Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:55 PM GMT

PDB ID	:	1Z2I
Title	:	CRYSTAL STRUCTURE OF Agrobacterium tumefaciens MALATE DEHYDROGENASE, NEW YORK STRUCTURAL GENOMICS CONSORTIUM
Authors	:	Patskovsky, Y.; Almo, S.C.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2005-03-08
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
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:

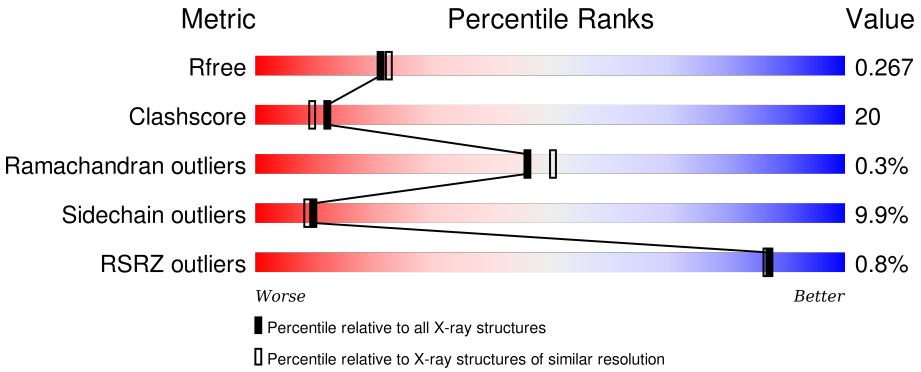
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	358	% 66% 27% 5% •
1	B	358	% 60% 33% 5% •
1	C	358	% 64% 30% • •
1	D	358	62% 31% • •

2 Entry composition

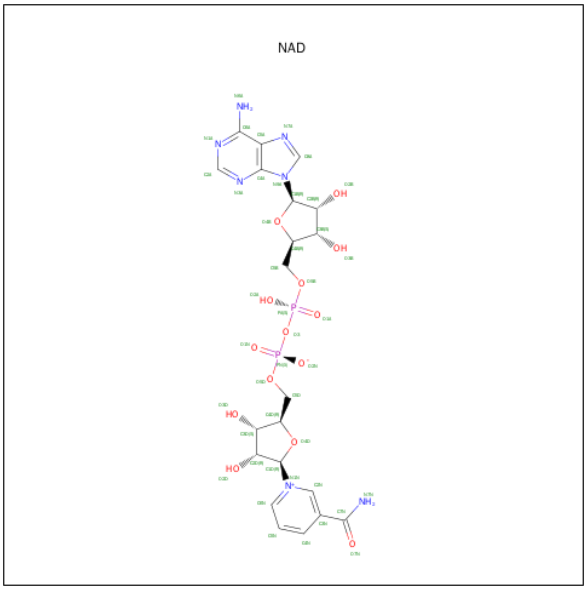
There are 3 unique types of molecules in this entry. The entry contains 11399 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	350	Total	C	N	O	S	0	0	0
			2631	1651	473	492	15			
1	B	350	Total	C	N	O	S	0	0	0
			2631	1651	473	492	15			
1	C	350	Total	C	N	O	S	0	0	0
			2631	1651	473	492	15			
1	D	350	Total	C	N	O	S	0	0	0
			2631	1651	473	492	15			

- 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		

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

- Molecule 3 is water.

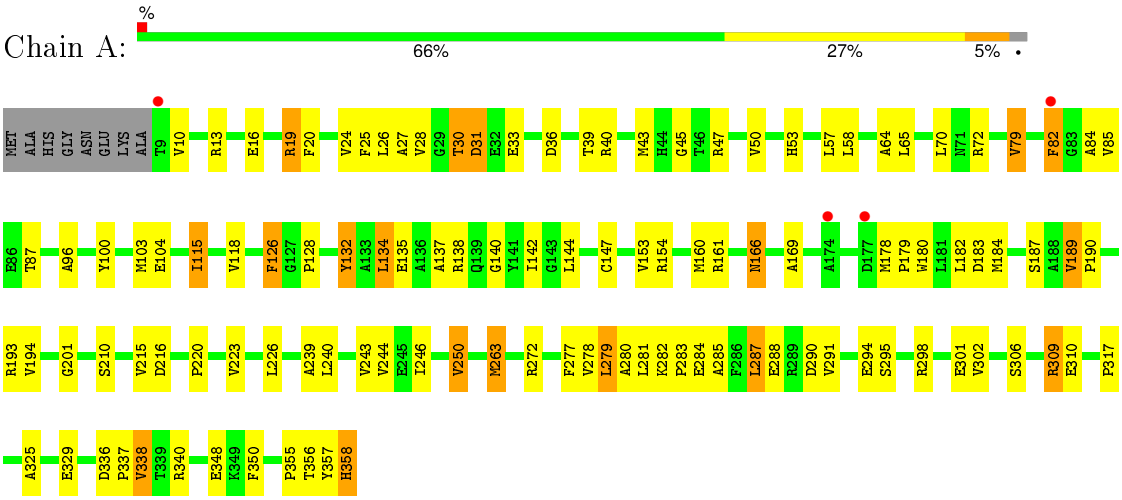
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	172	Total	O	0	0
			172	172		
3	B	188	Total	O	0	0
			188	188		
3	C	168	Total	O	0	0
			168	168		
3	D	171	Total	O	0	0
			171	171		

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.

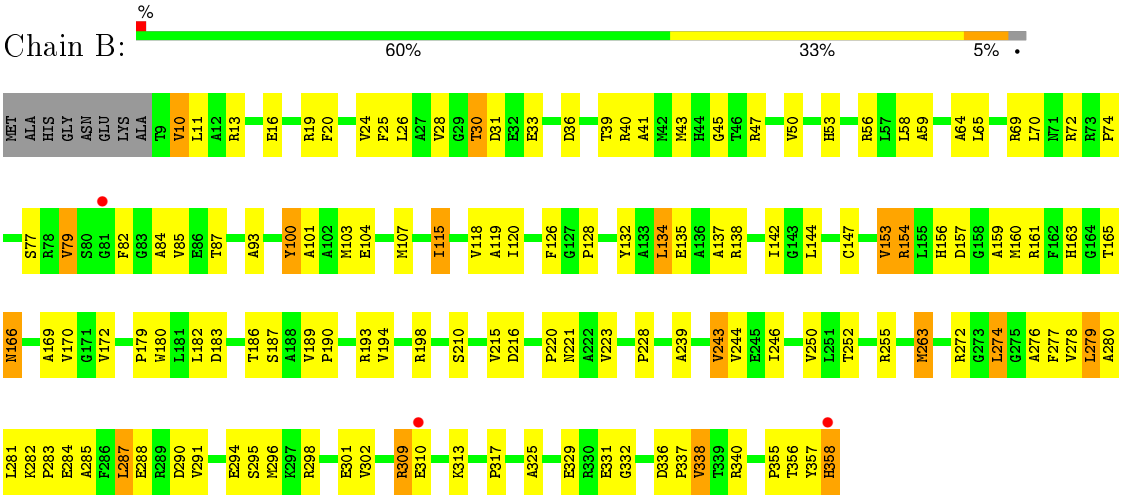
- Molecule 1: malate dehydrogenase

Chain A:



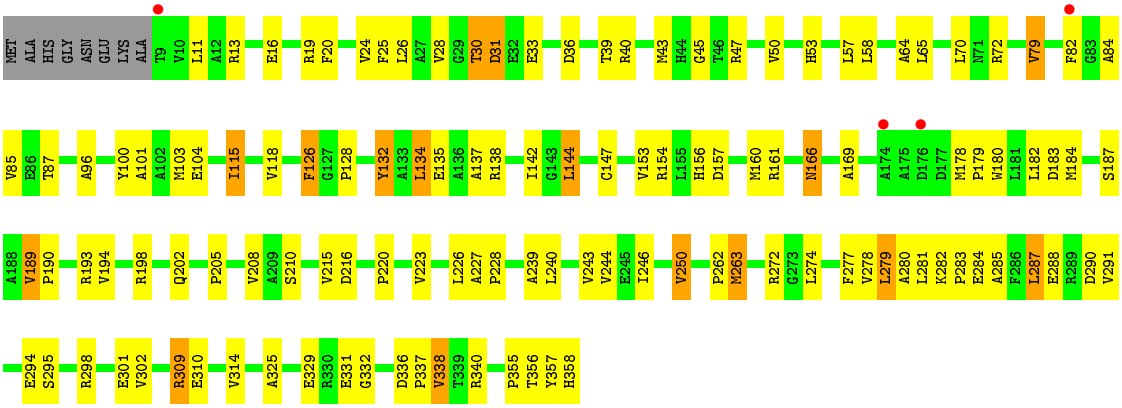
- Molecule 1: malate dehydrogenase

Chain B:



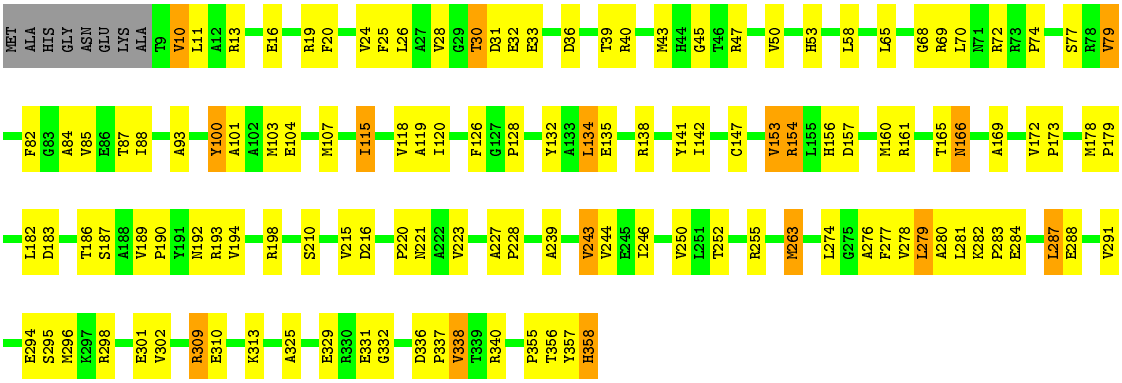
- Molecule 1: malate dehydrogenase

Chain C:



- Molecule 1: malate dehydrogenase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	98.22Å 98.22Å 146.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.83 – 2.20	Depositor EDS
% Data completeness (in resolution range)	88.6 (20.00-2.20) 89.1 (19.83-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.54 (at 2.21Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.239 , 0.265 0.241 , 0.267	Depositor DCC
R_{free} test set	2175 reflections (3.05%)	DCC
Wilson B-factor (Å^2)	23.8	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 32.2	EDS
Estimated twinning fraction	0.068 for -h,-k,l 0.469 for h,-h-k,-l 0.069 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Outliers	0 of 71317 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11399	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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	0.35	0/2688	0.60	0/3642
1	B	0.34	0/2688	0.60	0/3642
1	C	0.34	0/2688	0.59	0/3642
1	D	0.35	0/2688	0.60	0/3642
All	All	0.35	0/10752	0.60	0/14568

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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	TYR	Sidechain
1	B	132	TYR	Sidechain
1	C	132	TYR	Sidechain
1	D	132	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	2631	0	2573	111	0
1	B	2631	0	2573	125	0
1	C	2631	0	2573	115	0
1	D	2631	0	2573	112	0
2	A	44	0	26	2	0
2	B	44	0	26	3	0
2	C	44	0	26	3	0
2	D	44	0	26	3	0
3	A	172	0	0	7	0
3	B	188	0	0	15	0
3	C	168	0	0	7	0
3	D	171	0	0	16	0
All	All	11399	0	10396	417	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 20.

All (417) 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:115:ILE:HD11	1:B:84:ALA:HB3	1.34	1.09
1:C:115:ILE:HD11	1:D:84:ALA:HB3	1.36	1.07
1:A:84:ALA:HB3	1:B:115:ILE:HD11	1.40	1.02
1:C:166:ASN:HB3	1:C:244:VAL:HG21	1.38	1.01
1:A:144:LEU:HD12	1:A:279:LEU:HB3	1.39	1.00
1:A:166:ASN:HB3	1:A:244:VAL:HG21	1.42	1.00
1:C:84:ALA:HB3	1:D:115:ILE:HD11	1.41	1.00
1:B:220:PRO:HG2	3:B:879:HOH:O	1.69	0.93
1:A:285:ALA:HA	1:B:82:PHE:CZ	2.04	0.93
1:A:79:VAL:HG13	1:A:87:THR:HG23	1.51	0.92
1:D:166:ASN:HB3	1:D:244:VAL:HG21	1.50	0.92
1:B:166:ASN:HB3	1:B:244:VAL:HG21	1.53	0.90
1:D:32:GLU:HB2	3:D:860:HOH:O	1.72	0.89
1:A:285:ALA:HA	1:B:82:PHE:CE2	2.07	0.89
1:C:79:VAL:HG13	1:C:87:THR:HG23	1.53	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:VAL:HG22	1:B:190:PRO:HD2	1.58	0.84
1:A:189:VAL:HG22	1:A:190:PRO:HD2	1.60	0.84
1:C:189:VAL:HG22	1:C:190:PRO:HD2	1.61	0.83
1:D:189:VAL:HG22	1:D:190:PRO:HD2	1.59	0.82
1:D:79:VAL:HG13	1:D:87:THR:HG23	1.61	0.82
1:B:79:VAL:HG13	1:B:87:THR:HG23	1.61	0.82
1:B:10:VAL:HG22	1:B:358:HIS:O	1.79	0.81
1:A:144:LEU:HD12	1:A:279:LEU:CB	2.11	0.81
1:C:142:ILE:HB	1:C:281:LEU:HB2	1.65	0.78
1:C:166:ASN:HB3	1:C:244:VAL:CG2	2.14	0.76
1:A:325:ALA:O	1:A:329:GLU:HG2	1.86	0.76
1:A:142:ILE:HB	1:A:281:LEU:HB2	1.66	0.76
1:D:325:ALA:O	1:D:329:GLU:HG2	1.87	0.75
1:B:190:PRO:HD3	2:B:701:NAD:O2N	1.87	0.75
1:C:325:ALA:O	1:C:329:GLU:HG2	1.86	0.75
1:A:82:PHE:HE2	1:B:285:ALA:HB2	1.52	0.74
1:D:190:PRO:HD3	2:D:703:NAD:O2N	1.88	0.73
1:B:142:ILE:HB	1:B:281:LEU:HB2	1.71	0.73
1:B:36:ASP:O	1:B:40:ARG:HG3	1.89	0.73
1:C:309:ARG:HG3	1:C:309:ARG:HH21	1.54	0.73
1:B:325:ALA:O	1:B:329:GLU:HG2	1.88	0.73
1:A:144:LEU:CD1	1:A:279:LEU:HD13	2.20	0.72
1:D:198:ARG:HE	1:D:221:ASN:ND2	1.87	0.72
1:B:313:LYS:HG3	3:B:820:HOH:O	1.90	0.72
1:A:309:ARG:HH21	1:A:309:ARG:HG3	1.53	0.72
1:D:36:ASP:O	1:D:40:ARG:HG3	1.89	0.72
1:A:166:ASN:HB3	1:A:244:VAL:CG2	2.16	0.72
1:D:142:ILE:HB	1:D:281:LEU:HB2	1.71	0.71
1:C:169:ALA:HA	1:C:182:LEU:O	1.91	0.71
1:D:166:ASN:HB3	1:D:244:VAL:CG2	2.22	0.70
1:A:169:ALA:HA	1:A:182:LEU:O	1.93	0.69
1:B:103:MET:HE1	1:B:280:ALA:HB2	1.74	0.69
1:C:291:VAL:HA	1:C:294:GLU:HG2	1.76	0.68
1:A:291:VAL:HA	1:A:294:GLU:HG2	1.75	0.68
1:D:277:PHE:HE2	1:D:279:LEU:HD12	1.59	0.68
1:A:190:PRO:HD3	2:A:700:NAD:O2N	1.93	0.67
1:C:190:PRO:HD3	2:C:702:NAD:O2N	1.94	0.67
1:B:69:ARG:HD3	3:B:870:HOH:O	1.94	0.67
1:C:287:LEU:HD22	1:C:291:VAL:HG23	1.75	0.66
1:B:166:ASN:HB3	1:B:244:VAL:CG2	2.25	0.65
1:D:189:VAL:HG22	1:D:193:ARG:HG3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:LEU:HD22	1:A:291:VAL:HG23	1.78	0.65
1:C:153:VAL:HG21	3:C:865:HOH:O	1.97	0.65
1:B:277:PHE:HE2	1:B:279:LEU:HD12	1.59	0.65
1:A:201:GLY:HA2	3:A:830:HOH:O	1.96	0.65
1:A:153:VAL:HG21	3:A:862:HOH:O	1.95	0.65
1:A:36:ASP:O	1:A:40:ARG:HG3	1.97	0.65
1:D:103:MET:CE	1:D:280:ALA:HB2	2.27	0.64
1:D:198:ARG:HD2	3:D:723:HOH:O	1.97	0.64
1:C:19:ARG:HG2	3:C:721:HOH:O	1.98	0.64
1:A:65:LEU:HD23	1:A:70:LEU:HB2	1.80	0.64
1:B:189:VAL:HG22	1:B:193:ARG:HG3	1.79	0.64
1:A:161:ARG:HG3	3:A:740:HOH:O	1.97	0.64
1:A:277:PHE:HE2	1:A:279:LEU:HD12	1.62	0.63
1:C:36:ASP:O	1:C:40:ARG:HG3	1.98	0.63
1:B:198:ARG:HE	1:B:221:ASN:ND2	1.96	0.63
1:B:103:MET:CE	1:B:280:ALA:HB2	2.28	0.63
1:D:19:ARG:HD2	3:D:780:HOH:O	1.99	0.63
1:C:65:LEU:HD23	1:C:70:LEU:HB2	1.81	0.63
1:A:153:VAL:HG11	1:A:187:SER:HB3	1.81	0.63
1:C:153:VAL:HG11	1:C:187:SER:HB3	1.81	0.62
1:B:291:VAL:HA	1:B:294:GLU:HG2	1.80	0.62
1:D:156:HIS:HD2	3:D:856:HOH:O	1.82	0.62
1:D:291:VAL:HA	1:D:294:GLU:HG2	1.80	0.62
1:B:336:ASP:HB2	1:B:337:PRO:HD2	1.81	0.62
1:D:255:ARG:HG3	3:D:705:HOH:O	2.00	0.62
1:A:144:LEU:HD12	1:A:279:LEU:HD13	1.82	0.62
1:A:19:ARG:HG2	3:A:723:HOH:O	1.98	0.62
1:D:68:GLY:HA2	3:D:719:HOH:O	2.00	0.61
1:D:103:MET:HE1	1:D:280:ALA:HB2	1.80	0.61
1:C:53:HIS:HB3	1:C:128:PRO:HD3	1.83	0.61
1:B:77:SER:HB3	3:B:710:HOH:O	2.00	0.61
1:D:336:ASP:HB2	1:D:337:PRO:HD2	1.81	0.61
1:B:41:ALA:HB3	3:B:873:HOH:O	2.00	0.60
1:B:65:LEU:HD23	1:B:70:LEU:HB2	1.83	0.60
1:D:65:LEU:HD23	1:D:70:LEU:HB2	1.83	0.60
1:A:161:ARG:HD2	3:A:818:HOH:O	2.01	0.60
1:C:115:ILE:HD13	1:D:115:ILE:HD13	1.83	0.60
1:C:285:ALA:HA	1:D:82:PHE:CZ	2.37	0.60
1:B:134:LEU:O	1:B:138:ARG:HG3	2.02	0.60
1:D:134:LEU:O	1:D:138:ARG:HG3	2.02	0.59
1:C:277:PHE:HE2	1:C:279:LEU:HD12	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:VAL:HG21	3:B:884:HOH:O	2.02	0.59
1:D:198:ARG:HE	1:D:221:ASN:HD22	1.46	0.59
1:C:16:GLU:HG3	1:C:355:PRO:HA	1.84	0.59
1:B:255:ARG:HG3	3:B:705:HOH:O	2.02	0.59
1:D:10:VAL:HG22	1:D:358:HIS:O	2.02	0.59
1:A:115:ILE:HD13	1:B:115:ILE:HD13	1.84	0.59
1:C:182:LEU:HD13	1:D:239:ALA:HB1	1.85	0.59
1:A:53:HIS:HB3	1:A:128:PRO:HD3	1.84	0.59
1:C:183:ASP:O	2:C:702:NAD:H52A	2.02	0.59
1:B:288:GLU:O	1:B:291:VAL:HG22	2.02	0.59
1:B:274:LEU:HD22	3:B:877:HOH:O	2.02	0.59
1:B:56:ARG:HG2	3:B:761:HOH:O	2.02	0.59
1:C:16:GLU:CD	1:C:19:ARG:HH12	2.06	0.59
1:A:153:VAL:HG12	1:A:226:LEU:HB2	1.84	0.58
1:A:82:PHE:HE2	1:B:285:ALA:CB	2.15	0.58
1:D:288:GLU:O	1:D:291:VAL:HG22	2.03	0.58
1:A:183:ASP:O	2:A:700:NAD:H52A	2.04	0.58
1:D:169:ALA:HA	1:D:182:LEU:O	2.03	0.58
1:B:115:ILE:HG23	1:B:281:LEU:HD13	1.84	0.58
1:A:220:PRO:O	1:A:223:VAL:HG22	2.04	0.57
1:C:104:GLU:HB2	3:C:725:HOH:O	2.02	0.57
1:A:16:GLU:HG3	1:A:355:PRO:HA	1.86	0.57
1:B:13:ARG:HH11	1:B:332:GLY:HA2	1.69	0.57
1:C:161:ARG:HG3	3:C:777:HOH:O	2.03	0.57
1:A:100:TYR:HE2	1:A:135:GLU:HG3	1.69	0.57
1:D:77:SER:HB3	3:D:718:HOH:O	2.04	0.57
1:D:25:PHE:HB3	1:D:30:THR:HG21	1.87	0.57
1:B:169:ALA:HA	1:B:182:LEU:O	2.05	0.56
1:D:287:LEU:HD22	1:D:291:VAL:HG23	1.86	0.56
1:C:246:ILE:HD13	1:D:172:VAL:HG21	1.87	0.56
1:B:25:PHE:HB3	1:B:30:THR:HG21	1.88	0.56
1:B:115:ILE:CG2	1:B:281:LEU:HD13	2.35	0.56
1:C:153:VAL:HG12	1:C:226:LEU:HB2	1.87	0.56
1:D:19:ARG:HG2	3:D:817:HOH:O	2.04	0.56
1:C:39:THR:O	1:C:43:MET:HG2	2.06	0.56
1:A:336:ASP:HB2	1:A:337:PRO:HD2	1.86	0.56
1:D:69:ARG:HD3	3:D:869:HOH:O	2.05	0.56
1:D:309:ARG:HH21	1:D:309:ARG:HG3	1.71	0.56
1:A:246:ILE:HD13	1:B:172:VAL:HG21	1.87	0.55
1:A:115:ILE:CG2	1:A:281:LEU:HD13	2.37	0.55
1:C:336:ASP:HB2	1:C:337:PRO:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:ARG:HH11	1:D:332:GLY:HA2	1.70	0.55
1:B:103:MET:SD	1:B:278:VAL:HG13	2.47	0.55
1:A:288:GLU:O	1:A:291:VAL:HG22	2.05	0.55
1:D:153:VAL:HG11	1:D:187:SER:HB3	1.89	0.55
1:A:182:LEU:HD13	1:B:239:ALA:HB1	1.86	0.55
1:C:288:GLU:O	1:C:291:VAL:HG22	2.06	0.55
1:B:100:TYR:CE2	1:B:135:GLU:HG3	2.42	0.55
1:A:336:ASP:OD2	1:A:338:VAL:HG13	2.07	0.55
1:B:179:PRO:HG3	3:B:704:HOH:O	2.05	0.55
1:A:39:THR:O	1:A:43:MET:HG2	2.07	0.55
1:A:184:MET:O	1:A:184:MET:HG3	2.07	0.55
1:C:103:MET:SD	1:C:278:VAL:HG13	2.47	0.55
1:A:103:MET:HA	1:A:278:VAL:HG11	1.89	0.55
1:A:118:VAL:CG2	1:A:278:VAL:HB	2.37	0.55
1:D:263:MET:SD	3:D:753:HOH:O	2.58	0.55
1:A:285:ALA:CA	1:B:82:PHE:CZ	2.85	0.54
1:C:336:ASP:OD2	1:C:338:VAL:HG13	2.07	0.54
1:C:118:VAL:CG2	1:C:278:VAL:HB	2.37	0.54
1:C:103:MET:HA	1:C:278:VAL:HG11	1.90	0.54
1:B:287:LEU:HD22	1:B:291:VAL:HG23	1.88	0.54
1:B:309:ARG:HH21	1:B:309:ARG:HG3	1.71	0.54
1:D:24:VAL:O	1:D:28:VAL:HG23	2.07	0.54
1:B:100:TYR:HE2	1:B:135:GLU:HG3	1.72	0.54
1:A:103:MET:SD	1:A:278:VAL:HG13	2.48	0.54
1:B:45:GLY:HA2	1:B:50:VAL:HG13	1.88	0.54
1:C:285:ALA:CB	1:D:82:PHE:CZ	2.90	0.54
1:C:220:PRO:O	1:C:223:VAL:HG22	2.06	0.54
1:C:285:ALA:HA	1:D:82:PHE:CE2	2.43	0.54
1:B:103:MET:HA	1:B:278:VAL:HG11	1.90	0.54
1:D:179:PRO:HG3	3:D:704:HOH:O	2.08	0.54
1:B:153:VAL:HG11	1:B:187:SER:HB3	1.90	0.54
1:B:16:GLU:HG3	1:B:355:PRO:HA	1.90	0.54
1:B:24:VAL:O	1:B:28:VAL:HG23	2.08	0.54
1:A:82:PHE:CE2	1:B:285:ALA:CB	2.91	0.54
1:D:103:MET:HA	1:D:278:VAL:HG11	1.90	0.54
1:D:161:ARG:HD2	3:D:828:HOH:O	2.08	0.54
1:A:82:PHE:CE2	1:B:285:ALA:HB2	2.37	0.54
1:D:100:TYR:CE2	1:D:135:GLU:HG3	2.43	0.54
1:C:314:VAL:HA	3:C:855:HOH:O	2.08	0.54
1:D:189:VAL:CG2	1:D:190:PRO:HD2	2.35	0.53
1:C:115:ILE:CG2	1:C:281:LEU:HD13	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:336:ASP:OD2	1:D:338:VAL:HG13	2.08	0.53
1:B:189:VAL:CG2	1:B:190:PRO:HD2	2.34	0.53
1:D:103:MET:SD	1:D:278:VAL:HG13	2.49	0.53
1:C:13:ARG:HH11	1:C:332:GLY:HA2	1.72	0.53
1:D:309:ARG:HD2	1:D:310:GLU:H	1.73	0.53
1:B:336:ASP:OD2	1:B:338:VAL:HG13	2.09	0.53
1:D:100:TYR:HE2	1:D:135:GLU:HG3	1.73	0.53
1:C:115:ILE:HG23	1:C:281:LEU:HD13	1.91	0.53
1:A:100:TYR:CE2	1:A:135:GLU:HG3	2.44	0.53
1:D:45:GLY:HA2	1:D:50:VAL:HG13	1.90	0.53
1:C:96:ALA:HA	1:C:132:TYR:OH	2.09	0.53
1:B:13:ARG:HH11	1:B:332:GLY:CA	2.22	0.52
1:B:16:GLU:CD	1:B:19:ARG:HH12	2.13	0.52
1:C:100:TYR:HE2	1:C:135:GLU:HG3	1.74	0.52
1:C:309:ARG:HD2	1:C:310:GLU:H	1.75	0.52
1:D:16:GLU:HG3	1:D:355:PRO:HA	1.91	0.52
1:B:19:ARG:HD2	3:B:768:HOH:O	2.08	0.52
1:C:13:ARG:HH11	1:C:332:GLY:CA	2.21	0.52
1:D:16:GLU:CD	1:D:19:ARG:HH12	2.13	0.52
1:C:24:VAL:O	1:C:28:VAL:HG23	2.10	0.52
1:B:198:ARG:NH2	1:C:198:ARG:NH2	2.58	0.52
1:C:285:ALA:HB2	1:D:82:PHE:CZ	2.44	0.52
1:C:20:PHE:O	1:C:24:VAL:HG23	2.10	0.52
1:D:298:ARG:O	1:D:302:VAL:HG23	2.09	0.52
1:A:115:ILE:HG23	1:A:281:LEU:HD13	1.92	0.52
1:B:198:ARG:HE	1:B:221:ASN:HD22	1.58	0.52
1:C:100:TYR:CE2	1:C:135:GLU:HG3	2.45	0.51
1:B:298:ARG:O	1:B:302:VAL:HG23	2.10	0.51
1:A:96:ALA:HA	1:A:132:TYR:OH	2.10	0.51
1:C:156:HIS:O	1:C:157:ASP:HB2	2.09	0.51
1:B:228:PRO:HD2	3:B:777:HOH:O	2.09	0.51
1:D:119:ALA:HB1	1:D:252:THR:HG22	1.92	0.51
1:D:20:PHE:O	1:D:24:VAL:HG23	2.10	0.51
1:D:13:ARG:HH11	1:D:332:GLY:CA	2.24	0.51
1:D:313:LYS:HG3	3:D:801:HOH:O	2.10	0.51
1:C:144:LEU:HD13	1:C:279:LEU:HD13	1.93	0.51
1:D:13:ARG:HG2	3:D:766:HOH:O	2.09	0.51
1:A:24:VAL:O	1:A:28:VAL:HG23	2.11	0.51
1:C:25:PHE:HB3	1:C:30:THR:HG21	1.93	0.50
1:D:183:ASP:O	2:D:703:NAD:H52A	2.11	0.50
1:B:309:ARG:HD2	1:B:310:GLU:H	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ARG:HD2	1:A:310:GLU:H	1.76	0.50
1:B:13:ARG:NE	1:B:13:ARG:HA	2.27	0.50
1:A:134:LEU:O	1:A:138:ARG:HG3	2.12	0.50
1:B:115:ILE:HD12	1:B:115:ILE:H	1.75	0.50
1:B:183:ASP:O	2:B:701:NAD:H52A	2.12	0.50
1:C:13:ARG:NE	1:C:13:ARG:HA	2.26	0.49
1:C:285:ALA:HB1	1:D:85:VAL:HG21	1.94	0.49
1:C:189:VAL:HG22	1:C:193:ARG:HG3	1.93	0.49
1:D:13:ARG:NE	1:D:13:ARG:HA	2.27	0.49
1:B:20:PHE:O	1:B:24:VAL:HG23	2.11	0.49
1:A:317:PRO:HG3	3:A:810:HOH:O	2.12	0.49
1:D:115:ILE:H	1:D:115:ILE:HD12	1.78	0.49
1:C:103:MET:CE	1:C:280:ALA:HB2	2.42	0.49
1:B:119:ALA:HB1	1:B:252:THR:HG22	1.94	0.49
1:A:285:ALA:HB1	1:B:85:VAL:HG21	1.94	0.49
1:D:118:VAL:CG2	1:D:278:VAL:HB	2.43	0.49
1:B:39:THR:O	1:B:43:MET:HG2	2.13	0.49
1:A:25:PHE:HB3	1:A:30:THR:HG21	1.95	0.49
1:A:189:VAL:HG22	1:A:193:ARG:HG3	1.94	0.48
1:C:246:ILE:O	1:C:250:VAL:HG22	2.13	0.48
1:A:298:ARG:O	1:A:302:VAL:HG23	2.13	0.48
1:A:10:VAL:HG22	1:A:358:HIS:O	2.13	0.48
1:B:103:MET:O	1:B:107:MET:HG3	2.13	0.48
1:A:103:MET:CE	1:A:280:ALA:HB2	2.43	0.48
1:C:137:ALA:HB1	1:C:179:PRO:HB3	1.95	0.48
1:C:134:LEU:O	1:C:138:ARG:HG3	2.13	0.48
1:A:246:ILE:O	1:A:250:VAL:HG22	2.13	0.48
1:C:16:GLU:CG	1:C:356:THR:H	2.27	0.48
1:D:39:THR:O	1:D:43:MET:HG2	2.14	0.48
1:B:220:PRO:O	1:B:223:VAL:HG22	2.13	0.48
1:C:64:ALA:HB1	1:C:70:LEU:HG	1.95	0.48
1:C:288:GLU:HG3	1:C:290:ASP:H	1.78	0.48
1:B:246:ILE:O	1:B:250:VAL:HG22	2.14	0.47
1:A:85:VAL:HG13	1:B:115:ILE:HG13	1.97	0.47
1:A:210:SER:HA	1:A:216:ASP:HA	1.96	0.47
1:B:118:VAL:CG2	1:B:278:VAL:HB	2.44	0.47
1:A:20:PHE:O	1:A:24:VAL:HG23	2.14	0.47
1:A:115:ILE:CD1	1:B:115:ILE:HD13	2.45	0.47
1:A:288:GLU:HG3	1:A:290:ASP:H	1.79	0.47
1:A:239:ALA:HB1	1:B:182:LEU:HD13	1.97	0.47
1:D:246:ILE:O	1:D:250:VAL:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:PRO:O	1:D:223:VAL:HG22	2.15	0.47
1:B:159:ALA:HB1	3:B:785:HOH:O	2.13	0.47
1:C:309:ARG:HG3	1:C:309:ARG:NH2	2.27	0.47
1:A:137:ALA:HB1	1:A:179:PRO:HB3	1.95	0.47
1:C:118:VAL:HG23	1:C:278:VAL:HB	1.96	0.47
1:C:210:SER:HA	1:C:216:ASP:HA	1.96	0.47
1:A:285:ALA:HA	1:B:82:PHE:HZ	1.72	0.46
1:A:64:ALA:HB1	1:A:70:LEU:HG	1.96	0.46
1:C:115:ILE:CD1	1:D:115:ILE:HD13	2.45	0.46
1:D:101:ALA:O	1:D:104:GLU:HG2	2.15	0.46
1:B:263:MET:HG2	3:B:762:HOH:O	2.15	0.46
1:A:118:VAL:HG23	1:A:278:VAL:HB	1.97	0.46
1:A:189:VAL:CG2	1:A:190:PRO:HD2	2.40	0.46
1:D:165:THR:OG1	2:D:703:NAD:H5N	2.16	0.46
1:C:47:ARG:O	1:C:325:ALA:HA	2.16	0.46
1:A:16:GLU:CG	1:A:356:THR:H	2.28	0.46
1:D:282:LYS:HE2	1:D:284:GLU:HB2	1.98	0.46
1:C:189:VAL:CG2	1:C:190:PRO:HD2	2.41	0.45
1:C:340:ARG:HG3	1:C:357:TYR:CZ	2.51	0.45
1:A:357:TYR:O	1:A:358:HIS:HB3	2.17	0.45
1:D:210:SER:HA	1:D:216:ASP:HA	1.98	0.45
1:C:357:TYR:O	1:C:358:HIS:HB3	2.17	0.45
1:D:74:PRO:CB	1:D:93:ALA:HB2	2.46	0.45
1:C:282:LYS:HE3	1:C:284:GLU:HB2	1.98	0.45
1:D:103:MET:O	1:D:107:MET:HG3	2.16	0.45
1:D:156:HIS:CD2	3:D:856:HOH:O	2.63	0.45
1:C:28:VAL:HG12	1:C:72:ARG:HE	1.82	0.45
1:C:298:ARG:O	1:C:302:VAL:HG23	2.16	0.45
1:A:309:ARG:NH2	1:A:309:ARG:HG3	2.26	0.45
1:A:282:LYS:HE3	1:A:284:GLU:HB2	1.98	0.45
1:B:74:PRO:CB	1:B:93:ALA:HB2	2.46	0.45
1:D:47:ARG:O	1:D:325:ALA:HA	2.17	0.45
1:B:210:SER:HA	1:B:216:ASP:HA	1.99	0.45
1:C:85:VAL:HG13	1:D:115:ILE:HG13	1.98	0.45
1:D:115:ILE:HG23	1:D:281:LEU:HD13	1.98	0.45
1:B:101:ALA:O	1:B:104:GLU:HG2	2.16	0.45
1:B:74:PRO:HB2	1:B:93:ALA:HB2	1.98	0.45
1:D:120:ILE:HD12	1:D:276:ALA:HB3	1.98	0.45
1:A:115:ILE:HG13	1:B:85:VAL:CG1	2.47	0.44
1:C:160:MET:HG2	1:C:161:ARG:N	2.32	0.44
1:A:263:MET:HG2	1:A:272:ARG:NH2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:ASP:O	1:A:294:GLU:HG2	2.17	0.44
1:C:85:VAL:CG1	1:D:115:ILE:HG13	2.48	0.44
1:A:28:VAL:HG12	1:A:72:ARG:HE	1.81	0.44
1:A:85:VAL:CG1	1:B:115:ILE:HG13	2.47	0.44
1:C:115:ILE:HD12	1:C:115:ILE:H	1.82	0.44
1:D:115:ILE:CG2	1:D:281:LEU:HD13	2.48	0.44
1:D:166:ASN:O	1:D:186:THR:HG23	2.17	0.44
1:C:103:MET:HE1	1:C:280:ALA:HB2	1.98	0.44
1:B:282:LYS:HE2	1:B:284:GLU:HB2	1.99	0.44
1:A:47:ARG:O	1:A:325:ALA:HA	2.18	0.44
1:B:172:VAL:HG11	1:B:296:MET:HE1	1.99	0.44
1:B:120:ILE:HD12	1:B:276:ALA:HB3	1.99	0.44
1:C:290:ASP:O	1:C:294:GLU:HG2	2.17	0.44
1:C:263:MET:HG2	1:C:272:ARG:NH2	2.33	0.44
1:B:166:ASN:O	1:B:186:THR:HG23	2.18	0.44
1:C:178:MET:HA	1:C:179:PRO:HD3	1.88	0.44
1:B:160:MET:HG2	1:B:161:ARG:N	2.33	0.44
1:C:115:ILE:HG13	1:D:85:VAL:CG1	2.47	0.44
1:C:291:VAL:HA	1:C:294:GLU:CG	2.47	0.43
1:B:263:MET:HG2	1:B:272:ARG:NH2	2.33	0.43
1:D:154:ARG:O	1:D:228:PRO:HG3	2.18	0.43
1:A:140:GLY:HA3	3:A:825:HOH:O	2.18	0.43
1:B:165:THR:OG1	2:B:701:NAD:H5N	2.17	0.43
1:B:358:HIS:CD2	1:B:358:HIS:OXT	2.71	0.43
1:A:115:ILE:HG13	1:B:85:VAL:HG13	2.00	0.43
1:C:281:LEU:O	1:C:283:PRO:HD3	2.18	0.43
1:B:47:ARG:O	1:B:325:ALA:HA	2.18	0.43
1:A:53:HIS:HA	1:A:57:LEU:HD11	2.00	0.43
1:A:340:ARG:HG3	1:A:357:TYR:CZ	2.52	0.43
1:A:144:LEU:HD12	1:A:279:LEU:CD1	2.46	0.43
1:D:74:PRO:HB2	1:D:93:ALA:HB2	1.99	0.43
1:A:103:MET:O	1:A:103:MET:HE3	2.18	0.43
1:D:28:VAL:HG12	1:D:72:ARG:HE	1.84	0.43
1:D:53:HIS:HB3	1:D:128:PRO:HD3	2.00	0.43
1:C:239:ALA:HB1	1:D:182:LEU:HD13	2.00	0.43
1:D:161:ARG:HD3	3:D:809:HOH:O	2.17	0.43
1:A:178:MET:HA	1:A:179:PRO:HD3	1.87	0.43
1:D:141:TYR:O	1:D:173:PRO:HD3	2.19	0.43
1:A:240:LEU:O	1:A:243:VAL:HG22	2.19	0.43
1:A:281:LEU:O	1:A:283:PRO:HD3	2.18	0.42
1:D:172:VAL:HG11	1:D:296:MET:HE1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:ARG:HB2	1:C:16:GLU:HB2	2.01	0.42
1:A:160:MET:HG2	1:A:161:ARG:N	2.33	0.42
1:D:340:ARG:HG3	1:D:357:TYR:CZ	2.54	0.42
1:C:285:ALA:CA	1:D:82:PHE:CZ	3.02	0.42
1:B:340:ARG:HG3	1:B:357:TYR:CZ	2.53	0.42
1:B:180:TRP:NE1	1:B:317:PRO:HD2	2.34	0.42
1:A:27:ALA:HB1	1:A:350:PHE:HB3	2.01	0.42
1:B:142:ILE:O	1:B:280:ALA:HA	2.20	0.42
1:B:294:GLU:HG3	1:B:295:SER:N	2.34	0.42
1:B:103:MET:SD	1:B:278:VAL:CG1	3.07	0.42
1:C:205:PRO:O	1:C:208:VAL:HG22	2.19	0.42
1:A:263:MET:HG2	1:A:272:ARG:HH22	1.84	0.42
1:D:294:GLU:HG3	1:D:295:SER:N	2.34	0.42
1:C:161:ARG:H	1:C:161:ARG:HG3	1.66	0.42
1:C:45:GLY:HA2	1:C:50:VAL:HG13	2.02	0.42
1:D:227:ALA:HA	1:D:228:PRO:HD3	1.91	0.42
1:C:240:LEU:O	1:C:243:VAL:HG22	2.20	0.42
1:A:45:GLY:HA2	1:A:50:VAL:HG13	2.02	0.42
1:C:126:PHE:C	1:C:126:PHE:CD2	2.93	0.42
1:A:115:ILE:H	1:A:115:ILE:HD12	1.84	0.42
1:B:154:ARG:O	1:B:228:PRO:HG3	2.20	0.42
1:B:16:GLU:CG	1:B:356:THR:H	2.33	0.42
1:C:227:ALA:HA	1:C:228:PRO:HD3	1.91	0.42
1:D:160:MET:HG2	1:D:161:ARG:N	2.34	0.41
1:B:53:HIS:HB3	1:B:128:PRO:HD3	2.02	0.41
1:D:281:LEU:O	1:D:283:PRO:HD3	2.20	0.41
1:C:182:LEU:HD13	1:D:239:ALA:CB	2.50	0.41
1:A:126:PHE:C	1:A:126:PHE:HD2	2.24	0.41
1:B:156:HIS:O	1:B:157:ASP:HB2	2.20	0.41
1:B:281:LEU:O	1:B:283:PRO:HD3	2.20	0.41
1:C:115:ILE:HG13	1:D:85:VAL:HG13	2.01	0.41
1:B:198:ARG:HH22	1:C:198:ARG:NH2	2.19	0.41
1:D:156:HIS:O	1:D:157:ASP:HB2	2.20	0.41
1:B:134:LEU:HD22	1:B:134:LEU:O	2.20	0.41
1:C:101:ALA:O	1:C:104:GLU:HG2	2.20	0.41
1:C:180:TRP:HH2	1:D:243:VAL:HG12	1.85	0.41
1:D:166:ASN:CB	1:D:244:VAL:HG21	2.37	0.41
1:C:50:VAL:HG21	2:C:702:NAD:H4D	2.02	0.41
1:D:178:MET:HA	1:D:179:PRO:HD3	1.88	0.41
1:B:28:VAL:HG12	1:B:72:ARG:HE	1.85	0.41
1:C:263:MET:CE	3:C:703:HOH:O	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:LEU:HD13	1:D:331:GLU:HG2	2.03	0.41
1:A:144:LEU:HD13	1:A:279:LEU:HD13	1.99	0.41
1:C:53:HIS:HA	1:C:57:LEU:HD11	2.03	0.41
1:B:144:LEU:HD13	1:B:170:VAL:HG22	2.02	0.41
1:B:153:VAL:HG22	1:B:163:HIS:HB2	2.03	0.41
1:C:30:THR:HG23	1:C:31:ASP:O	2.20	0.41
1:C:126:PHE:HD2	1:C:126:PHE:C	2.24	0.41
1:A:309:ARG:CG	1:A:309:ARG:HH21	2.27	0.41
1:B:288:GLU:HG3	1:B:290:ASP:H	1.86	0.41
1:B:137:ALA:HB1	1:B:179:PRO:HB3	2.03	0.41
1:C:103:MET:O	1:C:103:MET:HE3	2.20	0.41
1:A:30:THR:HG23	1:A:31:ASP:O	2.21	0.41
1:C:11:LEU:HD13	1:C:331:GLU:HG2	2.01	0.41
1:B:161:ARG:HG3	3:B:789:HOH:O	2.20	0.40
1:C:184:MET:HG3	1:C:184:MET:O	2.20	0.40
1:B:11:LEU:HD13	1:B:331:GLU:HG2	2.03	0.40
1:A:285:ALA:CB	1:B:82:PHE:CZ	3.04	0.40
1:C:294:GLU:HG3	1:C:295:SER:N	2.36	0.40
1:D:16:GLU:CG	1:D:356:THR:H	2.34	0.40
1:B:64:ALA:HB1	1:B:70:LEU:HG	2.04	0.40
1:D:134:LEU:HD22	1:D:134:LEU:O	2.21	0.40
1:A:28:VAL:O	1:A:28:VAL:HG12	2.21	0.40
1:C:134:LEU:HD22	1:C:134:LEU:O	2.21	0.40
1:A:126:PHE:C	1:A:126:PHE:CD2	2.93	0.40
1:B:59:ALA:HB2	1:C:202:GLN:HE22	1.85	0.40
1:C:103:MET:SD	1:C:278:VAL:CG1	3.10	0.40
1:B:28:VAL:O	1:B:28:VAL:HG12	2.21	0.40
1:A:180:TRP:HH2	1:B:243:VAL:HG12	1.85	0.40
1:A:115:ILE:HD13	1:B:115:ILE:CD1	2.48	0.40
1:A:182:LEU:HD13	1:B:239:ALA:CB	2.52	0.40
1:A:294:GLU:HG3	1:A:295:SER:N	2.37	0.40
1:C:262:PRO:HG3	3:C:732:HOH:O	2.21	0.40
1:D:161:ARG:H	1:D:161:ARG:HG3	1.71	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	348/358 (97%)	331 (95%)	16 (5%)	1 (0%)	46	50
1	B	348/358 (97%)	332 (95%)	15 (4%)	1 (0%)	46	50
1	C	348/358 (97%)	330 (95%)	17 (5%)	1 (0%)	46	50
1	D	348/358 (97%)	333 (96%)	14 (4%)	1 (0%)	46	50
All	All	1392/1432 (97%)	1326 (95%)	62 (4%)	4 (0%)	46	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	ASN
1	B	166	ASN
1	C	166	ASN
1	D	166	ASN

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	262/267 (98%)	234 (89%)	28 (11%)	8	7
1	B	262/267 (98%)	237 (90%)	25 (10%)	11	10
1	C	262/267 (98%)	238 (91%)	24 (9%)	11	11
1	D	262/267 (98%)	235 (90%)	27 (10%)	9	8
All	All	1048/1068 (98%)	944 (90%)	104 (10%)	10	9

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	19	ARG
1	A	26	LEU
1	A	30	THR
1	A	31	ASP
1	A	33	GLU
1	A	58	LEU
1	A	79	VAL
1	A	82	PHE
1	A	104	GLU
1	A	115	ILE
1	A	126	PHE
1	A	134	LEU
1	A	147	CYS
1	A	154	ARG
1	A	189	VAL
1	A	194	VAL
1	A	215	VAL
1	A	250	VAL
1	A	263	MET
1	A	279	LEU
1	A	287	LEU
1	A	301	GLU
1	A	306	SER
1	A	309	ARG
1	A	338	VAL
1	A	348	GLU
1	A	358	HIS
1	B	10	VAL
1	B	26	LEU
1	B	30	THR
1	B	31	ASP
1	B	33	GLU
1	B	58	LEU
1	B	79	VAL
1	B	100	TYR
1	B	115	ILE
1	B	126	PHE
1	B	134	LEU
1	B	147	CYS
1	B	153	VAL
1	B	154	ARG

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Mol	Chain	Res	Type
1	B	194	VAL
1	B	215	VAL
1	B	243	VAL
1	B	263	MET
1	B	274	LEU
1	B	279	LEU
1	B	287	LEU
1	B	301	GLU
1	B	309	ARG
1	B	338	VAL
1	B	358	HIS
1	C	26	LEU
1	C	30	THR
1	C	31	ASP
1	C	33	GLU
1	C	58	LEU
1	C	79	VAL
1	C	82	PHE
1	C	115	ILE
1	C	126	PHE
1	C	134	LEU
1	C	144	LEU
1	C	147	CYS
1	C	154	ARG
1	C	189	VAL
1	C	194	VAL
1	C	215	VAL
1	C	250	VAL
1	C	263	MET
1	C	274	LEU
1	C	279	LEU
1	C	287	LEU
1	C	301	GLU
1	C	309	ARG
1	C	338	VAL
1	D	10	VAL
1	D	26	LEU
1	D	30	THR
1	D	31	ASP
1	D	33	GLU
1	D	58	LEU
1	D	79	VAL

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Mol	Chain	Res	Type
1	D	88	ILE
1	D	100	TYR
1	D	115	ILE
1	D	126	PHE
1	D	134	LEU
1	D	147	CYS
1	D	153	VAL
1	D	154	ARG
1	D	192	ASN
1	D	194	VAL
1	D	215	VAL
1	D	243	VAL
1	D	263	MET
1	D	274	LEU
1	D	279	LEU
1	D	287	LEU
1	D	301	GLU
1	D	309	ARG
1	D	338	VAL
1	D	358	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	202	GLN
1	A	221	ASN
1	B	122	ASN
1	B	202	GLN
1	B	221	ASN
1	B	358	HIS
1	C	122	ASN
1	C	202	GLN
1	C	221	ASN
1	D	122	ASN
1	D	221	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 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	700	-	38,48,48	1.08	4 (10%)	47,73,73	2.24	8 (17%)
2	NAD	B	701	-	38,48,48	1.15	4 (10%)	47,73,73	2.18	8 (17%)
2	NAD	C	702	-	38,48,48	1.07	4 (10%)	47,73,73	2.26	8 (17%)
2	NAD	D	703	-	38,48,48	1.18	5 (13%)	47,73,73	2.19	9 (19%)

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	700	-	-	0/22/62/62	0/5/5/5
2	NAD	B	701	-	-	0/22/62/62	0/5/5/5
2	NAD	C	702	-	-	0/22/62/62	0/5/5/5
2	NAD	D	703	-	-	0/22/62/62	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	703	NAD	C5A-N7A	-2.11	1.32	1.39
2	C	702	NAD	C5A-N7A	-2.07	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	NAD	C5A-N7A	-2.05	1.32	1.39
2	B	701	NAD	C5A-N7A	-2.04	1.32	1.39
2	D	703	NAD	C3N-C7N	2.11	1.53	1.50
2	B	701	NAD	O4D-C1D	2.13	1.43	1.41
2	D	703	NAD	O4D-C1D	2.22	1.44	1.41
2	D	703	NAD	C6N-N1N	2.57	1.42	1.35
2	B	701	NAD	C6N-N1N	2.57	1.42	1.35
2	A	700	NAD	C6N-N1N	2.60	1.42	1.35
2	C	702	NAD	C6N-N1N	2.61	1.42	1.35
2	C	702	NAD	O4D-C1D	2.65	1.44	1.41
2	A	700	NAD	O4D-C1D	2.66	1.44	1.41
2	A	700	NAD	O4B-C1B	3.19	1.45	1.41
2	C	702	NAD	O4B-C1B	3.24	1.45	1.41
2	D	703	NAD	O4B-C1B	3.88	1.46	1.41
2	B	701	NAD	O4B-C1B	3.90	1.46	1.41

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	702	NAD	N3A-C2A-N1A	-10.71	120.69	128.89
2	A	700	NAD	N3A-C2A-N1A	-10.65	120.74	128.89
2	D	703	NAD	N3A-C2A-N1A	-10.28	121.02	128.89
2	B	701	NAD	N3A-C2A-N1A	-10.27	121.03	128.89
2	B	701	NAD	C4D-O4D-C1D	-4.20	105.10	109.72
2	D	703	NAD	C4D-O4D-C1D	-4.18	105.12	109.72
2	A	700	NAD	C5B-C4B-C3B	-4.05	99.15	115.21
2	C	702	NAD	C5B-C4B-C3B	-4.03	99.22	115.21
2	D	703	NAD	C5B-C4B-C3B	-3.97	99.46	115.21
2	B	701	NAD	C5B-C4B-C3B	-3.96	99.48	115.21
2	C	702	NAD	C4D-O4D-C1D	-3.96	105.37	109.72
2	A	700	NAD	C4D-O4D-C1D	-3.88	105.46	109.72
2	D	703	NAD	PN-O3-PA	-3.26	123.56	132.73
2	C	702	NAD	PN-O3-PA	-3.18	123.80	132.73
2	B	701	NAD	PN-O3-PA	-3.13	123.94	132.73
2	A	700	NAD	PN-O3-PA	-3.06	124.14	132.73
2	C	702	NAD	C3N-C7N-N7N	-2.30	115.30	117.82
2	A	700	NAD	C3N-C7N-N7N	-2.19	115.42	117.82
2	D	703	NAD	C3N-C7N-N7N	-2.11	115.51	117.82
2	B	701	NAD	C3N-C7N-N7N	-2.05	115.57	117.82
2	D	703	NAD	O7N-C7N-C3N	2.10	121.88	119.59
2	D	703	NAD	O4B-C4B-C3B	2.31	109.80	105.15
2	B	701	NAD	O4B-C4B-C3B	2.31	109.80	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	700	NAD	O4B-C4B-C3B	2.36	109.90	105.15
2	C	702	NAD	O4B-C4B-C3B	2.36	109.90	105.15
2	D	703	NAD	O4D-C1D-N1N	2.80	111.21	108.13
2	B	701	NAD	O4D-C1D-N1N	2.94	111.36	108.13
2	C	702	NAD	O4D-C1D-N1N	3.26	111.71	108.13
2	A	700	NAD	O4D-C1D-N1N	3.36	111.82	108.13
2	B	701	NAD	O4B-C4B-C5B	5.90	130.41	109.32
2	D	703	NAD	O4B-C4B-C5B	5.90	130.42	109.32
2	A	700	NAD	O4B-C4B-C5B	5.93	130.52	109.32
2	C	702	NAD	O4B-C4B-C5B	5.93	130.53	109.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	700	NAD	2	0
2	B	701	NAD	3	0
2	C	702	NAD	3	0
2	D	703	NAD	3	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	350/358 (97%)	-0.21	4 (1%) 82 82	8, 25, 47, 68	0
1	B	350/358 (97%)	-0.29	3 (0%) 85 85	10, 24, 47, 82	0
1	C	350/358 (97%)	-0.24	4 (1%) 82 82	7, 26, 48, 72	0
1	D	350/358 (97%)	-0.30	0 100 100	10, 24, 47, 78	0
All	All	1400/1432 (97%)	-0.26	11 (0%) 87 87	7, 25, 48, 82	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	81	GLY	3.5
1	A	82	PHE	3.3
1	B	358	HIS	3.2
1	A	174	ALA	2.9
1	C	82	PHE	2.8
1	C	174	ALA	2.6
1	A	9	THR	2.5
1	C	9	THR	2.3
1	C	176	ASP	2.2
1	A	177	ASP	2.1
1	B	310	GLU	2.1

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

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	700	44/44	0.96	0.12	1.45	13,26,40,41	0
2	NAD	C	702	44/44	0.95	0.12	1.11	13,25,36,42	0
2	NAD	B	701	44/44	0.96	0.10	0.43	11,19,25,27	0
2	NAD	D	703	44/44	0.96	0.10	0.23	11,19,29,33	0

6.5 Other polymers

There are no such residues in this entry.