



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:26 AM GMT

PDB ID : 2X06  
Title : SULFOLACTATE DEHYDROGENASE FROM METHANOCALDOCOC-  
CUS JANNASCHII  
Authors : Irimia, A.; Madern, D.; Zaccai, G.; Vellieux, F.M.D.  
Deposited on : 2009-12-07  
Resolution : 2.50 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

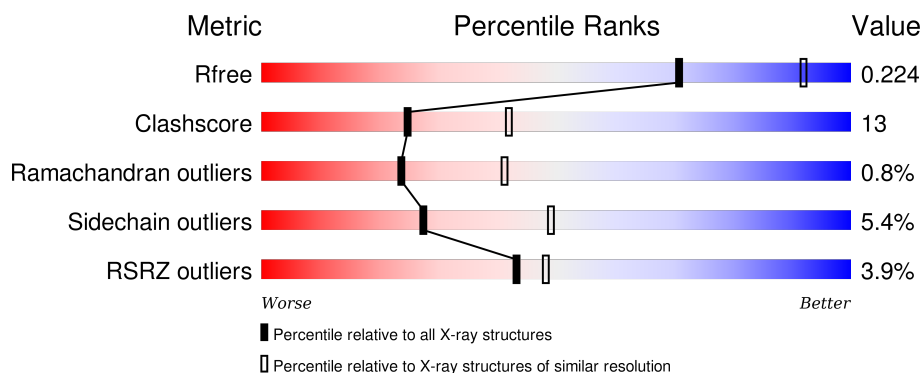
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	344	<div> <div>5%</div> <div>74%</div> <div>23%</div> <div>.</div> </div>
1	B	344	<div> <div>2%</div> <div>73%</div> <div>25%</div> <div>.</div> </div>
1	C	344	<div> <div>6%</div> <div>71%</div> <div>24%</div> <div>.</div> </div>
1	D	344	<div> <div>%</div> <div>78%</div> <div>20%</div> <div>.</div> </div>
1	E	344	<div> <div>3%</div> <div>73%</div> <div>25%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	344	<div><div></div><div>9%</div><div></div><div>72%</div><div></div><div>24%</div><div></div><div></div></div>
1	G	344	<div><div></div><div>4%</div><div></div><div>73%</div><div></div><div>25%</div><div></div><div></div></div>
1	H	344	<div><div></div><div>%</div><div></div><div>75%</div><div></div><div>23%</div><div></div><div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21878 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-SULFOLACTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	Se	0	2	0
			2635	1686	436	500	4	9			
1	B	344	Total	C	N	O	S	Se	0	1	0
			2631	1682	438	498	4	9			
1	C	344	Total	C	N	O	S	Se	0	1	0
			2628	1680	436	499	4	9			
1	D	344	Total	C	N	O	S	Se	0	2	0
			2635	1687	437	498	4	9			
1	E	344	Total	C	N	O	S	Se	0	0	0
			2623	1677	435	498	4	9			
1	F	344	Total	C	N	O	S	Se	0	0	0
			2623	1677	435	498	4	9			
1	G	344	Total	C	N	O	S	Se	0	1	0
			2628	1680	435	500	4	9			
1	H	344	Total	C	N	O	S	Se	0	0	0
			2623	1677	435	498	4	9			

- 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		
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		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	80	Total	O	0	0
			80	80		
3	B	68	Total	O	0	0
			68	68		
3	C	53	Total	O	0	0
			53	53		
3	D	60	Total	O	0	0
			60	60		

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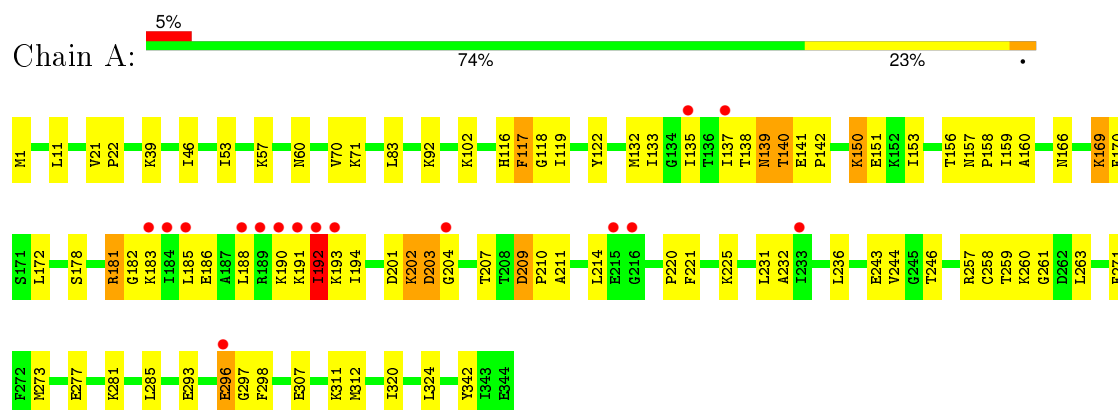
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	65	Total 65	O 65	0	0
3	F	53	Total 53	O 53	0	0
3	G	69	Total 69	O 69	0	0
3	H	52	Total 52	O 52	0	0

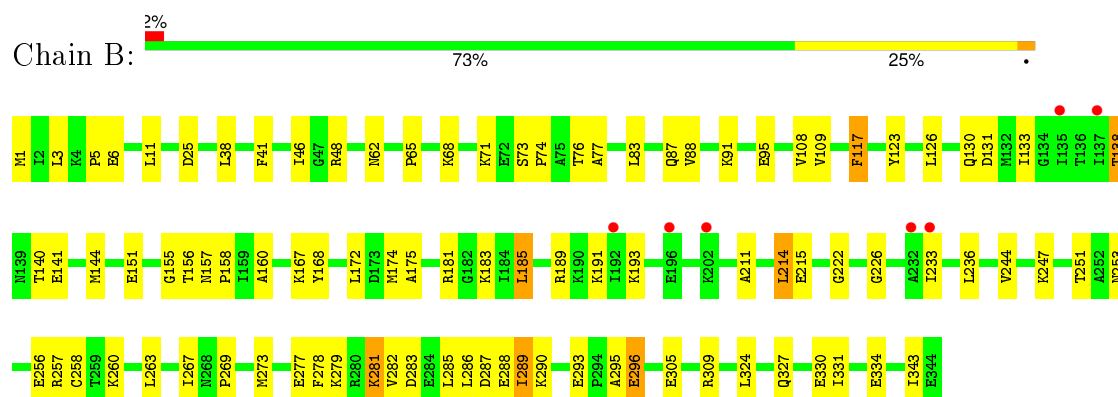
### 3 Residue-property plots [i](#)

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.

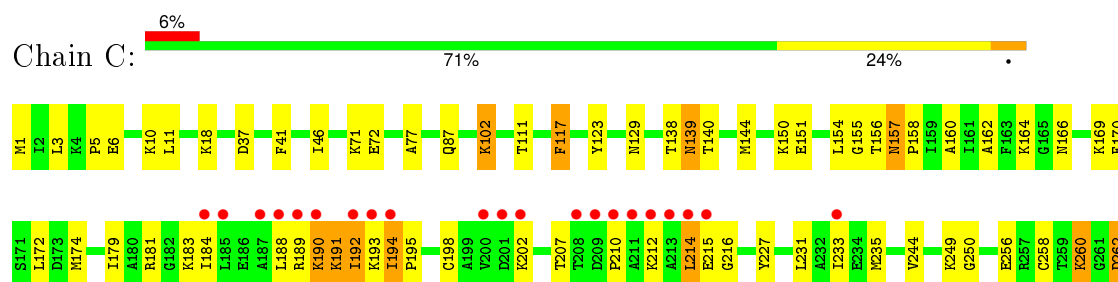
#### • Molecule 1: L-SULFOLACTATE DEHYDROGENASE



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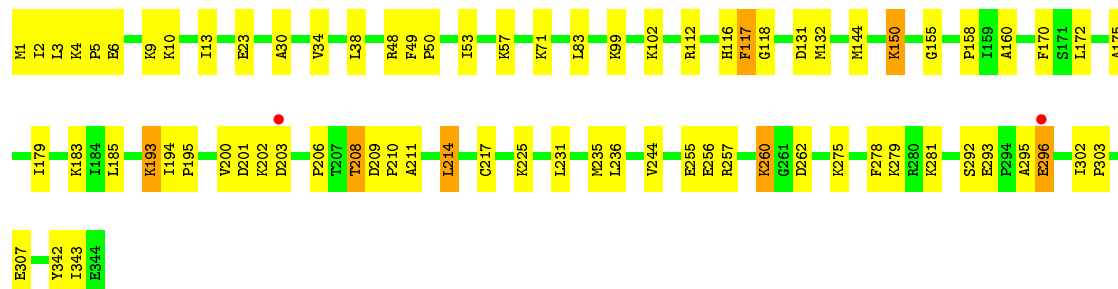
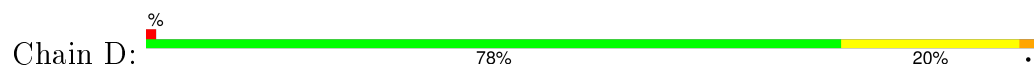


#### • Molecule 1: L-SULFOLACTATE DEHYDROGENASE

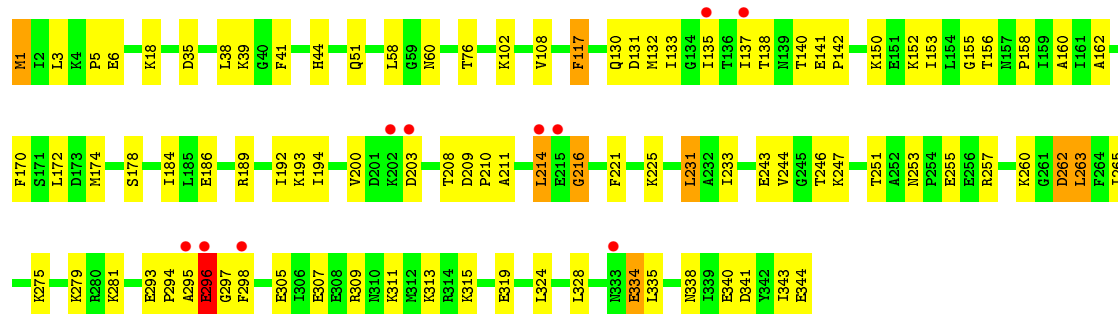




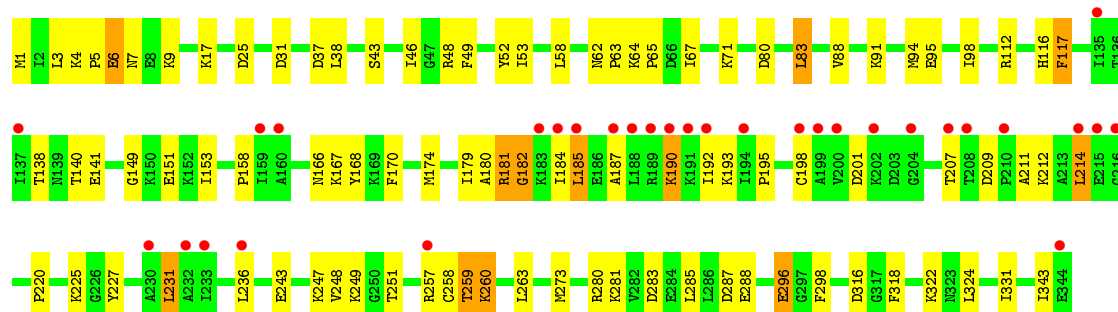
• Molecule 1: L-SULFOLACTATE DEHYDROGENASE



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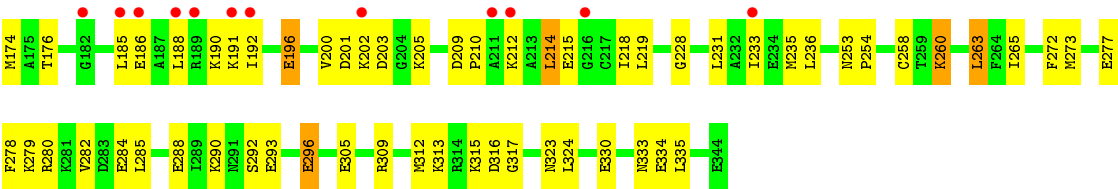
• Molecule 1: L-SULFOLACTATE DEHYDROGENASE



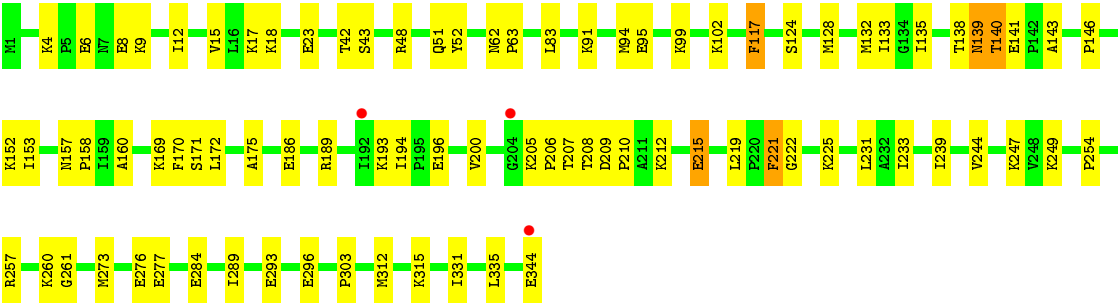
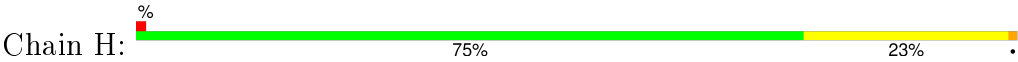
• Molecule 1: L-SULFOLACTATE DEHYDROGENASE







● Molecule 1: L-SULFOLACTATE DEHYDROGENASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.93Å 203.71Å 100.05Å 90.00° 112.05° 90.00°	Depositor
Resolution (Å)	32.83 – 2.50 32.89 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.1 (32.83-2.50) 96.1 (32.89-2.50)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.153 , 0.224 0.157 , 0.224	Depositor DCC
$R_{free}$ test set	4958 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.4	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 53.4	EDS
Estimated twinning fraction	0.048 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 99287 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	21878	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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: 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	0.40	0/2674	0.56	0/3577
1	B	0.39	0/2667	0.53	0/3568
1	C	0.41	0/2664	0.55	0/3565
1	D	0.40	0/2674	0.53	0/3576
1	E	0.39	0/2656	0.55	0/3554
1	F	0.38	0/2656	0.54	0/3554
1	G	0.39	0/2664	0.56	0/3565
1	H	0.38	0/2656	0.52	0/3554
All	All	0.39	0/21311	0.54	0/28513

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	2635	0	2734	73	0
1	B	2631	0	2728	87	0
1	C	2628	0	2721	91	0
1	D	2635	0	2741	52	0
1	E	2623	0	2715	83	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2623	0	2715	87	0
1	G	2628	0	2719	72	0
1	H	2623	0	2715	63	0
2	A	44	0	26	1	0
2	B	44	0	26	4	0
2	C	44	0	26	3	0
2	D	44	0	26	0	0
2	E	44	0	26	2	0
2	F	44	0	25	1	0
2	G	44	0	26	3	0
2	H	44	0	26	1	0
3	A	80	0	0	4	0
3	B	68	0	0	2	0
3	C	53	0	0	1	0
3	D	60	0	0	2	0
3	E	65	0	0	2	0
3	F	53	0	0	4	0
3	G	69	0	0	3	0
3	H	52	0	0	1	0
All	All	21878	0	21995	554	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 13.

All (554) 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:E:172:LEU:HD11	1:E:174:MSE:HE3	1.37	1.07
1:C:179:ILE:HG13	1:C:183:LYS:HE3	1.39	1.00
1:B:172:LEU:HD11	1:B:174:MSE:HE3	1.42	0.99
1:B:167:LYS:HE3	1:B:168:TYR:CE1	1.98	0.99
1:C:338:ASN:HD22	1:C:338:ASN:H	1.09	0.94
1:F:187:ALA:HA	1:F:190:LYS:HE2	1.52	0.89
1:D:83:LEU:HD11	1:D:257:ARG:HD3	1.56	0.88
1:C:202:LYS:HE2	1:C:215:GLU:HG2	1.56	0.86
1:D:202:LYS:HG3	3:D:2035:HOH:O	1.74	0.86
1:B:156:THR:CG2	2:B:4002:NAD:H5N	2.06	0.85
1:F:181:ARG:HH11	1:F:214:LEU:HD12	1.43	0.84
1:G:309:ARG:O	1:G:313:LYS:HD3	1.78	0.82
1:D:210:PRO:O	1:D:214:LEU:HD22	1.80	0.81
1:H:139:ASN:HD21	1:H:261:GLY:H	1.27	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:GLU:CD	1:D:6:GLU:H	1.83	0.80
1:E:194:ILE:O	1:E:208:THR:HG23	1.81	0.80
1:H:140:THR:HG22	1:H:141:GLU:O	1.82	0.79
1:B:156:THR:HG22	2:B:4002:NAD:H5N	1.64	0.79
1:C:172:LEU:HD11	1:C:174:MSE:HE3	1.64	0.78
1:C:179:ILE:CG1	1:C:183:LYS:HE3	2.13	0.77
1:G:1:MSE:HG3	1:G:2:ILE:H	1.48	0.77
1:G:201:ASP:HB2	1:G:205:LYS:H	1.49	0.76
1:A:296:GLU:HG3	1:A:297:GLY:H	1.51	0.76
1:F:207:THR:HG21	1:F:212:LYS:HB2	1.67	0.76
1:G:186:GLU:O	1:G:190:LYS:HB2	1.86	0.75
1:H:276:GLU:H	1:H:276:GLU:CD	1.90	0.74
1:C:338:ASN:ND2	1:C:338:ASN:H	1.85	0.74
1:G:292:SER:HB3	1:H:153:ILE:HD11	1.69	0.73
1:G:1:MSE:CG	1:G:2:ILE:H	2.00	0.73
1:B:172:LEU:HD11	1:B:174:MSE:CE	2.19	0.73
1:D:102:LYS:HG3	1:D:132:MSE:HE1	1.71	0.73
1:A:181:ARG:HH22	1:A:214:LEU:HA	1.52	0.73
1:C:140:THR:HG21	2:C:4003:NAD:H4N	1.71	0.72
1:E:174:MSE:HE2	1:F:225:LYS:HA	1.71	0.72
1:C:181:ARG:HH21	1:C:214:LEU:HD11	1.55	0.71
1:E:315:LYS:HE2	1:G:280:ARG:HG2	1.72	0.71
1:A:204:GLY:HA3	1:B:295:ALA:HB1	1.73	0.71
1:C:193:LYS:HE3	1:C:194:ILE:H	1.56	0.70
1:A:166:ASN:O	1:C:169:LYS:HE3	1.90	0.70
1:F:167:LYS:HE3	1:F:168:TYR:CE2	2.26	0.70
1:C:166:ASN:ND2	1:C:279:LYS:HD3	2.07	0.70
1:G:288:GLU:HG2	1:H:153:ILE:HD13	1.74	0.70
1:E:140:THR:HG22	1:E:141:GLU:O	1.92	0.70
1:F:187:ALA:CA	1:F:190:LYS:HE2	2.21	0.69
1:G:5:PRO:HG3	1:G:38:LEU:HD21	1.73	0.69
1:H:193:LYS:HB3	1:H:208:THR:CG2	2.22	0.69
1:C:285:LEU:HB2	1:D:244:VAL:HG21	1.74	0.69
1:C:166:ASN:HD21	1:C:279:LYS:HD3	1.57	0.69
1:B:167:LYS:HE3	1:B:168:TYR:HE1	1.55	0.69
1:C:174:MSE:HE1	1:D:225:LYS:O	1.93	0.69
1:E:343:ILE:HA	1:E:344:GLU:HB3	1.75	0.69
1:C:338:ASN:HD22	1:C:338:ASN:N	1.79	0.69
1:A:211:ALA:O	1:A:214:LEU:HG	1.93	0.68
1:H:51:GLN:HG3	1:H:254:PRO:HG3	1.74	0.68
1:E:193:LYS:HB3	1:E:208:THR:CG2	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:LEU:HD11	1:C:174:MSE:CE	2.24	0.68
1:E:172:LEU:HD11	1:E:174:MSE:CE	2.21	0.68
1:E:3:LEU:HD13	1:E:343:ILE:HD11	1.75	0.67
1:G:210:PRO:O	1:G:214:LEU:HD22	1.94	0.67
1:F:182:GLY:HA2	1:F:185:LEU:HD11	1.78	0.66
1:H:6:GLU:CD	1:H:6:GLU:H	1.99	0.66
1:H:207:THR:OG1	1:H:212:LYS:HE3	1.94	0.66
1:F:180:ALA:O	1:F:184:ILE:HG13	1.96	0.66
1:E:193:LYS:HB3	1:E:208:THR:HG22	1.76	0.66
1:D:170:PHE:CE1	1:D:303:PRO:HG2	2.30	0.65
1:G:200:VAL:HG13	1:G:219:LEU:HD11	1.77	0.65
1:G:258:CYS:SG	1:G:260:LYS:HG3	2.37	0.65
1:E:193:LYS:HD2	1:E:208:THR:HG22	1.78	0.65
1:G:201:ASP:HB3	1:G:203:ASP:H	1.61	0.65
1:B:327:GLN:O	1:B:331:ILE:HG13	1.96	0.65
1:E:102:LYS:HG3	1:E:132:MSE:HE1	1.78	0.65
1:F:190:LYS:O	1:F:192:ILE:HG23	1.97	0.64
1:B:156:THR:HG21	2:B:4002:NAD:H5N	1.78	0.64
1:C:184:ILE:HG12	1:C:194:ILE:HD11	1.79	0.64
1:E:60:ASN:ND2	1:E:257:ARG:HD2	2.12	0.64
1:E:275:LYS:O	1:E:279:LYS:HG3	1.99	0.63
1:C:179:ILE:HG13	1:C:183:LYS:CE	2.23	0.63
1:E:1:MSE:O	1:E:319:GLU:HA	1.99	0.63
1:F:17:LYS:HG3	3:F:2002:HOH:O	1.98	0.63
1:E:1:MSE:H3	1:E:1:MSE:SE	2.31	0.62
1:E:150:LYS:HD3	1:E:203:ASP:O	1.99	0.62
1:B:140:THR:HG22	1:B:141:GLU:O	1.99	0.62
1:B:283:ASP:O	1:B:287:ASP:HB2	1.99	0.62
1:B:258:CYS:SG	1:B:260:LYS:HG2	2.40	0.62
1:F:243:GLU:HB2	1:F:259:THR:CG2	2.29	0.62
1:C:172:LEU:HD21	1:C:174:MSE:HE3	1.81	0.62
1:E:160:ALA:HA	1:E:172:LEU:O	2.00	0.62
1:H:194:ILE:O	1:H:208:THR:HG23	2.00	0.61
1:A:83:LEU:HD11	1:A:257:ARG:HD3	1.80	0.61
1:B:48:ARG:NH2	1:B:251:THR:O	2.33	0.61
1:C:329:LYS:HB3	1:C:329:LYS:NZ	2.14	0.61
1:C:193:LYS:CG	1:C:194:ILE:H	2.14	0.61
1:E:178:SER:HB3	1:E:221:PHE:HA	1.83	0.61
1:A:158:PRO:HG3	2:A:4001:NAD:C4N	2.30	0.61
1:E:281:LYS:HD2	3:F:2039:HOH:O	2.00	0.61
1:A:293:GLU:CG	1:B:151:GLU:HB2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:ALA:HA	1:C:170:PHE:O	2.01	0.60
1:A:312:MSE:HE3	3:A:2070:HOH:O	2.00	0.60
1:C:194:ILE:HG12	1:C:195:PRO:HD2	1.82	0.60
1:D:275:LYS:HG3	3:D:2025:HOH:O	2.00	0.60
1:F:187:ALA:HA	1:F:190:LYS:HG2	1.84	0.60
1:F:62:ASN:HD22	1:F:63:PRO:HD2	1.66	0.60
1:A:60:ASN:OD1	1:A:257:ARG:HG2	2.02	0.60
3:E:2052:HOH:O	1:G:315:LYS:HE2	2.02	0.60
1:F:184:ILE:HG22	1:F:214:LEU:HD22	1.84	0.59
1:E:1:MSE:SE	1:E:1:MSE:N	2.85	0.59
1:C:129:ASN:HA	1:C:164:LYS:NZ	2.17	0.59
1:G:117:PHE:C	1:G:117:PHE:HD1	2.05	0.59
1:B:172:LEU:CD1	1:B:174:MSE:HE3	2.26	0.59
1:G:1:MSE:HG3	1:G:2:ILE:N	2.16	0.59
1:B:273:MSE:HE1	1:B:281:LYS:HD3	1.85	0.59
1:A:201:ASP:O	1:A:202:LYS:CB	2.51	0.59
1:C:193:LYS:HG2	1:C:194:ILE:H	1.68	0.59
1:A:178:SER:HB3	1:A:221:PHE:HA	1.85	0.59
1:F:5:PRO:HG3	1:F:38:LEU:HD21	1.85	0.59
1:D:5:PRO:HG3	1:D:38:LEU:HD21	1.84	0.59
1:G:188:LEU:HD22	1:G:214:LEU:HD23	1.85	0.59
1:A:53:ILE:HG22	1:A:57:LYS:HE2	1.84	0.59
1:A:140:THR:HG22	1:A:141:GLU:O	2.02	0.58
1:A:11:LEU:HD13	1:A:342:TYR:CD1	2.38	0.58
1:D:144:MSE:HE2	1:D:155:GLY:O	2.04	0.58
1:G:1:MSE:CG	1:G:2:ILE:N	2.66	0.58
1:C:156:THR:OG1	2:C:4003:NAD:H5N	2.03	0.58
1:E:186:GLU:HG2	1:E:189:ARG:HH12	1.68	0.58
1:D:9[B]:LYS:HG3	1:D:34:VAL:HG21	1.85	0.58
1:B:281:LYS:HB3	1:B:281:LYS:NZ	2.19	0.58
1:G:152:LYS:O	1:G:153:ILE:HD13	2.04	0.58
1:H:219:LEU:HD23	3:H:2030:HOH:O	2.03	0.57
1:E:192:ILE:HG22	1:E:193:LYS:N	2.19	0.57
1:A:201:ASP:O	1:A:202:LYS:HB2	2.04	0.57
1:F:181:ARG:HH11	1:F:214:LEU:CD1	2.16	0.57
1:G:117:PHE:CD1	1:G:117:PHE:C	2.77	0.57
1:G:24:GLU:O	1:G:28:ILE:HG13	2.05	0.57
1:E:324:LEU:O	1:E:328:LEU:HG	2.05	0.57
1:B:160:ALA:HA	1:B:172:LEU:O	2.05	0.57
1:C:138:THR:HG22	1:C:158:PRO:CG	2.35	0.57
1:F:248:VAL:HA	1:F:259:THR:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:GLU:HB3	1:D:150:LYS:HD2	1.87	0.57
1:H:99:LYS:O	1:H:102:LYS:HG2	2.05	0.56
1:A:225:LYS:O	1:B:174:MSE:HE1	2.04	0.56
1:B:138:THR:CG2	1:B:158:PRO:HG2	2.35	0.56
1:C:193:LYS:HE3	1:C:194:ILE:N	2.20	0.56
1:G:5:PRO:HD3	1:G:317:GLY:HA2	1.88	0.56
1:F:243:GLU:OE1	3:F:2040:HOH:O	2.16	0.56
1:E:133:ILE:HD13	1:F:236:LEU:HD22	1.87	0.56
1:A:220:PRO:HB2	3:A:2050:HOH:O	2.06	0.56
1:C:189:ARG:HB3	1:C:190:LYS:HE3	1.87	0.56
1:B:330:GLU:O	1:B:334:GLU:HG3	2.05	0.56
1:G:156:THR:OG1	2:G:4007:NAD:H5N	2.05	0.56
1:E:18:LYS:HE2	1:E:335:LEU:O	2.06	0.56
1:B:77:ALA:HB3	1:B:109:VAL:HG22	1.87	0.56
1:D:4:LYS:HB3	1:D:6:GLU:OE1	2.05	0.56
1:C:18:LYS:HE3	1:C:335:LEU:O	2.06	0.56
1:E:18:LYS:HG2	1:E:335:LEU:HB3	1.88	0.55
1:H:139:ASN:ND2	1:H:261:GLY:H	2.01	0.55
1:C:190:LYS:HD2	1:C:190:LYS:N	2.21	0.55
1:G:202:LYS:HD3	1:G:215:GLU:O	2.07	0.55
1:F:9:LYS:HE2	1:F:31:ASP:OD1	2.07	0.55
1:F:179:ILE:HG12	1:F:180:ALA:N	2.22	0.55
1:H:193:LYS:HB3	1:H:208:THR:HG22	1.88	0.55
1:A:181:ARG:HH22	1:A:214:LEU:CA	2.18	0.55
1:A:153:ILE:HG21	1:B:289:ILE:HG12	1.88	0.55
1:E:210:PRO:O	1:E:214:LEU:HD22	2.06	0.55
1:B:11:LEU:HD12	1:B:11:LEU:O	2.07	0.55
1:G:290:LYS:HE2	1:G:305:GLU:OE2	2.07	0.55
1:G:330:GLU:O	1:G:334:GLU:HG2	2.07	0.55
1:B:138:THR:HG23	1:B:158:PRO:HG2	1.87	0.55
1:A:116:HIS:CE1	1:A:118:GLY:HA2	2.42	0.54
1:F:3:LEU:HD13	1:F:343:ILE:HG12	1.89	0.54
1:F:192:ILE:HG13	1:F:193:LYS:O	2.08	0.54
1:B:91:LYS:O	1:B:95:GLU:HG2	2.07	0.54
1:F:179:ILE:HD13	1:F:184:ILE:HG12	1.89	0.54
1:D:160:ALA:HA	1:D:172:LEU:O	2.07	0.54
1:C:192:ILE:HD12	1:C:192:ILE:N	2.22	0.54
1:A:273:MSE:HE2	1:A:277:GLU:HB3	1.90	0.54
1:A:281:LYS:HE3	3:B:2050:HOH:O	2.07	0.54
1:A:160:ALA:HA	1:A:172:LEU:O	2.07	0.54
1:F:195:PRO:HB2	1:F:198:CYS:SG	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:209:ASP:HB3	1:H:212:LYS:HE2	1.90	0.53
1:G:8:GLU:HG3	1:G:46:ILE:HD12	1.90	0.53
1:A:293:GLU:HG2	1:B:151:GLU:HB2	1.90	0.53
1:E:51:GLN:HG3	3:E:2005:HOH:O	2.07	0.53
1:A:258:CYS:SG	1:A:260:LYS:HG2	2.48	0.53
1:F:83:LEU:HD11	1:F:257:ARG:CD	2.39	0.53
1:E:295:ALA:O	1:E:297:GLY:N	2.42	0.53
1:C:193:LYS:HG2	1:C:194:ILE:N	2.24	0.53
1:H:200:VAL:HA	1:H:207:THR:HG22	1.90	0.53
1:F:243:GLU:CG	1:F:259:THR:HG23	2.39	0.53
1:E:305:GLU:O	1:E:309:ARG:HG3	2.08	0.53
1:F:209:ASP:OD2	1:F:211:ALA:HB3	2.09	0.53
1:C:157:ASN:HB3	1:C:233:ILE:HG21	1.90	0.53
1:B:62:ASN:O	1:B:65:PRO:HD3	2.07	0.53
1:F:207:THR:HG22	1:F:209:ASP:H	1.74	0.53
1:G:284:GLU:OE2	1:H:247:LYS:HE3	2.09	0.53
1:D:260:LYS:C	1:D:260:LYS:HD2	2.29	0.53
1:D:194:ILE:O	1:D:208:THR:HG22	2.09	0.53
1:C:192:ILE:O	1:C:192:ILE:HG22	2.09	0.52
1:E:117:PHE:CD1	1:E:117:PHE:C	2.83	0.52
1:E:117:PHE:HD1	1:E:117:PHE:C	2.13	0.52
1:G:131:ASP:OD1	1:G:279:LYS:HE2	2.10	0.52
1:C:144:MSE:HE2	1:C:155:GLY:O	2.09	0.52
1:D:158:PRO:HA	1:D:175:ALA:HA	1.92	0.52
1:H:4:LYS:HB3	1:H:6:GLU:OE1	2.10	0.52
1:G:13:ILE:O	1:G:17:LYS:HG3	2.09	0.52
1:C:320:ILE:HB	1:C:324:LEU:HD23	1.91	0.52
1:E:35:ASP:OD2	1:E:311:LYS:NZ	2.40	0.52
1:B:156:THR:HG23	1:B:175:ALA:HB1	1.92	0.52
1:F:181:ARG:NH1	1:F:214:LEU:HD12	2.19	0.52
1:B:131:ASP:OD2	1:B:279:LYS:CE	2.58	0.52
1:A:236:LEU:HD22	1:B:133:ILE:HD13	1.90	0.52
1:C:172:LEU:HD11	1:C:174:MSE:HG2	1.91	0.52
1:H:94:MSE:HE3	1:H:124:SER:HA	1.91	0.52
1:D:194:ILE:HG22	1:D:208:THR:HA	1.92	0.51
1:C:326:ASN:HA	1:C:329:LYS:HZ2	1.75	0.51
1:F:138:THR:HG22	1:F:158:PRO:HG2	1.91	0.51
1:F:181:ARG:O	1:F:181:ARG:HG3	2.10	0.51
1:E:231:LEU:HD13	1:F:170:PHE:HE1	1.76	0.51
1:B:1:MSE:SE	1:B:1:MSE:N	2.93	0.51
1:E:5:PRO:HG3	1:E:38:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:184:ILE:HG22	1:E:214:LEU:HD22	1.92	0.51
1:A:260:LYS:HE2	3:A:2080:HOH:O	2.09	0.51
1:C:189:ARG:NH1	1:C:190:LYS:HE3	2.25	0.51
1:C:157:ASN:HB3	1:C:233:ILE:CG2	2.40	0.51
1:A:244:VAL:HG13	1:B:281:LYS:NZ	2.26	0.51
1:E:44:HIS:CE1	2:E:4005:NAD:C2N	2.93	0.51
1:G:209:ASP:OD2	1:G:212:LYS:HG2	2.10	0.51
1:C:172:LEU:CD1	1:C:174:MSE:HE3	2.39	0.51
1:D:193:LYS:HG2	1:D:208:THR:HB	1.92	0.51
1:H:273:MSE:HE2	1:H:277:GLU:HB3	1.92	0.51
1:G:196:GLU:H	1:G:196:GLU:CD	2.14	0.51
1:B:140:THR:HG21	1:B:156:THR:H	1.75	0.51
1:G:151:GLU:OE1	1:H:293:GLU:HG3	2.11	0.51
1:F:179:ILE:CD1	1:F:184:ILE:HG12	2.41	0.51
1:C:138:THR:HG22	1:C:158:PRO:HG2	1.93	0.51
1:B:305:GLU:O	1:B:309[B]:ARG:HD2	2.11	0.51
1:A:296:GLU:HG2	1:A:298:PHE:HD1	1.76	0.51
1:B:25:ASP:HB3	1:B:88:VAL:HG21	1.92	0.51
1:D:255:GLU:HG3	1:D:255:GLU:O	2.10	0.51
1:F:80:ASP:OD1	1:F:112:ARG:HD2	2.12	0.50
1:A:1:MSE:HG2	1:A:320:ILE:HG13	1.91	0.50
1:E:174:MSE:HE1	1:F:225:LYS:O	2.11	0.50
1:A:243:GLU:HG2	1:A:259:THR:HB	1.91	0.50
1:H:175:ALA:HB2	2:H:4008:NAD:H6N	1.93	0.50
1:D:131:ASP:OD1	1:D:279:LYS:HE2	2.11	0.50
1:F:167:LYS:HE3	1:F:168:TYR:HE2	1.75	0.50
1:B:3:LEU:HD13	1:B:343:ILE:HG12	1.93	0.50
1:F:151:GLU:O	1:F:153:ILE:HD12	2.12	0.50
1:C:338:ASN:N	1:C:338:ASN:ND2	2.45	0.50
1:B:138:THR:HG23	1:B:158:PRO:CG	2.42	0.50
1:D:209:ASP:OD2	1:D:211:ALA:HB3	2.11	0.50
1:A:119:ILE:HD12	1:A:122:TYR:H	1.77	0.50
1:C:322:LYS:O	1:C:325:TYR:HB3	2.12	0.50
1:E:192:ILE:CG2	1:E:193:LYS:N	2.74	0.49
1:B:156:THR:CG2	1:B:175:ALA:HB1	2.42	0.49
1:A:133:ILE:HD13	1:B:236:LEU:HD22	1.94	0.49
1:H:51:GLN:CG	1:H:254:PRO:HG3	2.41	0.49
1:G:174:MSE:HB3	2:G:4007:NAD:H52A	1.94	0.49
1:E:253:ASN:OD1	1:E:255:GLU:HG2	2.12	0.49
1:B:172:LEU:HD21	1:B:174:MSE:HE3	1.94	0.49
1:E:343:ILE:HA	1:E:344:GLU:CB	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:ASN:HD22	1:E:257:ARG:HD2	1.77	0.49
1:F:83:LEU:HD11	1:F:257:ARG:HD3	1.93	0.49
1:B:5:PRO:HG3	1:B:38:LEU:HD21	1.94	0.49
1:G:292:SER:HB3	1:H:153:ILE:CD1	2.41	0.49
1:A:201:ASP:HB3	1:A:207:THR:HG21	1.93	0.49
1:E:142:PRO:HG3	1:E:246:THR:HA	1.95	0.49
1:C:179:ILE:HD11	1:C:183:LYS:HG2	1.94	0.49
1:E:208:THR:O	1:E:208:THR:HG22	2.12	0.49
1:C:191:LYS:O	1:C:193:LYS:N	2.46	0.49
1:G:273:MSE:O	1:G:277:GLU:HG3	2.13	0.49
1:B:87:GLN:HA	1:B:123:TYR:OH	2.13	0.49
1:F:179:ILE:HG21	1:F:198:CYS:HB3	1.95	0.49
1:B:157:ASN:HB3	1:B:233:ILE:CG2	2.42	0.48
1:C:327:GLN:O	1:C:331:ILE:HG13	2.13	0.48
1:A:138:THR:HG22	1:A:158:PRO:HD2	1.96	0.48
1:G:312:MSE:O	1:G:315:LYS:HE3	2.13	0.48
1:A:137:ILE:CG2	1:A:159:ILE:HG13	2.43	0.48
1:E:296:GLU:OE1	1:E:297:GLY:N	2.45	0.48
1:A:320:ILE:HB	1:A:324:LEU:HD23	1.93	0.48
1:F:258:CYS:SG	1:F:260:LYS:HG3	2.53	0.48
1:G:176:THR:HG21	1:G:233:ILE:HD12	1.95	0.48
1:B:156:THR:CG2	1:B:156:THR:O	2.61	0.48
1:D:117:PHE:C	1:D:117:PHE:HD1	2.17	0.48
1:A:117:PHE:CD1	1:A:117:PHE:C	2.87	0.48
1:A:117:PHE:HD1	1:A:117:PHE:C	2.16	0.48
1:F:193:LYS:HB3	1:F:193:LYS:NZ	2.29	0.48
1:C:329:LYS:HZ2	1:C:329:LYS:HB3	1.77	0.48
1:C:293:GLU:HA	1:C:294:PRO:HD3	1.68	0.48
1:G:138:THR:HG22	1:G:158:PRO:HG2	1.95	0.48
1:C:193:LYS:CE	1:C:194:ILE:H	2.23	0.48
1:C:329:LYS:NZ	1:C:329:LYS:CB	2.76	0.48
1:D:194:ILE:HG13	1:D:195:PRO:HD2	1.96	0.48
1:B:278:PHE:O	1:B:282:VAL:HG23	2.14	0.48
1:F:273:MSE:HE1	1:F:281:LYS:HE2	1.96	0.48
1:F:179:ILE:CG2	1:F:198:CYS:HB3	2.44	0.48
1:C:193:LYS:HE2	1:C:193:LYS:HB3	1.66	0.48
1:A:139:ASN:HB2	1:A:261:GLY:H	1.79	0.48
1:G:285:LEU:HB2	1:H:244:VAL:HG21	1.96	0.48
1:C:278:PHE:CD1	1:D:235:MSE:HE2	2.49	0.48
1:A:203:ASP:OD2	1:A:203:ASP:N	2.46	0.48
1:E:140:THR:HB	1:E:155:GLY:HA3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:8:GLU:O	1:H:12:ILE:HD12	2.14	0.48
1:F:296:GLU:HB2	1:F:298:PHE:HD2	1.78	0.48
1:F:220:PRO:HG2	1:F:227:TYR:HB2	1.96	0.48
1:B:273:MSE:HE2	1:B:277:GLU:HB2	1.96	0.47
1:D:117:PHE:C	1:D:117:PHE:CD1	2.88	0.47
1:C:278:PHE:CE1	1:D:235:MSE:HE2	2.49	0.47
1:H:141:GLU:HG2	1:H:249:LYS:HA	1.95	0.47
1:F:259:THR:O	1:F:259:THR:CG2	2.62	0.47
1:F:65:PRO:HB2	1:F:67:ILE:HG13	1.95	0.47
1:F:190:LYS:HE3	1:F:192:ILE:HD11	1.97	0.47
1:D:102:LYS:CG	1:D:132:MSE:HE1	2.41	0.47
1:A:183:LYS:HD2	1:A:186:GLU:OE2	2.14	0.47
1:C:5:PRO:HD3	1:C:317:GLY:HA2	1.95	0.47
1:B:76:THR:HA	1:B:108:VAL:O	2.15	0.47
1:A:296:GLU:CG	1:A:297:GLY:H	2.22	0.47
1:E:338:ASN:HB3	1:E:341:ASP:OD1	2.15	0.47
1:A:192:ILE:O	1:A:193:LYS:HD3	2.15	0.47
1:B:73:SER:HB2	1:B:74:PRO:HD2	1.95	0.47
1:C:11:LEU:HD13	1:C:342:TYR:CD1	2.50	0.47
1:E:162:ALA:HA	1:E:170:PHE:O	2.14	0.47
1:B:141:GLU:HG3	1:B:251:THR:OG1	2.15	0.47
1:E:141:GLU:HG3	1:E:251:THR:OG1	2.15	0.47
1:F:140:THR:HG21	2:F:4006:NAD:H4N	1.97	0.47
1:H:186:GLU:HA	1:H:189:ARG:NH1	2.30	0.47
1:G:87:GLN:HA	1:G:123:TYR:OH	2.15	0.47
1:B:46:ILE:HG23	1:B:324:LEU:HD21	1.97	0.46
1:F:243:GLU:HB2	1:F:259:THR:HG23	1.97	0.46
1:A:46:ILE:HG23	1:A:324:LEU:HD21	1.96	0.46
1:A:190:LYS:HB3	1:A:192:ILE:HG12	1.97	0.46
1:F:166:ASN:HB2	1:F:283:ASP:OD2	2.16	0.46
1:G:138:THR:CG2	1:G:158:PRO:HG2	2.45	0.46
1:C:244:VAL:HG22	1:D:281:LYS:HD2	1.98	0.46
1:G:48:ARG:NH1	3:G:2012:HOH:O	2.46	0.46
1:G:190:LYS:HD3	1:G:192:ILE:HD13	1.97	0.46
1:E:76:THR:HA	1:E:108:VAL:O	2.16	0.46
1:E:6:GLU:CD	1:E:6:GLU:H	2.18	0.46
1:E:246:THR:HG23	1:F:288:GLU:OE1	2.16	0.46
1:A:209:ASP:HA	1:A:210:PRO:HD3	1.71	0.46
1:H:128:MSE:HE3	1:H:169:LYS:HE3	1.97	0.46
1:H:17:LYS:HD2	1:H:23:GLU:HG3	1.98	0.46
1:C:329:LYS:HZ2	1:C:329:LYS:CB	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:225:LYS:HE2	1:F:174:MSE:HB2	1.97	0.46
1:E:243:GLU:HB3	1:E:247:LYS:HB2	1.98	0.46
1:E:231:LEU:HD13	1:F:170:PHE:CE1	2.51	0.46
3:G:2063:HOH:O	1:H:146:PRO:HD2	2.16	0.46
1:B:126:LEU:O	1:B:130:GLN:HG2	2.15	0.46
1:F:4:LYS:HB2	1:F:7:ASN:HD22	1.81	0.46
1:C:250:GLY:HA2	1:C:256:GLU:HB2	1.98	0.46
1:E:137:ILE:HB	1:E:233:ILE:HG23	1.98	0.46
1:C:117:PHE:CD1	1:C:117:PHE:C	2.89	0.46
1:B:222:GLY:H	1:B:226:GLY:HA3	1.80	0.46
1:D:9[A]:LYS:HE2	1:D:13:ILE:HD11	1.98	0.46
1:B:83:LEU:HD11	1:B:257:ARG:HD2	1.98	0.46
1:E:192:ILE:HG22	1:E:193:LYS:O	2.16	0.45
1:F:62:ASN:ND2	1:F:64:LYS:H	2.15	0.45
1:A:236:LEU:CD2	1:B:133:ILE:HD13	2.47	0.45
1:A:137:ILE:HG22	1:A:159:ILE:HG13	1.98	0.45
1:D:200:VAL:CG2	1:D:217:CYS:HB2	2.46	0.45
1:E:307:GLU:H	1:E:307:GLU:CD	2.19	0.45
1:A:135:ILE:HA	1:A:160:ALA:O	2.16	0.45
1:E:296:GLU:OE1	1:E:298:PHE:CD1	2.69	0.45
1:H:157:ASN:HB3	1:H:233:ILE:CG2	2.47	0.45
1:F:201:ASP:HB3	1:F:207:THR:OG1	2.16	0.45
1:B:189:ARG:C	1:B:191:LYS:H	2.18	0.45
1:H:138:THR:O	1:H:158:PRO:HD2	2.17	0.45
1:G:296:GLU:OE2	1:H:205:LYS:HG2	2.16	0.45
1:E:152:LYS:O	1:E:153:ILE:HD13	2.17	0.45
1:E:172:LEU:CD1	1:E:174:MSE:HE3	2.26	0.45
1:G:167:LYS:HD3	1:G:168:TYR:CE2	2.51	0.45
1:E:244:VAL:HG21	1:F:285:LEU:HB2	1.97	0.45
1:C:3:LEU:HD13	1:C:343:ILE:HG12	1.98	0.45
1:F:247:LYS:O	1:F:259:THR:HG21	2.16	0.45
1:A:232:ALA:O	1:A:236:LEU:HG	2.16	0.45
1:H:221:PHE:CG	1:H:222:GLY:N	2.85	0.45
1:A:244:VAL:HG21	1:B:285:LEU:HB2	1.99	0.45
1:F:46:ILE:HG23	1:F:324:LEU:HD21	1.98	0.45
1:E:170:PHE:CE1	1:F:231:LEU:HD13	2.52	0.45
1:G:253:ASN:HA	1:G:254:PRO:HD2	1.77	0.45
1:C:139:ASN:HD22	1:C:139:ASN:HA	1.54	0.45
1:E:174:MSE:HE2	1:F:225:LYS:CA	2.43	0.44
1:H:331:ILE:O	1:H:335:LEU:HG	2.17	0.44
1:E:140:THR:HG21	1:E:156:THR:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:GLU:OE2	1:B:151:GLU:HB2	2.16	0.44
1:F:117:PHE:HD1	1:F:117:PHE:C	2.20	0.44
1:B:140:THR:CG2	1:B:156:THR:H	2.30	0.44
1:F:117:PHE:CD1	1:F:117:PHE:C	2.91	0.44
1:H:135:ILE:HA	1:H:160:ALA:O	2.18	0.44
1:C:258:CYS:SG	1:C:260:LYS:HG3	2.58	0.44
1:F:62:ASN:HD22	1:F:63:PRO:CD	2.30	0.44
1:E:294:PRO:HA	1:F:149:GLY:HA2	1.99	0.44
1:D:71:LYS:HB3	1:D:71:LYS:HE2	1.69	0.44
1:C:193:LYS:CG	1:C:194:ILE:N	2.79	0.44
1:G:46:ILE:HG23	1:G:324:LEU:HD21	1.99	0.44
1:D:48:ARG:O	1:D:48:ARG:HG3	2.18	0.44
1:H:200:VAL:HG12	1:H:206:PRO:HA	1.98	0.44
1:H:102:LYS:HB3	1:H:132:MSE:HE1	1.99	0.44
1:A:150:LYS:HG3	1:B:293:GLU:HG3	1.99	0.44
1:G:158:PRO:HD3	2:G:4007:NAD:C5N	2.48	0.44
1:G:236:LEU:HD22	1:H:133:ILE:HD13	1.99	0.44
1:C:195:PRO:HB2	1:C:198:CYS:SG	2.57	0.44
1:B:157:ASN:HB3	1:B:233:ILE:HG21	2.00	0.44
1:C:150:LYS:HG2	1:D:293:GLU:HB3	2.00	0.44
1:D:179:ILE:HD11	1:D:183:LYS:HD3	1.99	0.44
1:E:1:MSE:H1	1:E:1:MSE:HE3	1.82	0.43
1:A:39:LYS:HG2	1:A:307:GLU:HB3	1.99	0.43
1:E:263:LEU:HA	1:E:263:LEU:HD23	1.86	0.43
1:E:315:LYS:HD3	1:E:315:LYS:HA	1.71	0.43
1:A:182:GLY:HA2	1:A:185:LEU:HD21	1.99	0.43
1:H:117:PHE:HD1	1:H:117:PHE:C	2.21	0.43
1:D:53:ILE:HG22	1:D:57:LYS:HE3	2.00	0.43
1:D:116:HIS:CD2	1:D:118:GLY:H	2.36	0.43
1:G:272:PHE:HB3	1:H:239:ILE:O	2.19	0.43
1:G:323:ASN:HB2	3:G:2066:HOH:O	2.18	0.43
1:B:168:TYR:HB3	1:B:286:LEU:HD12	2.00	0.43
1:H:209:ASP:HA	1:H:210:PRO:HD3	1.85	0.43
1:B:144:MSE:HE2	1:B:155:GLY:O	2.18	0.43
1:H:128:MSE:CE	1:H:169:LYS:HE3	2.48	0.43
1:C:207:THR:OG1	1:C:212:LYS:HD2	2.18	0.43
1:G:28:ILE:HG23	1:G:91:LYS:HD3	2.01	0.43
1:G:157:ASN:O	1:G:176:THR:HG23	2.19	0.43
1:H:157:ASN:HB3	1:H:233:ILE:HG21	2.00	0.43
1:B:181:ARG:HG2	1:B:185:LEU:CD2	2.49	0.43
1:H:62:ASN:HA	1:H:63:PRO:HD3	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:LEU:HD12	1:B:214:LEU:HA	1.89	0.43
1:E:313:LYS:HD3	1:E:313:LYS:HA	1.72	0.43
1:H:117:PHE:CD1	1:H:117:PHE:C	2.91	0.43
1:F:53:ILE:HG13	1:F:331:ILE:HD13	2.00	0.43
1:B:267:ILE:O	1:B:269:PRO:HD3	2.19	0.43
1:F:243:GLU:HB2	1:F:259:THR:HG22	1.99	0.43
1:F:4:LYS:HB3	1:F:6:GLU:OE2	2.19	0.43
1:F:141:GLU:HG2	1:F:251:THR:OG1	2.17	0.43
1:F:283:ASP:O	1:F:287:ASP:HB2	2.18	0.43
1:D:194:ILE:HD12	1:D:194:ILE:HA	1.94	0.43
1:H:48:ARG:HD3	1:H:52:TYR:HE1	1.84	0.43
1:B:6:GLU:H	1:B:6:GLU:CD	2.22	0.43
1:G:278:PHE:O	1:G:282:VAL:HG23	2.19	0.42
1:G:228:GLY:HA3	1:H:172:LEU:HD13	2.01	0.42
1:H:83:LEU:HA	1:H:83:LEU:HD23	1.90	0.42
1:C:281:LYS:HE2	1:C:284:GLU:OE1	2.19	0.42
1:F:49:PHE:O	1:F:52:TYR:HB2	2.19	0.42
1:B:253:ASN:ND2	1:B:256:GLU:OE1	2.51	0.42
1:G:1:MSE:SE	1:G:2:ILE:H	2.51	0.42
1:B:295:ALA:O	1:B:296:GLU:C	2.58	0.42
1:E:184:ILE:HG22	1:E:214:LEU:CD2	2.49	0.42
1:B:83:LEU:HD21	1:B:257:ARG:HG2	2.02	0.42
1:E:209:ASP:OD2	1:E:211:ALA:HB3	2.19	0.42
1:A:285:LEU:HB2	1:B:244:VAL:HG21	2.01	0.42
1:E:262:ASP:OD1	1:E:262:ASP:N	2.52	0.42
1:H:193:LYS:CD	1:H:208:THR:HG22	2.50	0.42
1:C:170:PHE:CE1	1:C:303:PRO:HG2	2.54	0.42
1:G:263:LEU:HD23	1:G:263:LEU:HA	1.73	0.42
1:C:172:LEU:CD1	1:C:174:MSE:HG2	2.49	0.42
1:C:214:LEU:C	1:C:216:GLY:H	2.22	0.42
1:H:212:LYS:O	1:H:215:GLU:HG3	2.19	0.42
1:B:273:MSE:O	1:B:277:GLU:HG3	2.19	0.42
1:E:138:THR:HG22	1:E:158:PRO:HG2	2.01	0.42
1:A:70:VAL:HG12	1:A:71:LYS:HG3	2.01	0.42
1:E:338:ASN:OD1	1:E:340:GLU:HG2	2.19	0.42
1:A:102:LYS:HG3	1:A:132:MSE:HE1	2.00	0.42
1:D:307:GLU:CD	1:D:307:GLU:N	2.73	0.42
1:B:211:ALA:O	1:B:215:GLU:HG2	2.20	0.42
1:A:246:THR:HG23	1:B:288:GLU:OE1	2.19	0.42
1:H:200:VAL:CA	1:H:207:THR:HG22	2.49	0.42
1:G:218:ILE:HG22	1:G:219:LEU:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:174:MSE:SE	1:H:225:LYS:HG2	2.68	0.42
1:B:83:LEU:HD11	1:B:257:ARG:HG3	2.01	0.42
1:C:71:LYS:O	1:C:77:ALA:HA	2.18	0.42
1:F:25:ASP:HB3	1:F:88:VAL:HG21	2.01	0.42
1:C:37:ASP:OD2	1:C:46:ILE:N	2.50	0.42
1:B:131:ASP:OD2	1:B:279:LYS:HE3	2.20	0.42
1:H:143:ALA:HA	1:H:152:LYS:HD2	2.02	0.42
1:B:117:PHE:CD1	1:B:117:PHE:C	2.94	0.42
1:G:235:MSE:O	1:G:235:MSE:HE3	2.19	0.42
1:D:170:PHE:HE1	1:D:303:PRO:HG2	1.80	0.42
1:E:142:PRO:CG	1:E:246:THR:HA	2.50	0.42
1:C:150:LYS:HG2	1:D:293:GLU:CB	2.49	0.42
1:C:102:LYS:NZ	3:C:2015:HOH:O	2.53	0.42
1:F:187:ALA:HA	1:F:190:LYS:CG	2.49	0.41
1:H:139:ASN:H	1:H:139:ASN:ND2	2.18	0.41
1:C:160:ALA:HA	1:C:172:LEU:O	2.19	0.41
1:G:201:ASP:C	1:G:203:ASP:H	2.22	0.41
1:B:260:LYS:HE2	3:B:2030:HOH:O	2.20	0.41
1:A:151:GLU:OE1	1:B:293:GLU:HG2	2.20	0.41
1:H:312:MSE:O	1:H:315:LYS:HG2	2.19	0.41
1:B:290:LYS:HE2	1:B:305:GLU:OE2	2.20	0.41
1:B:189:ARG:C	1:B:191:LYS:N	2.74	0.41
1:C:151:GLU:HG2	1:D:292:SER:HB2	2.02	0.41
1:C:235:MSE:HE2	1:D:278:PHE:CE1	2.55	0.41
1:A:271:PHE:O	1:B:71:LYS:HD3	2.20	0.41
1:A:225:LYS:HA	1:B:174:MSE:CE	2.50	0.41
1:F:91:LYS:O	1:F:95:GLU:HG2	2.20	0.41
1:H:276:GLU:CD	1:H:276:GLU:N	2.66	0.41
1:B:131:ASP:OD2	1:B:279:LYS:HE2	2.21	0.41
1:E:41:PHE:CE2	2:E:4005:NAD:H52N	2.55	0.41
1:E:200:VAL:O	1:E:216:GLY:HA3	2.21	0.41
1:F:179:ILE:CG1	1:F:180:ALA:N	2.83	0.41
1:D:307:GLU:H	1:D:307:GLU:CD	2.24	0.41
1:D:49:PHE:HB3	1:D:50:PRO:HD3	2.02	0.41
1:A:293:GLU:H	1:A:293:GLU:HG2	1.70	0.41
1:C:188:LEU:C	1:C:190:LYS:H	2.24	0.41
1:F:151:GLU:HG3	1:F:153:ILE:HD11	2.02	0.41
1:C:10:LYS:HG2	1:C:342:TYR:HE2	1.85	0.41
1:G:18:LYS:HG2	1:G:335:LEU:HB3	2.03	0.41
1:D:3:LEU:HD13	1:D:343:ILE:HG12	2.02	0.41
1:H:170:PHE:CE1	1:H:303:PRO:HG2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:293:GLU:HG2	1:F:151:GLU:HG2	2.01	0.41
1:G:128:MSE:HG3	1:G:164:LYS:HG2	2.03	0.41
1:A:169[A]:LYS:HG2	1:A:170:PHE:N	2.34	0.41
1:A:21:VAL:HA	1:A:22:PRO:HD2	1.93	0.41
1:E:130:GLN:O	1:E:131:ASP:HB2	2.20	0.41
1:G:154:LEU:HD21	1:H:289:ILE:HD11	2.02	0.41
1:C:295:ALA:O	1:C:296:GLU:C	2.58	0.41
1:D:6:GLU:CD	1:D:6:GLU:N	2.62	0.41
1:C:191:LYS:C	1:C:193:LYS:H	2.22	0.41
1:H:15:VAL:O	1:H:18:LYS:HB2	2.21	0.41
1:B:41:PHE:CE1	2:B:4002:NAD:H52N	2.56	0.41
1:D:302:ILE:HG23	1:D:303:PRO:HD2	2.01	0.41
1:A:244:VAL:HG13	1:B:281:LYS:HZ1	1.85	0.41
1:D:9[A]:LYS:HD2	1:D:30:ALA:CB	2.51	0.41
1:G:273:MSE:HE2	1:G:277:GLU:HB2	2.02	0.41
1:C:249:LYS:HD3	1:C:256:GLU:OE1	2.21	0.41
1:F:280:ARG:NE	3:F:2046:HOH:O	2.52	0.41
1:D:10[B]:LYS:HG2	1:D:342:TYR:HE2	1.86	0.41
1:A:92:LYS:HE3	3:A:2019:HOH:O	2.21	0.41
1:C:188:LEU:O	1:C:190:LYS:N	2.54	0.41
1:C:262:ASP:N	1:C:262:ASP:OD1	2.54	0.41
1:C:41:PHE:CE2	2:C:4003:NAD:H52N	2.56	0.40
1:C:188:LEU:HB2	1:C:210:PRO:HB2	2.03	0.40
1:A:1:MSE:HB3	1:A:320:ILE:O	2.21	0.40
1:A:142:PRO:CG	1:A:246:THR:HA	2.50	0.40
1:F:249:LYS:H	1:F:259:THR:HB	1.86	0.40
1:G:108:VAL:HG22	1:G:265:ILE:HG12	2.02	0.40
1:F:94:MSE:O	1:F:98:ILE:HG13	2.21	0.40
1:D:201:ASP:O	1:D:202:LYS:C	2.60	0.40
1:G:28:ILE:CG2	1:G:91:LYS:HD3	2.52	0.40
1:F:187:ALA:HA	1:F:190:LYS:CE	2.38	0.40
1:B:156:THR:HG22	1:B:156:THR:O	2.22	0.40
1:A:296:GLU:HG2	1:A:298:PHE:CD1	2.57	0.40
1:F:260:LYS:HD2	1:F:260:LYS:C	2.42	0.40
1:C:117:PHE:HD1	1:C:117:PHE:C	2.25	0.40
1:E:39:LYS:HG2	1:E:307:GLU:HB3	2.03	0.40
1:H:83:LEU:HD11	1:H:257:ARG:HD2	2.03	0.40
1:C:87:GLN:HA	1:C:123:TYR:OH	2.21	0.40
1:E:135:ILE:HB	1:E:265:ILE:HB	2.02	0.40
1:G:201:ASP:N	1:G:205:LYS:O	2.54	0.40
1:A:140:THR:HG21	1:A:156:THR:H	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:138:THR:O	1:F:158:PRO:HD2	2.22	0.40
1:F:296:GLU:HB2	1:F:298:PHE:CD2	2.57	0.40
1:F:37:ASP:HB3	1:F:318:PHE:CZ	2.56	0.40
1:G:71:LYS:O	1:G:77:ALA:HA	2.21	0.40
1:H:91:LYS:O	1:H:95:GLU:HG2	2.21	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	344/344 (100%)	329 (96%)	11 (3%)	4 (1%)	16	29
1	B	343/344 (100%)	327 (95%)	15 (4%)	1 (0%)	46	68
1	C	343/344 (100%)	321 (94%)	18 (5%)	4 (1%)	16	29
1	D	344/344 (100%)	320 (93%)	20 (6%)	4 (1%)	16	29
1	E	342/344 (99%)	329 (96%)	10 (3%)	3 (1%)	21	37
1	F	342/344 (99%)	321 (94%)	18 (5%)	3 (1%)	21	37
1	G	343/344 (100%)	331 (96%)	10 (3%)	2 (1%)	30	50
1	H	342/344 (99%)	327 (96%)	13 (4%)	2 (1%)	30	50
All	All	2743/2752 (100%)	2605 (95%)	115 (4%)	23 (1%)	24	41

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	296	GLU
1	C	296	GLU
1	D	296	GLU
1	E	296	GLU
1	E	334	GLU

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Mol	Chain	Res	Type
1	G	296	GLU
1	A	192	ILE
1	A	202	LYS
1	C	191	LYS
1	C	192	ILE
1	E	216	GLY
1	F	190	LYS
1	G	191	LYS
1	H	296	GLU
1	D	203	ASP
1	F	296	GLU
1	H	221	PHE
1	A	296	GLU
1	D	295	ALA
1	C	157	ASN
1	D	206	PRO
1	F	182	GLY
1	A	157	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	279/268 (104%)	263 (94%)	16 (6%)	25	46
1	B	278/268 (104%)	267 (96%)	11 (4%)	38	64
1	C	278/268 (104%)	253 (91%)	25 (9%)	12	22
1	D	279/268 (104%)	262 (94%)	17 (6%)	23	42
1	E	277/268 (103%)	267 (96%)	10 (4%)	42	69
1	F	277/268 (103%)	259 (94%)	18 (6%)	21	39
1	G	278/268 (104%)	268 (96%)	10 (4%)	42	69
1	H	277/268 (103%)	264 (95%)	13 (5%)	32	56
All	All	2223/2144 (104%)	2103 (95%)	120 (5%)	27	49

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	PHE
1	A	139	ASN
1	A	140	THR
1	A	150	LYS
1	A	169[A]	LYS
1	A	169[B]	LYS
1	A	181	ARG
1	A	188	LEU
1	A	191	LYS
1	A	192	ILE
1	A	194	ILE
1	A	203	ASP
1	A	209	ASP
1	A	231	LEU
1	A	263	LEU
1	A	311	LYS
1	B	68	LYS
1	B	117	PHE
1	B	138	THR
1	B	183	LYS
1	B	185	LEU
1	B	193	LYS
1	B	214	LEU
1	B	247	LYS
1	B	263	LEU
1	B	281	LYS
1	B	289	ILE
1	C	1	MSE
1	C	6	GLU
1	C	72	GLU
1	C	102	LYS
1	C	111	THR
1	C	117	PHE
1	C	139	ASN
1	C	154	LEU
1	C	190	LYS
1	C	194	ILE
1	C	214	LEU
1	C	227	TYR
1	C	231	LEU
1	C	260	LYS
1	C	262	ASP
1	C	263	LEU

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Mol	Chain	Res	Type
1	C	268	ASN
1	C	290	LYS
1	C	293	GLU
1	C	313	LYS
1	C	321	ASP
1	C	329	LYS
1	C	330	GLU
1	C	338	ASN
1	C	344	GLU
1	D	1	MSE
1	D	2	ILE
1	D	23	GLU
1	D	99	LYS
1	D	112	ARG
1	D	117	PHE
1	D	150	LYS
1	D	185	LEU
1	D	193	LYS
1	D	208	THR
1	D	214	LEU
1	D	231	LEU
1	D	236	LEU
1	D	256	GLU
1	D	260	LYS
1	D	262	ASP
1	D	296	GLU
1	E	1	MSE
1	E	58	LEU
1	E	117	PHE
1	E	214	LEU
1	E	231	LEU
1	E	260	LYS
1	E	262	ASP
1	E	263	LEU
1	E	296	GLU
1	E	334	GLU
1	F	1	MSE
1	F	6	GLU
1	F	43	SER
1	F	48	ARG
1	F	58	LEU
1	F	71	LYS

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Mol	Chain	Res	Type
1	F	83	LEU
1	F	116	HIS
1	F	117	PHE
1	F	181	ARG
1	F	185	LEU
1	F	214	LEU
1	F	231	LEU
1	F	259	THR
1	F	260	LYS
1	F	263	LEU
1	F	316	ASP
1	F	322	LYS
1	G	117	PHE
1	G	169	LYS
1	G	185	LEU
1	G	196	GLU
1	G	214	LEU
1	G	231	LEU
1	G	260	LYS
1	G	263	LEU
1	G	293	GLU
1	G	333	ASN
1	H	9	LYS
1	H	42	THR
1	H	43	SER
1	H	117	PHE
1	H	139	ASN
1	H	140	THR
1	H	171	SER
1	H	196	GLU
1	H	215	GLU
1	H	231	LEU
1	H	260	LYS
1	H	284	GLU
1	H	344	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	166	ASN
1	A	333	ASN

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Mol	Chain	Res	Type
1	B	291	ASN
1	C	7	ASN
1	C	139	ASN
1	C	166	ASN
1	C	268	ASN
1	C	338	ASN
1	E	60	ASN
1	E	129	ASN
1	E	333	ASN
1	F	51	GLN
1	F	62	ASN
1	F	113	ASN
1	F	327	GLN
1	G	115	ASN
1	G	129	ASN
1	G	166	ASN
1	H	51	GLN
1	H	103	ASN
1	H	129	ASN
1	H	139	ASN
1	H	166	ASN
1	H	323	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

8 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	4001	-	38,48,48	1.92	8 (21%)	47,73,73	2.68	11 (23%)
2	NAD	B	4002	-	38,48,48	1.84	8 (21%)	47,73,73	2.51	10 (21%)
2	NAD	C	4003	-	38,48,48	1.85	7 (18%)	47,73,73	2.52	12 (25%)
2	NAD	D	4004	-	38,48,48	1.84	8 (21%)	47,73,73	2.53	12 (25%)
2	NAD	E	4005	-	38,48,48	1.88	7 (18%)	47,73,73	2.57	13 (27%)
2	NAD	F	4006	-	38,48,48	1.85	7 (18%)	47,73,73	2.44	9 (19%)
2	NAD	G	4007	-	38,48,48	1.80	8 (21%)	47,73,73	2.39	12 (25%)
2	NAD	H	4008	-	38,48,48	1.91	9 (23%)	47,73,73	2.54	12 (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
2	NAD	A	4001	-	-	0/22/62/62	0/5/5/5
2	NAD	B	4002	-	-	0/22/62/62	0/5/5/5
2	NAD	C	4003	-	-	0/22/62/62	0/5/5/5
2	NAD	D	4004	-	-	0/22/62/62	0/5/5/5
2	NAD	E	4005	-	-	0/22/62/62	0/5/5/5
2	NAD	F	4006	-	-	0/22/62/62	0/5/5/5
2	NAD	G	4007	-	-	0/22/62/62	0/5/5/5
2	NAD	H	4008	-	-	0/22/62/62	0/5/5/5

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4004	NAD	O4D-C4D	-3.20	1.37	1.45
2	C	4003	NAD	O4D-C4D	-3.00	1.38	1.45
2	F	4006	NAD	O4D-C4D	-2.99	1.38	1.45
2	B	4002	NAD	O4D-C4D	-2.96	1.38	1.45
2	G	4007	NAD	O4D-C4D	-2.95	1.38	1.45
2	A	4001	NAD	O4D-C4D	-2.86	1.38	1.45
2	H	4008	NAD	C2B-C3B	-2.73	1.46	1.53
2	E	4005	NAD	O4D-C4D	-2.68	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4002	NAD	C2B-C3B	-2.61	1.46	1.53
2	F	4006	NAD	O3D-C3D	-2.59	1.36	1.43
2	C	4003	NAD	C2B-C3B	-2.58	1.46	1.53
2	H	4008	NAD	O4D-C4D	-2.55	1.39	1.45
2	D	4004	NAD	O3D-C3D	-2.54	1.36	1.43
2	H	4008	NAD	O3D-C3D	-2.52	1.36	1.43
2	E	4005	NAD	O4B-C1B	-2.50	1.38	1.41
2	F	4006	NAD	C2B-C3B	-2.49	1.46	1.53
2	E	4005	NAD	C2B-C3B	-2.46	1.46	1.53
2	A	4001	NAD	O3D-C3D	-2.42	1.37	1.43
2	D	4004	NAD	C2B-C3B	-2.42	1.46	1.53
2	D	4004	NAD	C2D-C3D	-2.35	1.47	1.53
2	G	4007	NAD	C2B-C3B	-2.31	1.47	1.53
2	D	4004	NAD	O2D-C2D	-2.31	1.37	1.43
2	G	4007	NAD	O3D-C3D	-2.29	1.37	1.43
2	G	4007	NAD	C2D-C3D	-2.28	1.47	1.53
2	B	4002	NAD	O3D-C3D	-2.25	1.37	1.43
2	B	4002	NAD	O4B-C1B	-2.23	1.38	1.41
2	H	4008	NAD	O4B-C1B	-2.20	1.38	1.41
2	E	4005	NAD	O3D-C3D	-2.19	1.37	1.43
2	C	4003	NAD	O3D-C3D	-2.18	1.37	1.43
2	B	4002	NAD	O2D-C2D	-2.18	1.37	1.43
2	G	4007	NAD	O4B-C1B	-2.16	1.38	1.41
2	A	4001	NAD	C2B-C3B	-2.16	1.47	1.53
2	C	4003	NAD	O2D-C2D	-2.12	1.37	1.43
2	A	4001	NAD	O2D-C2D	-2.07	1.38	1.43
2	F	4006	NAD	O2D-C2D	-2.05	1.38	1.43
2	H	4008	NAD	O2D-C2D	-2.05	1.38	1.43
2	H	4008	NAD	O2B-C2B	-2.03	1.38	1.43
2	A	4001	NAD	O4B-C1B	-2.01	1.38	1.41
2	F	4006	NAD	C6A-N6A	2.80	1.43	1.34
2	E	4005	NAD	C6A-N6A	2.81	1.43	1.34
2	H	4008	NAD	C6A-N6A	2.86	1.43	1.34
2	G	4007	NAD	C6A-N6A	2.86	1.43	1.34
2	A	4001	NAD	C6A-N6A	2.87	1.43	1.34
2	B	4002	NAD	C6A-N6A	2.88	1.43	1.34
2	C	4003	NAD	C6A-N6A	2.88	1.43	1.34
2	D	4004	NAD	C6A-N6A	2.95	1.44	1.34
2	G	4007	NAD	O4D-C1D	5.35	1.48	1.41
2	G	4007	NAD	C7N-N7N	5.36	1.43	1.33
2	C	4003	NAD	C7N-N7N	5.39	1.43	1.33
2	D	4004	NAD	C7N-N7N	5.46	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	4006	NAD	C7N-N7N	5.46	1.44	1.33
2	H	4008	NAD	C7N-N7N	5.46	1.44	1.33
2	E	4005	NAD	C7N-N7N	5.53	1.44	1.33
2	D	4004	NAD	O4D-C1D	5.55	1.48	1.41
2	B	4002	NAD	C7N-N7N	5.58	1.44	1.33
2	A	4001	NAD	C7N-N7N	5.59	1.44	1.33
2	B	4002	NAD	O4D-C1D	5.62	1.48	1.41
2	F	4006	NAD	O4D-C1D	5.78	1.48	1.41
2	C	4003	NAD	O4D-C1D	5.96	1.48	1.41
2	E	4005	NAD	O4D-C1D	6.34	1.49	1.41
2	H	4008	NAD	O4D-C1D	6.47	1.49	1.41
2	A	4001	NAD	O4D-C1D	6.89	1.49	1.41

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4001	NAD	N3A-C2A-N1A	-9.65	121.50	128.89
2	F	4006	NAD	N3A-C2A-N1A	-9.38	121.72	128.89
2	E	4005	NAD	N3A-C2A-N1A	-9.24	121.82	128.89
2	F	4006	NAD	O3-PA-O5B	-8.94	79.23	102.94
2	C	4003	NAD	N3A-C2A-N1A	-8.90	122.08	128.89
2	A	4001	NAD	O3-PA-O5B	-8.74	79.75	102.94
2	D	4004	NAD	N3A-C2A-N1A	-8.71	122.23	128.89
2	B	4002	NAD	N3A-C2A-N1A	-8.50	122.39	128.89
2	H	4008	NAD	O3-PA-O5B	-8.40	80.65	102.94
2	D	4004	NAD	O3-PA-O5B	-8.21	81.15	102.94
2	G	4007	NAD	N3A-C2A-N1A	-8.21	122.61	128.89
2	E	4005	NAD	O3-PA-O5B	-7.97	81.79	102.94
2	G	4007	NAD	O3-PA-O5B	-7.81	82.20	102.94
2	H	4008	NAD	N3A-C2A-N1A	-7.79	122.93	128.89
2	B	4002	NAD	O3-PA-O5B	-7.68	82.57	102.94
2	C	4003	NAD	O3-PA-O5B	-6.95	84.49	102.94
2	A	4001	NAD	O2A-PA-O3	-4.92	82.76	105.09
2	C	4003	NAD	O2A-PA-O3	-4.85	83.11	105.09
2	G	4007	NAD	O2A-PA-O3	-4.77	83.46	105.09
2	C	4003	NAD	C4D-O4D-C1D	-4.74	104.51	109.72
2	H	4008	NAD	O2A-PA-O3	-4.67	83.92	105.09
2	D	4004	NAD	O2A-PA-O3	-4.66	83.96	105.09
2	E	4005	NAD	O2A-PA-O3	-4.51	84.62	105.09
2	F	4006	NAD	O2A-PA-O3	-4.45	84.89	105.09
2	B	4002	NAD	O2A-PA-O3	-4.43	85.02	105.09
2	B	4002	NAD	C4D-O4D-C1D	-3.39	106.00	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4002	NAD	C1B-N9A-C4A	-3.17	122.16	126.94
2	E	4005	NAD	C2B-C1B-N9A	-2.87	109.90	114.29
2	G	4007	NAD	O7N-C7N-N7N	-2.80	118.66	122.59
2	H	4008	NAD	O7N-C7N-N7N	-2.77	118.70	122.59
2	D	4004	NAD	O7N-C7N-N7N	-2.56	118.99	122.59
2	C	4003	NAD	C2B-C1B-N9A	-2.39	110.63	114.29
2	G	4007	NAD	C4A-C5A-N7A	-2.35	107.31	109.48
2	G	4007	NAD	C4D-O4D-C1D	-2.29	107.20	109.72
2	D	4004	NAD	C2B-C1B-N9A	-2.29	110.80	114.29
2	G	4007	NAD	C1B-N9A-C4A	-2.20	123.62	126.94
2	G	4007	NAD	C2B-C1B-N9A	-2.19	110.94	114.29
2	A	4001	NAD	PN-O3-PA	-2.18	126.62	132.73
2	E	4005	NAD	O7N-C7N-N7N	-2.16	119.55	122.59
2	E	4005	NAD	PN-O3-PA	-2.13	126.74	132.73
2	C	4003	NAD	C1B-N9A-C4A	-2.10	123.77	126.94
2	D	4004	NAD	C1B-N9A-C4A	-2.05	123.85	126.94
2	E	4005	NAD	C1B-N9A-C4A	-2.02	123.89	126.94
2	H	4008	NAD	C2B-C1B-N9A	-2.01	111.22	114.29
2	C	4003	NAD	C3N-C7N-N7N	2.02	120.03	117.82
2	D	4004	NAD	O2A-PA-O5B	2.03	118.72	108.46
2	H	4008	NAD	O2A-PA-O5B	2.05	118.80	108.46
2	C	4003	NAD	O5D-C5D-C4D	2.08	116.77	109.12
2	F	4006	NAD	O5B-C5B-C4B	2.09	116.82	109.12
2	A	4001	NAD	O5B-PA-O1A	2.10	117.75	109.62
2	H	4008	NAD	O5B-C5B-C4B	2.10	116.87	109.12
2	E	4005	NAD	O2A-PA-O5B	2.11	119.09	108.46
2	D	4004	NAD	O5B-C5B-C4B	2.13	116.95	109.12
2	D	4004	NAD	C2D-C3D-C4D	2.16	107.05	102.61
2	G	4007	NAD	O5D-C5D-C4D	2.17	117.11	109.12
2	B	4002	NAD	O4B-C1B-N9A	2.20	112.70	108.10
2	F	4006	NAD	O5D-C5D-C4D	2.21	117.28	109.12
2	F	4006	NAD	O2A-PA-O5B	2.21	119.63	108.46
2	E	4005	NAD	O5D-C5D-C4D	2.22	117.29	109.12
2	A	4001	NAD	O3-PN-O5D	2.24	108.88	102.94
2	H	4008	NAD	O3-PN-O5D	2.30	109.04	102.94
2	E	4005	NAD	C3N-C7N-N7N	2.37	120.41	117.82
2	F	4006	NAD	C2D-C3D-C4D	2.39	107.52	102.61
2	C	4003	NAD	O3-PN-O5D	2.50	109.57	102.94
2	A	4001	NAD	O2A-PA-O5B	2.52	121.19	108.46
2	B	4002	NAD	O5B-C5B-C4B	2.53	118.45	109.12
2	A	4001	NAD	O5B-C5B-C4B	2.58	118.62	109.12
2	A	4001	NAD	C3N-C7N-N7N	2.62	120.69	117.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4005	NAD	O5B-C5B-C4B	2.62	118.79	109.12
2	H	4008	NAD	C2D-C3D-C4D	2.65	108.05	102.61
2	D	4004	NAD	O4B-C1B-N9A	2.66	113.67	108.10
2	D	4004	NAD	O5B-PA-O1A	2.68	120.03	109.62
2	E	4005	NAD	O5B-PA-O1A	2.75	120.30	109.62
2	B	4002	NAD	C3N-C7N-N7N	2.77	120.84	117.82
2	H	4008	NAD	O5B-PA-O1A	2.79	120.43	109.62
2	C	4003	NAD	O5B-PA-O1A	2.83	120.61	109.62
2	G	4007	NAD	C3N-C7N-N7N	2.85	120.94	117.82
2	F	4006	NAD	O5B-PA-O1A	2.88	120.81	109.62
2	G	4007	NAD	O5B-PA-O1A	2.98	121.19	109.62
2	C	4003	NAD	O4B-C1B-N9A	3.04	114.47	108.10
2	B	4002	NAD	O5B-PA-O1A	3.06	121.50	109.62
2	A	4001	NAD	O5D-C5D-C4D	3.18	120.85	109.12
2	H	4008	NAD	C3N-C7N-N7N	3.71	121.87	117.82
2	G	4007	NAD	O4D-C1D-N1N	5.54	114.22	108.13
2	F	4006	NAD	O4D-C1D-N1N	5.81	114.51	108.13
2	C	4003	NAD	O4D-C1D-N1N	7.08	115.91	108.13
2	D	4004	NAD	O4D-C1D-N1N	7.30	116.15	108.13
2	B	4002	NAD	O4D-C1D-N1N	7.46	116.33	108.13
2	A	4001	NAD	O4D-C1D-N1N	7.96	116.88	108.13
2	E	4005	NAD	O4D-C1D-N1N	7.99	116.91	108.13
2	H	4008	NAD	O4D-C1D-N1N	8.36	117.31	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4001	NAD	1	0
2	B	4002	NAD	4	0
2	C	4003	NAD	3	0
2	E	4005	NAD	2	0
2	F	4006	NAD	1	0
2	G	4007	NAD	3	0
2	H	4008	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	335/344 (97%)	-0.13	16 (4%) 34 39	15, 30, 85, 112	0
1	B	335/344 (97%)	-0.24	7 (2%) 67 71	12, 31, 57, 87	0
1	C	335/344 (97%)	-0.09	21 (6%) 23 26	15, 33, 86, 125	0
1	D	335/344 (97%)	-0.35	2 (0%) 90 91	14, 31, 63, 89	0
1	E	335/344 (97%)	-0.24	10 (2%) 54 59	14, 35, 63, 87	0
1	F	335/344 (97%)	0.06	31 (9%) 11 11	16, 36, 81, 121	0
1	G	335/344 (97%)	-0.13	14 (4%) 40 45	16, 33, 63, 91	0
1	H	335/344 (97%)	-0.20	3 (0%) 85 88	16, 37, 67, 98	0
All	All	2680/2752 (97%)	-0.17	104 (3%) 43 48	12, 33, 71, 125	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	184	ILE	7.5
1	A	192	ILE	5.3
1	A	184	ILE	4.7
1	C	188	LEU	4.5
1	F	188	LEU	4.3
1	F	192	ILE	4.3
1	A	191	LYS	4.2
1	C	211	ALA	4.2
1	C	212	LYS	4.1
1	F	215	GLU	4.1
1	C	192	ILE	4.0
1	A	188	LEU	3.4
1	G	185	LEU	3.3
1	A	215	GLU	3.3
1	F	344	GLU	3.2
1	F	198	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	135	ILE	3.2
1	F	187	ALA	3.2
1	F	210	PRO	3.2
1	F	191	LYS	3.1
1	F	233	ILE	3.1
1	F	207	THR	3.1
1	G	191	LYS	3.1
1	C	210	PRO	3.1
1	G	188	LEU	3.1
1	C	209	ASP	3.1
1	C	189	ARG	3.0
1	A	185	LEU	3.0
1	H	344	GLU	3.0
1	A	216	GLY	3.0
1	F	135	ILE	3.0
1	F	194	ILE	3.0
1	C	187	ALA	2.9
1	A	204	GLY	2.9
1	A	189	ARG	2.9
1	E	202	LYS	2.9
1	A	183	LYS	2.9
1	C	208	THR	2.9
1	E	295	ALA	2.9
1	C	190	LYS	2.8
1	E	296	GLU	2.8
1	F	202	LYS	2.8
1	F	204	GLY	2.8
1	C	194	ILE	2.7
1	C	213	ALA	2.7
1	F	199	ALA	2.7
1	B	233	ILE	2.6
1	C	202	LYS	2.6
1	F	190	LYS	2.6
1	C	200	VAL	2.6
1	G	186	GLU	2.6
1	F	200	VAL	2.5
1	G	189	ARG	2.5
1	C	193	LYS	2.5
1	C	184	ILE	2.5
1	F	159	ILE	2.5
1	G	192	ILE	2.5
1	F	183	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	135	ILE	2.5
1	A	296	GLU	2.4
1	F	214	LEU	2.4
1	F	137	ILE	2.4
1	G	211	ALA	2.4
1	A	233	ILE	2.3
1	E	214	LEU	2.3
1	B	135	ILE	2.3
1	F	216	GLY	2.3
1	A	193	LYS	2.3
1	F	189	ARG	2.3
1	B	202	LYS	2.3
1	G	137	ILE	2.3
1	G	233	ILE	2.3
1	F	236	LEU	2.3
1	B	192	ILE	2.2
1	C	233	ILE	2.2
1	B	196	GLU	2.2
1	A	190	LYS	2.2
1	C	215	GLU	2.2
1	B	232	ALA	2.2
1	E	137	ILE	2.1
1	D	203	ASP	2.1
1	G	202	LYS	2.1
1	A	137	ILE	2.1
1	F	230	ALA	2.1
1	H	192	ILE	2.1
1	C	185	LEU	2.1
1	D	296	GLU	2.1
1	F	232	ALA	2.1
1	B	137	ILE	2.1
1	E	298	PHE	2.1
1	G	216	GLY	2.1
1	G	212	LYS	2.1
1	G	135	ILE	2.1
1	E	215	GLU	2.1
1	C	214	LEU	2.1
1	F	185	LEU	2.1
1	F	208	THR	2.1
1	E	333	ASN	2.0
1	F	257	ARG	2.0
1	H	204	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	203	ASP	2.0
1	G	182	GLY	2.0
1	F	160	ALA	2.0
1	C	201	ASP	2.0

## 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( $\text{\AA}^2$ )	Q<0.9
2	NAD	H	4008	44/44	0.96	0.14	0.16	36,50,63,276	0
2	NAD	D	4004	44/44	0.97	0.12	0.08	33,44,56,179	0
2	NAD	G	4007	44/44	0.92	0.14	-0.24	48,56,71,275	0
2	NAD	F	4006	44/44	0.95	0.12	-0.66	32,49,69,79	0
2	NAD	A	4001	44/44	0.97	0.11	-0.76	23,39,52,189	0
2	NAD	B	4002	44/44	0.96	0.12	-0.78	36,47,59,256	0
2	NAD	C	4003	44/44	0.96	0.12	-0.81	35,51,59,87	0
2	NAD	E	4005	44/44	0.96	0.11	-1.06	34,50,54,275	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.