Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:25 AM GMT

PDB ID	:	3OX4
Title	:	Structures of iron-dependent alcohol dehydrogenase 2 from Zymomonas mobilis ZM4 complexed with NAD cofactor
Authors	:	Moon, J.H.; Lee, H.J.; Song, J.M.; Park, S.Y.; Park, M.Y.; Park, H.M.; Sun, J.; Park, J.H.; Kim, J.S.
Deposited on	:	2010-09-21
Resolution	:	2.00 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:

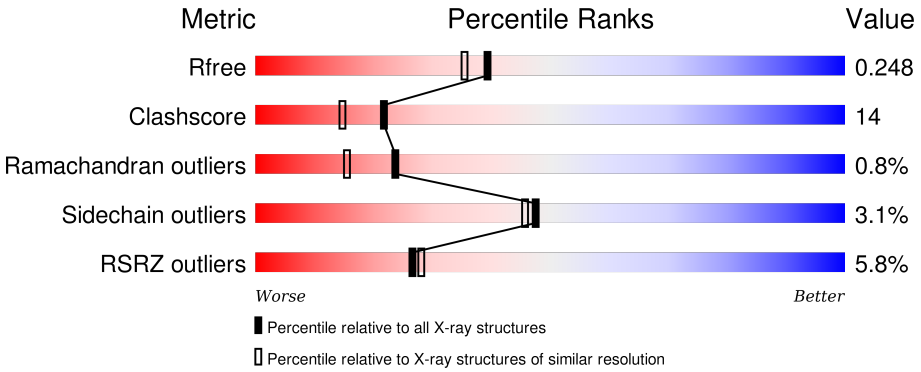
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	383	6% 70% 28%
1	B	383	2% 75% 22%
1	C	383	11% 73% 26%
1	D	383	4% 73% 24%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAD	D	1385	-	-	-	X

2 Entry composition

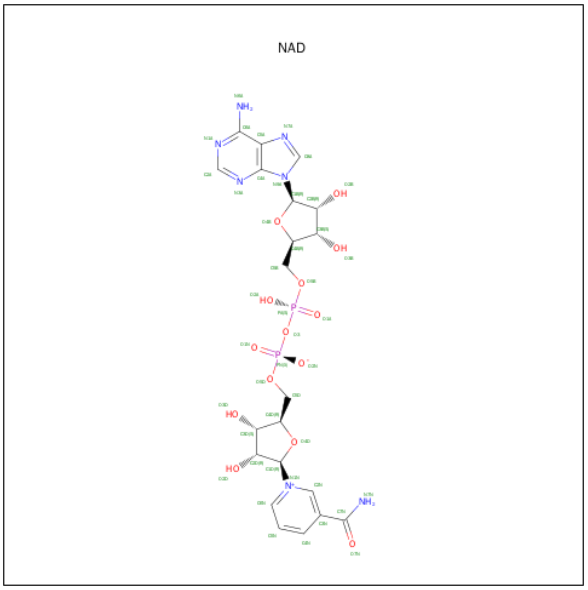
There are 4 unique types of molecules in this entry. The entry contains 11923 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alcohol dehydrogenase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			2797	1759	474	542	22			
1	B	382	Total	C	N	O	S	0	0	0
			2797	1759	474	542	22			
1	C	382	Total	C	N	O	S	0	0	0
			2797	1759	474	542	22			
1	D	382	Total	C	N	O	S	0	0	0
			2797	1759	474	542	22			

- 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 FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Fe	0	0
			1	1		
3	A	1	Total	Fe	0	0
			1	1		
3	D	1	Total	Fe	0	0
			1	1		
3	C	1	Total	Fe	0	0
			1	1		

- Molecule 4 is water.

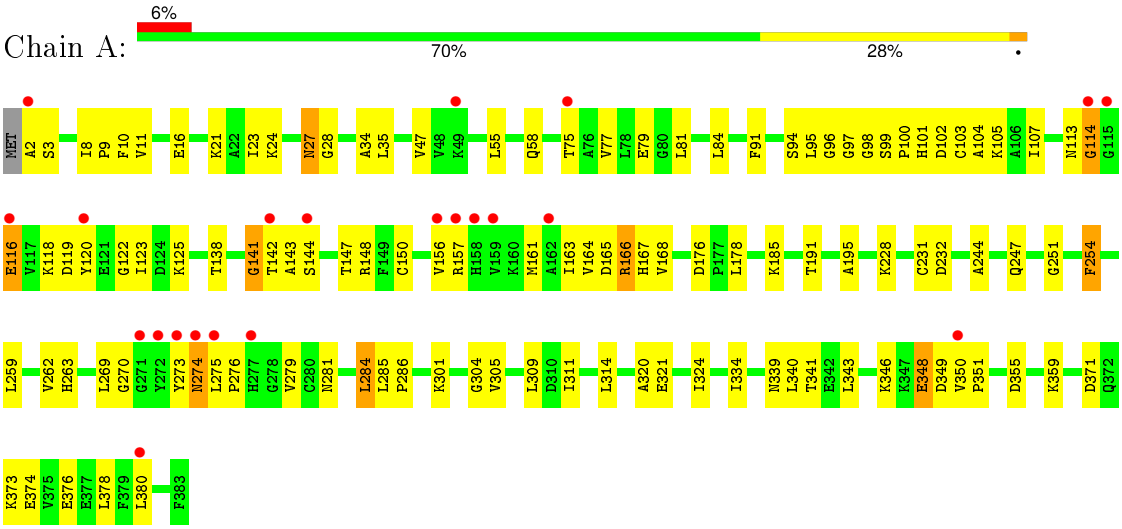
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	128	Total	O	0	0
			128	128		
4	B	181	Total	O	0	0
			181	181		
4	C	92	Total	O	0	0
			92	92		
4	D	154	Total	O	0	0
			154	154		

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.

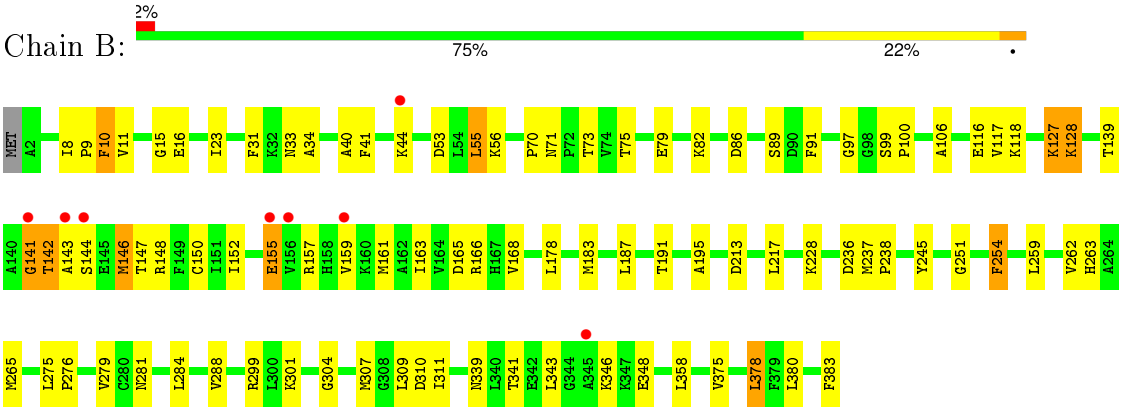
- Molecule 1: Alcohol dehydrogenase 2

Chain A:



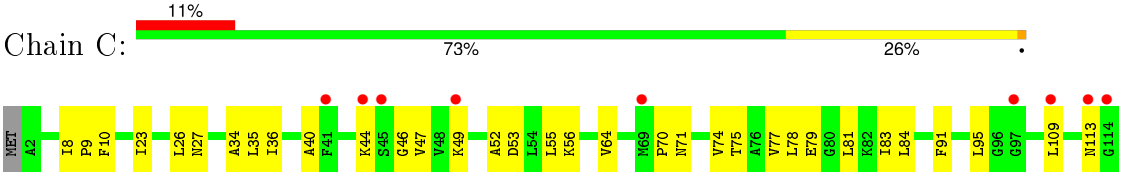
- Molecule 1: Alcohol dehydrogenase 2

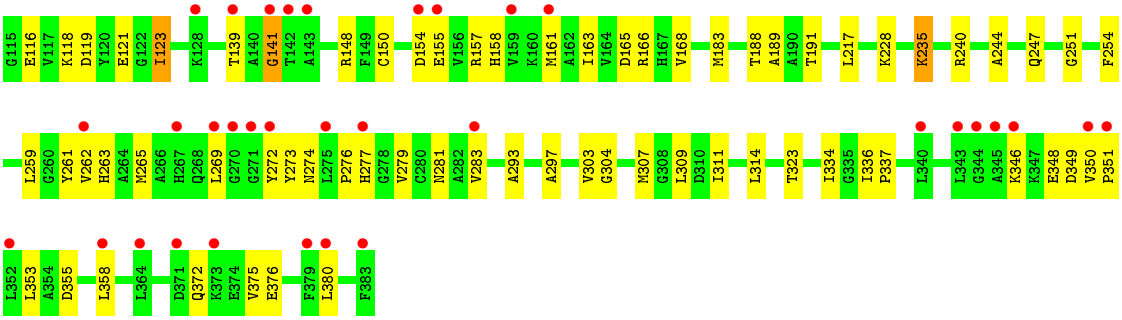
Chain B:



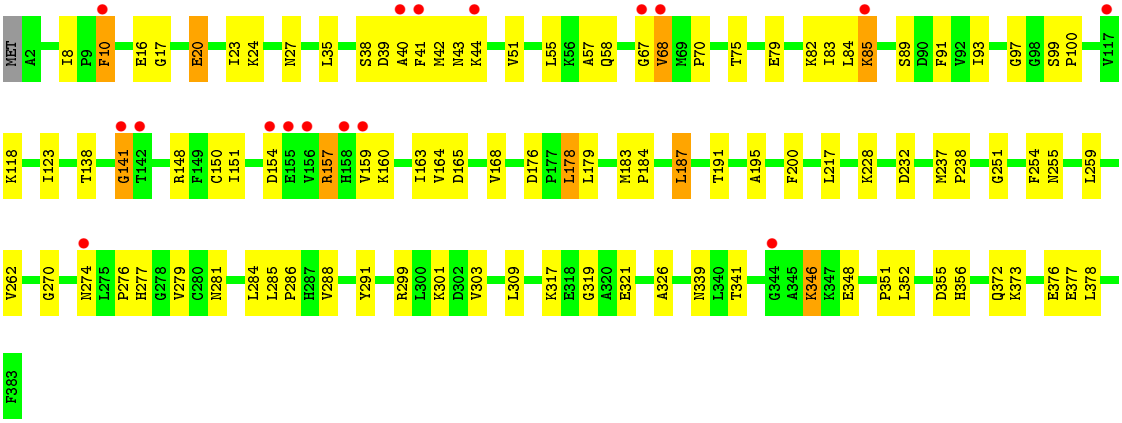
- Molecule 1: Alcohol dehydrogenase 2

Chain C:





- Molecule 1: Alcohol dehydrogenase 2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	60.51Å 86.97Å 124.47Å 90.00° 94.83° 90.00°	Depositor
Resolution (Å)	28.75 – 2.00 28.75 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.9 (28.75-2.00) 95.1 (28.75-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.252 0.209 , 0.248	Depositor DCC
R_{free} test set	4308 reflections (5.50%)	DCC
Wilson B-factor (Å^2)	20.9	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 63.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 84722 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11923	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.09 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.2036e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: FE2, 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	0.31	0/2841	0.56	0/3851
1	B	0.33	0/2841	0.57	0/3851
1	C	0.28	0/2841	0.53	0/3851
1	D	0.31	0/2841	0.57	0/3851
All	All	0.31	0/11364	0.56	0/15404

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2797	0	2820	88	0
1	B	2797	0	2820	82	0
1	C	2797	0	2820	77	0
1	D	2797	0	2820	81	0
2	A	44	0	26	0	0
2	B	44	0	26	1	0
2	C	44	0	26	1	0
2	D	44	0	26	1	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	128	0	0	3	0
4	B	181	0	0	3	0
4	C	92	0	0	3	0
4	D	154	0	0	8	0
All	All	11923	0	11384	319	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 14.

All (319) 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:142:THR:HG22	1:A:144:SER:H	1.21	1.02
1:B:106:ALA:HB2	1:B:152:ILE:HD11	1.43	0.98
1:D:41:PHE:HA	1:D:44:LYS:HE2	1.43	0.98
1:B:16:GLU:HG3	1:B:178:LEU:HD21	1.42	0.96
1:A:16:GLU:HG3	1:A:178:LEU:HD21	1.51	0.91
1:B:143:ALA:HB1	1:B:146:MET:HE2	1.54	0.89
1:B:146:MET:HE2	1:B:251:GLY:HA3	1.55	0.88
1:A:118:LYS:HE3	1:A:157:ARG:HH11	1.38	0.88
1:B:142:THR:HG22	1:B:144:SER:H	1.39	0.86
1:B:16:GLU:HG3	1:B:178:LEU:CD2	2.06	0.85
1:A:270:GLY:HA2	1:A:275:LEU:H	1.47	0.80
1:C:123:ILE:H	1:C:123:ILE:HD13	1.47	0.79
1:B:183:MET:SD	1:B:187:LEU:HD12	2.23	0.79
1:A:47:VAL:HG12	1:A:95:LEU:HD21	1.65	0.78
1:B:276:PRO:HB2	1:B:279:VAL:HG22	1.64	0.78
1:A:185:LYS:HE3	1:A:231:CYS:HB3	1.64	0.78
1:B:106:ALA:CB	1:B:152:ILE:HD11	2.13	0.78
1:A:276:PRO:HG2	1:A:279:VAL:HG22	1.66	0.77
1:C:188:THR:HG22	1:C:240:ARG:HH12	1.48	0.77
1:C:165:ASP:O	1:C:168:VAL:HG22	1.85	0.76
1:D:372:GLN:O	1:D:376:GLU:HG3	1.86	0.76
1:C:52:ALA:O	1:C:56:LYS:HG2	1.87	0.75
1:A:142:THR:HB	4:A:452:HOH:O	1.86	0.74
1:A:142:THR:HG22	1:A:144:SER:N	2.02	0.74
1:B:262:VAL:HG12	1:B:281:ASN:HD22	1.53	0.74
1:D:285:LEU:HB3	1:D:286:PRO:HD3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:LEU:HG	1:D:89:SER:HB2	1.71	0.73
1:A:77:VAL:HG13	1:A:107:ILE:HD13	1.71	0.72
1:A:16:GLU:CG	1:A:178:LEU:HD21	2.20	0.72
1:C:34:ALA:HB2	1:C:91:PHE:CE1	2.25	0.71
1:A:113:ASN:HB3	1:A:120:TYR:OH	1.90	0.71
1:A:285:LEU:HB3	1:A:286:PRO:HD3	1.72	0.71
1:B:33:ASN:HD22	1:B:89:SER:HA	1.55	0.70
1:C:150:CYS:HB3	1:C:163:ILE:HB	1.71	0.70
1:A:118:LYS:HG2	1:A:161:MET:SD	2.31	0.70
1:B:141:GLY:HA2	1:B:195:ALA:HB2	1.73	0.69
1:D:262:VAL:HG12	1:D:281:ASN:HD22	1.58	0.68
1:A:99:SER:HB2	1:A:100:PRO:HD3	1.76	0.68
1:A:176:ASP:OD2	1:A:178:LEU:HD23	1.92	0.68
1:B:141:GLY:HA3	1:B:191:THR:O	1.93	0.68
1:B:82:LYS:HE2	1:B:86:ASP:OD2	1.94	0.68
1:D:40:ALA:HB2	1:D:67:GLY:HA2	1.76	0.68
1:A:276:PRO:HG2	1:A:279:VAL:CG2	2.24	0.67
1:A:103:CYS:O	1:A:107:ILE:HG12	1.95	0.67
1:A:77:VAL:HA	1:A:107:ILE:HD11	1.75	0.67
1:D:99:SER:HB2	1:D:100:PRO:HD3	1.77	0.66
1:B:142:THR:CG2	1:B:144:SER:H	2.07	0.66
1:A:284:LEU:HD13	1:A:340:LEU:HD21	1.77	0.66
1:C:355:ASP:HB2	1:C:372:GLN:HE22	1.60	0.66
1:C:262:VAL:HG12	1:C:281:ASN:ND2	2.11	0.66
1:C:188:THR:CG2	1:C:240:ARG:HH12	2.08	0.66
1:B:34:ALA:HB2	1:B:91:PHE:CE1	2.31	0.66
1:C:35:LEU:HD22	1:C:84:LEU:HB2	1.77	0.66
1:A:27:ASN:HD22	1:A:28:GLY:N	1.93	0.65
1:D:20:GLU:O	1:D:24:LYS:HG3	1.96	0.65
1:A:24:LYS:NZ	1:A:24:LYS:HB3	2.12	0.65
1:B:40:ALA:O	1:B:44:LYS:HG2	1.97	0.64
1:C:346:LYS:HB2	1:C:349:ASP:OD2	1.97	0.64
1:B:143:ALA:HB1	1:B:146:MET:CE	2.27	0.64
1:C:10:PHE:CZ	1:D:10:PHE:HB2	2.32	0.64
1:C:293:ALA:O	1:C:297:ALA:HB2	1.98	0.64
1:D:42:MET:HE2	1:D:138:THR:HG21	1.80	0.63
1:B:143:ALA:O	1:B:146:MET:HE3	1.99	0.63
1:D:291:TYR:HB2	1:D:378:LEU:HD21	1.79	0.63
1:C:276:PRO:HG2	1:C:279:VAL:CG2	2.29	0.63
1:C:276:PRO:HG2	1:C:279:VAL:HG22	1.81	0.63
1:B:99:SER:HB2	1:B:100:PRO:HD3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:MET:CE	1:B:251:GLY:HA3	2.28	0.62
1:C:350:VAL:HB	1:C:351:PRO:HD3	1.81	0.62
1:D:165:ASP:O	1:D:168:VAL:HG22	2.00	0.61
1:A:350:VAL:HB	1:A:351:PRO:HD3	1.82	0.61
1:D:79:GLU:O	1:D:82:LYS:HG2	2.00	0.61
1:C:49:LYS:HE3	1:C:53:ASP:OD1	2.01	0.60
1:A:2:ALA:N	1:B:245:TYR:HH	1.98	0.60
1:C:189:ALA:HB1	1:C:334:ILE:HD12	1.82	0.59
1:C:244:ALA:O	1:C:247:GLN:HG3	2.02	0.59
1:A:34:ALA:HB2	1:A:91:PHE:CE1	2.38	0.59
1:B:146:MET:HE3	1:B:147:THR:HG23	1.83	0.59
1:B:142:THR:HB	4:B:399:HOH:O	2.02	0.59
1:D:317:LYS:HB2	1:D:317:LYS:NZ	2.17	0.58
1:B:75:THR:O	1:B:79:GLU:HG3	2.04	0.58
1:A:24:LYS:HZ2	1:A:24:LYS:HB3	1.69	0.58
1:C:262:VAL:HG12	1:C:281:ASN:HD22	1.69	0.57
1:A:185:LYS:HE2	1:A:334:ILE:O	2.03	0.57
1:B:33:ASN:ND2	1:B:89:SER:HA	2.18	0.56
1:B:127:LYS:O	1:B:128:LYS:HD2	2.05	0.56
1:C:358:LEU:HD21	1:C:375:VAL:HG21	1.87	0.56
1:A:350:VAL:HG12	1:A:376:GLU:HG2	1.88	0.56
1:D:97:GLY:O	1:D:100:PRO:HD2	2.05	0.56
1:B:44:LYS:HE2	1:C:274:ASN:HD22	1.70	0.56
1:B:236:ASP:OD2	1:B:238:PRO:HD2	2.05	0.56
1:A:166:ARG:HH11	1:A:166:ARG:HB3	1.70	0.56
1:B:165:ASP:O	1:B:168:VAL:HG22	2.04	0.56
1:D:351:PRO:HA	1:D:376:GLU:OE2	2.06	0.56
1:B:139:THR:HB	1:B:191:THR:HG21	1.89	0.55
1:C:118:LYS:HA	1:C:161:MET:HE1	1.88	0.55
1:A:97:GLY:O	1:A:100:PRO:HD2	2.07	0.55
1:D:42:MET:CE	1:D:138:THR:HG21	2.36	0.55
1:A:118:LYS:HE3	1:A:157:ARG:NH1	2.16	0.55
1:A:21:LYS:HA	1:A:24:LYS:HZ2	1.71	0.55
1:D:148:ARG:HG2	1:D:255:ASN:OD1	2.08	0.54
1:C:279:VAL:O	1:C:283:VAL:HG12	2.06	0.54
1:D:187:LEU:HD22	1:D:191:THR:HG23	1.89	0.54
1:C:348:GLU:H	1:C:348:GLU:CD	2.11	0.54
1:C:376:GLU:O	1:C:380:LEU:HD13	2.07	0.54
1:C:46:GLY:HA2	4:C:451:HOH:O	2.08	0.54
1:C:77:VAL:O	1:C:81:LEU:HB2	2.08	0.54
1:D:317:LYS:O	1:D:321:GLU:HG2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:PRO:HB2	1:D:279:VAL:HG22	1.89	0.53
1:A:269:LEU:O	1:A:273:TYR:HB2	2.07	0.53
1:A:3:SER:H	1:B:15:GLY:HA3	1.73	0.53
1:A:165:ASP:O	1:A:168:VAL:HG22	2.08	0.53
1:D:41:PHE:HA	1:D:44:LYS:CE	2.30	0.53
1:B:97:GLY:O	1:B:100:PRO:HD2	2.08	0.53
1:A:8:ILE:O	1:B:10:PHE:HA	2.08	0.53
1:B:155:GLU:CD	1:B:155:GLU:H	2.11	0.53
1:A:98:GLY:HA2	1:A:144:SER:OG	2.08	0.53
1:D:38:SER:OG	1:D:42:MET:HB2	2.09	0.53
1:D:67:GLY:O	1:D:68:VAL:C	2.47	0.53
1:C:40:ALA:O	1:C:44:LYS:HG3	2.08	0.53
1:B:147:THR:HG21	2:B:1385:NAD:N7N	2.24	0.53
1:B:127:LYS:C	1:B:128:LYS:HD2	2.29	0.52
1:A:259:LEU:HD13	1:A:263:HIS:CG	2.45	0.52
1:D:352:LEU:HD23	1:D:352:LEU:C	2.29	0.52
1:A:346:LYS:HB2	1:A:349:ASP:OD2	2.10	0.52
1:D:141:GLY:HA2	1:D:195:ALA:HB2	1.92	0.52
1:C:259:LEU:HD13	1:C:263:HIS:CG	2.45	0.52
1:B:358:LEU:HD21	1:B:375:VAL:HG21	1.91	0.52
1:B:262:VAL:HG22	1:B:288:VAL:HB	1.92	0.52
1:A:8:ILE:HG13	1:A:9:PRO:HD2	1.92	0.52
1:B:23:ILE:HD12	1:B:55:LEU:HD13	1.91	0.52
1:A:141:GLY:HA3	1:A:191:THR:O	2.10	0.52
1:C:123:ILE:N	1:C:123:ILE:HD13	2.23	0.51
1:A:34:ALA:HB2	1:A:91:PHE:CZ	2.45	0.51
1:A:166:ARG:NH1	1:A:166:ARG:HB3	2.25	0.51
1:D:35:LEU:HD22	1:D:84:LEU:HB2	1.92	0.51
1:B:304:GLY:O	1:B:309:LEU:HD13	2.10	0.51
1:B:213:ASP:OD1	1:B:299:ARG:NH2	2.44	0.51
1:A:141:GLY:HA2	1:A:195:ALA:HB2	1.92	0.51
1:A:23:ILE:HD12	1:A:55:LEU:HD13	1.92	0.51
1:C:139:THR:HB	1:C:191:THR:HG21	1.92	0.51
1:A:143:ALA:O	1:A:147:THR:HG23	2.11	0.51
1:B:53:ASP:HA	1:B:56:LYS:HD3	1.93	0.50
1:D:57:ALA:HB3	4:D:510:HOH:O	2.11	0.50
1:A:339:ASN:O	1:A:343:LEU:HD23	2.11	0.50
1:A:166:ARG:HG2	1:A:167:HIS:N	2.26	0.50
1:B:259:LEU:HD13	1:B:263:HIS:CG	2.47	0.50
1:C:157:ARG:HG3	1:C:157:ARG:HH11	1.75	0.50
1:A:373:LYS:HG3	4:A:523:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:GLY:HA2	1:B:254:PHE:CD1	2.47	0.49
1:D:42:MET:HE1	4:D:478:HOH:O	2.11	0.49
1:C:311:ILE:HG22	1:C:314:LEU:HD12	1.94	0.49
1:A:339:ASN:OD1	1:A:341:THR:HB	2.12	0.49
1:A:228:LYS:HE3	1:A:232:ASP:OD2	2.12	0.49
1:B:150:CYS:HB3	1:B:163:ILE:HB	1.95	0.49
1:A:350:VAL:HG21	1:A:380:LEU:CD2	2.42	0.49
1:D:55:LEU:HD21	1:D:93:ILE:HD12	1.94	0.49
1:A:118:LYS:CE	1:A:157:ARG:HH11	2.16	0.49
1:D:51:VAL:O	1:D:55:LEU:HD13	2.12	0.49
1:D:254:PHE:HB2	1:D:259:LEU:CD2	2.43	0.49
1:C:109:LEU:HD13	1:C:113:ASN:HD22	1.78	0.49
1:B:82:LYS:HE3	4:B:521:HOH:O	2.13	0.48
1:A:346:LYS:HB3	1:A:348:GLU:OE1	2.13	0.48
1:B:339:ASN:OD1	1:B:341:THR:HB	2.12	0.48
1:D:299:ARG:HG3	4:D:461:HOH:O	2.13	0.48
1:A:75:THR:HG23	4:A:454:HOH:O	2.12	0.48
1:D:123:ILE:HD13	1:D:164:VAL:HB	1.94	0.48
1:B:146:MET:HE3	1:B:147:THR:CG2	2.43	0.48
1:C:23:ILE:HG23	1:C:55:LEU:HD23	1.94	0.48
1:D:270:GLY:O	1:D:274:ASN:HA	2.13	0.48
1:B:73:THR:HB	1:B:155:GLU:HG3	1.95	0.48
1:A:123:ILE:HA	1:A:164:VAL:O	2.13	0.48
1:A:116:GLU:HG2	1:A:119:ASP:OD1	2.14	0.48
1:B:228:LYS:HB2	4:B:409:HOH:O	2.12	0.48
1:B:117:VAL:CG1	1:B:152:ILE:HD12	2.43	0.48
1:C:49:LYS:HD2	1:C:52:ALA:HB3	1.96	0.48
1:C:261:TYR:O	1:C:265:MET:HG3	2.13	0.48
1:A:122:GLY:HA3	1:A:125:LYS:NZ	2.28	0.48
1:C:74:VAL:O	1:C:78:LEU:HG	2.13	0.48
1:A:81:LEU:HD22	1:A:107:ILE:HD12	1.96	0.48
1:C:23:ILE:O	1:C:26:LEU:HB2	2.14	0.48
1:A:27:ASN:HB2	1:A:58:GLN:OE1	2.13	0.48
1:A:371:ASP:OD1	1:A:374:GLU:HG3	2.13	0.48
1:C:269:LEU:O	1:C:273:TYR:HB2	2.14	0.48
1:D:151:ILE:CG2	1:D:160:LYS:HB3	2.44	0.48
1:B:70:PRO:O	1:B:71:ASN:HB2	2.13	0.48
1:D:254:PHE:HB2	1:D:259:LEU:HD21	1.95	0.47
1:D:339:ASN:OD1	1:D:341:THR:HB	2.14	0.47
1:C:123:ILE:HG12	1:C:123:ILE:O	2.14	0.47
1:D:75:THR:O	1:D:79:GLU:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:GLY:O	1:D:20:GLU:HG2	2.15	0.47
1:B:44:LYS:HD2	1:C:273:TYR:O	2.14	0.47
1:A:114:GLY:N	1:A:120:TYR:OH	2.45	0.47
1:C:10:PHE:CD2	1:D:10:PHE:CD1	3.03	0.47
1:D:176:ASP:OD2	1:D:178:LEU:HB2	2.13	0.47
1:B:275:LEU:HD13	1:B:343:LEU:HB3	1.97	0.47
1:C:8:ILE:HG13	1:C:9:PRO:HD2	1.96	0.47
1:C:269:LEU:HD21	1:C:353:LEU:HD13	1.97	0.47
1:A:348:GLU:CD	1:A:348:GLU:H	2.18	0.47
1:C:109:LEU:HD13	1:C:109:LEU:C	2.35	0.47
1:D:159:VAL:HG11	1:D:356:HIS:HD2	1.80	0.47
1:C:75:THR:HG23	1:C:155:GLU:OE1	2.13	0.47
1:D:237:MET:HB3	1:D:238:PRO:HD3	1.95	0.47
1:B:346:LYS:HE3	1:B:348:GLU:OE2	2.15	0.47
1:D:262:VAL:HG22	1:D:288:VAL:HB	1.97	0.46
1:C:276:PRO:HB2	4:C:436:HOH:O	2.16	0.46
1:D:187:LEU:HD22	1:D:191:THR:CG2	2.45	0.46
1:D:23:ILE:HD12	1:D:55:LEU:HD12	1.97	0.46
1:D:85:LYS:NZ	1:D:85:LYS:HB3	2.31	0.46
1:C:118:LYS:HB2	1:C:161:MET:HE3	1.98	0.46
1:B:56:LYS:NZ	1:B:56:LYS:HB3	2.31	0.46
1:B:339:ASN:O	1:B:343:LEU:HD23	2.14	0.46
1:C:116:GLU:HB2	1:C:119:ASP:OD1	2.15	0.46
1:A:94:SER:HB3	1:A:104:ALA:CB	2.45	0.46
1:C:79:GLU:O	1:C:83:ILE:HG12	2.15	0.46
1:B:157:ARG:O	1:B:159:VAL:HG23	2.15	0.46
1:B:8:ILE:HG13	1:B:9:PRO:HD2	1.98	0.46
1:B:275:LEU:CD1	1:B:343:LEU:HB3	2.46	0.46
1:A:262:VAL:HG12	1:A:281:ASN:HD22	1.81	0.46
1:D:23:ILE:HD12	1:D:55:LEU:CD1	2.46	0.46
1:D:348:GLU:HG3	4:D:487:HOH:O	2.15	0.46
1:C:235:LYS:HD2	1:C:235:LYS:N	2.31	0.46
1:B:118:LYS:HB2	1:B:161:MET:HE1	1.98	0.45
1:C:34:ALA:HB2	1:C:91:PHE:CZ	2.52	0.45
1:C:84:LEU:O	1:C:84:LEU:HD23	2.17	0.45
1:A:122:GLY:HA3	1:A:125:LYS:HZ3	1.80	0.45
1:C:121:GLU:OE2	1:C:161:MET:HE2	2.17	0.45
1:A:320:ALA:O	1:A:324:ILE:HG13	2.17	0.45
1:B:10:PHE:CD2	1:B:11:VAL:HG23	2.52	0.45
1:C:254:PHE:HB2	1:C:259:LEU:CD2	2.47	0.45
1:C:158:HIS:HB2	1:C:272:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:LEU:HD23	1:A:84:LEU:C	2.37	0.45
1:B:117:VAL:HG13	1:B:152:ILE:HD12	1.98	0.44
1:C:351:PRO:HG3	1:C:376:GLU:OE1	2.18	0.44
1:D:301:LYS:HG3	1:D:319:GLY:HA3	1.99	0.44
1:D:355:ASP:CA	1:D:372:GLN:HE21	2.31	0.44
1:B:31:PHE:HB3	1:B:91:PHE:CE1	2.52	0.44
1:B:34:ALA:HB2	1:B:91:PHE:CZ	2.53	0.44
1:D:317:LYS:HB2	1:D:317:LYS:HZ3	1.82	0.44
1:C:309:LEU:N	1:C:309:LEU:HD12	2.31	0.44
1:C:141:GLY:HA3	1:C:191:THR:HB	1.99	0.44
1:D:151:ILE:HG21	1:D:160:LYS:HD3	2.00	0.44
1:A:10:PHE:HA	1:B:8:ILE:O	2.17	0.44
1:B:116:GLU:OE1	1:B:118:LYS:HE2	2.17	0.44
1:B:23:ILE:HD12	1:B:55:LEU:CD1	2.47	0.44
1:B:265:MET:SD	1:B:378:LEU:HD13	2.58	0.44
1:C:304:GLY:HA3	1:C:323:THR:OG1	2.18	0.44
1:B:146:MET:CE	1:B:147:THR:CG2	2.96	0.43
1:D:91:PHE:CE1	1:D:93:ILE:HD11	2.53	0.43
1:D:346:LYS:HE3	4:D:509:HOH:O	2.18	0.43
1:D:277:HIS:CG	2:D:1385:NAD:H2D	2.53	0.43
1:A:270:GLY:HA2	1:A:275:LEU:HB2	1.99	0.43
1:D:373:LYS:O	1:D:377:GLU:HG3	2.18	0.43
1:D:70:PRO:HA	1:D:99:SER:OG	2.19	0.43
1:C:36:ILE:HB	1:C:64:VAL:HG22	1.99	0.43
1:A:244:ALA:O	1:A:247:GLN:HG3	2.19	0.43
1:A:16:GLU:HA	1:A:178:LEU:HD23	2.00	0.43
1:C:334:ILE:HG13	1:C:336:ILE:HG12	2.00	0.43
1:A:101:HIS:O	1:A:105:LYS:HG3	2.19	0.43
1:B:41:PHE:C	1:B:41:PHE:CD1	2.91	0.43
1:A:251:GLY:HA2	1:A:254:PHE:CD1	2.53	0.43
1:C:303:VAL:O	1:C:307:MET:HG3	2.18	0.43
1:A:355:ASP:O	1:A:359:LYS:HG3	2.19	0.43
1:A:150:CYS:HB3	1:A:163:ILE:HB	1.99	0.43
1:A:11:VAL:HG11	1:B:166:ARG:NH2	2.33	0.43
1:D:228:LYS:HE3	1:D:232:ASP:OD2	2.18	0.43
1:D:200:PHE:CE1	1:D:303:VAL:HG11	2.54	0.43
1:B:237:MET:HB2	1:B:238:PRO:HD3	2.01	0.43
1:D:187:LEU:HD23	1:D:187:LEU:HA	1.86	0.43
1:B:380:LEU:HA	1:B:383:PHE:CD1	2.54	0.43
1:D:154:ASP:OD2	1:D:157:ARG:HD2	2.18	0.42
1:C:116:GLU:O	1:C:119:ASP:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:LYS:O	1:A:185:LYS:HD3	2.20	0.42
1:A:77:VAL:HA	1:A:107:ILE:CD1	2.44	0.42
1:A:75:THR:O	1:A:79:GLU:HB2	2.19	0.42
1:A:304:GLY:O	1:A:309:LEU:HB2	2.18	0.42
1:B:146:MET:CE	1:B:147:THR:HG22	2.48	0.42
1:D:176:ASP:HB3	1:D:179:LEU:HD13	2.01	0.42
1:B:187:LEU:O	1:B:187:LEU:HD13	2.20	0.42
1:D:85:LYS:HD2	1:D:85:LYS:C	2.40	0.42
1:A:35:LEU:HD22	1:A:84:LEU:HB2	2.00	0.42
1:D:118:LYS:HG2	4:D:486:HOH:O	2.20	0.42
1:C:263:HIS:CD2	1:C:277:HIS:HE2	2.37	0.42
1:D:27:ASN:HB2	1:D:58:GLN:OE1	2.20	0.42
1:D:183:MET:HA	1:D:184:PRO:HD3	1.91	0.42
1:D:38:SER:OG	1:D:39:ASP:N	2.53	0.41
1:C:251:GLY:HA2	1:C:254:PHE:CE1	2.55	0.41
1:D:16:GLU:OE2	1:D:178:LEU:HD11	2.20	0.41
1:B:146:MET:HE1	1:B:147:THR:HG22	2.02	0.41
1:A:77:VAL:HG12	1:A:81:LEU:HD23	2.02	0.41
1:C:10:PHE:HA	1:D:8:ILE:O	2.20	0.41
1:D:157:ARG:H	1:D:157:ARG:HG3	1.63	0.41
1:B:139:THR:HG22	1:B:187:LEU:HD11	2.02	0.41
1:D:82:LYS:HG3	1:D:83:ILE:N	2.35	0.41
2:C:1385:NAD:H2B	4:C:461:HOH:O	2.20	0.41
1:D:41:PHE:O	1:D:44:LYS:HG2	2.21	0.41
1:B:307:MET:HB2	1:B:309:LEU:HD13	2.02	0.41
1:D:346:LYS:HZ2	1:D:346:LYS:HB3	1.85	0.41
1:D:228:LYS:HB3	4:D:406:HOH:O	2.20	0.41
1:C:139:THR:HA	1:C:183:MET:SD	2.61	0.41
1:D:179:LEU:HD12	1:D:179:LEU:N	2.35	0.41
1:C:47:VAL:HG12	1:C:95:LEU:HD21	2.01	0.41
1:D:372:GLN:HB2	4:D:475:HOH:O	2.20	0.41
1:D:309:LEU:HD21	1:D:326:ALA:HB2	2.02	0.41
1:A:301:LYS:O	1:A:305:VAL:HG23	2.21	0.41
1:A:96:GLY:HA2	1:A:138:THR:OG1	2.20	0.41
1:D:251:GLY:HA2	1:D:254:PHE:CD1	2.56	0.41
1:B:118:LYS:CB	1:B:161:MET:HE1	2.50	0.41
1:A:311:ILE:HB	1:A:314:LEU:HD12	2.03	0.41
1:B:301:LYS:HE3	1:B:311:ILE:O	2.20	0.41
1:A:273:TYR:O	1:A:274:ASN:C	2.59	0.40
1:C:70:PRO:O	1:C:71:ASN:HB2	2.22	0.40
1:C:157:ARG:HG3	1:C:157:ARG:NH1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:ASP:O	1:C:158:HIS:N	2.54	0.40
1:C:355:ASP:HB2	1:C:372:GLN:NE2	2.33	0.40
1:C:109:LEU:HD22	1:C:113:ASN:ND2	2.35	0.40
1:C:84:LEU:C	1:C:84:LEU:HD23	2.41	0.40
1:A:8:ILE:HG13	1:A:9:PRO:CD	2.52	0.40
1:D:150:CYS:HB3	1:D:163:ILE:HB	2.03	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	380/383 (99%)	355 (93%)	20 (5%)	5 (1%)	15	7
1	B	380/383 (99%)	366 (96%)	13 (3%)	1 (0%)	46	41
1	C	380/383 (99%)	360 (95%)	17 (4%)	3 (1%)	24	15
1	D	380/383 (99%)	364 (96%)	13 (3%)	3 (1%)	24	15
All	All	1520/1532 (99%)	1445 (95%)	63 (4%)	12 (1%)	24	15

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	157	ARG
1	A	114	GLY
1	A	116	GLU
1	D	68	VAL
1	A	141	GLY
1	A	274	ASN
1	B	141	GLY
1	C	141	GLY
1	D	141	GLY

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Mol	Chain	Res	Type
1	C	27	ASN
1	C	337	PRO
1	A	156	VAL

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	294/295 (100%)	285 (97%)	9 (3%)	47 46
1	B	294/295 (100%)	281 (96%)	13 (4%)	35 30
1	C	294/295 (100%)	288 (98%)	6 (2%)	63 65
1	D	294/295 (100%)	285 (97%)	9 (3%)	47 46
All	All	1176/1180 (100%)	1139 (97%)	37 (3%)	47 46

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	102	ASP
1	A	148	ARG
1	A	166	ARG
1	A	254	PHE
1	A	284	LEU
1	A	321	GLU
1	A	348	GLU
1	A	378	LEU
1	B	10	PHE
1	B	55	LEU
1	B	127	LYS
1	B	128	LYS
1	B	142	THR
1	B	146	MET
1	B	148	ARG
1	B	155	GLU
1	B	217	LEU

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Mol	Chain	Res	Type
1	B	254	PHE
1	B	284	LEU
1	B	310	ASP
1	B	378	LEU
1	C	123	ILE
1	C	148	ARG
1	C	166	ARG
1	C	217	LEU
1	C	228	LYS
1	C	235	LYS
1	D	10	PHE
1	D	20	GLU
1	D	43	ASN
1	D	85	LYS
1	D	178	LEU
1	D	187	LEU
1	D	217	LEU
1	D	284	LEU
1	D	346	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	61	ASN
1	A	281	ASN
1	B	33	ASN
1	B	58	GLN
1	B	61	ASN
1	B	71	ASN
1	B	281	ASN
1	C	274	ASN
1	C	281	ASN
1	C	372	GLN
1	D	43	ASN
1	D	50	GLN
1	D	88	ASN
1	D	158	HIS
1	D	281	ASN
1	D	372	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

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	1385	-	38,48,48	1.68	7 (18%)	47,73,73	2.12	12 (25%)
2	NAD	B	1385	-	38,48,48	1.63	6 (15%)	47,73,73	2.12	12 (25%)
2	NAD	C	1385	-	38,48,48	1.63	6 (15%)	47,73,73	2.12	12 (25%)
2	NAD	D	1385	-	38,48,48	1.75	6 (15%)	47,73,73	2.16	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	NAD	A	1385	-	-	0/22/62/62	0/5/5/5
2	NAD	B	1385	-	-	0/22/62/62	0/5/5/5
2	NAD	C	1385	-	-	0/22/62/62	0/5/5/5
2	NAD	D	1385	-	-	0/22/62/62	0/5/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1385	NAD	C2A-N3A	2.01	1.35	1.32
2	B	1385	NAD	PA-O5B	2.01	1.68	1.59
2	D	1385	NAD	C2A-N3A	2.08	1.35	1.32
2	C	1385	NAD	C4N-C3N	2.08	1.42	1.39
2	C	1385	NAD	PA-O5B	2.12	1.68	1.59
2	B	1385	NAD	C2A-N3A	2.19	1.36	1.32
2	D	1385	NAD	PA-O5B	2.20	1.69	1.59
2	A	1385	NAD	C4N-C3N	2.25	1.43	1.39
2	A	1385	NAD	PA-O5B	2.30	1.69	1.59
2	C	1385	NAD	O4D-C1D	2.45	1.44	1.41
2	B	1385	NAD	C4N-C3N	2.47	1.43	1.39
2	A	1385	NAD	O4D-C1D	2.81	1.44	1.41
2	D	1385	NAD	C6N-N1N	2.96	1.43	1.35
2	C	1385	NAD	C6N-N1N	3.12	1.43	1.35
2	A	1385	NAD	C6N-N1N	3.30	1.44	1.35
2	B	1385	NAD	C6N-N1N	3.35	1.44	1.35
2	D	1385	NAD	O4D-C1D	3.40	1.45	1.41
2	C	1385	NAD	C4A-N3A	3.94	1.41	1.35
2	B	1385	NAD	C4A-N3A	4.02	1.41	1.35
2	A	1385	NAD	C4A-N3A	4.12	1.41	1.35
2	D	1385	NAD	C4A-N3A	4.30	1.42	1.35
2	B	1385	NAD	C2N-C3N	5.05	1.46	1.39
2	A	1385	NAD	C2N-C3N	5.14	1.46	1.39
2	C	1385	NAD	C2N-C3N	5.20	1.46	1.39
2	D	1385	NAD	C2N-C3N	5.89	1.47	1.39

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1385	NAD	N3A-C2A-N1A	-6.30	124.07	128.89
2	A	1385	NAD	O2A-PA-O3	-6.27	76.63	105.09
2	D	1385	NAD	O2A-PA-O3	-6.21	76.91	105.09
2	C	1385	NAD	N3A-C2A-N1A	-6.05	124.26	128.89
2	B	1385	NAD	O2A-PA-O3	-6.03	77.74	105.09
2	C	1385	NAD	O2A-PA-O3	-5.95	78.11	105.09
2	D	1385	NAD	N3A-C2A-N1A	-5.87	124.40	128.89
2	B	1385	NAD	N3A-C2A-N1A	-5.79	124.46	128.89
2	C	1385	NAD	O3-PA-O5B	-4.79	90.23	102.94
2	D	1385	NAD	O7N-C7N-N7N	-4.75	115.92	122.59
2	B	1385	NAD	O7N-C7N-N7N	-4.75	115.92	122.59
2	D	1385	NAD	O3-PA-O5B	-4.67	90.54	102.94
2	B	1385	NAD	O3-PA-O5B	-4.66	90.57	102.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1385	NAD	O3-PA-O5B	-4.54	90.89	102.94
2	A	1385	NAD	O7N-C7N-N7N	-4.42	116.37	122.59
2	C	1385	NAD	O7N-C7N-N7N	-4.41	116.39	122.59
2	D	1385	NAD	C3N-C2N-N1N	-3.20	116.68	120.36
2	A	1385	NAD	C4B-O4B-C1B	-3.04	106.38	109.72
2	C	1385	NAD	C3N-C2N-N1N	-2.91	117.01	120.36
2	A	1385	NAD	C3N-C2N-N1N	-2.82	117.11	120.36
2	B	1385	NAD	C3N-C2N-N1N	-2.74	117.21	120.36
2	D	1385	NAD	C4B-O4B-C1B	-2.73	106.72	109.72
2	B	1385	NAD	C4B-O4B-C1B	-2.63	106.82	109.72
2	A	1385	NAD	O3-PN-O5D	-2.32	96.78	102.94
2	B	1385	NAD	O3-PN-O5D	-2.28	96.88	102.94
2	C	1385	NAD	O3-PN-O5D	-2.13	97.30	102.94
2	D	1385	NAD	O3-PN-O5D	-2.12	97.31	102.94
2	A	1385	NAD	C3N-C7N-N7N	2.05	120.06	117.82
2	C	1385	NAD	O2B-C2B-C3B	2.13	118.76	111.83
2	D	1385	NAD	C3N-C7N-N7N	2.15	120.17	117.82
2	A	1385	NAD	O2B-C2B-C3B	2.26	119.16	111.83
2	C	1385	NAD	C3N-C7N-N7N	2.32	120.36	117.82
2	C	1385	NAD	C4D-O4D-C1D	2.39	112.34	109.72
2	D	1385	NAD	O2B-C2B-C3B	2.42	119.70	111.83
2	B	1385	NAD	O2B-C2B-C3B	2.46	119.83	111.83
2	B	1385	NAD	C3N-C7N-N7N	2.57	120.63	117.82
2	A	1385	NAD	C5N-C4N-C3N	2.74	123.78	120.33
2	C	1385	NAD	C5N-C4N-C3N	2.77	123.82	120.33
2	B	1385	NAD	C5N-C4N-C3N	2.94	124.03	120.33
2	D	1385	NAD	C5N-C4N-C3N	2.99	124.10	120.33
2	C	1385	NAD	O7N-C7N-C3N	3.36	123.25	119.59
2	B	1385	NAD	O7N-C7N-C3N	3.54	123.45	119.59
2	A	1385	NAD	O7N-C7N-C3N	3.65	123.57	119.59
2	D	1385	NAD	O7N-C7N-C3N	3.97	123.92	119.59
2	C	1385	NAD	O2A-PA-O1A	4.58	137.33	112.53
2	A	1385	NAD	O2A-PA-O1A	4.60	137.45	112.53
2	D	1385	NAD	O2A-PA-O1A	4.66	137.80	112.53
2	B	1385	NAD	O2A-PA-O1A	4.69	137.95	112.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1385	NAD	1	0
2	C	1385	NAD	1	0
2	D	1385	NAD	1	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	382/383 (99%)	0.24	22 (5%) 26 28	11, 30, 66, 100	0
1	B	382/383 (99%)	-0.13	8 (2%) 67 67	6, 24, 50, 71	0
1	C	382/383 (99%)	0.73	42 (10%) 7 8	14, 44, 81, 103	0
1	D	382/383 (99%)	0.06	17 (4%) 37 38	10, 28, 56, 97	0
All	All	1528/1532 (99%)	0.23	89 (5%) 26 28	6, 30, 69, 103	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	272	TYR	8.0
1	A	272	TYR	6.8
1	D	156	VAL	6.3
1	A	274	ASN	6.1
1	C	114	GLY	5.4
1	A	273	TYR	5.2
1	A	275	LEU	5.2
1	C	340	LEU	4.9
1	B	156	VAL	4.9
1	A	2	ALA	4.7
1	D	67	GLY	4.6
1	C	159	VAL	4.5
1	C	343	LEU	4.4
1	D	44	LYS	4.3
1	D	159	VAL	4.3
1	A	271	GLY	4.2
1	C	277	HIS	4.0
1	D	274	ASN	3.9
1	C	383	PHE	3.7
1	B	159	VAL	3.6
1	C	350	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	159	VAL	3.5
1	C	373	LYS	3.4
1	D	68	VAL	3.3
1	C	142	THR	3.3
1	B	144	SER	3.2
1	C	352	LEU	3.2
1	C	344	GLY	3.2
1	C	379	PHE	3.2
1	A	49	LYS	3.2
1	D	155	GLU	3.2
1	D	154	ASP	3.1
1	A	277	HIS	3.0
1	C	41	PHE	3.0
1	A	114	GLY	3.0
1	C	44	LYS	3.0
1	D	158	HIS	3.0
1	A	120	TYR	2.9
1	C	161	MET	2.9
1	B	141	GLY	2.8
1	A	144	SER	2.7
1	C	380	LEU	2.6
1	A	156	VAL	2.6
1	C	283	VAL	2.6
1	C	271	GLY	2.6
1	D	41	PHE	2.5
1	A	75	THR	2.5
1	C	49	LYS	2.5
1	D	141	GLY	2.5
1	C	275	LEU	2.4
1	A	115	GLY	2.4
1	C	269	LEU	2.4
1	A	142	THR	2.4
1	C	69	MET	2.4
1	D	142	THR	2.3
1	C	45	SER	2.3
1	A	158	HIS	2.3
1	C	128	LYS	2.3
1	A	162	ALA	2.3
1	C	154	ASP	2.3
1	C	270	GLY	2.3
1	A	116	GLU	2.3
1	D	344	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	346	LYS	2.3
1	D	85	LYS	2.3
1	C	371	ASP	2.2
1	B	345	ALA	2.2
1	A	380	LEU	2.2
1	A	157	ARG	2.2
1	B	143	ALA	2.2
1	B	155	GLU	2.2
1	C	143	ALA	2.2
1	D	10	PHE	2.2
1	B	44	LYS	2.2
1	C	358	LEU	2.2
1	C	139	THR	2.2
1	C	262	VAL	2.2
1	C	364	LEU	2.1
1	C	141	GLY	2.1
1	C	97	GLY	2.1
1	D	117	VAL	2.1
1	C	113	ASN	2.1
1	C	267	HIS	2.1
1	C	351	PRO	2.1
1	C	155	GLU	2.1
1	D	40	ALA	2.1
1	A	350	VAL	2.1
1	C	345	ALA	2.0
1	C	109	LEU	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	NAD	D	1385	44/44	0.85	0.25	2.45	41,47,53,55	0
2	NAD	A	1385	44/44	0.82	0.21	1.04	39,49,55,56	0
2	NAD	C	1385	44/44	0.83	0.21	0.45	44,48,53,55	0
2	NAD	B	1385	44/44	0.89	0.16	0.36	38,44,50,53	0
3	FE2	A	501	1/1	0.99	0.12	-1.02	24,24,24,24	0
3	FE2	C	501	1/1	0.99	0.08	-	26,26,26,26	0
3	FE2	D	501	1/1	1.00	0.09	-	20,20,20,20	0
3	FE2	B	501	1/1	1.00	0.09	-	14,14,14,14	0

6.5 Other polymers (i)

There are no such residues in this entry.