



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:38 PM GMT

PDB ID : 1Y3I
Title : Crystal Structure of Mycobacterium tuberculosis NAD kinase-NAD complex
Authors : Mori, S.; Yamasaki, M.; Maruyama, Y.; Momma, K.; Kawai, S.; Hashimoto, W.; Mikami, B.; Murata, K.
Deposited on : 2004-11-25
Resolution : 2.60 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

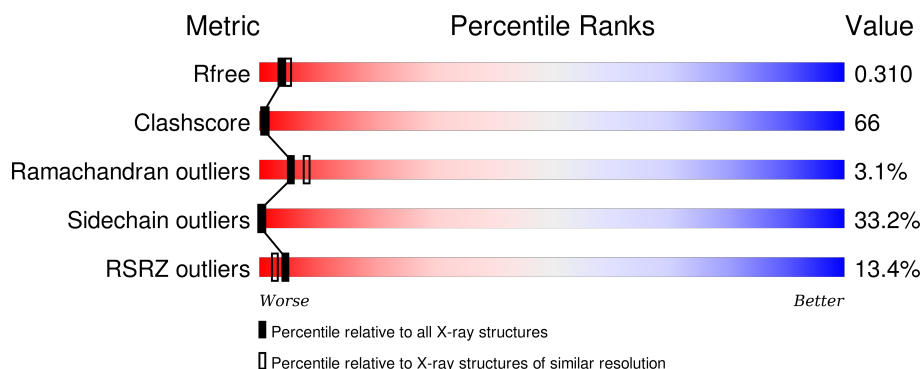
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 ≥ 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	307	<div> <div>9%</div> <div>17%</div> <div>38%</div> <div>18%</div> <div>•</div> <div>25%</div> </div>
1	B	307	<div> <div>11%</div> <div>21%</div> <div>40%</div> <div>13%</div> <div>•</div> <div>25%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	701	-	-	X	-
4	GOL	A	601	-	X	-	-
4	GOL	A	602	-	X	-	-
4	GOL	B	1601	-	X	-	-
4	GOL	B	603	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3636 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 Inorganic polyphosphate/ATP-NAD kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1738	1105	310	318	5			
1	B	231	Total	C	N	O	S	0	0	0
			1738	1105	310	318	5			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

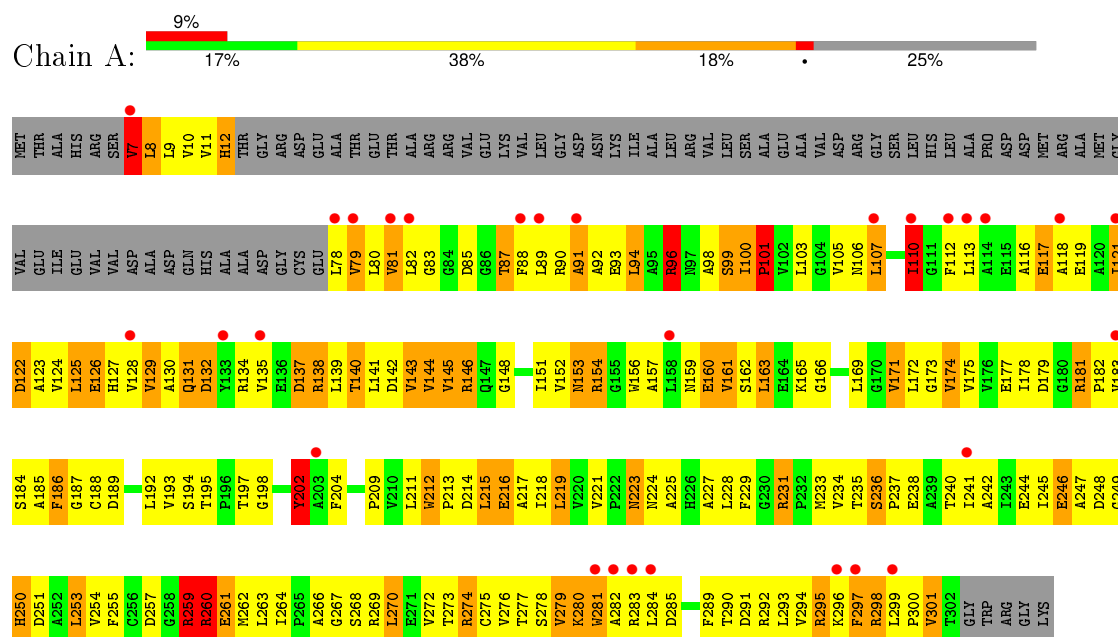
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	26	Total	O	0	0
			26	26		
5	B	17	Total	O	0	0
			17	17		

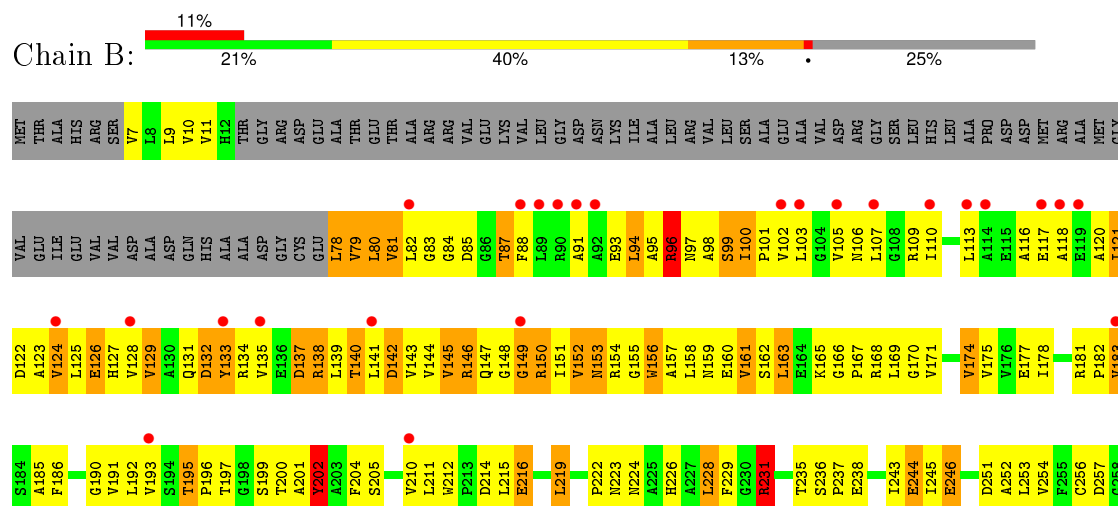
3 Residue-property plots

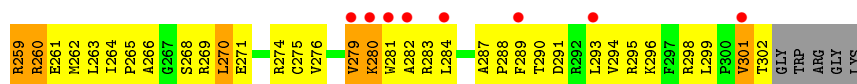
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Inorganic polyphosphate/ATP-NAD kinase



- Molecule 1: Inorganic polyphosphate/ATP-NAD kinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	110.45Å 110.45Å 108.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.60 28.92 – 2.40	Depositor EDS
% Data completeness (in resolution range)	91.0 (10.00-2.60) 89.7 (28.92-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.39Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.191 , 0.215 0.283 , 0.310	Depositor DCC
R_{free} test set	1110 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 251.6	EDS
Estimated twinning fraction	0.489 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 26613 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3636	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GOL, SO4, NAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.76	3/1768 (0.2%)	1.37	13/2410 (0.5%)
1	B	0.31	0/1768	1.13	10/2410 (0.4%)
All	All	1.27	3/3536 (0.1%)	1.25	23/4820 (0.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	7	VAL	CB-CG1	42.57	2.42	1.52
1	A	7	VAL	CB-CG2	42.35	2.41	1.52
1	A	7	VAL	CA-CB	41.27	2.41	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	VAL	CA-CB-CG1	-19.51	81.64	110.90
1	A	7	VAL	CA-CB-CG2	-19.18	82.13	110.90
1	A	7	VAL	CG1-CB-CG2	-18.34	81.55	110.90
1	B	260	ARG	NE-CZ-NH2	16.52	128.56	120.30
1	A	260	ARG	NE-CZ-NH1	15.85	128.23	120.30
1	A	260	ARG	CD-NE-CZ	15.24	144.94	123.60
1	A	202	TYR	CB-CG-CD1	14.05	129.43	121.00
1	A	260	ARG	NE-CZ-NH2	-13.88	113.36	120.30
1	B	260	ARG	CD-NE-CZ	13.46	142.44	123.60
1	A	202	TYR	CB-CG-CD2	-13.35	112.99	121.00
1	B	260	ARG	NE-CZ-NH1	-12.90	113.85	120.30
1	B	202	TYR	CB-CG-CD2	10.20	127.12	121.00
1	B	202	TYR	CB-CG-CD1	-9.30	115.42	121.00
1	A	96	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	B	96	ARG	NE-CZ-NH1	8.61	124.60	120.30
1	A	7	VAL	N-CA-CB	-8.14	93.58	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	ARG	CD-NE-CZ	7.20	133.67	123.60
1	B	231	ARG	NE-CZ-NH1	-7.10	116.75	120.30
1	A	96	ARG	CD-NE-CZ	6.48	132.68	123.60
1	B	149	GLY	C-N-CA	5.30	134.96	121.70
1	B	231	ARG	NE-CZ-NH2	5.25	122.93	120.30
1	A	96	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	181	ARG	NE-CZ-NH1	5.15	122.88	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1738	0	1776	253	0
1	B	1738	0	1776	246	0
2	B	5	0	0	2	0
3	A	44	0	26	3	0
3	B	44	0	26	7	0
4	A	12	0	8	0	0
4	B	12	0	8	1	0
5	A	26	0	0	3	0
5	B	17	0	0	1	0
All	All	3636	0	3620	477	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 66.

All (477) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:GLY:HA2	1:A:107:LEU:HD22	1.32	1.09
1:B:106:ASN:HB3	1:B:117:GLU:HA	1.37	1.05
1:A:78:LEU:HD21	1:A:80:LEU:HD11	1.35	1.04
1:A:217:ALA:HA	1:A:237:PRO:HD3	1.39	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:ASP:HB3	1:B:263:LEU:HD21	1.45	0.98
1:A:7:VAL:CG1	1:A:7:VAL:CB	2.42	0.98
1:A:7:VAL:CA	1:A:7:VAL:CB	2.41	0.98
1:B:147:GLN:HG3	1:B:152:VAL:HG21	1.45	0.97
1:A:7:VAL:CG2	1:A:7:VAL:CB	2.41	0.97
1:A:110:ILE:HD13	1:A:295:ARG:HH22	1.33	0.93
1:B:163:LEU:HD11	1:B:245:ILE:HD11	1.49	0.92
1:B:79:VAL:HG21	1:B:95:ALA:CB	2.03	0.89
1:B:163:LEU:HG	1:B:270:LEU:HD12	1.54	0.89
1:A:211:LEU:HB3	1:A:215:LEU:HD23	1.55	0.88
1:A:7:VAL:HG13	1:A:78:LEU:HB3	1.53	0.88
1:A:140:THR:HG23	1:A:278:SER:HA	1.55	0.86
1:A:83:GLY:CA	1:A:107:LEU:HD22	2.05	0.86
1:A:79:VAL:HG22	1:A:100:ILE:HD13	1.57	0.85
1:B:141:LEU:HD12	1:B:195:THR:HG22	1.59	0.85
1:A:103:LEU:HB2	1:A:282:ALA:HB3	1.60	0.84
1:B:146:ARG:HB3	1:B:151:ILE:HA	1.58	0.84
1:A:7:VAL:HA	1:A:78:LEU:O	1.78	0.83
1:B:101:PRO:HA	1:B:280:LYS:HB2	1.61	0.83
1:A:141:LEU:HD12	1:A:195:THR:HG22	1.61	0.82
1:A:141:LEU:HD21	1:A:218:ILE:HG12	1.59	0.82
1:B:145:VAL:HG22	1:B:152:VAL:HG23	1.62	0.82
1:A:7:VAL:HG12	1:A:80:LEU:HD21	1.60	0.81
1:B:96:ARG:HB2	1:B:279:VAL:HG23	1.61	0.80
1:B:105:VAL:HG22	1:B:116:ALA:HB3	1.62	0.80
1:A:153:ASN:HD22	1:A:154:ARG:H	1.25	0.79
1:B:105:VAL:HG21	1:B:124:VAL:HG11	1.64	0.78
1:A:83:GLY:O	1:A:107:LEU:HB2	1.84	0.76
1:B:145:VAL:HG13	1:B:153:ASN:HB3	1.66	0.76
1:A:105:VAL:HG11	1:A:121:ILE:HG23	1.65	0.76
1:A:78:LEU:CD2	1:A:80:LEU:HD11	2.13	0.76
1:B:134:ARG:O	1:B:282:ALA:HA	1.86	0.76
1:A:11:VAL:HG22	1:A:82:LEU:HB2	1.66	0.76
1:A:79:VAL:HG23	1:A:101:PRO:O	1.85	0.76
1:A:112:PHE:O	1:A:296:LYS:HE3	1.85	0.75
1:B:79:VAL:HG21	1:B:95:ALA:HB1	1.69	0.75
1:B:79:VAL:HG21	1:B:95:ALA:HB2	1.68	0.75
1:A:91:ALA:O	1:A:94:LEU:HG	1.86	0.75
1:B:95:ALA:O	1:B:280:LYS:HE2	1.88	0.74
1:B:165:LYS:HG3	1:B:166:GLY:O	1.87	0.74
1:A:98:ALA:O	1:A:100:ILE:HG22	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:SER:HA	1:B:301:VAL:HA	1.70	0.74
1:B:279:VAL:HA	1:B:280:LYS:HZ3	1.52	0.74
1:A:240:THR:HA	1:A:273:THR:HG22	1.69	0.74
1:A:163:LEU:HD11	1:A:245:ILE:HD12	1.69	0.73
1:B:226:HIS:ND1	4:B:1601:GOL:H12	2.04	0.73
1:B:125:LEU:O	1:B:128:VAL:HG13	1.88	0.72
1:B:157:ALA:HB2	1:B:256:CYS:HB3	1.71	0.72
1:B:146:ARG:NH2	1:B:149:GLY:H	1.88	0.72
1:A:293:LEU:O	1:A:297:PHE:HB2	1.89	0.72
1:A:237:PRO:O	1:A:274:ARG:HB2	1.89	0.71
1:A:93:GLU:O	1:A:96:ARG:HB3	1.89	0.71
1:A:127:HIS:ND1	1:A:132:ASP:HB2	2.05	0.71
1:B:146:ARG:HH22	1:B:149:GLY:H	1.38	0.71
1:B:83:GLY:HA2	1:B:107:LEU:HB2	1.70	0.71
1:A:105:VAL:HA	1:A:116:ALA:O	1.89	0.71
1:B:157:ALA:HA	1:B:260:ARG:HH22	1.54	0.70
1:B:82:LEU:O	1:B:107:LEU:HD22	1.90	0.70
1:A:8:LEU:HD21	1:A:10:VAL:HG22	1.73	0.70
1:B:245:ILE:HG22	1:B:266:ALA:HA	1.72	0.70
1:B:9:LEU:HD11	1:B:82:LEU:HD23	1.73	0.70
1:A:90:ARG:HB2	1:A:259:ARG:HH22	1.56	0.70
1:B:147:GLN:HB2	1:B:150:ARG:HD3	1.73	0.70
1:B:295:ARG:HH22	1:B:296:LYS:HZ3	1.39	0.70
1:B:96:ARG:HD2	1:B:156:TRP:CE2	2.27	0.70
3:B:1501:NAD:O4D	3:B:1501:NAD:H52A	1.90	0.69
1:B:147:GLN:CG	1:B:152:VAL:HG21	2.22	0.69
1:B:177:GLU:HG2	1:B:182:PRO:HB3	1.74	0.69
1:B:279:VAL:HA	1:B:280:LYS:NZ	2.07	0.69
1:B:79:VAL:HG23	1:B:101:PRO:O	1.92	0.69
1:A:140:THR:CG2	1:A:278:SER:HA	2.23	0.69
1:B:78:LEU:HD12	1:B:101:PRO:O	1.93	0.69
1:B:263:LEU:HD22	1:B:264:ILE:N	2.08	0.69
1:A:90:ARG:O	1:A:93:GLU:HB3	1.92	0.69
1:A:125:LEU:HA	1:A:128:VAL:HG13	1.75	0.68
1:A:209:PRO:HD2	1:A:219:LEU:HD11	1.74	0.68
1:A:178:ILE:O	1:B:290:THR:HG21	1.93	0.68
1:B:177:GLU:HA	1:B:182:PRO:HA	1.75	0.68
1:B:178:ILE:HD13	1:B:235:THR:HG21	1.76	0.68
1:A:101:PRO:HA	1:A:280:LYS:HB2	1.76	0.68
1:B:175:VAL:HG22	1:B:185:ALA:HB2	1.76	0.67
1:A:126:GLU:HA	1:A:129:VAL:HG13	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:VAL:HG12	1:A:80:LEU:CD2	2.24	0.67
1:A:125:LEU:O	1:A:128:VAL:HG13	1.94	0.67
1:B:147:GLN:O	1:B:150:ARG:HB3	1.95	0.67
1:A:130:ALA:HB3	1:A:132:ASP:OD2	1.95	0.67
1:B:79:VAL:HG22	1:B:100:ILE:HD13	1.76	0.66
1:A:11:VAL:HG13	1:A:82:LEU:O	1.94	0.66
1:B:138:ARG:HH22	1:B:283:ARG:HH11	1.42	0.66
1:A:143:VAL:HG11	1:A:161:VAL:HG11	1.76	0.66
1:A:139:LEU:HD11	1:A:237:PRO:HB3	1.77	0.66
1:B:200:THR:HG22	1:B:210:VAL:HG13	1.77	0.66
1:B:120:ALA:O	1:B:124:VAL:HG23	1.96	0.66
1:A:291:ASP:OD1	1:B:181:ARG:HG3	1.96	0.66
1:A:153:ASN:HD22	1:A:154:ARG:N	1.94	0.65
1:A:244:GLU:OE1	1:A:269:ARG:HB2	1.96	0.65
1:B:153:ASN:HD22	1:B:154:ARG:H	1.43	0.65
1:A:135:VAL:HA	1:A:281:TRP:O	1.96	0.65
1:B:244:GLU:OE1	1:B:269:ARG:HD2	1.96	0.65
1:B:254:VAL:O	1:B:261:GLU:HA	1.96	0.64
1:B:127:HIS:HB3	1:B:132:ASP:HB2	1.80	0.64
1:B:138:ARG:HH22	1:B:283:ARG:NH1	1.96	0.64
1:A:212:TRP:HB2	1:B:235:THR:HA	1.80	0.64
1:B:80:LEU:HD12	1:B:103:LEU:HD23	1.79	0.64
1:A:212:TRP:O	1:A:215:LEU:HB2	1.97	0.64
1:B:216:GLU:O	1:B:237:PRO:HD3	1.98	0.64
1:B:106:ASN:O	1:B:118:ALA:HB2	1.98	0.64
1:B:166:GLY:HA3	1:B:169:LEU:HD13	1.79	0.63
1:A:79:VAL:O	1:A:80:LEU:HD13	1.98	0.63
1:A:122:ASP:O	1:A:125:LEU:HD13	1.99	0.63
1:A:137:ASP:HB3	1:A:278:SER:HB2	1.81	0.63
1:B:290:THR:O	1:B:294:VAL:HG12	1.97	0.63
1:B:216:GLU:HB3	1:B:237:PRO:HG3	1.81	0.63
1:A:295:ARG:O	1:A:298:ARG:HG2	1.98	0.63
1:B:96:ARG:HA	1:B:280:LYS:NZ	2.15	0.62
1:A:110:ILE:HD13	1:A:295:ARG:NH2	2.09	0.62
1:A:166:GLY:HA3	1:A:169:LEU:HD22	1.80	0.62
1:A:290:THR:HG23	1:B:183:VAL:HG23	1.81	0.62
1:B:231:ARG:HB2	2:B:701:SO4:O1	1.99	0.61
1:B:133:TYR:HA	1:B:283:ARG:O	2.00	0.61
1:B:141:LEU:CD1	1:B:195:THR:HG22	2.29	0.61
1:A:85:ASP:O	1:A:89:LEU:HG	2.01	0.61
1:B:202:TYR:O	1:B:205:SER:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:THR:O	1:A:294:VAL:HG12	2.01	0.61
1:B:163:LEU:O	1:B:190:GLY:HA3	2.01	0.61
1:A:106:ASN:O	1:A:118:ALA:HB2	2.00	0.61
1:A:110:ILE:HG22	5:A:610:HOH:O	2.01	0.61
1:A:212:TRP:CZ3	1:B:235:THR:HG22	2.35	0.61
1:B:163:LEU:HD12	1:B:243:ILE:HG21	1.83	0.61
1:B:125:LEU:HD12	1:B:125:LEU:H	1.66	0.60
1:A:175:VAL:HG22	1:A:185:ALA:HB2	1.82	0.60
1:A:295:ARG:NH2	1:A:296:LYS:HA	2.17	0.60
1:B:96:ARG:HD2	1:B:156:TRP:CZ2	2.37	0.60
1:B:216:GLU:CB	1:B:237:PRO:HG3	2.31	0.60
1:A:12:HIS:HB2	1:A:83:GLY:HA2	1.84	0.60
1:B:11:VAL:HG22	1:B:82:LEU:HB2	1.84	0.60
1:B:102:VAL:HG12	1:B:280:LYS:O	2.02	0.59
1:B:107:LEU:HA	1:B:118:ALA:HB2	1.83	0.59
1:A:139:LEU:HD13	1:A:217:ALA:H	1.67	0.59
1:B:246:GLU:O	1:B:266:ALA:HB1	2.02	0.59
1:A:259:ARG:HG3	1:A:260:ARG:NH1	2.17	0.59
1:B:143:VAL:HG21	1:B:161:VAL:HG11	1.85	0.59
1:B:126:GLU:HA	1:B:129:VAL:HG13	1.85	0.59
1:B:79:VAL:C	1:B:80:LEU:HD13	2.24	0.58
1:B:263:LEU:HD22	1:B:264:ILE:H	1.67	0.58
1:B:243:ILE:HD13	1:B:270:LEU:HD13	1.85	0.58
1:A:234:VAL:HG12	1:B:215:LEU:HD21	1.84	0.58
1:A:78:LEU:C	1:A:100:ILE:HD11	2.24	0.58
1:A:143:VAL:HB	1:A:272:VAL:HG22	1.83	0.58
1:A:166:GLY:HA3	1:A:169:LEU:HD13	1.86	0.58
1:A:12:HIS:HB2	1:A:83:GLY:CA	2.34	0.58
1:A:80:LEU:CD1	1:A:103:LEU:HD23	2.33	0.58
1:B:270:LEU:HD23	1:B:271:GLU:H	1.68	0.58
1:B:9:LEU:HG	1:B:11:VAL:HG23	1.86	0.57
1:A:231:ARG:HG2	1:B:204:PHE:HE1	1.69	0.57
1:A:217:ALA:CA	1:A:237:PRO:HD3	2.25	0.57
1:A:259:ARG:HG3	1:A:260:ARG:HH11	1.69	0.57
1:B:79:VAL:HG22	1:B:100:ILE:CD1	2.34	0.57
1:B:245:ILE:CG2	1:B:266:ALA:HA	2.34	0.57
1:B:289:PHE:CE2	1:B:293:LEU:HD22	2.39	0.57
1:A:173:GLY:O	1:A:174:VAL:HG23	2.04	0.57
1:A:139:LEU:CD1	1:A:237:PRO:HB3	2.34	0.57
1:B:159:ASN:HB2	1:B:257:ASP:OD1	2.05	0.57
1:A:9:LEU:HD11	1:A:82:LEU:CD2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:SER:HA	1:B:280:LYS:HE3	1.87	0.57
1:A:245:ILE:HG13	1:A:264:ILE:HG21	1.86	0.57
1:A:216:GLU:C	1:A:237:PRO:HG3	2.25	0.57
1:A:184:SER:CA	1:B:301:VAL:HA	2.35	0.57
1:A:145:VAL:HG22	1:A:152:VAL:CG2	2.35	0.57
1:A:143:VAL:O	1:A:154:ARG:HG3	2.05	0.56
1:A:139:LEU:HD12	1:A:216:GLU:HG3	1.87	0.56
1:A:125:LEU:CA	1:A:128:VAL:HG13	2.34	0.56
1:B:186:PHE:CZ	1:B:222:PRO:HB3	2.40	0.56
1:B:295:ARG:NH2	1:B:296:LYS:HZ3	2.03	0.56
1:A:212:TRP:O	1:A:215:LEU:HD22	2.05	0.56
3:B:1501:NAD:H51A	3:B:1501:NAD:O5D	2.06	0.56
1:B:256:CYS:HB3	1:B:260:ARG:NH2	2.21	0.56
1:A:212:TRP:CE3	1:B:235:THR:HG22	2.40	0.56
1:B:165:LYS:HD2	1:B:170:GLY:O	2.07	0.55
1:B:263:LEU:O	1:B:265:PRO:HD3	2.07	0.55
1:A:216:GLU:O	1:A:237:PRO:HG3	2.06	0.55
1:B:200:THR:CG2	1:B:210:VAL:HG13	2.36	0.55
1:A:172:LEU:O	1:A:187:GLY:HA2	2.06	0.55
1:A:10:VAL:O	1:A:81:VAL:HA	2.07	0.55
1:B:146:ARG:HH12	1:B:149:GLY:HA2	1.71	0.55
1:B:140:THR:CG2	1:B:279:VAL:H	2.20	0.55
1:B:93:GLU:O	1:B:96:ARG:HD3	2.07	0.55
1:B:252:ALA:HB3	1:B:264:ILE:HB	1.90	0.54
1:B:9:LEU:CD1	1:B:80:LEU:HB2	2.37	0.54
1:A:7:VAL:CG1	1:A:80:LEU:HD21	2.32	0.54
1:A:189:ASP:HB2	1:A:224:ASN:HB2	1.89	0.54
1:B:157:ALA:HB1	1:B:257:ASP:OD1	2.07	0.54
1:A:255:PHE:CE2	1:A:261:GLU:HB2	2.42	0.54
1:A:171:VAL:HG22	1:A:188:CYS:N	2.22	0.54
1:B:196:PRO:HA	1:B:211:LEU:HD12	1.88	0.54
1:B:229:PHE:CZ	1:B:231:ARG:HB3	2.43	0.54
1:B:96:ARG:HA	1:B:280:LYS:HE2	1.90	0.54
1:A:144:VAL:HB	1:A:153:ASN:O	2.08	0.54
1:B:289:PHE:HE2	1:B:293:LEU:HD22	1.72	0.54
1:B:174:VAL:HG13	1:B:243:ILE:HG23	1.90	0.53
1:A:140:THR:O	1:A:275:CYS:HB3	2.08	0.53
1:A:121:ILE:HD12	1:A:121:ILE:H	1.73	0.53
1:A:101:PRO:CA	1:A:280:LYS:HB2	2.39	0.53
1:A:143:VAL:O	1:A:154:ARG:HA	2.09	0.53
1:B:216:GLU:CG	1:B:237:PRO:HG3	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ASP:OD1	1:A:154:ARG:HD3	2.07	0.53
1:A:246:GLU:HG2	1:A:246:GLU:O	2.07	0.53
1:A:159:ASN:O	1:A:198:GLY:HA3	2.09	0.53
1:A:229:PHE:HE1	1:B:204:PHE:HZ	1.55	0.53
1:B:9:LEU:HD21	1:B:11:VAL:HG21	1.90	0.53
1:A:219:LEU:HD13	1:A:221:VAL:HG23	1.91	0.53
1:B:146:ARG:HA	1:B:152:VAL:H	1.74	0.53
1:B:288:PRO:HD2	1:B:291:ASP:OD2	2.08	0.53
1:A:78:LEU:CD2	1:A:128:VAL:HB	2.38	0.53
1:A:182:PRO:HG2	1:B:301:VAL:HG21	1.90	0.53
1:A:124:VAL:HG13	1:A:284:LEU:CD1	2.39	0.52
1:A:78:LEU:CA	1:A:100:ILE:HD11	2.39	0.52
1:B:106:ASN:OD1	1:B:117:GLU:HG3	2.09	0.52
1:B:138:ARG:HG3	1:B:281:TRP:CD1	2.44	0.52
1:A:8:LEU:HG	1:A:9:LEU:N	2.24	0.52
1:A:8:LEU:HD21	1:A:10:VAL:CG2	2.39	0.52
1:A:301:VAL:HG23	1:A:301:VAL:O	2.10	0.52
1:A:213:PRO:HG3	1:A:289:PHE:CD1	2.45	0.52
1:A:117:GLU:HB3	1:A:119:GLU:OE1	2.08	0.52
1:B:127:HIS:HA	1:B:132:ASP:OD2	2.10	0.52
1:B:96:ARG:CB	1:B:279:VAL:HG23	2.36	0.52
1:A:189:ASP:HB2	1:A:223:ASN:O	2.10	0.52
1:A:295:ARG:HG3	1:A:296:LYS:N	2.24	0.52
1:A:93:GLU:O	1:A:96:ARG:HD3	2.10	0.52
1:A:212:TRP:N	1:A:215:LEU:HD22	2.25	0.51
1:B:95:ALA:HA	1:B:100:ILE:HG23	1.91	0.51
1:A:122:ASP:O	1:A:125:LEU:HB2	2.10	0.51
1:A:246:GLU:HG2	1:A:249:GLY:H	1.75	0.51
1:A:112:PHE:HB3	1:A:113:LEU:HD23	1.91	0.51
1:B:98:ALA:HB3	1:B:100:ILE:HG22	1.93	0.51
1:B:9:LEU:HD12	1:B:80:LEU:HB2	1.91	0.51
1:A:124:VAL:HG13	1:A:284:LEU:HD11	1.92	0.51
1:A:96:ARG:HD2	1:A:156:TRP:CZ2	2.45	0.51
1:A:163:LEU:HA	1:A:254:VAL:HG22	1.92	0.51
1:A:163:LEU:HD11	1:A:245:ILE:CD1	2.37	0.51
1:B:175:VAL:O	1:B:243:ILE:HA	2.11	0.50
1:B:82:LEU:HD12	1:B:107:LEU:CD1	2.42	0.50
1:A:103:LEU:HB2	1:A:282:ALA:CB	2.35	0.50
1:B:301:VAL:O	1:B:302:THR:O	2.29	0.50
1:B:96:ARG:HA	1:B:280:LYS:CE	2.41	0.50
1:A:127:HIS:HA	1:A:132:ASP:OD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:SER:CB	1:B:211:LEU:H	2.23	0.50
1:A:145:VAL:HG22	1:A:152:VAL:HG23	1.94	0.50
1:B:135:VAL:HG23	1:B:135:VAL:O	2.12	0.50
1:B:7:VAL:HG13	1:B:80:LEU:HD21	1.93	0.50
1:B:177:GLU:HG2	1:B:182:PRO:CB	2.39	0.50
1:A:234:VAL:HB	1:B:211:LEU:HD23	1.93	0.50
1:A:236:SER:HB3	1:B:214:ASP:OD1	2.12	0.50
1:B:299:LEU:O	1:B:301:VAL:HG13	2.12	0.50
1:A:247:ALA:HA	1:A:267:GLY:N	2.27	0.50
1:A:163:LEU:HD23	1:A:253:LEU:O	2.12	0.49
1:A:134:ARG:O	1:A:281:TRP:O	2.30	0.49
1:A:7:VAL:HG13	1:A:78:LEU:CB	2.35	0.49
1:A:135:VAL:O	1:A:135:VAL:HG23	2.12	0.49
1:A:144:VAL:CG2	1:A:151:ILE:HG23	2.42	0.49
1:A:78:LEU:HD11	1:A:103:LEU:HB3	1.95	0.49
1:A:144:VAL:HG23	1:A:146:ARG:HG2	1.95	0.49
1:A:250:HIS:HB2	5:A:606:HOH:O	2.11	0.49
1:B:157:ALA:HB2	1:B:256:CYS:CB	2.41	0.49
1:B:122:ASP:O	1:B:126:GLU:HB2	2.12	0.49
1:A:212:TRP:CH2	1:B:178:ILE:HD12	2.48	0.49
1:B:133:TYR:HB3	1:B:284:LEU:CD2	2.43	0.49
1:B:100:ILE:C	1:B:280:LYS:HD3	2.34	0.49
1:B:150:ARG:O	1:B:150:ARG:HG2	2.12	0.49
1:B:143:VAL:CG2	1:B:161:VAL:HG11	2.43	0.49
1:B:246:GLU:HG2	1:B:246:GLU:O	2.12	0.48
1:A:217:ALA:HA	1:A:237:PRO:CD	2.28	0.48
1:A:113:LEU:HD21	3:A:501:NAD:N6A	2.28	0.48
1:B:147:GLN:HG3	1:B:152:VAL:CG2	2.30	0.48
1:A:146:ARG:NH2	5:A:627:HOH:O	2.45	0.48
1:B:121:ILE:O	1:B:124:VAL:HB	2.13	0.48
1:B:177:GLU:HG2	1:B:182:PRO:CA	2.43	0.48
1:B:79:VAL:HB	1:B:102:VAL:HA	1.95	0.48
1:B:7:VAL:HG22	1:B:78:LEU:N	2.29	0.48
1:A:122:ASP:HA	1:A:125:LEU:HD13	1.95	0.48
1:B:126:GLU:O	1:B:129:VAL:HG13	2.14	0.48
1:B:301:VAL:O	1:B:301:VAL:HG23	2.12	0.48
1:A:90:ARG:HA	1:A:259:ARG:NH2	2.29	0.48
1:B:186:PHE:HZ	1:B:222:PRO:HB3	1.79	0.48
1:A:125:LEU:C	1:A:128:VAL:HG13	2.33	0.48
1:A:194:SER:OG	1:A:195:THR:O	2.30	0.48
1:A:100:ILE:C	1:A:280:LYS:HD3	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ALA:HA	1:B:260:ARG:NH2	2.26	0.47
1:B:192:LEU:HD21	1:B:202:TYR:CD1	2.49	0.47
1:B:78:LEU:HD12	1:B:79:VAL:N	2.28	0.47
1:A:157:ALA:HA	1:A:257:ASP:OD1	2.14	0.47
3:B:1501:NAD:C8A	3:B:1501:NAD:H4D	2.45	0.47
1:B:9:LEU:CD2	1:B:11:VAL:HG21	2.44	0.47
1:A:105:VAL:HG11	1:A:121:ILE:CG2	2.37	0.47
1:A:125:LEU:HA	1:A:128:VAL:CG1	2.43	0.47
1:A:202:TYR:HB2	3:A:501:NAD:O2D	2.15	0.47
1:B:147:GLN:N	1:B:152:VAL:HG22	2.29	0.47
1:A:212:TRP:CG	1:B:235:THR:HA	2.48	0.47
1:A:93:GLU:HG2	1:A:94:LEU:N	2.28	0.47
1:B:244:GLU:OE1	1:B:269:ARG:HB2	2.15	0.47
1:B:94:LEU:HA	1:B:97:ASN:HB3	1.96	0.47
1:B:139:LEU:HD21	1:B:141:LEU:HG	1.96	0.47
1:A:143:VAL:HG11	1:A:161:VAL:CG1	2.45	0.47
1:A:126:GLU:CA	1:A:129:VAL:HG13	2.44	0.47
1:A:107:LEU:HA	1:A:118:ALA:HB2	1.96	0.47
1:B:195:THR:OG1	1:B:197:THR:OG1	2.29	0.47
1:A:7:VAL:HG22	1:A:78:LEU:N	2.30	0.47
1:B:146:ARG:HA	1:B:152:VAL:HG22	1.96	0.47
1:B:126:GLU:CA	1:B:129:VAL:HG13	2.45	0.47
1:A:141:LEU:HD22	1:A:272:VAL:CG1	2.45	0.46
1:A:244:GLU:CD	1:A:269:ARG:HB2	2.35	0.46
1:A:219:LEU:HD23	1:A:234:VAL:HG22	1.97	0.46
1:A:166:GLY:C	1:A:169:LEU:HD13	2.35	0.46
1:A:166:GLY:CA	1:A:169:LEU:HD13	2.46	0.46
1:A:127:HIS:O	1:A:131:GLN:HA	2.14	0.46
1:B:200:THR:HG21	1:B:289:PHE:HZ	1.81	0.46
1:A:189:ASP:CG	1:A:224:ASN:HD22	2.19	0.46
1:A:117:GLU:HG2	1:A:119:GLU:OE1	2.16	0.46
1:A:121:ILE:CD1	1:A:121:ILE:H	2.25	0.46
1:A:212:TRP:CH2	1:B:235:THR:HG22	2.50	0.46
1:A:96:ARG:HD2	1:A:156:TRP:CE2	2.51	0.46
1:B:287:ALA:HB1	1:B:288:PRO:HD2	1.96	0.46
1:A:125:LEU:CD1	1:A:125:LEU:H	2.29	0.46
1:A:178:ILE:HD11	1:A:233:MET:SD	2.56	0.46
1:A:181:ARG:HB2	1:B:290:THR:CG2	2.46	0.46
1:B:231:ARG:NH1	2:B:701:SO4:O1	2.49	0.46
1:B:143:VAL:HG23	1:B:270:LEU:HD21	1.96	0.46
1:A:144:VAL:HG21	1:A:151:ILE:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ASN:O	1:B:195:THR:HG23	2.15	0.46
1:B:121:ILE:HD12	1:B:122:ASP:H	1.80	0.46
1:B:169:LEU:HD12	1:B:169:LEU:N	2.31	0.46
1:A:132:ASP:N	1:A:132:ASP:OD2	2.49	0.46
1:B:294:VAL:HG23	1:B:299:LEU:HB2	1.98	0.45
1:A:80:LEU:HD22	1:A:80:LEU:N	2.30	0.45
1:A:96:ARG:HG3	1:A:96:ARG:HH11	1.81	0.45
1:A:204:PHE:O	1:B:231:ARG:NH2	2.48	0.45
1:A:214:ASP:OD1	1:B:236:SER:HB3	2.16	0.45
1:B:106:ASN:ND2	1:B:109:ARG:O	2.49	0.45
1:B:205:SER:OG	3:B:1501:NAD:N7N	2.49	0.45
1:A:11:VAL:CG2	1:A:82:LEU:HB2	2.41	0.45
1:A:88:PHE:O	1:A:92:ALA:N	2.49	0.45
1:B:140:THR:HG21	1:B:279:VAL:H	1.81	0.45
1:A:122:ASP:CA	1:A:125:LEU:HD13	2.47	0.45
1:A:294:VAL:O	1:A:298:ARG:N	2.49	0.45
1:A:218:ILE:HB	1:A:235:THR:OG1	2.16	0.45
1:A:231:ARG:NH2	1:B:204:PHE:O	2.50	0.45
1:A:12:HIS:ND1	1:A:87:THR:OG1	2.50	0.45
1:B:91:ALA:O	1:B:94:LEU:HG	2.15	0.45
1:A:80:LEU:HD12	1:A:103:LEU:HD23	1.97	0.45
1:B:147:GLN:NE2	5:B:1611:HOH:O	2.50	0.45
1:A:245:ILE:N	1:A:245:ILE:HD13	2.32	0.45
1:A:166:GLY:CA	1:A:169:LEU:HD22	2.45	0.45
1:B:81:VAL:HG13	1:B:103:LEU:O	2.17	0.45
1:B:143:VAL:O	1:B:155:GLY:N	2.50	0.45
1:B:85:ASP:OD2	1:B:113:LEU:N	2.50	0.45
1:B:79:VAL:O	1:B:103:LEU:N	2.50	0.45
1:A:9:LEU:HA	1:A:80:LEU:O	2.16	0.45
1:A:290:THR:CG2	1:B:183:VAL:HG23	2.45	0.45
1:A:127:HIS:ND1	1:A:132:ASP:O	2.50	0.45
1:B:238:GLU:H	1:B:238:GLU:HG2	1.67	0.45
1:B:78:LEU:HD12	1:B:79:VAL:H	1.82	0.45
1:A:292:ARG:HG2	1:A:296:LYS:HE2	1.97	0.45
1:A:139:LEU:HD13	1:A:217:ALA:N	2.31	0.45
1:A:137:ASP:N	1:A:137:ASP:OD2	2.50	0.45
1:A:177:GLU:HA	1:A:181:ARG:O	2.16	0.45
1:A:7:VAL:CG1	1:A:78:LEU:HD23	2.46	0.44
1:B:88:PHE:O	1:B:91:ALA:HB3	2.17	0.44
1:A:225:ALA:O	1:A:227:ALA:N	2.50	0.44
1:B:140:THR:HG21	1:B:279:VAL:HB	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:VAL:HG23	1:B:101:PRO:C	2.37	0.44
1:B:80:LEU:HD13	1:B:80:LEU:N	2.33	0.44
1:B:94:LEU:O	1:B:97:ASN:N	2.51	0.44
1:B:84:GLY:O	1:B:87:THR:N	2.50	0.44
1:A:83:GLY:HA2	1:A:107:LEU:CD2	2.24	0.44
1:B:201:ALA:O	1:B:204:PHE:N	2.50	0.44
1:B:132:ASP:OD2	1:B:132:ASP:N	2.50	0.44
1:B:80:LEU:N	1:B:80:LEU:HD22	2.33	0.44
1:A:144:VAL:HA	1:A:154:ARG:HA	2.00	0.44
1:B:296:LYS:O	1:B:298:ARG:NH1	2.50	0.44
1:B:147:GLN:N	1:B:150:ARG:O	2.50	0.44
1:A:90:ARG:HB2	1:A:259:ARG:HH12	1.82	0.44
1:B:142:ASP:HB2	1:B:275:CYS:HB2	2.00	0.44
1:B:132:ASP:O	1:B:284:LEU:HD22	2.17	0.44
1:B:146:ARG:HB3	1:B:151:ILE:CA	2.39	0.44
1:B:228:LEU:HD22	1:B:228:LEU:HA	1.82	0.44
1:A:105:VAL:HG13	1:A:117:GLU:C	2.38	0.44
1:B:252:ALA:O	1:B:263:LEU:HD22	2.18	0.44
1:B:254:VAL:HG23	1:B:264:ILE:CG1	2.48	0.43
1:B:82:LEU:HD12	1:B:107:LEU:HD11	2.00	0.43
1:A:122:ASP:C	1:A:125:LEU:HD13	2.38	0.43
1:A:135:VAL:HG12	1:A:281:TRP:O	2.18	0.43
1:A:174:VAL:N	1:A:186:PHE:O	2.50	0.43
1:A:242:ALA:HA	1:A:270:LEU:O	2.18	0.43
1:A:159:ASN:OD1	3:A:501:NAD:N6A	2.50	0.43
1:B:280:LYS:HD2	1:B:280:LYS:H	1.84	0.43
1:B:263:LEU:C	1:B:264:ILE:HD13	2.39	0.43
1:A:90:ARG:HB2	1:A:259:ARG:NH2	2.29	0.43
1:A:231:ARG:HH11	1:A:231:ARG:HD3	1.66	0.43
1:A:78:LEU:HD12	1:A:79:VAL:N	2.33	0.43
1:B:163:LEU:HG	1:B:270:LEU:CD1	2.37	0.43
1:A:137:ASP:HB3	1:A:278:SER:CB	2.47	0.43
1:A:182:PRO:O	1:B:301:VAL:HG11	2.18	0.43
1:A:103:LEU:HD13	1:A:284:LEU:HD21	2.00	0.43
1:A:113:LEU:O	1:A:281:TRP:HH2	2.01	0.43
1:B:137:ASP:N	1:B:137:ASP:OD2	2.49	0.43
1:B:143:VAL:CG2	1:B:270:LEU:HD21	2.49	0.43
1:A:144:VAL:HG12	1:A:154:ARG:CG	2.49	0.43
1:A:179:ASP:OD2	1:B:288:PRO:HB2	2.19	0.43
1:A:121:ILE:O	1:A:124:VAL:HB	2.18	0.43
1:A:280:LYS:H	1:A:280:LYS:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:VAL:HA	1:B:219:LEU:O	2.18	0.43
1:A:160:GLU:HB2	1:A:193:VAL:O	2.18	0.43
1:B:138:ARG:HG3	1:B:281:TRP:HB2	2.00	0.42
1:A:78:LEU:HD12	1:A:79:VAL:H	1.85	0.42
1:A:90:ARG:CB	1:A:259:ARG:HH22	2.29	0.42
1:A:88:PHE:O	1:A:92:ALA:HB3	2.19	0.42
1:B:163:LEU:HB3	1:B:191:VAL:H	1.84	0.42
1:A:212:TRP:CB	1:B:235:THR:HA	2.47	0.42
1:A:247:ALA:HA	1:A:266:ALA:C	2.39	0.42
1:B:279:VAL:HG13	1:B:280:LYS:N	2.34	0.42
1:A:125:LEU:H	1:A:125:LEU:HD12	1.85	0.42
1:A:7:VAL:HA	1:A:78:LEU:N	2.35	0.42
1:B:138:ARG:HG3	1:B:281:TRP:CG	2.54	0.42
1:A:163:LEU:HD23	1:A:254:VAL:HG23	2.01	0.42
1:B:123:ALA:HB1	1:B:127:HIS:NE2	2.35	0.42
1:B:101:PRO:CA	1:B:280:LYS:HB2	2.43	0.42
1:A:279:VAL:HG13	1:A:280:LYS:N	2.33	0.42
1:B:153:ASN:ND2	1:B:154:ARG:H	2.14	0.42
1:A:259:ARG:HB2	1:A:260:ARG:HG3	2.01	0.42
1:A:263:LEU:HD22	1:A:264:ILE:H	1.84	0.42
1:B:295:ARG:HG3	1:B:296:LYS:N	2.34	0.42
1:B:9:LEU:HD12	1:B:80:LEU:O	2.19	0.42
1:B:156:TRP:O	1:B:260:ARG:NH2	2.50	0.42
1:B:139:LEU:O	1:B:197:THR:HG21	2.20	0.42
1:A:284:LEU:HD23	1:A:284:LEU:N	2.34	0.42
1:B:128:VAL:HG23	1:B:128:VAL:O	2.18	0.42
1:B:98:ALA:HB3	1:B:100:ILE:CG2	2.50	0.42
1:A:78:LEU:HG	1:A:80:LEU:CD2	2.49	0.42
1:B:101:PRO:CG	1:B:135:VAL:HG11	2.50	0.42
1:B:257:ASP:HA	3:B:1501:NAD:O3D	2.19	0.42
1:B:162:SER:O	1:B:254:VAL:HA	2.20	0.42
1:A:138:ARG:HG3	1:A:281:TRP:CD1	2.55	0.42
1:B:143:VAL:CB	1:B:161:VAL:HG11	2.51	0.41
1:A:240:THR:HG23	1:A:273:THR:CG2	2.49	0.41
1:A:234:VAL:HB	1:B:211:LEU:CD2	2.50	0.41
3:B:1501:NAD:H8A	3:B:1501:NAD:H4D	2.01	0.41
1:B:138:ARG:HD2	1:B:281:TRP:CG	2.56	0.41
1:B:259:ARG:HB2	1:B:260:ARG:HG3	2.02	0.41
1:A:122:ASP:OD2	1:A:123:ALA:N	2.53	0.41
1:B:79:VAL:O	1:B:103:LEU:HB3	2.21	0.41
1:B:125:LEU:HA	1:B:128:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:GLU:HG2	1:B:182:PRO:HA	2.01	0.41
1:A:162:SER:HB2	1:A:192:LEU:HD23	2.02	0.41
1:B:158:LEU:HD21	1:B:281:TRP:HE1	1.86	0.41
1:B:101:PRO:N	1:B:280:LYS:HD3	2.36	0.41
1:A:113:LEU:HD23	1:A:113:LEU:N	2.35	0.41
1:A:11:VAL:HG22	1:A:82:LEU:CB	2.44	0.41
1:A:218:ILE:O	1:A:235:THR:N	2.49	0.41
1:A:241:ILE:N	1:A:272:VAL:O	2.50	0.41
1:B:201:ALA:O	1:B:204:PHE:HB3	2.21	0.41
1:B:117:GLU:HG3	1:B:118:ALA:H	1.85	0.40
1:B:158:LEU:O	1:B:195:THR:HG21	2.21	0.40
1:A:82:LEU:CD1	1:A:105:VAL:HB	2.52	0.40
1:A:103:LEU:CD1	1:A:284:LEU:HD21	2.52	0.40
1:B:143:VAL:HG23	1:B:270:LEU:CD2	2.51	0.40
1:A:229:PHE:CE1	1:A:231:ARG:HB2	2.56	0.40
1:A:251:ASP:OD2	1:A:266:ALA:N	2.50	0.40
1:B:159:ASN:OD1	3:B:1501:NAD:N6A	2.50	0.40
1:B:153:ASN:HD22	1:B:154:ARG:N	2.12	0.40
1:A:189:ASP:CB	1:A:224:ASN:HB2	2.51	0.40
1:A:299:LEU:HA	1:A:300:PRO:HD3	1.94	0.40
1:A:125:LEU:O	1:A:128:VAL:N	2.52	0.40
1:A:125:LEU:O	1:A:129:VAL:HG12	2.22	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	227/307 (74%)	187 (82%)	32 (14%)	8 (4%)	4	6
1	B	227/307 (74%)	190 (84%)	31 (14%)	6 (3%)	7	11
All	All	454/614 (74%)	377 (83%)	63 (14%)	14 (3%)	5	8

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	SER
1	A	125	LEU
1	A	110	ILE
1	A	148	GLY
1	A	268	SER
1	B	148	GLY
1	B	167	PRO
1	B	268	SER
1	B	224	ASN
1	B	133	TYR
1	A	91	ALA
1	A	259	ARG
1	A	101	PRO
1	B	124	VAL

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	184/242 (76%)	115 (62%)	69 (38%)	0	0
1	B	184/242 (76%)	131 (71%)	53 (29%)	0	1
All	All	368/484 (76%)	246 (67%)	122 (33%)	0	0

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	8	LEU
1	A	12	HIS
1	A	79	VAL
1	A	81	VAL
1	A	87	THR
1	A	94	LEU
1	A	96	ARG
1	A	99	SER

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Mol	Chain	Res	Type
1	A	100	ILE
1	A	101	PRO
1	A	107	LEU
1	A	110	ILE
1	A	117	GLU
1	A	121	ILE
1	A	122	ASP
1	A	126	GLU
1	A	129	VAL
1	A	131	GLN
1	A	132	ASP
1	A	137	ASP
1	A	138	ARG
1	A	140	THR
1	A	143	VAL
1	A	144	VAL
1	A	145	VAL
1	A	146	ARG
1	A	153	ASN
1	A	154	ARG
1	A	160	GLU
1	A	161	VAL
1	A	163	LEU
1	A	165	LYS
1	A	171	VAL
1	A	174	VAL
1	A	183	VAL
1	A	186	PHE
1	A	197	THR
1	A	202	TYR
1	A	212	TRP
1	A	215	LEU
1	A	216	GLU
1	A	219	LEU
1	A	223	ASN
1	A	228	LEU
1	A	231	ARG
1	A	236	SER
1	A	238	GLU
1	A	246	GLU
1	A	248	ASP
1	A	250	HIS

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Mol	Chain	Res	Type
1	A	253	LEU
1	A	259	ARG
1	A	260	ARG
1	A	261	GLU
1	A	262	MET
1	A	270	LEU
1	A	274	ARG
1	A	276	VAL
1	A	277	THR
1	A	279	VAL
1	A	280	LYS
1	A	281	TRP
1	A	283	ARG
1	A	285	ASP
1	A	295	ARG
1	A	297	PHE
1	A	298	ARG
1	A	301	VAL
1	B	10	VAL
1	B	78	LEU
1	B	79	VAL
1	B	80	LEU
1	B	81	VAL
1	B	87	THR
1	B	94	LEU
1	B	96	ARG
1	B	99	SER
1	B	100	ILE
1	B	110	ILE
1	B	121	ILE
1	B	126	GLU
1	B	129	VAL
1	B	131	GLN
1	B	132	ASP
1	B	137	ASP
1	B	138	ARG
1	B	140	THR
1	B	142	ASP
1	B	144	VAL
1	B	145	VAL
1	B	146	ARG
1	B	150	ARG

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Mol	Chain	Res	Type
1	B	152	VAL
1	B	153	ASN
1	B	156	TRP
1	B	160	GLU
1	B	161	VAL
1	B	163	LEU
1	B	168	ARG
1	B	171	VAL
1	B	174	VAL
1	B	183	VAL
1	B	195	THR
1	B	202	TYR
1	B	212	TRP
1	B	216	GLU
1	B	219	LEU
1	B	223	ASN
1	B	228	LEU
1	B	231	ARG
1	B	244	GLU
1	B	246	GLU
1	B	253	LEU
1	B	259	ARG
1	B	262	MET
1	B	270	LEU
1	B	274	ARG
1	B	276	VAL
1	B	279	VAL
1	B	280	LYS
1	B	301	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	ASN
1	A	131	GLN
1	A	153	ASN
1	A	223	ASN
1	B	97	ASN
1	B	147	GLN
1	B	153	ASN
1	B	223	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAD	A	501	-	38,48,48	1.55	2 (5%)	47,73,73	2.33	9 (19%)
4	GOL	A	601	-	5,5,5	4.70	5 (100%)	5,5,5	5.04	3 (60%)
4	GOL	A	602	-	5,5,5	4.65	5 (100%)	5,5,5	4.71	3 (60%)
3	NAD	B	1501	-	38,48,48	1.57	2 (5%)	47,73,73	2.16	7 (14%)
4	GOL	B	1601	-	5,5,5	4.78	5 (100%)	5,5,5	5.61	3 (60%)
4	GOL	B	603	-	5,5,5	4.73	5 (100%)	5,5,5	4.74	3 (60%)
2	SO4	B	701	-	4,4,4	3.37	2 (50%)	6,6,6	0.94	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	A	501	-	-	0/22/62/62	0/5/5/5
4	GOL	A	601	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	602	-	-	0/4/4/4	0/0/0/0
3	NAD	B	1501	-	-	0/22/62/62	0/5/5/5
4	GOL	B	1601	-	-	0/4/4/4	0/0/0/0
4	GOL	B	603	-	-	0/4/4/4	0/0/0/0
2	SO4	B	701	-	-	0/0/0/0	0/0/0/0

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1601	GOL	C3-C2	-8.10	1.21	1.52
4	B	603	GOL	C3-C2	-7.90	1.22	1.52
4	A	601	GOL	C3-C2	-7.87	1.22	1.52
4	A	602	GOL	C3-C2	-7.80	1.22	1.52
2	B	701	SO4	O3-S	-4.80	1.30	1.47
4	B	1601	GOL	C1-C2	-3.28	1.39	1.52
4	B	603	GOL	C1-C2	-3.24	1.39	1.52
4	A	601	GOL	C1-C2	-3.14	1.40	1.52
4	A	602	GOL	C1-C2	-3.07	1.40	1.52
4	B	1601	GOL	O2-C2	-2.80	1.35	1.43
4	A	601	GOL	O2-C2	-2.65	1.35	1.43
4	B	603	GOL	O2-C2	-2.65	1.35	1.43
4	A	602	GOL	O2-C2	-2.54	1.35	1.43
3	A	501	NAD	C3N-C7N	2.05	1.53	1.50
3	B	1501	NAD	C6N-N1N	2.12	1.41	1.35
4	B	1601	GOL	O3-C3	3.36	1.56	1.42
4	B	603	GOL	O3-C3	3.48	1.57	1.42
4	A	601	GOL	O3-C3	3.48	1.57	1.42
4	A	602	GOL	O3-C3	3.52	1.57	1.42
4	B	1601	GOL	O1-C1	4.34	1.61	1.42
4	A	602	GOL	O1-C1	4.38	1.61	1.42
4	A	601	GOL	O1-C1	4.39	1.61	1.42
4	B	603	GOL	O1-C1	4.45	1.61	1.42
2	B	701	SO4	O1-S	4.66	1.63	1.47
3	A	501	NAD	C4N-C3N	8.04	1.53	1.39
3	B	1501	NAD	C4N-C3N	8.25	1.53	1.39

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1501	NAD	N3A-C2A-N1A	-9.52	121.61	128.89
3	A	501	NAD	N3A-C2A-N1A	-9.41	121.69	128.89
3	B	1501	NAD	C5N-C4N-C3N	-7.82	110.50	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	NAD	C4D-O4D-C1D	-6.62	102.44	109.72
3	A	501	NAD	C5N-C4N-C3N	-6.35	112.35	120.33
3	A	501	NAD	C3N-C7N-N7N	-3.55	113.93	117.82
3	A	501	NAD	C1B-N9A-C4A	-3.37	121.85	126.94
3	B	1501	NAD	C3N-C7N-N7N	-3.22	114.29	117.82
3	A	501	NAD	C4A-C5A-N7A	-2.68	107.01	109.48
3	B	1501	NAD	C1B-N9A-C4A	-2.62	122.99	126.94
3	B	1501	NAD	C4A-C5A-N7A	-2.33	107.34	109.48
3	A	501	NAD	C2N-C3N-C4N	2.03	120.55	118.29
3	B	1501	NAD	O4D-C1D-N1N	2.16	110.51	108.13
3	A	501	NAD	O7N-C7N-C3N	2.91	122.76	119.59
3	B	1501	NAD	O7N-C7N-C3N	2.93	122.78	119.59
3	A	501	NAD	C6N-C5N-C4N	2.98	123.95	119.44
4	B	603	GOL	O1-C1-C2	3.15	125.46	110.18
4	A	601	GOL	O1-C1-C2	3.19	125.67	110.18
4	B	1601	GOL	O1-C1-C2	3.55	127.39	110.18
4	A	602	GOL	O1-C1-C2	3.69	128.06	110.18
4	A	602	GOL	O2-C2-C3	4.88	131.02	108.65
4	B	603	GOL	O2-C2-C3	5.58	134.25	108.65
4	A	601	GOL	O2-C2-C3	6.08	136.53	108.65
4	B	1601	GOL	O2-C2-C3	6.84	140.01	108.65
4	B	603	GOL	O3-C3-C2	8.39	150.90	110.18
4	A	602	GOL	O3-C3-C2	8.52	151.50	110.18
4	A	601	GOL	O3-C3-C2	8.85	153.10	110.18
4	B	1601	GOL	O3-C3-C2	9.87	158.06	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	NAD	3	0
3	B	1501	NAD	7	0
4	B	1601	GOL	1	0
2	B	701	SO4	2	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, 95th 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 ²)	Q<0.9
1	A	231/307 (75%)	0.83	29 (12%) 5 3	17, 51, 121, 143	0
1	B	231/307 (75%)	0.77	33 (14%) 4 2	18, 51, 121, 143	0
All	All	462/614 (75%)	0.80	62 (13%) 4 2	17, 51, 121, 143	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	282	ALA	11.1
1	B	279	VAL	7.9
1	A	118	ALA	7.4
1	A	78	LEU	6.4
1	A	281	TRP	6.4
1	A	133	TYR	6.1
1	A	82	LEU	5.9
1	A	299	LEU	5.9
1	B	88	PHE	5.7
1	A	88	PHE	5.6
1	B	118	ALA	5.5
1	A	7	VAL	5.2
1	A	113	LEU	5.0
1	B	282	ALA	5.0
1	B	82	LEU	4.9
1	B	117	GLU	4.7
1	A	128	VAL	4.7
1	B	284	LEU	4.6
1	B	133	TYR	4.6
1	B	113	LEU	4.4
1	B	124	VAL	4.3
1	A	135	VAL	3.8
1	B	107	LEU	3.6
1	B	293	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	89	LEU	3.5
1	A	121	ILE	3.4
1	B	135	VAL	3.4
1	B	110	ILE	3.4
1	A	110	ILE	3.3
1	B	102	VAL	3.3
1	A	112	PHE	3.2
1	B	210	VAL	3.0
1	A	284	LEU	3.0
1	B	149	GLY	3.0
1	A	107	LEU	3.0
1	B	114	ALA	2.9
1	B	103	LEU	2.9
1	B	89	LEU	2.9
1	A	296	LYS	2.7
1	A	79	VAL	2.7
1	B	128	VAL	2.7
1	B	289	PHE	2.7
1	B	301	VAL	2.6
1	B	183	VAL	2.6
1	A	283	ARG	2.4
1	B	90	ARG	2.4
1	A	114	ALA	2.3
1	A	241	ILE	2.3
1	B	280	LYS	2.2
1	B	92	ALA	2.2
1	B	105	VAL	2.2
1	A	81	VAL	2.2
1	B	141	LEU	2.1
1	A	203	ALA	2.1
1	B	281	TRP	2.1
1	B	91	ALA	2.1
1	A	183	VAL	2.1
1	B	119	GLU	2.1
1	A	91	ALA	2.1
1	A	297	PHE	2.1
1	A	158	LEU	2.0
1	B	193	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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(\AA^2)	Q<0.9
2	SO4	B	701	5/5	0.97	0.23	0.39	22,74,85,93	0
4	GOL	A	602	6/6	0.88	0.28	-0.09	33,64,68,83	0
3	NAD	A	501	44/44	0.96	0.21	-0.13	18,47,63,87	0
4	GOL	B	1601	6/6	0.94	0.20	-0.21	17,21,26,37	0
3	NAD	B	1501	44/44	0.95	0.18	-0.33	19,47,64,87	0
4	GOL	A	601	6/6	0.85	0.27	-	34,65,69,70	0
4	GOL	B	603	6/6	0.98	0.16	-	28,35,42,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.