Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:54 AM GMT

PDB ID	:	2OME
Title	:	Crystal structure of human CTBP2 dehydrogenase complexed with NAD(H)
Authors	:	Pilka, E.S.; Guo, K.; Rojkova, A.; Debreczeni, J.E.; Kavanagh, K.L.; von Delft, F.; Arrowsmith, C.H.; Weigelt, J.; Edwards, A.; Sundstrom, M.; Oppermann, U.; Structural Genomics Consortium (SGC)
Deposited on	:	2007-01-22
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

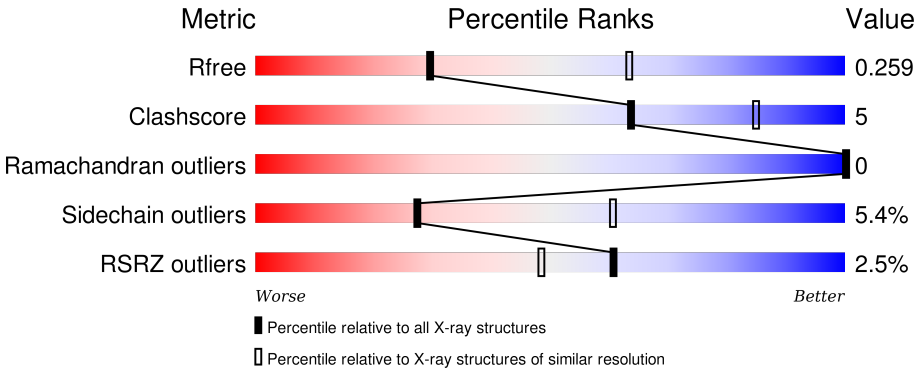
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	336	87% 10%
1	B	336	3% 87% 10%
1	C	336	85% 12%
1	D	336	2% 81% 16%
1	E	336	7% 82% 14%

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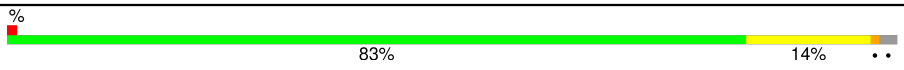
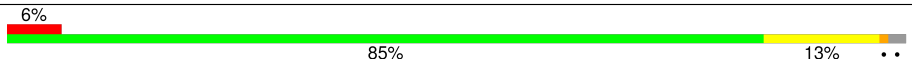
Mol	Chain	Length	Quality of chain
1	F	336	
1	G	336	
1	H	336	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20793 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 C-terminal-binding protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	1	0
			2554	1601	458	482	13			
1	B	330	Total	C	N	O	S	0	0	0
			2520	1586	445	476	13			
1	C	330	Total	C	N	O	S	0	1	0
			2561	1607	461	480	13			
1	D	330	Total	C	N	O	S	0	0	0
			2532	1589	455	475	13			
1	E	330	Total	C	N	O	S	0	0	0
			2487	1560	447	467	13			
1	F	330	Total	C	N	O	S	0	2	0
			2551	1599	457	482	13			
1	G	330	Total	C	N	O	S	0	3	0
			2508	1570	449	476	13			
1	H	330	Total	C	N	O	S	0	1	0
			2544	1593	457	481	13			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	SER	-	CLONING ARTIFACT	UNP P56545
A	30	MET	-	CLONING ARTIFACT	UNP P56545
B	29	SER	-	CLONING ARTIFACT	UNP P56545
B	30	MET	-	CLONING ARTIFACT	UNP P56545
C	29	SER	-	CLONING ARTIFACT	UNP P56545
C	30	MET	-	CLONING ARTIFACT	UNP P56545
D	29	SER	-	CLONING ARTIFACT	UNP P56545
D	30	MET	-	CLONING ARTIFACT	UNP P56545
E	29	SER	-	CLONING ARTIFACT	UNP P56545
E	30	MET	-	CLONING ARTIFACT	UNP P56545
F	29	SER	-	CLONING ARTIFACT	UNP P56545
F	30	MET	-	CLONING ARTIFACT	UNP P56545
G	29	SER	-	CLONING ARTIFACT	UNP P56545

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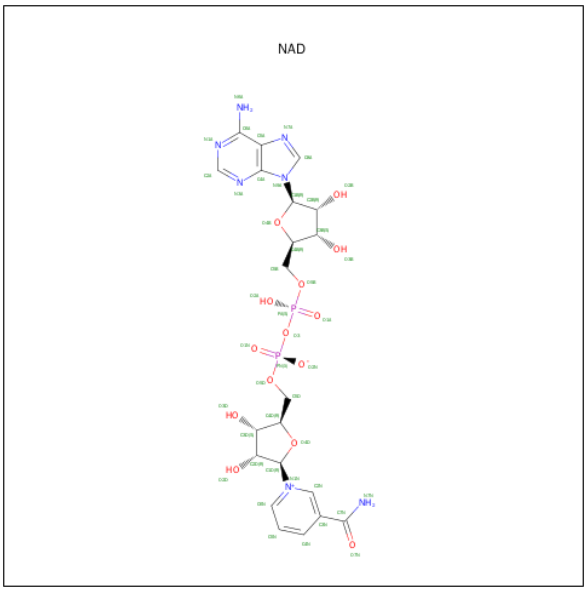
Chain	Residue	Modelled	Actual	Comment	Reference
G	30	MET	-	CLONING ARTIFACT	UNP P56545
H	29	SER	-	CLONING ARTIFACT	UNP P56545
H	30	MET	-	CLONING ARTIFACT	UNP P56545

- 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		
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		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is water.

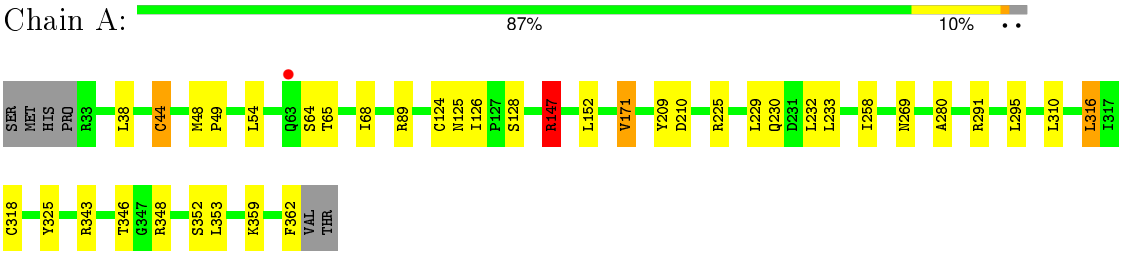
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	28	Total O 28 28	0	0
3	B	19	Total O 19 19	0	0
3	C	29	Total O 29 29	0	0
3	D	23	Total O 23 23	0	0
3	E	9	Total O 9 9	0	0
3	F	30	Total O 30 30	0	0
3	G	17	Total O 17 17	0	0
3	H	29	Total O 29 29	0	0

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.

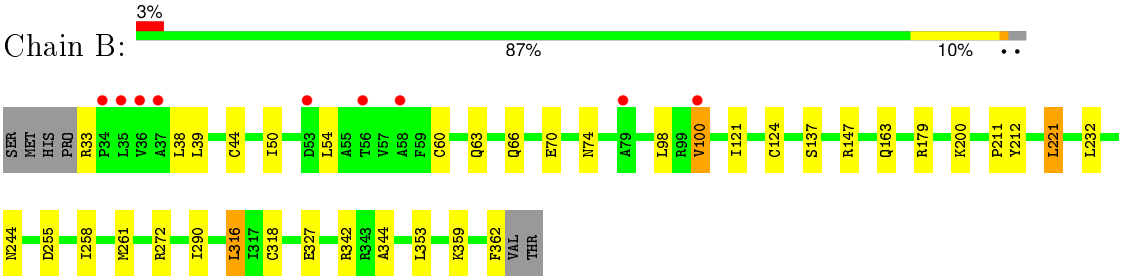
- Molecule 1: C-terminal-binding protein 2

Chain A:



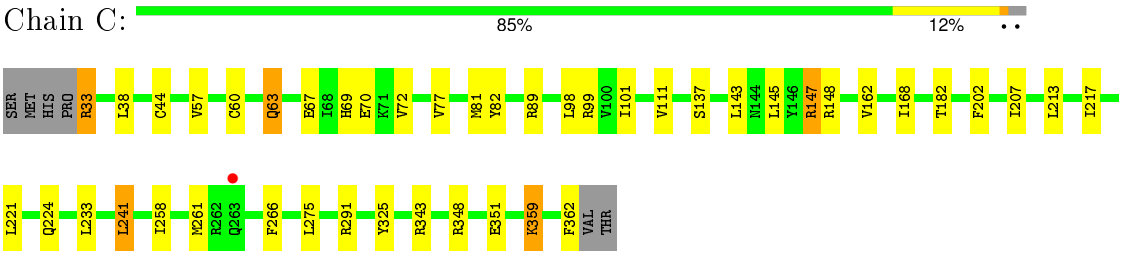
- Molecule 1: C-terminal-binding protein 2

Chain B:



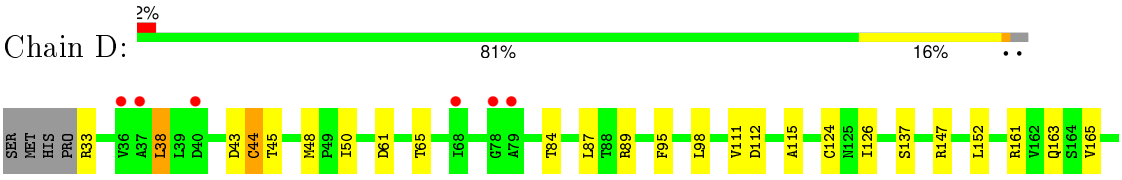
- Molecule 1: C-terminal-binding protein 2

Chain C:

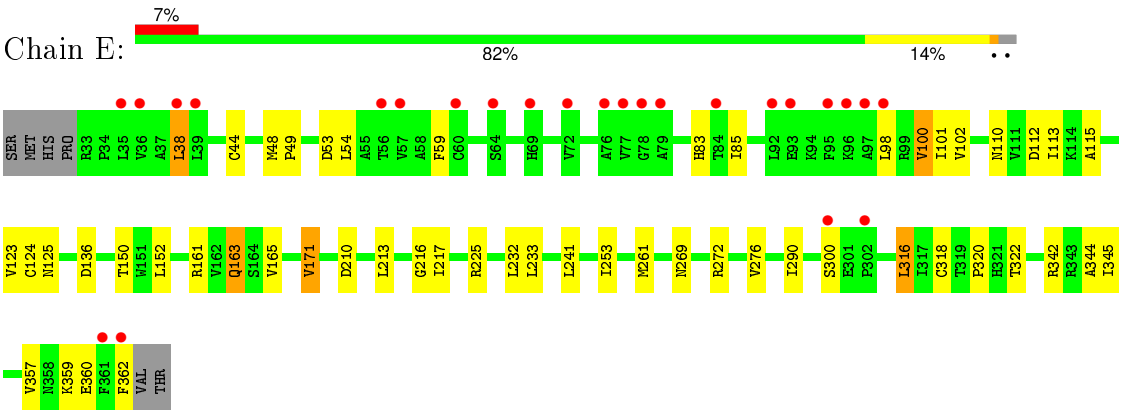


- Molecule 1: C-terminal-binding protein 2

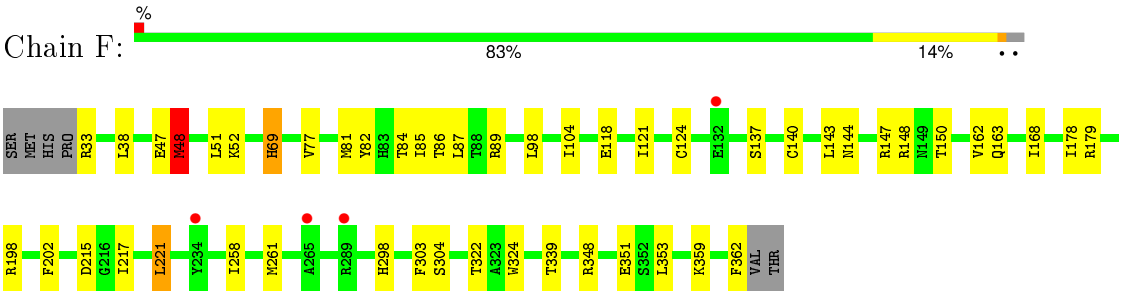
Chain D:



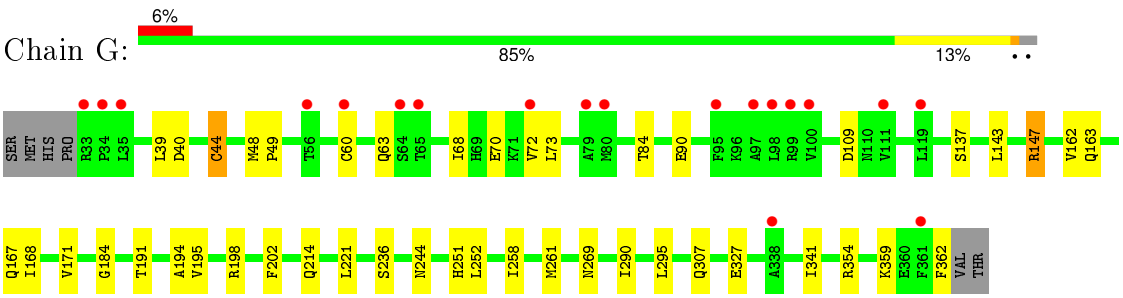
• Molecule 1: C-terminal-binding protein 2



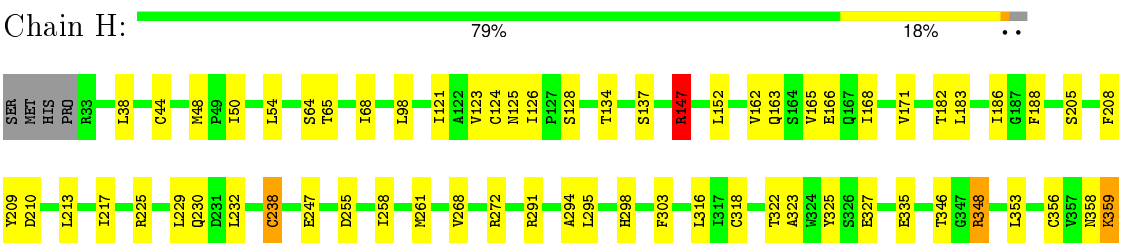
• Molecule 1: C-terminal-binding protein 2



• Molecule 1: C-terminal-binding protein 2



• Molecule 1: C-terminal-binding protein 2

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VAL
THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.75Å 141.57Å 138.22Å 90.00° 98.93° 90.00°	Depositor
Resolution (Å)	43.31 – 2.80 43.33 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.31-2.80) 100.0 (43.33-2.80)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.207 , 0.257 0.213 , 0.259	Depositor DCC
R_{free} test set	4104 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	56.5	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 50.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 82108 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	20793	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.68	0/2601	0.76	3/3525 (0.1%)
1	B	0.64	0/2561	0.73	1/3474 (0.0%)
1	C	0.73	0/2609	0.77	3/3533 (0.1%)
1	D	0.62	0/2573	0.72	2/3488 (0.1%)
1	E	0.56	0/2528	0.70	1/3434 (0.0%)
1	F	0.68	2/2603 (0.1%)	0.77	3/3530 (0.1%)
1	G	0.59	0/2558	0.68	1/3472 (0.0%)
1	H	0.65	2/2592 (0.1%)	0.76	3/3516 (0.1%)
All	All	0.65	4/20625 (0.0%)	0.74	17/27972 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
All	All	0	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	356	CYS	CB-SG	-6.05	1.72	1.82
1	H	238	CYS	CB-SG	-5.59	1.72	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	48	MET	CB-CG	5.49	1.69	1.51
1	F	48	MET	CG-SD	5.42	1.95	1.81

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	147	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	G	147	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	A	147	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	147	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	F	147	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	H	147	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	C	343	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	C	147	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	E	272	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	H	272	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	F	48	MET	CB-CG-SD	5.35	128.44	112.40
1	C	147	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	272	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	D	169	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	A	343	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	H	147	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	D	272	ARG	NE-CZ-NH1	5.05	122.83	120.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	359	LYS	Peptide
1	B	33	ARG	Peptide
1	B	359	LYS	Peptide
1	C	359	LYS	Peptide
1	D	359	LYS	Peptide
1	E	359	LYS	Peptide
1	F	359	LYS	Peptide
1	G	359	LYS	Peptide
1	H	359	LYS	Peptide

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	2554	0	2507	20	0
1	B	2520	0	2464	22	0
1	C	2561	0	2542	24	0
1	D	2532	0	2497	35	0
1	E	2487	0	2403	37	0
1	F	2551	0	2499	31	0
1	G	2508	0	2414	24	0
1	H	2544	0	2491	33	0
2	A	44	0	26	0	0
2	B	44	0	26	1	0
2	C	44	0	26	0	0
2	D	44	0	26	2	0
2	E	44	0	26	0	0
2	F	44	0	26	1	0
2	G	44	0	26	1	0
2	H	44	0	26	0	0
3	A	28	0	0	0	0
3	B	19	0	0	0	0
3	C	29	0	0	1	0
3	D	23	0	0	1	0
3	E	9	0	0	0	0
3	F	30	0	0	0	0
3	G	17	0	0	1	0
3	H	29	0	0	1	0
All	All	20793	0	20025	210	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 5.

All (210) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:LEU:HD13	1:D:217:ILE:HD12	1.41	1.01
1:F:81:MET:CE	1:F:85:ILE:HG23	1.93	0.98
1:F:81:MET:HE3	1:F:85:ILE:HG23	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:MET:CE	1:C:111:VAL:HG22	2.03	0.87
1:H:124:CYS:SG	1:H:353:LEU:HD13	2.15	0.86
1:H:98:LEU:HD23	1:H:121:ILE:HD13	1.59	0.84
1:E:44:CYS:HG	1:E:59:PHE:HB3	1.43	0.83
1:D:213:LEU:CD1	1:D:217:ILE:HD12	2.11	0.80
1:C:81:MET:HE3	1:C:111:VAL:HG22	1.64	0.79
1:H:213:LEU:HD13	1:H:217:ILE:HD12	1.64	0.79
1:D:261:MET:HE1	1:D:290:ILE:HD11	1.67	0.77
1:E:44:CYS:SG	1:E:59:PHE:HB3	2.28	0.72
1:D:261:MET:CE	1:D:290:ILE:HD11	2.20	0.71
1:C:81:MET:CE	1:C:111:VAL:CG2	2.69	0.70
1:D:229:LEU:HD22	1:D:252:LEU:HD11	1.72	0.70
1:G:147:ARG:NH2	1:H:325:TYR:O	2.24	0.69
1:F:98:LEU:HD23	1:F:121:ILE:HD13	1.73	0.69
1:B:258:ILE:HA	1:B:261:MET:HE2	1.75	0.68
1:B:261:MET:CE	1:B:290:ILE:HD11	2.25	0.67
1:F:81:MET:HE3	1:F:85:ILE:CG2	2.24	0.65
1:F:81:MET:CE	1:F:85:ILE:CG2	2.73	0.63
1:G:40:ASP:OD2	1:G:84:THR:OG1	2.14	0.63
1:C:63:GLN:NE2	1:C:67:GLU:OE2	2.31	0.63
1:B:261:MET:HE1	1:B:290:ILE:HD11	1.80	0.63
1:A:310:LEU:HD13	1:A:316:LEU:HD11	1.81	0.61
1:E:113:ILE:HG22	1:E:123:VAL:HG11	1.82	0.61
1:H:54:LEU:HD11	1:H:346:THR:HG23	1.81	0.61
1:G:162:VAL:HG22	1:G:171:VAL:HG21	1.81	0.60
1:D:258:ILE:HA	1:D:261:MET:HE2	1.83	0.60
1:G:70:GLU:HA	1:G:73:LEU:HD12	1.83	0.60
1:E:232:LEU:C	1:E:232:LEU:HD23	2.22	0.60
1:C:82:TYR:CG	1:D:165:VAL:HG21	2.36	0.60
1:E:150:THR:HG23	1:F:150:THR:HG23	1.84	0.60
1:F:298:HIS:CD2	1:F:303:PHE:CD1	2.91	0.58
1:E:83:HIS:HA	1:E:110:ASN:ND2	2.19	0.58
1:E:98:LEU:HD21	1:E:101:ILE:HG12	1.87	0.57
1:A:124:CYS:SG	1:A:353:LEU:HD13	2.45	0.57
1:C:325:TYR:O	1:D:147:ARG:NH2	2.37	0.57
1:B:124:CYS:SG	1:B:353:LEU:HD13	2.45	0.57
1:A:209:TYR:HB3	1:A:232:LEU:HD13	1.86	0.57
1:H:44:CYS:SG	1:H:48:MET:CE	2.93	0.56
1:H:152:LEU:HD23	1:H:171:VAL:HG12	1.88	0.56
1:F:81:MET:HE2	1:F:85:ILE:HG23	1.84	0.56
1:D:112:ASP:OD2	1:D:115:ALA:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:GLU:O	1:B:74:ASN:ND2	2.39	0.56
1:E:152:LEU:CD2	1:E:171:VAL:HG13	2.37	0.55
1:B:258:ILE:HG23	1:B:261:MET:HE3	1.89	0.55
1:G:137:SER:OG	1:H:147:ARG:HD3	2.07	0.55
1:A:125:ASN:O	1:A:126:ILE:HD13	2.07	0.55
1:G:162:VAL:CG2	1:G:171:VAL:HG21	2.37	0.54
1:F:124:CYS:SG	1:F:353:LEU:HD13	2.46	0.54
1:H:348:ARG:HA	3:H:903:HOH:O	2.07	0.54
1:G:44:CYS:O	1:G:44:CYS:SG	2.65	0.54
1:C:241:LEU:HD22	1:C:275:LEU:HD13	1.89	0.54
1:H:123:VAL:HG23	1:H:358:ASN:ND2	2.22	0.54
1:C:60:CYS:SG	1:C:72:VAL:HG21	2.47	0.54
1:H:44:CYS:SG	1:H:48:MET:HE2	2.48	0.53
1:E:165:VAL:HG21	1:F:82:TYR:CG	2.43	0.53
1:E:44:CYS:HG	1:E:59:PHE:CB	2.18	0.53
1:D:213:LEU:HD13	1:D:217:ILE:CD1	2.27	0.53
1:H:54:LEU:HD11	1:H:346:THR:CG2	2.37	0.53
1:C:33:ARG:N	3:C:909:HOH:O	2.41	0.53
1:B:100:VAL:HG11	1:B:344:ALA:HB1	1.89	0.53
1:D:87:LEU:HD12	1:D:111:VAL:HG22	1.90	0.53
1:H:258:ILE:HG12	1:H:261:MET:HE3	1.90	0.53
1:C:143:LEU:HD11	1:C:202:PHE:CE2	2.45	0.52
1:E:152:LEU:HD22	1:E:171:VAL:CG1	2.40	0.52
1:E:112:ASP:OD2	1:E:115:ALA:HB2	2.10	0.52
1:D:269:ASN:HB3	1:D:295:LEU:HD22	1.91	0.52
1:G:184:GLY:HA3	1:G:236:SER:OG	2.10	0.52
1:H:134:THR:HG23	1:H:323:ALA:HB1	1.92	0.52
1:E:261:MET:CE	1:E:290:ILE:HD11	2.40	0.52
1:F:86:THR:O	1:F:87:LEU:HD23	2.10	0.51
1:B:100:VAL:HG11	1:B:344:ALA:CB	2.40	0.51
1:A:258:ILE:HD12	1:A:280:ALA:HB1	1.93	0.51
1:D:316:LEU:HD22	1:D:318:CYS:SG	2.51	0.51
1:B:221:LEU:HD23	1:B:221:LEU:N	2.25	0.51
1:D:311:LYS:O	3:D:909:HOH:O	2.19	0.51
1:G:167:GLN:O	1:G:171:VAL:HG23	2.11	0.50
1:F:221:LEU:HD21	1:G:221:LEU:HD21	1.93	0.50
1:E:136:ASP:OD2	1:F:178:ILE:HD12	2.11	0.50
1:H:165:VAL:HA	1:H:168:ILE:HD12	1.94	0.50
1:A:229:LEU:O	1:A:233:LEU:HG	2.12	0.50
1:F:217:ILE:HG22	1:F:221:LEU:CD1	2.42	0.50
1:F:143:LEU:HD11	1:F:202:PHE:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:CYS:SG	1:D:353:LEU:HD13	2.51	0.50
1:E:102:VAL:HG22	1:E:124:CYS:HB2	1.94	0.50
1:A:38:LEU:C	1:A:38:LEU:HD23	2.32	0.49
1:C:147:ARG:HD3	1:D:137:SER:OG	2.12	0.49
1:F:217:ILE:HG22	1:F:221:LEU:HD12	1.95	0.49
1:C:182:THR:HG21	1:C:207:ILE:HD13	1.94	0.49
1:G:48:MET:N	1:G:49:PRO:HD2	2.28	0.49
1:E:152:LEU:CD2	1:E:171:VAL:CG1	2.91	0.48
1:D:44:CYS:HG	1:D:48:MET:HG3	1.77	0.48
1:D:244:ASN:HA	2:D:901:NAD:O3D	2.13	0.48
1:B:98:LEU:HD23	1:B:121:ILE:HD13	1.94	0.48
1:A:152:LEU:CD2	1:A:171:VAL:CG1	2.91	0.48
1:A:210:ASP:O	1:A:225:ARG:NH2	2.46	0.48
1:F:348:ARG:HG3	1:F:351:GLU:HB2	1.96	0.48
1:E:125:ASN:ND2	1:E:357:VAL:HG11	2.28	0.48
1:E:44:CYS:HG	1:E:59:PHE:HD2	1.62	0.48
1:H:50:ILE:HD11	1:H:335:GLU:HG2	1.96	0.47
1:E:163:GLN:HE21	1:E:163:GLN:C	2.18	0.47
1:H:162:VAL:HG22	1:H:171:VAL:HG21	1.96	0.47
1:G:143:LEU:HD11	1:G:202:PHE:CE2	2.49	0.47
1:F:47:GLU:O	1:F:51:LEU:HD12	2.14	0.47
1:H:152:LEU:CD2	1:H:171:VAL:HG12	2.43	0.47
1:E:125:ASN:ND2	1:E:357:VAL:CG1	2.78	0.47
1:B:54:LEU:HD12	1:B:342:ARG:NH1	2.29	0.47
1:D:126:ILE:HD12	1:D:336:ALA:CB	2.44	0.47
1:C:162:VAL:HG12	1:C:168:ILE:HG13	1.97	0.47
1:E:320:PRO:HD2	1:E:322:THR:HG23	1.97	0.47
1:C:217:ILE:CG2	1:C:221:LEU:HD12	2.45	0.47
1:E:83:HIS:HA	1:E:110:ASN:HD21	1.80	0.46
1:D:152:LEU:CD2	1:D:171:VAL:HG12	2.44	0.46
1:B:244:ASN:HA	2:B:901:NAD:O3D	2.15	0.46
1:H:65:THR:HA	1:H:68:ILE:HD12	1.97	0.46
1:E:38:LEU:CD2	1:E:38:LEU:C	2.84	0.46
1:G:307:GLN:HA	3:G:917:HOH:O	2.16	0.46
1:E:54:LEU:HD11	1:E:342:ARG:NE	2.31	0.46
1:D:126:ILE:HD12	1:D:336:ALA:HB1	1.98	0.46
1:A:65:THR:HA	1:A:68:ILE:HD12	1.96	0.46
1:E:320:PRO:HD2	1:E:322:THR:CG2	2.45	0.46
1:A:325:TYR:O	1:B:147:ARG:NH2	2.34	0.46
1:B:258:ILE:HG23	1:B:261:MET:CE	2.45	0.46
1:D:43:ASP:OD2	1:D:45:THR:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:89:ARG:NH2	1:F:118:GLU:OE1	2.48	0.46
1:F:198:ARG:HG3	1:F:198:ARG:NH1	2.31	0.46
1:C:182:THR:CG2	1:C:207:ILE:HD13	2.45	0.46
1:G:60:CYS:SG	1:G:72:VAL:HG21	2.56	0.46
1:D:233:LEU:HD22	1:D:261:MET:CG	2.46	0.46
1:H:268:VAL:HG22	1:H:294:ALA:HB3	1.98	0.45
1:A:269:ASN:HB3	1:A:295:LEU:HD22	1.98	0.45
1:E:152:LEU:HD13	1:F:322:THR:HG21	1.98	0.45
1:D:38:LEU:HD12	1:D:44:CYS:HB2	1.98	0.45
1:B:261:MET:HE3	1:B:290:ILE:HD11	1.95	0.45
1:G:261:MET:CE	1:G:290:ILE:HD11	2.46	0.45
1:F:258:ILE:HG12	1:F:261:MET:HE3	1.99	0.45
1:A:147:ARG:HD3	1:B:137:SER:OG	2.17	0.45
1:G:48:MET:HE3	1:G:48:MET:HB2	1.73	0.44
1:B:211:PRO:HG2	1:B:212:TYR:CE1	2.52	0.44
1:D:95:PHE:CG	1:D:98:LEU:HD22	2.52	0.44
1:D:95:PHE:CD2	1:D:98:LEU:HD22	2.52	0.44
1:E:253:ILE:HB	1:E:276:VAL:HG22	2.00	0.44
1:D:310:LEU:HD13	1:D:316:LEU:HD11	1.99	0.44
1:E:261:MET:HE1	1:E:290:ILE:HD11	1.99	0.44
1:B:200:LYS:NZ	1:B:221:LEU:O	2.50	0.44
1:E:316:LEU:HD22	1:E:318:CYS:SG	2.57	0.44
1:E:213:LEU:HD22	1:E:217:ILE:HD12	1.99	0.44
1:E:233:LEU:HD22	1:E:261:MET:HG2	1.99	0.44
1:B:50:ILE:O	1:B:342:ARG:NH1	2.51	0.44
1:C:233:LEU:HD22	1:C:261:MET:HG2	1.99	0.44
1:F:81:MET:HE2	1:F:85:ILE:CG2	2.45	0.43
1:D:191:THR:O	1:D:195:VAL:HG23	2.17	0.43
1:A:128:SER:HB2	1:D:216:GLY:HA2	2.00	0.43
1:A:48:MET:HB3	1:A:49:PRO:HD3	2.00	0.43
1:G:269:ASN:HB3	1:G:295:LEU:HD22	1.99	0.43
1:C:98:LEU:HD21	1:C:101:ILE:CG1	2.48	0.43
1:E:100:VAL:HG11	1:E:344:ALA:HB1	2.00	0.43
1:G:168:ILE:HG23	1:H:322:THR:HG22	2.01	0.43
1:H:186:ILE:HD13	1:H:229:LEU:CD1	2.48	0.43
1:D:324:TRP:HB3	2:D:901:NAD:H4N	2.01	0.43
1:D:44:CYS:SG	1:D:48:MET:HG3	2.58	0.43
1:B:211:PRO:HG2	1:B:212:TYR:CD1	2.54	0.43
1:F:221:LEU:HD21	1:G:221:LEU:CD2	2.49	0.43
1:A:44:CYS:SG	1:A:44:CYS:O	2.77	0.43
1:C:98:LEU:HD21	1:C:101:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:VAL:HG13	1:C:99:ARG:HG3	2.01	0.43
1:E:216:GLY:HA2	1:H:128:SER:HB2	2.01	0.42
1:D:295:LEU:O	1:D:318:CYS:HA	2.19	0.42
1:C:207:ILE:HG22	1:C:224:GLN:HB2	2.01	0.42
1:E:261:MET:HE1	1:E:290:ILE:CD1	2.48	0.42
1:B:39:LEU:O	1:B:60:CYS:HB2	2.19	0.42
1:G:341:ILE:HA	1:G:341:ILE:HD13	1.92	0.42
1:D:89:ARG:NH1	1:D:115:ALA:HB2	2.34	0.42
1:A:295:LEU:O	1:A:318:CYS:HA	2.20	0.42
1:H:210:ASP:O	1:H:225:ARG:NH2	2.49	0.42
1:F:162:VAL:HG12	1:F:168:ILE:HG13	2.02	0.42
1:H:298:HIS:CD2	1:H:303:PHE:CD1	3.08	0.42
1:G:194:ALA:O	1:G:198:ARG:HD2	2.19	0.42
1:F:198:ARG:HH11	1:F:198:ARG:HG3	1.84	0.42
1:C:145:LEU:HD13	1:C:266:PHE:HB3	2.01	0.42
1:F:324:TRP:HB3	2:F:901:NAD:H4N	2.01	0.42
1:F:48:MET:O	1:F:52:LYS:N	2.53	0.42
1:F:140:CYS:O	1:F:144:ASN:ND2	2.52	0.42
1:D:50:ILE:O	1:D:50:ILE:HG22	2.20	0.41
1:C:44:CYS:SG	1:C:57:VAL:HG12	2.60	0.41
1:H:183:LEU:HD12	1:H:238:CYS:O	2.20	0.41
1:A:48:MET:HE3	1:A:48:MET:HB2	1.70	0.41
1:C:348:ARG:HB2	1:C:351:GLU:OE1	2.20	0.41
1:E:48:MET:N	1:E:49:PRO:HD2	2.35	0.41
1:H:210:ASP:CG	1:H:213:LEU:HG	2.40	0.41
1:F:82:TYR:CZ	1:F:104:ILE:HD13	2.55	0.41
1:G:244:ASN:HA	2:G:901:NAD:O3D	2.21	0.41
1:B:316:LEU:HD22	1:B:318:CYS:SG	2.60	0.41
1:D:233:LEU:HD22	1:D:261:MET:HG3	2.02	0.41
1:E:210:ASP:O	1:E:225:ARG:NH2	2.53	0.41
1:H:209:TYR:HB3	1:H:232:LEU:HD13	2.03	0.41
1:G:191:THR:O	1:G:195:VAL:HG23	2.21	0.41
1:H:166:GLU:N	1:H:166:GLU:OE1	2.54	0.41
1:E:241:LEU:HD12	1:E:269:ASN:HB2	2.03	0.41
1:A:54:LEU:HD11	1:A:346:THR:CG2	2.51	0.41
1:H:295:LEU:O	1:H:318:CYS:HA	2.21	0.40
1:A:152:LEU:CD2	1:A:171:VAL:HG13	2.51	0.40
1:C:81:MET:HE1	1:C:111:VAL:HG22	1.96	0.40
1:H:188:PHE:HB2	1:H:208:PHE:CD1	2.57	0.40
1:H:125:ASN:O	1:H:126:ILE:HD13	2.22	0.40
1:G:39:LEU:HD22	1:G:68:ILE:CD1	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:38:LEU:HD23	1:H:38:LEU:C	2.42	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	329/336 (98%)	315 (96%)	14 (4%)	0	100	100
1	B	328/336 (98%)	315 (96%)	13 (4%)	0	100	100
1	C	329/336 (98%)	316 (96%)	13 (4%)	0	100	100
1	D	328/336 (98%)	314 (96%)	14 (4%)	0	100	100
1	E	328/336 (98%)	314 (96%)	14 (4%)	0	100	100
1	F	330/336 (98%)	317 (96%)	13 (4%)	0	100	100
1	G	331/336 (98%)	315 (95%)	16 (5%)	0	100	100
1	H	329/336 (98%)	312 (95%)	17 (5%)	0	100	100
All	All	2632/2688 (98%)	2518 (96%)	114 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	261/276 (95%)	250 (96%)	11 (4%)	36	71
1	B	254/276 (92%)	241 (95%)	13 (5%)	29	63
1	C	267/276 (97%)	252 (94%)	15 (6%)	26	59
1	D	259/276 (94%)	240 (93%)	19 (7%)	17	44
1	E	247/276 (90%)	235 (95%)	12 (5%)	31	65
1	F	263/276 (95%)	247 (94%)	16 (6%)	23	55
1	G	252/276 (91%)	240 (95%)	12 (5%)	31	66
1	H	262/276 (95%)	247 (94%)	15 (6%)	25	58
All	All	2065/2208 (94%)	1952 (94%)	113 (6%)	27	59

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	CYS
1	A	64	SER
1	A	89	ARG
1	A	147	ARG
1	A	171	VAL
1	A	230	GLN
1	A	291	ARG
1	A	316	LEU
1	A	348	ARG
1	A	352	SER
1	A	362	PHE
1	B	38	LEU
1	B	44	CYS
1	B	63	GLN
1	B	66	GLN
1	B	100	VAL
1	B	163	GLN
1	B	179	ARG
1	B	221	LEU
1	B	232	LEU
1	B	255	ASP
1	B	316	LEU
1	B	327	GLU
1	B	362	PHE
1	C	33	ARG
1	C	38	LEU
1	C	63	GLN

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Mol	Chain	Res	Type
1	C	69[A]	HIS
1	C	69[B]	HIS
1	C	70	GLU
1	C	89	ARG
1	C	137	SER
1	C	148	ARG
1	C	213	LEU
1	C	241	LEU
1	C	258	ILE
1	C	291	ARG
1	C	359	LYS
1	C	362	PHE
1	D	33	ARG
1	D	38	LEU
1	D	44	CYS
1	D	61	ASP
1	D	65	THR
1	D	84	THR
1	D	161	ARG
1	D	163	GLN
1	D	205	SER
1	D	214	GLN
1	D	311	LYS
1	D	316	LEU
1	D	327	GLU
1	D	331	LEU
1	D	345	ILE
1	D	346	THR
1	D	359	LYS
1	D	360	GLU
1	D	362	PHE
1	E	38	LEU
1	E	53	ASP
1	E	85	ILE
1	E	100	VAL
1	E	161	ARG
1	E	163	GLN
1	E	171	VAL
1	E	300	SER
1	E	316	LEU
1	E	345	ILE
1	E	360	GLU

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Mol	Chain	Res	Type
1	E	362	PHE
1	F	33	ARG
1	F	38	LEU
1	F	48	MET
1	F	69[A]	HIS
1	F	69[B]	HIS
1	F	77	VAL
1	F	84	THR
1	F	137	SER
1	F	148	ARG
1	F	163	GLN
1	F	179	ARG
1	F	215	ASP
1	F	221	LEU
1	F	304	SER
1	F	339	THR
1	F	362	PHE
1	G	44	CYS
1	G	63	GLN
1	G	90	GLU
1	G	109	ASP
1	G	163	GLN
1	G	214	GLN
1	G	251	HIS
1	G	252	LEU
1	G	258	ILE
1	G	327	GLU
1	G	354	ARG
1	G	362	PHE
1	H	64	SER
1	H	137	SER
1	H	147	ARG
1	H	163	GLN
1	H	182	THR
1	H	205	SER
1	H	230	GLN
1	H	247	GLU
1	H	255	ASP
1	H	291	ARG
1	H	316	LEU
1	H	327	GLU
1	H	348	ARG

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Mol	Chain	Res	Type
1	H	359	LYS
1	H	362	PHE

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

Mol	Chain	Res	Type
1	B	63	GLN
1	B	74	ASN
1	B	149	ASN
1	B	224	GLN
1	C	63	GLN
1	C	230	GLN
1	D	230	GLN
1	D	283	GLN
1	E	163	GLN
1	E	248	HIS
1	F	74	ASN
1	G	251	HIS
1	G	283	GLN
1	G	355	ASN
1	H	149	ASN
1	H	246	ASN
1	H	283	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

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAD	A	901	-	38,48,48	1.51	3 (7%)	47,73,73	2.13	8 (17%)
2	NAD	B	901	-	38,48,48	1.64	3 (7%)	47,73,73	2.05	8 (17%)
2	NAD	C	901	-	38,48,48	1.79	4 (10%)	47,73,73	2.15	9 (19%)
2	NAD	D	901	-	38,48,48	1.71	3 (7%)	47,73,73	1.90	5 (10%)
2	NAD	E	901	-	38,48,48	1.76	3 (7%)	47,73,73	2.15	8 (17%)
2	NAD	F	901	-	38,48,48	1.66	4 (10%)	47,73,73	2.28	9 (19%)
2	NAD	G	901	-	38,48,48	1.73	3 (7%)	47,73,73	1.99	6 (12%)
2	NAD	H	901	-	38,48,48	1.57	4 (10%)	47,73,73	2.23	8 (17%)

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	901	-	-	0/22/62/62	0/5/5/5
2	NAD	B	901	-	-	0/22/62/62	0/5/5/5
2	NAD	C	901	-	-	0/22/62/62	0/5/5/5
2	NAD	D	901	-	-	0/22/62/62	0/5/5/5
2	NAD	E	901	-	-	0/22/62/62	0/5/5/5
2	NAD	F	901	-	-	0/22/62/62	0/5/5/5
2	NAD	G	901	-	-	0/22/62/62	0/5/5/5
2	NAD	H	901	-	-	0/22/62/62	0/5/5/5

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	901	NAD	O4D-C4D	-2.47	1.39	1.45
2	H	901	NAD	O4D-C4D	-2.18	1.40	1.45
2	F	901	NAD	O4D-C4D	-2.10	1.40	1.45
2	E	901	NAD	C2A-N1A	2.36	1.38	1.33
2	H	901	NAD	C2A-N1A	2.39	1.38	1.33
2	A	901	NAD	C2A-N1A	2.53	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	901	NAD	C2A-N1A	2.55	1.38	1.33
2	C	901	NAD	C2A-N1A	2.70	1.39	1.33
2	D	901	NAD	C2A-N1A	2.72	1.39	1.33
2	A	901	NAD	C2A-N3A	3.17	1.37	1.32
2	B	901	NAD	C2A-N1A	3.18	1.39	1.33
2	G	901	NAD	C2A-N1A	3.40	1.40	1.33
2	H	901	NAD	C2A-N3A	3.87	1.39	1.32
2	G	901	NAD	C2A-N3A	3.91	1.39	1.32
2	E	901	NAD	C2A-N3A	4.06	1.39	1.32
2	B	901	NAD	C2A-N3A	4.15	1.39	1.32
2	F	901	NAD	C2A-N3A	4.20	1.39	1.32
2	D	901	NAD	C2A-N3A	4.30	1.39	1.32
2	C	901	NAD	C2A-N3A	4.31	1.39	1.32
2	H	901	NAD	O7N-C7N	6.29	1.37	1.24
2	A	901	NAD	O7N-C7N	6.62	1.38	1.24
2	B	901	NAD	O7N-C7N	7.12	1.39	1.24
2	F	901	NAD	O7N-C7N	7.17	1.39	1.24
2	C	901	NAD	O7N-C7N	7.58	1.40	1.24
2	G	901	NAD	O7N-C7N	7.60	1.40	1.24
2	D	901	NAD	O7N-C7N	7.93	1.41	1.24
2	E	901	NAD	O7N-C7N	8.53	1.42	1.24

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	901	NAD	N3A-C2A-N1A	-11.12	120.38	128.89
2	D	901	NAD	N3A-C2A-N1A	-10.45	120.90	128.89
2	H	901	NAD	N3A-C2A-N1A	-10.34	120.98	128.89
2	E	901	NAD	N3A-C2A-N1A	-10.22	121.07	128.89
2	C	901	NAD	N3A-C2A-N1A	-10.20	121.09	128.89
2	B	901	NAD	N3A-C2A-N1A	-10.02	121.22	128.89
2	A	901	NAD	N3A-C2A-N1A	-9.63	121.52	128.89
2	G	901	NAD	N3A-C2A-N1A	-9.58	121.56	128.89
2	A	901	NAD	PN-O3-PA	-5.68	116.77	132.73
2	H	901	NAD	PN-O3-PA	-5.08	118.45	132.73
2	C	901	NAD	PN-O3-PA	-4.85	119.10	132.73
2	C	901	NAD	C4B-O4B-C1B	-3.98	105.34	109.72
2	G	901	NAD	PN-O3-PA	-3.84	121.94	132.73
2	F	901	NAD	O7N-C7N-C3N	-3.67	115.58	119.59
2	H	901	NAD	C1B-N9A-C4A	-3.64	121.44	126.94
2	D	901	NAD	C4A-C5A-N7A	-3.56	106.21	109.48
2	E	901	NAD	C4A-C5A-N7A	-3.55	106.21	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	901	NAD	PN-O3-PA	-3.34	123.36	132.73
2	F	901	NAD	PN-O3-PA	-3.34	123.36	132.73
2	F	901	NAD	C4B-O4B-C1B	-3.12	106.29	109.72
2	A	901	NAD	C4A-C5A-N7A	-2.96	106.76	109.48
2	F	901	NAD	O3-PN-O5D	-2.94	95.13	102.94
2	B	901	NAD	O7N-C7N-C3N	-2.87	116.46	119.59
2	B	901	NAD	PN-O3-PA	-2.86	124.70	132.73
2	G	901	NAD	C4D-O4D-C1D	-2.81	106.63	109.72
2	F	901	NAD	C4D-O4D-C1D	-2.74	106.71	109.72
2	E	901	NAD	C1B-N9A-C4A	-2.61	123.00	126.94
2	C	901	NAD	O5B-PA-O1A	-2.60	99.51	109.62
2	E	901	NAD	C4B-O4B-C1B	-2.35	107.14	109.72
2	H	901	NAD	C4A-C5A-N7A	-2.34	107.33	109.48
2	C	901	NAD	O3D-C3D-C2D	-2.31	104.31	111.83
2	C	901	NAD	O3-PN-O5D	-2.30	96.84	102.94
2	D	901	NAD	PN-O3-PA	-2.27	126.34	132.73
2	D	901	NAD	C1B-N9A-C4A	-2.15	123.70	126.94
2	B	901	NAD	O3D-C3D-C2D	-2.01	105.30	111.83
2	G	901	NAD	C2N-C3N-C4N	2.05	120.58	118.29
2	C	901	NAD	C2N-C3N-C4N	2.07	120.59	118.29
2	F	901	NAD	C2B-C1B-N9A	2.07	117.45	114.29
2	B	901	NAD	C2N-C3N-C4N	2.14	120.67	118.29
2	A	901	NAD	O2A-PA-O3	2.19	115.02	105.09
2	C	901	NAD	O4B-C4B-C3B	2.19	109.56	105.15
2	A	901	NAD	C2B-C1B-N9A	2.33	117.86	114.29
2	H	901	NAD	C2B-C1B-N9A	2.45	118.04	114.29
2	G	901	NAD	N6A-C6A-N1A	2.53	124.62	119.20
2	H	901	NAD	C2N-C3N-C4N	2.62	121.21	118.29
2	B	901	NAD	O4B-C1B-N9A	2.65	113.64	108.10
2	E	901	NAD	C3N-C7N-N7N	2.65	120.72	117.82
2	D	901	NAD	O2A-PA-O3	2.67	117.20	105.09
2	A	901	NAD	C3N-C7N-N7N	2.73	120.80	117.82
2	B	901	NAD	O2A-PA-O3	2.75	117.57	105.09
2	F	901	NAD	O4D-C1D-N1N	2.93	111.35	108.13
2	A	901	NAD	C2N-C3N-C4N	2.93	121.56	118.29
2	E	901	NAD	O2A-PA-O3	3.15	119.38	105.09
2	H	901	NAD	C3N-C7N-N7N	3.16	121.27	117.82
2	C	901	NAD	O4B-C1B-N9A	3.70	115.85	108.10
2	F	901	NAD	C3N-C7N-N7N	4.21	122.43	117.82
2	A	901	NAD	O4D-C1D-N1N	4.97	113.59	108.13
2	G	901	NAD	O4D-C1D-N1N	5.19	113.84	108.13
2	H	901	NAD	O4D-C1D-N1N	5.34	113.99	108.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	901	NAD	O4D-C1D-N1N	5.50	114.17	108.13
2	B	901	NAD	O4D-C1D-N1N	5.70	114.39	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	NAD	1	0
2	D	901	NAD	2	0
2	F	901	NAD	1	0
2	G	901	NAD	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	330/336 (98%)	0.06	1 (0%) 94 92	46, 49, 52, 57	0
1	B	330/336 (98%)	-0.02	9 (2%) 58 45	46, 49, 52, 57	0
1	C	330/336 (98%)	-0.03	1 (0%) 94 92	46, 49, 52, 56	0
1	D	330/336 (98%)	0.13	7 (2%) 67 56	46, 49, 51, 56	0
1	E	330/336 (98%)	0.40	25 (7%) 17 9	47, 49, 51, 54	0
1	F	330/336 (98%)	0.11	4 (1%) 81 73	46, 49, 52, 56	0
1	G	330/336 (98%)	0.23	19 (5%) 26 16	46, 49, 51, 56	0
1	H	330/336 (98%)	-0.05	0 100 100	47, 49, 51, 56	0
All	All	2640/2688 (98%)	0.10	66 (2%) 61 48	46, 49, 52, 57	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	79	ALA	6.3
1	E	78	GLY	4.9
1	G	33	ARG	4.7
1	E	36	VAL	4.5
1	G	99	ARG	4.5
1	G	97	ALA	4.4
1	G	100	VAL	4.1
1	E	77	VAL	4.0
1	G	98	LEU	4.0
1	E	79	ALA	4.0
1	E	35	LEU	3.9
1	G	361	PHE	3.7
1	E	56	THR	3.6
1	G	95	PHE	3.5
1	B	35	LEU	3.3
1	G	35	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	362	PHE	3.3
1	E	60	CYS	3.2
1	E	64	SER	3.0
1	G	72	VAL	3.0
1	E	302	PRO	2.8
1	G	65	THR	2.8
1	B	53	ASP	2.8
1	E	98	LEU	2.7
1	G	111	VAL	2.7
1	G	34	PRO	2.7
1	B	56	THR	2.7
1	E	361	PHE	2.6
1	E	96	LYS	2.6
1	D	78	GLY	2.6
1	G	338	ALA	2.6
1	B	58	ALA	2.5
1	A	63	GLN	2.5
1	G	60	CYS	2.5
1	F	234	TYR	2.4
1	E	76	ALA	2.4
1	D	37	ALA	2.4
1	E	300	SER	2.4
1	G	80	MET	2.4
1	D	362	PHE	2.4
1	B	36	VAL	2.4
1	G	56	THR	2.4
1	D	79	ALA	2.3
1	E	72	VAL	2.3
1	E	97	ALA	2.3
1	G	119	LEU	2.3
1	B	34	PRO	2.3
1	E	39	LEU	2.2
1	E	38	LEU	2.2
1	B	37	ALA	2.2
1	D	68	ILE	2.2
1	E	93	GLU	2.1
1	G	64	SER	2.1
1	F	265	ALA	2.1
1	B	100	VAL	2.1
1	E	84	THR	2.1
1	E	95	PHE	2.1
1	C	263	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	92	LEU	2.1
1	B	79	ALA	2.1
1	F	132[A]	GLU	2.1
1	E	69	HIS	2.1
1	D	40	ASP	2.0
1	E	57	VAL	2.0
1	F	289	ARG	2.0
1	D	36	VAL	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	G	901	44/44	0.96	0.14	-1.16	35,41,46,50	0
2	NAD	E	901	44/44	0.96	0.15	-1.28	37,41,56,59	0
2	NAD	F	901	44/44	0.97	0.12	-1.78	27,34,38,41	0
2	NAD	D	901	44/44	0.96	0.12	-1.93	35,40,48,49	0
2	NAD	B	901	44/44	0.97	0.12	-2.21	24,35,42,46	0
2	NAD	H	901	44/44	0.98	0.11	-2.80	30,35,38,40	0
2	NAD	C	901	44/44	0.98	0.11	-2.99	20,27,31,33	0
2	NAD	A	901	44/44	0.97	0.10	-3.53	25,33,34,40	0

6.5 Other polymers (i)

There are no such residues in this entry.