



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:11 PM GMT

PDB ID : 1NTO  
Title : N249Y MUTANT OF ALCOHOL DEHYDROGENASE FROM THE ARCHAEON SULFOLOBUS SOLFATARICUS-MONOCLINIC CRYSTAL FORM  
Authors : Esposito, L.; Bruno, I.; Sica, F.; Raia, C.A.; Giordano, A.; Rossi, M.; Mazarella, L.; Zagari, A.  
Deposited on : 2003-01-30  
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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

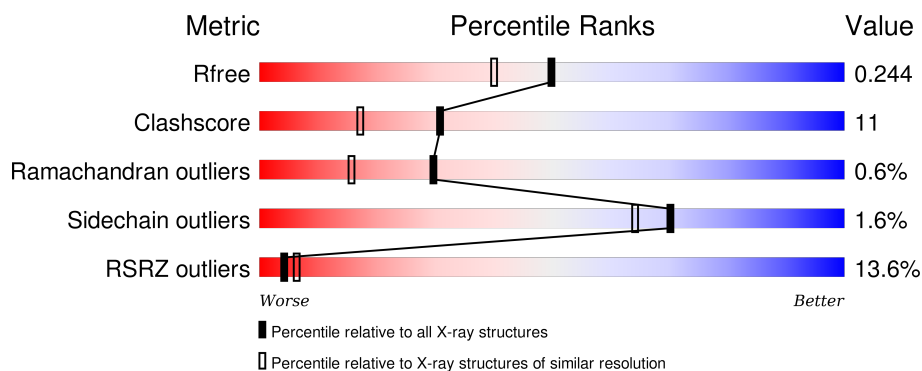
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.94 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))
$R_{free}$	91344	2910 (1.96-1.92)
Clashscore	102246	3095 (1.96-1.92)
Ramachandran outliers	100387	3062 (1.96-1.92)
Sidechain outliers	100360	3062 (1.96-1.92)
RSRZ outliers	91569	2915 (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	347	<div> <div>7%</div> <div>80%</div> <div>19%</div> <div>.</div> </div>
1	B	347	<div> <div>19%</div> <div>78%</div> <div>22%</div> <div>.</div> </div>
1	C	347	<div> <div>16%</div> <div>82%</div> <div>18%</div> </div>
1	D	347	<div> <div>11%</div> <div>80%</div> <div>19%</div> <div>.</div> </div>
1	E	347	<div> <div>13%</div> <div>79%</div> <div>20%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	H	347	<div><div></div><div>16%</div><div></div><div>80%</div><div></div><div>20%</div><div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16354 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 NAD-dependent alcohol dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2620	1666	454	486	14			
1	B	347	Total	C	N	O	S	0	0	0
			2604	1656	448	486	14			
1	C	347	Total	C	N	O	S	0	0	0
			2617	1665	450	488	14			
1	D	347	Total	C	N	O	S	0	0	0
			2620	1668	452	486	14			
1	E	347	Total	C	N	O	S	0	0	0
			2628	1671	455	488	14			
1	H	347	Total	C	N	O	S	0	0	0
			2620	1667	451	488	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	249	TYR	ASN	ENGINEERED	UNP P39462
B	249	TYR	ASN	ENGINEERED	UNP P39462
C	249	TYR	ASN	ENGINEERED	UNP P39462
D	249	TYR	ASN	ENGINEERED	UNP P39462
E	249	TYR	ASN	ENGINEERED	UNP P39462
H	249	TYR	ASN	ENGINEERED	UNP P39462

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Zn	0	0
			2	2		
2	E	2	Total	Zn	0	0
			2	2		
2	H	2	Total	Zn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	Zn 2	0	0
2	C	2	Total 2	Zn 2	0	0
2	A	2	Total 2	Zn 2	0	0

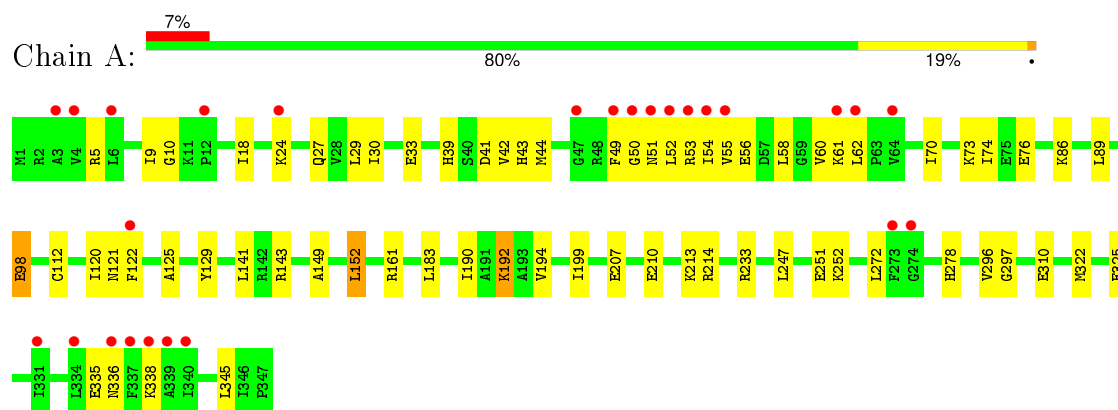
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	142	Total 142	O 142	0	0
3	B	83	Total 83	O 83	0	0
3	C	92	Total 92	O 92	0	0
3	D	138	Total 138	O 138	0	0
3	E	101	Total 101	O 101	0	0
3	H	77	Total 77	O 77	0	0

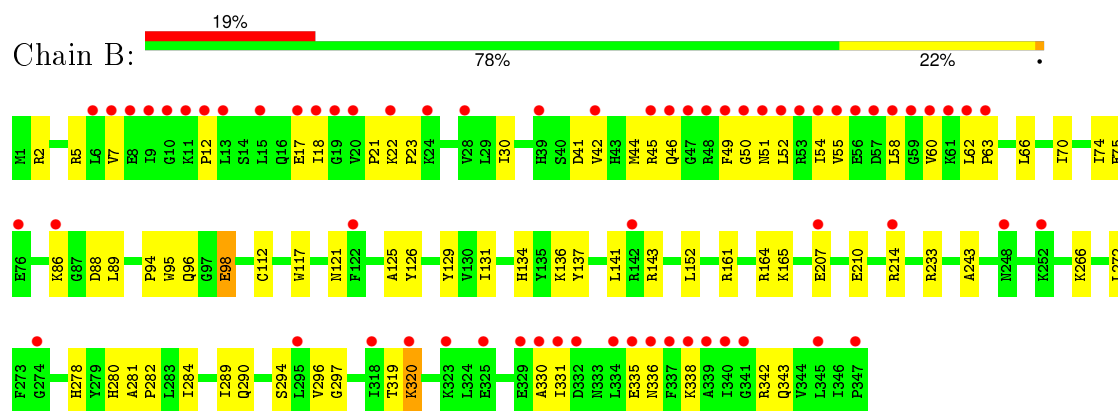
### 3 Residue-property plots [i](#)

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.

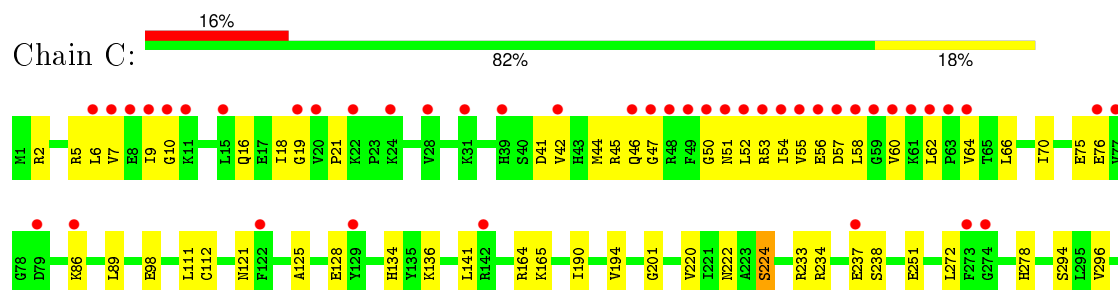
#### • Molecule 1: NAD-dependent alcohol dehydrogenase

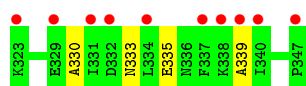


#### • Molecule 1: NAD-dependent alcohol dehydrogenase



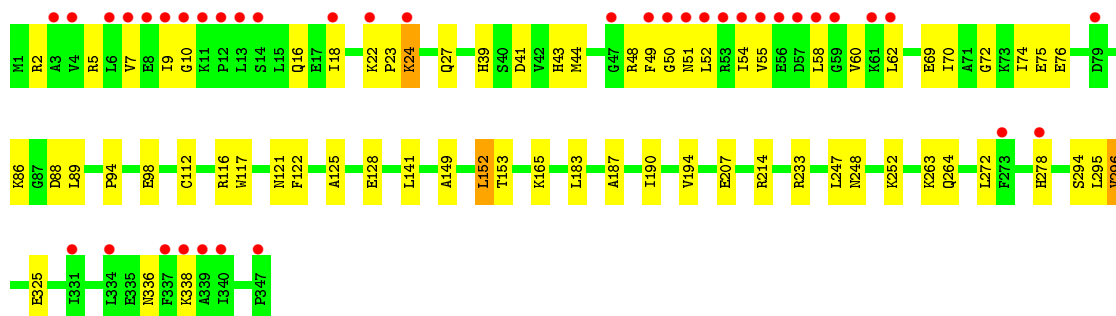
#### • Molecule 1: NAD-dependent alcohol dehydrogenase





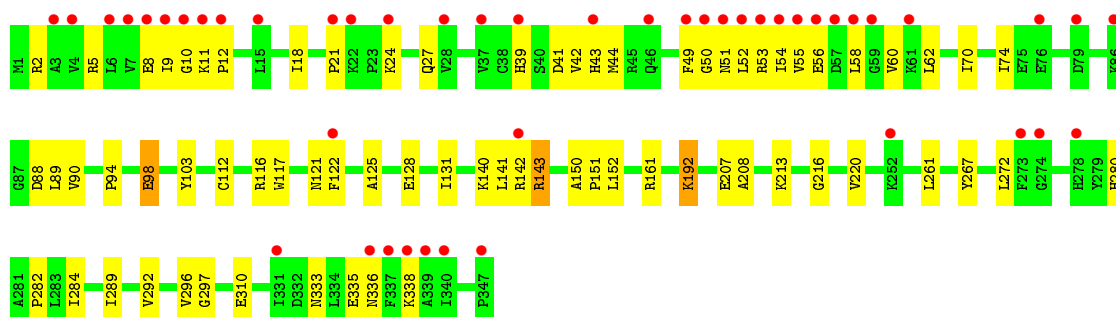
- Molecule 1: NAD-dependent alcohol dehydrogenase

Chain D: 11% 80% 19%



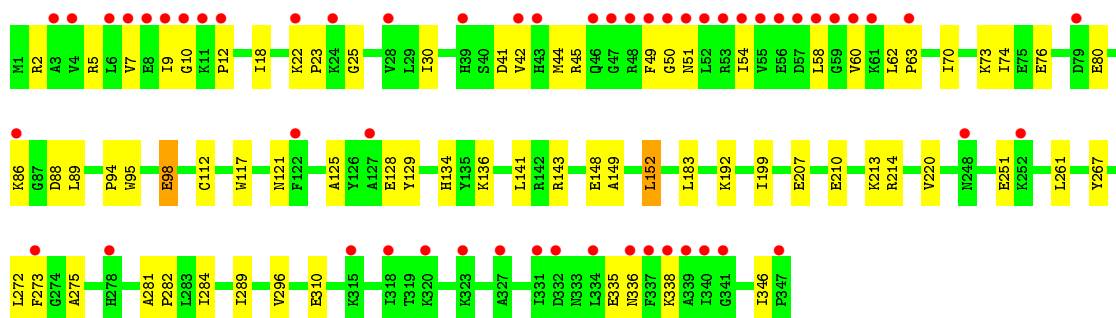
- Molecule 1: NAD-dependent alcohol dehydrogenase

Chain E: 13% 79% 20%



- Molecule 1: NAD-dependent alcohol dehydrogenase

Chain H: 16% 80% 20%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	215.33Å 91.59Å 118.24Å 90.00° 99.20° 90.00°	Depositor
Resolution (Å)	15.00 – 1.94 14.98 – 1.94	Depositor EDS
% Data completeness (in resolution range)	86.9 (15.00-1.94) 87.0 (14.98-1.94)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.52 (at 1.94Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.210 , 0.244 0.210 , 0.244	Depositor DCC
$R_{free}$ test set	7341 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.5	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.46 , 65.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 146709 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	16354	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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: ZN

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	0.51	0/2665	0.68	0/3606
1	B	0.44	0/2648	0.64	0/3585
1	C	0.46	0/2662	0.68	0/3604
1	D	0.51	0/2665	0.67	0/3605
1	E	0.45	0/2673	0.65	0/3615
1	H	0.44	0/2665	0.64	0/3606
All	All	0.47	0/15978	0.66	0/21621

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	103	TYR	Sidechain

### 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	2620	0	2670	55	0
1	B	2604	0	2645	68	0
1	C	2617	0	2657	60	0
1	D	2620	0	2674	65	0
1	E	2628	0	2685	56	0
1	H	2620	0	2667	51	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	H	2	0	0	0	0
3	A	142	0	0	4	0
3	B	83	0	0	2	0
3	C	92	0	0	2	0
3	D	138	0	0	1	0
3	E	101	0	0	1	0
3	H	77	0	0	1	0
All	All	16354	0	15998	344	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 11.

All (344) 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:8:GLU:HB3	1:E:11:LYS:HE2	1.51	0.93
1:B:42:VAL:HG13	1:B:335:GLU:HG2	1.55	0.88
1:D:54:ILE:HB	1:D:60:VAL:HG21	1.58	0.86
1:E:192:LYS:HE3	1:E:216:GLY:O	1.78	0.84
1:B:54:ILE:HB	1:B:60:VAL:HG21	1.58	0.83
1:C:54:ILE:HB	1:C:60:VAL:HG21	1.59	0.83
1:C:60:VAL:HG12	1:C:62:LEU:HD12	1.62	0.81
1:B:60:VAL:HG12	1:B:62:LEU:HD12	1.62	0.81
1:H:60:VAL:HG12	1:H:62:LEU:HD12	1.61	0.81
1:H:2:ARG:HG3	1:H:128:GLU:OE2	1.80	0.81
1:A:54:ILE:HB	1:A:60:VAL:HG21	1.62	0.80
1:E:338:LYS:HB2	1:E:338:LYS:HZ2	1.46	0.79
1:H:54:ILE:HB	1:H:60:VAL:HG21	1.63	0.79
1:A:76:GLU:OE1	1:A:86:LYS:HE2	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:ASN:HD22	1:A:338:LYS:HE3	1.50	0.76
1:C:222:ASN:OD1	1:C:224:SER:HB2	1.86	0.76
1:H:76:GLU:OE1	1:H:86:LYS:HE2	1.86	0.75
1:A:60:VAL:HG22	1:A:121:ASN:HA	1.66	0.75
1:E:11:LYS:HG3	1:E:12:PRO:HD2	1.70	0.73
1:D:60:VAL:HG12	1:D:62:LEU:HD12	1.70	0.73
1:D:60:VAL:HG22	1:D:121:ASN:HA	1.71	0.73
1:E:336:ASN:HD22	1:E:338:LYS:HE3	1.54	0.72
1:E:5:ARG:HH11	1:E:18:ILE:HG21	1.55	0.72
1:E:143:ARG:HD2	1:E:310:GLU:O	1.89	0.72
1:H:338:LYS:HZ2	1:H:338:LYS:HB2	1.52	0.72
1:A:336:ASN:HB2	1:A:338:LYS:HE3	1.73	0.71
1:A:60:VAL:HG12	1:A:62:LEU:HD12	1.72	0.71
1:B:338:LYS:HZ2	1:B:338:LYS:HB2	1.56	0.70
1:E:70:ILE:HG12	1:E:125:ALA:HB2	1.74	0.70
1:C:98:GLU:HG3	1:C:112:CYS:SG	2.32	0.69
1:D:338:LYS:HB2	1:D:338:LYS:NZ	2.06	0.69
1:C:278:HIS:CE1	1:D:278:HIS:CE1	2.81	0.69
1:D:278:HIS:NE2	1:H:73:LYS:HE2	2.08	0.68
1:A:33:GLU:OE2	1:A:73:LYS:HG3	1.94	0.68
1:A:5:ARG:HH11	1:A:18:ILE:HG21	1.59	0.68
1:B:50:GLY:CA	1:B:272:LEU:HD13	2.23	0.67
1:B:42:VAL:CG1	1:B:335:GLU:HG2	2.23	0.67
1:H:44:MET:HE1	1:H:54:ILE:HG21	1.76	0.67
1:D:54:ILE:HB	1:D:60:VAL:CG2	2.26	0.66
1:C:70:ILE:HG12	1:C:125:ALA:HB2	1.77	0.66
1:H:338:LYS:NZ	1:H:338:LYS:HB2	2.11	0.66
1:B:207:GLU:CD	1:B:207:GLU:H	1.97	0.66
1:A:41:ASP:HA	1:A:44:MET:HB2	1.78	0.65
1:C:5:ARG:HH11	1:C:18:ILE:HG21	1.61	0.65
1:C:54:ILE:HB	1:C:60:VAL:CG2	2.28	0.64
1:C:278:HIS:CE1	1:D:278:HIS:HE1	2.14	0.64
1:A:143:ARG:HD2	1:A:310:GLU:O	1.98	0.64
1:H:42:VAL:HG13	1:H:335:GLU:HG2	1.78	0.63
1:A:5:ARG:NH1	1:A:18:ILE:HG21	2.14	0.63
1:D:295:LEU:HG	1:D:296:VAL:HG13	1.81	0.63
1:E:41:ASP:HA	1:E:44:MET:HB2	1.81	0.62
1:B:319:THR:HG22	1:B:342:ARG:HB3	1.80	0.62
1:H:54:ILE:HB	1:H:60:VAL:CG2	2.28	0.62
1:B:134:HIS:ND1	1:B:136:LYS:HG2	2.15	0.62
1:H:210:GLU:HG3	1:H:214:ARG:NH1	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:LEU:HG	1:B:141:LEU:HD12	1.82	0.62
1:B:54:ILE:HB	1:B:60:VAL:CG2	2.27	0.61
1:D:278:HIS:HE2	1:H:73:LYS:HE2	1.64	0.61
1:C:5:ARG:NH1	1:C:18:ILE:HG21	2.14	0.61
1:E:336:ASN:HD22	1:E:338:LYS:CE	2.13	0.61
1:B:58:LEU:HD12	1:B:58:LEU:N	2.14	0.61
1:C:58:LEU:N	1:C:58:LEU:HD12	2.15	0.61
1:A:50:GLY:CA	1:A:272:LEU:HD13	2.30	0.61
1:H:336:ASN:HD22	1:H:338:LYS:HE3	1.66	0.60
1:C:42:VAL:HG13	1:C:335:GLU:HG2	1.82	0.60
1:H:284:ILE:HA	1:H:289:ILE:HG12	1.82	0.60
1:B:62:LEU:N	1:B:62:LEU:HD12	2.16	0.60
1:H:143:ARG:HD2	1:H:310:GLU:O	2.02	0.60
1:E:336:ASN:HB2	1:E:338:LYS:HE3	1.83	0.60
1:B:74:ILE:HD12	1:B:88:ASP:HB2	1.84	0.60
1:E:338:LYS:NZ	1:E:338:LYS:HB2	2.14	0.59
1:E:5:ARG:NH1	1:E:18:ILE:HG21	2.17	0.59
1:A:336:ASN:O	1:A:338:LYS:HG3	2.03	0.59
1:H:49:PHE:CE2	1:H:117:TRP:HZ3	2.20	0.59
1:H:273:PHE:CE2	1:H:275:ALA:HB2	2.38	0.59
1:D:70:ILE:HG12	1:D:125:ALA:HB2	1.84	0.59
1:A:70:ILE:HG12	1:A:125:ALA:HB2	1.85	0.58
1:H:41:ASP:HA	1:H:44:MET:HB3	1.85	0.58
1:A:54:ILE:HB	1:A:60:VAL:CG2	2.31	0.58
1:B:5:ARG:HH11	1:B:18:ILE:HD13	1.68	0.58
1:A:89:LEU:HG	1:A:141:LEU:HD12	1.84	0.58
1:B:60:VAL:HG22	1:B:121:ASN:HA	1.84	0.58
1:B:49:PHE:CE2	1:B:117:TRP:HZ3	2.22	0.58
1:C:330:ALA:HA	1:C:333:ASN:HD22	1.69	0.58
1:H:60:VAL:HG22	1:H:121:ASN:HA	1.86	0.58
1:B:60:VAL:HG12	1:B:62:LEU:CD1	2.34	0.58
1:B:98:GLU:HG3	1:B:112:CYS:SG	2.44	0.58
1:B:50:GLY:HA3	1:B:272:LEU:HD13	1.86	0.57
1:B:210:GLU:HG3	1:B:214:ARG:HH11	1.67	0.57
1:C:60:VAL:HG22	1:C:121:ASN:HA	1.86	0.57
1:B:336:ASN:HB2	1:B:338:LYS:HE3	1.86	0.57
1:H:98:GLU:HG3	1:H:112:CYS:SG	2.45	0.57
1:D:338:LYS:HB2	1:D:338:LYS:HZ2	1.67	0.57
1:C:233:ARG:HG2	3:C:564:HOH:O	2.04	0.57
1:A:207:GLU:H	1:A:207:GLU:CD	2.08	0.57
1:H:42:VAL:CG1	1:H:335:GLU:HG2	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:ARG:HG2	3:C:552:HOH:O	2.04	0.56
1:C:53:ARG:HB2	1:C:56:GLU:HB2	1.85	0.56
1:C:278:HIS:HE1	1:D:278:HIS:HE1	1.52	0.56
1:C:134:HIS:ND1	1:C:136:LYS:HG2	2.20	0.56
1:D:2:ARG:HG3	1:D:128:GLU:OE2	2.06	0.56
1:E:8:GLU:HB3	1:E:11:LYS:CE	2.31	0.56
1:A:5:ARG:NH1	1:A:18:ILE:HD13	2.19	0.56
1:D:22:LYS:HD2	1:D:23:PRO:HD2	1.87	0.55
1:H:281:ALA:HB3	1:H:282:PRO:HD3	1.89	0.55
1:D:50:GLY:CA	1:D:272:LEU:HD13	2.37	0.55
1:D:24:LYS:HD3	1:D:27:GLN:OE1	2.07	0.55
1:B:52:LEU:HD12	1:B:52:LEU:N	2.22	0.54
1:A:247:LEU:HD12	1:A:247:LEU:H	1.73	0.54
1:H:89:LEU:HG	1:H:141:LEU:HD12	1.89	0.54
1:E:2:ARG:HG3	1:E:128:GLU:OE2	2.07	0.54
1:H:12:PRO:HA	1:H:45:ARG:HD2	1.89	0.54
1:B:22:LYS:HD2	1:B:23:PRO:HD2	1.90	0.54
1:B:207:GLU:N	1:B:207:GLU:CD	2.62	0.54
1:D:50:GLY:HA2	1:D:272:LEU:HB3	1.90	0.54
1:C:76:GLU:OE1	1:C:86:LYS:HE2	2.08	0.53
1:D:55:VAL:HG22	1:D:62:LEU:HD11	1.90	0.53
1:C:57:ASP:HB2	1:C:58:LEU:HD12	1.90	0.53
1:E:55:VAL:HA	1:E:60:VAL:HG12	1.90	0.53
1:A:42:VAL:HG13	1:A:335:GLU:HG2	1.90	0.53
1:D:336:ASN:HB2	1:D:338:LYS:HE3	1.90	0.53
1:H:149:ALA:O	1:H:152:LEU:HB2	2.09	0.53
1:H:207:GLU:CD	1:H:207:GLU:H	2.11	0.52
1:B:336:ASN:HD22	1:B:338:LYS:HE3	1.74	0.52
1:E:58:LEU:HD12	1:E:58:LEU:N	2.24	0.52
1:E:208:ALA:HA	3:E:565:HOH:O	2.09	0.52
1:D:98:GLU:HG3	1:D:112:CYS:SG	2.49	0.52
1:H:336:ASN:HB2	1:H:338:LYS:HG3	1.91	0.52
1:B:55:VAL:HG22	1:B:62:LEU:HD11	1.91	0.52
1:E:336:ASN:HB2	1:E:338:LYS:HG3	1.91	0.52
1:E:39:HIS:NE2	1:E:43:HIS:NE2	2.56	0.52
1:D:336:ASN:CB	1:D:338:LYS:HE3	2.39	0.52
1:E:98:GLU:HG3	1:E:112:CYS:SG	2.49	0.52
1:A:336:ASN:ND2	1:A:338:LYS:HE3	2.23	0.52
1:C:42:VAL:CG1	1:C:335:GLU:HG2	2.40	0.52
1:E:50:GLY:HA3	1:E:272:LEU:HD22	1.90	0.52
1:D:62:LEU:N	1:D:62:LEU:HD12	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:MET:C	1:B:46:GLN:H	2.13	0.52
1:H:134:HIS:ND1	1:H:136:LYS:HG2	2.25	0.51
1:H:22:LYS:HD2	1:H:23:PRO:HD2	1.93	0.51
1:D:183:LEU:HD22	1:D:248:ASN:ND2	2.26	0.51
1:H:44:MET:CE	1:H:54:ILE:HG21	2.41	0.51
1:C:53:ARG:HB3	1:C:56:GLU:OE1	2.11	0.51
1:H:338:LYS:NZ	1:H:338:LYS:CB	2.74	0.51
1:H:50:GLY:HA3	1:H:272:LEU:HD22	1.93	0.51
1:A:98:GLU:HG3	1:A:112:CYS:SG	2.51	0.50
1:D:75:GLU:O	1:D:86:LYS:HG3	2.12	0.50
1:A:30:ILE:HD13	1:A:74:ILE:HA	1.93	0.50
1:H:70:ILE:HG12	1:H:125:ALA:HB2	1.92	0.50
1:E:74:ILE:HD12	1:E:88:ASP:HB2	1.92	0.50
1:B:70:ILE:HG12	1:B:125:ALA:HB2	1.93	0.50
1:A:251:GLU:HG3	3:A:603:HOH:O	2.11	0.50
1:C:7:VAL:HG22	1:C:16:GLN:NE2	2.27	0.50
1:C:60:VAL:CG2	1:C:121:ASN:HA	2.41	0.50
1:C:41:ASP:HA	1:C:44:MET:HB2	1.94	0.50
1:H:25:GLY:C	1:H:80:GLU:HB2	2.31	0.50
1:A:336:ASN:HB2	1:A:338:LYS:HG3	1.93	0.50
1:H:58:LEU:N	1:H:58:LEU:HD12	2.27	0.50
1:B:75:GLU:O	1:B:86:LYS:HG3	2.12	0.50
1:D:207:GLU:CD	1:D:207:GLU:H	2.15	0.49
1:D:55:VAL:HG22	1:D:62:LEU:CD1	2.42	0.49
1:D:41:ASP:HA	1:D:44:MET:HB2	1.93	0.49
1:B:62:LEU:H	1:B:62:LEU:HD12	1.76	0.49
1:A:44:MET:SD	1:A:54:ILE:HG21	2.51	0.49
1:C:278:HIS:HE1	1:D:278:HIS:CE1	2.27	0.49
1:H:346:ILE:HD13	3:H:571:HOH:O	2.13	0.49
1:B:165:LYS:HD2	1:B:294:SER:HB2	1.94	0.49
1:A:39:HIS:NE2	1:A:43:HIS:NE2	2.61	0.49
1:C:6:LEU:HB2	1:C:66:LEU:HD11	1.95	0.49
1:B:336:ASN:O	1:B:338:LYS:HG3	2.12	0.49
1:B:210:GLU:HG3	1:B:214:ARG:NH1	2.26	0.49
1:B:41:ASP:HA	1:B:44:MET:HB2	1.95	0.49
1:H:192:LYS:HE3	1:H:199:ILE:HD12	1.94	0.49
1:B:66:LEU:HB2	1:B:126:TYR:CD2	2.47	0.49
1:C:52:LEU:N	1:C:52:LEU:HD12	2.28	0.49
1:D:44:MET:SD	1:D:54:ILE:HG21	2.52	0.49
1:C:89:LEU:HG	1:C:141:LEU:HD12	1.95	0.49
1:E:207:GLU:H	1:E:207:GLU:CD	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:90:VAL:HG12	1:E:140:LYS:HA	1.96	0.48
1:D:74:ILE:HD12	1:D:88:ASP:HB2	1.94	0.48
1:B:336:ASN:HB2	1:B:338:LYS:HG3	1.95	0.48
1:C:75:GLU:O	1:C:86:LYS:HG3	2.14	0.48
1:C:54:ILE:HA	1:C:58:LEU:HB2	1.95	0.48
1:E:60:VAL:HG13	1:E:62:LEU:HD12	1.94	0.48
1:A:53:ARG:NH1	1:A:56:GLU:HG2	2.29	0.48
1:D:5:ARG:NH1	1:D:18:ILE:HG21	2.28	0.48
1:E:24:LYS:HG2	1:E:27:GLN:OE1	2.14	0.48
1:D:52:LEU:HD12	1:D:52:LEU:N	2.28	0.48
1:B:42:VAL:HG13	1:B:335:GLU:CG	2.36	0.48
1:C:44:MET:C	1:C:46:GLN:H	2.17	0.48
1:E:52:LEU:HD12	1:E:52:LEU:N	2.29	0.48
1:A:149:ALA:O	1:A:152:LEU:HB2	2.14	0.48
1:B:281:ALA:HB3	1:B:282:PRO:HD3	1.96	0.47
1:B:17:GLU:O	1:B:17:GLU:HG3	2.14	0.47
1:H:94:PRO:HG2	1:H:95:TRP:CE2	2.49	0.47
1:B:62:LEU:CD1	1:B:62:LEU:H	2.25	0.47
1:C:60:VAL:HG12	1:C:62:LEU:CD1	2.38	0.47
1:A:58:LEU:HD12	1:A:58:LEU:N	2.29	0.47
1:C:165:LYS:HD2	1:C:294:SER:HB2	1.95	0.47
1:A:322:MET:O	1:A:345:LEU:HA	2.14	0.47
1:E:161:ARG:HD2	1:E:297:GLY:HA2	1.96	0.47
1:B:284:ILE:HA	1:B:289:ILE:HG12	1.95	0.47
1:E:333:ASN:OD1	1:E:338:LYS:NZ	2.46	0.47
1:D:76:GLU:OE1	1:D:86:LYS:HE2	2.15	0.47
1:E:336:ASN:O	1:E:338:LYS:HG3	2.15	0.47
1:B:319:THR:CG2	1:B:342:ARG:HB3	2.45	0.47
1:H:273:PHE:CD2	1:H:275:ALA:HB2	2.50	0.47
1:D:39:HIS:NE2	1:D:43:HIS:NE2	2.63	0.47
1:D:214:ARG:HB3	3:D:624:HOH:O	2.14	0.47
1:H:60:VAL:CG1	1:H:62:LEU:HD12	2.40	0.47
1:D:9:ILE:HG22	1:D:10:GLY:N	2.29	0.47
1:A:52:LEU:N	1:A:52:LEU:HD12	2.30	0.47
1:C:45:ARG:NH2	1:C:335:GLU:OE2	2.39	0.46
1:B:44:MET:C	1:B:46:GLN:N	2.68	0.46
1:C:234:ARG:HH11	1:C:234:ARG:HG2	1.80	0.46
1:B:45:ARG:NH2	1:B:331:ILE:HG22	2.29	0.46
1:B:320:LYS:NZ	1:B:320:LYS:HB3	2.30	0.46
1:D:7:VAL:HG21	1:D:16:GLN:HE21	1.79	0.46
1:E:60:VAL:HG23	1:E:121:ASN:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:GLY:O	1:C:21:PRO:HD3	2.15	0.46
1:D:58:LEU:HD12	1:D:58:LEU:N	2.31	0.46
1:C:2:ARG:HG3	1:C:128:GLU:OE2	2.16	0.46
1:C:44:MET:C	1:C:46:GLN:N	2.69	0.46
1:E:70:ILE:HG12	1:E:125:ALA:CB	2.44	0.46
1:E:49:PHE:CE2	1:E:117:TRP:HZ3	2.33	0.46
1:H:261:LEU:HD11	1:H:267:TYR:HB2	1.98	0.46
1:C:50:GLY:HA2	1:C:272:LEU:HB3	1.98	0.46
1:A:24:LYS:HG2	1:A:27:GLN:OE1	2.16	0.46
1:A:190:ILE:O	1:A:194:VAL:HG22	2.15	0.45
1:E:53:ARG:NH1	1:E:56:GLU:HG2	2.32	0.45
1:B:12:PRO:HA	1:B:45:ARG:HD2	1.98	0.45
1:B:55:VAL:HG22	1:B:62:LEU:CD1	2.46	0.45
1:E:2:ARG:HG3	1:E:2:ARG:HH11	1.80	0.45
1:D:121:ASN:OD1	1:D:122:PHE:HD1	1.98	0.45
1:D:116:ARG:HA	1:D:122:PHE:CE1	2.51	0.45
1:D:49:PHE:CE2	1:D:117:TRP:HZ3	2.34	0.45
1:D:48:ARG:HA	1:D:52:LEU:O	2.17	0.45
1:D:72:GLY:O	1:D:89:LEU:HD12	2.17	0.45
1:H:5:ARG:NH1	1:H:18:ILE:HD13	2.31	0.45
1:E:150:ALA:HB3	1:E:151:PRO:HD3	1.98	0.45
1:B:280:HIS:CD2	1:B:282:PRO:HD2	2.51	0.45
1:H:30:ILE:O	1:H:129:TYR:HA	2.17	0.45
1:D:60:VAL:CG2	1:D:121:ASN:HA	2.45	0.45
1:B:62:LEU:CD1	1:B:62:LEU:N	2.79	0.45
1:C:54:ILE:HA	1:C:58:LEU:HD13	1.98	0.45
1:B:2:ARG:HH11	1:B:2:ARG:HG3	1.81	0.45
1:B:54:ILE:O	1:B:60:VAL:N	2.44	0.45
1:D:2:ARG:HH11	1:D:2:ARG:HG3	1.81	0.45
1:C:234:ARG:NH1	1:C:234:ARG:HG2	2.32	0.45
1:D:165:LYS:HD2	1:D:294:SER:HB2	1.99	0.44
1:E:11:LYS:HG3	1:E:12:PRO:CD	2.45	0.44
1:C:64:VAL:O	1:C:64:VAL:HG13	2.16	0.44
1:A:336:ASN:CB	1:A:338:LYS:HE3	2.46	0.44
1:E:89:LEU:HG	1:E:141:LEU:HD12	1.99	0.44
1:A:55:VAL:HG23	3:A:611:HOH:O	2.18	0.44
1:H:213:LYS:HG3	1:H:220:VAL:HG11	1.99	0.44
1:B:58:LEU:N	1:B:58:LEU:CD1	2.80	0.44
1:A:50:GLY:HA2	1:A:272:LEU:HD13	1.99	0.44
1:B:164:ARG:NE	3:B:516:HOH:O	2.50	0.44
1:A:233:ARG:HA	1:A:233:ARG:HD3	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:LYS:HE3	1:A:199:ILE:HD12	1.99	0.44
1:C:9:ILE:HG22	1:C:10:GLY:N	2.33	0.44
1:D:252:LYS:NZ	1:H:148:GLU:OE1	2.51	0.44
1:E:336:ASN:HB2	1:E:338:LYS:CD	2.48	0.44
1:D:183:LEU:HD22	1:D:248:ASN:HD21	1.81	0.44
1:E:5:ARG:NH1	1:E:18:ILE:HD13	2.31	0.44
1:B:319:THR:HG22	1:B:342:ARG:O	2.18	0.44
1:B:330:ALA:HA	1:B:343:GLN:OE1	2.17	0.44
1:A:161:ARG:HD2	1:A:297:GLY:HA2	1.99	0.43
1:D:5:ARG:HH11	1:D:18:ILE:HG21	1.82	0.43
1:E:336:ASN:HB2	1:E:338:LYS:CE	2.47	0.43
1:H:7:VAL:HG22	1:H:63:PRO:HB3	2.00	0.43
1:E:213:LYS:HG3	1:E:220:VAL:HG11	2.00	0.43
1:E:42:VAL:HG13	1:E:335:GLU:HG2	2.00	0.43
1:H:74:ILE:HD12	1:H:88:ASP:HB2	2.00	0.43
1:B:320:LYS:HZ2	1:B:320:LYS:HB3	1.83	0.43
1:A:278:HIS:ND1	1:B:278:HIS:ND1	2.56	0.43
1:H:9:ILE:HG22	1:H:10:GLY:N	2.34	0.43
1:A:42:VAL:CG1	1:A:335:GLU:HG2	2.48	0.43
1:C:111:LEU:HD13	1:D:264:GLN:HG3	2.00	0.43
1:E:21:PRO:HB2	1:E:131:ILE:CG1	2.49	0.43
1:A:60:VAL:CG1	1:A:62:LEU:HD12	2.47	0.43
1:A:149:ALA:HA	1:A:152:LEU:HD22	2.00	0.43
1:D:69:GLU:HA	1:D:153:THR:OG1	2.18	0.43
1:C:58:LEU:N	1:C:58:LEU:CD1	2.82	0.42
1:C:42:VAL:HG13	1:C:335:GLU:CG	2.48	0.42
1:C:57:ASP:CB	1:C:58:LEU:HD12	2.49	0.42
1:H:336:ASN:HB2	1:H:338:LYS:HE3	2.00	0.42
1:C:278:HIS:ND1	1:D:278:HIS:CE1	2.88	0.42
1:H:5:ARG:HH11	1:H:18:ILE:HG21	1.84	0.42
1:B:161:ARG:HD2	1:B:297:GLY:HA2	2.01	0.42
1:E:116:ARG:HG2	1:E:122:PHE:CZ	2.54	0.42
1:A:338:LYS:HB2	1:A:338:LYS:HZ2	1.84	0.42
1:C:333:ASN:HB3	1:C:339:ALA:HB2	2.00	0.42
1:E:280:HIS:CD2	1:E:282:PRO:HD2	2.53	0.42
1:B:54:ILE:HD12	1:B:60:VAL:HG11	2.02	0.42
1:C:7:VAL:CG2	1:C:16:GLN:NE2	2.82	0.42
1:C:52:LEU:H	1:C:52:LEU:HD12	1.84	0.42
1:D:187:ALA:HB2	1:D:247:LEU:HD11	2.02	0.42
1:A:9:ILE:HG22	1:A:10:GLY:N	2.34	0.42
1:B:60:VAL:CG2	1:B:121:ASN:HA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LYS:HG3	3:A:601:HOH:O	2.19	0.42
1:C:54:ILE:O	1:C:60:VAL:N	2.52	0.41
1:E:50:GLY:HA2	1:E:272:LEU:HB3	2.01	0.41
1:A:210:GLU:OE2	1:A:213:LYS:HE2	2.20	0.41
1:B:96:GLN:HG2	1:B:137:TYR:CD1	2.56	0.41
1:A:338:LYS:NZ	1:A:338:LYS:CB	2.83	0.41
1:E:44:MET:SD	1:E:54:ILE:HG21	2.60	0.41
1:E:54:ILE:HA	1:E:58:LEU:HB2	2.02	0.41
1:D:89:LEU:HG	1:D:141:LEU:HD12	2.02	0.41
1:B:21:PRO:HB2	1:B:131:ILE:CG1	2.50	0.41
1:B:7:VAL:HG22	1:B:63:PRO:HB3	2.01	0.41
1:E:261:LEU:HD11	1:E:267:TYR:HB2	2.01	0.41
1:A:29:LEU:HD11	1:A:129:TYR:HB3	2.02	0.41
1:C:62:LEU:HD12	1:C:62:LEU:N	2.35	0.41
1:D:338:LYS:NZ	1:D:338:LYS:CB	2.81	0.41
1:D:263:LYS:O	1:D:264:GLN:HB2	2.20	0.41
1:D:325:GLU:CD	1:D:325:GLU:H	2.24	0.41
1:D:60:VAL:HG12	1:D:62:LEU:CD1	2.45	0.41
1:E:9:ILE:HG22	1:E:10:GLY:N	2.35	0.41
1:A:325:GLU:CD	1:A:325:GLU:H	2.23	0.41
1:C:201:GLY:O	1:C:220:VAL:HA	2.21	0.41
1:C:54:ILE:C	1:C:60:VAL:HB	2.41	0.41
1:C:55:VAL:HG22	1:C:62:LEU:CD1	2.51	0.41
1:A:121:ASN:OD1	1:A:122:PHE:HD1	2.04	0.41
1:E:55:VAL:CA	1:E:60:VAL:HG12	2.50	0.41
1:C:190:ILE:O	1:C:194:VAL:HG22	2.21	0.41
1:D:278:HIS:CE1	1:H:73:LYS:HE2	2.56	0.41
1:A:214:ARG:NH1	3:A:535:HOH:O	2.35	0.41
1:A:49:PHE:CE1	1:A:120:ILE:HD13	2.56	0.41
1:B:243:ALA:HA	1:B:266:LYS:O	2.21	0.41
1:D:149:ALA:O	1:D:152:LEU:HB2	2.21	0.41
1:E:54:ILE:O	1:E:60:VAL:N	2.49	0.41
1:B:30:ILE:O	1:B:129:TYR:HA	2.21	0.41
1:E:60:VAL:CG1	1:E:60:VAL:O	2.69	0.40
1:D:233:ARG:HA	1:D:233:ARG:HD3	1.84	0.40
1:B:94:PRO:HG2	1:B:95:TRP:CE2	2.56	0.40
1:E:284:ILE:HA	1:E:289:ILE:HG12	2.04	0.40
1:D:295:LEU:O	1:D:296:VAL:C	2.60	0.40
1:C:237:GLU:O	1:C:238:SER:HB2	2.22	0.40
1:D:70:ILE:HG12	1:D:125:ALA:CB	2.50	0.40
1:A:76:GLU:CD	1:A:86:LYS:HE2	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:GLN:NE2	3:B:562:HOH:O	2.54	0.40
1:D:190:ILE:O	1:D:194:VAL:HG22	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	345/347 (99%)	333 (96%)	10 (3%)	2 (1%)	30	16
1	B	345/347 (99%)	325 (94%)	18 (5%)	2 (1%)	30	16
1	C	345/347 (99%)	330 (96%)	12 (4%)	3 (1%)	21	9
1	D	345/347 (99%)	330 (96%)	13 (4%)	2 (1%)	30	16
1	E	345/347 (99%)	333 (96%)	10 (3%)	2 (1%)	30	16
1	H	345/347 (99%)	327 (95%)	16 (5%)	2 (1%)	30	16
All	All	2070/2082 (99%)	1978 (96%)	79 (4%)	13 (1%)	30	16

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	51	ASN
1	C	51	ASN
1	H	51	ASN
1	A	51	ASN
1	A	296	VAL
1	B	296	VAL
1	D	51	ASN
1	D	296	VAL
1	E	51	ASN
1	E	296	VAL

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Mol	Chain	Res	Type
1	H	296	VAL
1	C	296	VAL
1	C	47	GLY

### 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	273/278 (98%)	268 (98%)	5 (2%)	66	58
1	B	270/278 (97%)	265 (98%)	5 (2%)	65	56
1	C	272/278 (98%)	270 (99%)	2 (1%)	88	87
1	D	273/278 (98%)	270 (99%)	3 (1%)	80	76
1	E	275/278 (99%)	268 (98%)	7 (2%)	55	44
1	H	273/278 (98%)	269 (98%)	4 (2%)	72	66
All	All	1636/1668 (98%)	1610 (98%)	26 (2%)	70	64

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LYS
1	A	98	GLU
1	A	152	LEU
1	A	183	LEU
1	A	192	LYS
1	B	98	GLU
1	B	143	ARG
1	B	152	LEU
1	B	233	ARG
1	B	320	LYS
1	C	224	SER
1	C	251	GLU
1	D	24	LYS
1	D	94	PRO
1	D	152	LEU

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Mol	Chain	Res	Type
1	E	94	PRO
1	E	98	GLU
1	E	142	ARG
1	E	143	ARG
1	E	152	LEU
1	E	192	LYS
1	E	292	VAL
1	H	98	GLU
1	H	152	LEU
1	H	183	LEU
1	H	251	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	336	ASN
1	B	16	GLN
1	B	336	ASN
1	C	16	GLN
1	C	39	HIS
1	C	333	ASN
1	D	16	GLN
1	D	248	ASN
1	D	336	ASN
1	E	16	GLN
1	E	278	HIS
1	E	336	ASN
1	H	16	GLN
1	H	290	GLN
1	H	336	ASN

### 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](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	347/347 (100%)	0.39	26 (7%)	17 25	12, 26, 72, 87	0
1	B	347/347 (100%)	0.83	65 (18%)	2 2	17, 35, 75, 88	0
1	C	347/347 (100%)	0.76	54 (15%)	3 4	16, 32, 74, 89	0
1	D	347/347 (100%)	0.41	38 (10%)	7 11	12, 27, 73, 88	0
1	E	347/347 (100%)	0.53	46 (13%)	4 7	17, 31, 74, 88	0
1	H	347/347 (100%)	0.65	55 (15%)	3 4	16, 33, 75, 89	0
All	All	2082/2082 (100%)	0.59	284 (13%)	4 6	12, 31, 75, 89	0

All (284) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	337	PHE	12.5
1	C	47	GLY	11.6
1	A	338	LYS	10.8
1	B	340	ILE	10.6
1	E	337	PHE	10.6
1	E	340	ILE	10.4
1	A	337	PHE	9.6
1	H	52	LEU	9.2
1	H	340	ILE	8.9
1	C	52	LEU	8.9
1	H	339	ALA	8.8
1	C	56	GLU	8.7
1	E	339	ALA	7.8
1	C	337	PHE	7.8
1	C	7	VAL	7.6
1	C	61	LYS	7.4
1	D	337	PHE	7.3
1	B	338	LYS	7.3
1	H	61	LYS	7.2

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Mol	Chain	Res	Type	RSRZ
1	A	54	ILE	6.9
1	B	52	LEU	6.8
1	D	54	ILE	6.8
1	C	59	GLY	6.6
1	C	55	VAL	6.5
1	C	48	ARG	6.3
1	B	58	LEU	6.2
1	B	55	VAL	6.1
1	B	59	GLY	6.0
1	B	61	LYS	6.0
1	C	340	ILE	5.9
1	B	51	ASN	5.9
1	A	340	ILE	5.9
1	C	51	ASN	5.8
1	A	339	ALA	5.7
1	C	60	VAL	5.7
1	D	52	LEU	5.7
1	B	50	GLY	5.6
1	H	10	GLY	5.5
1	B	62	LEU	5.5
1	E	61	LYS	5.5
1	C	53	ARG	5.5
1	E	338	LYS	5.4
1	B	337	PHE	5.4
1	B	47	GLY	5.3
1	D	6	LEU	5.2
1	D	340	ILE	5.2
1	H	56	GLU	5.0
1	C	58	LEU	5.0
1	H	338	LYS	4.9
1	C	347	PRO	4.8
1	E	12	PRO	4.8
1	B	46	GLN	4.7
1	B	12	PRO	4.6
1	B	56	GLU	4.6
1	H	51	ASN	4.6
1	B	54	ILE	4.5
1	B	334	LEU	4.5
1	D	339	ALA	4.5
1	C	57	ASP	4.5
1	B	48	ARG	4.5
1	A	51	ASN	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	53	ARG	4.4
1	B	339	ALA	4.4
1	H	331	ILE	4.4
1	C	62	LEU	4.4
1	E	336	ASN	4.4
1	B	18	ILE	4.4
1	A	331	ILE	4.4
1	H	50	GLY	4.4
1	C	54	ILE	4.3
1	A	3	ALA	4.2
1	E	54	ILE	4.2
1	E	331	ILE	4.2
1	D	55	VAL	4.2
1	C	63	PRO	4.2
1	B	53	ARG	4.2
1	A	61	LYS	4.2
1	C	339	ALA	4.2
1	C	9	ILE	4.2
1	H	53	ARG	4.2
1	D	347	PRO	4.1
1	H	58	LEU	4.1
1	A	4	VAL	4.1
1	E	52	LEU	4.1
1	H	54	ILE	4.1
1	H	12	PRO	4.1
1	E	274	GLY	4.0
1	B	318	ILE	4.0
1	H	55	VAL	4.0
1	B	7	VAL	4.0
1	B	60	VAL	4.0
1	B	142	ARG	4.0
1	D	53	ARG	4.0
1	B	248	ASN	3.9
1	A	53	ARG	3.9
1	D	50	GLY	3.9
1	E	273	PHE	3.9
1	B	9	ILE	3.9
1	A	50	GLY	3.9
1	B	122	PHE	3.9
1	H	59	GLY	3.8
1	D	47	GLY	3.8
1	B	28	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	61	LYS	3.8
1	B	347	PRO	3.7
1	C	10	GLY	3.7
1	H	6	LEU	3.7
1	H	8	GLU	3.7
1	A	52	LEU	3.7
1	H	9	ILE	3.7
1	E	56	GLU	3.7
1	B	57	ASP	3.7
1	D	10	GLY	3.6
1	D	57	ASP	3.6
1	C	142	ARG	3.6
1	E	51	ASN	3.6
1	H	11	LYS	3.5
1	D	51	ASN	3.5
1	E	28	VAL	3.5
1	H	341	GLY	3.4
1	B	331	ILE	3.4
1	H	22	LYS	3.4
1	C	273	PHE	3.4
1	H	347	PRO	3.4
1	D	4	VAL	3.4
1	B	8	GLU	3.4
1	B	11	LYS	3.4
1	D	338	LYS	3.4
1	D	9	ILE	3.3
1	C	49	PHE	3.3
1	D	24	LYS	3.3
1	A	274	GLY	3.3
1	E	79	ASP	3.3
1	B	323	LYS	3.3
1	H	248	ASN	3.3
1	H	7	VAL	3.3
1	C	331	ILE	3.3
1	E	24	LYS	3.2
1	B	63	PRO	3.2
1	H	49	PHE	3.2
1	C	6	LEU	3.2
1	C	39	HIS	3.2
1	D	79	ASP	3.2
1	H	334	LEU	3.2
1	C	11	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	274	GLY	3.2
1	B	39	HIS	3.2
1	A	6	LEU	3.1
1	A	273	PHE	3.1
1	C	79	ASP	3.1
1	C	50	GLY	3.1
1	D	7	VAL	3.1
1	C	46	GLN	3.1
1	A	334	LEU	3.1
1	E	10	GLY	3.1
1	B	49	PHE	3.1
1	H	47	GLY	3.0
1	D	22	LYS	3.0
1	H	278	HIS	3.0
1	H	28	VAL	3.0
1	H	332	ASP	3.0
1	C	15	LEU	3.0
1	D	13	LEU	3.0
1	B	325	GLU	2.9
1	C	334	LEU	2.9
1	C	19	GLY	2.9
1	B	336	ASN	2.9
1	E	6	LEU	2.9
1	H	57	ASP	2.9
1	D	56	GLU	2.9
1	H	43	HIS	2.9
1	E	278	HIS	2.8
1	H	3	ALA	2.8
1	E	347	PRO	2.8
1	E	122	PHE	2.8
1	D	278	HIS	2.8
1	H	273	PHE	2.8
1	C	28	VAL	2.8
1	E	55	VAL	2.8
1	E	39	HIS	2.8
1	A	24	LYS	2.8
1	B	22	LYS	2.8
1	A	55	VAL	2.8
1	B	274	GLY	2.8
1	B	10	GLY	2.7
1	D	11	LYS	2.7
1	C	20	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	17	GLU	2.7
1	E	9	ILE	2.7
1	B	42	VAL	2.7
1	E	3	ALA	2.7
1	B	320	LYS	2.6
1	H	24	LYS	2.6
1	B	207	GLU	2.6
1	D	59	GLY	2.6
1	B	86	LYS	2.6
1	C	8	GLU	2.6
1	D	331	ILE	2.6
1	B	332	ASP	2.6
1	E	58	LEU	2.6
1	E	76	GLU	2.5
1	B	15	LEU	2.5
1	C	64	VAL	2.5
1	H	318	ILE	2.5
1	E	46	GLN	2.5
1	C	86	LYS	2.5
1	E	142	ARG	2.5
1	D	273	PHE	2.5
1	C	332	ASP	2.5
1	A	64	VAL	2.5
1	H	320	LYS	2.5
1	B	345	LEU	2.5
1	D	12	PRO	2.5
1	H	60	VAL	2.4
1	C	338	LYS	2.4
1	H	46	GLN	2.4
1	C	76	GLU	2.4
1	H	336	ASN	2.4
1	B	295	LEU	2.4
1	E	252	LYS	2.4
1	D	8	GLU	2.4
1	E	50	GLY	2.4
1	C	129	TYR	2.4
1	A	12	PRO	2.4
1	D	14	SER	2.4
1	A	122	PHE	2.4
1	E	49	PHE	2.4
1	C	22	LYS	2.4
1	E	11	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	252	LYS	2.4
1	H	323	LYS	2.4
1	B	20	VAL	2.4
1	B	24	LYS	2.3
1	C	42	VAL	2.3
1	E	7	VAL	2.3
1	D	49	PHE	2.3
1	B	13	LEU	2.3
1	D	62	LEU	2.3
1	H	39	HIS	2.3
1	C	122	PHE	2.3
1	D	58	LEU	2.3
1	E	43	HIS	2.3
1	A	336	ASN	2.3
1	H	122	PHE	2.3
1	C	323	LYS	2.2
1	H	4	VAL	2.2
1	B	214	ARG	2.2
1	B	252	LYS	2.2
1	H	127	ALA	2.2
1	B	341	GLY	2.2
1	H	315	LYS	2.2
1	E	8	GLU	2.2
1	E	86	LYS	2.2
1	B	335	GLU	2.2
1	B	19	GLY	2.2
1	E	59	GLY	2.1
1	A	49	PHE	2.1
1	B	330	ALA	2.1
1	E	21	PRO	2.1
1	H	63	PRO	2.1
1	C	31	LYS	2.1
1	H	327	ALA	2.1
1	H	79	ASP	2.1
1	B	76	GLU	2.1
1	B	329	GLU	2.1
1	E	37	VAL	2.1
1	B	45	ARG	2.1
1	A	47	GLY	2.1
1	D	3	ALA	2.1
1	E	15	LEU	2.1
1	H	42	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	57	ASP	2.1
1	H	86	LYS	2.0
1	C	329	GLU	2.0
1	A	62	LEU	2.0
1	E	4	VAL	2.0
1	C	24	LYS	2.0
1	C	237	GLU	2.0
1	E	22	LYS	2.0
1	B	6	LEU	2.0
1	D	334	LEU	2.0
1	C	77	VAL	2.0
1	H	48	ARG	2.0
1	D	18	ILE	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(Å <sup>2</sup> )	Q<0.9
2	ZN	A	400	1/1	0.99	0.06	-0.71	20,20,20,20	0
2	ZN	H	400	1/1	1.00	0.04	-1.30	24,24,24,24	0
2	ZN	B	400	1/1	0.99	0.06	-1.84	24,24,24,24	0
2	ZN	C	400	1/1	1.00	0.05	-2.03	21,21,21,21	0
2	ZN	D	400	1/1	1.00	0.05	-2.04	22,22,22,22	0
2	ZN	E	400	1/1	0.99	0.04	-2.06	23,23,23,23	0
2	ZN	E	500	1/1	0.99	0.04	-2.07	32,32,32,32	0
2	ZN	B	500	1/1	0.95	0.04	-2.70	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	H	500	1/1	0.99	0.03	-2.74	35,35,35,35	0
2	ZN	A	500	1/1	0.99	0.03	-3.08	28,28,28,28	0
2	ZN	C	500	1/1	0.99	0.03	-3.51	33,33,33,33	0
2	ZN	D	500	1/1	1.00	0.03	-4.45	26,26,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.