



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:38 AM GMT

PDB ID : 3PLZ  
Title : Human LRH1 LBD bound to GR470  
Authors : Williams, S.P.; Xu, R.; Zuercher, W.J.  
Deposited on : 2010-11-15  
Resolution : 1.75 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

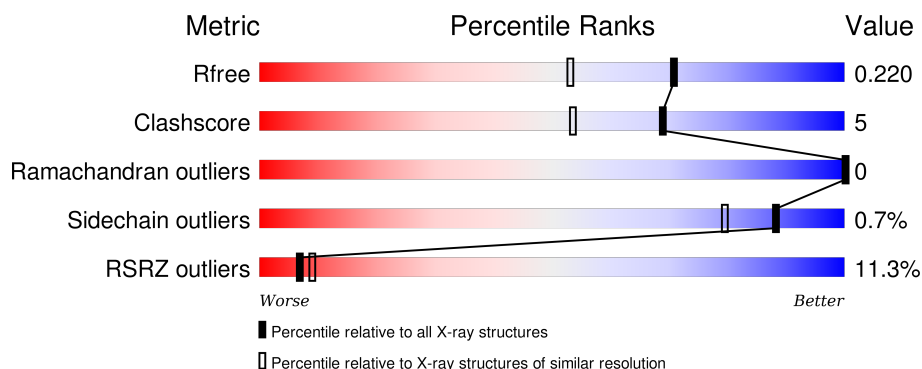
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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))
$R_{free}$	91344	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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	257	<div> <div>13%</div> <div>84%</div> <div>5%</div> <div>10%</div> </div>
1	B	257	<div> <div>8%</div> <div>84%</div> <div>9%</div> <div>7%</div> </div>
2	C	14	<div> <div>14%</div> <div>71%</div> <div>14%</div> <div>14%</div> </div>
2	D	14	<div> <div>7%</div> <div>79%</div> <div>7%</div> <div>14%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	B	2	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4332 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 FTZ-F1 related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	5	0
			1852	1204	300	334	14			
1	B	240	Total	C	N	O	S	0	2	0
			1907	1231	318	345	13			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	285	MET	-	EXPRESSION TAG	UNP Q9UEC0
A	286	LYS	-	EXPRESSION TAG	UNP Q9UEC0
A	287	LYS	-	EXPRESSION TAG	UNP Q9UEC0
A	288	GLY	-	EXPRESSION TAG	UNP Q9UEC0
A	289	HIS	-	EXPRESSION TAG	UNP Q9UEC0
A	290	HIS	-	EXPRESSION TAG	UNP Q9UEC0
A	291	HIS	-	EXPRESSION TAG	UNP Q9UEC0
A	292	HIS	-	EXPRESSION TAG	UNP Q9UEC0
A	293	HIS	-	EXPRESSION TAG	UNP Q9UEC0
A	294	HIS	-	EXPRESSION TAG	UNP Q9UEC0
A	295	LEU	-	EXPRESSION TAG	UNP Q9UEC0
A	296	VAL	-	EXPRESSION TAG	UNP Q9UEC0
A	297	PRO	-	EXPRESSION TAG	UNP Q9UEC0
A	298	ARG	-	EXPRESSION TAG	UNP Q9UEC0
A	299	GLY	-	EXPRESSION TAG	UNP Q9UEC0
B	285	MET	-	EXPRESSION TAG	UNP Q9UEC0
B	286	LYS	-	EXPRESSION TAG	UNP Q9UEC0
B	287	LYS	-	EXPRESSION TAG	UNP Q9UEC0
B	288	GLY	-	EXPRESSION TAG	UNP Q9UEC0
B	289	HIS	-	EXPRESSION TAG	UNP Q9UEC0
B	290	HIS	-	EXPRESSION TAG	UNP Q9UEC0
B	291	HIS	-	EXPRESSION TAG	UNP Q9UEC0
B	292	HIS	-	EXPRESSION TAG	UNP Q9UEC0
B	293	HIS	-	EXPRESSION TAG	UNP Q9UEC0
B	294	HIS	-	EXPRESSION TAG	UNP Q9UEC0

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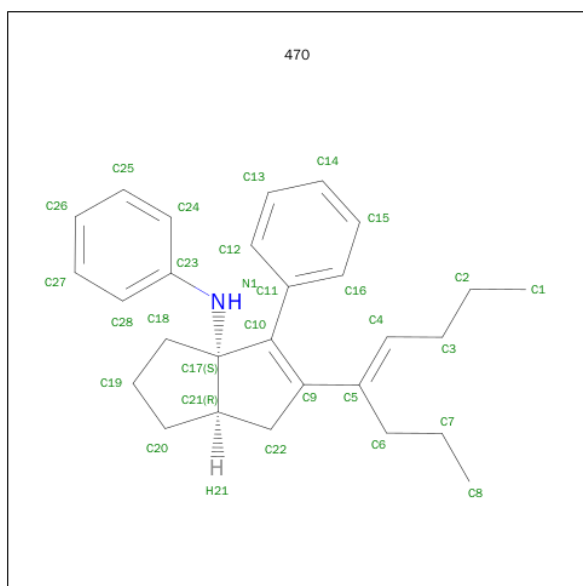
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Chain	Residue	Modelled	Actual	Comment	Reference
B	295	LEU	-	EXPRESSION TAG	UNP Q9UEC0
B	296	VAL	-	EXPRESSION TAG	UNP Q9UEC0
B	297	PRO	-	EXPRESSION TAG	UNP Q9UEC0
B	298	ARG	-	EXPRESSION TAG	UNP Q9UEC0
B	299	GLY	-	EXPRESSION TAG	UNP Q9UEC0

- Molecule 2 is a protein called Nuclear receptor coactivator 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	12	Total	C	N	O	0	0	0
			99	65	18	16			
2	D	12	Total	C	N	O	0	0	0
			103	67	18	18			

- Molecule 3 is (3AS,6AR)-5-[(4E)-OCT-4-EN-4-YL]-N,4-DIPHENYL-2,3,6,6A-TETRAHYDRO PENTALEN-3A(1H)-AMINE (three-letter code: 470) (formula: C<sub>28</sub>H<sub>35</sub>N).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N		0	0
			29	28	1			
3	B	1	Total	C	N		0	0
			29	28	1			

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

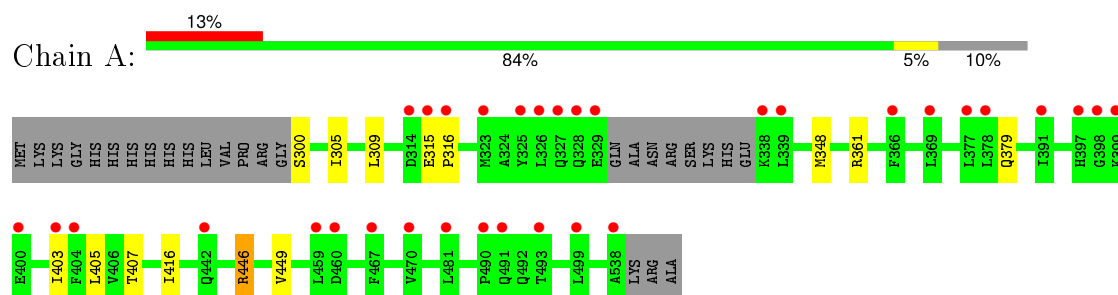
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	137	Total	O	0	0
			137	137		
5	C	10	Total	O	0	0
			10	10		
5	B	148	Total	O	0	0
			148	148		
5	D	10	Total	O	0	0
			10	10		

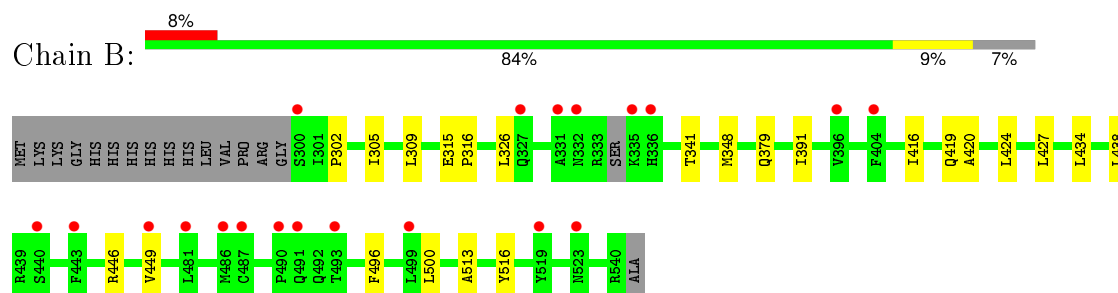
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

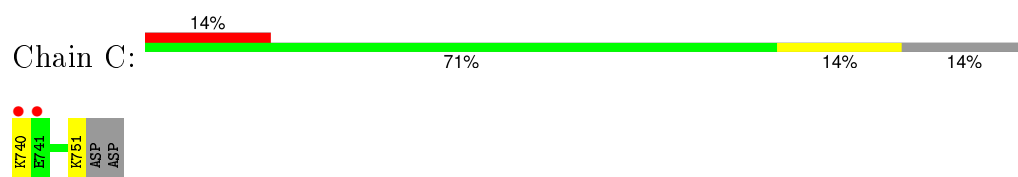
- Molecule 1: FTZ-F1 related protein



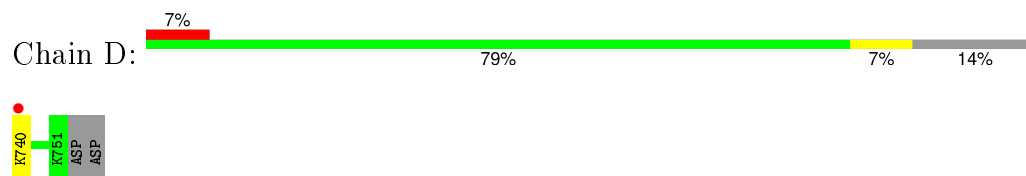
- Molecule 1: FTZ-F1 related protein



- Molecule 2: Nuclear receptor coactivator 2



- Molecule 2: Nuclear receptor coactivator 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.67Å 89.05Å 65.45Å 90.00° 101.71° 90.00°	Depositor
Resolution (Å)	19.94 – 1.75 19.47 – 1.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.94-1.75) 91.2 (19.47-1.75)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.79 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.5.0053	Depositor
R, $R_{free}$	0.185 , 0.214 0.194 , 0.220	Depositor DCC
$R_{free}$ test set	3905 reflections (7.75%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.1	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 53.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 54325 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4332	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 470, EDO

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	0.35	0/1903	0.48	0/2579
1	B	0.35	0/1947	0.50	0/2637
2	C	0.45	0/99	0.53	0/131
2	D	0.39	0/103	0.53	0/136
All	All	0.36	0/4052	0.49	0/5483

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 [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	1852	0	1833	15	0
1	B	1907	0	1889	22	0
2	C	99	0	108	2	0
2	D	103	0	112	1	0
3	A	29	0	35	2	0
3	B	29	0	35	0	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
5	A	137	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	148	0	0	4	0
5	C	10	0	0	0	0
5	D	10	0	0	0	0
All	All	4332	0	4024	37	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 (37) 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:403:ILE:HD13	3:A:1:470:H27	1.49	0.95
1:B:305:ILE:O	1:B:309:LEU:HD13	1.77	0.84
1:B:309:LEU:HD12	1:B:449[B]:VAL:HG21	1.59	0.83
1:A:403:ILE:HD12	1:A:416:ILE:HD12	1.58	0.82
1:A:309:LEU:CD1	1:A:449[B]:VAL:HG11	2.14	0.78
1:B:513:ALA:HB2	5:B:100:HOH:O	1.85	0.77
1:B:420:ALA:HB1	1:B:424:LEU:HB3	1.69	0.74
1:B:309:LEU:HD12	1:B:449[A]:VAL:HG11	1.73	0.71
1:A:309:LEU:HD12	1:A:449[B]:VAL:HG11	1.73	0.69
1:A:361:ARG:NH1	2:C:751:LYS:O	2.27	0.67
1:A:348[B]:MET:CE	1:A:405:LEU:HD13	2.25	0.66
1:B:309:LEU:CD1	1:B:449[B]:VAL:HG21	2.26	0.65
1:B:348:MET:HE2	1:B:348:MET:HA	1.84	0.59
1:B:326:LEU:HD11	1:B:348:MET:HE1	1.85	0.59
1:B:434:LEU:CD1	5:B:154:HOH:O	2.51	0.58
1:A:379:GLN:HE22	2:C:740:LYS:N	2.05	0.55
1:B:391:ILE:HG21	1:B:438:LEU:HD12	1.92	0.51
1:B:326:LEU:HD11	1:B:348:MET:CE	2.40	0.51
1:A:348[B]:MET:SD	1:A:405:LEU:HD13	2.53	0.48
1:A:348[B]:MET:HE3	1:A:405:LEU:HD13	1.93	0.47
1:A:446:ARG:O	1:A:449[B]:VAL:HG12	2.14	0.47
1:B:341:THR:HG22	1:B:416[B]:ILE:HD13	1.96	0.47
1:B:315:GLU:HB3	1:B:316:PRO:HD3	1.97	0.47
1:A:403:ILE:CD1	1:A:416:ILE:HD12	2.37	0.46
1:B:434:LEU:HD13	5:B:154:HOH:O	2.14	0.46
1:B:496:PHE:CZ	1:B:500:LEU:HD11	2.50	0.46
1:B:302:PRO:HD2	1:B:305:ILE:HD12	1.97	0.46
1:A:305:ILE:O	1:A:309:LEU:HD13	2.15	0.45
1:B:379:GLN:HE22	2:D:740:LYS:N	2.13	0.45
1:B:348:MET:CE	1:B:348:MET:HA	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348[A]:MET:HE1	1:A:407:THR:HG21	1.99	0.44
1:B:309:LEU:CD1	1:B:449[A]:VAL:HG11	2.43	0.43
1:A:403:ILE:CD1	3:A:1:470:H27	2.34	0.43
1:B:427:LEU:HD22	5:B:100:HOH:O	2.19	0.43
1:B:341:THR:N	1:B:419:GLN:HE22	2.19	0.41
1:B:424:LEU:HD13	1:B:516:TYR:CE2	2.56	0.41
1:A:315:GLU:N	1:A:316:PRO:CD	2.85	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	232/257 (90%)	228 (98%)	4 (2%)	0	100	100
1	B	238/257 (93%)	236 (99%)	2 (1%)	0	100	100
2	C	10/14 (71%)	9 (90%)	1 (10%)	0	100	100
2	D	10/14 (71%)	10 (100%)	0	0	100	100
All	All	490/542 (90%)	483 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	199/231 (86%)	197 (99%)	2 (1%)	82	69
1	B	203/231 (88%)	202 (100%)	1 (0%)	92	87
2	C	10/13 (77%)	10 (100%)	0	100	100
2	D	11/13 (85%)	11 (100%)	0	100	100
All	All	423/488 (87%)	420 (99%)	3 (1%)	88	79

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	300	SER
1	A	446	ARG
1	B	446	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	379	GLN
1	A	419	GLN
1	A	426	ASN
1	A	432	GLN
1	A	478	ASN
1	A	512	GLN
1	B	327	GLN
1	B	330	GLN
1	B	379	GLN
1	B	419	GLN
1	B	521	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules 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

4 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	470	A	1	-	29,32,32	0.51	0	28,44,44	1.31	2 (7%)
4	EDO	A	2	-	3,3,3	0.47	0	2,2,2	0.39	0
3	470	B	1	-	29,32,32	0.46	0	28,44,44	1.30	1 (3%)
4	EDO	B	2	-	3,3,3	0.44	0	2,2,2	0.38	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	470	A	1	-	-	0/16/47/47	0/4/4/4
4	EDO	A	2	-	-	0/1/1/1	0/0/0/0
3	470	B	1	-	-	0/16/47/47	0/4/4/4
4	EDO	B	2	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	470	C18-C17-N1	-4.64	105.77	112.87
3	A	1	470	C18-C17-N1	-4.64	105.78	112.87
3	A	1	470	C22-C21-C17	2.44	107.41	103.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	470	2	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 ⓘ

### 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	231/257 (89%)	0.77	33 (14%) 4 5	12, 18, 29, 44	0
1	B	240/257 (93%)	0.68	20 (8%) 14 17	12, 18, 27, 36	0
2	C	12/14 (85%)	0.88	2 (16%) 2 4	11, 14, 25, 31	0
2	D	12/14 (85%)	0.59	1 (8%) 14 17	11, 15, 26, 27	0
All	All	495/542 (91%)	0.73	56 (11%) 7 9	11, 18, 28, 44	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	339	LEU	9.0
1	A	493	THR	7.0
1	A	338	LYS	6.0
1	B	336	HIS	5.8
1	B	490	PRO	5.5
1	A	316	PRO	4.4
1	B	491	GLN	4.4
1	A	327	GLN	4.3
1	A	400	GLU	4.2
1	B	335	LYS	4.1
1	A	467	PHE	4.0
1	B	332	ASN	3.9
1	A	398	GLY	3.9
1	B	487	CYS	3.8
1	A	491	GLN	3.7
1	A	329	GLU	3.7
1	A	538	ALA	3.6
1	A	325	TYR	3.5
1	B	331	ALA	3.5
1	A	470	VAL	3.3
1	A	404[A]	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	486	MET	3.3
1	B	481	LEU	3.2
2	C	741	GLU	3.1
1	A	399	LYS	3.0
1	B	327	GLN	2.9
2	C	740	LYS	3.0
1	B	396	VAL	2.9
1	A	481	LEU	2.8
1	A	377	LEU	2.8
1	A	314	ASP	2.7
1	B	440	SER	2.7
1	A	328	GLN	2.7
1	A	490	PRO	2.7
1	B	493	THR	2.6
1	B	300	SER	2.6
1	A	366	PHE	2.5
1	B	523	ASN	2.5
1	A	323	MET	2.4
1	B	499	LEU	2.4
1	A	326	LEU	2.4
1	A	459	LEU	2.4
1	A	397	HIS	2.3
1	B	519	TYR	2.3
1	B	404	PHE	2.3
1	A	403	ILE	2.3
1	A	460	ASP	2.2
1	A	315	GLU	2.2
1	A	369	LEU	2.2
1	A	499	LEU	2.2
1	A	442	GLN	2.1
1	A	391	ILE	2.1
1	B	443	PHE	2.1
1	A	378	LEU	2.1
1	B	449[A]	VAL	2.0
2	D	740	LYS	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 [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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	B	2	4/4	0.85	0.21	5.04	52,53,53,53	0
3	470	A	1	29/29	0.89	0.13	1.02	21,23,27,29	0
3	470	B	1	29/29	0.96	0.12	0.05	13,15,23,28	0
4	EDO	A	2	4/4	0.83	0.10	-	59,59,59,59	0

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

There are no such residues in this entry.