



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 07:30 pm GMT

PDB ID : 4L2O  
Title : Crystal structure of human ALDH3A1 with its selective inhibitor 1-(4-fluorophenyl)sulfonyl-2-methylbenzimidazole  
Authors : Hurley, T.D.; Parajuli, B.  
Deposited on : 2013-06-04  
Resolution : 1.94 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

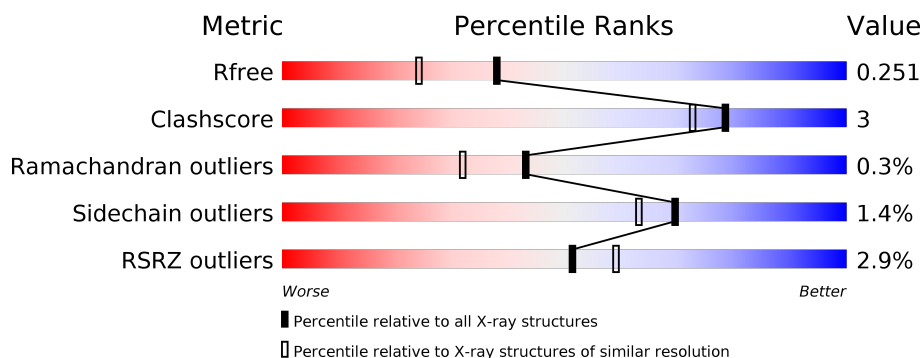
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.94 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))
$R_{free}$	111664	3622 (1.96-1.92)
Clashscore	122126	3795 (1.96-1.92)
Ramachandran outliers	120053	3757 (1.96-1.92)
Sidechain outliers	120020	3757 (1.96-1.92)
RSRZ outliers	108989	3554 (1.96-1.92)

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	469	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>5%</div> </div> </div>
1	B	469	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>5%</div> </div> </div>
1	E	469	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>5%</div> </div> </div>
1	G	469	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>5%</div> </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
5	1DD	A	506	-	-	-	X
5	1DD	B	504	-	-	-	X
5	1DD	E	504	-	-	-	X
5	1DD	G	505	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15234 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 Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	6	0
			3519	2242	598	661	18			
1	B	447	Total	C	N	O	S	0	2	0
			3498	2230	593	657	18			
1	E	447	Total	C	N	O	S	0	6	0
			3521	2244	598	661	18			
1	G	447	Total	C	N	O	S	0	5	0
			3509	2236	594	661	18			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	HIS	-	EXPRESSION TAG	UNP P30838
A	-15	HIS	-	EXPRESSION TAG	UNP P30838
A	-14	HIS	-	EXPRESSION TAG	UNP P30838
A	-13	HIS	-	EXPRESSION TAG	UNP P30838
A	-12	HIS	-	EXPRESSION TAG	UNP P30838
A	-11	HIS	-	EXPRESSION TAG	UNP P30838
A	-10	SER	-	EXPRESSION TAG	UNP P30838
A	-9	SER	-	EXPRESSION TAG	UNP P30838
A	-8	GLY	-	EXPRESSION TAG	UNP P30838
A	-7	LEU	-	EXPRESSION TAG	UNP P30838
A	-6	VAL	-	EXPRESSION TAG	UNP P30838
A	-5	PRO	-	EXPRESSION TAG	UNP P30838
A	-4	ARG	-	EXPRESSION TAG	UNP P30838
A	-3	GLY	-	EXPRESSION TAG	UNP P30838
A	-2	SER	-	EXPRESSION TAG	UNP P30838
A	-1	HIS	-	EXPRESSION TAG	UNP P30838
A	133	ALA	SER	NATURAL VARIANT	UNP P30838
B	-16	HIS	-	EXPRESSION TAG	UNP P30838
B	-15	HIS	-	EXPRESSION TAG	UNP P30838
B	-14	HIS	-	EXPRESSION TAG	UNP P30838
B	-13	HIS	-	EXPRESSION TAG	UNP P30838

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	EXPRESSION TAG	UNP P30838
B	-11	HIS	-	EXPRESSION TAG	UNP P30838
B	-10	SER	-	EXPRESSION TAG	UNP P30838
B	-9	SER	-	EXPRESSION TAG	UNP P30838
B	-8	GLY	-	EXPRESSION TAG	UNP P30838
B	-7	LEU	-	EXPRESSION TAG	UNP P30838
B	-6	VAL	-	EXPRESSION TAG	UNP P30838
B	-5	PRO	-	EXPRESSION TAG	UNP P30838
B	-4	ARG	-	EXPRESSION TAG	UNP P30838
B	-3	GLY	-	EXPRESSION TAG	UNP P30838
B	-2	SER	-	EXPRESSION TAG	UNP P30838
B	-1	HIS	-	EXPRESSION TAG	UNP P30838
B	133	ALA	SER	NATURAL VARIANT	UNP P30838
E	-16	HIS	-	EXPRESSION TAG	UNP P30838
E	-15	HIS	-	EXPRESSION TAG	UNP P30838
E	-14	HIS	-	EXPRESSION TAG	UNP P30838
E	-13	HIS	-	EXPRESSION TAG	UNP P30838
E	-12	HIS	-	EXPRESSION TAG	UNP P30838
E	-11	HIS	-	EXPRESSION TAG	UNP P30838
E	-10	SER	-	EXPRESSION TAG	UNP P30838
E	-9	SER	-	EXPRESSION TAG	UNP P30838
E	-8	GLY	-	EXPRESSION TAG	UNP P30838
E	-7	LEU	-	EXPRESSION TAG	UNP P30838
E	-6	VAL	-	EXPRESSION TAG	UNP P30838
E	-5	PRO	-	EXPRESSION TAG	UNP P30838
E	-4	ARG	-	EXPRESSION TAG	UNP P30838
E	-3	GLY	-	EXPRESSION TAG	UNP P30838
E	-2	SER	-	EXPRESSION TAG	UNP P30838
E	-1	HIS	-	EXPRESSION TAG	UNP P30838
E	133	ALA	SER	NATURAL VARIANT	UNP P30838
G	-16	HIS	-	EXPRESSION TAG	UNP P30838
G	-15	HIS	-	EXPRESSION TAG	UNP P30838
G	-14	HIS	-	EXPRESSION TAG	UNP P30838
G	-13	HIS	-	EXPRESSION TAG	UNP P30838
G	-12	HIS	-	EXPRESSION TAG	UNP P30838
G	-11	HIS	-	EXPRESSION TAG	UNP P30838
G	-10	SER	-	EXPRESSION TAG	UNP P30838
G	-9	SER	-	EXPRESSION TAG	UNP P30838
G	-8	GLY	-	EXPRESSION TAG	UNP P30838
G	-7	LEU	-	EXPRESSION TAG	UNP P30838
G	-6	VAL	-	EXPRESSION TAG	UNP P30838
G	-5	PRO	-	EXPRESSION TAG	UNP P30838

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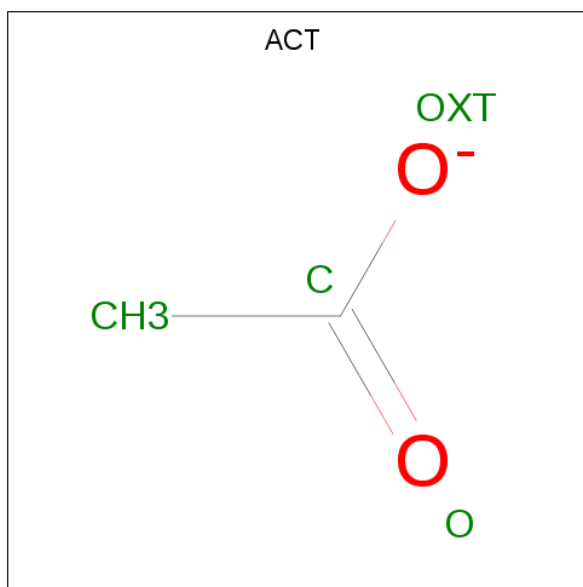
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Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	ARG	-	EXPRESSION TAG	UNP P30838
G	-3	GLY	-	EXPRESSION TAG	UNP P30838
G	-2	SER	-	EXPRESSION TAG	UNP P30838
G	-1	HIS	-	EXPRESSION TAG	UNP P30838
G	133	ALA	SER	NATURAL VARIANT	UNP P30838

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total K 2 2	0	0
2	B	2	Total K 2 2	0	0
2	A	2	Total K 2 2	0	0
2	E	1	Total K 1 1	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



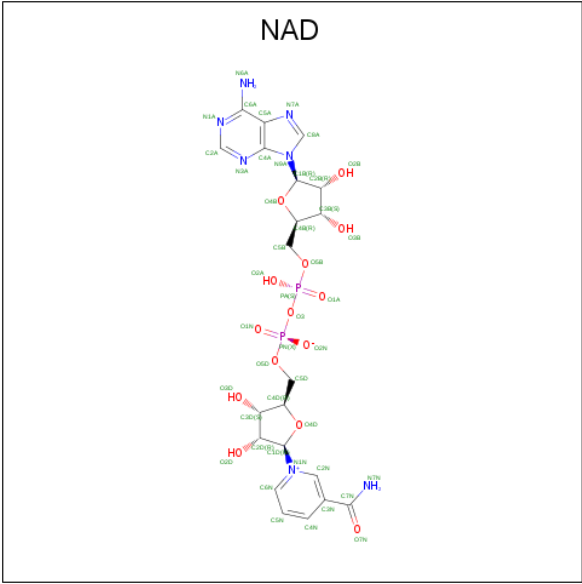
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0

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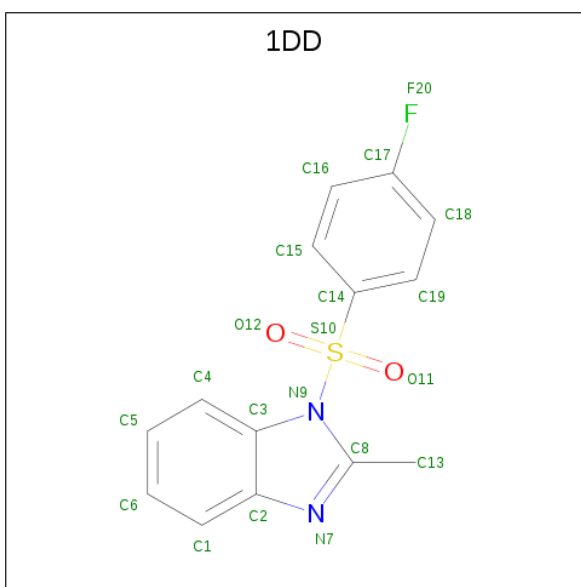
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 5 is 1-[(4-fluorophenyl)sulfonyl]-2-methyl-1H-benzimidazole (three-letter code: 1DD) (formula: C<sub>14</sub>H<sub>11</sub>FN<sub>2</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 20	C 14	F 1	N 2	O 2	S 1	0	0
5	B	1	Total 20	C 14	F 1	N 2	O 2	S 1	0	0
5	E	1	Total 20	C 14	F 1	N 2	O 2	S 1	0	0
5	G	1	Total 20	C 14	F 1	N 2	O 2	S 1	0	0

- Molecule 6 is water.

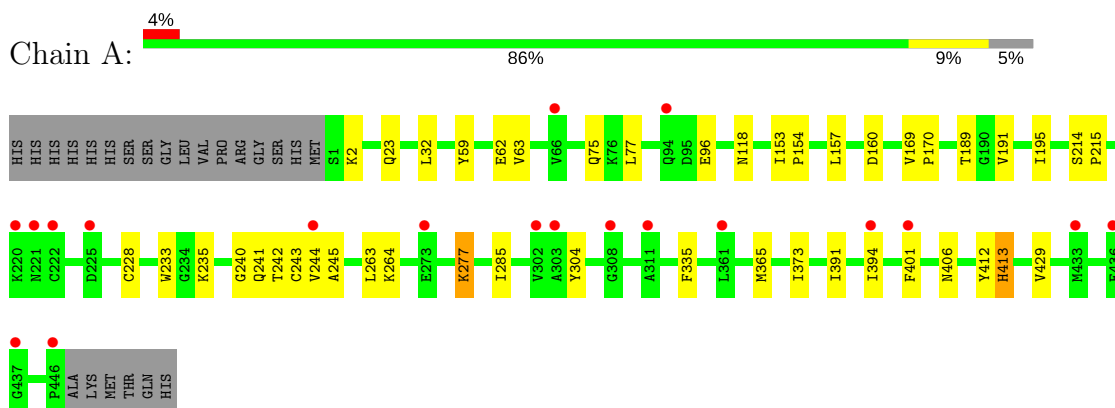
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	212	Total	O	0	0
			212	212		
6	B	256	Total	O	0	0
			256	256		
6	E	235	Total	O	0	0
			235	235		
6	G	205	Total	O	0	0
			205	205		



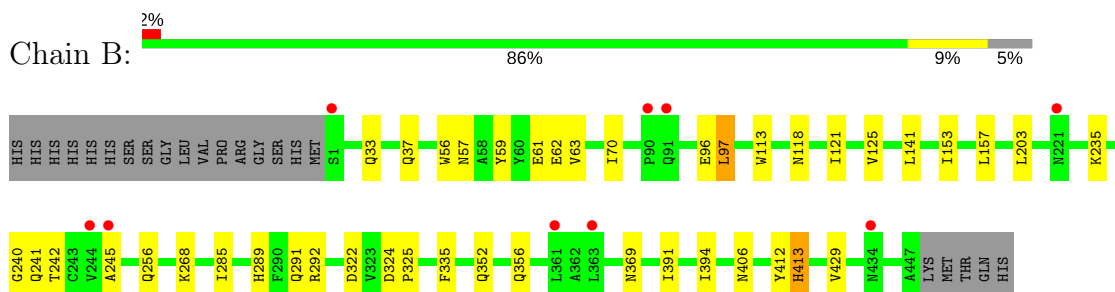
### 3 Residue-property plots [i](#)

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

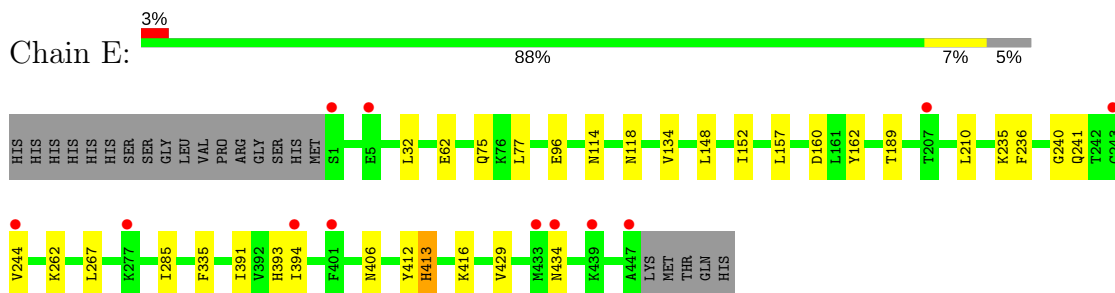
- Molecule 1: Aldehyde dehydrogenase



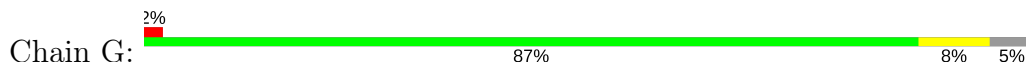
- Molecule 1: Aldehyde dehydrogenase

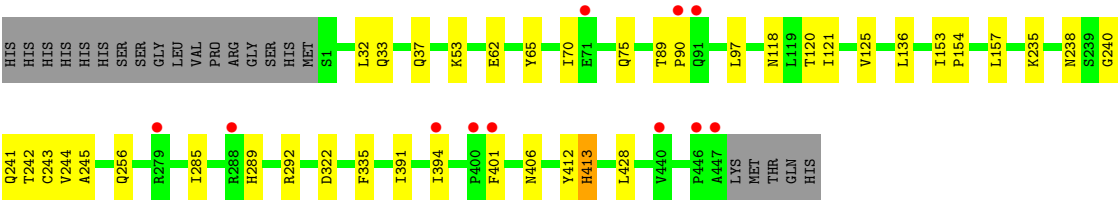


- Molecule 1: Aldehyde dehydrogenase



- Molecule 1: Aldehyde dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.22Å 90.92Å 117.92Å 90.00° 112.48° 90.00°	Depositor
Resolution (Å)	40.00 – 1.94 41.95 – 1.94	Depositor EDS
% Data completeness (in resolution range)	95.7 (40.00-1.94) 95.7 (41.95-1.94)	Depositor EDS
$R_{merge}$	0.34	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.215 , 0.250 0.215 , 0.251	Depositor DCC
$R_{free}$ test set	6642 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.1	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 30.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15234	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.66 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.4431e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.333 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: 1DD, K, NAD, ACT

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	0.49	1/3604 (0.0%)	0.49	1/4885 (0.0%)
1	B	0.39	1/3577 (0.0%)	0.48	1/4850 (0.0%)
1	E	0.39	0/3609	0.48	1/4892 (0.0%)
1	G	0.39	0/3594	0.48	0/4873
All	All	0.41	2/14384 (0.0%)	0.48	3/19500 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	56	TRP	CD2-CE2	5.15	1.47	1.41
1	A	233	TRP	CD2-CE2	5.04	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	97	LEU	CA-CB-CG	5.44	127.81	115.30
1	E	160	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	160	ASP	CB-CG-OD2	5.16	122.94	118.30

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	3519	0	3559	25	0
1	B	3498	0	3535	21	0
1	E	3521	0	3565	17	0
1	G	3509	0	3547	26	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	E	1	0	0	0	0
2	G	2	0	0	0	0
3	A	8	0	6	0	0
3	E	4	0	3	0	0
3	G	4	0	3	0	0
4	A	44	0	26	0	0
4	B	44	0	26	1	0
4	E	44	0	26	0	0
4	G	44	0	26	1	0
5	A	20	0	11	3	0
5	B	20	0	11	1	0
5	E	20	0	11	1	0
5	G	20	0	11	4	0
6	A	212	0	0	1	0
6	B	256	0	0	0	0
6	E	235	0	0	2	0
6	G	205	0	0	1	0
All	All	15234	0	14366	90	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 3.

All (90) 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:G:256:GLN:HE22	1:G:322:ASP:H	1.19	0.91
1:B:256:GLN:HE22	1:B:322:ASP:H	1.26	0.83
1:B:289:HIS:HD2	1:B:292:ARG:HE	1.42	0.67
1:G:412:TYR:O	1:G:413:HIS:HB2	1.94	0.67
1:G:289:HIS:HD2	1:G:292:ARG:HE	1.44	0.64
1:G:53:LYS:HE3	1:G:238:ASN:ND2	2.12	0.64
1:E:412:TYR:O	1:E:413:HIS:HB2	1.96	0.63
1:A:412:TYR:O	1:A:413:HIS:HB2	1.99	0.63
1:A:241:GLN:HE22	1:A:285:ILE:H	1.48	0.61
1:A:243:CYS:SG	6:A:812:HOH:O	2.15	0.60
1:G:241:GLN:HE22	1:G:285:ILE:H	1.47	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:53:LYS:HE3	1:G:238:ASN:HD22	1.67	0.59
1:B:412:TYR:O	1:B:413:HIS:HB2	2.01	0.59
1:B:62:GLU:HG3	1:B:118:ASN:HB2	1.84	0.58
1:A:62:GLU:HG3	1:A:118:ASN:HB2	1.85	0.58
1:B:241:GLN:HE22	1:B:285:ILE:H	1.50	0.57
1:B:33:GLN:HG3	1:B:70:ILE:HG21	1.86	0.57
1:E:391:ILE:O	1:E:394:ILE:HG12	2.05	0.56
1:A:391:ILE:O	1:A:394:ILE:HG12	2.05	0.56
1:G:244:VAL:HG22	6:G:779:HOH:O	2.05	0.56
1:A:264:LYS:HE2	1:A:304:TYR:CD1	2.41	0.56
1:G:256:GLN:NE2	1:G:322:ASP:H	1.97	0.55
1:B:256:GLN:NE2	1:B:322:ASP:H	2.00	0.54
1:A:96:GLU:HB2	1:A:429:VAL:HB	1.89	0.54
1:B:391:ILE:O	1:B:394:ILE:HG12	2.08	0.54
1:B:352:GLN:O	1:B:356:GLN:HG2	2.07	0.53
1:G:401:PHE:CE2	5:G:505:1DD:H11	2.44	0.53
1:G:243:CYS:SG	4:G:504:NAD:C4N	2.97	0.52
1:G:391:ILE:O	1:G:394:ILE:HG12	2.10	0.52
1:E:32[A]:LEU:HG	1:E:157:LEU:HD21	1.92	0.52
1:E:241:GLN:HE22	1:E:285:ILE:H	1.56	0.52
1:E:96:GLU:HB2	1:E:429:VAL:HB	1.92	0.52
1:G:244:VAL:HG23	1:G:391:ILE:HD13	1.92	0.52
1:G:32:LEU:HG	1:G:157:LEU:HD21	1.93	0.51
1:A:32[A]:LEU:HG	1:A:157:LEU:HD21	1.92	0.50
1:A:242:THR:HB	1:A:245:ALA:HB2	1.94	0.50
1:B:96:GLU:HB2	1:B:429:VAL:HB	1.95	0.48
1:A:394:ILE:HD12	5:A:506:1DD:C2	2.43	0.48
1:E:394:ILE:HD12	5:E:504:1DD:C2	2.44	0.47
1:A:401:PHE:CE2	5:A:506:1DD:H11	2.49	0.47
1:E:244:VAL:HG21	1:E:394:ILE:HD13	1.96	0.47
1:G:394:ILE:HD12	5:G:505:1DD:C2	2.45	0.47
1:B:394:ILE:HD12	5:B:504:1DD:C2	2.44	0.47
1:G:235:LYS:O	1:G:240:GLY:HA2	2.15	0.46
1:A:153:ILE:HB	1:A:154:PRO:HD3	1.97	0.46
1:E:393:HIS:HE1	6:E:771:HOH:O	1.98	0.46
1:A:235:LYS:O	1:A:240:GLY:HA2	2.16	0.46
1:A:191:VAL:O	1:A:195:ILE:HG12	2.16	0.46
1:A:153:ILE:HG23	1:A:157:LEU:HD12	1.98	0.45
1:A:412:TYR:O	1:A:413:HIS:CB	2.65	0.45
1:G:97:LEU:CD2	1:G:428:LEU:HD13	2.47	0.45
1:G:412:TYR:O	1:G:413:HIS:CB	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:121:ILE:O	1:G:125:VAL:HG23	2.17	0.44
1:B:235:LYS:O	1:B:240:GLY:HA2	2.18	0.44
1:A:59:TYR:HA	1:A:63:VAL:HB	1.99	0.44
1:G:33:GLN:HG3	1:G:70:ILE:HG21	2.00	0.43
1:E:235:LYS:O	1:E:240:GLY:HA2	2.19	0.43
1:G:289:HIS:CD2	1:G:292:ARG:HE	2.31	0.43
1:G:89:THR:HB	1:G:90:PRO:HD2	2.01	0.42
1:A:277:LYS:N	1:A:277:LYS:HD2	2.33	0.42
1:E:236:PHE:CD2	1:E:267:LEU:HD21	2.53	0.42
1:B:153:ILE:HG23	1:B:157:LEU:HD12	2.01	0.42
1:A:228:CYS:HB3	1:A:263:LEU:HD23	2.00	0.42
1:A:23[A]:GLN:HA	1:A:23[A]:GLN:OE1	2.18	0.42
1:E:114:ASN:ND2	6:E:808:HOH:O	2.47	0.42
1:E:148:LEU:O	1:E:152:ILE:HG12	2.19	0.42
1:B:113:TRP:CD1	1:B:141:LEU:HD12	2.54	0.42
1:A:244:VAL:HG21	1:A:394:ILE:HD13	2.02	0.42
1:G:62:GLU:HG3	1:G:118:ASN:HB2	2.01	0.42
1:A:365:MET:SD	1:A:373:ILE:HG23	2.59	0.41
1:G:153:ILE:HB	1:G:154:PRO:HD3	2.01	0.41
5:G:505:1DD:C13	5:G:505:1DD:O12	2.68	0.41
1:G:242:THR:HB	1:G:245:ALA:HB2	2.02	0.41
1:A:189:THR:HG23	1:B:203:LEU:HD11	2.03	0.41
1:G:120:THR:HB	1:G:136[A]:LEU:HD11	2.03	0.41
1:E:134:VAL:O	1:E:162:TYR:HA	2.19	0.41
5:A:506:1DD:C13	5:A:506:1DD:O12	2.68	0.41
1:B:324:ASP:HA	1:B:325:PRO:HD2	1.96	0.41
1:B:57:ASN:O	1:B:61:GLU:HB2	2.20	0.41
1:E:62:GLU:HG3	1:E:118:ASN:HB2	2.03	0.41
1:B:121:ILE:O	1:B:125:VAL:HG23	2.20	0.41
1:A:214:SER:HA	1:A:215:PRO:HD3	1.94	0.41
1:E:412:TYR:O	1:E:413:HIS:CB	2.64	0.41
1:G:65:TYR:CD2	5:G:505:1DD:H4	2.56	0.41
1:B:242:THR:HB	1:B:245:ALA:HB2	2.02	0.40
1:B:59:TYR:HA	1:B:63:VAL:HB	2.03	0.40
1:A:169:VAL:HB	1:A:170:PRO:HD3	2.03	0.40
1:E:416:LYS:HD2	1:E:416:LYS:HA	1.89	0.40
1:B:289:HIS:HE1	4:B:503:NAD:O2A	2.05	0.40
1:E:189:THR:HA	1:E:210:LEU:HD13	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	450/469 (96%)	440 (98%)	9 (2%)	1 (0%)	49	39
1	B	447/469 (95%)	436 (98%)	10 (2%)	1 (0%)	49	39
1	E	451/469 (96%)	444 (98%)	5 (1%)	2 (0%)	36	24
1	G	450/469 (96%)	444 (99%)	5 (1%)	1 (0%)	49	39
All	All	1798/1876 (96%)	1764 (98%)	29 (2%)	5 (0%)	43	32

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	413	HIS
1	B	413	HIS
1	E	413	HIS
1	G	413	HIS
1	E	434	ASN

### 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	386/400 (96%)	380 (98%)	6 (2%)	65	59
1	B	382/400 (96%)	375 (98%)	7 (2%)	62	54
1	E	386/400 (96%)	381 (99%)	5 (1%)	71	66
1	G	385/400 (96%)	381 (99%)	4 (1%)	78	75
All	All	1539/1600 (96%)	1517 (99%)	22 (1%)	69	63



All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	75	GLN
1	A	77	LEU
1	A	277	LYS
1	A	335	PHE
1	A	406	ASN
1	B	37	GLN
1	B	97	LEU
1	B	268	LYS
1	B	291	GLN
1	B	335	PHE
1	B	369	ASN
1	B	406	ASN
1	E	75	GLN
1	E	77	LEU
1	E	262	LYS
1	E	335	PHE
1	E	406	ASN
1	G	37	GLN
1	G	75	GLN
1	G	335	PHE
1	G	406	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	118	ASN
1	A	241	GLN
1	A	291	GLN
1	A	393	HIS
1	A	397	HIS
1	A	423	HIS
1	B	33	GLN
1	B	37	GLN
1	B	93	GLN
1	B	118	ASN
1	B	122	GLN
1	B	238	ASN
1	B	241	GLN
1	B	256	GLN

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Mol	Chain	Res	Type
1	B	289	HIS
1	B	291	GLN
1	B	369	ASN
1	B	406	ASN
1	B	423	HIS
1	E	27	GLN
1	E	37	GLN
1	E	241	GLN
1	E	393	HIS
1	E	397	HIS
1	E	406	ASN
1	E	423	HIS
1	G	27	GLN
1	G	33	GLN
1	G	37	GLN
1	G	75	GLN
1	G	118	ASN
1	G	122	GLN
1	G	238	ASN
1	G	241	GLN
1	G	256	GLN
1	G	289	HIS
1	G	406	ASN
1	G	423	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 ⓘ

Of 19 ligands modelled in this entry, 7 are monoatomic - leaving 12 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	$\# Z  > 2$
3	ACT	A	503	-	1,3,3	1.24	0	0,3,3	0.00	-
3	ACT	A	504	-	1,3,3	1.31	0	0,3,3	0.00	-
4	NAD	A	505	-	40,48,48	0.86	1 (2%)	44,73,73	1.43	4 (9%)
5	1DD	A	506	-	18,22,22	1.26	1 (5%)	27,33,33	1.81	6 (22%)
4	NAD	B	503	-	40,48,48	0.87	1 (2%)	44,73,73	1.41	4 (9%)
5	1DD	B	504	-	18,22,22	1.25	1 (5%)	27,33,33	1.79	7 (25%)
3	ACT	E	502	-	1,3,3	1.23	0	0,3,3	0.00	-
4	NAD	E	503	-	40,48,48	0.88	1 (2%)	44,73,73	1.40	3 (6%)
5	1DD	E	504	-	18,22,22	1.26	1 (5%)	27,33,33	1.79	6 (22%)
3	ACT	G	503	-	1,3,3	1.28	0	0,3,3	0.00	-
4	NAD	G	504	-	40,48,48	0.88	1 (2%)	44,73,73	1.42	5 (11%)
5	1DD	G	505	-	18,22,22	1.26	1 (5%)	27,33,33	1.84	7 (25%)

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	ACT	A	503	-	-	0/0/0/0	0/0/0/0
3	ACT	A	504	-	-	0/0/0/0	0/0/0/0
4	NAD	A	505	-	-	0/22/62/62	0/5/5/5
5	1DD	A	506	-	-	0/6/12/12	0/3/3/3
4	NAD	B	503	-	-	0/22/62/62	0/5/5/5
5	1DD	B	504	-	-	0/6/12/12	0/3/3/3
3	ACT	E	502	-	-	0/0/0/0	0/0/0/0
4	NAD	E	503	-	-	0/22/62/62	0/5/5/5
5	1DD	E	504	-	-	0/6/12/12	0/3/3/3
3	ACT	G	503	-	-	0/0/0/0	0/0/0/0
4	NAD	G	504	-	-	0/22/62/62	0/5/5/5
5	1DD	G	505	-	-	0/6/12/12	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	503	NAD	C5A-C4A	3.13	1.47	1.40
4	A	505	NAD	C5A-C4A	3.18	1.47	1.40
4	B	503	NAD	C5A-C4A	3.20	1.47	1.40
4	G	504	NAD	C5A-C4A	3.26	1.47	1.40
5	B	504	1DD	C3-C2	3.90	1.48	1.40
5	A	506	1DD	C3-C2	3.93	1.48	1.40
5	G	505	1DD	C3-C2	3.94	1.48	1.40
5	E	504	1DD	C3-C2	3.99	1.48	1.40

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	505	NAD	N3A-C2A-N1A	-6.88	122.98	128.86
4	B	503	NAD	N3A-C2A-N1A	-6.77	123.07	128.86
4	E	503	NAD	N3A-C2A-N1A	-6.70	123.13	128.86
4	G	504	NAD	N3A-C2A-N1A	-6.65	123.17	128.86
4	E	503	NAD	C4A-C5A-N7A	-2.80	106.70	109.41
4	A	505	NAD	PN-O3-PA	-2.79	123.26	132.63
4	G	504	NAD	C4A-C5A-N7A	-2.74	106.76	109.41
4	G	504	NAD	PN-O3-PA	-2.71	123.53	132.63
4	B	503	NAD	C4A-C5A-N7A	-2.61	106.89	109.41
4	A	505	NAD	C4A-C5A-N7A	-2.45	107.04	109.41
4	E	503	NAD	PN-O3-PA	-2.45	124.41	132.63
4	B	503	NAD	PN-O3-PA	-2.32	124.83	132.63
5	A	506	1DD	O11-S10-O12	-2.23	109.20	117.30
5	G	505	1DD	O11-S10-O12	-2.21	109.28	117.30
5	B	504	1DD	O11-S10-O12	-2.20	109.30	117.30
5	E	504	1DD	O11-S10-O12	-2.17	109.44	117.30
5	B	504	1DD	C16-C17-C18	-2.06	120.04	122.86
5	G	505	1DD	C16-C17-C18	-2.05	120.06	122.86
4	G	504	NAD	C2A-N1A-C6A	2.01	122.17	118.75
4	G	504	NAD	C3N-C7N-N7N	2.04	120.13	117.76
4	B	503	NAD	C2A-N1A-C6A	2.14	122.39	118.75
5	E	504	1DD	C13-C8-N9	2.14	127.07	124.56
5	B	504	1DD	C13-C8-N9	2.18	127.11	124.56
5	G	505	1DD	C13-C8-N9	2.22	127.16	124.56
4	A	505	NAD	C2A-N1A-C6A	2.26	122.59	118.75
5	A	506	1DD	C13-C8-N9	2.29	127.24	124.56
5	G	505	1DD	C4-C3-N9	2.59	136.43	131.28
5	A	506	1DD	C4-C3-N9	2.62	136.49	131.28
5	B	504	1DD	C4-C3-N9	2.66	136.58	131.28
5	E	504	1DD	C4-C3-N9	2.70	136.67	131.28
5	B	504	1DD	O11-S10-N9	3.76	109.00	105.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	506	1DD	O12-S10-N9	3.81	109.03	105.86
5	A	506	1DD	O11-S10-N9	3.99	109.19	105.86
5	B	504	1DD	C14-S10-N9	4.04	110.86	104.61
5	E	504	1DD	O11-S10-N9	4.06	109.24	105.86
5	E	504	1DD	O12-S10-N9	4.17	109.34	105.86
5	G	505	1DD	O11-S10-N9	4.24	109.40	105.86
5	G	505	1DD	C14-S10-N9	4.26	111.20	104.61
5	G	505	1DD	O12-S10-N9	4.30	109.44	105.86
5	E	504	1DD	C14-S10-N9	4.31	111.28	104.61
5	B	504	1DD	O12-S10-N9	4.41	109.54	105.86
5	A	506	1DD	C14-S10-N9	4.89	112.18	104.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	506	1DD	3	0
4	B	503	NAD	1	0
5	B	504	1DD	1	0
5	E	504	1DD	1	0
4	G	504	NAD	1	0
5	G	505	1DD	4	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	446/469 (95%)	0.36	19 (4%) 35 43	21, 32, 49, 55	2 (0%)
1	B	447/469 (95%)	0.15	9 (2%) 65 72	20, 30, 41, 57	0
1	E	447/469 (95%)	0.19	12 (2%) 54 62	22, 30, 39, 54	0
1	G	447/469 (95%)	0.20	11 (2%) 57 65	21, 31, 42, 53	1 (0%)
All	All	1787/1876 (95%)	0.23	51 (2%) 51 59	20, 31, 44, 57	3 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	447	ALA	5.5
1	E	434	ASN	4.8
1	A	220	LYS	4.4
1	A	244	VAL	3.8
1	E	447	ALA	3.5
1	A	446	PRO	3.5
1	A	94	GLN	3.4
1	G	446	PRO	3.4
1	B	221	ASN	3.3
1	G	401	PHE	3.3
1	G	440	VAL	3.3
1	A	437	GLY	3.2
1	A	221	ASN	3.1
1	B	91	GLN	3.1
1	A	433	MET	3.1
1	A	394	ILE	2.9
1	G	90	PRO	2.9
1	A	308	GLY	2.8
1	E	244	VAL	2.8
1	E	243	CYS	2.8
1	E	277	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	394	ILE	2.7
1	E	401	PHE	2.7
1	E	433	MET	2.6
1	B	90	PRO	2.6
1	E	1	SER	2.5
1	A	436	GLU	2.5
1	G	279	ARG	2.4
1	E	5	GLU	2.4
1	A	303	ALA	2.4
1	G	288	ARG	2.4
1	A	222	CYS	2.4
1	A	225	ASP	2.2
1	G	400	PRO	2.2
1	B	244	VAL	2.2
1	G	71	GLU	2.2
1	E	439	LYS	2.2
1	A	361	LEU	2.2
1	B	363	LEU	2.2
1	B	1	SER	2.1
1	B	245	ALA	2.1
1	E	394	ILE	2.1
1	B	361	LEU	2.1
1	E	207	THR	2.1
1	B	434	ASN	2.1
1	G	91	GLN	2.0
1	A	66	VAL	2.0
1	A	302	VAL	2.0
1	A	311	ALA	2.0
1	A	401	PHE	2.0
1	A	273	GLU	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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	K	A	502	1/1	0.23	0.16	62,62,62,62	0
2	K	G	502	1/1	0.46	0.20	64,64,64,64	0
2	K	B	502	1/1	0.52	0.20	61,61,61,61	0
5	1DD	E	504	20/20	0.66	0.70	34,35,35,36	20
2	K	G	501	1/1	0.70	0.35	53,53,53,53	0
5	1DD	G	505	20/20	0.70	0.59	35,35,36,36	20
5	1DD	B	504	20/20	0.71	0.49	33,33,34,34	20
5	1DD	A	506	20/20	0.73	0.61	34,34,35,35	20
2	K	E	501	1/1	0.75	0.18	48,48,48,48	0
2	K	A	501	1/1	0.84	0.20	67,67,67,67	0
2	K	B	501	1/1	0.85	0.34	51,51,51,51	0
3	ACT	A	504	4/4	0.86	0.12	44,45,45,45	0
3	ACT	E	502	4/4	0.88	0.16	37,39,39,39	0
4	NAD	A	505	44/44	0.88	0.12	32,35,43,44	0
4	NAD	B	503	44/44	0.89	0.12	27,31,34,35	0
4	NAD	G	504	44/44	0.90	0.13	28,36,38,39	0
4	NAD	E	503	44/44	0.91	0.11	30,37,39,40	0
3	ACT	G	503	4/4	0.93	0.10	38,38,38,39	0
3	ACT	A	503	4/4	0.96	0.15	46,46,46,47	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.