Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:51 PM GMT

PDB ID	:	1HLP
Title	:	STRUCTURAL FEATURES STABILIZING HALOPHILIC MALATE DEHYDROGENASE FROM AN ARCHAEBACTERIUM
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Deposited on	:	1994-10-04
Resolution	:	3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

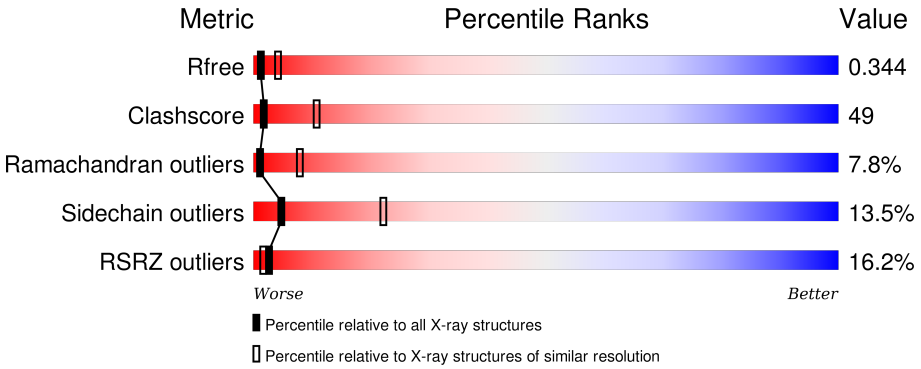
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 <=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	303	19% 39% 46% 14% .
1	B	303	14% 34% 52% 12% .

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	NAD	A	330	-	-	-	X
2	NAD	B	330	-	-	-	X

2 Entry composition

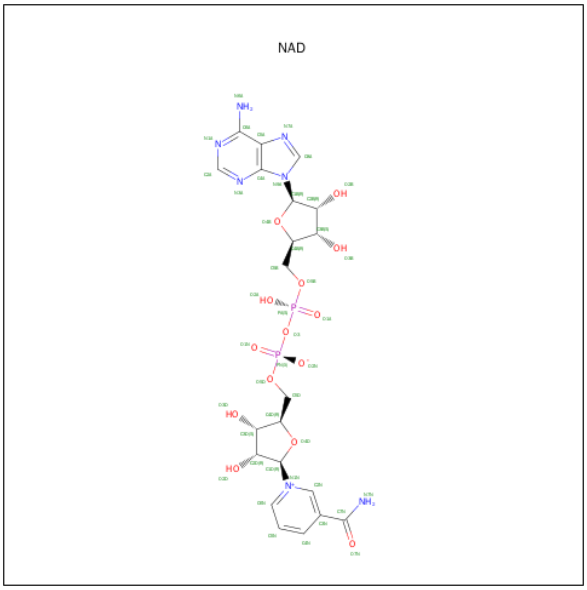
There are 2 unique types of molecules in this entry. The entry contains 4690 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MALATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	0	0
			2301	1415	393	489	4			
1	B	303	Total	C	N	O	S	0	0	0
			2301	1415	393	489	4			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



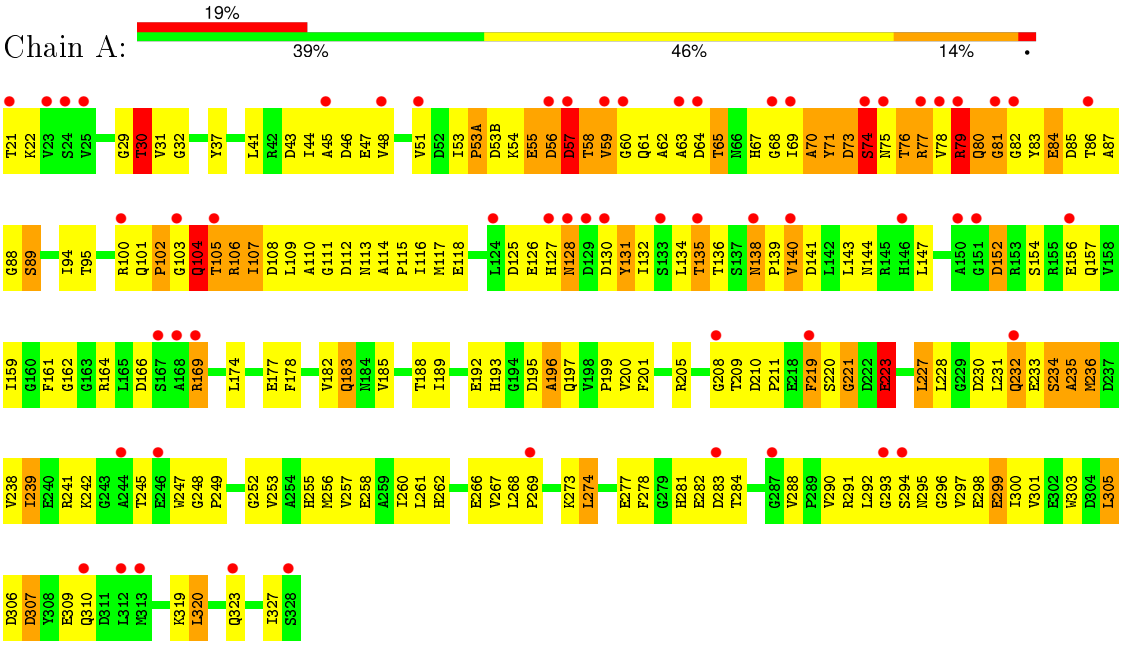
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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.

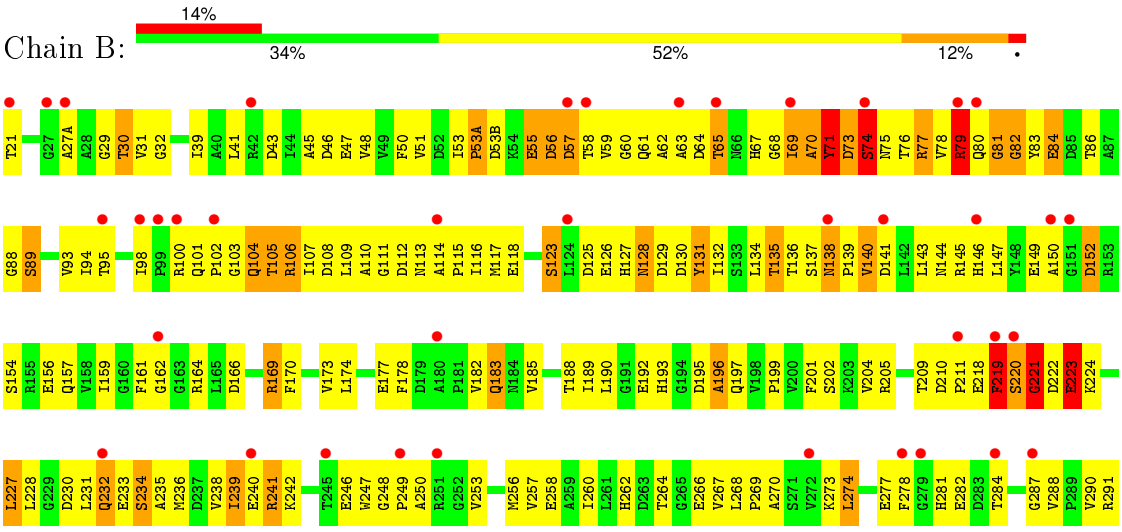
- Molecule 1: MALATE DEHYDROGENASE

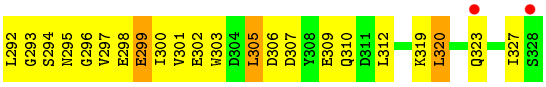
Chain A:



- Molecule 1: MALATE DEHYDROGENASE

Chain B:




L292
G293
S294
N295
G296
V297
E298
E299
I300
V301
E302
W303
D304
L305
D306
D307
Y308
E309
Q310
D311
L312
K319
L320
Q323
I327
S328

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	114.60Å 130.60Å 123.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.20 20.15 – 2.81	Depositor EDS
% Data completeness (in resolution range)	84.0 (10.00-3.20) 63.0 (20.15-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.83Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.182 , 0.280 0.335 , 0.344	Depositor DCC
R_{free} test set	1143 reflections (11.06%)	DCC
Wilson B-factor (Å^2)	32.6	Xtriage
Anisotropy	1.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 76.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	3 of 14335 reflections (0.021%)	Xtriage
F_o,F_c correlation	0.78	EDS
Total number of atoms	4690	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.74	0/2338	0.92	6/3175 (0.2%)
1	B	0.73	0/2338	0.92	5/3175 (0.2%)
All	All	0.74	0/4676	0.92	11/6350 (0.2%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	221	GLY	N-CA-C	-8.26	92.45	113.10
1	B	138	ASN	N-CA-C	7.59	131.49	111.00
1	B	221	GLY	N-CA-C	-7.27	94.92	113.10
1	A	138	ASN	N-CA-C	7.09	130.15	111.00
1	A	223	GLU	N-CA-C	6.68	129.05	111.00
1	B	74	SER	N-CA-C	6.31	128.03	111.00
1	A	74	SER	N-CA-C	6.25	127.87	111.00
1	B	223	GLU	N-CA-C	5.77	126.58	111.00
1	A	219	PHE	N-CA-C	-5.60	95.88	111.00
1	B	219	PHE	N-CA-C	-5.45	96.28	111.00
1	A	57	ASP	N-CA-C	-5.29	96.71	111.00

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	2301	0	2165	215	0
1	B	2301	0	2165	246	0
2	A	44	0	26	10	0
2	B	44	0	26	12	0
All	All	4690	0	4382	441	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 49.

All (441) 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:B:48:VAL:HB	1:B:77:ARG:HB2	1.50	0.94
1:B:291:ARG:HG2	1:B:298:GLU:HB2	1.51	0.92
1:A:249:PRO:O	1:A:253:VAL:HG23	1.70	0.92
1:A:79:ARG:HH11	1:A:79:ARG:HB3	1.32	0.90
1:A:62:ALA:H	1:A:79:ARG:HH12	1.19	0.90
1:A:29:GLY:HA3	2:A:330:NAD:O5B	1.73	0.89
1:B:29:GLY:HA3	2:B:330:NAD:O5B	1.73	0.88
1:B:79:ARG:HB3	1:B:79:ARG:HH11	1.39	0.87
1:B:32:GLY:HA2	1:B:95:THR:HG21	1.54	0.86
1:A:63:ALA:H	1:A:79:ARG:NH2	1.74	0.86
1:B:249:PRO:O	1:B:253:VAL:HG23	1.77	0.85
1:A:291:ARG:HG2	1:A:298:GLU:HB2	1.56	0.85
1:B:189:ILE:HD11	1:B:231:LEU:HD21	1.58	0.83
1:A:69:ILE:HG13	1:A:70:ALA:H	1.43	0.83
1:A:79:ARG:H	1:A:79:ARG:HD2	1.43	0.82
1:B:113:ASN:HA	1:B:116:ILE:HD12	1.60	0.82
1:A:182:VAL:HG21	1:B:70:ALA:HB1	1.60	0.82
1:A:189:ILE:HD11	1:A:231:LEU:HD21	1.61	0.82
1:A:48:VAL:HB	1:A:77:ARG:HB2	1.62	0.82
1:B:78:VAL:HG12	1:B:80:GLN:HG3	1.60	0.81
1:B:65:THR:HB	1:B:77:ARG:CZ	2.11	0.80
1:A:65:THR:HB	1:A:77:ARG:CZ	2.11	0.80
1:A:65:THR:HG23	1:B:247:TRP:CD1	2.17	0.80
1:A:114:ALA:HB3	1:A:115:PRO:HD3	1.63	0.79
1:A:177:GLU:HG2	1:A:227:LEU:HD11	1.62	0.79
1:A:62:ALA:HB3	1:A:79:ARG:NH1	1.98	0.79
1:B:136:THR:HB	2:B:330:NAD:H2N	1.63	0.78
1:B:290:VAL:HG21	1:B:297:VAL:HG22	1.66	0.78
1:B:183:GLN:HE21	1:B:183:GLN:HA	1.50	0.77
1:B:69:ILE:HG13	1:B:70:ALA:H	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ALA:H	1:B:79:ARG:NH2	1.83	0.76
1:B:43:ASP:HA	1:B:75:ASN:ND2	2.01	0.75
1:A:183:GLN:HA	1:A:183:GLN:HE21	1.51	0.75
1:A:65:THR:HB	1:A:77:ARG:NH1	2.01	0.75
1:A:228:LEU:HG	1:A:232:GLN:OE1	1.86	0.74
1:A:43:ASP:HA	1:A:75:ASN:HD22	1.52	0.74
1:B:94:ILE:HB	1:B:135:THR:HB	1.70	0.73
1:B:62:ALA:HB3	1:B:79:ARG:NH1	2.03	0.73
1:B:62:ALA:H	1:B:79:ARG:HH12	1.34	0.73
1:A:77:ARG:O	1:A:77:ARG:HD2	1.89	0.73
1:A:62:ALA:N	1:A:79:ARG:HH12	1.86	0.72
1:B:21:THR:OG1	1:B:45:ALA:HA	1.89	0.72
1:A:242:LYS:HE2	1:B:64:ASP:OD2	1.89	0.72
1:A:319:LYS:HG2	1:A:323:GLN:OE1	1.89	0.71
1:A:247:TRP:CD1	1:B:65:THR:HG23	2.25	0.71
1:B:59:VAL:HA	1:B:79:ARG:HG3	1.72	0.70
1:A:79:ARG:HB3	1:A:79:ARG:NH1	2.05	0.70
1:B:136:THR:O	2:B:330:NAD:H2N	1.91	0.70
1:B:177:GLU:HG2	1:B:227:LEU:HD11	1.72	0.70
1:B:78:VAL:CG1	1:B:80:GLN:HG3	2.22	0.70
1:B:77:ARG:O	1:B:77:ARG:HD2	1.91	0.70
1:A:238:VAL:HG13	1:A:239:ILE:HG12	1.73	0.70
1:B:65:THR:HB	1:B:77:ARG:NH1	2.06	0.69
1:B:192:GLU:HG3	1:B:320:LEU:HD11	1.73	0.69
1:B:273:LYS:HD2	1:B:284:THR:O	1.91	0.69
1:A:56:ASP:OD1	1:B:241:ARG:HD2	1.92	0.69
1:A:59:VAL:HA	1:A:79:ARG:HG3	1.75	0.68
1:A:169:ARG:HD3	1:B:67:HIS:ND1	2.08	0.68
1:A:136:THR:O	2:A:330:NAD:H2N	1.94	0.68
1:B:128:ASN:HD22	1:B:128:ASN:N	1.92	0.68
1:A:256:MET:HG2	1:A:268:LEU:HD13	1.76	0.68
1:A:136:THR:HB	2:A:330:NAD:H2N	1.76	0.67
1:A:32:GLY:HA2	1:A:95:THR:HG21	1.76	0.67
1:B:257:VAL:HA	1:B:260:ILE:HD12	1.77	0.67
1:A:257:VAL:HA	1:A:260:ILE:HD12	1.76	0.67
1:B:236:MET:O	1:B:239:ILE:HG13	1.95	0.67
1:B:199:PRO:HG3	1:B:228:LEU:HD11	1.77	0.66
1:A:69:ILE:HG13	1:A:70:ALA:N	2.11	0.66
1:A:112:ASP:O	1:A:115:PRO:HD2	1.95	0.66
1:B:189:ILE:CD1	1:B:231:LEU:HD21	2.24	0.66
1:B:69:ILE:HB	1:B:74:SER:OG	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ALA:H	1:A:79:ARG:NH1	1.93	0.65
1:B:238:VAL:HG13	1:B:239:ILE:HG12	1.78	0.65
1:B:115:PRO:O	1:B:118:GLU:HB2	1.97	0.64
1:B:166:ASP:OD2	1:B:193:HIS:HD2	1.80	0.64
1:A:54:LYS:O	1:A:56:ASP:N	2.31	0.64
1:A:113:ASN:HA	1:A:116:ILE:HD12	1.80	0.64
1:A:59:VAL:HG13	1:A:79:ARG:HG3	1.80	0.63
1:B:268:LEU:O	1:B:290:VAL:HG12	1.97	0.63
1:B:306:ASP:O	1:B:310:GLN:HG3	1.98	0.63
1:B:31:VAL:HG12	2:B:330:NAD:PN	2.38	0.63
1:A:268:LEU:HD12	1:A:292:LEU:HD12	1.79	0.63
1:A:104:GLN:O	1:A:108:ASP:HB2	1.97	0.63
1:B:79:ARG:HD2	1:B:79:ARG:H	1.64	0.63
1:B:138:ASN:C	1:B:140:VAL:H	2.00	0.63
1:B:319:LYS:HG2	1:B:323:GLN:OE1	1.98	0.63
1:A:138:ASN:O	1:A:140:VAL:HG12	1.99	0.63
1:A:241:ARG:HD2	1:B:56:ASP:OD1	1.99	0.63
1:B:59:VAL:HG12	1:B:59:VAL:O	1.99	0.62
1:B:268:LEU:HD12	1:B:292:LEU:HD12	1.81	0.62
1:A:234:SER:C	1:A:236:MET:H	2.01	0.62
1:B:112:ASP:O	1:B:115:PRO:HD2	2.00	0.62
1:B:62:ALA:N	1:B:79:ARG:HH12	1.97	0.62
1:B:233:GLU:O	1:B:235:ALA:N	2.33	0.62
1:A:138:ASN:C	1:A:140:VAL:H	2.02	0.62
1:A:59:VAL:HG12	1:A:59:VAL:O	1.99	0.61
1:A:51:VAL:HG21	1:A:86:THR:CG2	2.29	0.61
1:B:43:ASP:HA	1:B:75:ASN:HD22	1.65	0.61
1:B:65:THR:HB	1:B:77:ARG:NH2	2.15	0.61
1:B:219:PHE:O	1:B:221:GLY:N	2.34	0.61
1:B:266:GLU:O	1:B:291:ARG:HA	2.00	0.61
1:B:69:ILE:HG13	1:B:70:ALA:N	2.15	0.61
1:B:88:GLY:H	1:B:128:ASN:HB3	1.64	0.61
1:B:78:VAL:HB	1:B:80:GLN:HE21	1.65	0.60
1:B:105:THR:O	1:B:107:ILE:N	2.33	0.60
1:B:197:GLN:HE22	1:B:232:GLN:HG3	1.65	0.60
1:B:51:VAL:HG21	1:B:86:THR:CG2	2.32	0.60
1:A:43:ASP:HA	1:A:75:ASN:ND2	2.16	0.60
1:B:114:ALA:HB3	1:B:115:PRO:HD3	1.84	0.59
1:A:273:LYS:HD2	1:A:284:THR:O	2.02	0.59
1:B:107:ILE:HG22	1:B:327:ILE:CD1	2.33	0.59
1:A:62:ALA:CB	1:A:79:ARG:NH1	2.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:GLN:HG3	1:B:109:LEU:HB2	1.83	0.59
1:A:21:THR:OG1	1:A:45:ALA:HA	2.03	0.59
1:A:21:THR:O	1:A:46:ASP:HB2	2.02	0.59
1:B:136:THR:HB	2:B:330:NAD:C2N	2.33	0.59
1:A:209:THR:O	1:A:211:PRO:HD3	2.03	0.59
1:B:267:VAL:HA	1:B:290:VAL:O	2.02	0.59
1:B:107:ILE:O	1:B:110:ALA:HB3	2.01	0.59
1:A:47:GLU:HA	1:A:76:THR:O	2.03	0.59
1:B:125:ASP:O	1:B:126:GLU:HG2	2.03	0.59
1:B:140:VAL:HG21	1:B:161:PHE:O	2.03	0.58
1:A:189:ILE:CD1	1:A:231:LEU:HD21	2.33	0.58
1:B:139:PRO:HD2	1:B:143:LEU:HD21	1.83	0.58
1:A:51:VAL:HG22	1:A:81:GLY:O	2.03	0.58
1:B:128:ASN:ND2	1:B:128:ASN:N	2.52	0.58
1:B:27(A):ALA:CB	1:B:50:PHE:HB3	2.34	0.58
1:B:228:LEU:HG	1:B:232:GLN:OE1	2.04	0.58
1:B:211:PRO:HB3	1:B:219:PHE:CE2	2.39	0.57
1:B:230:ASP:HA	1:B:234:SER:HB2	1.85	0.57
1:A:94:ILE:HB	1:A:135:THR:HB	1.85	0.57
1:B:107:ILE:HG22	1:B:327:ILE:HD11	1.87	0.57
1:B:58:THR:O	1:B:79:ARG:NH1	2.38	0.57
1:A:273:LYS:HE3	1:A:283:ASP:HA	1.87	0.56
1:A:138:ASN:C	1:A:140:VAL:N	2.58	0.56
1:A:58:THR:O	1:A:79:ARG:NH1	2.39	0.56
1:A:69:ILE:HD12	1:A:74:SER:HB2	1.86	0.56
1:A:268:LEU:O	1:A:290:VAL:HG12	2.05	0.56
1:B:47:GLU:HA	1:B:76:THR:O	2.06	0.56
1:B:59:VAL:HA	1:B:79:ARG:CG	2.36	0.56
1:A:30:THR:HG23	2:A:330:NAD:O1N	2.04	0.56
1:A:306:ASP:O	1:A:310:GLN:HG3	2.05	0.56
1:B:182:VAL:O	1:B:182:VAL:HG22	2.05	0.56
1:B:305:LEU:H	1:B:305:LEU:HD12	1.71	0.56
1:B:293:GLY:O	1:B:295:ASN:N	2.39	0.56
1:B:62:ALA:H	1:B:79:ARG:NH1	2.03	0.56
1:A:117:MET:HB3	1:A:147:LEU:HG	1.87	0.56
1:B:256:MET:HG2	1:B:268:LEU:HD13	1.88	0.56
1:A:107:ILE:CG2	1:A:327:ILE:HD13	2.35	0.56
1:A:79:ARG:C	1:A:81:GLY:H	2.09	0.55
1:B:113:ASN:HA	1:B:116:ILE:CD1	2.33	0.55
1:B:78:VAL:HB	1:B:80:GLN:NE2	2.21	0.55
1:A:107:ILE:HG22	1:A:327:ILE:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ILE:HD12	1:B:132:ILE:H	1.71	0.55
1:B:138:ASN:C	1:B:140:VAL:N	2.59	0.55
1:A:233:GLU:O	1:A:235:ALA:N	2.40	0.55
1:A:301:VAL:HG12	1:A:303:TRP:CD1	2.41	0.55
1:A:62:ALA:HA	1:A:65:THR:OG1	2.07	0.55
1:A:65:THR:HB	1:A:77:ARG:NH2	2.21	0.55
1:A:69:ILE:HB	1:A:74:SER:OG	2.07	0.55
1:A:162:GLY:HA2	2:A:330:NAD:O7N	2.07	0.54
1:B:166:ASP:O	1:B:169:ARG:HB2	2.08	0.54
1:B:278:PHE:HE2	1:B:305:LEU:HD11	1.72	0.54
1:A:78:VAL:HB	1:A:80:GLN:HE21	1.72	0.54
1:B:201:PHE:CZ	1:B:228:LEU:HD13	2.42	0.54
1:B:77:ARG:O	1:B:78:VAL:HG23	2.07	0.54
1:A:65:THR:CB	1:A:77:ARG:NH1	2.69	0.54
1:A:37:TYR:HB2	1:A:65:THR:CG2	2.38	0.54
1:A:107:ILE:HG22	1:A:327:ILE:CD1	2.37	0.54
1:B:62:ALA:HA	1:B:65:THR:OG1	2.07	0.54
1:B:138:ASN:O	1:B:140:VAL:HG12	2.06	0.54
1:A:298:GLU:O	1:A:299:GLU:HB3	2.07	0.54
1:A:62:ALA:N	1:A:79:ARG:NH1	2.52	0.54
1:A:51:VAL:HG21	1:A:86:THR:HG22	1.89	0.54
1:A:290:VAL:HG21	1:A:297:VAL:HG22	1.90	0.54
1:A:64:ASP:HB2	1:B:238:VAL:HG23	1.90	0.54
1:B:53:ILE:HG23	2:B:330:NAD:C4A	2.38	0.54
1:A:63:ALA:HB2	1:A:79:ARG:HH21	1.73	0.54
1:B:134:LEU:HD22	1:B:253:VAL:HG13	1.90	0.54
1:A:65:THR:O	1:A:68:GLY:N	2.41	0.53
1:A:31:VAL:HG13	1:A:95:THR:HB	1.90	0.53
1:A:230:ASP:HA	1:A:234:SER:OG	2.07	0.53
1:A:113:ASN:HA	1:A:116:ILE:CD1	2.38	0.53
1:A:140:VAL:HG13	1:A:141:ASP:H	1.74	0.53
1:A:84:GLU:HA	1:A:127:HIS:CE1	2.43	0.53
1:B:134:LEU:HD21	1:B:161:PHE:HB2	1.89	0.53
1:B:190:LEU:HB3	1:B:287:GLY:O	2.09	0.53
1:B:298:GLU:O	1:B:299:GLU:HB3	2.09	0.53
1:A:78:VAL:HG12	1:A:80:GLN:HG3	1.91	0.53
1:B:144:ASN:O	1:B:147:LEU:HB2	2.08	0.53
1:A:166:ASP:OD2	1:A:193:HIS:HD2	1.91	0.52
1:B:31:VAL:HG12	2:B:330:NAD:O2N	2.10	0.52
1:A:164:ARG:HD3	1:A:268:LEU:HD22	1.90	0.52
1:B:59:VAL:C	1:B:79:ARG:CZ	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:THR:O	1:B:89:SER:HB2	2.10	0.52
1:B:236:MET:SD	1:B:239:ILE:HD11	2.50	0.52
1:B:83:TYR:CD2	1:B:123:SER:HB2	2.45	0.52
1:A:88:GLY:H	1:A:128:ASN:HB3	1.74	0.52
1:A:236:MET:O	1:A:239:ILE:HG13	2.10	0.52
1:B:223:GLU:HA	1:B:223:GLU:OE1	2.10	0.52
1:A:236:MET:HA	1:A:238:VAL:HG12	1.91	0.52
1:A:136:THR:HB	2:A:330:NAD:C2N	2.40	0.52
1:B:274:LEU:HD13	1:B:277:GLU:HB2	1.91	0.52
1:B:100:ARG:NH2	1:B:102:PRO:O	2.43	0.51
1:B:59:VAL:HG13	1:B:79:ARG:HG3	1.91	0.51
1:A:64:ASP:OD2	1:B:242:LYS:HE2	2.11	0.51
1:B:270:ALA:HB3	1:B:290:VAL:HG11	1.92	0.51
1:B:201:PHE:HZ	1:B:228:LEU:HD13	1.74	0.51
1:B:195:ASP:O	1:B:196:ALA:CB	2.59	0.51
1:A:107:ILE:O	1:A:110:ALA:HB3	2.11	0.51
1:A:293:GLY:O	1:A:295:ASN:N	2.43	0.51
1:A:31:VAL:HG12	2:A:330:NAD:PN	2.51	0.51
1:A:292:LEU:HA	1:A:296:GLY:O	2.10	0.51
1:A:144:ASN:O	1:A:147:LEU:HB2	2.11	0.51
1:A:134:LEU:HA	1:A:159:ILE:O	2.10	0.51
1:A:242:LYS:NZ	1:B:61:GLN:OE1	2.44	0.51
1:B:174:LEU:O	1:B:178:PHE:HD1	1.93	0.51
1:A:134:LEU:HD21	1:A:161:PHE:HB2	1.92	0.50
1:B:31:VAL:HG13	1:B:95:THR:HB	1.92	0.50
1:A:139:PRO:HD2	1:A:143:LEU:HD21	1.93	0.50
1:A:267:VAL:HA	1:A:290:VAL:O	2.11	0.50
1:A:195:ASP:O	1:A:196:ALA:CB	2.60	0.50
1:B:21:THR:O	1:B:46:ASP:HB2	2.11	0.50
1:B:241:ARG:NH1	1:B:241:ARG:HG3	2.27	0.50
1:B:88:GLY:N	1:B:128:ASN:HB3	2.26	0.50
1:B:78:VAL:CB	1:B:80:GLN:HE21	2.24	0.50
1:A:63:ALA:N	1:A:79:ARG:NH2	2.53	0.50
1:A:169:ARG:HD3	1:B:67:HIS:CE1	2.47	0.50
1:B:63:ALA:HB2	1:B:79:ARG:HH21	1.77	0.50
1:B:62:ALA:N	1:B:79:ARG:NH1	2.60	0.50
1:A:59:VAL:HA	1:A:79:ARG:CG	2.41	0.50
1:B:211:PRO:HA	1:B:219:PHE:CZ	2.46	0.50
1:B:264:THR:OG1	1:B:266:GLU:HG3	2.12	0.50
1:B:95:THR:O	2:B:330:NAD:H51N	2.11	0.50
1:B:80:GLN:O	1:B:81:GLY:C	2.50	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:PHE:HA	1:B:204:VAL:HG23	1.94	0.49
1:B:62:ALA:CB	1:B:79:ARG:NH1	2.74	0.49
1:B:106:ARG:O	1:B:109:LEU:HB3	2.12	0.49
1:A:305:LEU:HD12	1:A:305:LEU:H	1.78	0.49
1:B:62:ALA:HB1	1:B:77:ARG:HD3	1.94	0.49
1:B:32:GLY:HA2	1:B:95:THR:CG2	2.34	0.49
1:B:241:ARG:HG3	1:B:241:ARG:HH11	1.77	0.49
1:A:22:LYS:HA	1:A:47:GLU:O	2.12	0.49
1:A:154:SER:OG	1:A:156:GLU:HG2	2.11	0.49
1:A:86:THR:O	1:A:89:SER:HB2	2.13	0.49
1:B:27(A):ALA:HB1	1:B:50:PHE:HB3	1.94	0.49
1:B:136:THR:HG22	1:B:161:PHE:HB3	1.95	0.49
1:B:53:ILE:HB	1:B:53(A):PRO:HD2	1.95	0.49
1:B:209:THR:O	1:B:211:PRO:HD3	2.13	0.49
1:B:100:ARG:HG2	1:B:101:GLN:N	2.27	0.49
1:A:115:PRO:O	1:A:118:GLU:HB2	2.12	0.48
1:B:305:LEU:HB3	1:B:309:GLU:OE1	2.12	0.48
1:B:197:GLN:NE2	1:B:232:GLN:HG3	2.28	0.48
1:B:154:SER:OG	1:B:156:GLU:HG2	2.13	0.48
1:B:205:ARG:HG3	1:B:210:ASP:OD2	2.13	0.48
1:B:281:HIS:O	1:B:282:GLU:HG3	2.13	0.48
1:A:134:LEU:CD2	1:A:161:PHE:HB2	2.44	0.48
1:B:253:VAL:O	1:B:257:VAL:HG23	2.13	0.48
1:A:197:GLN:NE2	1:A:232:GLN:HG3	2.29	0.48
1:B:77:ARG:C	1:B:77:ARG:HD2	2.33	0.48
1:A:199:PRO:HG3	1:A:228:LEU:HD21	1.96	0.48
1:B:169:ARG:O	1:B:173:VAL:HG22	2.14	0.48
1:B:84:GLU:HA	1:B:127:HIS:CE1	2.49	0.48
1:B:59:VAL:O	1:B:79:ARG:NH2	2.47	0.48
1:A:108:ASP:O	1:A:111:GLY:N	2.47	0.48
1:B:211:PRO:C	1:B:219:PHE:H	2.18	0.48
1:B:258:GLU:O	1:B:262:HIS:HB2	2.14	0.48
1:A:197:GLN:HE22	1:A:232:GLN:HG3	1.79	0.47
1:A:199:PRO:HG3	1:A:228:LEU:HD11	1.95	0.47
1:A:67:HIS:HE1	1:B:235:ALA:O	1.97	0.47
1:A:143:LEU:HD22	1:A:143:LEU:H	1.79	0.47
1:B:134:LEU:HA	1:B:159:ILE:O	2.13	0.47
1:A:234:SER:C	1:A:236:MET:N	2.66	0.47
1:B:111:GLY:O	1:B:114:ALA:HB3	2.13	0.47
1:A:44:ILE:CD1	1:A:261:LEU:HD12	2.44	0.47
1:B:189:ILE:HD11	1:B:231:LEU:CD2	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:MET:O	1:A:260:ILE:HG13	2.15	0.47
1:A:128:ASN:N	1:A:128:ASN:HD22	2.10	0.47
1:A:201:PHE:CZ	1:A:228:LEU:HD13	2.49	0.47
1:B:309:GLU:O	1:B:312:LEU:N	2.46	0.47
1:A:164:ARG:N	1:A:269:PRO:HG2	2.29	0.47
1:B:106:ARG:HG3	1:B:106:ARG:HH11	1.80	0.47
1:A:105:THR:O	1:A:107:ILE:N	2.47	0.47
1:B:69:ILE:O	1:B:71:TYR:N	2.48	0.47
1:B:164:ARG:N	1:B:269:PRO:HG2	2.28	0.47
1:A:230:ASP:HA	1:A:234:SER:CB	2.44	0.47
1:A:219:PHE:O	1:A:221:GLY:N	2.46	0.47
1:A:192:GLU:HG3	1:A:320:LEU:HD11	1.95	0.47
1:A:100:ARG:NH2	1:A:103:GLY:O	2.48	0.47
1:B:117:MET:HB3	1:B:147:LEU:HG	1.96	0.47
1:B:83:TYR:CE2	1:B:123:SER:HB2	2.49	0.47
1:A:69:ILE:CG1	1:A:70:ALA:H	2.22	0.47
1:A:101:GLN:HB3	1:A:102:PRO:HD2	1.97	0.47
1:B:82:GLY:C	1:B:84:GLU:N	2.68	0.47
1:A:132:ILE:HA	1:A:157:GLN:HB3	1.96	0.46
1:A:59:VAL:HG22	1:A:79:ARG:HG3	1.98	0.46
1:B:115:PRO:HA	1:B:118:GLU:CD	2.36	0.46
1:A:80:GLN:O	1:A:81:GLY:C	2.53	0.46
1:B:221:GLY:HA2	1:B:224:LYS:HE3	1.98	0.46
1:A:164:ARG:HH11	1:A:164:ARG:HG3	1.80	0.46
1:A:125:ASP:O	1:A:126:GLU:HG2	2.15	0.46
1:A:61:GLN:N	1:A:79:ARG:HH22	2.14	0.46
1:A:305:LEU:HB3	1:A:309:GLU:OE1	2.16	0.46
1:A:100:ARG:HG2	1:A:101:GLN:N	2.30	0.46
1:A:104:GLN:HG3	1:A:109:LEU:HB2	1.97	0.46
1:B:205:ARG:HG2	1:B:209:THR:O	2.15	0.46
1:B:134:LEU:CD2	1:B:161:PHE:HB2	2.46	0.46
1:B:174:LEU:CB	1:B:185:VAL:HG11	2.46	0.46
1:B:230:ASP:HA	1:B:234:SER:CB	2.47	0.45
1:A:307:ASP:HA	1:A:310:GLN:HB2	1.98	0.45
1:B:234:SER:C	1:B:236:MET:H	2.19	0.45
1:A:245:THR:OG1	2:A:330:NAD:H6N	2.16	0.45
1:B:132:ILE:HA	1:B:157:GLN:HB3	1.98	0.45
1:B:236:MET:HA	1:B:238:VAL:HG12	1.98	0.45
1:B:143:LEU:H	1:B:143:LEU:HD22	1.82	0.45
1:B:164:ARG:HD3	1:B:268:LEU:HD22	1.99	0.45
1:B:62:ALA:HB1	1:B:77:ARG:CD	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:GLY:O	1:B:105:THR:N	2.47	0.45
1:B:195:ASP:O	1:B:196:ALA:HB3	2.17	0.45
1:B:59:VAL:O	1:B:59:VAL:CG1	2.64	0.45
1:A:61:GLN:OE1	1:B:242:LYS:NZ	2.48	0.45
1:A:128:ASN:ND2	1:A:128:ASN:N	2.64	0.45
1:A:64:ASP:OD2	1:B:246:GLU:HB3	2.17	0.45
1:A:73:ASP:HA	1:B:183:GLN:OE1	2.17	0.45
1:A:205:ARG:HD2	1:A:208:GLY:HA2	1.98	0.45
1:B:301:VAL:HG12	1:B:303:TRP:CD1	2.52	0.45
1:A:94:ILE:HG22	1:A:94:ILE:O	2.17	0.45
1:B:79:ARG:NH1	1:B:79:ARG:HB3	2.18	0.44
1:B:305:LEU:N	1:B:305:LEU:HD12	2.33	0.44
1:A:87:ALA:HB2	1:A:127:HIS:HB3	1.99	0.44
1:A:77:ARG:O	1:A:78:VAL:HG23	2.18	0.44
1:A:274:LEU:HD13	1:A:277:GLU:HB2	1.99	0.44
1:B:108:ASP:O	1:B:111:GLY:N	2.51	0.44
1:A:174:LEU:HB3	1:A:185:VAL:HG11	2.00	0.44
1:A:174:LEU:CB	1:A:185:VAL:HG11	2.48	0.44
1:B:211:PRO:HA	1:B:219:PHE:CE1	2.53	0.44
1:B:101:GLN:HB3	1:B:102:PRO:HD2	2.00	0.44
1:A:274:LEU:HD12	1:A:277:GLU:O	2.18	0.44
1:B:51:VAL:HG21	1:B:86:THR:HG22	1.99	0.44
1:B:62:ALA:CB	1:B:77:ARG:HD3	2.48	0.44
1:B:51:VAL:HG22	1:B:81:GLY:O	2.18	0.44
1:B:113:ASN:HB2	1:B:143:LEU:HD11	2.00	0.44
1:A:183:GLN:OE1	1:B:73:ASP:HA	2.17	0.44
1:A:169:ARG:HD2	1:A:236:MET:HE1	2.00	0.44
1:A:290:VAL:HG23	1:A:297:VAL:HG13	1.99	0.44
1:B:174:LEU:HB3	1:B:185:VAL:HG11	2.00	0.44
1:A:139:PRO:HB2	1:A:143:LEU:CD2	2.47	0.44
1:A:29:GLY:O	1:A:32:GLY:N	2.50	0.44
1:A:105:THR:O	1:A:106:ARG:C	2.56	0.44
1:A:277:GLU:O	1:A:278:PHE:HB2	2.18	0.44
1:B:130:ASP:O	1:B:131:TYR:C	2.56	0.44
1:A:78:VAL:CG1	1:A:79:ARG:N	2.81	0.44
1:A:62:ALA:HB3	1:A:79:ARG:CZ	2.48	0.43
1:A:77:ARG:C	1:A:77:ARG:HD2	2.37	0.43
1:B:103:GLY:C	1:B:105:THR:H	2.22	0.43
1:A:63:ALA:H	1:A:79:ARG:HH22	1.58	0.43
1:A:230:ASP:HA	1:A:234:SER:HB2	2.01	0.43
1:A:100:ARG:NH2	1:A:102:PRO:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:HIS:CE1	2:A:330:NAD:O7N	2.71	0.43
1:B:114:ALA:O	1:B:118:GLU:HG3	2.18	0.43
1:B:59:VAL:O	1:B:79:ARG:CZ	2.67	0.43
1:B:107:ILE:CG2	1:B:327:ILE:HD13	2.48	0.43
1:B:202:SER:HA	1:B:218:GLU:OE1	2.19	0.43
1:A:252:GLY:O	1:A:255:HIS:HB3	2.19	0.43
1:B:60:GLY:CA	1:B:79:ARG:NH2	2.81	0.43
1:B:117:MET:HG3	1:B:143:LEU:HD12	1.99	0.43
1:B:69:ILE:CG1	1:B:70:ALA:H	2.23	0.43
1:A:57:ASP:OD1	1:A:57:ASP:N	2.51	0.43
1:A:62:ALA:HB1	1:A:77:ARG:HD3	1.99	0.43
1:B:188:THR:HG22	1:B:189:ILE:H	1.83	0.43
1:B:201:PHE:HA	1:B:204:VAL:CG2	2.47	0.43
1:A:281:HIS:O	1:A:282:GLU:HG3	2.19	0.43
1:B:292:LEU:HA	1:B:296:GLY:O	2.19	0.43
1:B:59:VAL:C	1:B:79:ARG:NH2	2.72	0.43
1:A:182:VAL:HG21	1:B:70:ALA:CB	2.41	0.43
1:A:201:PHE:HZ	1:A:228:LEU:HD13	1.84	0.43
1:A:211:PRO:C	1:A:219:PHE:H	2.22	0.43
1:A:174:LEU:O	1:A:178:PHE:HD1	2.02	0.43
1:A:60:GLY:C	1:A:79:ARG:HH22	2.23	0.42
1:A:136:THR:HG22	1:A:161:PHE:HB3	2.01	0.42
1:B:139:PRO:HB2	1:B:143:LEU:CD2	2.49	0.42
1:B:58:THR:C	1:B:60:GLY:H	2.22	0.42
1:B:83:TYR:OH	2:B:330:NAD:N1A	2.53	0.42
1:B:79:ARG:C	1:B:81:GLY:H	2.21	0.42
1:A:62:ALA:HB1	1:A:77:ARG:CD	2.49	0.42
1:B:210:ASP:HA	1:B:211:PRO:HD3	1.74	0.42
1:B:146:HIS:O	1:B:150:ALA:CB	2.67	0.42
1:B:55:GLU:HG3	1:B:55:GLU:O	2.18	0.42
1:A:78:VAL:HB	1:A:80:GLN:NE2	2.35	0.42
1:A:266:GLU:O	1:A:291:ARG:HA	2.20	0.42
1:A:56:ASP:O	1:B:241:ARG:CB	2.67	0.42
1:B:162:GLY:HA2	2:B:330:NAD:O7N	2.20	0.42
1:A:83:TYR:OH	2:A:330:NAD:N1A	2.53	0.42
1:B:300:ILE:HD12	1:B:300:ILE:H	1.85	0.42
1:B:65:THR:CB	1:B:77:ARG:NH1	2.80	0.42
1:A:105:THR:HG23	1:A:105:THR:O	2.20	0.42
1:B:274:LEU:HD12	1:B:277:GLU:O	2.20	0.42
1:A:53:ILE:HB	1:A:53(A):PRO:HD2	2.02	0.42
1:B:39:ILE:HD11	1:B:93:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:GLU:OE1	1:A:223:GLU:HA	2.19	0.42
1:A:106:ARG:O	1:A:107:ILE:C	2.59	0.41
1:B:281:HIS:C	1:B:282:GLU:HG3	2.40	0.41
1:B:63:ALA:N	1:B:79:ARG:NH2	2.62	0.41
1:A:210:ASP:HA	1:A:211:PRO:HD3	1.69	0.41
1:B:278:PHE:CE1	1:B:302:GLU:HA	2.55	0.41
1:B:146:HIS:O	1:B:150:ALA:HB3	2.20	0.41
1:B:145:ARG:O	1:B:149:GLU:HG2	2.19	0.41
1:A:281:HIS:HB3	1:A:284:THR:HG21	2.01	0.41
1:A:301:VAL:HG12	1:A:303:TRP:HD1	1.83	0.41
1:A:73:ASP:O	1:A:74:SER:CB	2.67	0.41
1:B:69:ILE:HD13	1:B:69:ILE:HG21	1.89	0.41
1:B:170:PHE:O	1:B:173:VAL:HG23	2.21	0.41
1:A:248:GLY:HA2	1:B:68:GLY:HA2	2.02	0.41
1:A:247:TRP:CE3	1:A:247:TRP:HA	2.55	0.41
1:A:59:VAL:CG1	1:A:59:VAL:O	2.68	0.41
1:A:60:GLY:CA	1:A:79:ARG:NH2	2.84	0.41
1:A:235:ALA:O	1:B:67:HIS:HE1	2.03	0.41
1:A:241:ARG:H	1:A:241:ARG:HG2	1.69	0.41
1:B:131:TYR:CG	1:B:131:TYR:O	2.73	0.41
1:A:130:ASP:O	1:A:131:TYR:C	2.59	0.41
1:B:98:ILE:O	1:B:109:LEU:HD11	2.21	0.41
1:A:85:ASP:C	1:A:87:ALA:H	2.24	0.41
1:B:247:TRP:O	1:B:248:GLY:C	2.59	0.41
1:A:234:SER:O	1:A:236:MET:N	2.53	0.41
1:A:258:GLU:O	1:A:262:HIS:HB2	2.21	0.41
1:B:219:PHE:N	1:B:219:PHE:CD1	2.88	0.40
1:A:79:ARG:O	1:A:81:GLY:N	2.49	0.40
1:B:136:THR:O	1:B:137:SER:C	2.59	0.40
1:B:57:ASP:OD1	1:B:57:ASP:N	2.54	0.40
1:B:51:VAL:HG13	1:B:81:GLY:O	2.22	0.40
1:A:114:ALA:O	1:A:118:GLU:HG3	2.20	0.40
1:B:218:GLU:C	1:B:220:SER:N	2.72	0.40
1:B:60:GLY:C	1:B:79:ARG:HH22	2.25	0.40
1:A:60:GLY:N	1:A:79:ARG:NH2	2.69	0.40
1:B:138:ASN:HB2	2:B:330:NAD:O2D	2.21	0.40
1:B:140:VAL:HG13	1:B:141:ASP:H	1.86	0.40
1:B:29:GLY:O	1:B:32:GLY:N	2.47	0.40
1:A:290:VAL:CG2	1:A:297:VAL:HG13	2.51	0.40
1:B:100:ARG:NH2	1:B:103:GLY:O	2.55	0.40
1:A:300:ILE:HD12	1:A:300:ILE:H	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:VAL:HG11	2:B:330:NAD:H72N	1.87	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	301/303 (99%)	230 (76%)	46 (15%)	25 (8%)	1 7
1	B	301/303 (99%)	232 (77%)	47 (16%)	22 (7%)	1 9
All	All	602/606 (99%)	462 (77%)	93 (15%)	47 (8%)	1 8

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	THR
1	A	55	GLU
1	A	70	ALA
1	A	71	TYR
1	A	106	ARG
1	A	131	TYR
1	A	140	VAL
1	A	152	ASP
1	A	196	ALA
1	A	234	SER
1	A	294	SER
1	B	30	THR
1	B	70	ALA
1	B	81	GLY
1	B	104	GLN
1	B	106	ARG
1	B	131	TYR

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Mol	Chain	Res	Type
1	B	140	VAL
1	B	152	ASP
1	B	196	ALA
1	B	234	SER
1	B	294	SER
1	A	81	GLY
1	A	82	GLY
1	A	200	VAL
1	B	71	TYR
1	B	79	ARG
1	B	82	GLY
1	B	220	SER
1	A	73	ASP
1	A	80	GLN
1	A	104	GLN
1	B	105	THR
1	B	299	GLU
1	A	56	ASP
1	A	105	THR
1	A	107	ILE
1	A	220	SER
1	A	299	GLU
1	B	73	ASP
1	A	235	ALA
1	B	56	ASP
1	B	250	ALA
1	A	79	ARG
1	A	59	VAL
1	B	221	GLY
1	B	69	ILE

5.3.2 Protein sidechains (i)

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	244/244 (100%)	211 (86%)	33 (14%)	5 22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	244/244 (100%)	211 (86%)	33 (14%)	5 22
All	All	488/488 (100%)	422 (86%)	66 (14%)	5 22

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	THR
1	A	41	LEU
1	A	53(A)	PRO
1	A	53(B)	ASP
1	A	55	GLU
1	A	57	ASP
1	A	58	THR
1	A	65	THR
1	A	71	TYR
1	A	74	SER
1	A	76	THR
1	A	77	ARG
1	A	79	ARG
1	A	84	GLU
1	A	89	SER
1	A	102	PRO
1	A	104	GLN
1	A	128	ASN
1	A	135	THR
1	A	152	ASP
1	A	169	ARG
1	A	183	GLN
1	A	188	THR
1	A	223	GLU
1	A	227	LEU
1	A	232	GLN
1	A	236	MET
1	A	239	ILE
1	A	274	LEU
1	A	288	VAL
1	A	305	LEU
1	A	307	ASP
1	A	320	LEU
1	B	30	THR
1	B	41	LEU
1	B	53(A)	PRO

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Mol	Chain	Res	Type
1	B	53(B)	ASP
1	B	55	GLU
1	B	57	ASP
1	B	65	THR
1	B	71	TYR
1	B	74	SER
1	B	77	ARG
1	B	79	ARG
1	B	84	GLU
1	B	89	SER
1	B	123	SER
1	B	128	ASN
1	B	129	ASP
1	B	135	THR
1	B	152	ASP
1	B	169	ARG
1	B	183	GLN
1	B	219	PHE
1	B	222	ASP
1	B	223	GLU
1	B	227	LEU
1	B	232	GLN
1	B	239	ILE
1	B	240	GLU
1	B	241	ARG
1	B	274	LEU
1	B	288	VAL
1	B	305	LEU
1	B	307	ASP
1	B	320	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	80	GLN
1	A	128	ASN
1	A	138	ASN
1	A	157	GLN
1	A	183	GLN
1	A	184	ASN
1	A	193	HIS

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Mol	Chain	Res	Type
1	A	281	HIS
1	B	75	ASN
1	B	80	GLN
1	B	128	ASN
1	B	138	ASN
1	B	157	GLN
1	B	183	GLN
1	B	184	ASN
1	B	193	HIS
1	B	281	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 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	330	-	38,48,48	1.04	4 (10%)	47,73,73	2.48	10 (21%)
2	NAD	B	330	-	38,48,48	1.07	2 (5%)	47,73,73	2.43	14 (29%)

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	330	-	-	0/22/62/62	0/5/5/5
2	NAD	B	330	-	-	0/22/62/62	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	330	NAD	O3D-C3D	2.01	1.47	1.43
2	B	330	NAD	O4D-C1D	2.08	1.43	1.41
2	A	330	NAD	C6N-N1N	2.12	1.41	1.35
2	A	330	NAD	O4D-C1D	2.40	1.44	1.41
2	A	330	NAD	O4B-C1B	2.43	1.44	1.41
2	B	330	NAD	O4B-C1B	2.98	1.45	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	330	NAD	C4B-O4B-C1B	-8.13	100.78	109.72
2	A	330	NAD	C4D-O4D-C1D	-8.09	100.83	109.72
2	B	330	NAD	C4D-O4D-C1D	-7.45	101.53	109.72
2	A	330	NAD	N3A-C2A-N1A	-7.43	123.21	128.89
2	B	330	NAD	N3A-C2A-N1A	-7.39	123.24	128.89
2	B	330	NAD	C4B-O4B-C1B	-4.50	104.78	109.72
2	B	330	NAD	O2B-C2B-C3B	-4.10	98.50	111.83
2	B	330	NAD	O7N-C7N-C3N	-3.88	115.35	119.59
2	B	330	NAD	C1B-N9A-C4A	-3.87	121.10	126.94
2	B	330	NAD	O5D-PN-O1N	-2.98	98.04	109.62
2	A	330	NAD	PN-O3-PA	-2.95	124.45	132.73
2	B	330	NAD	C4N-C3N-C7N	-2.52	114.43	121.09
2	A	330	NAD	C1B-N9A-C4A	-2.44	123.26	126.94
2	A	330	NAD	O7N-C7N-C3N	-2.18	117.20	119.59
2	B	330	NAD	O4D-C1D-N1N	2.06	110.40	108.13
2	A	330	NAD	C4A-C5A-N7A	2.08	111.39	109.48
2	B	330	NAD	C3N-C2N-N1N	2.25	122.96	120.36
2	B	330	NAD	C6N-C5N-C4N	2.44	123.13	119.44
2	A	330	NAD	O4D-C1D-N1N	3.02	111.45	108.13
2	B	330	NAD	C2B-C1B-N9A	3.19	119.17	114.29
2	B	330	NAD	O3-PN-O5D	3.22	111.47	102.94
2	A	330	NAD	O4B-C1B-N9A	3.44	115.29	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	330	NAD	O4B-C1B-N9A	3.57	115.58	108.10
2	A	330	NAD	C2B-C1B-N9A	4.58	121.30	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	330	NAD	10	0
2	B	330	NAD	12	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	303/303 (100%)	1.17	57 (18%)	2	1	2, 16, 35, 46	0
1	B	303/303 (100%)	1.07	41 (13%)	4	2	2, 16, 35, 47	0
All	All	606/606 (100%)	1.12	98 (16%)	3	2	2, 16, 35, 47	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	232	GLN	7.2
1	B	232	GLN	6.4
1	A	74	SER	5.4
1	A	57	ASP	5.1
1	B	150	ALA	4.4
1	A	219	PHE	4.3
1	A	130	ASP	4.2
1	B	211	PRO	4.2
1	A	323	GLN	4.0
1	B	57	ASP	4.0
1	B	27	GLY	4.0
1	A	150	ALA	3.9
1	A	146	HIS	3.9
1	B	58	THR	3.8
1	A	140	VAL	3.8
1	A	124	LEU	3.8
1	B	79	ARG	3.7
1	A	127	HIS	3.6
1	A	82	GLY	3.4
1	B	99	PRO	3.3
1	B	245	THR	3.3
1	B	272	VAL	3.2
1	A	24	SER	3.2
1	A	244	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	180	ALA	3.1
1	A	64	ASP	3.1
1	A	21	THR	3.1
1	A	283	ASP	3.1
1	A	81	GLY	3.1
1	B	102	PRO	3.1
1	B	328	SER	3.1
1	B	124	LEU	3.0
1	A	138	ASN	3.0
1	B	219	PHE	3.0
1	A	129	ASP	3.0
1	B	141	ASP	2.9
1	B	249	PRO	2.8
1	B	98	ILE	2.8
1	B	63	ALA	2.8
1	B	74	SER	2.8
1	B	21	THR	2.8
1	A	78	VAL	2.7
1	A	86	THR	2.7
1	A	23	VAL	2.7
1	A	156	GLU	2.6
1	A	68	GLY	2.6
1	A	313	MET	2.6
1	B	65	THR	2.6
1	A	79	ARG	2.5
1	B	278	PHE	2.5
1	A	105	THR	2.5
1	A	60	GLY	2.5
1	B	100	ARG	2.4
1	B	138	ASN	2.4
1	A	169	ARG	2.4
1	A	25	VAL	2.3
1	A	48	VAL	2.3
1	B	279	GLY	2.3
1	A	167	SER	2.3
1	A	246	GLU	2.3
1	A	56	ASP	2.3
1	A	51	VAL	2.3
1	A	128	ASN	2.3
1	A	269	PRO	2.3
1	A	293	GLY	2.3
1	A	63	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	100	ARG	2.2
1	A	59	VAL	2.2
1	A	208	GLY	2.2
1	B	287	GLY	2.2
1	A	310	GLN	2.2
1	A	294	SER	2.2
1	B	27(A)	ALA	2.2
1	A	77	ARG	2.2
1	A	151	GLY	2.2
1	A	69	ILE	2.1
1	B	146	HIS	2.1
1	A	328	SER	2.1
1	B	220	SER	2.1
1	B	151	GLY	2.1
1	B	42	ARG	2.1
1	A	45	ALA	2.1
1	A	75	ASN	2.1
1	A	135	THR	2.1
1	B	284	THR	2.1
1	B	69	ILE	2.1
1	A	103	GLY	2.1
1	B	80	GLN	2.1
1	B	323	GLN	2.0
1	B	95	THR	2.0
1	B	162	GLY	2.0
1	A	133	SER	2.0
1	A	312	LEU	2.0
1	A	287	GLY	2.0
1	A	168	ALA	2.0
1	B	114	ALA	2.0
1	B	251	ARG	2.0
1	B	240	GLU	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

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^{th} 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^2)	Q<0.9
2	NAD	A	330	44/44	0.61	0.46	1.24	20,29,34,36	0
2	NAD	B	330	44/44	0.65	0.43	0.66	21,31,36,39	0

6.5 Other polymers

There are no such residues in this entry.