Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:05 PM GMT

PDB ID : 1NFB
Title : Ternary complex of the human type II Inosine Monophosphate Dedhydroge-
nase with 6Cl-IMP and NAD
Authors : Risal, D.; Strickler, M.D.; Goldstein, B.M.
Deposited on : 2002-12-13
Resolution : 2.90 Å(reported)

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 2.90 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	Percentile Ranks	Value
Rfree		0.266
Clashscore		34
Ramachandran outliers		7.3%
Sidechain outliers		11.4%
RSRZ outliers		10.0%

Worse *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
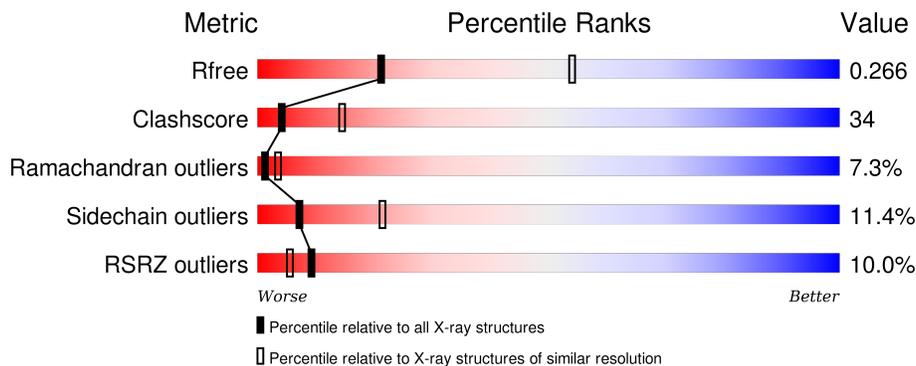
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	514	8% / 37% 34% 6% 23%
1	B	514	8% / 37% 34% 6% 23%

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
3	NAD	B	702	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5885 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 Inosine-5'-monophosphate dehydrogenase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			2833	1783	489	545	16			
1	B	396	Total	C	N	O	S	0	0	0
			2833	1783	489	545	16			

- Molecule 2 is 6-CHLOROPURINE RIBOSIDE, 5'-MONOPHOSPHATE (three-letter code: CPR) (formula: $C_{10}H_{13}ClN_4O_7P$).
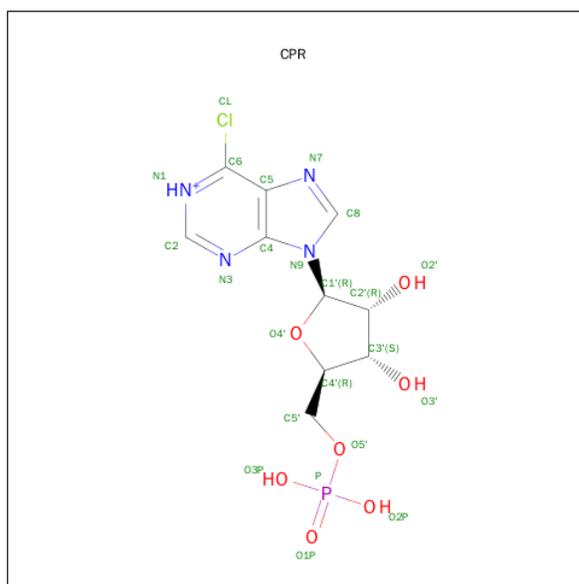
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	10	4	7	1		
2	B	1	Total	C	N	O	P	0	0
			22	10	4	7	1		

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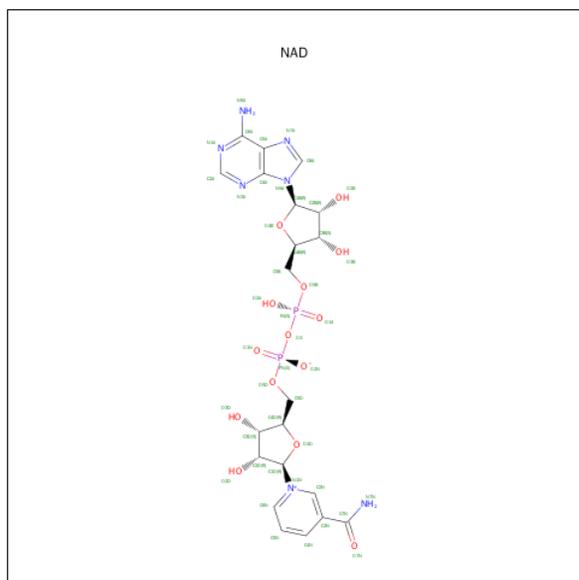
NAD

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		

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total	O	0	0
			43	43		
4	B	44	Total	O	0	0
			44	44		

3 Residue-property plots ⓘ

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: Inosine-5'-monophosphate dehydrogenase 2
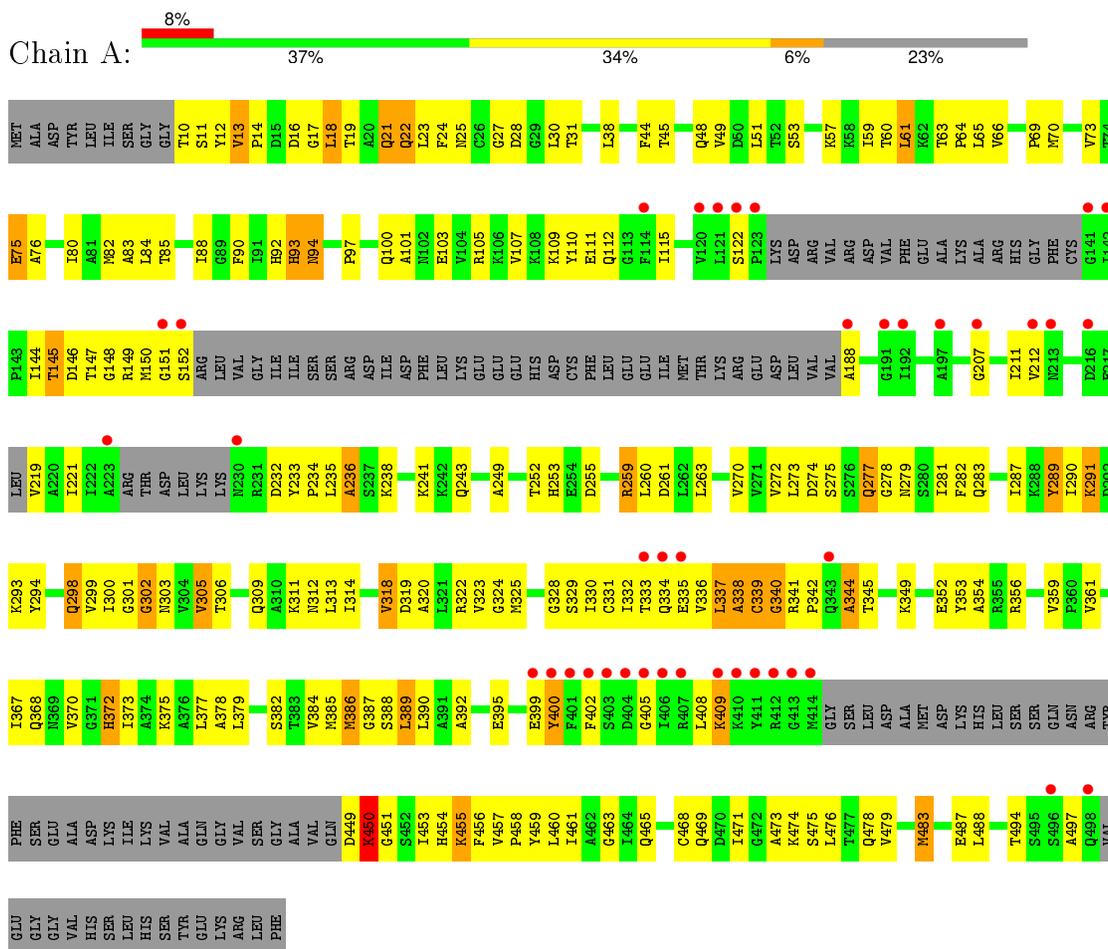
- Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

4   Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	145.19Å 145.19Å 127.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.82 – 2.90 51.33 – 2.90	Depositor EDS
% Data completeness (in resolution range)	66.5 (47.82-2.90) 74.6 (51.33-2.90)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	0.03	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.274 0.245 , 0.266	Depositor DCC
R_{free} test set	2190 reflections (11.11%)	DCC
Wilson B-factor (Å^2)	60.9	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 39.0	EDS
Estimated twinning fraction	0.447 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	0 of 24769 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	5885	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CPR, 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	0.49	0/2870	0.74	1/3881 (0.0%)
1	B	0.50	0/2870	0.75	0/3881
All	All	0.49	0/5740	0.75	1/7762 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	450	LYS	CB-CG-CD	5.17	125.05	111.60

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	2833	0	2702	189	0
1	B	2833	0	2702	186	0
2	A	22	0	11	2	0
2	B	22	0	11	3	0
3	A	44	0	26	4	0
3	B	44	0	26	5	0
4	A	43	0	0	8	0
4	B	44	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5885	0	5478	379	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 34.

All (379) 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:270:VAL:HG12	1:B:298:GLN:HB2	1.30	1.10
1:B:334:GLN:HB3	1:B:337:LEU:HB3	1.42	1.02
1:A:270:VAL:HG12	1:A:298:GLN:HB2	1.43	1.00
1:B:305:VAL:H	1:B:309:GLN:NE2	1.61	0.97
1:A:28:ASP:HB3	1:A:30:LEU:HG	1.48	0.94
1:A:332:ILE:HG12	1:A:333:THR:H	1.33	0.93
1:B:28:ASP:HB3	1:B:30:LEU:HG	1.54	0.90
1:B:332:ILE:HG12	1:B:333:THR:H	1.39	0.87
1:A:45:THR:H	1:A:48:GLN:NE2	1.76	0.84
1:B:305:VAL:H	1:B:309:GLN:HE22	1.28	0.82
1:A:303:ASN:OD1	1:A:322:ARG:HD3	1.78	0.81
1:B:473:ALA:HA	1:B:478:GLN:HE21	1.45	0.81
1:B:486:GLY:O	1:B:489:LYS:HE2	1.80	0.80
1:A:298:GLN:HE21	1:A:298:GLN:HA	1.47	0.80
1:A:45:THR:H	1:A:48:GLN:HE21	1.27	0.79
1:A:105:ARG:HH12	1:A:109:LYS:HE3	1.48	0.78
1:B:291:LYS:NZ	1:B:291:LYS:HA	1.98	0.77
1:B:92:HIS:HD2	1:B:94:ASN:H	1.33	0.76
1:A:337:LEU:HD12	1:A:339:CYS:H	1.49	0.76
1:B:291:LYS:HZ1	1:B:291:LYS:HA	1.51	0.76
1:A:252:THR:HG21	1:A:283:GLN:HG2	1.68	0.75
1:B:303:ASN:OD1	1:B:322:ARG:HD3	1.87	0.74
1:B:82:MET:HE3	1:B:390:LEU:HD13	1.69	0.74
1:B:253:HIS:HA	3:B:702:NAD:H61A	1.53	0.74
1:B:257:LYS:HG2	1:B:289:TYR:CE2	2.23	0.73
1:A:253:HIS:HA	3:A:701:NAD:H61A	1.51	0.73
3:A:701:NAD:H3D	3:A:701:NAD:O3	1.89	0.73
3:B:702:NAD:O3	3:B:702:NAD:H3D	1.89	0.72
1:A:253:HIS:HA	3:A:701:NAD:N6A	2.04	0.72
1:B:253:HIS:HA	3:B:702:NAD:N6A	2.05	0.71
1:A:92:HIS:CD2	1:A:94:ASN:H	2.08	0.71
1:B:330:ILE:HG23	1:B:335:GLU:HB2	1.71	0.71
1:A:330:ILE:HG23	1:A:335:GLU:HB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:GLN:HB2	1:A:337:LEU:HB3	1.71	0.71
1:A:277:GLN:HE21	1:A:277:GLN:CA	2.04	0.70
1:B:105:ARG:HH12	1:B:109:LYS:HG2	1.57	0.70
1:B:305:VAL:N	1:B:309:GLN:HE22	1.90	0.70
1:A:291:LYS:HA	1:A:291:LYS:NZ	2.07	0.69
1:A:483:MET:HB3	1:A:488:LEU:HD23	1.74	0.69
1:A:105:ARG:HH22	1:A:109:LYS:HE3	1.56	0.69
1:B:232:ASP:OD1	1:B:234:PRO:HD3	1.93	0.68
1:B:241:LYS:O	1:B:243:GLN:HG3	1.94	0.67
1:A:84:LEU:HB3	1:A:233:TYR:CD2	2.29	0.67
1:B:305:VAL:N	1:B:309:GLN:NE2	2.41	0.67
1:B:300:ILE:HG12	1:B:320:ALA:HB3	1.76	0.67
1:A:334:GLN:CB	1:A:337:LEU:HB3	2.25	0.66
1:B:257:LYS:HG2	1:B:289:TYR:HE2	1.61	0.65
1:B:386:MET:CE	1:B:389:LEU:HD23	2.26	0.65
1:A:311:LYS:HD3	4:A:709:HOH:O	1.97	0.65
1:B:66:VAL:O	1:B:385:MET:HA	1.96	0.65
1:B:84:LEU:HB3	1:B:233:TYR:CD2	2.31	0.65
1:A:82:MET:HE3	1:A:390:LEU:HD13	1.78	0.65
1:A:28:ASP:HB2	4:A:705:HOH:O	1.95	0.65
1:B:270:VAL:CG1	1:B:298:GLN:HB2	2.18	0.65
1:A:57:LYS:HE3	1:A:319:ASP:HA	1.79	0.65
1:A:69:PRO:HG3	1:A:90:PHE:HB3	1.79	0.64
1:A:19:THR:HB	1:A:22:GLN:HG2	1.80	0.64
1:A:306:THR:OG1	1:A:309:GLN:HG3	1.98	0.64
1:A:66:VAL:O	1:A:385:MET:HA	1.98	0.64
1:A:30:LEU:O	1:A:344:ALA:HB3	1.97	0.63
1:A:293:LYS:HG2	1:A:294:TYR:CE2	2.33	0.63
1:B:337:LEU:HD12	1:B:339:CYS:H	1.62	0.63
1:A:298:GLN:HA	1:A:298:GLN:NE2	2.14	0.63
1:A:323:VAL:HG23	1:A:361:VAL:HG13	1.80	0.63
1:B:275:SER:O	1:B:303:ASN:HB2	1.99	0.63
1:B:70:MET:SD	2:B:631:CPR:H8	2.38	0.63
1:A:270:VAL:CG1	1:A:298:GLN:HB2	2.26	0.63
3:B:702:NAD:PN	3:B:702:NAD:H3D	2.39	0.62
1:B:314:ILE:HA	1:B:318:VAL:HG22	1.81	0.62
1:A:473:ALA:HA	1:A:478:GLN:HE21	1.65	0.62
1:A:377:LEU:HD13	1:A:476:LEU:HD13	1.82	0.62
1:B:36:LEU:HG	1:B:493:ARG:NH1	2.14	0.62
1:A:188:ALA:HB3	1:A:211:ILE:HA	1.82	0.61
1:A:332:ILE:CG1	1:A:333:THR:H	2.11	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:SER:O	1:A:303:ASN:HB2	2.01	0.61
1:A:61:LEU:HD23	1:A:61:LEU:N	2.15	0.61
1:A:241:LYS:O	1:A:243:GLN:HG3	1.99	0.61
1:A:73:VAL:HG11	1:A:387:GLY:HA2	1.81	0.61
1:B:395:GLU:OE1	1:B:453:ILE:HG12	2.00	0.61
1:A:59:ILE:CD1	1:A:270:VAL:HG13	2.30	0.61
3:A:701:NAD:PN	3:A:701:NAD:H3D	2.40	0.61
1:A:59:ILE:HD12	1:A:270:VAL:HG13	1.82	0.61
1:B:30:LEU:O	1:B:344:ALA:HB3	2.01	0.61
1:B:303:ASN:ND2	1:B:324:GLY:O	2.34	0.60
1:B:69:PRO:HG3	1:B:90:PHE:HB3	1.84	0.60
1:B:76:ALA:O	1:B:80:ILE:HG13	2.02	0.60
1:B:45:THR:H	1:B:48:GLN:NE2	2.00	0.60
1:A:66:VAL:HG13	1:A:88:ILE:HG23	1.84	0.60
1:A:59:ILE:HD12	1:A:270:VAL:CG1	2.32	0.60
1:A:105:ARG:NH1	1:A:109:LYS:HE3	2.16	0.60
1:B:370:VAL:HG11	1:B:463:GLY:HA3	1.84	0.59
1:A:332:ILE:HG12	1:A:333:THR:N	2.10	0.59
1:B:188:ALA:HB3	1:B:211:ILE:HA	1.83	0.59
1:B:188:ALA:CB	1:B:211:ILE:HA	2.32	0.59
1:A:328:GLY:HA2	4:A:744:HOH:O	2.02	0.59
1:A:494:THR:OG1	1:A:497:ALA:HB2	2.02	0.59
1:B:245:LEU:HD11	4:B:705:HOH:O	2.02	0.59
1:B:461:ILE:O	1:B:465:GLN:HG3	2.03	0.59
1:B:23:LEU:HD12	1:B:23:LEU:O	2.03	0.59
1:A:314:ILE:HA	1:A:318:VAL:HG22	1.84	0.58
1:B:483:MET:HB3	1:B:488:LEU:HD23	1.85	0.58
1:A:303:ASN:ND2	1:A:324:GLY:O	2.36	0.58
1:B:325:MET:HG2	1:B:340:GLY:HA2	1.86	0.58
1:B:92:HIS:CD2	1:B:94:ASN:H	2.18	0.58
1:A:75:GLU:HG2	4:A:741:HOH:O	2.02	0.58
1:B:36:LEU:HD12	1:B:493:ARG:HD3	1.86	0.57
1:A:188:ALA:CB	1:A:211:ILE:HA	2.34	0.57
1:A:28:ASP:HB3	1:A:30:LEU:CG	2.27	0.57
1:A:333:THR:HG22	1:A:334:GLN:N	2.19	0.57
1:A:69:PRO:HG3	1:A:90:PHE:CB	2.35	0.57
1:A:330:ILE:HG12	1:A:335:GLU:HG2	1.86	0.57
1:B:252:THR:HG21	1:B:283:GLN:HG2	1.86	0.57
1:A:277:GLN:C	1:A:277:GLN:HE21	2.09	0.56
1:B:242:LYS:N	1:B:242:LYS:HD2	2.20	0.56
1:B:452:SER:HB3	1:B:455:LYS:HE3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:LEU:CB	1:B:283:GLN:HE22	2.17	0.56
1:B:71:ASP:HA	1:B:92:HIS:ND1	2.20	0.56
1:B:69:PRO:HG3	1:B:90:PHE:CB	2.36	0.56
1:A:300:ILE:HG12	1:A:320:ALA:HB3	1.87	0.56
1:B:333:THR:HG22	1:B:334:GLN:N	2.20	0.56
1:B:12:TYR:O	1:B:13:VAL:HG22	2.05	0.56
1:B:71:ASP:HA	1:B:92:HIS:CE1	2.41	0.56
1:B:67:SER:HB3	1:B:82:MET:HE3	1.87	0.56
1:A:313:LEU:O	1:A:318:VAL:HG22	2.05	0.56
1:B:453:ILE:HG23	1:B:457:VAL:HG23	1.87	0.56
1:B:10:THR:HG22	1:B:12:TYR:H	1.70	0.55
1:A:298:GLN:HE21	1:A:298:GLN:CA	2.18	0.55
1:A:392:ALA:HB1	1:A:449:ASP:OD2	2.07	0.55
1:B:378:ALA:O	1:B:483:MET:HG2	2.05	0.55
1:A:333:THR:HG22	1:A:334:GLN:H	1.71	0.55
1:B:386:MET:HE3	1:B:389:LEU:HD23	1.88	0.55
1:A:370:VAL:HG11	1:A:463:GLY:HA3	1.89	0.55
1:A:105:ARG:NH2	1:A:109:LYS:HE3	2.21	0.54
1:B:260:LEU:HD21	1:B:294:TYR:HE2	1.72	0.54
1:B:273:LEU:HB2	1:B:283:GLN:HE22	1.71	0.54
1:A:44:PHE:CZ	1:A:474:LYS:HG3	2.42	0.54
1:A:105:ARG:HH12	1:A:109:LYS:CE	2.17	0.54
1:A:273:LEU:HB3	1:A:283:GLN:NE2	2.22	0.54
1:B:330:ILE:HG23	4:B:741:HOH:O	2.06	0.54
1:B:13:VAL:O	1:B:13:VAL:CG2	2.56	0.54
1:A:386:MET:HE2	1:A:389:LEU:HD23	1.90	0.54
1:B:49:VAL:HG11	1:B:465:GLN:HA	1.89	0.54
1:B:480:ARG:HD2	4:B:708:HOH:O	2.06	0.54
1:B:483:MET:HE3	1:B:484:TYR:CZ	2.42	0.54
1:A:100:GLN:OE1	1:A:263:LEU:HD21	2.06	0.54
1:B:493:ARG:HG3	1:B:493:ARG:HH11	1.73	0.54
1:B:115:ILE:HG22	1:B:222:ILE:HA	1.89	0.54
1:A:457:VAL:HB	1:A:458:PRO:HD3	1.90	0.53
1:A:312:ASN:HD22	1:A:312:ASN:N	2.06	0.53
1:B:334:GLN:O	1:B:337:LEU:HD23	2.08	0.53
1:B:101:ALA:HA	1:B:263:LEU:HD23	1.89	0.53
1:A:345:THR:HG23	4:A:705:HOH:O	2.07	0.53
1:A:70:MET:SD	2:A:631:CPR:H8	2.49	0.53
1:B:334:GLN:CB	1:B:337:LEU:HB3	2.28	0.53
1:A:49:VAL:HG11	1:A:465:GLN:HA	1.91	0.53
1:A:105:ARG:HG2	1:A:105:ARG:HH11	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ILE:HG12	1:B:298:GLN:HG3	1.89	0.53
1:B:61:LEU:HD23	1:B:61:LEU:N	2.23	0.53
1:B:473:ALA:HA	1:B:478:GLN:NE2	2.20	0.52
1:B:259:ARG:HB2	4:B:712:HOH:O	2.09	0.52
1:A:277:GLN:HA	1:A:277:GLN:HE21	1.73	0.52
1:B:333:THR:HG22	1:B:334:GLN:H	1.75	0.52
1:B:305:VAL:H	1:B:309:GLN:HE21	1.52	0.52
1:B:287:ILE:HD13	1:B:299:VAL:HG11	1.92	0.51
1:B:41:TYR:CE2	1:B:43:ASP:HB3	2.45	0.51
1:B:370:VAL:HA	1:B:373:ILE:HD12	1.92	0.51
1:A:273:LEU:CB	1:A:283:GLN:HE22	2.24	0.51
1:B:82:MET:HE3	1:B:390:LEU:CD1	2.39	0.51
1:A:93:HIS:HB3	1:A:100:GLN:NE2	2.25	0.51
1:A:373:ILE:HG23	1:A:384:VAL:HG21	1.93	0.51
1:B:21:GLN:HE21	1:B:22:GLN:N	2.08	0.51
1:B:341:ARG:HG2	1:B:342:PRO:HD2	1.91	0.51
1:B:269:ASP:HB3	4:B:706:HOH:O	2.10	0.51
1:B:323:VAL:HG23	1:B:361:VAL:HG13	1.92	0.51
1:B:103:GLU:OE1	1:B:106:LYS:HD3	2.10	0.51
1:B:18:LEU:HB3	1:B:22:GLN:HG3	1.92	0.51
1:B:494:THR:OG1	1:B:497:ALA:HB2	2.12	0.50
1:A:375:LYS:O	1:A:379:LEU:HG	2.11	0.50
1:B:493:ARG:HG3	1:B:493:ARG:NH1	2.27	0.50
1:B:335:GLU:HG3	4:B:717:HOH:O	2.10	0.50
1:A:473:ALA:CB	1:A:479:VAL:HG22	2.42	0.50
1:B:103:GLU:O	1:B:107:VAL:HG23	2.12	0.50
1:A:293:LYS:HE2	1:A:294:TYR:OH	2.11	0.50
1:B:51:LEU:HD12	1:B:461:ILE:HG23	1.94	0.50
1:B:305:VAL:HG11	1:B:325:MET:HB3	1.93	0.50
1:A:330:ILE:HG22	1:A:331:CYS:N	2.27	0.50
1:A:454:HIS:O	1:A:455:LYS:HE3	2.11	0.50
1:B:494:THR:N	1:B:497:ALA:HB3	2.27	0.50
1:A:10:THR:HG22	1:A:12:TYR:H	1.77	0.50
1:B:386:MET:HE1	1:B:389:LEU:HD23	1.94	0.49
1:A:494:THR:OG1	1:A:497:ALA:CB	2.60	0.49
1:A:53:SER:OG	1:A:64:PRO:HB3	2.12	0.49
1:B:332:ILE:HG12	1:B:333:THR:N	2.17	0.49
1:B:93:HIS:HB3	1:B:100:GLN:HE22	1.77	0.49
1:A:65:LEU:HD13	1:A:460:LEU:HD12	1.94	0.49
1:A:273:LEU:HD11	1:A:287:ILE:HD13	1.93	0.49
1:A:305:VAL:HG11	1:A:325:MET:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:LEU:HG	1:B:493:ARG:HH11	1.78	0.49
1:A:395:GLU:OE1	1:A:453:ILE:HG12	2.11	0.49
1:B:93:HIS:ND1	1:B:250:ILE:HA	2.26	0.49
1:B:332:ILE:CG1	1:B:333:THR:H	2.16	0.49
1:B:454:HIS:O	1:B:458:PRO:HG2	2.12	0.49
1:B:212:VAL:HA	1:B:219:VAL:N	2.27	0.49
1:A:212:VAL:HA	1:A:219:VAL:N	2.27	0.49
1:A:13:VAL:O	1:A:13:VAL:CG2	2.60	0.49
1:A:461:ILE:O	1:A:465:GLN:HG3	2.13	0.48
1:B:60:THR:C	1:B:61:LEU:HD23	2.33	0.48
1:B:80:ILE:HG12	1:B:107:VAL:HG13	1.94	0.48
1:A:314:ILE:HA	1:A:318:VAL:CG2	2.43	0.48
1:A:80:ILE:HG12	1:A:107:VAL:HG13	1.95	0.48
1:A:234:PRO:HG2	1:A:235:LEU:HG	1.95	0.48
1:B:455:LYS:C	1:B:458:PRO:HD2	2.33	0.48
1:A:63:THR:HG21	1:A:461:ILE:HD11	1.95	0.48
1:B:330:ILE:HG12	1:B:335:GLU:HG2	1.95	0.48
1:B:300:ILE:HD13	1:B:362:ILE:HD11	1.96	0.48
1:A:241:LYS:NZ	4:A:729:HOH:O	2.46	0.48
1:A:454:HIS:O	1:A:458:PRO:HG2	2.14	0.48
1:A:408:LEU:C	1:A:408:LEU:HD13	2.34	0.48
1:B:21:GLN:O	1:B:23:LEU:N	2.46	0.48
1:A:277:GLN:NE2	1:A:279:ASN:H	2.12	0.48
1:B:495:SER:C	1:B:497:ALA:H	2.17	0.48
1:B:47:ASP:OD1	1:B:48:GLN:HG3	2.14	0.48
1:A:44:PHE:CE2	1:A:474:LYS:HG3	2.49	0.47
1:B:392:ALA:HB1	1:B:449:ASP:OD2	2.14	0.47
1:A:60:THR:C	1:A:61:LEU:HD23	2.34	0.47
1:A:334:GLN:HA	1:A:334:GLN:HE21	1.79	0.47
1:B:255:ASP:OD1	1:B:255:ASP:N	2.36	0.47
1:B:144:ILE:O	1:B:152:SER:N	2.47	0.47
1:B:289:TYR:CE1	1:B:293:LYS:HD3	2.49	0.47
1:B:483:MET:HB3	1:B:488:LEU:CD2	2.43	0.47
1:A:345:THR:O	1:A:349:LYS:HG2	2.14	0.47
1:A:337:LEU:HD12	1:A:339:CYS:N	2.24	0.47
1:B:21:GLN:C	1:B:23:LEU:H	2.18	0.47
1:A:105:ARG:HB3	1:A:105:ARG:CZ	2.45	0.47
1:A:283:GLN:O	1:A:287:ILE:HG12	2.14	0.47
1:A:144:ILE:O	1:A:152:SER:N	2.47	0.47
1:A:241:LYS:HE2	4:A:729:HOH:O	2.15	0.47
1:A:368:GLN:H	1:A:372:HIS:CD2	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:GLN:O	1:A:23:LEU:N	2.48	0.47
1:A:249:ALA:HB1	1:A:274:ASP:HB2	1.97	0.47
1:B:353:TYR:O	1:B:356:ARG:HB2	2.15	0.47
1:B:274:ASP:OD1	3:B:702:NAD:N7N	2.48	0.46
1:A:277:GLN:CA	1:A:277:GLN:NE2	2.76	0.46
1:B:480:ARG:O	1:B:484:TYR:HD2	1.98	0.46
1:A:293:LYS:HG2	1:A:294:TYR:CD2	2.50	0.46
1:B:83:ALA:O	1:B:236:ALA:HA	2.16	0.46
1:B:19:THR:H	1:B:22:GLN:CD	2.18	0.46
1:B:337:LEU:O	1:B:338:ALA:C	2.54	0.46
1:A:337:LEU:O	1:A:338:ALA:C	2.54	0.46
1:A:283:GLN:OE1	1:A:302:GLY:N	2.43	0.46
1:B:273:LEU:HD11	1:B:287:ILE:HD13	1.97	0.46
1:B:44:PHE:O	1:B:469:GLN:NE2	2.48	0.46
1:B:13:VAL:O	1:B:13:VAL:HG23	2.14	0.46
1:A:278:GLY:HA3	1:A:302:GLY:HA3	1.98	0.46
1:A:291:LYS:HZ3	1:A:291:LYS:HA	1.79	0.46
1:A:83:ALA:O	1:A:236:ALA:HA	2.15	0.46
1:B:45:THR:H	1:B:48:GLN:HE21	1.63	0.46
1:A:312:ASN:ND2	1:A:312:ASN:N	2.64	0.46
1:B:93:HIS:HB3	1:B:100:GLN:NE2	2.31	0.46
1:A:23:LEU:HG	1:A:23:LEU:O	2.14	0.45
1:A:273:LEU:CB	1:A:283:GLN:NE2	2.80	0.45
1:B:457:VAL:HB	1:B:458:PRO:HD3	1.99	0.45
1:A:471:ILE:HD11	1:A:479:VAL:HG13	1.96	0.45
1:B:492:LYS:HG2	1:B:493:ARG:N	2.31	0.45
1:A:483:MET:CB	1:A:488:LEU:HD23	2.44	0.45
1:B:273:LEU:HB3	1:B:283:GLN:NE2	2.31	0.45
1:A:325:MET:HG2	1:A:340:GLY:HA2	1.97	0.45
1:B:104:VAL:HG21	1:B:263:LEU:HD22	1.99	0.45
1:A:333:THR:CG2	1:A:334:GLN:H	2.28	0.45
1:A:85:THR:HB	1:A:457:VAL:HG11	1.98	0.45
1:A:146:ASP:O	1:A:148:GLY:N	2.50	0.45
1:A:287:ILE:HD13	1:A:299:VAL:HG11	1.98	0.45
1:B:483:MET:HE3	1:B:484:TYR:CE1	2.52	0.45
1:A:92:HIS:HD2	1:A:94:ASN:H	1.61	0.45
1:A:97:PRO:HG3	1:A:259:ARG:CZ	2.46	0.45
1:A:51:LEU:HD12	1:A:461:ILE:HG23	1.98	0.45
1:B:67:SER:HB3	1:B:82:MET:CE	2.46	0.45
1:A:19:THR:HB	1:A:22:GLN:CG	2.44	0.45
1:A:93:HIS:HB3	1:A:100:GLN:HE22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:GLN:C	1:A:23:LEU:H	2.20	0.45
1:A:241:LYS:CE	4:A:729:HOH:O	2.65	0.45
1:A:13:VAL:O	1:A:13:VAL:HG22	2.17	0.45
1:A:103:GLU:O	1:A:107:VAL:HG23	2.17	0.45
1:A:23:LEU:O	1:A:28:ASP:OD2	2.35	0.44
1:B:249:ALA:HB1	1:B:274:ASP:HB2	1.98	0.44
1:B:273:LEU:CB	1:B:283:GLN:NE2	2.81	0.44
1:B:456:PHE:O	1:B:459:TYR:HB3	2.16	0.44
1:A:49:VAL:HG11	1:A:468:CYS:HB2	2.00	0.44
1:A:18:LEU:N	1:A:18:LEU:HD22	2.33	0.44
1:B:242:LYS:HD2	1:B:242:LYS:H	1.83	0.44
1:B:146:ASP:O	1:B:148:GLY:N	2.49	0.44
1:A:84:LEU:HA	1:A:236:ALA:CB	2.48	0.44
1:B:68:SER:HA	1:B:69:PRO:HD3	1.85	0.44
1:A:475:SER:O	1:A:479:VAL:HG23	2.18	0.44
1:B:10:THR:HG22	1:B:12:TYR:N	2.32	0.44
1:B:278:GLY:HA3	1:B:302:GLY:HA3	1.98	0.44
1:B:53:SER:O	1:B:60:THR:HG23	2.18	0.44
1:A:289:TYR:HD2	1:A:290:ILE:N	2.15	0.44
1:B:51:LEU:HD22	1:B:476:LEU:HD11	1.99	0.44
1:A:453:ILE:HG23	1:A:457:VAL:HG23	1.99	0.44
1:B:23:LEU:O	1:B:28:ASP:OD2	2.36	0.43
1:B:105:ARG:HH11	1:B:105:ARG:HG2	1.83	0.43
1:A:455:LYS:HE3	1:A:455:LYS:HA	2.00	0.43
1:B:341:ARG:HA	1:B:342:PRO:HD3	1.87	0.43
1:B:20:ALA:O	1:B:24:PHE:HD2	2.01	0.43
1:B:63:THR:HG23	1:B:86:GLY:HA3	2.00	0.43
1:B:354:ALA:HB1	1:B:359:VAL:O	2.18	0.43
1:A:408:LEU:HD13	1:A:409:LYS:N	2.32	0.43
1:B:70:MET:HE2	1:B:70:MET:HB3	1.85	0.43
1:B:13:VAL:O	1:B:14:PRO:O	2.36	0.43
1:B:301:GLY:O	1:B:302:GLY:O	2.36	0.43
1:B:21:GLN:C	1:B:23:LEU:N	2.71	0.43
1:A:76:ALA:O	1:A:80:ILE:HG13	2.18	0.43
1:A:386:MET:CE	1:A:389:LEU:HD23	2.49	0.43
1:A:289:TYR:CD2	1:A:290:ILE:N	2.86	0.43
1:B:53:SER:OG	1:B:64:PRO:HB3	2.19	0.43
1:A:341:ARG:CG	1:A:342:PRO:HD2	2.49	0.43
1:A:45:THR:N	1:A:48:GLN:HE21	2.05	0.42
1:B:333:THR:CG2	1:B:334:GLN:H	2.30	0.42
1:A:260:LEU:O	1:A:263:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:GLY:O	1:A:302:GLY:O	2.38	0.42
1:A:277:GLN:HE22	1:A:279:ASN:H	1.67	0.42
1:B:292:ASP:O	1:B:295:PRO:HD3	2.18	0.42
1:B:260:LEU:O	1:B:263:LEU:HB2	2.20	0.42
1:A:101:ALA:HA	1:A:263:LEU:HD23	2.02	0.42
1:B:452:SER:O	1:B:455:LYS:HG2	2.20	0.42
1:A:323:VAL:CG2	1:A:361:VAL:HG13	2.47	0.42
1:B:105:ARG:NH1	1:B:109:LYS:HG2	2.29	0.42
1:A:272:VAL:HG13	1:A:272:VAL:O	2.20	0.42
1:B:233:TYR:HE2	1:B:454:HIS:CE1	2.37	0.42
1:A:353:TYR:O	1:A:356:ARG:HB2	2.20	0.42
1:B:390:LEU:O	1:B:393:THR:HG23	2.19	0.42
1:A:395:GLU:CD	1:A:453:ILE:H	2.23	0.42
2:A:631:CPR:H3'	2:A:631:CPR:H8	2.02	0.42
1:A:334:GLN:O	1:A:337:LEU:HD23	2.20	0.42
1:A:330:ILE:HG22	1:A:331:CYS:H	1.85	0.42
1:A:367:ILE:HD13	1:A:372:HIS:HB3	2.02	0.42
1:A:97:PRO:HB3	1:A:259:ARG:HA	2.02	0.42
1:B:364:ASP:OD2	2:B:631:CPR:O2'	2.35	0.42
1:A:378:ALA:O	1:A:483:MET:HG2	2.20	0.41
1:B:238:LYS:HA	1:B:243:GLN:O	2.20	0.41
1:B:311:LYS:HG2	1:B:315:ASP:OD2	2.20	0.41
1:A:456:PHE:O	1:A:459:TYR:HB3	2.19	0.41
1:B:63:THR:HG21	1:B:461:ILE:HD11	2.02	0.41
1:A:21:GLN:C	1:A:23:LEU:N	2.72	0.41
1:B:19:THR:O	1:B:22:GLN:HG2	2.20	0.41
1:A:388:SER:O	1:A:390:LEU:N	2.54	0.41
1:A:238:LYS:HB2	1:A:238:LYS:HE2	1.73	0.41
1:A:354:ALA:HB1	1:A:359:VAL:O	2.20	0.41
1:B:18:LEU:HB3	1:B:22:GLN:HE21	1.84	0.41
1:B:330:ILE:HG22	1:B:331:CYS:N	2.36	0.41
1:A:305:VAL:HG22	1:A:309:GLN:NE2	2.36	0.41
1:A:487:GLU:HA	1:B:12:TYR:CE1	2.55	0.41
1:A:44:PHE:O	1:A:469:GLN:NE2	2.53	0.41
1:A:455:LYS:C	1:A:458:PRO:HD2	2.41	0.41
1:B:73:VAL:HG21	1:B:387:GLY:CA	2.51	0.41
1:A:281:ILE:HG23	1:A:282:PHE:N	2.35	0.41
1:B:331:CYS:HB2	2:B:631:CPR:HN1	1.76	0.41
1:A:305:VAL:HG22	1:A:309:GLN:HE22	1.85	0.41
1:B:377:LEU:HA	1:B:381:ALA:HB3	2.02	0.41
1:B:18:LEU:HA	1:B:22:GLN:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:ILE:CD1	1:A:479:VAL:HG13	2.51	0.41
1:A:23:LEU:HD23	1:A:24:PHE:CE2	2.56	0.41
1:A:332:ILE:CG1	1:A:333:THR:N	2.76	0.41
1:A:45:THR:N	1:A:48:GLN:NE2	2.57	0.41
1:B:388:SER:O	1:B:390:LEU:N	2.54	0.41
1:A:352:GLU:O	1:A:352:GLU:CD	2.59	0.41
1:A:145:THR:HA	1:A:151:GLY:HA3	2.02	0.41
1:A:273:LEU:HB2	1:A:283:GLN:HE22	1.86	0.41
1:B:238:LYS:HB2	1:B:243:GLN:N	2.36	0.41
1:B:375:LYS:NZ	4:B:709:HOH:O	2.53	0.41
1:B:145:THR:HA	1:B:151:GLY:HA3	2.02	0.41
1:B:260:LEU:HD21	1:B:294:TYR:CE2	2.53	0.40
1:B:272:VAL:HG13	1:B:272:VAL:O	2.21	0.40
1:B:108:LYS:HD2	1:B:244:LEU:O	2.21	0.40
1:A:291:LYS:HA	1:A:291:LYS:CE	2.51	0.40
1:A:115:ILE:HG22	1:A:221:ILE:C	2.42	0.40
1:B:72:THR:HG22	1:B:411:TYR:CE1	2.56	0.40
1:B:51:LEU:HD21	1:B:464:ILE:HG22	2.04	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	384/514 (75%)	304 (79%)	52 (14%)	28 (7%)	1	3
1	B	384/514 (75%)	301 (78%)	55 (14%)	28 (7%)	1	3
All	All	768/1028 (75%)	605 (79%)	107 (14%)	56 (7%)	1	3

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	PRO
1	A	147	THR
1	A	400	TYR
1	A	450	LYS
1	B	14	PRO
1	B	147	THR
1	B	400	TYR
1	B	450	LYS
1	A	17	GLY
1	A	145	THR
1	A	150	MET
1	A	302	GLY
1	A	337	LEU
1	A	451	GLY
1	B	17	GLY
1	B	145	THR
1	B	150	MET
1	B	302	GLY
1	B	337	LEU
1	B	451	GLY
1	A	13	VAL
1	A	22	GLN
1	A	27	GLY
1	A	236	ALA
1	B	13	VAL
1	B	22	GLN
1	B	27	GLY
1	B	112	GLN
1	B	236	ALA
1	A	112	GLN
1	A	122	SER
1	A	207	GLY
1	A	289	TYR
1	B	207	GLY
1	B	289	TYR
1	B	344	ALA
1	A	110	TYR
1	A	149	ARG
1	A	338	ALA
1	A	344	ALA
1	A	389	LEU
1	A	399	GLU
1	A	405	GLY

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Mol	Chain	Res	Type
1	B	122	SER
1	B	149	ARG
1	B	338	ALA
1	B	399	GLU
1	B	405	GLY
1	B	496	SER
1	A	340	GLY
1	B	110	TYR
1	B	340	GLY
1	B	389	LEU
1	B	305	VAL
1	A	305	VAL
1	A	318	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	271/420 (64%)	240 (89%)	31 (11%)	7	21
1	B	271/420 (64%)	240 (89%)	31 (11%)	7	21
All	All	542/840 (64%)	480 (89%)	62 (11%)	7	21

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	16	ASP
1	A	18	LEU
1	A	21	GLN
1	A	25	ASN
1	A	31	THR
1	A	38	LEU
1	A	61	LEU
1	A	75	GLU
1	A	93	HIS

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Mol	Chain	Res	Type
1	A	94	ASN
1	A	111	GLU
1	A	232	ASP
1	A	255	ASP
1	A	259	ARG
1	A	261	ASP
1	A	277	GLN
1	A	291	LYS
1	A	298	GLN
1	A	329	SER
1	A	336	VAL
1	A	339	CYS
1	A	372	HIS
1	A	382	SER
1	A	386	MET
1	A	400	TYR
1	A	402	PHE
1	A	409	LYS
1	A	450	LYS
1	A	455	LYS
1	A	483	MET
1	B	13	VAL
1	B	16	ASP
1	B	18	LEU
1	B	21	GLN
1	B	38	LEU
1	B	61	LEU
1	B	63	THR
1	B	93	HIS
1	B	94	ASN
1	B	111	GLU
1	B	232	ASP
1	B	238	LYS
1	B	255	ASP
1	B	260	LEU
1	B	268	VAL
1	B	277	GLN
1	B	291	LYS
1	B	329	SER
1	B	334	GLN
1	B	339	CYS
1	B	372	HIS

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Mol	Chain	Res	Type
1	B	386	MET
1	B	388	SER
1	B	400	TYR
1	B	402	PHE
1	B	406	ILE
1	B	409	LYS
1	B	450	LYS
1	B	483	MET
1	B	495	SER
1	B	498	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	48	GLN
1	A	92	HIS
1	A	94	ASN
1	A	112	GLN
1	A	243	GLN
1	A	265	GLN
1	A	277	GLN
1	A	309	GLN
1	A	312	ASN
1	A	334	GLN
1	A	372	HIS
1	A	454	HIS
1	A	478	GLN
1	B	21	GLN
1	B	22	GLN
1	B	33	ASN
1	B	48	GLN
1	B	92	HIS
1	B	94	ASN
1	B	112	GLN
1	B	265	GLN
1	B	309	GLN
1	B	312	ASN
1	B	372	HIS
1	B	454	HIS
1	B	478	GLN
1	B	498	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	CPR	A	631	1	19,24,25	1.48	1 (5%)	22,36,38	1.89	4 (18%)
3	NAD	A	701	-	38,48,48	1.72	5 (13%)	47,73,73	2.18	5 (10%)
2	CPR	B	631	1	19,24,25	1.44	1 (5%)	22,36,38	1.89	4 (18%)
3	NAD	B	702	-	38,48,48	1.73	5 (13%)	47,73,73	2.11	4 (8%)

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	CPR	A	631	1	-	0/6/26/26	0/3/3/3
3	NAD	A	701	-	-	0/22/62/62	0/5/5/5
2	CPR	B	631	1	-	0/6/26/26	0/3/3/3
3	NAD	B	702	-	-	0/22/62/62	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	NAD	C6N-C5N	2.07	1.43	1.38
3	A	701	NAD	C4N-C3N	2.15	1.43	1.39
3	A	701	NAD	C6N-C5N	2.17	1.43	1.38
3	B	702	NAD	C4N-C3N	2.29	1.43	1.39
3	A	701	NAD	C6N-N1N	3.96	1.46	1.35
3	B	702	NAD	C6N-N1N	3.98	1.46	1.35
2	B	631	CPR	O4'-C1'	4.53	1.46	1.41
2	A	631	CPR	O4'-C1'	4.81	1.47	1.41
3	A	701	NAD	O4D-C1D	4.85	1.47	1.41
3	B	702	NAD	O4D-C1D	4.89	1.47	1.41
3	B	702	NAD	O4B-C1B	5.66	1.48	1.41
3	A	701	NAD	O4B-C1B	5.81	1.48	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	NAD	N3A-C2A-N1A	-12.18	119.57	128.89
3	B	702	NAD	N3A-C2A-N1A	-12.15	119.59	128.89
2	A	631	CPR	N1-C2-N3	-5.82	120.64	127.82
2	B	631	CPR	N1-C2-N3	-5.77	120.70	127.82
3	A	701	NAD	C3N-C7N-N7N	-3.52	113.96	117.82
3	A	701	NAD	PN-O3-PA	-3.49	122.94	132.73
3	B	702	NAD	PN-O3-PA	-3.43	123.10	132.73
2	A	631	CPR	C5-C4-N3	-3.24	119.81	125.77
2	B	631	CPR	C5-C4-N3	-3.20	119.88	125.77
3	B	702	NAD	O7N-C7N-C3N	2.25	122.04	119.59
2	A	631	CPR	O2P-P-O1P	2.50	118.63	110.58
2	B	631	CPR	O2P-P-O1P	2.50	118.64	110.58
3	A	701	NAD	O7N-C7N-C3N	2.67	122.50	119.59
3	A	701	NAD	O4D-C1D-N1N	3.34	111.80	108.13
3	B	702	NAD	O4D-C1D-N1N	3.37	111.83	108.13
2	A	631	CPR	C6-N1-C2	3.97	121.37	115.89
2	B	631	CPR	C6-N1-C2	4.00	121.41	115.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	631	CPR	2	0
3	A	701	NAD	4	0
2	B	631	CPR	3	0
3	B	702	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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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(Å²)	Q<0.9
1	A	396/514 (77%)	0.69	40 (10%)	9	5	18, 52, 110, 143	0
1	B	396/514 (77%)	0.72	39 (9%)	10	6	17, 52, 112, 148	0
All	All	792/1028 (77%)	0.70	79 (9%)	9	5	17, 52, 111, 148	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	411	TYR	14.1
1	A	411	TYR	13.0
1	B	403	SER	12.4
1	B	413	GLY	10.8
1	B	402	PHE	10.7
1	B	122	SER	10.1
1	A	141	GLY	8.5
1	A	191	GLY	8.3
1	A	414	MET	7.9
1	A	333	THR	7.9
1	A	402	PHE	7.4
1	A	403	SER	7.3
1	A	413	GLY	7.2
1	A	334	GLN	7.0
1	B	406	ILE	6.9
1	A	152	SER	6.9
1	B	412	ARG	6.9
1	B	207	GLY	6.7
1	A	401	PHE	6.4
1	B	335	GLU	6.3
1	A	400	TYR	6.3
1	B	333	THR	6.1
1	B	141	GLY	6.1
1	A	122	SER	5.7

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Mol	Chain	Res	Type	RSRZ
1	B	408	LEU	5.7
1	B	404	ASP	5.3
1	B	230	ASN	5.2
1	A	123	PRO	5.2
1	A	207	GLY	5.0
1	A	223	ALA	5.0
1	B	405	GLY	4.8
1	B	334	GLN	4.5
1	A	213	ASN	4.4
1	B	216	ASP	4.3
1	A	212	VAL	4.3
1	A	335	GLU	4.3
1	B	496	SER	4.2
1	B	142	ILE	4.2
1	B	152	SER	4.1
1	B	123	PRO	4.0
1	A	192	ILE	3.9
1	B	191	GLY	3.9
1	B	401	PHE	3.9
1	A	412	ARG	3.9
1	A	230	ASN	3.8
1	B	198	ASN	3.7
1	B	414	MET	3.6
1	B	498	GLN	3.6
1	A	142	ILE	3.4
1	B	337	LEU	3.2
1	A	188	ALA	3.2
1	A	496	SER	3.2
1	A	410	LYS	3.1
1	B	197	ALA	3.0
1	B	399	GLU	3.0
1	A	197	ALA	2.9
1	B	400	TYR	2.8
1	B	407	ARG	2.8
1	A	406	ILE	2.8
1	B	215	ASP	2.8
1	A	409	LYS	2.7
1	A	151	GLY	2.6
1	B	188	ALA	2.6
1	A	399	GLU	2.5
1	B	146	ASP	2.5
1	A	404	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	114	PHE	2.5
1	A	343	GLN	2.4
1	B	120	VAL	2.3
1	B	336	VAL	2.2
1	A	405	GLY	2.2
1	B	189	PRO	2.2
1	A	121	LEU	2.2
1	A	216	ASP	2.1
1	B	151	GLY	2.1
1	A	498	GLN	2.1
1	A	407	ARG	2.0
1	A	120	VAL	2.0
1	B	190	ALA	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, 95th 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	B	702	44/44	0.77	0.44	1.15	138,138,138,138	0
3	NAD	A	701	44/44	0.82	0.36	0.46	126,126,126,126	0
2	CPR	A	631	22/23	0.93	0.23	-0.20	74,75,75,76	0
2	CPR	B	631	22/23	0.93	0.19	-0.34	69,70,70,70	0

6.5 Other polymers (i)

There are no such residues in this entry.