Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:06 AM GMT

PDB ID	:	2ZIZ
Title	:	Crystal structure of Mycobacterium tuberculosis S-adenosyl-L-homocysteine hydrolase in ternary complex with NAD and 3-deazaadenosine
Authors	:	Reddy, M.C.M.; Gokulan, K.; Shetty, N.D.; Owen, J.L.; Ioerger, T.R.; Sacchettini, J.C.
Deposited on	:	2008-02-29
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 (i) symbol.

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

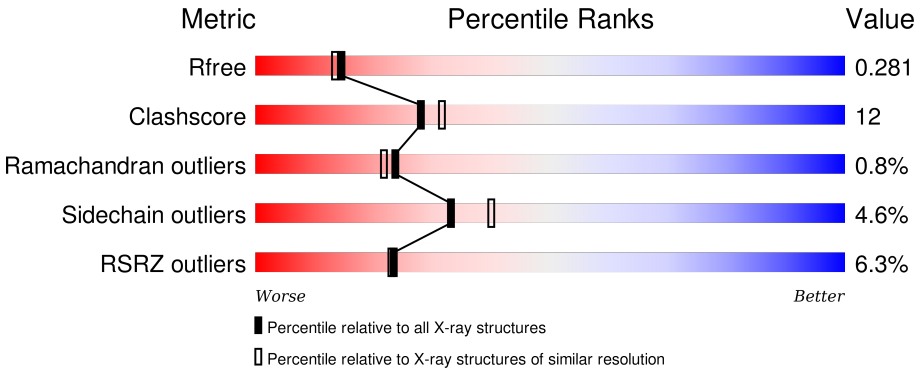
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 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	495	2% 75% 21%
1	B	495	6% 70% 26%
1	C	495	5% 77% 19%
1	D	495	12% 70% 25%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16004 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.

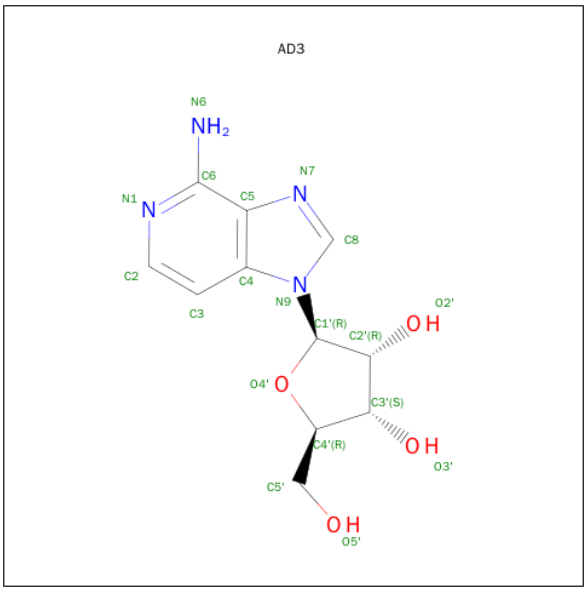
- Molecule 1 is a protein called Adenosylhomocysteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	0	0
			3748	2364	643	724	17			
1	B	485	Total	C	N	O	S	0	0	0
			3748	2364	643	724	17			
1	C	485	Total	C	N	O	S	0	0	0
			3748	2364	643	724	17			
1	D	485	Total	C	N	O	S	0	0	0
			3748	2364	643	724	17			

There are 4 discrepancies between the modelled and reference sequences:

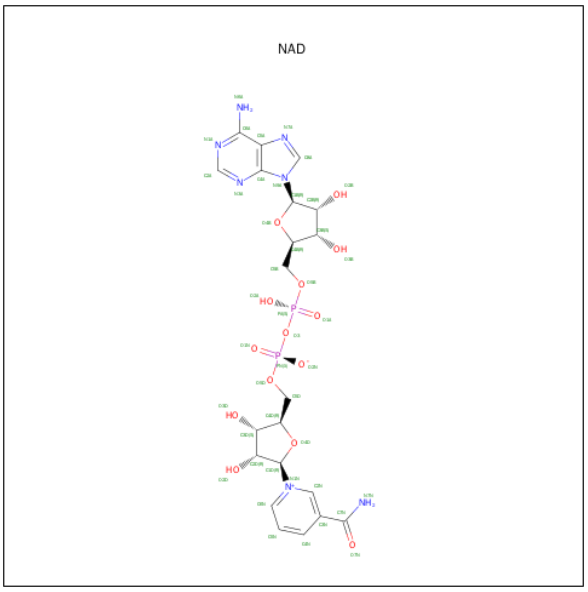
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP P60176
B	1	MET	-	EXPRESSION TAG	UNP P60176
C	1	MET	-	EXPRESSION TAG	UNP P60176
D	1	MET	-	EXPRESSION TAG	UNP P60176

- Molecule 2 is 3-DEAZA-ADENOSINE (three-letter code: AD3) (formula: $C_{11}H_{14}N_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	11	4	4		
2	B	1	Total	C	N	O	0	0
			19	11	4	4		
2	C	1	Total	C	N	O	0	0
			19	11	4	4		
2	D	1	Total	C	N	O	0	0
			19	11	4	4		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is water.

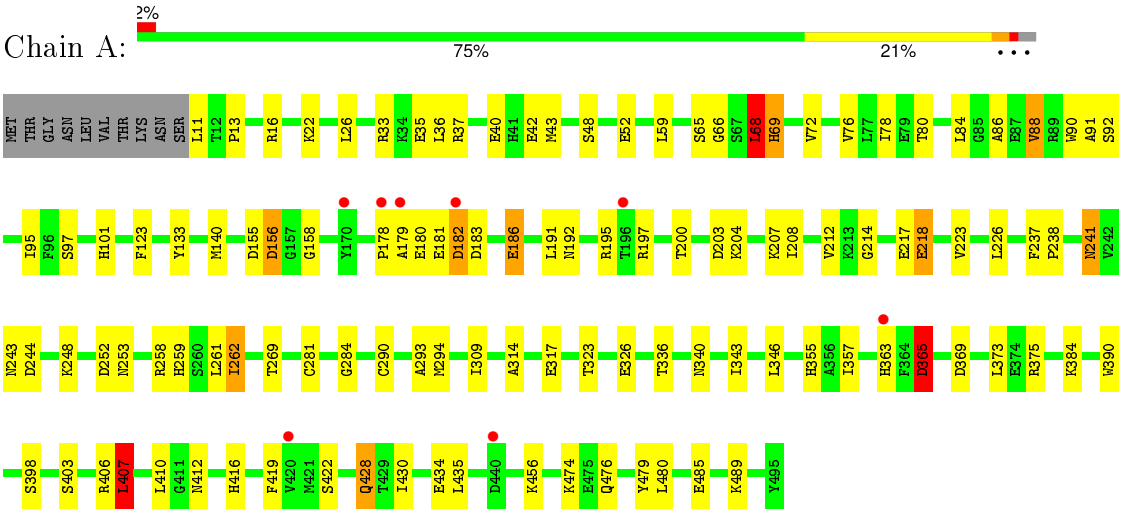
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	209	Total	O	0	0
			209	209		
4	B	154	Total	O	0	0
			154	154		
4	C	215	Total	O	0	0
			215	215		
4	D	182	Total	O	0	0
			182	182		

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.

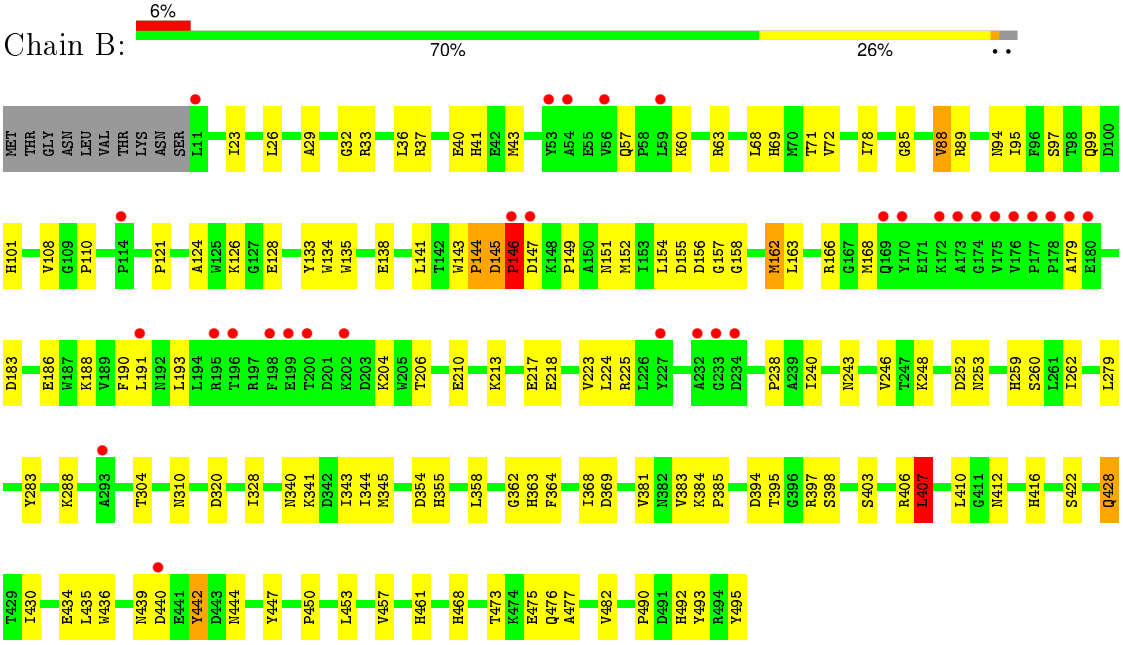
- Molecule 1: Adenosylhomocysteinase

Chain A:



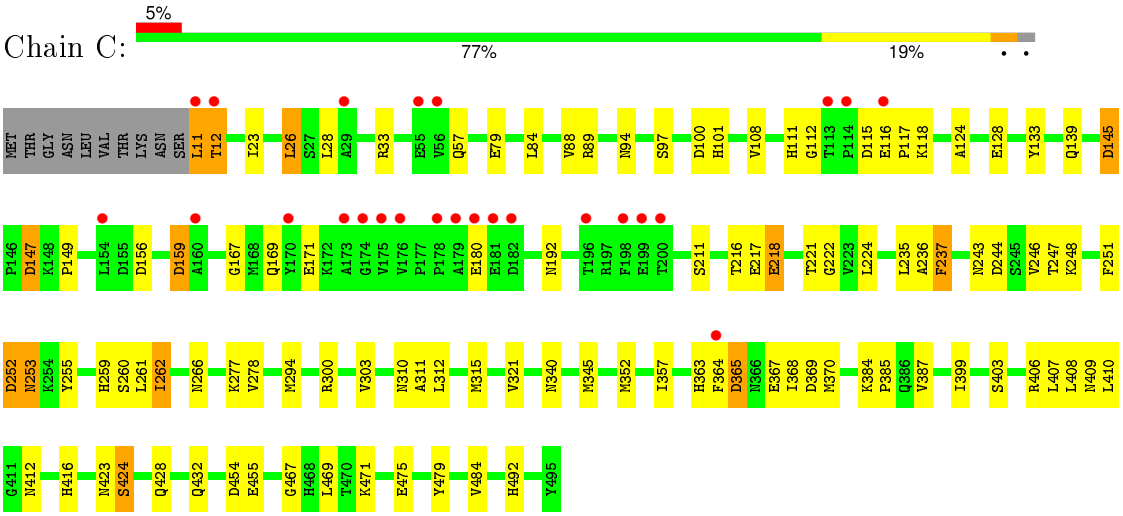
- Molecule 1: Adenosylhomocysteinase

Chain B:



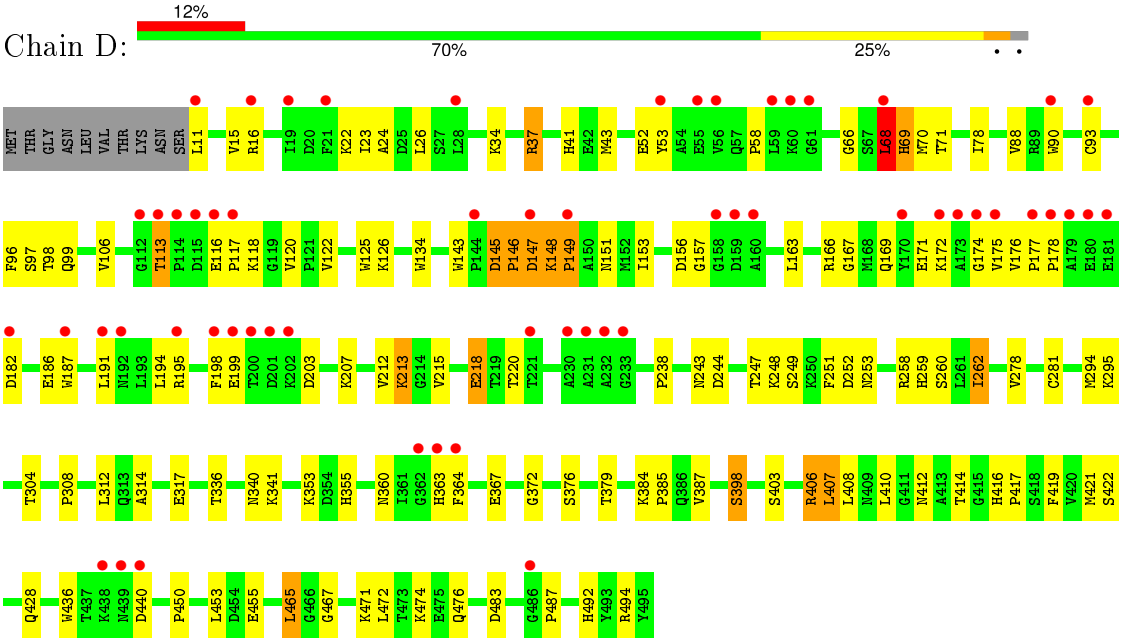
- Molecule 1: Adenosylhomocysteinase

Chain C:



• Molecule 1: Adenosylhomocysteinase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	100.55Å 111.32Å 94.47Å 90.00° 96.77° 90.00°	Depositor
Resolution (Å)	38.18 – 2.20 38.18 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.4 (38.18-2.20) 94.4 (38.18-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.198 , 0.285 0.195 , 0.281	Depositor DCC
R_{free} test set	4899 reflections (5.23%)	DCC
Wilson B-factor (Å^2)	37.2	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 56.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 98497 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16004	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.66% 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: AD3, 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	0.97	3/3824 (0.1%)	0.94	7/5186 (0.1%)
1	B	0.85	0/3824	0.85	3/5186 (0.1%)
1	C	0.87	1/3824 (0.0%)	0.88	7/5186 (0.1%)
1	D	0.81	1/3824 (0.0%)	0.87	5/5186 (0.1%)
All	All	0.88	5/15296 (0.0%)	0.89	22/20744 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	GLU	CB-CG	6.00	1.63	1.52
1	A	485	GLU	CG-CD	5.24	1.59	1.51
1	D	314	ALA	CA-CB	5.23	1.63	1.52
1	A	314	ALA	CA-CB	5.16	1.63	1.52
1	C	455	GLU	CG-CD	5.01	1.59	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	100	ASP	CB-CG-OD1	6.98	124.58	118.30
1	C	156	ASP	CB-CG-OD2	6.78	124.40	118.30
1	A	156	ASP	CB-CG-OD1	6.68	124.32	118.30
1	D	406	ARG	NE-CZ-NH1	-6.58	117.01	120.30
1	C	252	ASP	CB-CG-OD2	6.54	124.19	118.30
1	A	68	LEU	CA-CB-CG	6.29	129.78	115.30
1	C	159	ASP	CB-CG-OD2	6.09	123.79	118.30
1	D	465	LEU	CB-CG-CD1	-5.96	100.87	111.00
1	B	407	LEU	CA-CB-CG	5.84	128.74	115.30
1	A	407	LEU	CA-CB-CG	5.75	128.53	115.30
1	A	26	LEU	CB-CG-CD2	-5.75	101.23	111.00
1	A	365	ASP	N-CA-C	5.66	126.27	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	26	LEU	CA-CB-CG	5.64	128.28	115.30
1	D	467	GLY	N-CA-C	-5.59	99.11	113.10
1	C	467	GLY	N-CA-C	-5.50	99.34	113.10
1	D	68	LEU	CA-CB-CG	5.44	127.81	115.30
1	D	258	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	A	183	ASP	CB-CG-OD1	5.26	123.03	118.30
1	C	365	ASP	N-CA-C	5.14	124.87	111.00
1	B	435	LEU	CA-CB-CG	5.09	127.01	115.30
1	B	156	ASP	CB-CG-OD2	5.07	122.86	118.30
1	C	156	ASP	CB-CG-OD1	-5.02	113.79	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3748	0	3693	78	0
1	B	3748	0	3693	106	0
1	C	3748	0	3693	80	0
1	D	3748	0	3693	111	0
2	A	19	0	14	3	0
2	B	19	0	14	1	0
2	C	19	0	14	1	0
2	D	19	0	14	1	0
3	A	44	0	26	2	0
3	B	44	0	26	2	0
3	C	44	0	26	2	0
3	D	44	0	26	2	0
4	A	209	0	0	3	0
4	B	154	0	0	4	1
4	C	215	0	0	4	1
4	D	182	0	0	6	2
All	All	16004	0	14932	352	2

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 12.

All (352) 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:D:146:PRO:CB	1:D:147:ASP:HB2	1.52	1.38
1:A:68:LEU:HD22	1:A:156:ASP:HB2	1.35	1.08
1:B:262:ILE:HD11	1:D:262:ILE:HD11	1.09	1.04
1:D:146:PRO:HB3	1:D:147:ASP:CB	1.92	1.00
1:D:146:PRO:HB3	1:D:147:ASP:HB2	1.01	0.98
1:B:262:ILE:CD1	1:D:262:ILE:HD11	1.95	0.97
1:D:146:PRO:HB2	1:D:147:ASP:HB2	1.46	0.97
1:C:368:ILE:HG22	1:C:370:MET:HE2	1.47	0.97
1:D:146:PRO:CB	1:D:147:ASP:CB	2.42	0.96
1:B:358:LEU:HD11	1:B:368:ILE:HD13	1.44	0.95
1:A:218:GLU:HG3	1:A:428:GLN:HE22	1.33	0.93
1:B:262:ILE:HD11	1:D:262:ILE:CD1	1.98	0.92
1:D:259:HIS:HE1	4:D:838:HOH:O	1.53	0.91
1:B:145:ASP:H	1:B:146:PRO:CD	1.84	0.91
1:A:262:ILE:HD11	1:C:262:ILE:HD11	1.52	0.90
1:D:218:GLU:HG3	1:D:428:GLN:NE2	1.87	0.90
1:D:145:ASP:OD2	1:D:146:PRO:HD2	1.77	0.84
1:D:384:LYS:HB2	1:D:385:PRO:CD	2.10	0.82
1:B:57:GLN:HE22	1:B:85:GLY:HA2	1.45	0.81
1:C:368:ILE:CG2	1:C:370:MET:HE2	2.12	0.80
3:C:550:NAD:C4N	2:C:500:AD3:H3'	2.10	0.79
1:C:112:GLY:HA2	1:C:118:LYS:HG3	1.64	0.79
1:D:384:LYS:HB2	1:D:385:PRO:HD2	1.64	0.78
1:C:243:ASN:HD21	1:C:253:ASN:HD21	1.31	0.78
1:D:295:LYS:HE3	4:D:736:HOH:O	1.83	0.77
1:D:218:GLU:HG3	1:D:428:GLN:HE22	1.49	0.74
1:A:68:LEU:HD22	1:A:156:ASP:CB	2.16	0.73
1:B:157:GLY:HA3	1:B:363:HIS:HE2	1.54	0.73
1:D:450:PRO:HD2	1:D:453:LEU:HD12	1.70	0.73
1:D:70:MET:HB3	1:D:98:THR:HG23	1.70	0.72
1:B:218:GLU:O	1:B:248:LYS:HE3	1.89	0.72
1:C:260:SER:HB2	1:C:409:ASN:HB2	1.71	0.72
1:B:358:LEU:CD1	1:B:368:ILE:HD13	2.17	0.72
1:D:218:GLU:CG	1:D:428:GLN:HE22	2.03	0.71
1:D:407:LEU:H	1:D:407:LEU:HD23	1.56	0.71
1:A:218:GLU:CG	1:A:428:GLN:HE22	2.02	0.70
1:B:33:ARG:O	1:B:37:ARG:HG3	1.91	0.70
1:A:243:ASN:HD21	1:A:253:ASN:HD21	1.37	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:ILE:CG2	1:C:370:MET:CE	2.69	0.70
2:A:500:AD3:H3'	3:A:550:NAD:C4N	2.22	0.70
1:C:218:GLU:HG3	1:C:428:GLN:NE2	2.08	0.68
1:B:162:MET:O	1:B:166:ARG:HB2	1.94	0.68
1:C:368:ILE:HG22	1:C:370:MET:CE	2.23	0.68
2:B:500:AD3:H3'	3:B:550:NAD:C4N	2.23	0.67
1:B:157:GLY:HA3	1:B:363:HIS:NE2	2.10	0.67
1:B:138:GLU:OE2	1:B:204:LYS:NZ	2.28	0.67
1:C:218:GLU:CG	1:C:428:GLN:HE22	2.06	0.67
1:A:479:TYR:CD1	1:B:341:LYS:HD2	2.30	0.67
1:A:22:LYS:HE3	4:A:640:HOH:O	1.94	0.66
1:B:145:ASP:O	1:B:147:ASP:N	2.23	0.66
3:D:550:NAD:C4N	2:D:500:AD3:H3'	2.26	0.66
1:C:11:LEU:HD22	1:C:12:THR:H	1.60	0.65
1:D:153:ILE:O	1:D:215:VAL:HA	1.97	0.65
1:C:368:ILE:HG21	1:C:370:MET:HE3	1.78	0.65
1:C:216:THR:CG2	1:C:432:GLN:NE2	2.60	0.65
1:B:260:SER:OG	1:B:416:HIS:HD2	1.80	0.64
1:C:236:ALA:O	4:C:869:HOH:O	2.14	0.64
1:B:358:LEU:HD11	1:B:368:ILE:CD1	2.25	0.64
1:B:403:SER:OG	1:B:412:ASN:ND2	2.30	0.64
1:A:252:ASP:OD1	1:A:416:HIS:CE1	2.51	0.64
1:B:68:LEU:O	1:B:69:HIS:C	2.37	0.64
1:B:145:ASP:H	1:B:146:PRO:HD3	1.62	0.63
1:A:241:ASN:C	1:A:241:ASN:HD22	2.02	0.63
1:D:146:PRO:HB2	1:D:147:ASP:CB	2.17	0.62
1:C:57:GLN:HA	1:C:57:GLN:NE2	2.15	0.62
1:D:472:LEU:HD22	1:D:476:GLN:HB3	1.80	0.62
1:C:384:LYS:HB2	1:C:385:PRO:HD2	1.82	0.62
1:C:133:TYR:OH	1:C:159:ASP:OD1	2.12	0.62
1:A:252:ASP:OD1	1:A:416:HIS:HE1	1.84	0.61
1:D:187:TRP:NE1	1:D:191:LEU:HD11	2.16	0.61
1:B:213:LYS:HB3	1:B:439:ASN:ND2	2.15	0.61
1:C:218:GLU:HG3	1:C:428:GLN:HE22	1.64	0.61
1:B:381:VAL:HG12	1:D:34:LYS:HE2	1.81	0.61
1:B:145:ASP:H	1:B:146:PRO:HD2	1.66	0.61
1:A:261:LEU:HD21	1:A:294:MET:HE3	1.82	0.60
1:B:168:MET:HG3	1:B:206:THR:HA	1.83	0.60
1:D:403:SER:OG	1:D:412:ASN:ND2	2.34	0.60
1:C:112:GLY:CA	1:C:118:LYS:HG3	2.30	0.60
1:C:365:ASP:HB3	1:C:406:ARG:HG3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ARG:O	1:A:37:ARG:HG3	2.02	0.60
1:C:368:ILE:HG21	1:C:370:MET:CE	2.32	0.60
1:C:255:TYR:OH	1:D:317:GLU:OE2	2.16	0.60
1:B:213:LYS:HB3	1:B:439:ASN:HD21	1.66	0.60
1:D:145:ASP:HB3	1:D:148:LYS:HG3	1.84	0.59
1:D:96:PHE:O	1:D:126:LYS:NZ	2.28	0.59
1:A:340:ASN:HB3	1:A:343:ILE:HD11	1.84	0.59
1:C:340:ASN:O	1:C:367:GLU:HG2	2.03	0.59
1:B:29:ALA:HB2	1:B:108:VAL:HG21	1.84	0.59
1:B:155:ASP:OD2	1:B:158:GLY:HA2	2.01	0.59
1:D:207:LYS:HE2	4:D:681:HOH:O	2.03	0.58
1:C:384:LYS:HB2	1:C:385:PRO:CD	2.34	0.58
1:C:167:GLY:O	1:C:171:GLU:HG3	2.02	0.58
1:D:23:ILE:HD11	1:D:26:LEU:HD11	1.84	0.58
1:B:383:VAL:HA	1:D:34:LYS:HD3	1.86	0.58
1:D:260:SER:OG	1:D:416:HIS:HD2	1.87	0.58
1:A:403:SER:OG	1:A:412:ASN:ND2	2.37	0.58
1:B:43:MET:HA	1:B:422:SER:HB2	1.86	0.58
1:C:310:ASN:H	1:C:310:ASN:HD22	1.52	0.58
1:D:78:ILE:HG23	1:D:88:VAL:HG21	1.86	0.57
1:D:167:GLY:O	1:D:171:GLU:HG3	2.04	0.57
1:C:403:SER:OG	1:C:412:ASN:ND2	2.37	0.57
1:B:134:TRP:HE1	1:B:186:GLU:HG3	1.69	0.57
1:C:216:THR:HG23	1:C:432:GLN:NE2	2.19	0.57
1:B:468:HIS:HB3	4:B:660:HOH:O	2.05	0.57
1:B:63:ARG:NH2	1:B:149:PRO:O	2.24	0.57
1:A:218:GLU:O	1:A:248:LYS:HE3	2.05	0.56
1:A:214:GLY:HA3	1:A:435:LEU:HD13	1.86	0.56
1:C:260:SER:OG	1:C:416:HIS:HD2	1.88	0.56
1:D:106:VAL:HG12	1:D:120:VAL:HG22	1.87	0.56
1:D:99:GLN:HE22	1:D:414:THR:HB	1.70	0.56
1:D:145:ASP:CB	1:D:146:PRO:HD2	2.35	0.56
1:D:384:LYS:CB	1:D:385:PRO:CD	2.78	0.56
1:B:354:ASP:HB2	1:B:397:ARG:HG2	1.87	0.56
1:C:97:SER:HB3	1:C:410:LEU:HB3	1.88	0.56
1:B:340:ASN:HB3	1:B:343:ILE:HD11	1.86	0.56
1:D:213:LYS:O	1:D:238:PRO:HD2	2.06	0.55
1:B:95:ILE:HG22	1:B:133:TYR:HB2	1.86	0.55
1:D:203:ASP:O	1:D:207:LYS:HG2	2.07	0.55
1:B:36:LEU:HD12	1:B:72:VAL:HG13	1.88	0.55
1:D:37:ARG:NH2	4:D:764:HOH:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:ILE:HD12	1:C:266:ASN:ND2	2.22	0.54
1:A:80:THR:O	1:A:84:LEU:HG	2.08	0.54
1:C:57:GLN:NE2	1:C:84:LEU:C	2.61	0.54
1:C:244:ASP:OD2	1:D:492:HIS:HE1	1.91	0.54
1:C:252:ASP:OD2	1:C:416:HIS:HE1	1.90	0.54
1:C:246:VAL:HG22	1:D:494:ARG:CZ	2.38	0.54
1:B:57:GLN:HE22	1:B:85:GLY:CA	2.19	0.53
1:A:42:GLU:O	1:A:419:PHE:HA	2.07	0.53
1:A:262:ILE:CD1	1:C:262:ILE:HD11	2.32	0.53
1:B:358:LEU:CD1	1:B:368:ILE:CD1	2.86	0.53
1:D:384:LYS:HE3	1:D:387:VAL:HG21	1.91	0.53
1:D:78:ILE:HD11	1:D:90:TRP:CD2	2.43	0.53
1:A:197:ARG:HD2	1:A:204:LYS:HD2	1.91	0.53
1:B:145:ASP:N	1:B:146:PRO:CD	2.60	0.53
1:B:252:ASP:OD1	1:B:416:HIS:CE1	2.62	0.52
1:A:65:SER:HB3	1:A:140:MET:SD	2.49	0.52
1:C:115:ASP:C	1:C:117:PRO:HD3	2.30	0.52
1:D:248:LYS:C	1:D:248:LYS:HD3	2.29	0.52
1:B:407:LEU:HD22	1:B:410:LEU:HD12	1.91	0.52
1:C:492:HIS:HE1	1:D:244:ASP:OD2	1.92	0.52
1:A:223:VAL:HG21	1:A:241:ASN:ND2	2.25	0.52
1:B:450:PRO:HD2	1:B:453:LEU:HD12	1.91	0.52
1:D:11:LEU:HD22	1:D:22:LYS:HE3	1.92	0.52
1:C:261:LEU:HD12	1:C:408:LEU:HD11	1.91	0.51
1:B:243:ASN:HD21	1:B:253:ASN:HD21	1.58	0.51
1:A:489:LYS:HE2	1:B:310:ASN:HD21	1.75	0.51
1:A:35:GLU:OE1	1:A:101:HIS:HE1	1.94	0.51
1:A:363:HIS:ND1	2:A:500:AD3:O5'	2.34	0.51
1:A:178:PRO:HA	1:A:195:ARG:NH2	2.26	0.51
4:A:732:HOH:O	1:C:259:HIS:HE1	1.92	0.51
1:D:243:ASN:O	1:D:249:SER:HB3	2.10	0.51
1:B:381:VAL:CG1	1:D:34:LYS:HE2	2.41	0.51
1:B:240:ILE:HG12	1:B:447:TYR:HB2	1.93	0.51
1:A:179:ALA:HB2	1:A:191:LEU:HD12	1.92	0.51
1:A:59:LEU:HB3	1:A:86:ALA:HB2	1.92	0.51
1:A:309:ILE:HG21	1:B:246:VAL:HG11	1.93	0.51
1:B:218:GLU:HG3	1:B:428:GLN:HE22	1.75	0.51
1:A:269:THR:HG21	1:A:357:ILE:HD13	1.93	0.51
1:D:455:GLU:OE2	1:D:487:PRO:HA	2.10	0.50
1:B:206:THR:O	1:B:210:GLU:HG3	2.10	0.50
1:A:241:ASN:C	1:A:241:ASN:ND2	2.65	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ILE:HG23	1:B:88:VAL:HG21	1.93	0.50
1:D:145:ASP:CG	1:D:146:PRO:HD2	2.30	0.50
1:B:144:PRO:O	1:B:145:ASP:HB2	2.12	0.49
1:D:23:ILE:HD11	1:D:26:LEU:CD1	2.42	0.49
1:B:283:TYR:CE2	1:B:288:LYS:HE3	2.47	0.49
1:B:283:TYR:CD2	1:B:288:LYS:HE3	2.47	0.49
1:B:141:LEU:HD12	1:B:163:LEU:HD23	1.95	0.49
1:D:69:HIS:CE1	1:D:93:CYS:SG	3.05	0.49
1:D:178:PRO:HA	1:D:195:ARG:HH21	1.76	0.49
1:A:43:MET:HA	1:A:422:SER:HB2	1.94	0.49
1:D:407:LEU:HD12	1:D:410:LEU:HD12	1.94	0.49
1:C:23:ILE:HD11	1:C:26:LEU:HD13	1.94	0.49
1:D:146:PRO:HB2	1:D:147:ASP:CA	2.42	0.49
1:D:143:TRP:HB2	1:D:149:PRO:HA	1.93	0.49
1:D:166:ARG:HA	1:D:169:GLN:HB3	1.95	0.49
1:D:53:TYR:HD2	1:D:58:PRO:HG3	1.77	0.49
1:C:145:ASP:OD1	1:C:147:ASP:HB2	2.13	0.49
1:D:43:MET:HA	1:D:422:SER:HB2	1.95	0.49
1:C:218:GLU:HG2	1:C:428:GLN:HE22	1.77	0.49
1:A:192:ASN:OD1	1:A:195:ARG:NH1	2.45	0.48
1:B:163:LEU:HD13	1:B:190:PHE:CE1	2.48	0.48
1:C:124:ALA:HA	1:C:128:GLU:OE2	2.14	0.48
1:D:68:LEU:HB2	1:D:156:ASP:HB3	1.96	0.48
1:B:252:ASP:OD1	1:B:416:HIS:HE1	1.96	0.48
1:D:218:GLU:CG	1:D:428:GLN:NE2	2.63	0.48
1:D:23:ILE:O	1:D:24:ALA:C	2.52	0.48
1:A:78:ILE:HG23	1:A:88:VAL:HG21	1.96	0.48
1:A:284:GLY:HA3	3:A:550:NAD:O5B	2.14	0.48
1:B:430:ILE:O	1:B:434:GLU:HG2	2.13	0.48
1:C:247:THR:HA	1:C:251:PHE:CD2	2.49	0.48
1:D:15:VAL:O	1:D:16:ARG:NH1	2.47	0.48
1:A:155:ASP:OD2	1:A:158:GLY:HA2	2.13	0.48
1:A:238:PRO:HB2	1:A:435:LEU:HD21	1.94	0.47
1:B:457:VAL:O	1:B:461:HIS:ND1	2.38	0.47
1:C:471:LYS:NZ	1:C:484:VAL:HG11	2.29	0.47
1:A:340:ASN:HD21	1:B:476:GLN:HB3	1.79	0.47
1:B:71:THR:HG22	1:B:99:GLN:NE2	2.30	0.47
1:C:28:LEU:HB3	1:C:101:HIS:HA	1.97	0.47
1:B:57:GLN:NE2	1:B:85:GLY:HA2	2.22	0.47
1:C:221:THR:HG1	3:C:550:NAD:HO3N	1.60	0.47
1:B:29:ALA:CB	1:B:108:VAL:HG21	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:HIS:HD2	4:B:685:HOH:O	1.96	0.47
1:B:384:LYS:HB2	1:B:385:PRO:CD	2.44	0.47
1:D:52:GLU:HB3	1:D:53:TYR:CD1	2.50	0.47
1:B:57:GLN:HB3	1:B:60:LYS:HG3	1.97	0.47
1:B:394:ASP:OD1	1:B:395:THR:HG23	2.15	0.47
1:B:23:ILE:HD11	1:B:26:LEU:HD13	1.97	0.47
1:A:281:CYS:HB2	1:A:336:THR:HA	1.96	0.46
1:B:124:ALA:HA	1:B:128:GLU:OE2	2.15	0.46
1:C:252:ASP:OD2	1:C:416:HIS:CE1	2.67	0.46
1:B:213:LYS:HG3	1:B:436:TRP:CZ3	2.51	0.46
1:D:151:ASN:HA	1:D:212:VAL:HA	1.97	0.46
1:B:179:ALA:HB2	1:B:191:LEU:HD12	1.97	0.46
1:C:479:TYR:CD1	1:D:341:LYS:HD2	2.50	0.46
1:D:360:ASN:ND2	1:D:364:PHE:O	2.48	0.46
1:B:68:LEU:HD22	1:B:154:LEU:CD2	2.46	0.46
1:C:423:ASN:HD21	1:D:312:LEU:CD2	2.28	0.46
1:C:363:HIS:CD2	1:C:364:PHE:CE1	3.04	0.46
1:C:469:LEU:HD11	1:D:308:PRO:HB3	1.98	0.46
1:D:146:PRO:CB	1:D:147:ASP:CA	2.94	0.46
1:A:197:ARG:HG3	1:A:197:ARG:O	2.16	0.46
1:D:22:LYS:HG3	1:D:125:TRP:CZ3	2.51	0.46
1:A:95:ILE:HG22	1:A:133:TYR:HB2	1.98	0.46
1:A:262:ILE:HD11	1:C:262:ILE:CD1	2.34	0.46
1:C:57:GLN:HA	1:C:57:GLN:HE21	1.81	0.46
1:C:345:MET:HA	1:C:369:ASP:HB2	1.97	0.46
1:B:442:TYR:N	1:B:442:TYR:CD1	2.84	0.46
1:D:406:ARG:O	1:D:407:LEU:C	2.52	0.46
1:B:69:HIS:CE1	1:B:410:LEU:HD13	2.51	0.45
1:C:33:ARG:NH2	1:C:79:GLU:OE2	2.23	0.45
1:D:483:ASP:HB3	4:D:733:HOH:O	2.14	0.45
1:C:216:THR:HG23	1:C:432:GLN:HE22	1.80	0.45
1:A:13:PRO:HB3	1:A:123:PHE:HE1	1.80	0.45
1:D:113:THR:HG23	1:D:116:GLU:HB3	1.98	0.45
1:D:88:VAL:CG2	1:D:120:VAL:HG21	2.46	0.45
1:D:16:ARG:HB2	1:D:117:PRO:HG2	1.98	0.45
1:A:182:ASP:OD1	1:A:375:ARG:NH1	2.49	0.45
1:D:408:LEU:C	1:D:408:LEU:HD12	2.37	0.45
1:B:248:LYS:HD3	1:B:252:ASP:HB3	1.99	0.45
1:D:106:VAL:CG1	1:D:120:VAL:HG22	2.47	0.45
1:B:320:ASP:OD1	1:C:300:ARG:HD2	2.16	0.45
1:C:311:ALA:O	1:C:315:MET:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ASN:ND2	1:A:244:ASP:H	2.15	0.45
1:D:157:GLY:HA3	1:D:363:HIS:NE2	2.32	0.45
1:D:259:HIS:ND1	1:D:417:PRO:HD3	2.32	0.45
1:A:323:THR:OG1	1:A:326:GLU:HG2	2.17	0.45
1:B:246:VAL:HG21	1:B:495:TYR:CE1	2.52	0.44
1:B:259:HIS:HE1	4:D:673:HOH:O	2.00	0.44
1:B:225:ARG:HE	1:B:364:PHE:HE2	1.64	0.44
1:B:32:GLY:HA2	1:B:101:HIS:HD2	1.82	0.44
1:C:217:GLU:OE2	1:C:222:GLY:HA3	2.18	0.44
1:C:312:LEU:HG	1:D:251:PHE:CE2	2.52	0.44
1:A:72:VAL:O	1:A:76:VAL:HG23	2.17	0.44
1:C:216:THR:CG2	1:C:432:GLN:HE21	2.29	0.44
1:A:259:HIS:HE1	4:C:850:HOH:O	2.00	0.44
1:B:145:ASP:C	1:B:147:ASP:H	2.15	0.44
1:D:97:SER:HB2	1:D:410:LEU:HB3	1.98	0.44
1:D:340:ASN:O	1:D:367:GLU:HG2	2.17	0.44
1:B:213:LYS:O	1:B:238:PRO:HD2	2.17	0.44
1:D:88:VAL:HG23	1:D:120:VAL:HG21	2.00	0.44
1:A:261:LEU:HD22	1:A:290:CYS:SG	2.58	0.44
1:D:416:HIS:HB2	1:D:421:MET:SD	2.58	0.44
1:C:278:VAL:HG11	1:C:294:MET:HG3	2.00	0.44
1:C:89:ARG:NH2	1:C:139:GLN:O	2.37	0.44
1:B:88:VAL:O	1:B:121:PRO:HD2	2.17	0.44
1:C:235:LEU:HG	1:C:237:PHE:O	2.16	0.44
1:C:352:MET:HB2	1:C:399:ILE:HD11	1.99	0.44
1:A:59:LEU:HA	1:A:59:LEU:HD23	1.84	0.43
1:A:52:GLU:OE1	1:A:456:LYS:NZ	2.32	0.43
1:D:252:ASP:OD1	1:D:416:HIS:CE1	2.71	0.43
1:A:91:ALA:HB2	1:A:140:MET:HB2	2.00	0.43
1:A:248:LYS:HD3	1:A:252:ASP:HB3	1.99	0.43
1:D:218:GLU:HG3	1:D:428:GLN:HE21	1.74	0.43
1:A:363:HIS:CE1	2:A:500:AD3:HO5'	2.31	0.43
1:A:489:LYS:NZ	3:B:550:NAD:O3B	2.35	0.43
1:B:95:ILE:CG2	1:B:133:TYR:HB2	2.49	0.43
1:B:57:GLN:NE2	1:B:85:GLY:CA	2.80	0.43
1:D:71:THR:HA	1:D:99:GLN:HG3	1.99	0.43
1:C:423:ASN:HD21	1:D:312:LEU:HD21	1.84	0.43
1:B:345:MET:HA	1:B:369:ASP:HB3	2.00	0.43
1:A:69:HIS:ND1	1:A:97:SER:CB	2.82	0.43
1:D:281:CYS:HB2	1:D:336:THR:HA	2.01	0.43
1:B:394:ASP:OD1	1:B:395:THR:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:TRP:O	1:A:398:SER:HA	2.19	0.43
1:D:134:TRP:CZ3	1:D:163:LEU:HD22	2.54	0.43
1:A:428:GLN:HE21	1:A:428:GLN:HB2	1.55	0.43
1:C:57:GLN:HE22	1:C:84:LEU:C	2.23	0.42
1:D:99:GLN:NE2	1:D:414:THR:HB	2.33	0.42
1:A:384:LYS:NZ	4:A:591:HOH:O	2.51	0.42
1:B:89:ARG:HD3	1:B:143:TRP:CE2	2.54	0.42
1:D:23:ILE:HG23	1:D:122:VAL:O	2.19	0.42
1:A:258:ARG:HA	1:A:293:ALA:HB2	2.00	0.42
1:A:217:GLU:HG3	1:A:223:VAL:HG23	2.01	0.42
1:D:213:LYS:HG3	1:D:436:TRP:HZ3	1.85	0.42
1:A:36:LEU:HD12	1:A:72:VAL:HG13	2.01	0.42
1:A:36:LEU:O	1:A:40:GLU:HG3	2.19	0.42
1:A:69:HIS:CD2	1:A:410:LEU:HD13	2.55	0.42
1:A:203:ASP:O	1:A:207:LYS:HG3	2.20	0.42
1:A:476:GLN:HB3	1:B:340:ASN:HD21	1.83	0.42
1:A:480:LEU:HA	1:B:224:LEU:HD21	2.01	0.42
1:C:108:VAL:O	1:C:112:GLY:HA3	2.19	0.42
1:B:94:ASN:ND2	1:B:407:LEU:CD1	2.83	0.42
1:C:357:ILE:HD11	4:C:849:HOH:O	2.19	0.42
1:B:126:LYS:HE2	4:B:697:HOH:O	2.18	0.42
1:A:346:LEU:HD13	1:A:373:LEU:HA	2.02	0.42
1:C:218:GLU:CG	1:C:428:GLN:NE2	2.73	0.42
1:D:471:LYS:HG2	1:D:472:LEU:O	2.20	0.42
1:B:36:LEU:O	1:B:40:GLU:HG3	2.20	0.42
1:D:163:LEU:HD12	1:D:194:LEU:HD21	2.01	0.42
1:A:244:ASP:OD2	1:B:492:HIS:HE1	2.03	0.42
1:B:355:HIS:NE2	1:D:41:HIS:ND1	2.68	0.42
1:D:419:PHE:CZ	1:D:465:LEU:HG	2.55	0.42
1:C:248:LYS:HG2	1:C:424:SER:HB3	2.02	0.41
1:A:406:ARG:O	1:A:407:LEU:C	2.58	0.41
1:C:115:ASP:HB3	4:C:779:HOH:O	2.19	0.41
1:C:149:PRO:HG2	1:C:211:SER:HB2	2.02	0.41
1:D:174:GLY:O	1:D:198:PHE:CE2	2.74	0.41
1:C:216:THR:HG21	1:C:432:GLN:NE2	2.32	0.41
1:B:328:ILE:CD1	1:B:344:ILE:HD12	2.50	0.41
1:A:403:SER:O	1:A:406:ARG:CG	2.68	0.41
1:A:66:GLY:HA3	1:A:90:TRP:CZ3	2.55	0.41
1:D:278:VAL:HG11	1:D:294:MET:HG3	2.01	0.41
1:D:355:HIS:N	1:D:398:SER:O	2.47	0.41
1:B:477:ALA:HB1	1:B:482:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ASN:O	1:B:152:MET:HG2	2.20	0.41
1:D:163:LEU:CD1	1:D:194:LEU:HD21	2.50	0.41
1:D:176:VAL:HA	1:D:177:PRO:HD3	1.85	0.41
1:A:430:ILE:O	1:A:434:GLU:HG2	2.21	0.41
1:C:303:VAL:O	1:C:321:VAL:HA	2.20	0.41
1:D:66:GLY:HA3	1:D:90:TRP:CZ3	2.55	0.41
1:C:94:ASN:HB3	1:C:97:SER:OG	2.21	0.41
1:B:490:PRO:HD2	1:B:493:TYR:HB2	2.02	0.41
1:B:473:THR:OG1	1:B:476:GLN:HG3	2.21	0.41
1:D:26:LEU:N	1:D:26:LEU:HD12	2.36	0.41
1:D:252:ASP:OD1	1:D:416:HIS:HE1	2.03	0.41
1:A:66:GLY:HA3	1:A:90:TRP:CE3	2.56	0.41
1:B:279:LEU:HD11	1:B:304:THR:CG2	2.51	0.41
1:D:372:GLY:O	1:D:376:SER:HB3	2.21	0.41
1:B:260:SER:OG	1:B:416:HIS:CD2	2.66	0.40
1:B:94:ASN:HB3	1:B:97:SER:HB3	2.04	0.40
1:B:110:PRO:HD2	4:B:598:HOH:O	2.20	0.40
1:B:217:GLU:HG3	1:B:223:VAL:HG23	2.01	0.40
1:A:223:VAL:O	1:A:226:LEU:HB2	2.21	0.40
1:B:213:LYS:HG3	1:B:436:TRP:HZ3	1.87	0.40
1:C:97:SER:CB	1:C:410:LEU:HB3	2.50	0.40
1:B:135:TRP:O	1:B:138:GLU:HB3	2.21	0.40
1:D:304:THR:OG1	3:D:550:NAD:H2A	2.21	0.40
1:C:384:LYS:HE3	1:C:387:VAL:HG21	2.02	0.40
1:A:355:HIS:N	1:A:398:SER:O	2.40	0.40
1:A:208:ILE:O	1:A:212:VAL:HG23	2.21	0.40
1:D:247:THR:HA	1:D:251:PHE:CD1	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:847:HOH:O	4:D:691:HOH:O[1_455]	2.08	0.12
4:B:679:HOH:O	4:D:689:HOH:O[1_556]	2.16	0.04

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	483/495 (98%)	456 (94%)	22 (5%)	5 (1%)	19	16
1	B	483/495 (98%)	455 (94%)	23 (5%)	5 (1%)	19	16
1	C	483/495 (98%)	456 (94%)	25 (5%)	2 (0%)	39	42
1	D	483/495 (98%)	454 (94%)	25 (5%)	4 (1%)	24	22
All	All	1932/1980 (98%)	1821 (94%)	95 (5%)	16 (1%)	24	22

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	365	ASP
1	B	145	ASP
1	B	146	PRO
1	D	146	PRO
1	A	181	GLU
1	B	362	GLY
1	D	69	HIS
1	D	149	PRO
1	A	369	ASP
1	B	407	LEU
1	C	145	ASP
1	A	69	HIS
1	A	474	LYS
1	D	147	ASP
1	C	116	GLU
1	B	144	PRO

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	395/404 (98%)	377 (95%)	18 (5%)	33	40
1	B	395/404 (98%)	381 (96%)	14 (4%)	43	53
1	C	395/404 (98%)	376 (95%)	19 (5%)	31	37
1	D	395/404 (98%)	373 (94%)	22 (6%)	26	29
All	All	1580/1616 (98%)	1507 (95%)	73 (5%)	33	40

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	16	ARG
1	A	48	SER
1	A	68	LEU
1	A	88	VAL
1	A	92	SER
1	A	180	GLU
1	A	182	ASP
1	A	186	GLU
1	A	200	THR
1	A	218	GLU
1	A	237	PHE
1	A	241	ASN
1	A	262	ILE
1	A	317	GLU
1	A	365	ASP
1	A	407	LEU
1	A	428	GLN
1	B	88	VAL
1	B	146	PRO
1	B	162	MET
1	B	183	ASP
1	B	188	LYS
1	B	193	LEU
1	B	398	SER
1	B	406	ARG
1	B	407	LEU
1	B	428	GLN
1	B	440	ASP
1	B	442	TYR

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Mol	Chain	Res	Type
1	B	444	ASN
1	B	475	GLU
1	C	11	LEU
1	C	12	THR
1	C	26	LEU
1	C	88	VAL
1	C	111	HIS
1	C	147	ASP
1	C	169	GLN
1	C	180	GLU
1	C	192	ASN
1	C	218	GLU
1	C	224	LEU
1	C	237	PHE
1	C	253	ASN
1	C	262	ILE
1	C	277	LYS
1	C	407	LEU
1	C	424	SER
1	C	454	ASP
1	C	475	GLU
1	D	37	ARG
1	D	68	LEU
1	D	113	THR
1	D	118	LYS
1	D	145	ASP
1	D	148	LYS
1	D	172	LYS
1	D	175	VAL
1	D	182	ASP
1	D	186	GLU
1	D	199	GLU
1	D	213	LYS
1	D	218	GLU
1	D	220	THR
1	D	253	ASN
1	D	262	ILE
1	D	353	LYS
1	D	379	THR
1	D	398	SER
1	D	407	LEU
1	D	440	ASP

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Mol	Chain	Res	Type
1	D	474	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	101	HIS
1	A	241	ASN
1	A	243	ASN
1	A	259	HIS
1	A	310	ASN
1	A	412	ASN
1	A	416	HIS
1	A	428	GLN
1	A	492	HIS
1	B	57	GLN
1	B	243	ASN
1	B	259	HIS
1	B	310	ASN
1	B	386	GLN
1	B	412	ASN
1	B	416	HIS
1	B	439	ASN
1	B	492	HIS
1	C	57	GLN
1	C	192	ASN
1	C	243	ASN
1	C	259	HIS
1	C	310	ASN
1	C	355	HIS
1	C	412	ASN
1	C	416	HIS
1	C	427	ASN
1	C	428	GLN
1	C	432	GLN
1	C	492	HIS
1	D	259	HIS
1	D	310	ASN
1	D	412	ASN
1	D	416	HIS
1	D	427	ASN
1	D	428	GLN

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Mol	Chain	Res	Type
1	D	492	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

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	AD3	A	500	-	17,21,21	2.02	4 (23%)	19,31,31	2.42	7 (36%)
3	NAD	A	550	-	38,48,48	1.34	4 (10%)	47,73,73	2.81	10 (21%)
2	AD3	B	500	-	17,21,21	1.58	3 (17%)	19,31,31	1.98	4 (21%)
3	NAD	B	550	-	38,48,48	1.49	8 (21%)	47,73,73	3.03	14 (29%)
2	AD3	C	500	-	17,21,21	1.69	3 (17%)	19,31,31	2.04	4 (21%)
3	NAD	C	550	-	38,48,48	1.41	7 (18%)	47,73,73	2.27	7 (14%)
2	AD3	D	500	-	17,21,21	1.51	3 (17%)	19,31,31	2.36	6 (31%)
3	NAD	D	550	-	38,48,48	1.34	3 (7%)	47,73,73	2.68	12 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AD3	A	500	-	-	0/2/22/22	0/3/3/3
3	NAD	A	550	-	-	0/22/62/62	0/5/5/5
2	AD3	B	500	-	-	0/2/22/22	0/3/3/3
3	NAD	B	550	-	-	0/22/62/62	0/5/5/5
2	AD3	C	500	-	-	0/2/22/22	0/3/3/3
3	NAD	C	550	-	-	0/22/62/62	0/5/5/5
2	AD3	D	500	-	-	0/2/22/22	0/3/3/3
3	NAD	D	550	-	-	0/22/62/62	0/5/5/5

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	AD3	C4-N9	-5.70	1.31	1.38
2	C	500	AD3	C4-N9	-3.95	1.33	1.38
2	D	500	AD3	C4-N9	-3.40	1.34	1.38
2	B	500	AD3	C4-N9	-2.59	1.35	1.38
3	C	550	NAD	C7N-N7N	-2.53	1.27	1.33
3	A	550	NAD	C7N-N7N	-2.36	1.28	1.33
3	B	550	NAD	C7N-N7N	-2.29	1.28	1.33
3	D	550	NAD	C7N-N7N	-2.02	1.28	1.33
3	C	550	NAD	O4D-C1D	2.02	1.43	1.41
3	B	550	NAD	C4A-N3A	2.05	1.38	1.35
3	C	550	NAD	C3N-C7N	2.09	1.53	1.50
3	B	550	NAD	O2B-C2B	2.22	1.48	1.43
3	C	550	NAD	O3D-C3D	2.25	1.48	1.43
3	A	550	NAD	C2A-N3A	2.29	1.36	1.32
3	C	550	NAD	C2N-C3N	2.31	1.42	1.39
2	D	500	AD3	C3-C2	2.32	1.39	1.36
3	B	550	NAD	C5A-C4A	2.32	1.45	1.40
2	A	500	AD3	C3-C2	2.34	1.39	1.36
3	C	550	NAD	O4B-C1B	2.62	1.44	1.41
2	A	500	AD3	O4'-C1'	2.75	1.44	1.41
3	B	550	NAD	O4B-C1B	2.92	1.44	1.41
3	B	550	NAD	O4D-C1D	3.09	1.45	1.41
3	A	550	NAD	O4D-C1D	3.38	1.45	1.41
2	C	500	AD3	C3-C2	3.58	1.41	1.36
2	D	500	AD3	C4-C5	3.61	1.47	1.40
2	B	500	AD3	C3-C2	3.63	1.41	1.36
2	C	500	AD3	C4-C5	3.65	1.47	1.40
3	D	550	NAD	O7N-C7N	3.80	1.32	1.24
3	B	550	NAD	C2A-N3A	3.82	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	AD3	C4-C5	3.90	1.48	1.40
3	B	550	NAD	O7N-C7N	4.04	1.32	1.24
2	A	500	AD3	C4-C5	4.17	1.48	1.40
3	C	550	NAD	O7N-C7N	4.38	1.33	1.24
3	A	550	NAD	O7N-C7N	4.86	1.34	1.24
3	D	550	NAD	O4D-C1D	5.15	1.47	1.41

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	550	NAD	N3A-C2A-N1A	-16.24	116.46	128.89
3	A	550	NAD	N3A-C2A-N1A	-14.98	117.43	128.89
3	D	550	NAD	N3A-C2A-N1A	-14.42	117.85	128.89
3	C	550	NAD	N3A-C2A-N1A	-12.70	119.17	128.89
2	D	500	AD3	C4'-O4'-C1'	-6.96	102.08	109.72
2	C	500	AD3	C4'-O4'-C1'	-6.24	102.86	109.72
2	A	500	AD3	C3-C2-N1	-6.19	118.44	123.91
3	A	550	NAD	C1B-N9A-C4A	-4.84	119.64	126.94
2	B	500	AD3	C4'-O4'-C1'	-4.56	104.70	109.72
3	A	550	NAD	C4A-C5A-N7A	-4.07	105.73	109.48
3	B	550	NAD	C1B-N9A-C4A	-4.03	120.87	126.94
3	B	550	NAD	C4A-C5A-N7A	-4.02	105.78	109.48
3	D	550	NAD	C1B-N9A-C4A	-3.74	121.30	126.94
3	D	550	NAD	C4B-O4B-C1B	-3.73	105.62	109.72
3	B	550	NAD	PN-O3-PA	-3.72	122.28	132.73
2	C	500	AD3	O5'-C5'-C4'	-3.71	99.07	111.33
3	C	550	NAD	C4A-C5A-N7A	-3.65	106.12	109.48
3	A	550	NAD	PN-O3-PA	-3.45	123.05	132.73
3	B	550	NAD	C5N-C4N-C3N	-3.42	116.03	120.33
3	D	550	NAD	C4A-C5A-N7A	-3.38	106.37	109.48
2	D	500	AD3	C3-C2-N1	-3.37	120.94	123.91
2	B	500	AD3	C3-C2-N1	-3.33	120.97	123.91
3	C	550	NAD	O7N-C7N-N7N	-3.12	118.20	122.59
3	B	550	NAD	O7N-C7N-N7N	-3.00	118.38	122.59
3	C	550	NAD	C4B-O4B-C1B	-2.89	106.54	109.72
2	D	500	AD3	O2'-C2'-C3'	-2.83	102.63	111.83
3	C	550	NAD	C2B-C1B-N9A	-2.69	110.18	114.29
3	D	550	NAD	C5B-C4B-C3B	-2.62	104.82	115.21
3	B	550	NAD	C4B-O4B-C1B	-2.61	106.85	109.72
2	A	500	AD3	C2'-C1'-N9	-2.52	110.44	114.29
2	A	500	AD3	C4'-O4'-C1'	-2.47	107.01	109.72
3	D	550	NAD	C5N-C4N-C3N	-2.42	117.29	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	550	NAD	PN-O3-PA	-2.35	126.12	132.73
2	A	500	AD3	C2-C3-C4	-2.27	117.52	119.64
3	A	550	NAD	C5N-C4N-C3N	-2.27	117.48	120.33
2	D	500	AD3	C2-C3-C4	-2.22	117.56	119.64
3	B	550	NAD	C5D-C4D-C3D	-2.04	107.10	115.21
3	D	550	NAD	C2N-C3N-C4N	2.04	120.57	118.29
2	C	500	AD3	C2-N1-C6	2.08	121.29	117.78
2	D	500	AD3	C3-C4-N9	2.11	134.28	131.94
3	B	550	NAD	C2A-N1A-C6A	2.14	122.59	118.77
3	C	550	NAD	O2N-PN-O1N	2.20	124.43	112.53
3	D	550	NAD	C4D-O4D-C1D	2.39	112.34	109.72
3	A	550	NAD	O2A-PA-O1A	2.51	126.13	112.53
2	A	500	AD3	N6-C6-N1	2.60	124.79	119.20
3	D	550	NAD	O4B-C4B-C3B	2.63	110.44	105.15
2	A	500	AD3	O4'-C1'-N9	2.68	113.72	108.10
3	C	550	NAD	O7N-C7N-C3N	2.71	122.55	119.59
3	B	550	NAD	O5B-PA-O1A	2.74	120.26	109.62
3	D	550	NAD	C3N-C7N-N7N	2.82	120.90	117.82
3	B	550	NAD	C2N-C3N-C4N	2.89	121.51	118.29
3	B	550	NAD	C2B-C3B-C4B	2.89	108.56	102.61
2	B	500	AD3	C2-N1-C6	3.00	122.84	117.78
2	C	500	AD3	C3-C4-N9	3.04	135.32	131.94
3	A	550	NAD	C2B-C1B-N9A	3.25	119.26	114.29
3	A	550	NAD	C2A-N1A-C6A	3.43	124.90	118.77
3	A	550	NAD	C4D-O4D-C1D	3.54	113.61	109.72
3	B	550	NAD	O4B-C1B-N9A	3.57	115.57	108.10
3	D	550	NAD	C2A-N1A-C6A	3.60	125.20	118.77
2	B	500	AD3	C3-C4-N9	3.82	136.18	131.94
3	A	550	NAD	C2N-C3N-C4N	3.89	122.62	118.29
2	D	500	AD3	C2-N1-C6	4.28	125.01	117.78
3	B	550	NAD	C3N-C7N-N7N	4.68	122.94	117.82
2	A	500	AD3	C2-N1-C6	5.05	126.30	117.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	AD3	3	0
3	A	550	NAD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	AD3	1	0
3	B	550	NAD	2	0
2	C	500	AD3	1	0
3	C	550	NAD	2	0
2	D	500	AD3	1	0
3	D	550	NAD	2	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	485/495 (97%)	-0.05	8 (1%) 74 73	19, 33, 58, 81	0
1	B	485/495 (97%)	0.26	32 (6%) 22 21	22, 43, 82, 103	0
1	C	485/495 (97%)	0.10	25 (5%) 31 30	21, 37, 65, 98	0
1	D	485/495 (97%)	0.53	58 (11%) 6 5	19, 46, 86, 116	0
All	All	1940/1980 (97%)	0.21	123 (6%) 23 23	19, 39, 76, 116	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	175	VAL	7.0
1	D	117	PRO	6.3
1	C	175	VAL	6.1
1	C	11	LEU	5.9
1	D	114	PRO	5.9
1	B	199	GLU	5.8
1	B	175	VAL	5.7
1	D	174	GLY	5.6
1	B	170	TYR	5.3
1	D	147	ASP	5.3
1	D	182	ASP	5.2
1	D	180	GLU	4.9
1	D	440	ASP	4.9
1	A	182	ASP	4.9
1	D	181	GLU	4.7
1	D	11	LEU	4.6
1	D	231	ALA	4.1
1	D	116	GLU	4.1
1	B	54	ALA	4.0
1	D	179	ALA	4.0
1	D	170	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	59	LEU	3.9
1	B	11	LEU	3.9
1	C	181	GLU	3.8
1	D	199	GLU	3.8
1	D	200	THR	3.8
1	B	56	VAL	3.7
1	B	176	VAL	3.6
1	D	364	PHE	3.6
1	B	232	ALA	3.6
1	D	486	GLY	3.6
1	D	178	PRO	3.5
1	C	176	VAL	3.5
1	C	182	ASP	3.5
1	D	232	ALA	3.5
1	D	53	TYR	3.5
1	D	198	PHE	3.5
1	B	177	PRO	3.5
1	B	196	THR	3.4
1	D	173	ALA	3.4
1	D	177	PRO	3.3
1	D	233	GLY	3.3
1	C	114	PRO	3.3
1	D	21	PHE	3.2
1	C	200	THR	3.2
1	B	200	THR	3.2
1	B	53	TYR	3.1
1	B	202	LYS	3.1
1	D	172	LYS	3.1
1	D	191	LEU	3.1
1	B	440	ASP	3.1
1	C	180	GLU	3.1
1	D	187	TRP	3.1
1	D	60	LYS	3.0
1	B	195	ARG	3.0
1	B	179	ALA	3.0
1	D	112	GLY	2.9
1	B	147	ASP	2.9
1	B	178	PRO	2.9
1	C	174	GLY	2.9
1	C	198	PHE	2.9
1	D	93	CYS	2.8
1	B	169	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	180	GLU	2.8
1	B	227	TYR	2.8
1	D	160	ALA	2.8
1	C	116	GLU	2.8
1	C	12	THR	2.8
1	D	202	LYS	2.8
1	C	160	ALA	2.8
1	A	420	VAL	2.7
1	B	173	ALA	2.7
1	A	440	ASP	2.7
1	C	179	ALA	2.7
1	C	173	ALA	2.7
1	B	172	LYS	2.7
1	A	179	ALA	2.6
1	D	115	ASP	2.6
1	B	191	LEU	2.6
1	D	192	ASN	2.6
1	D	113	THR	2.5
1	C	29	ALA	2.5
1	D	230	ALA	2.5
1	B	146	PRO	2.5
1	C	113	THR	2.5
1	D	195	ARG	2.5
1	D	68	LEU	2.4
1	D	144	PRO	2.4
1	D	438	LYS	2.4
1	D	201	ASP	2.4
1	D	59	LEU	2.4
1	C	199	GLU	2.4
1	B	174	GLY	2.4
1	C	170	TYR	2.4
1	C	55	GLU	2.3
1	D	61	GLY	2.3
1	A	170	TYR	2.3
1	C	196	THR	2.3
1	D	28	LEU	2.3
1	B	293	ALA	2.3
1	C	56	VAL	2.3
1	B	114	PRO	2.2
1	D	55	GLU	2.2
1	B	198	PHE	2.2
1	B	233	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	158	GLY	2.2
1	D	149	PRO	2.2
1	D	19	ILE	2.2
1	C	364	PHE	2.2
1	D	159	ASP	2.1
1	D	362	GLY	2.1
1	D	221	THR	2.1
1	B	234	ASP	2.1
1	D	56	VAL	2.1
1	A	196	THR	2.1
1	C	178	PRO	2.1
1	C	154	LEU	2.0
1	A	363	HIS	2.0
1	D	90	TRP	2.0
1	D	439	ASN	2.0
1	D	363	HIS	2.0
1	A	178	PRO	2.0
1	D	16	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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	AD3	A	500	19/19	0.96	0.18	0.46	15,24,33,44	0
2	AD3	C	500	19/19	0.94	0.17	0.20	18,26,36,45	0
2	AD3	B	500	19/19	0.96	0.14	-0.37	21,33,53,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	AD3	D	500	19/19	0.94	0.17	-0.63	21,27,35,46	0
3	NAD	B	550	44/44	0.96	0.11	-0.70	30,36,41,46	0
3	NAD	D	550	44/44	0.96	0.11	-0.84	24,33,40,41	0
3	NAD	A	550	44/44	0.96	0.10	-0.86	20,29,33,36	0
3	NAD	C	550	44/44	0.97	0.10	-0.98	24,31,36,39	0

6.5 Other polymers (i)

There are no such residues in this entry.