



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 22, 2016 – 02:52 PM EDT

PDB ID : 4ZVV  
Title : Lactate dehydrogenase A in complex with a trisubstituted piperidine-2,4-dione inhibitor GNE-140  
Authors : Li, Y.; Chen, Z.; Eigenbrot, C.  
Deposited on : 2015-05-18  
Resolution : 2.20 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
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) : rb-20027939

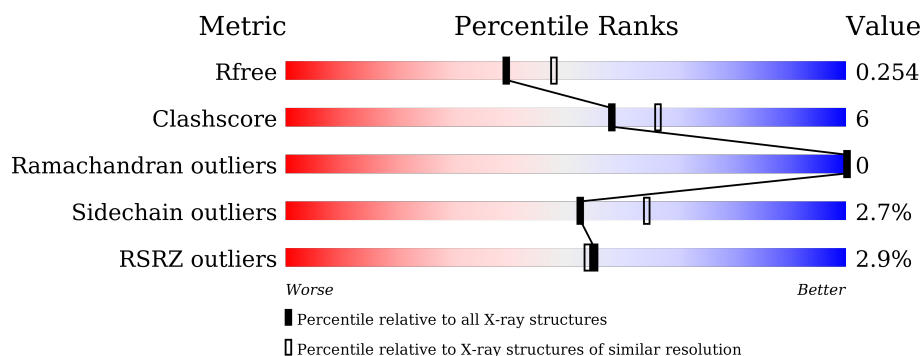
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	332	<div> <div>3%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
1	B	332	<div> <div>2%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
1	C	332	<div> <div>2%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>
1	D	332	<div> <div>4%</div> <div>89%</div> <div>9%</div> <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
3	SO4	A	402	-	-	-	X
3	SO4	A	403	-	-	-	X
3	SO4	B	402	-	-	-	X

## 2 Entry composition i

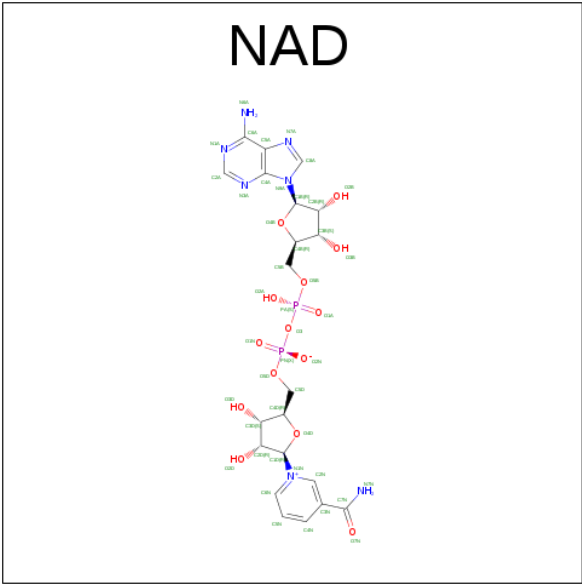
There are 5 unique types of molecules in this entry. The entry contains 10928 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-lactate dehydrogenase A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	B	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	C	331	Total	C	N	O	S	0	0	0
			2568	1639	439	477	13			
1	D	331	Total	C	N	O	S	0	1	0
			2572	1642	439	478	13			

- Molecule 2 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
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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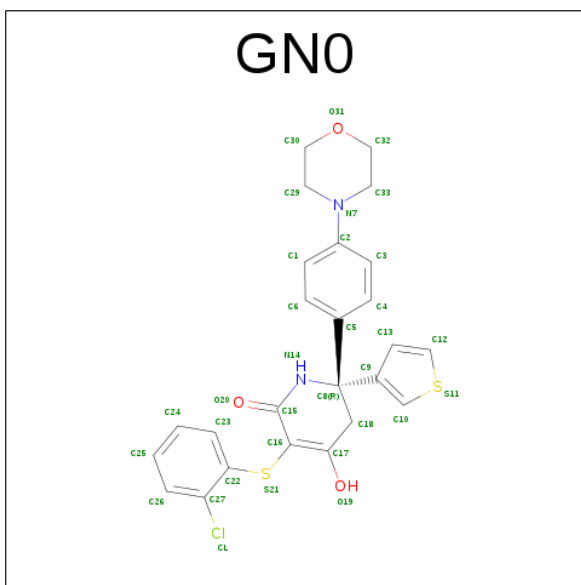
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is (2 {R})-5-(2-chlorophenyl)sulfanyl-2-(4-morpholin-4-ylphenyl)-4-oxidanyl-2-thiophen-3-yl-1,3-dihydropyridin-6-one (three-letter code: GN0) (formula: C<sub>25</sub>H<sub>23</sub>ClN<sub>2</sub>O<sub>3</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 33	C 25	Cl 1	N 2	O 3	S 2	0	0
4	B	1	Total 33	C 25	Cl 1	N 2	O 3	S 2	0	0
4	C	1	Total 33	C 25	Cl 1	N 2	O 3	S 2	0	0
4	D	1	Total 33	C 25	Cl 1	N 2	O 3	S 2	0	0

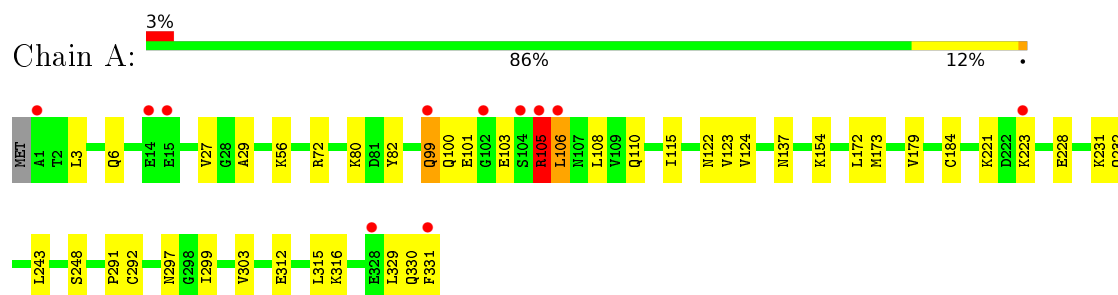
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	72	Total O 72 72	0	0
5	B	71	Total O 71 71	0	0
5	C	82	Total O 82 82	0	0
5	D	84	Total O 84 84	0	0

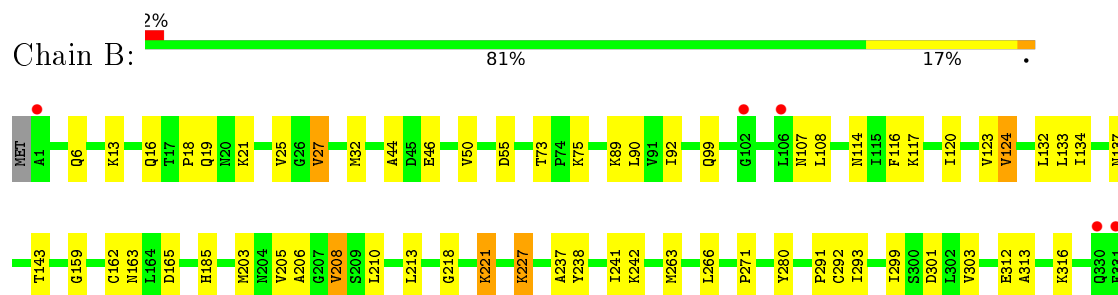
### 3 Residue-property plots

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.

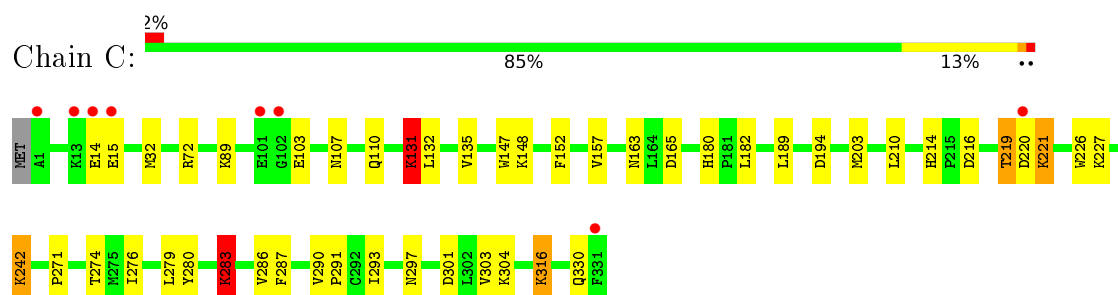
- Molecule 1: L-lactate dehydrogenase A chain



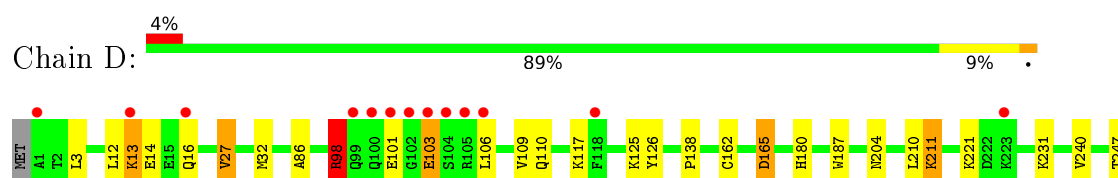
- Molecule 1: L-lactate dehydrogenase A chain

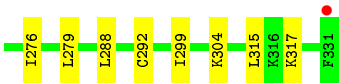


- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.16 Å 81.29 Å 102.47 Å 90.00° 98.31° 90.00°	Depositor
Resolution (Å)	38.45 – 2.20 38.45 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (38.45-2.20) 85.8 (38.45-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.64 (at 2.20 Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.232 , 0.259 0.229 , 0.254	Depositor DCC
$R_{free}$ test set	1152 reflections (2.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.0	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 24.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10928	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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, 0.333 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: GN0, SO4, NAD

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	0.67	10/2612 (0.4%)	0.55	2/3532 (0.1%)
1	B	0.50	1/2612 (0.0%)	0.50	1/3532 (0.0%)
1	C	0.59	9/2612 (0.3%)	0.51	1/3532 (0.0%)
1	D	0.73	13/2619 (0.5%)	0.61	4/3541 (0.1%)
All	All	0.63	33/10455 (0.3%)	0.54	8/14137 (0.1%)

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	13	LYS	CA-C	16.53	1.96	1.52
1	B	13	LYS	CB-CG	-11.04	1.22	1.52
1	D	13	LYS	CB-CG	-10.90	1.23	1.52
1	A	101	GLU	CG-CD	-10.49	1.36	1.51
1	A	101	GLU	CD-OE1	10.43	1.37	1.25
1	C	242	LYS	CE-NZ	10.06	1.74	1.49
1	C	283	LYS	CE-NZ	9.08	1.71	1.49
1	D	98	ARG	CZ-NH2	8.29	1.43	1.33
1	D	103	GLU	CD-OE1	8.11	1.34	1.25
1	A	105	ARG	CG-CD	7.10	1.69	1.51
1	A	99	GLN	CD-NE2	6.79	1.49	1.32
1	D	117	LYS	CE-NZ	6.51	1.65	1.49
1	A	80	LYS	CE-NZ	6.50	1.65	1.49
1	D	101	GLU	CB-CG	6.41	1.64	1.52
1	C	15	GLU	CB-CG	-6.26	1.40	1.52
1	A	99	GLN	CG-CD	6.06	1.65	1.51
1	A	231	LYS	CD-CE	5.99	1.66	1.51
1	A	106	LEU	CG-CD1	5.97	1.74	1.51
1	D	13	LYS	C-N	-5.84	1.20	1.34
1	D	231	LYS	CD-CE	5.82	1.65	1.51
1	C	242	LYS	CD-CE	5.77	1.65	1.51
1	C	221	LYS	CE-NZ	5.67	1.63	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	211	LYS	CE-NZ	5.59	1.63	1.49
1	C	14	GLU	CB-CG	-5.55	1.41	1.52
1	D	14	GLU	CB-CG	5.38	1.62	1.52
1	C	227	LYS	CE-NZ	5.34	1.62	1.49
1	A	154	LYS	CE-NZ	5.33	1.62	1.49
1	D	103	GLU	CG-CD	-5.27	1.44	1.51
1	D	103	GLU	CD-OE2	5.24	1.31	1.25
1	A	223	LYS	CE-NZ	5.10	1.61	1.49
1	C	131	LYS	CD-CE	5.09	1.64	1.51
1	C	148	LYS	CD-CE	5.06	1.63	1.51
1	D	103	GLU	CB-CG	5.04	1.61	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	13	LYS	CB-CA-C	12.89	136.18	110.40
1	D	13	LYS	CB-CG-CD	9.71	136.84	111.60
1	D	98	ARG	NE-CZ-NH1	-8.77	115.92	120.30
1	A	105	ARG	NE-CZ-NH2	6.50	123.55	120.30
1	D	13	LYS	CA-CB-CG	-5.79	100.66	113.40
1	A	101	GLU	OE1-CD-OE2	-5.62	116.56	123.30
1	C	242	LYS	CD-CE-NZ	-5.55	98.92	111.70
1	B	13	LYS	CA-CB-CG	5.54	125.59	113.40

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	2568	0	2656	35	0
1	B	2568	0	2656	46	0
1	C	2568	0	2656	31	0
1	D	2572	0	2660	30	0
2	A	44	0	26	2	0
2	B	44	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	44	0	26	1	0
2	D	44	0	26	0	0
3	A	15	0	0	0	0
3	B	10	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	33	0	0	0	0
4	B	33	0	0	0	0
4	C	33	0	0	0	0
4	D	33	0	0	0	0
5	A	72	0	0	0	0
5	B	71	0	0	1	0
5	C	82	0	0	0	0
5	D	84	0	0	0	0
All	All	10928	0	10732	126	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 6.

All (126) 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:C:283:LYS:NZ	1:C:283:LYS:CE	1.71	1.50
1:C:242:LYS:CE	1:C:242:LYS:NZ	1.74	1.49
1:D:13:LYS:C	1:D:13:LYS:CA	1.95	1.34
1:A:99:GLN:NE2	1:A:103:GLU:OE2	1.91	1.03
1:B:227:LYS:HE3	1:B:227:LYS:N	1.81	0.95
1:A:106:LEU:O	1:A:106:LEU:HD13	1.72	0.89
1:A:99:GLN:HE21	1:A:100:GLN:H	1.24	0.85
1:B:227:LYS:HE3	1:B:227:LYS:H	1.47	0.78
1:A:99:GLN:HE21	1:A:100:GLN:N	1.81	0.77
1:B:134:ILE:CG2	1:B:159:GLY:HA2	2.15	0.76
1:A:99:GLN:NE2	1:A:100:GLN:H	1.84	0.75
1:A:105:ARG:HD2	1:A:106:LEU:H	1.52	0.74
1:A:27:VAL:O	1:A:27:VAL:HG12	1.88	0.73
1:B:134:ILE:HG22	1:B:159:GLY:HA2	1.70	0.73
1:B:90:LEU:HB2	1:B:263:MET:CE	2.24	0.67
1:C:242:LYS:CD	1:C:242:LYS:NZ	2.58	0.66
1:B:313:ALA:HA	1:B:316:LYS:HE3	1.77	0.66
1:B:44:ALA:O	1:B:73:THR:HG22	1.96	0.65
1:C:103:GLU:HG3	1:C:107:ASN:HD22	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ILE:HD12	1:B:301:ASP:HB2	1.78	0.64
1:B:116:PHE:HZ	1:B:134:ILE:HD11	1.62	0.64
1:C:291:PRO:HG2	1:C:303:VAL:HB	1.82	0.62
1:A:110:GLN:HE21	1:A:330:GLN:H	1.45	0.61
1:B:134:ILE:HG21	1:B:143:THR:OG1	2.01	0.61
1:C:283:LYS:CD	1:C:283:LYS:NZ	2.63	0.61
1:B:218:GLY:H	1:B:227:LYS:HZ1	1.49	0.59
1:B:292:CYS:HB3	1:B:299:ILE:HG23	1.85	0.59
1:C:110:GLN:HE22	1:C:330:GLN:H	1.49	0.59
1:A:27:VAL:O	1:A:27:VAL:CG1	2.51	0.58
1:A:110:GLN:NE2	1:A:330:GLN:H	2.02	0.57
1:D:98:ARG:CD	1:D:103:GLU:OE1	2.52	0.57
1:C:214:HIS:HB2	1:D:3:LEU:HD13	1.87	0.57
1:C:203:MET:HG2	1:C:210:LEU:HD22	1.87	0.57
1:A:105:ARG:HD2	1:A:106:LEU:N	2.19	0.56
1:C:219:THR:HG23	1:C:221:LYS:H	1.70	0.56
1:B:90:LEU:HB2	1:B:263:MET:HE3	1.87	0.56
1:A:173:MET:SD	1:A:184:CYS:HB3	2.46	0.56
1:D:276:ILE:HG22	1:D:279:LEU:HB2	1.87	0.56
1:D:27:VAL:HG13	1:D:27:VAL:O	2.07	0.55
1:D:27:VAL:HG22	1:D:32:MET:SD	2.48	0.54
1:A:3:LEU:CD1	1:B:213:LEU:HD11	2.36	0.54
1:C:180:HIS:CE1	1:C:182:LEU:HD12	2.42	0.54
1:D:240:VAL:HG11	1:D:247:THR:HG22	1.89	0.54
1:B:206:ALA:HA	1:D:187:TRP:CZ2	2.43	0.54
1:D:276:ILE:HG13	1:D:288:LEU:HB2	1.89	0.54
1:A:291:PRO:HB2	1:A:303:VAL:HB	1.89	0.54
1:D:292:CYS:HB3	1:D:299:ILE:HG23	1.89	0.53
1:B:116:PHE:CZ	1:B:134:ILE:HD11	2.45	0.52
1:B:203:MET:HB3	1:B:210:LEU:HD12	1.91	0.52
1:D:98:ARG:HD3	1:D:103:GLU:OE1	2.10	0.52
1:B:120:ILE:O	1:B:124:VAL:HG13	2.09	0.52
1:B:291:PRO:HB2	1:B:303:VAL:HB	1.92	0.52
1:C:274:THR:O	1:C:287:PHE:HA	2.10	0.52
1:D:98:ARG:NE	1:D:103:GLU:OE1	2.42	0.52
1:A:99:GLN:NE2	1:A:100:GLN:N	2.51	0.52
1:A:292:CYS:HB3	1:A:299:ILE:HG23	1.91	0.51
1:B:114:ASN:HA	1:B:117:LYS:HE2	1.91	0.51
1:A:297:ASN:ND2	1:D:16:GLN:NE2	2.58	0.51
1:A:297:ASN:OD1	1:D:16:GLN:NE2	2.40	0.51
1:A:115:ILE:HG23	2:A:401:NAD:N6A	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:VAL:O	2:C:401:NAD:H2N	2.09	0.51
1:C:293:ILE:HD12	1:C:301:ASP:HB2	1.93	0.51
1:B:92:ILE:HG12	1:B:133:LEU:HD23	1.93	0.50
1:B:134:ILE:HG23	1:B:159:GLY:HA2	1.92	0.48
1:B:25:VAL:HG13	1:B:50:VAL:HG22	1.93	0.48
1:A:297:ASN:CG	1:D:16:GLN:HE22	2.16	0.48
1:C:163:ASN:HA	1:C:271:PRO:HG2	1.95	0.48
1:B:99:GLN:HB2	1:B:108:LEU:HD22	1.95	0.48
1:B:16:GLN:OE1	1:C:297:ASN:ND2	2.47	0.47
1:C:132:LEU:HD13	1:C:152:PHE:HE2	1.79	0.47
1:D:125:LYS:HE3	1:D:126:TYR:CZ	2.48	0.47
1:D:98:ARG:HD2	1:D:98:ARG:N	2.30	0.47
1:C:32:MET:HA	1:C:32:MET:CE	2.44	0.47
1:A:137:ASN:HB2	2:A:401:NAD:O2D	2.15	0.47
1:C:32:MET:HA	1:C:32:MET:HE2	1.97	0.46
1:B:19:GLN:O	1:B:89:LYS:HE2	2.15	0.46
1:A:312:GLU:HG2	1:A:316:LYS:NZ	2.31	0.46
1:A:179:VAL:HG13	1:A:184:CYS:SG	2.56	0.45
1:A:297:ASN:CG	1:D:16:GLN:NE2	2.70	0.45
1:A:106:LEU:HD13	1:A:106:LEU:C	2.37	0.45
1:C:219:THR:HG23	1:C:221:LYS:N	2.32	0.45
1:C:216:ASP:O	1:C:219:THR:HG22	2.17	0.45
1:D:86:ALA:HA	1:D:126:TYR:HB3	1.99	0.45
1:B:221:LYS:HD2	1:B:221:LYS:H	1.82	0.45
1:C:316:LYS:HE3	1:C:316:LYS:HB2	1.68	0.45
1:B:218:GLY:H	1:B:227:LYS:NZ	2.14	0.44
1:D:276:ILE:HG22	1:D:276:ILE:O	2.17	0.44
1:B:46:GLU:OE1	1:B:75:LYS:HD3	2.18	0.44
1:A:297:ASN:ND2	1:D:16:GLN:HE21	2.16	0.44
1:B:266:LEU:O	1:D:180:HIS:HB2	2.18	0.44
1:C:89:LYS:O	1:C:131:LYS:HE2	2.18	0.44
1:D:106:LEU:HD22	1:D:110:GLN:HB3	2.00	0.44
1:B:27:VAL:O	1:B:27:VAL:HG13	2.18	0.43
1:A:172:LEU:HD13	1:A:232:GLN:HB3	2.00	0.43
1:A:6:GLN:O	1:D:304:LYS:HE2	2.18	0.43
1:A:82:TYR:CG	1:A:122:ASN:HB3	2.54	0.43
1:D:162:CYS:HA	1:D:165:ASP:OD1	2.19	0.43
1:D:204:ASN:HA	1:D:210:LEU:HD13	2.00	0.43
1:B:137:ASN:HB2	2:B:401:NAD:O2D	2.19	0.43
1:B:162:CYS:HA	1:B:165:ASP:OD1	2.19	0.42
1:A:243:LEU:HB3	1:B:55:ASP:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:GLN:O	1:C:304:LYS:HE3	2.19	0.42
1:D:109:VAL:HG22	1:D:138:PRO:HG2	2.01	0.42
1:B:27:VAL:HG22	1:B:32:MET:SD	2.60	0.42
1:A:228:GLU:O	1:A:232:GLN:HB2	2.20	0.42
1:B:238:TYR:O	1:B:242:LYS:HG3	2.20	0.42
1:B:280:TYR:HB3	1:B:312:GLU:HG2	2.01	0.41
1:B:237:ALA:O	1:B:241:ILE:HG12	2.19	0.41
1:C:276:ILE:HG22	1:C:286:VAL:HG13	2.02	0.41
1:B:185:HIS:O	1:B:203:MET:HA	2.20	0.41
1:A:99:GLN:OE1	1:A:108:LEU:HD22	2.21	0.41
1:C:132:LEU:HD13	1:C:152:PHE:CE2	2.54	0.41
1:C:147:TRP:HA	1:C:157:VAL:HG21	2.03	0.41
1:C:279:LEU:HD13	1:C:280:TYR:CD2	2.55	0.41
1:A:29:ALA:HB1	1:A:248:SER:HB3	2.03	0.41
1:A:297:ASN:HD21	1:D:16:GLN:HE21	1.68	0.41
1:C:189:LEU:HD22	1:C:290:VAL:HA	2.03	0.40
1:B:123:VAL:HG11	1:B:132:LEU:HD21	2.03	0.40
1:A:297:ASN:HD21	1:D:16:GLN:NE2	2.18	0.40
1:C:226:TRP:CE2	1:D:3:LEU:HD23	2.57	0.40
1:B:205:VAL:O	1:B:208:VAL:HG13	2.21	0.40
1:C:132:LEU:CD1	1:C:152:PHE:HE2	2.34	0.40
1:B:163:ASN:HA	1:B:271:PRO:HG2	2.03	0.40
1:B:18:PRO:HB2	1:B:21:LYS:HB2	2.03	0.40
1:B:218:GLY:H	1:B:227:LYS:HE2	1.86	0.40
1:B:73:THR:HG23	5:B:514:HOH:O	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	329/332 (99%)	321 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	329/332 (99%)	323 (98%)	6 (2%)	0	100	100
1	C	329/332 (99%)	322 (98%)	7 (2%)	0	100	100
1	D	330/332 (99%)	323 (98%)	7 (2%)	0	100	100
All	All	1317/1328 (99%)	1289 (98%)	28 (2%)	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	287/288 (100%)	278 (97%)	9 (3%)	47	59
1	B	287/288 (100%)	281 (98%)	6 (2%)	61	74
1	C	287/288 (100%)	279 (97%)	8 (3%)	51	63
1	D	288/288 (100%)	280 (97%)	8 (3%)	51	63
All	All	1149/1152 (100%)	1118 (97%)	31 (3%)	52	64

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LYS
1	A	72	ARG
1	A	105	ARG
1	A	123	VAL
1	A	124	VAL
1	A	221	LYS
1	A	315	LEU
1	A	329	LEU
1	A	331	PHE
1	B	27	VAL
1	B	107	ASN
1	B	124	VAL
1	B	208	VAL

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Mol	Chain	Res	Type
1	B	221	LYS
1	B	227	LYS
1	C	72	ARG
1	C	131	LYS
1	C	165	ASP
1	C	194	ASP
1	C	219	THR
1	C	220	ASP
1	C	283	LYS
1	C	316	LYS
1	D	12	LEU
1	D	27	VAL
1	D	98	ARG
1	D	165	ASP
1	D	211	LYS
1	D	221	LYS
1	D	315	LEU
1	D	317	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	110	GLN
1	A	297	ASN
1	C	107	ASN
1	C	110	GLN
1	C	297	ASN
1	D	16	GLN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

15 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$
2	NAD	A	401	-	42,48,48	0.95	1 (2%)	46,73,73	1.42	7 (15%)
3	SO4	A	402	-	4,4,4	0.17	0	6,6,6	0.10	0
3	SO4	A	403	-	4,4,4	0.20	0	6,6,6	0.11	0
3	SO4	A	404	-	4,4,4	0.21	0	6,6,6	0.10	0
4	GN0	A	405	-	32,37,37	1.49	7 (21%)	35,53,53	2.21	8 (22%)
2	NAD	B	401	-	42,48,48	0.95	1 (2%)	46,73,73	1.60	6 (13%)
3	SO4	B	402	-	4,4,4	0.22	0	6,6,6	0.08	0
3	SO4	B	403	-	4,4,4	0.17	0	6,6,6	0.05	0
4	GN0	B	404	-	32,37,37	1.35	7 (21%)	35,53,53	2.28	5 (14%)
2	NAD	C	401	-	42,48,48	1.00	2 (4%)	46,73,73	1.70	10 (21%)
3	SO4	C	402	-	4,4,4	0.21	0	6,6,6	0.15	0
4	GN0	C	403	-	32,37,37	1.28	5 (15%)	35,53,53	2.43	6 (17%)
2	NAD	D	401	-	42,48,48	0.96	2 (4%)	46,73,73	1.43	8 (17%)
3	SO4	D	402	-	4,4,4	0.18	0	6,6,6	0.07	0
4	GN0	D	403	-	32,37,37	1.38	6 (18%)	35,53,53	2.39	7 (20%)

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	NAD	A	401	-	-	0/22/62/62	0/5/5/5
3	SO4	A	402	-	-	0/0/0/0	0/0/0/0
3	SO4	A	403	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	404	-	-	0/0/0/0	0/0/0/0
4	GN0	A	405	-	-	0/14/46/46	0/5/5/5
2	NAD	B	401	-	-	0/22/62/62	0/5/5/5
3	SO4	B	402	-	-	0/0/0/0	0/0/0/0
3	SO4	B	403	-	-	0/0/0/0	0/0/0/0
4	GN0	B	404	-	-	0/14/46/46	0/5/5/5
2	NAD	C	401	-	-	0/22/62/62	0/5/5/5
3	SO4	C	402	-	-	0/0/0/0	0/0/0/0
4	GN0	C	403	-	-	0/14/46/46	0/5/5/5
2	NAD	D	401	-	-	0/22/62/62	0/5/5/5
3	SO4	D	402	-	-	0/0/0/0	0/0/0/0
4	GN0	D	403	-	-	0/14/46/46	0/5/5/5

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	405	GN0	C8-C9	-4.11	1.48	1.53
4	D	403	GN0	C8-C9	-3.96	1.48	1.53
4	B	404	GN0	C8-C9	-3.90	1.48	1.53
4	C	403	GN0	C8-C9	-3.86	1.48	1.53
4	A	405	GN0	C8-N14	-2.77	1.43	1.46
4	B	404	GN0	O19-C17	-2.76	1.25	1.32
4	A	405	GN0	O19-C17	-2.75	1.25	1.32
4	C	403	GN0	O19-C17	-2.74	1.25	1.32
4	A	405	GN0	C16-S21	-2.73	1.71	1.76
4	D	403	GN0	O19-C17	-2.71	1.25	1.32
4	A	405	GN0	C8-C5	-2.71	1.50	1.53
4	D	403	GN0	C8-N14	-2.66	1.44	1.46
4	D	403	GN0	C8-C5	-2.63	1.50	1.53
4	B	404	GN0	C8-N14	-2.53	1.44	1.46
4	B	404	GN0	C8-C5	-2.50	1.50	1.53
2	C	401	NAD	C3N-C7N	-2.47	1.46	1.50
4	C	403	GN0	C8-N14	-2.37	1.44	1.46
4	B	404	GN0	C16-S21	-2.23	1.72	1.76
2	D	401	NAD	C3N-C7N	-2.16	1.47	1.50
4	D	403	GN0	C16-S21	-2.10	1.72	1.76
4	A	405	GN0	C10-C9	2.20	1.38	1.37
4	B	404	GN0	C15-N14	2.22	1.38	1.35
4	C	403	GN0	C15-N14	2.23	1.38	1.35
2	A	401	NAD	C7N-N7N	2.28	1.37	1.33
2	D	401	NAD	C7N-N7N	2.29	1.37	1.33
2	C	401	NAD	C7N-N7N	2.32	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	403	GN0	C10-C9	2.33	1.38	1.37
2	B	401	NAD	C7N-N7N	2.34	1.37	1.33
4	B	404	GN0	C10-C9	2.38	1.38	1.37
4	A	405	GN0	C15-N14	2.41	1.38	1.35
4	D	403	GN0	C10-C9	2.46	1.38	1.37

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NAD	C4B-O4B-C1B	-6.83	102.40	109.64
2	C	401	NAD	O5D-PN-O1N	-4.98	88.81	109.21
2	C	401	NAD	C3N-C7N-N7N	-4.24	113.03	117.82
2	A	401	NAD	C4B-O4B-C1B	-4.18	105.21	109.64
2	D	401	NAD	C3N-C7N-N7N	-4.00	113.30	117.82
2	D	401	NAD	C4B-O4B-C1B	-3.97	105.43	109.64
2	C	401	NAD	C4B-O4B-C1B	-3.67	105.76	109.64
4	A	405	GN0	O31-C32-C33	-3.34	104.12	111.83
2	B	401	NAD	C3N-C7N-N7N	-3.32	114.07	117.82
2	A	401	NAD	C3N-C7N-N7N	-3.31	114.08	117.82
2	A	401	NAD	C4D-O4D-C1D	-3.04	106.42	109.64
4	A	405	GN0	O31-C30-C29	-3.02	104.86	111.83
4	C	403	GN0	O19-C17-C18	-2.99	108.06	114.63
2	D	401	NAD	C4D-O4D-C1D	-2.86	106.61	109.64
2	B	401	NAD	C4D-O4D-C1D	-2.75	106.72	109.64
4	B	404	GN0	O19-C17-C18	-2.71	108.67	114.63
2	C	401	NAD	O2N-PN-O5D	-2.63	95.69	108.24
4	D	403	GN0	O19-C17-C18	-2.53	109.05	114.63
4	D	403	GN0	O31-C30-C29	-2.40	106.28	111.83
4	A	405	GN0	O19-C17-C18	-2.37	109.42	114.63
2	C	401	NAD	C4D-O4D-C1D	-2.19	107.32	109.64
4	D	403	GN0	O31-C32-C33	-2.17	106.80	111.83
2	A	401	NAD	C1B-N9A-C4A	-2.03	124.55	126.81
4	C	403	GN0	O31-C30-C29	-2.02	107.16	111.83
2	D	401	NAD	C2N-C3N-C4N	2.03	120.57	118.27
2	B	401	NAD	O7N-C7N-N7N	2.05	125.50	122.58
2	A	401	NAD	O4B-C1B-N9A	2.08	112.03	108.11
2	A	401	NAD	O7N-C7N-N7N	2.09	125.56	122.58
2	D	401	NAD	N6A-C6A-N1A	2.10	122.04	118.52
2	D	401	NAD	O4B-C1B-N9A	2.10	112.08	108.11
2	C	401	NAD	O4D-C1D-N1N	2.15	110.42	108.10
2	D	401	NAD	O7N-C7N-N7N	2.18	125.69	122.58
2	B	401	NAD	O4B-C1B-N9A	2.20	112.27	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	NAD	C2N-C3N-C4N	2.22	120.78	118.27
2	C	401	NAD	O4B-C1B-N9A	2.23	112.32	108.11
4	C	403	GN0	C18-C8-N14	2.39	110.04	107.86
2	D	401	NAD	O4D-C1D-N1N	2.53	110.83	108.10
4	A	405	GN0	C22-S21-C16	2.59	105.93	102.40
2	C	401	NAD	O7N-C7N-N7N	2.74	126.48	122.58
2	B	401	NAD	O4D-C1D-N1N	2.84	111.17	108.10
2	A	401	NAD	O4D-C1D-N1N	3.16	111.52	108.10
4	B	404	GN0	C18-C8-N14	3.29	110.86	107.86
4	A	405	GN0	C18-C8-N14	3.35	110.91	107.86
2	C	401	NAD	O2N-PN-O1N	3.50	130.78	112.56
4	D	403	GN0	C18-C8-N14	3.62	111.15	107.86
4	B	404	GN0	C33-N7-C29	4.33	120.50	111.54
4	D	403	GN0	C33-N7-C29	4.33	120.52	111.54
4	D	403	GN0	O19-C17-C16	4.39	130.23	121.89
4	C	403	GN0	C33-N7-C29	4.50	120.86	111.54
4	B	404	GN0	O19-C17-C16	4.53	130.51	121.89
4	A	405	GN0	C33-N7-C29	4.54	120.93	111.54
4	A	405	GN0	O19-C17-C16	4.55	130.54	121.89
4	C	403	GN0	O19-C17-C16	4.77	130.97	121.89
4	A	405	GN0	C8-N14-C15	8.38	122.05	117.28
4	B	404	GN0	C8-N14-C15	10.06	123.00	117.28
4	D	403	GN0	C8-N14-C15	10.86	123.45	117.28
4	C	403	GN0	C8-N14-C15	11.40	123.76	117.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAD	2	0
2	B	401	NAD	1	0
2	C	401	NAD	1	0

## 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	331/332 (99%)	0.08	11 (3%) 50 49	28, 35, 50, 66	0
1	B	331/332 (99%)	0.07	5 (1%) 76 75	26, 34, 48, 57	1 (0%)
1	C	331/332 (99%)	0.08	8 (2%) 62 61	26, 33, 46, 55	2 (0%)
1	D	331/332 (99%)	0.10	14 (4%) 40 39	27, 32, 49, 62	1 (0%)
All	All	1324/1328 (99%)	0.08	38 (2%) 55 54	26, 34, 49, 66	4 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	ALA	6.6
1	D	331	PHE	5.5
1	A	105	ARG	5.1
1	D	102	GLY	4.9
1	D	104	SER	4.9
1	D	105	ARG	4.0
1	C	331	PHE	3.9
1	D	1	ALA	3.8
1	A	331	PHE	3.5
1	D	118	PHE	3.4
1	B	106	LEU	3.4
1	D	100	GLN	3.4
1	D	99	GLN	3.3
1	A	106	LEU	3.3
1	C	101	GLU	3.2
1	A	1	ALA	3.1
1	A	223	LYS	3.1
1	C	15	GLU	2.9
1	D	101	GLU	2.9
1	B	331	PHE	2.8
1	A	104	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	106	LEU	2.8
1	D	13	LYS	2.7
1	D	223	LYS	2.6
1	B	1	ALA	2.6
1	A	102	GLY	2.5
1	A	15	GLU	2.5
1	B	102	GLY	2.5
1	A	328	GLU	2.4
1	D	103	GLU	2.3
1	C	13	LYS	2.3
1	B	330	GLN	2.3
1	A	99	GLN	2.3
1	C	14	GLU	2.2
1	A	14	GLU	2.2
1	C	102	GLY	2.1
1	C	220	ASP	2.1
1	D	16	GLN	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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(Å <sup>2</sup> )	Q<0.9
3	SO4	B	402	5/5	0.77	0.38	9.07	31,32,32,32	5
3	SO4	A	402	5/5	0.91	0.24	3.88	56,56,57,57	0
3	SO4	A	403	5/5	0.89	0.22	2.48	51,52,52,53	0
3	SO4	D	402	5/5	0.93	0.16	0.56	50,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAD	C	401	44/44	0.94	0.12	-0.34	30,32,35,35	0
4	GN0	D	403	33/33	0.93	0.12	-0.35	32,34,35,35	0
4	GN0	A	405	33/33	0.93	0.11	-0.41	34,35,36,38	0
4	GN0	B	404	33/33	0.95	0.11	-0.50	34,36,40,40	0
4	GN0	C	403	33/33	0.91	0.12	-0.62	34,36,36,38	0
2	NAD	A	401	44/44	0.94	0.12	-0.65	34,35,40,40	0
2	NAD	B	401	44/44	0.95	0.10	-0.69	31,33,35,35	0
2	NAD	D	401	44/44	0.96	0.09	-0.69	28,31,34,34	0
3	SO4	A	404	5/5	0.95	0.11	-	50,50,51,51	5
3	SO4	C	402	5/5	0.94	0.12	-	49,50,50,51	0
3	SO4	B	403	5/5	0.89	0.15	-	45,46,47,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.