]	HIS	3.6
1	A	256	SER	3.4
1	A	261	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	305	ASN	3.3
1	B	367	CYS	3.2
1	A	218	SER	3.0
1	A	225	TRP	2.9
1	A	260	PRO	2.9
1	B	384	TYR	2.9
1	A	310	GLY	2.8
1	B	362	HIS	2.7
1	A	419	ALA	2.7
1	B	252	GLN	2.6
1	B	355	GLY	2.6
1	A	252	GLN	2.6
1	B	239	PRO	2.6
1	B	381	PRO	2.6
1	B	217	ARG	2.6
1	A	421	GLU	2.6
1	B	313	PHE	2.5
1	B	311	SER	2.5
1	B	380	LEU	2.5
1	A	254	SER	2.4
1	B	433	LYS	2.3
1	A	354	ASN	2.2
2	C	5	LEU	2.2
1	B	361	ILE	2.2
1	A	227	LEU	2.2
1	A	287[A]	ARG	2.1
1	A	345	VAL	2.1
1	B	341	VAL	2.0
1	A	251	GLY	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, 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
2	6CW	C	3	15/16	0.84	0.12	36,40,44,49	0
2	6CW	D	3	15/16	0.85	0.20	41,56,59,60	0
2	ALN	D	13	15/16	0.93	0.14	40,47,54,56	0
2	NLE	C	8	8/9	0.94	0.10	38,40,42,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ALN	C	13	15/16	0.95	0.10	40,47,51,54	0
2	NLE	D	8	8/9	0.96	0.08	39,40,44,47	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	A	505	4/4	0.66	0.30	44,52,53,57	4
3	EDO	A	503	4/4	0.73	0.26	57,65,71,71	0
3	EDO	A	504	4/4	0.77	0.17	53,55,55,60	0
3	EDO	A	501	4/4	0.80	0.15	62,62,62,64	0
3	EDO	A	509	4/4	0.81	0.18	49,54,61,66	0
3	EDO	A	507	4/4	0.83	0.24	50,56,56,67	0
3	EDO	B	502	4/4	0.85	0.18	44,56,57,58	0
4	MYR	A	502	16/16	0.88	0.21	41,52,73,74	0
4	MYR	B	501	16/16	0.88	0.23	48,56,97,99	0
3	EDO	A	506	4/4	0.92	0.22	65,66,66,75	4
3	EDO	A	510	4/4	0.93	0.12	41,44,47,51	0
5	PO4	B	503	5/5	0.93	0.10	44,44,55,55	0
3	EDO	A	508	4/4	0.95	0.10	43,44,46,48	4

6.5 Other polymers [i](#)

There are no such residues in this entry.