Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:01 PM GMT

PDB ID	:	1IB6
Title	:	CRYSTAL STRUCTURE OF R153C E. COLI MALATE DEHYDROGENASE
Authors	:	Bell, J.K.; Yennawar, H.P.; Wright, S.K.; Thompson, J.R.; Viola, R.E.; Banaszak, L.J.
Deposited on	:	2001-03-27
Resolution	:	2.10 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:

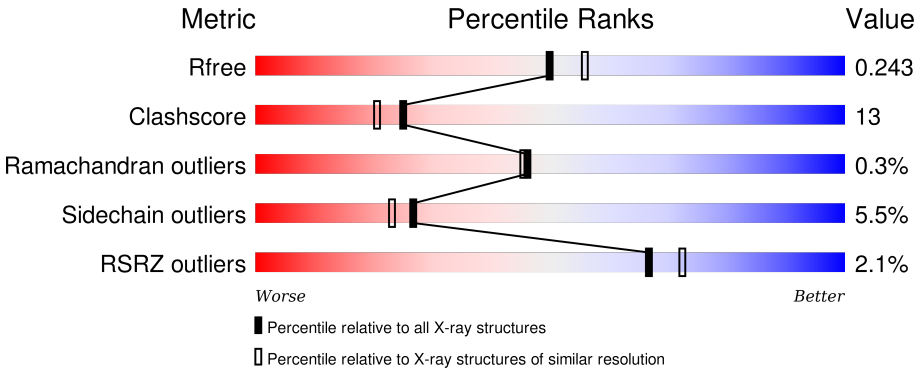
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	312	2% 69% 29%
1	B	312	5% 66% 31%
1	C	312	81% 17%
1	D	312	% 81% 17%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9508 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.

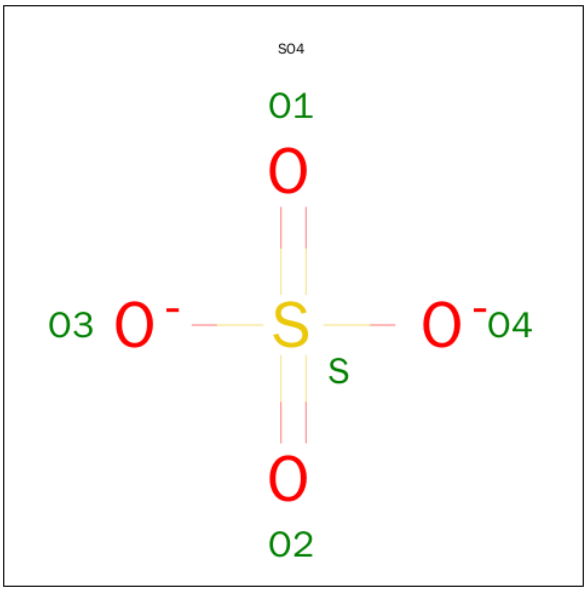
- Molecule 1 is a protein called MALATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	0	0
			2267	1435	384	440	8			
1	B	312	Total	C	N	O	S	0	0	0
			2267	1435	384	440	8			
1	C	312	Total	C	N	O	S	0	0	0
			2267	1435	384	440	8			
1	D	312	Total	C	N	O	S	0	0	0
			2267	1435	384	440	8			

There are 8 discrepancies between the modelled and reference sequences:

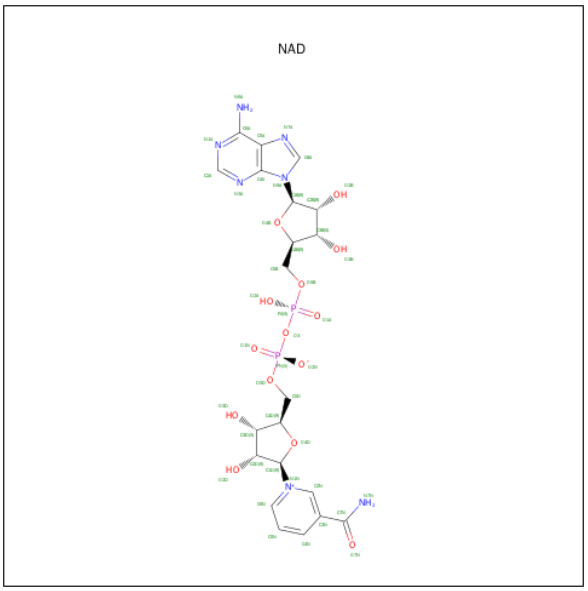
Chain	Residue	Modelled	Actual	Comment	Reference
A	153	CYS	ARG	ENGINEERED	UNP P61889
A	307	GLN	GLU	SEE REMARK 999	UNP P61889
B	153	CYS	ARG	ENGINEERED	UNP P61889
B	307	GLN	GLU	SEE REMARK 999	UNP P61889
C	153	CYS	ARG	ENGINEERED	UNP P61889
C	307	GLN	GLU	SEE REMARK 999	UNP P61889
D	153	CYS	ARG	ENGINEERED	UNP P61889
D	307	GLN	GLU	SEE REMARK 999	UNP P61889

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- 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	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.

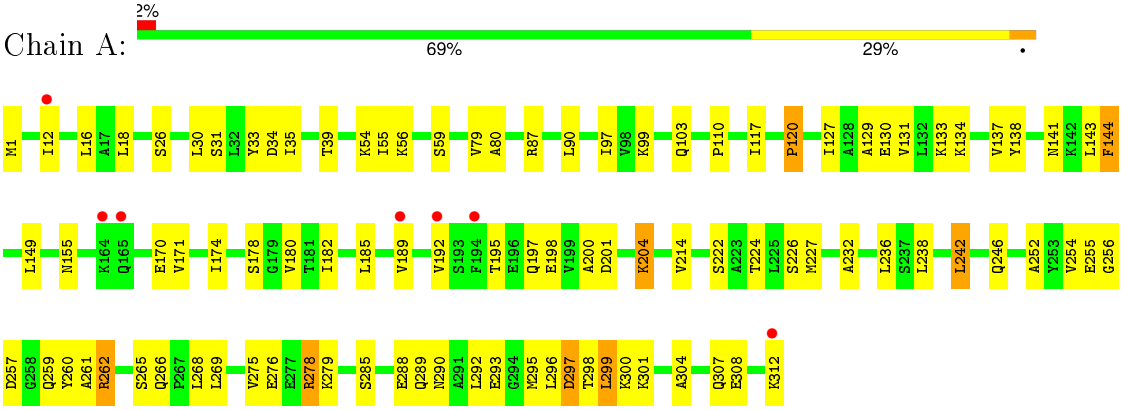
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	75	Total	O	0	0
			75	75		
4	B	54	Total	O	0	0
			54	54		
4	C	75	Total	O	0	0
			75	75		
4	D	74	Total	O	0	0
			74	74		

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.

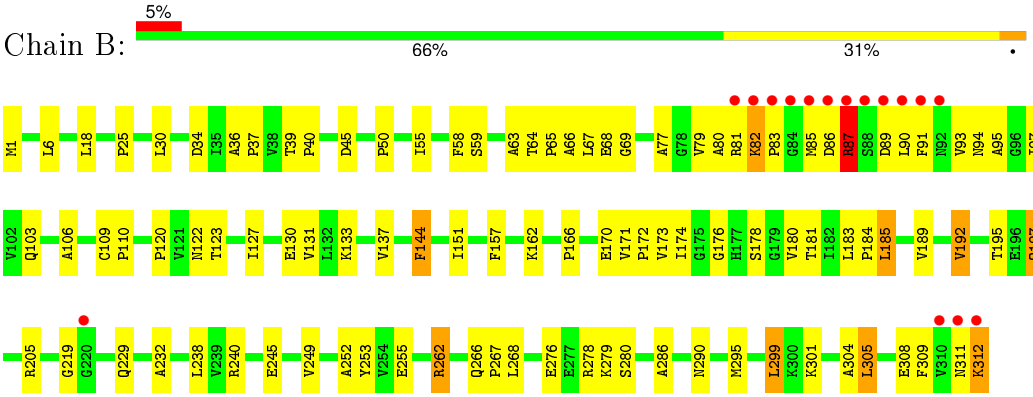
- Molecule 1: MALATE DEHYDROGENASE

Chain A:



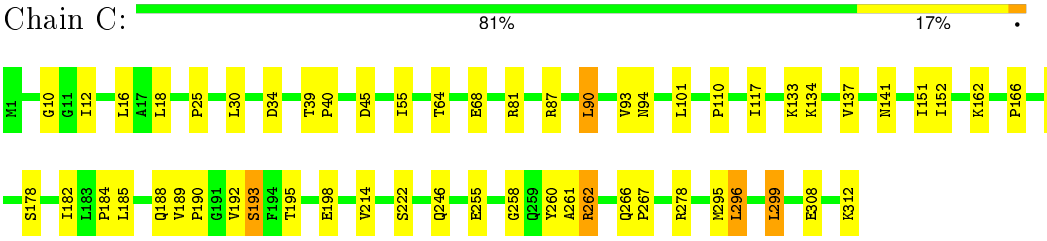
- Molecule 1: MALATE DEHYDROGENASE

Chain B:



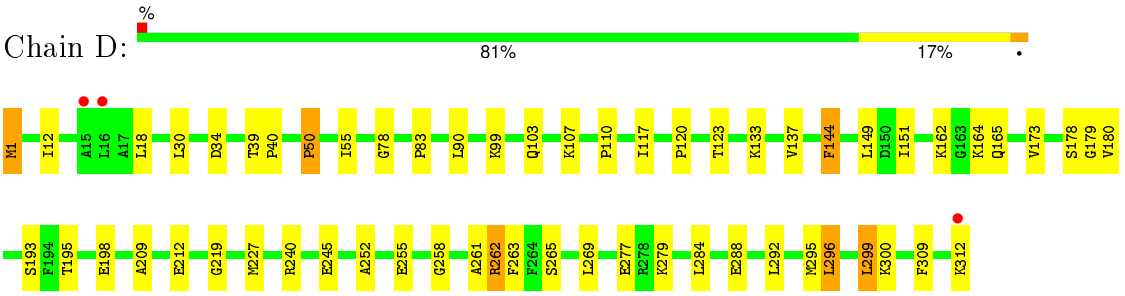
- Molecule 1: MALATE DEHYDROGENASE

Chain C:



- Molecule 1: MALATE DEHYDROGENASE

Chain D:


%
81%
17%
M1
I12
A15
L16
A17
L18
L30
D34
T39
P40
P50
I55
G78
P83
L90
K99
Q103
K107
P110
I117
P120
T123
K133
V137
F144
L149
D150
I151
K162
G163
K164
Q165
V173
S178
G179
V180
S193
F194
T195
E198
A209
E212
G219
M227
R240
E245
A252
E255
G258
A261
R262
F263
F264
S265
L269
E277
R278
K279
L284
E288
L292
M295
L296
L299
K300
F309
K312

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	148.14Å 53.08Å 164.29Å 90.00° 95.26° 90.00°	Depositor
Resolution (Å)	37.42 – 2.10 37.41 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.4 (37.42-2.10) 96.9 (37.41-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.00Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.192 , 0.244 0.191 , 0.243	Depositor DCC
R_{free} test set	7418 reflections (10.06%)	DCC
Wilson B-factor (Å^2)	35.4	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 50.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	2 of 83908 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9508	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% 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: SO4, NAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.73	1/2295 (0.0%)	0.83	1/3108 (0.0%)
1	B	0.88	3/2295 (0.1%)	0.80	3/3108 (0.1%)
1	C	1.00	4/2295 (0.2%)	0.84	5/3108 (0.2%)
1	D	0.75	1/2295 (0.0%)	0.84	3/3108 (0.1%)
All	All	0.85	9/9180 (0.1%)	0.83	12/12432 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	172	PRO	N-CD	-18.10	1.22	1.47
1	C	190	PRO	N-CD	-18.06	1.22	1.47
1	B	50	PRO	N-CD	-18.06	1.22	1.47
1	B	166	PRO	N-CD	-18.05	1.22	1.47
1	C	25	PRO	N-CD	-18.04	1.22	1.47
1	C	166	PRO	N-CD	-18.04	1.22	1.47
1	A	120	PRO	N-CD	-18.02	1.22	1.47
1	C	184	PRO	N-CD	-18.02	1.22	1.47
1	D	40	PRO	N-CD	-18.01	1.22	1.47

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1	MET	CG-SD-CE	5.97	109.75	100.20
1	C	45	ASP	CB-CG-OD1	5.72	123.45	118.30
1	C	184	PRO	N-CD-CG	5.54	111.51	103.20
1	B	50	PRO	N-CD-CG	5.54	111.51	103.20
1	C	25	PRO	N-CD-CG	5.51	111.47	103.20
1	B	172	PRO	N-CD-CG	5.51	111.46	103.20
1	C	166	PRO	N-CD-CG	5.50	111.46	103.20
1	C	190	PRO	N-CD-CG	5.50	111.45	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	40	PRO	N-CD-CG	5.49	111.44	103.20
1	B	166	PRO	N-CD-CG	5.49	111.44	103.20
1	A	120	PRO	N-CD-CG	5.47	111.41	103.20
1	D	227	MET	CG-SD-CE	5.36	108.77	100.20

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	2267	0	2351	79	0
1	B	2267	0	2351	78	0
1	C	2267	0	2351	42	0
1	D	2267	0	2351	40	0
2	A	10	0	0	0	0
2	C	10	0	0	1	0
2	D	10	0	0	0	0
3	A	44	0	26	5	0
3	C	44	0	26	5	0
3	D	44	0	26	5	0
4	A	75	0	0	8	0
4	B	54	0	0	4	0
4	C	75	0	0	2	0
4	D	74	0	0	1	0
All	All	9508	0	9482	237	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 13.

All (237) 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:110:PRO:HB3	1:B:137:VAL:HG21	1.44	0.99
1:B:82:LYS:HB3	1:B:83:PRO:HD2	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:GLN:HE21	1:A:289:GLN:HA	1.37	0.90
1:B:106:ALA:O	1:B:110:PRO:HG3	1.72	0.90
1:C:30:LEU:HD23	1:C:55:ILE:HD12	1.55	0.88
1:A:174:ILE:HG22	1:A:266:GLN:HA	1.58	0.84
1:C:81:ARG:HB3	1:C:90:LEU:HD21	1.58	0.83
1:B:266:GLN:NE2	1:B:278:ARG:HB3	1.94	0.83
1:A:129:ALA:O	1:A:133:LYS:HG3	1.80	0.82
1:B:83:PRO:HD3	1:B:219:GLY:HA2	1.62	0.81
1:C:12:ILE:HD12	3:C:314:NAD:H51N	1.63	0.79
1:A:238:LEU:O	1:A:242:LEU:HD22	1.83	0.79
1:D:12:ILE:HD12	3:D:315:NAD:H51N	1.62	0.78
1:A:224:THR:HG21	4:B:351:HOH:O	1.84	0.77
1:A:260:TYR:CE1	1:A:292:LEU:HD21	2.19	0.77
1:A:296:LEU:O	1:A:300:LYS:HG3	1.86	0.75
1:B:81:ARG:HD3	1:B:86:ASP:O	1.86	0.75
1:B:286:ALA:HB3	4:B:446:HOH:O	1.85	0.74
1:A:295:MET:CE	1:A:299:LEU:HD12	2.18	0.72
1:A:255:GLU:CD	1:A:262:ARG:HH11	1.92	0.72
1:B:311:ASN:O	1:B:312:LYS:HB3	1.88	0.71
1:C:134:LYS:HB3	1:C:134:LYS:NZ	2.04	0.71
1:A:289:GLN:HA	1:A:289:GLN:NE2	2.04	0.71
1:A:97:ILE:HG23	3:A:313:NAD:N6A	2.06	0.70
1:A:197:GLN:HG3	4:A:376:HOH:O	1.89	0.70
1:B:266:GLN:HE21	1:B:278:ARG:HB3	1.55	0.70
1:D:295:MET:HE2	1:D:299:LEU:HD12	1.74	0.70
1:A:110:PRO:HB2	1:A:137:VAL:HG21	1.74	0.69
1:C:110:PRO:CB	1:C:137:VAL:HG21	2.23	0.69
1:B:99:LYS:O	1:B:103:GLN:HG3	1.93	0.69
1:C:110:PRO:HB2	1:C:137:VAL:HG21	1.75	0.69
1:B:127:ILE:O	1:B:131:VAL:HG23	1.92	0.68
1:D:195:THR:OG1	1:D:198:GLU:HG3	1.93	0.67
1:A:130:GLU:OE2	1:A:262:ARG:NH2	2.28	0.67
1:A:222:SER:HB2	4:A:353:HOH:O	1.94	0.67
1:D:110:PRO:HB2	1:D:137:VAL:HG21	1.77	0.66
1:B:90:LEU:O	1:B:93:VAL:HB	1.97	0.65
1:B:77:ALA:HB1	1:B:97:ILE:CD1	2.27	0.65
1:A:35:ILE:HD11	4:A:396:HOH:O	1.96	0.65
1:A:285:SER:OG	1:A:288:GLU:HG3	1.98	0.64
1:A:143:LEU:O	1:A:254:VAL:HG12	1.97	0.64
1:C:117:ILE:O	3:C:314:NAD:H2N	1.97	0.63
1:D:255:GLU:OE2	1:D:262:ARG:HD3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ILE:HD12	3:A:313:NAD:H51N	1.81	0.63
1:B:151:ILE:HD13	1:B:173:VAL:HB	1.81	0.63
1:A:297:ASP:HB2	4:A:371:HOH:O	1.99	0.62
1:B:137:VAL:O	1:B:137:VAL:HG22	2.00	0.62
1:A:269:LEU:HD23	1:A:276:GLU:HG2	1.81	0.61
1:B:37:PRO:HD2	4:B:406:HOH:O	1.99	0.61
1:C:195:THR:OG1	1:C:198:GLU:HG3	2.01	0.61
1:A:127:ILE:O	1:A:131:VAL:HG23	2.01	0.60
1:C:260:TYR:HB3	1:C:296:LEU:HD11	1.82	0.60
1:A:134:LYS:HG3	4:A:365:HOH:O	2.01	0.60
1:A:87:ARG:O	1:A:120:PRO:HG3	2.01	0.60
1:B:151:ILE:CD1	1:B:173:VAL:HB	2.31	0.60
1:B:6:LEU:HD13	1:B:101:LEU:HD22	1.83	0.60
1:B:162:LYS:HG3	1:B:192:VAL:CG1	2.32	0.59
1:A:133:LYS:NZ	1:A:133:LYS:HB3	2.17	0.59
1:D:30:LEU:O	1:D:55:ILE:HA	2.02	0.59
1:B:34:ASP:HB3	1:B:39:THR:OG1	2.03	0.59
1:A:259:GLN:O	1:A:259:GLN:HG2	2.02	0.59
1:B:58:PHE:CD1	1:B:66:ALA:HB2	2.38	0.59
1:A:149:LEU:HD22	1:A:227:MET:SD	2.43	0.58
1:A:30:LEU:HD23	1:A:55:ILE:HD12	1.85	0.58
1:B:83:PRO:HD3	1:B:219:GLY:CA	2.33	0.58
1:B:110:PRO:CB	1:B:137:VAL:HG21	2.25	0.58
1:D:99:LYS:HE2	1:D:103:GLN:NE2	2.18	0.58
1:D:309:PHE:HA	1:D:312:LYS:HE3	1.85	0.58
1:B:94:ASN:O	1:B:97:ILE:HG22	2.03	0.58
1:A:232:ALA:O	1:A:236:LEU:HG	2.05	0.57
1:B:195:THR:O	1:B:199:VAL:HG23	2.05	0.57
1:C:64:THR:O	1:C:68:GLU:HG3	2.05	0.57
1:B:255:GLU:OE2	1:B:262:ARG:HD3	2.05	0.57
1:A:26:SER:OG	1:C:246:GLN:HG3	2.05	0.56
1:C:185:LEU:HD23	1:C:188:GLN:NE2	2.19	0.56
1:D:255:GLU:HB2	1:D:263:PHE:CE1	2.41	0.56
1:B:39:THR:HB	1:B:40:PRO:HD3	1.86	0.56
1:B:77:ALA:HB1	1:B:97:ILE:HD13	1.86	0.56
1:C:222:SER:HB2	4:C:472:HOH:O	2.06	0.56
1:B:240:ARG:CZ	1:B:245:GLU:OE1	2.54	0.56
1:B:151:ILE:HD13	1:B:173:VAL:CG2	2.36	0.55
1:B:109:CYS:N	1:B:110:PRO:HD3	2.22	0.55
1:B:144:PHE:CD1	1:B:144:PHE:N	2.74	0.55
1:C:110:PRO:HB2	1:C:137:VAL:CG2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:VAL:HG22	1:A:222:SER:HB3	1.87	0.55
1:B:106:ALA:O	1:B:110:PRO:CG	2.53	0.54
1:A:266:GLN:NE2	1:A:278:ARG:HB2	2.23	0.54
1:C:87:ARG:HD3	2:C:318:SO4:O1	2.08	0.53
1:A:79:VAL:HG12	1:A:80:ALA:O	2.07	0.53
1:A:255:GLU:CD	1:A:262:ARG:NH1	2.61	0.53
1:A:97:ILE:HG23	3:A:313:NAD:H61A	1.73	0.53
1:B:276:GLU:HA	1:B:276:GLU:OE1	2.08	0.52
1:A:226:SER:HB3	1:B:45:ASP:O	2.09	0.52
1:D:83:PRO:HD2	1:D:219:GLY:HA2	1.91	0.52
1:A:99:LYS:O	1:A:103:GLN:HG3	2.09	0.52
1:B:162:LYS:HG3	1:B:192:VAL:HG11	1.91	0.52
1:A:201:ASP:HB3	4:A:377:HOH:O	2.10	0.52
1:D:110:PRO:HB2	1:D:137:VAL:CG2	2.38	0.52
1:B:94:ASN:HA	1:B:97:ILE:HG22	1.92	0.52
1:C:295:MET:HE2	1:C:299:LEU:HD12	1.92	0.52
1:A:252:ALA:O	1:A:265:SER:HA	2.10	0.51
1:C:178:SER:O	1:C:182:ILE:HG13	2.10	0.51
1:A:110:PRO:CB	1:A:137:VAL:HG21	2.40	0.51
1:A:30:LEU:O	1:A:55:ILE:HA	2.09	0.51
1:B:197:GLN:NE2	1:B:201:ASP:OD2	2.44	0.51
1:C:110:PRO:HB3	1:C:137:VAL:HG21	1.93	0.51
1:B:122:ASN:HA	1:B:253:TYR:CZ	2.46	0.51
1:C:87:ARG:HA	1:C:90:LEU:HD23	1.93	0.51
1:A:189:VAL:CG1	1:A:192:VAL:HG22	2.41	0.51
1:C:152:ILE:HB	1:D:50:PRO:HD3	1.93	0.50
1:D:120:PRO:HG2	1:D:123:THR:HB	1.93	0.50
1:B:189:VAL:HG12	1:B:192:VAL:HG23	1.92	0.50
1:C:30:LEU:CD2	1:C:55:ILE:HD12	2.34	0.50
1:B:85:MET:CE	1:B:89:ASP:HB3	2.41	0.50
1:B:89:ASP:C	1:B:91:PHE:H	2.15	0.50
1:B:77:ALA:HB1	1:B:97:ILE:HD11	1.92	0.50
1:A:295:MET:HE1	1:A:299:LEU:HD12	1.94	0.49
1:C:133:LYS:HE3	1:C:262:ARG:HH12	1.77	0.49
1:B:82:LYS:HB3	1:B:83:PRO:CD	2.32	0.49
1:C:189:VAL:HB	1:C:192:VAL:CG2	2.42	0.49
1:B:189:VAL:HG12	1:B:192:VAL:CG2	2.42	0.49
1:D:240:ARG:NH1	1:D:245:GLU:OE2	2.45	0.49
1:B:130:GLU:OE1	1:B:130:GLU:HA	2.11	0.49
1:C:255:GLU:CD	1:C:262:ARG:HH11	2.16	0.49
1:B:130:GLU:OE1	1:B:133:LYS:HE3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:LYS:HE2	4:D:576:HOH:O	2.12	0.49
1:A:141:ASN:OD1	1:A:278:ARG:NH2	2.46	0.49
1:B:301:LYS:O	1:B:304:ALA:HB3	2.13	0.48
1:A:34:ASP:O	1:A:59:SER:HA	2.13	0.48
1:C:134:LYS:HZ2	1:C:134:LYS:HB3	1.76	0.48
1:D:292:LEU:O	1:D:295:MET:HG2	2.14	0.48
1:A:304:ALA:HA	1:A:307:GLN:NE2	2.29	0.48
1:B:64:THR:N	1:B:65:PRO:HD2	2.29	0.48
1:A:34:ASP:HB3	1:A:39:THR:OG1	2.13	0.48
1:C:34:ASP:OD2	3:C:314:NAD:H1B	2.14	0.48
1:A:178:SER:H	1:A:182:ILE:HG13	1.79	0.48
1:C:308:GLU:O	1:C:312:LYS:HB3	2.13	0.48
3:C:314:NAD:H6N	4:C:474:HOH:O	2.13	0.47
1:A:144:PHE:CE2	1:A:275:VAL:HG23	2.50	0.47
1:B:267:PRO:HB2	1:B:279:LYS:HB2	1.94	0.47
1:B:151:ILE:HD13	1:B:173:VAL:CB	2.44	0.47
1:B:85:MET:HE1	1:B:89:ASP:HB3	1.97	0.47
1:B:67:LEU:O	1:B:68:GLU:C	2.52	0.47
1:B:252:ALA:HB3	1:B:268:LEU:CD1	2.45	0.47
1:A:174:ILE:HG22	1:A:265:SER:O	2.14	0.47
1:A:54:LYS:NZ	1:A:56:LYS:HE3	2.30	0.47
1:A:133:LYS:HZ3	1:A:133:LYS:HB3	1.79	0.47
1:D:103:GLN:O	1:D:107:LYS:HG2	2.15	0.46
1:B:91:PHE:CE1	1:B:305:LEU:HD23	2.50	0.46
1:C:39:THR:HB	1:C:40:PRO:HD3	1.97	0.46
1:A:298:THR:O	1:A:301:LYS:HB3	2.16	0.46
1:A:308:GLU:O	1:A:312:LYS:HB3	2.15	0.46
1:D:110:PRO:CB	1:D:137:VAL:HG21	2.42	0.46
1:B:63:ALA:C	1:B:65:PRO:HD2	2.35	0.46
1:D:252:ALA:O	1:D:265:SER:HA	2.16	0.46
1:A:304:ALA:HA	1:A:307:GLN:HE21	1.81	0.46
1:A:54:LYS:HZ3	1:A:56:LYS:HE3	1.81	0.46
1:D:34:ASP:HB3	1:D:39:THR:OG1	2.15	0.45
1:B:308:GLU:OE1	1:B:312:LYS:HG2	2.16	0.45
1:D:269:LEU:HB3	1:D:277:GLU:HG2	1.98	0.45
1:A:224:THR:CG2	4:B:351:HOH:O	2.54	0.45
1:D:295:MET:CE	1:D:299:LEU:HD12	2.44	0.45
1:A:204:LYS:HB2	1:A:204:LYS:HE3	1.84	0.45
1:A:144:PHE:N	1:A:144:PHE:CD1	2.84	0.45
1:A:246:GLN:OE1	1:D:165:GLN:HG2	2.17	0.45
1:D:144:PHE:CD1	1:D:144:PHE:N	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:GLY:HA3	3:C:314:NAD:O5B	2.17	0.44
1:D:284:LEU:HB3	1:D:288:GLU:HB2	1.99	0.44
1:A:189:VAL:HG12	1:A:192:VAL:HG22	2.00	0.44
1:D:295:MET:HG2	1:D:296:LEU:HD23	1.99	0.44
1:C:174:ILE:HG22	1:C:266:GLN:HA	2.00	0.44
1:C:134:LYS:HB3	1:C:134:LYS:HZ3	1.78	0.44
1:A:97:ILE:HD13	3:A:313:NAD:N7A	2.33	0.44
1:C:266:GLN:HB2	1:C:267:PRO:HD2	2.00	0.44
1:D:78:GLY:O	3:D:315:NAD:H51A	2.18	0.44
1:A:260:TYR:O	1:A:261:ALA:HB2	2.18	0.44
1:B:240:ARG:NH1	1:B:245:GLU:OE1	2.51	0.44
1:C:214:VAL:HG22	1:C:222:SER:HB3	1.99	0.44
1:C:101:LEU:HD23	1:C:101:LEU:HA	1.79	0.44
1:D:162:LYS:NZ	1:D:193:SER:O	2.47	0.44
1:B:176:GLY:HA3	1:B:181:THR:HB	1.99	0.44
1:B:249:VAL:HA	1:B:268:LEU:O	2.17	0.43
1:A:257:ASP:N	1:A:257:ASP:OD1	2.47	0.43
1:B:110:PRO:HB3	1:B:137:VAL:CG2	2.31	0.43
1:B:87:ARG:O	1:B:120:PRO:HB3	2.18	0.43
1:A:268:LEU:HD13	1:A:275:VAL:CG2	2.49	0.43
1:A:103:GLN:HG2	1:A:131:VAL:CG1	2.49	0.43
1:C:141:ASN:OD1	1:C:278:ARG:NH2	2.49	0.43
1:D:258:GLY:HA2	1:D:261:ALA:O	2.19	0.43
1:A:261:ALA:O	1:A:262:ARG:C	2.56	0.43
1:B:36:ALA:HA	1:B:37:PRO:HD3	1.83	0.43
1:B:174:ILE:HD13	1:B:185:LEU:HD21	2.01	0.43
1:C:30:LEU:O	1:C:55:ILE:HA	2.18	0.43
1:D:99:LYS:HG2	1:D:103:GLN:HE21	1.84	0.43
1:C:93:VAL:HG23	1:C:94:ASN:N	2.34	0.43
1:B:183:LEU:HA	1:B:184:PRO:HD3	1.87	0.43
1:D:300:LYS:HB3	1:D:300:LYS:HE2	1.59	0.42
1:B:229:GLN:O	1:B:232:ALA:HB3	2.17	0.42
1:B:90:LEU:O	1:B:93:VAL:CB	2.65	0.42
1:B:295:MET:CE	1:B:299:LEU:HD12	2.49	0.42
1:C:258:GLY:HA2	1:C:261:ALA:O	2.19	0.42
1:A:138:TYR:CE2	1:A:255:GLU:OE1	2.73	0.42
1:D:83:PRO:CD	1:D:219:GLY:HA2	2.49	0.42
1:D:209:ALA:O	1:D:212:GLU:HB3	2.20	0.42
1:A:260:TYR:N	4:A:361:HOH:O	2.49	0.42
1:C:162:LYS:HE3	1:C:193:SER:O	2.19	0.42
1:C:255:GLU:O	1:C:278:ARG:NH1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:TYR:C	1:A:33:TYR:CD1	2.93	0.42
1:D:99:LYS:HE2	1:D:103:GLN:HE21	1.85	0.41
1:B:30:LEU:HD23	1:B:55:ILE:HD12	2.02	0.41
1:B:79:VAL:HG12	1:B:80:ALA:N	2.35	0.41
1:A:268:LEU:HD13	1:A:275:VAL:HG22	2.02	0.41
1:B:290:ASN:HA	1:B:290:ASN:HD22	1.66	0.41
1:A:117:ILE:O	3:A:313:NAD:H2N	2.19	0.41
1:D:292:LEU:O	1:D:296:LEU:HD23	2.21	0.41
1:A:155:ASN:ND2	1:A:170:GLU:OE2	2.54	0.41
1:A:195:THR:OG1	1:A:198:GLU:HG3	2.20	0.41
1:B:157:PHE:CE1	1:B:205:ARG:CZ	3.04	0.41
1:B:91:PHE:CE1	1:B:123:THR:HG21	2.56	0.41
1:C:151:ILE:HD13	1:C:173:VAL:HG23	2.02	0.41
1:A:289:GLN:O	1:A:293:GLU:HG2	2.20	0.41
3:D:315:NAD:H2D	3:D:315:NAD:H6N	1.86	0.41
1:D:117:ILE:O	3:D:315:NAD:H2N	2.20	0.41
1:D:178:SER:O	1:D:180:VAL:N	2.54	0.41
1:D:151:ILE:CD1	1:D:173:VAL:HB	2.51	0.41
1:A:256:GLY:HA3	4:A:359:HOH:O	2.20	0.41
1:B:130:GLU:CD	1:B:133:LYS:HE3	2.41	0.40
1:D:12:ILE:HD12	3:D:315:NAD:C5D	2.42	0.40
1:A:90:LEU:HB2	1:A:120:PRO:HD3	2.03	0.40
1:B:34:ASP:O	1:B:59:SER:HA	2.19	0.40
1:B:133:LYS:NZ	1:B:262:ARG:NH2	2.70	0.40
1:C:151:ILE:HD13	1:C:173:VAL:CG2	2.51	0.40
1:A:289:GLN:HE21	1:A:289:GLN:CA	2.10	0.40
1:A:197:GLN:O	1:A:200:ALA:HB3	2.21	0.40
1:D:149:LEU:HD12	1:D:149:LEU:HA	1.93	0.40
1:B:94:ASN:O	1:B:95:ALA:C	2.60	0.40
1:B:195:THR:OG1	1:B:198:GLU:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	310/312 (99%)	291 (94%)	19 (6%)	0	100 100
1	B	310/312 (99%)	280 (90%)	27 (9%)	3 (1%)	19 13
1	C	310/312 (99%)	303 (98%)	7 (2%)	0	100 100
1	D	310/312 (99%)	299 (96%)	10 (3%)	1 (0%)	46 45
All	All	1240/1248 (99%)	1173 (95%)	63 (5%)	4 (0%)	46 45

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	179	GLY
1	B	69	GLY
1	B	87	ARG
1	B	309	PHE

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	241/241 (100%)	225 (93%)	16 (7%)	21 17
1	B	241/241 (100%)	222 (92%)	19 (8%)	15 11
1	C	241/241 (100%)	233 (97%)	8 (3%)	45 47
1	D	241/241 (100%)	231 (96%)	10 (4%)	37 36
All	All	964/964 (100%)	911 (94%)	53 (6%)	27 23

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	16	LEU
1	A	18	LEU
1	A	31	SER

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Mol	Chain	Res	Type
1	A	144	PHE
1	A	171	VAL
1	A	180	VAL
1	A	185	LEU
1	A	204	LYS
1	A	242	LEU
1	A	262	ARG
1	A	278	ARG
1	A	279	LYS
1	A	290	ASN
1	A	297	ASP
1	A	299	LEU
1	B	1	MET
1	B	18	LEU
1	B	25	PRO
1	B	82	LYS
1	B	87	ARG
1	B	144	PHE
1	B	170	GLU
1	B	171	VAL
1	B	178	SER
1	B	180	VAL
1	B	185	LEU
1	B	192	VAL
1	B	197	GLN
1	B	238	LEU
1	B	262	ARG
1	B	280	SER
1	B	299	LEU
1	B	305	LEU
1	B	312	LYS
1	C	16	LEU
1	C	18	LEU
1	C	90	LEU
1	C	171	VAL
1	C	193	SER
1	C	262	ARG
1	C	296	LEU
1	C	299	LEU
1	D	1	MET
1	D	18	LEU
1	D	50	PRO

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Mol	Chain	Res	Type
1	D	90	LEU
1	D	144	PHE
1	D	164	LYS
1	D	262	ARG
1	D	279	LYS
1	D	296	LEU
1	D	299	LEU

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

Mol	Chain	Res	Type
1	A	23	GLN
1	A	208	ASN
1	A	243	GLN
1	A	259	GLN
1	A	266	GLN
1	A	289	GLN
1	A	307	GLN
1	A	311	ASN
1	B	259	GLN
1	B	266	GLN
1	B	290	ASN
1	B	307	GLN
1	D	103	GLN
1	D	259	GLN
1	D	307	GLN

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 (i)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAD	A	313	-	38,48,48	2.14	7 (18%)	47,73,73	1.85	8 (17%)
2	SO4	A	316	-	4,4,4	3.28	2 (50%)	6,6,6	1.01	0
2	SO4	A	317	-	4,4,4	3.34	2 (50%)	6,6,6	0.96	0
3	NAD	C	314	-	38,48,48	2.27	8 (21%)	47,73,73	1.83	9 (19%)
2	SO4	C	318	-	4,4,4	3.25	2 (50%)	6,6,6	1.01	0
2	SO4	C	319	-	4,4,4	3.32	2 (50%)	6,6,6	0.92	0
3	NAD	D	315	-	38,48,48	2.28	8 (21%)	47,73,73	1.79	7 (14%)
2	SO4	D	320	-	4,4,4	3.30	2 (50%)	6,6,6	1.06	1 (16%)
2	SO4	D	321	-	4,4,4	3.34	2 (50%)	6,6,6	0.89	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	A	313	-	-	0/22/62/62	0/5/5/5
2	SO4	A	316	-	-	0/0/0/0	0/0/0/0
2	SO4	A	317	-	-	0/0/0/0	0/0/0/0
3	NAD	C	314	-	-	0/22/62/62	0/5/5/5
2	SO4	C	318	-	-	0/0/0/0	0/0/0/0
2	SO4	C	319	-	-	0/0/0/0	0/0/0/0
3	NAD	D	315	-	-	0/22/62/62	0/5/5/5
2	SO4	D	320	-	-	0/0/0/0	0/0/0/0
2	SO4	D	321	-	-	0/0/0/0	0/0/0/0

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	321	SO4	O3-S	-4.58	1.30	1.47
2	A	317	SO4	O3-S	-4.58	1.30	1.47
2	C	319	SO4	O3-S	-4.49	1.31	1.47
2	C	318	SO4	O3-S	-4.42	1.31	1.47
2	D	320	SO4	O3-S	-4.26	1.32	1.47
2	A	316	SO4	O3-S	-4.24	1.32	1.47
3	A	313	NAD	C6N-C5N	-2.90	1.32	1.38
3	D	315	NAD	C3N-C7N	-2.82	1.46	1.50
3	C	314	NAD	C6N-C5N	-2.62	1.32	1.38
3	D	315	NAD	C6N-C5N	-2.49	1.33	1.38
3	C	314	NAD	O4B-C1B	-2.41	1.38	1.41
3	D	315	NAD	O4B-C1B	-2.25	1.38	1.41
3	C	314	NAD	O4D-C4D	2.03	1.49	1.45
3	C	314	NAD	C2A-N1A	2.06	1.37	1.33
3	A	313	NAD	C2A-N1A	2.21	1.38	1.33
3	D	315	NAD	C2A-N1A	2.40	1.38	1.33
3	A	313	NAD	O2B-C2B	2.46	1.48	1.43
3	A	313	NAD	C6N-N1N	3.27	1.44	1.35
3	C	314	NAD	C6N-N1N	3.55	1.45	1.35
3	D	315	NAD	C6N-N1N	3.65	1.45	1.35
2	C	319	SO4	O1-S	4.70	1.63	1.47
2	C	318	SO4	O1-S	4.73	1.63	1.47
2	A	317	SO4	O1-S	4.81	1.63	1.47
2	D	321	SO4	O1-S	4.84	1.63	1.47
2	A	316	SO4	O1-S	4.92	1.64	1.47
2	D	320	SO4	O1-S	4.96	1.64	1.47
3	A	313	NAD	C5N-C4N	5.26	1.49	1.38
3	D	315	NAD	C5N-C4N	5.57	1.50	1.38
3	C	314	NAD	C5N-C4N	5.73	1.50	1.38
3	A	313	NAD	C2N-C3N	6.21	1.48	1.39
3	D	315	NAD	C2N-C3N	6.57	1.49	1.39
3	C	314	NAD	C2N-C3N	7.11	1.49	1.39
3	A	313	NAD	C4N-C3N	7.63	1.52	1.39
3	C	314	NAD	C4N-C3N	7.88	1.52	1.39
3	D	315	NAD	C4N-C3N	7.99	1.53	1.39

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	313	NAD	C5N-C4N-C3N	-6.03	112.75	120.33
3	D	315	NAD	C5N-C4N-C3N	-5.79	113.06	120.33
3	C	314	NAD	C5N-C4N-C3N	-5.75	113.10	120.33
3	C	314	NAD	C4B-O4B-C1B	-3.85	105.49	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	313	NAD	C4B-O4B-C1B	-3.79	105.55	109.72
3	A	313	NAD	O7N-C7N-C3N	-3.56	115.70	119.59
3	D	315	NAD	C4B-O4B-C1B	-3.43	105.95	109.72
3	D	315	NAD	O7N-C7N-C3N	-3.26	116.03	119.59
3	C	314	NAD	O3-PN-O5D	-2.93	95.17	102.94
3	C	314	NAD	O7N-C7N-C3N	-2.80	116.53	119.59
3	A	313	NAD	O3-PN-O5D	-2.35	96.69	102.94
3	C	314	NAD	O7N-C7N-N7N	-2.21	119.49	122.59
3	D	315	NAD	O3-PN-O5D	-2.20	97.09	102.94
2	D	320	SO4	O2-S-O1	-2.13	102.73	109.50
3	A	313	NAD	O2N-PN-O5D	2.00	118.57	108.46
3	C	314	NAD	O2N-PN-O5D	2.01	118.58	108.46
3	A	313	NAD	O4D-C1D-N1N	2.48	110.86	108.13
3	C	314	NAD	O4D-C1D-N1N	2.97	111.39	108.13
3	D	315	NAD	C6N-C5N-C4N	3.38	124.55	119.44
3	C	314	NAD	C6N-C5N-C4N	3.77	125.14	119.44
3	D	315	NAD	O4D-C1D-N1N	3.91	112.43	108.13
3	A	313	NAD	C6N-C5N-C4N	4.00	125.48	119.44
3	D	315	NAD	C3N-C7N-N7N	5.46	123.79	117.82
3	C	314	NAD	C3N-C7N-N7N	5.63	123.98	117.82
3	A	313	NAD	C3N-C7N-N7N	6.08	124.47	117.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	313	NAD	5	0
3	C	314	NAD	5	0
2	C	318	SO4	1	0
3	D	315	NAD	5	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	312/312 (100%)	-0.16	7 (2%) 65 71	29, 45, 76, 93	0
1	B	312/312 (100%)	0.02	16 (5%) 32 40	27, 50, 80, 100	7 (2%)
1	C	312/312 (100%)	-0.44	0 100 100	25, 39, 62, 94	0
1	D	312/312 (100%)	-0.33	3 (0%) 84 87	25, 41, 61, 92	0
All	All	1248/1248 (100%)	-0.23	26 (2%) 67 72	25, 44, 74, 100	7 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	84	GLY	13.2
1	B	88	SER	6.6
1	B	90	LEU	5.2
1	B	83	PRO	5.2
1	B	85	MET	4.8
1	B	91	PHE	4.1
1	B	312	LYS	4.0
1	B	82	LYS	3.8
1	B	310	VAL	3.8
1	A	192	VAL	3.7
1	B	311	ASN	3.5
1	D	312	LYS	3.5
1	B	89	ASP	3.1
1	B	86	ASP	3.0
1	B	220	GLY	2.9
1	B	81	ARG	2.8
1	A	165	GLN	2.7
1	B	87	ARG	2.6
1	A	12	ILE	2.5
1	A	189	VAL	2.5
1	A	312	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	194	PHE	2.4
1	B	92	ASN	2.3
1	D	16	LEU	2.1
1	D	15	ALA	2.0
1	A	164	LYS	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
3	NAD	D	315	44/44	0.96	0.15	1.46	22,34,49,56	43
3	NAD	A	313	44/44	0.90	0.18	1.38	37,61,74,80	20
2	SO4	A	317	5/5	0.86	0.16	0.56	46,48,54,57	5
2	SO4	C	318	5/5	0.97	0.12	0.36	56,58,62,67	5
3	NAD	C	314	44/44	0.96	0.11	-0.22	35,44,54,56	44
2	SO4	D	321	5/5	0.93	0.12	-0.41	55,61,66,69	5
2	SO4	A	316	5/5	0.94	0.10	-0.49	97,100,100,100	0
2	SO4	C	319	5/5	0.98	0.09	-1.15	27,39,45,47	5
2	SO4	D	320	5/5	0.97	0.07	-1.43	52,55,67,67	0

6.5 Other polymers (i)

There are no such residues in this entry.