Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2023 – 05:28 PM JST

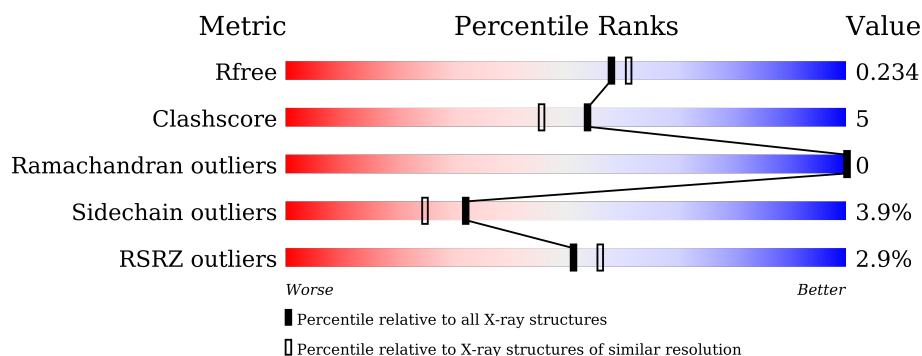|		
PDB ID	:	6LSD
Title	:	Crystal Structure of YEATS domain of human YEATS2 in complex with H3K27bz peptide
Authors	:	Li, H.T.; Ren, X.L.
Deposited on	:	2020-01-17
Resolution	:	2.05 Å(reported)

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 2.05 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	Percentile Ranks	Value
Rfree		0.234
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		3.9%
RSRZ outliers		2.9%

Worse　　　　　　　　　　　　　　Better

∎ Percentile relative to all X-ray structures
⫿ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	135	.% / 88% / 7% · ·
1	B	135	4% / 83% / 13% ·
2	C	9	78% / 22%
2	D	9	78% / 22%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 2583 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 YEATS domain-containing protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	130	Total	C	N	O	S	0	0	0
			1096	703	204	188	1			
1	B	135	Total	C	N	O	S	0	0	0
			1138	727	213	196	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	198	SER	-	expression tag	UNP Q9ULM3
A	199	HIS	-	expression tag	UNP Q9ULM3
A	200	MET	-	expression tag	UNP Q9ULM3
B	-2	SER	-	expression tag	UNP Q9ULM3
B	-1	HIS	-	expression tag	UNP Q9ULM3
B	0	MET	-	expression tag	UNP Q9ULM3

- Molecule 2 is a protein called 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	0	0	0
			65	41	12	12			
2	D	9	Total	C	N	O	0	0	0
			65	41	12	12			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1

O

O3 O⁻ — S — O⁻ O4

S

O

O2
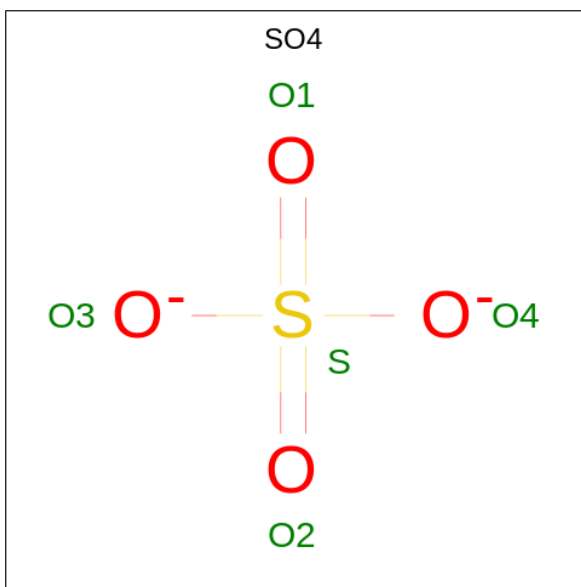
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	C	1	Total 5	O 4	S 1	0	0
3	D	1	Total 5	O 4	S 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL
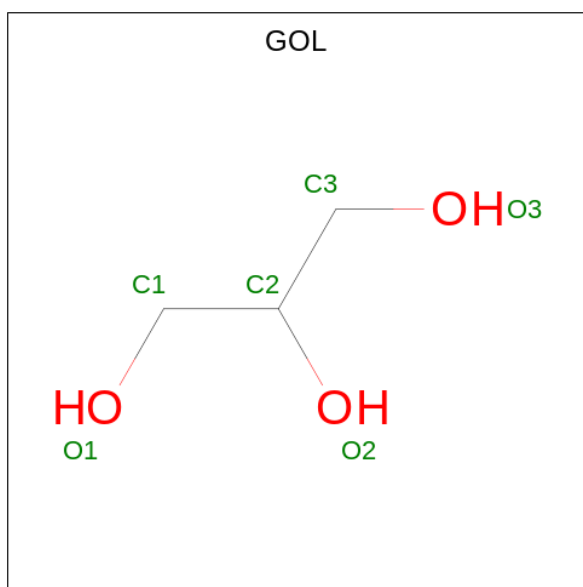
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 3	O 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	69	Total 69	O 69	0	0
5	B	80	Total 80	O 80	0	0
5	C	10	Total 10	O 10	0	0
5	D	9	Total 9	O 9	0	0

3 Residue-property plots ⓘ

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: YEATS domain-containing protein 2

Chain A:

• Molecule 1: YEATS domain-containing protein 2

Chain B:

• Molecule 2: 2

Chain C:

• Molecule 2: 2

Chain D:
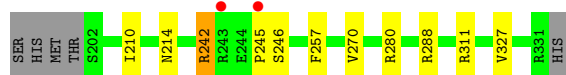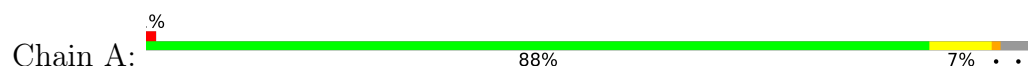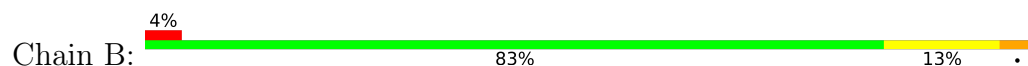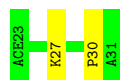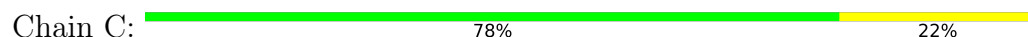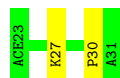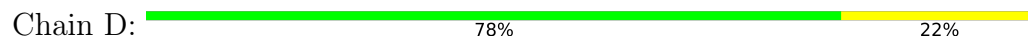
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	89.67Å 89.67Å 86.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.84 – 2.05 44.84 – 2.05	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.84-2.05) 100.0 (44.84-2.05)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.191 , 0.234 0.191 , 0.234	Depositor DCC
R_{free} test set	1563 reflections (6.82%)	wwPDB-VP
Wilson B-factor (Å^2)	36.1	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 52.0	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.020 for -h,-l,-k 0.015 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2583	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 8.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: GOL, ACE, SO4, LBZ

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	0.40	0/1127	0.55	0/1525
1	B	0.41	0/1171	0.56	0/1583
2	C	0.46	0/45	0.57	0/58
2	D	0.48	0/45	0.59	0/58
All	All	0.41	0/2388	0.56	0/3224

There are no bond length outliers.

There are no bond angle outliers.

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	1096	0	1101	10	0
1	B	1138	0	1139	15	0
2	C	65	0	48	1	0
2	D	65	0	48	1	0
3	A	10	0	0	1	0
3	B	25	0	0	1	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	6	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	69	0	0	5	0
5	B	80	0	0	1	0
5	C	10	0	0	0	0
5	D	9	0	0	0	0
All	All	2583	0	2344	25	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 5.

All (25) 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:246:SER:HA	4:A:403:GOL:H31	1.56	0.88
1:B:279:ARG:NH1	5:B:501:HOH:O	2.15	0.78
1:B:203:ARG:NH1	3:B:402:SO4:O4	2.24	0.68
1:A:242:ARG:NH2	5:A:503:HOH:O	2.21	0.67
1:A:311:ARG:NE	5:A:502:HOH:O	2.21	0.60
1:B:311:ARG:CZ	2:D:30:PRO:HB3	2.35	0.56
1:B:220:PRO:HG2	1:B:223:LYS:HG3	1.88	0.55
1:A:280:ARG:NH2	3:A:401:SO4:O3	2.33	0.55
1:B:252:LYS:HD3	1:B:271:ARG:HH12	1.72	0.55
1:A:246:SER:HA	4:A:403:GOL:H11	1.92	0.52
1:B:299:LYS:N	1:B:299:LYS:HD3	2.24	0.52
1:A:257:PHE:HB2	1:A:288:ARG:HB3	1.92	0.51
1:B:331:ARG:O	1:B:332:HIS:HB2	2.12	0.50
5:A:536:HOH:O	2:C:30:PRO:HD2	2.11	0.49
1:B:257:PHE:HB2	1:B:288:ARG:HB3	1.94	0.49
1:A:270:VAL:HG13	1:B:243:ARG:HH11	1.79	0.47
1:B:225:GLU:HG3	1:B:226:GLU:N	2.31	0.45
1:A:210:ILE:HD12	1:A:327:VAL:HG11	1.98	0.44
1:B:299:LYS:HD3	1:B:299:LYS:H	1.85	0.42
1:A:245:PRO:O	5:A:501:HOH:O	2.21	0.42
1:B:301:ILE:HD13	1:B:327:VAL:HG12	2.02	0.42
1:B:242:ARG:HD3	1:B:242:ARG:H	1.84	0.41
1:A:280:ARG:NE	5:A:511:HOH:O	2.51	0.41
1:B:252:LYS:HD3	1:B:271:ARG:NH1	2.35	0.41
1:B:297:GLN:HB3	1:B:330:HIS:ND1	2.35	0.41

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	128/135 (95%)	125 (98%)	3 (2%)	0	100	100
1	B	133/135 (98%)	127 (96%)	6 (4%)	0	100	100
2	C	6/9 (67%)	6 (100%)	0	0	100	100
2	D	6/9 (67%)	6 (100%)	0	0	100	100
All	All	273/288 (95%)	264 (97%)	9 (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	123/128 (96%)	121 (98%)	2 (2%)	62	59
1	B	128/128 (100%)	120 (94%)	8 (6%)	18	9
2	C	3/3 (100%)	3 (100%)	0	100	100
2	D	3/3 (100%)	3 (100%)	0	100	100
All	All	257/262 (98%)	247 (96%)	10 (4%)	32	25

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	ASN
1	A	242	ARG

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Mol	Chain	Res	Type
1	B	202	SER
1	B	214	ASN
1	B	225	GLU
1	B	242	ARG
1	B	267	LEU
1	B	271	ARG
1	B	299	LYS
1	B	332	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	248	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	LBZ	D	27	2	16,17,18	1.53	1 (6%)	15,20,22	1.02	1 (6%)
2	LBZ	C	27	2	16,17,18	1.51	1 (6%)	15,20,22	1.20	2 (13%)

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	LBZ	D	27	2	-	0/13/14/16	0/1/1/1
2	LBZ	C	27	2	-	0/13/14/16	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	27	LBZ	C7-N1	4.68	1.44	1.33
2	C	27	LBZ	C7-N1	4.31	1.43	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	27	LBZ	C8-N1-C7	-2.46	116.47	122.08
2	C	27	LBZ	O1-C7-N1	-2.41	117.80	122.61
2	D	27	LBZ	C1-C2-C3	2.02	121.47	118.59

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 ⓘ

There are no monosaccharides in this entry.

5.6　Ligand geometry ⓘ

10 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	SO4	A	401	-	4,4,4	0.14	0	6,6,6	0.22	0
3	SO4	B	403	-	4,4,4	0.16	0	6,6,6	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	SO4	A	402	-	4,4,4	0.16	0	6,6,6	0.14	0
3	SO4	B	401	-	4,4,4	0.15	0	6,6,6	0.22	0
4	GOL	A	403	-	5,5,5	1.00	0	5,5,5	0.90	0
3	SO4	D	101	-	4,4,4	0.16	0	6,6,6	0.16	0
3	SO4	B	402	-	4,4,4	0.15	0	6,6,6	0.21	0
3	SO4	B	405	-	4,4,4	0.22	0	6,6,6	0.32	0
3	SO4	B	404	-	4,4,4	0.14	0	6,6,6	0.17	0
3	SO4	C	101	-	4,4,4	0.13	0	6,6,6	0.31	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	GOL	A	403	-	-	4/4/4/4	-

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
4	A	403	GOL	C1-C2-C3-O3
4	A	403	GOL	O2-C2-C3-O3
4	A	403	GOL	O1-C1-C2-C3
4	A	403	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	SO4	1	0
4	A	403	GOL	2	0
3	B	402	SO4	1	0

5.7 Other polymers ⓘ

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, 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(Å²)	Q<0.9
1	A	130/135 (96%)	0.38	2 (1%)	73	76	22, 39, 60, 64	0
1	B	135/135 (100%)	0.21	6 (4%)	34	37	23, 38, 59, 77	0
2	C	7/9 (77%)	0.43	0	100	100	28, 32, 38, 39	0
2	D	7/9 (77%)	-0.08	0	100	100	29, 33, 39, 39	0
All	All	279/288 (96%)	0.29	8 (2%)	51	56	22, 38, 60, 77	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	245	PRO	5.2
1	A	243	ARG	4.0
1	B	332	HIS	3.6
1	B	226	GLU	3.1
1	B	271	ARG	2.8
1	B	272	GLU	2.4
1	B	-1	HIS	2.3
1	B	313	TYR	2.3

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(Å²)	Q<0.9
2	LBZ	D	27	17/18	0.96	0.13	24,30,35,38	0
2	LBZ	C	27	17/18	0.97	0.12	22,28,31,34	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
4	GOL	A	403	6/6	0.64	0.24	46,57,60,62	0
3	SO4	B	404	5/5	0.77	0.33	62,70,87,92	0
3	SO4	B	405	5/5	0.88	0.24	46,59,62,78	0
3	SO4	A	401	5/5	0.90	0.15	53,60,65,72	0
3	SO4	C	101	5/5	0.93	0.20	54,57,60,62	0
3	SO4	B	403	5/5	0.93	0.12	52,57,68,72	0
3	SO4	B	402	5/5	0.95	0.11	47,50,53,54	0
3	SO4	A	402	5/5	0.95	0.14	56,62,69,71	0
3	SO4	D	101	5/5	0.96	0.13	51,51,61,64	0
3	SO4	B	401	5/5	0.99	0.18	44,46,51,52	0

6.5 Other polymers ⓘ

There are no such residues in this entry.