



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:35 AM GMT

PDB ID : 2UXX  
Title : Human LSD1 Histone Demethylase-CoREST in complex with an FAD- tranyl-  
cypromine adduct  
Authors : Yang, M.; Culhane, J.C.; Machius, M.; Cole, P.A.; Yu, H.  
Deposited on : 2007-03-30  
Resolution : 2.74 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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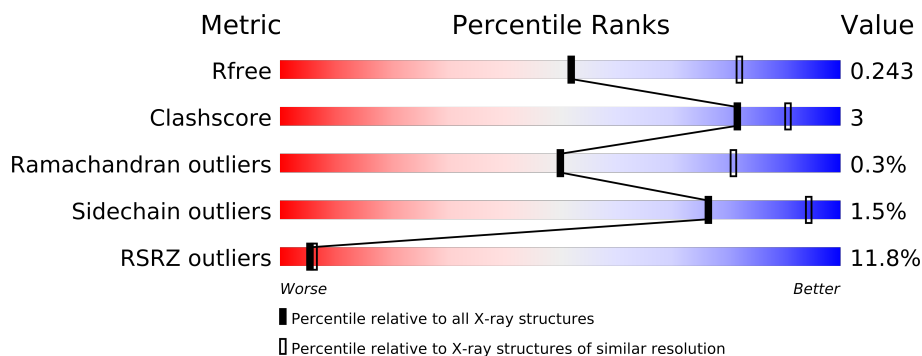
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.74 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))
$R_{free}$	66092	2164 (2.78-2.70)
Clashscore	79885	2639 (2.78-2.70)
Ramachandran outliers	78287	2594 (2.78-2.70)
Sidechain outliers	78261	2595 (2.78-2.70)
RSRZ outliers	66119	2166 (2.78-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	666	
2	B	235	

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 6379 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

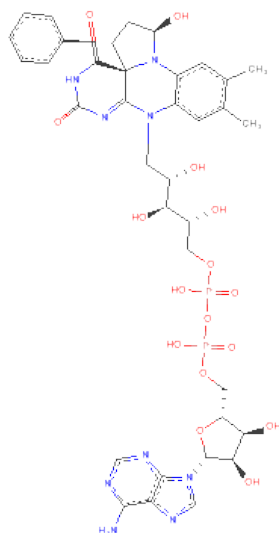
- Molecule 1 is a protein called LYSINE-SPECIFIC HISTONE DEMETHYLASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	665	5209	3318	905	966	20	0	0	0

- Molecule 2 is a protein called REST COREPRESSOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	134	1086	682	197	204	3	0	0	0

- Molecule 3 is FAD-TRANS-2-PHENYLCYCLOPROPYLAMINEADDUCT (three-letter code: FAJ) (formula: C<sub>36</sub>H<sub>43</sub>N<sub>9</sub>O<sub>16</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	63	36	9	16	2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

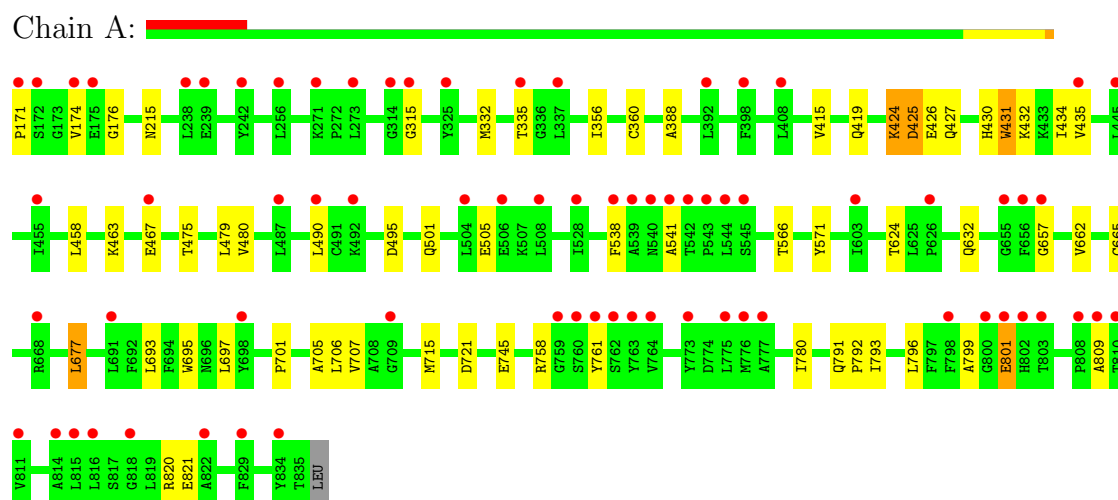
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	7	Total	O	0	0
			7	7		
6	B	1	Total	O	0	0
			1	1		

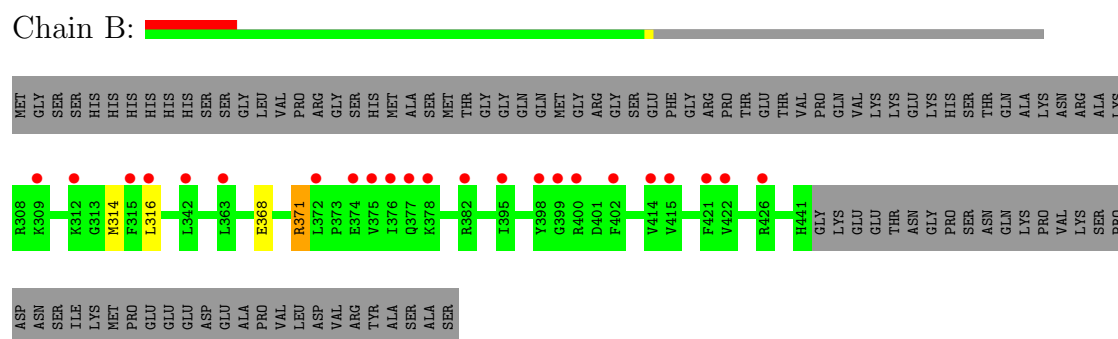
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: LYSINE-SPECIFIC HISTONE DEMETHYLASE 1



#### • Molecule 2: REST COREPRESSOR 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.80Å 178.50Å 235.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 2.74 49.20 – 2.74	Depositor EDS
% Data completeness (in resolution range)	97.5 (49.00-2.74) 97.5 (49.20-2.74)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.74 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.235 , 0.260 0.223 , 0.243	Depositor DCC
$R_{free}$ test set	1529 reflections (2.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	76.8	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 50.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 65173 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6379	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAJ, GOL, 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	0.56	3/5323 (0.1%)	0.59	4/7221 (0.1%)
2	B	0.32	0/1102	0.46	0/1486
All	All	0.53	3/6425 (0.0%)	0.57	4/8707 (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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	424	LYS	C-N	20.70	1.81	1.34
1	A	425	ASP	C-N	19.86	1.79	1.34
1	A	431	TRP	C-N	-16.88	0.95	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	431	TRP	O-C-N	14.13	145.31	122.70
1	A	431	TRP	CA-C-N	-10.40	94.31	117.20
1	A	431	TRP	C-N-CA	-9.35	98.32	121.70
1	A	424	LYS	O-C-N	-6.32	112.58	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	430	HIS	Mainchain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5209	0	5238	40	0
2	B	1086	0	1098	2	0
3	A	63	0	41	2	0
4	A	12	0	16	0	0
5	A	1	0	0	0	0
6	A	7	0	0	0	0
6	B	1	0	0	0	0
All	All	6379	0	6393	41	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (41) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:425:ASP:C	1:A:426:GLU:N	1.79	1.35
1:A:424:LYS:C	1:A:425:ASP:N	1.81	1.33
1:A:427:GLN:O	1:A:431:TRP:CD1	2.18	0.97
1:A:427:GLN:O	1:A:431:TRP:HD1	1.64	0.78
1:A:695:TRP:HE1	1:A:706:LEU:HD11	1.54	0.71
1:A:801:GLU:HG2	1:A:809:ALA:H	1.54	0.70
1:A:801:GLU:HG3	1:A:809:ALA:HA	1.74	0.68
1:A:566:THR:HG21	1:A:697:LEU:HD13	1.78	0.64
1:A:801:GLU:CG	1:A:809:ALA:H	2.16	0.59
1:A:479:LEU:O	1:A:480:VAL:HB	2.05	0.57
1:A:801:GLU:HG3	1:A:809:ALA:CA	2.38	0.54
1:A:360:CYS:SG	1:A:677:LEU:HD22	2.48	0.54
1:A:761:TYR:CD1	1:A:809:ALA:HB1	2.45	0.51
1:A:415:VAL:O	1:A:419:GLN:HG2	2.12	0.50
1:A:677:LEU:HD23	1:A:693:LEU:HD11	1.94	0.49
1:A:801:GLU:CG	1:A:809:ALA:N	2.77	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:171:PRO:HB2	1:A:176:GLY:HA2	1.97	0.47
1:A:431:TRP:CE3	1:A:434:ILE:HD12	2.50	0.47
1:A:356:ILE:HD11	1:A:566:THR:HG23	1.96	0.47
1:A:624:THR:HG22	1:A:799:ALA:HB3	1.96	0.47
1:A:495:ASP:OD1	2:B:371:ARG:NH2	2.49	0.46
1:A:458:LEU:HD12	1:A:490:LEU:HD12	1.98	0.46
1:A:425:ASP:C	1:A:426:GLU:CA	2.79	0.46
1:A:425:ASP:CA	1:A:426:GLU:N	2.74	0.46
1:A:463:LYS:O	1:A:467:GLU:HG3	2.16	0.45
1:A:665:CYS:HB2	1:A:745:GLU:HB2	1.99	0.45
1:A:541:ALA:O	1:A:657:GLY:HA3	2.17	0.45
1:A:174:VAL:HB	1:A:215:ASN:HB3	1.99	0.44
1:A:793:ILE:H	1:A:793:ILE:HD12	1.83	0.44
1:A:791:GLN:HA	1:A:792:PRO:HD3	1.92	0.43
1:A:662:VAL:HB	1:A:705:ALA:HB3	2.00	0.43
1:A:335:THR:HG21	3:A:900:FAJ:H7	2.00	0.43
1:A:707:VAL:HG11	1:A:715:MET:HG3	2.01	0.43
1:A:388:ALA:HB1	2:B:316:LEU:HD11	1.99	0.43
1:A:820:ARG:NE	1:A:821:GLU:OE2	2.47	0.42
1:A:780:ILE:HB	1:A:796:LEU:HB3	2.00	0.42
1:A:632:GLN:CD	1:A:758:ARG:HE	2.23	0.42
1:A:432:LYS:HA	1:A:435:VAL:HG22	2.02	0.42
1:A:801:GLU:HG2	1:A:809:ALA:N	2.27	0.41
3:A:900:FAJ:H10	3:A:900:FAJ:H5	1.87	0.41
1:A:501:GLN:O	1:A:505:GLU:HB2	2.21	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	663/666 (100%)	644 (97%)	17 (3%)	2 (0%)	50	81
2	B	132/235 (56%)	128 (97%)	4 (3%)	0	100	100
All	All	795/901 (88%)	772 (97%)	21 (3%)	2 (0%)	50	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	315	GLY
1	A	701	PRO

### 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	565/566 (100%)	558 (99%)	7 (1%)	82	95
2	B	118/203 (58%)	115 (98%)	3 (2%)	60	88
All	All	683/769 (89%)	673 (98%)	10 (2%)	76	94

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

Mol	Chain	Res	Type
1	A	332	MET
1	A	475	THR
1	A	538	PHE
1	A	571	TYR
1	A	677	LEU
1	A	721	ASP
1	A	801	GLU
2	B	314	MET
2	B	368	GLU
2	B	371	ARG

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 chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\# Z  > 2$
4	GOL	A	1837	-	5,5,5	0.34	0	5,5,5	0.25	0
4	GOL	A	1838	-	5,5,5	0.32	0	5,5,5	0.26	0
3	FAJ	A	900	-	70,70,70	1.00	5 (7%)	107,109,109	1.58	16 (14%)

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	1837	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1838	-	-	0/4/4/4	0/0/0/0
3	FAJ	A	900	-	-	0/38/106/106	0/2/8/8

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	FAJ	C34-N5	-3.02	1.33	1.37
3	A	900	FAJ	C3-N2	2.97	1.41	1.32
3	A	900	FAJ	C4-C1	2.09	1.55	1.53
3	A	900	FAJ	C1-N1	2.03	1.40	1.37
3	A	900	FAJ	C6-C5	2.02	1.54	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	FAJ	N7-C35-N8	-8.95	121.23	128.71
3	A	900	FAJ	N7-C34-N5	4.23	133.08	125.43
3	A	900	FAJ	C12-C5-C6	-3.85	107.80	115.40
3	A	900	FAJ	C28-O14-C31	-3.65	105.79	109.75
3	A	900	FAJ	C1-C4-C3	-3.49	104.14	112.79
3	A	900	FAJ	C15-C14-N3	-3.26	117.20	122.02
3	A	900	FAJ	O14-C31-C30	-3.05	102.09	106.77
3	A	900	FAJ	C33-C34-N7	-2.71	119.81	125.70
3	A	900	FAJ	P2-O10-P1	-2.70	123.76	131.68
3	A	900	FAJ	C4-C3-N4	2.50	121.57	115.60
3	A	900	FAJ	C1-N1-C2	-2.48	120.91	125.59
3	A	900	FAJ	C35-N7-C34	2.31	120.57	114.01
3	A	900	FAJ	C4-C1-N1	2.18	120.24	117.11
3	A	900	FAJ	O14-C31-N5	-2.17	106.42	108.44
3	A	900	FAJ	C34-C33-N6	-2.17	107.66	109.52
3	A	900	FAJ	C26-C25-C24	-2.14	108.02	112.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	665/666 (99%)	0.89	72 (10%) 6 7	70, 100, 117, 125	0
2	B	134/235 (57%)	0.90	23 (17%) 2 2	77, 98, 117, 126	0
All	All	799/901 (88%)	0.89	95 (11%) 5 6	70, 99, 118, 126	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	376	ILE	6.0
2	B	378	LYS	5.5
1	A	172	SER	5.2
2	B	375	VAL	5.0
1	A	171	PRO	4.6
2	B	312	LYS	3.7
1	A	504	LEU	3.4
1	A	242	TYR	3.4
2	B	374	GLU	3.4
2	B	395	ILE	3.4
2	B	316	LEU	3.2
2	B	414	VAL	3.2
2	B	309	LYS	3.2
2	B	402	PHE	3.0
1	A	808	PRO	3.0
2	B	422	VAL	3.0
1	A	809	ALA	2.9
2	B	399	GLY	2.9
2	B	382	ARG	2.9
1	A	763	TYR	2.8
2	B	421	PHE	2.8
1	A	762	SER	2.8
1	A	773	TYR	2.8
1	A	273	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	834	TYR	2.7
1	A	668	ARG	2.7
1	A	238	LEU	2.7
1	A	490	LEU	2.7
1	A	656	PHE	2.7
1	A	506	GLU	2.7
2	B	426	ARG	2.6
1	A	508	LEU	2.6
1	A	816	LEU	2.6
1	A	798	PHE	2.6
1	A	815	LEU	2.5
1	A	528	ILE	2.5
1	A	603	ILE	2.5
1	A	539	ALA	2.5
1	A	776	MET	2.4
1	A	271	LYS	2.4
1	A	392	LEU	2.4
2	B	363	LEU	2.4
1	A	655	GLY	2.4
1	A	698	TYR	2.4
2	B	400	ARG	2.4
1	A	542	THR	2.3
2	B	377	GLN	2.3
1	A	801	GLU	2.3
1	A	545	SER	2.3
1	A	760	SER	2.3
2	B	415	VAL	2.3
1	A	764	VAL	2.3
1	A	777	ALA	2.3
1	A	810	THR	2.3
1	A	492	LYS	2.3
1	A	800	GLY	2.3
1	A	540	ASN	2.2
1	A	802	HIS	2.2
1	A	811	VAL	2.2
1	A	822	ALA	2.2
1	A	175	GLU	2.2
1	A	538	PHE	2.2
1	A	691	LEU	2.2
1	A	325	TYR	2.2
1	A	174	VAL	2.2
1	A	543	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	315	GLY	2.1
2	B	372	LEU	2.1
1	A	487	LEU	2.1
1	A	759	GLY	2.1
1	A	829	PHE	2.1
1	A	445	LEU	2.1
1	A	314	GLY	2.1
1	A	408	LEU	2.1
1	A	814	ALA	2.1
1	A	626	PRO	2.1
1	A	761	TYR	2.1
1	A	239	GLU	2.1
1	A	337	LEU	2.1
1	A	467	GLU	2.1
1	A	435	VAL	2.1
1	A	398	PHE	2.1
2	B	315	PHE	2.1
2	B	398	TYR	2.1
1	A	818	GLY	2.1
1	A	775	LEU	2.0
2	B	342	LEU	2.0
1	A	335	THR	2.0
1	A	455	ILE	2.0
1	A	657	GLY	2.0
1	A	256	LEU	2.0
1	A	544	LEU	2.0
1	A	803	THR	2.0
1	A	709	GLY	2.0
1	A	541	ALA	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	A	1838	6/6	0.31	1.33	133,134,134,134	0
5	CL	A	1840	1/1	0.25	-0.61	109,109,109,109	0
4	GOL	A	1837	6/6	0.22	-0.94	83,84,85,85	0
3	FAJ	A	900	63/63	0.19	-1.76	58,67,74,74	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.