Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:40 PM GMT

PDB ID	:	3RHD
Title	:	Crystal structure of glyceraldehyde-3-phosphate dehydrogenase GapN from Methanocaldococcus jannaschii DSM 2661 complexed with NADP
Authors	:	Malashkevich, V.N.; Toro, R.; Seidel, R.; Garrett, S.; Foti, R.; Almo, S.C.; New York Structural Genomics Research Consortium (NYSGRC)
Deposited on	:	2011-04-11
Resolution	:	2.20 Å(reported)

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

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

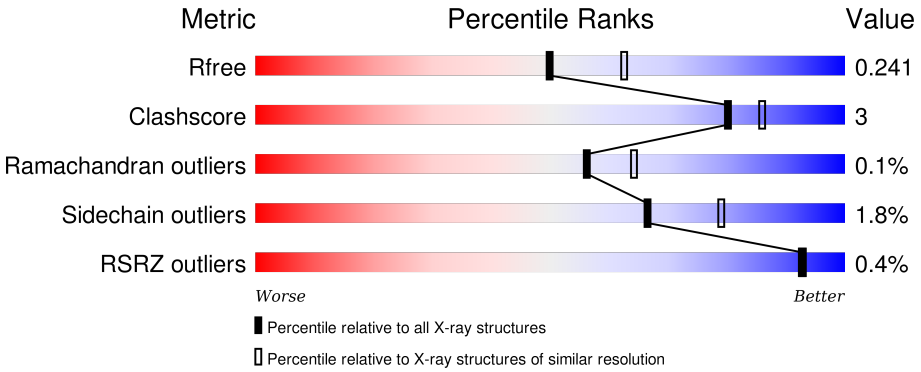
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	486	% 83% 10% 6%
1	B	486	86% 8% 6%
1	C	486	84% 10% 6%
1	D	486	% 84% 10% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15019 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 Lactaldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	8	0
			3579	2299	596	668	16			
1	B	456	Total	C	N	O	S	0	8	0
			3580	2300	596	668	16			
1	C	456	Total	C	N	O	S	0	6	0
			3566	2290	594	667	15			
1	D	456	Total	C	N	O	S	0	5	0
			3560	2286	592	667	15			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	VAL	-	EXPRESSION TAG	UNP Q58806
A	465	ALA	-	EXPRESSION TAG	UNP Q58806
A	466	GLU	-	EXPRESSION TAG	UNP Q58806
A	467	ASN	-	EXPRESSION TAG	UNP Q58806
A	468	LEU	-	EXPRESSION TAG	UNP Q58806
A	469	TYR	-	EXPRESSION TAG	UNP Q58806
A	470	PHE	-	EXPRESSION TAG	UNP Q58806
A	471	GLN	-	EXPRESSION TAG	UNP Q58806
A	472	SER	-	EXPRESSION TAG	UNP Q58806
A	473	HIS	-	EXPRESSION TAG	UNP Q58806
A	474	HIS	-	EXPRESSION TAG	UNP Q58806
A	475	HIS	-	EXPRESSION TAG	UNP Q58806
A	476	HIS	-	EXPRESSION TAG	UNP Q58806
A	477	HIS	-	EXPRESSION TAG	UNP Q58806
A	478	HIS	-	EXPRESSION TAG	UNP Q58806
A	479	TRP	-	EXPRESSION TAG	UNP Q58806
A	480	SER	-	EXPRESSION TAG	UNP Q58806
A	481	HIS	-	EXPRESSION TAG	UNP Q58806
A	482	PRO	-	EXPRESSION TAG	UNP Q58806
A	483	GLN	-	EXPRESSION TAG	UNP Q58806
A	484	PHE	-	EXPRESSION TAG	UNP Q58806

Continued on next page...

Continued from previous page...

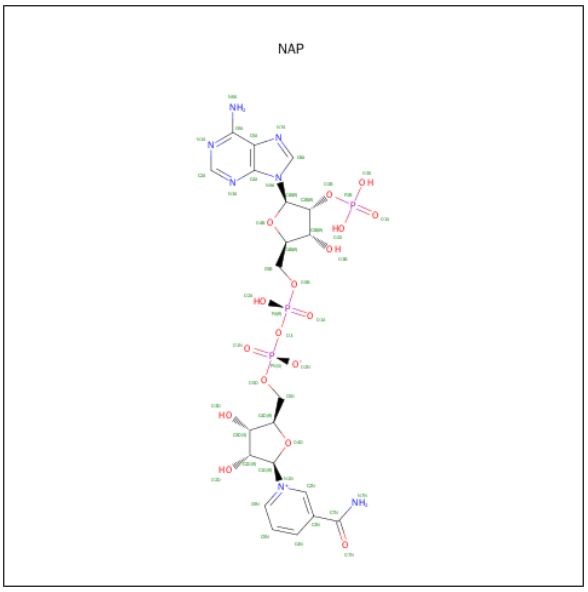
Chain	Residue	Modelled	Actual	Comment	Reference
A	485	GLU	-	EXPRESSION TAG	UNP Q58806
A	486	LYS	-	EXPRESSION TAG	UNP Q58806
B	1	VAL	-	EXPRESSION TAG	UNP Q58806
B	465	ALA	-	EXPRESSION TAG	UNP Q58806
B	466	GLU	-	EXPRESSION TAG	UNP Q58806
B	467	ASN	-	EXPRESSION TAG	UNP Q58806
B	468	LEU	-	EXPRESSION TAG	UNP Q58806
B	469	TYR	-	EXPRESSION TAG	UNP Q58806
B	470	PHE	-	EXPRESSION TAG	UNP Q58806
B	471	GLN	-	EXPRESSION TAG	UNP Q58806
B	472	SER	-	EXPRESSION TAG	UNP Q58806
B	473	HIS	-	EXPRESSION TAG	UNP Q58806
B	474	HIS	-	EXPRESSION TAG	UNP Q58806
B	475	HIS	-	EXPRESSION TAG	UNP Q58806
B	476	HIS	-	EXPRESSION TAG	UNP Q58806
B	477	HIS	-	EXPRESSION TAG	UNP Q58806
B	478	HIS	-	EXPRESSION TAG	UNP Q58806
B	479	TRP	-	EXPRESSION TAG	UNP Q58806
B	480	SER	-	EXPRESSION TAG	UNP Q58806
B	481	HIS	-	EXPRESSION TAG	UNP Q58806
B	482	PRO	-	EXPRESSION TAG	UNP Q58806
B	483	GLN	-	EXPRESSION TAG	UNP Q58806
B	484	PHE	-	EXPRESSION TAG	UNP Q58806
B	485	GLU	-	EXPRESSION TAG	UNP Q58806
B	486	LYS	-	EXPRESSION TAG	UNP Q58806
C	1	VAL	-	EXPRESSION TAG	UNP Q58806
C	465	ALA	-	EXPRESSION TAG	UNP Q58806
C	466	GLU	-	EXPRESSION TAG	UNP Q58806
C	467	ASN	-	EXPRESSION TAG	UNP Q58806
C	468	LEU	-	EXPRESSION TAG	UNP Q58806
C	469	TYR	-	EXPRESSION TAG	UNP Q58806
C	470	PHE	-	EXPRESSION TAG	UNP Q58806
C	471	GLN	-	EXPRESSION TAG	UNP Q58806
C	472	SER	-	EXPRESSION TAG	UNP Q58806
C	473	HIS	-	EXPRESSION TAG	UNP Q58806
C	474	HIS	-	EXPRESSION TAG	UNP Q58806
C	475	HIS	-	EXPRESSION TAG	UNP Q58806
C	476	HIS	-	EXPRESSION TAG	UNP Q58806
C	477	HIS	-	EXPRESSION TAG	UNP Q58806
C	478	HIS	-	EXPRESSION TAG	UNP Q58806
C	479	TRP	-	EXPRESSION TAG	UNP Q58806
C	480	SER	-	EXPRESSION TAG	UNP Q58806

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	481	HIS	-	EXPRESSION TAG	UNP Q58806
C	482	PRO	-	EXPRESSION TAG	UNP Q58806
C	483	GLN	-	EXPRESSION TAG	UNP Q58806
C	484	PHE	-	EXPRESSION TAG	UNP Q58806
C	485	GLU	-	EXPRESSION TAG	UNP Q58806
C	486	LYS	-	EXPRESSION TAG	UNP Q58806
D	1	VAL	-	EXPRESSION TAG	UNP Q58806
D	465	ALA	-	EXPRESSION TAG	UNP Q58806
D	466	GLU	-	EXPRESSION TAG	UNP Q58806
D	467	ASN	-	EXPRESSION TAG	UNP Q58806
D	468	LEU	-	EXPRESSION TAG	UNP Q58806
D	469	TYR	-	EXPRESSION TAG	UNP Q58806
D	470	PHE	-	EXPRESSION TAG	UNP Q58806
D	471	GLN	-	EXPRESSION TAG	UNP Q58806
D	472	SER	-	EXPRESSION TAG	UNP Q58806
D	473	HIS	-	EXPRESSION TAG	UNP Q58806
D	474	HIS	-	EXPRESSION TAG	UNP Q58806
D	475	HIS	-	EXPRESSION TAG	UNP Q58806
D	476	HIS	-	EXPRESSION TAG	UNP Q58806
D	477	HIS	-	EXPRESSION TAG	UNP Q58806
D	478	HIS	-	EXPRESSION TAG	UNP Q58806
D	479	TRP	-	EXPRESSION TAG	UNP Q58806
D	480	SER	-	EXPRESSION TAG	UNP Q58806
D	481	HIS	-	EXPRESSION TAG	UNP Q58806
D	482	PRO	-	EXPRESSION TAG	UNP Q58806
D	483	GLN	-	EXPRESSION TAG	UNP Q58806
D	484	PHE	-	EXPRESSION TAG	UNP Q58806
D	485	GLU	-	EXPRESSION TAG	UNP Q58806
D	486	LYS	-	EXPRESSION TAG	UNP Q58806

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is water.

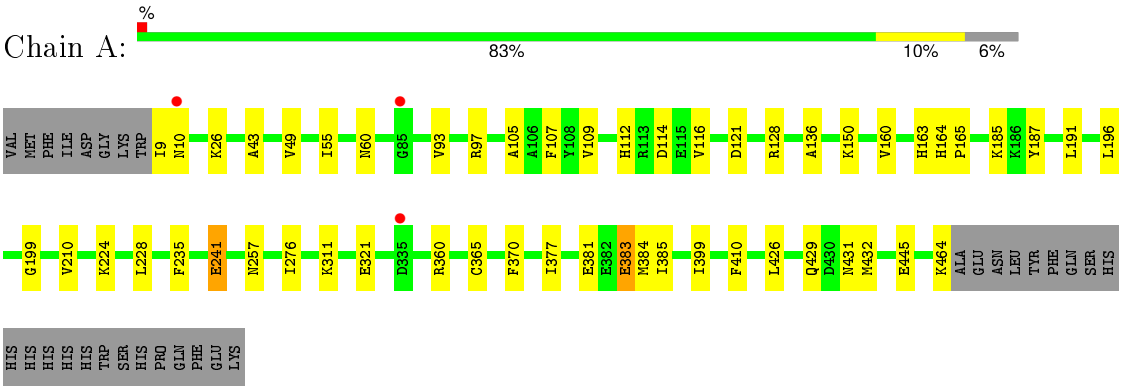
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	170	Total	O	0	0
			170	170		
3	B	181	Total	O	0	0
			181	181		
3	C	152	Total	O	0	0
			152	152		
3	D	107	Total	O	0	0
			107	107		

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.

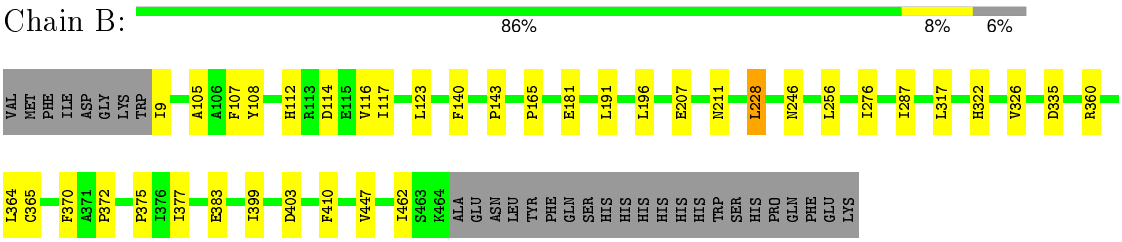
- Molecule 1: Lactaldehyde dehydrogenase

Chain A:



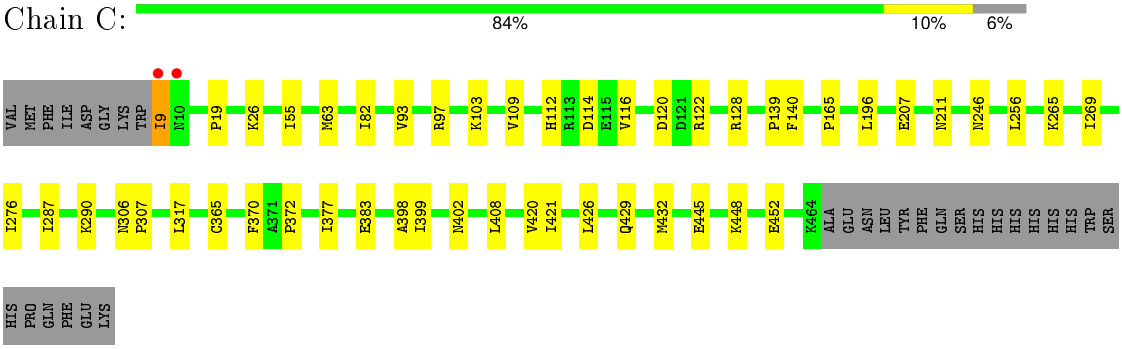
- Molecule 1: Lactaldehyde dehydrogenase

Chain B:



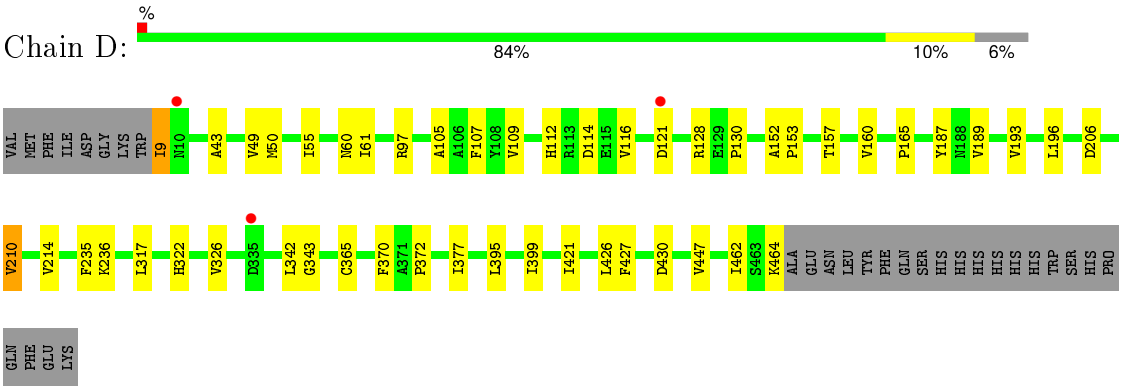
- Molecule 1: Lactaldehyde dehydrogenase

Chain C:



- Molecule 1: Lactaldehyde dehydrogenase

Chain D:


%
84%
10%
6%
VAL MET PHE ILE ASP GLY LYS TRP I9 N10 A43 V49 M50 I55 N60 I61 R97 A105 A106 F107 Y108 V109 H112 R113 D114 E115 V116 D121 R128 E129 P130 A152 P153 T157 V160 P165 Y187 N188 V189 V193 L196 D206
V210 V214 F235 K236 L317 H322 V326 D335 L342 G343 C365 F370 A371 P372 I377 L395 I399 I421 L426 F427 D430 V447 I462 S463 K464 ALA GLU ASN LEU TYR PHE GLN SER HIS HIS HIS HIS HIS TRP SER HIS PRO
GLN PHE GLU LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	164.24Å 77.38Å 167.39Å 90.00° 118.29° 90.00°	Depositor
Resolution (Å)	19.96 – 2.20 19.96 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.96-2.20) 99.6 (19.96-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.179 , 0.238 0.182 , 0.241	Depositor DCC
R_{free} test set	4688 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	37.2	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 33.5	EDS
Estimated twinning fraction	0.004 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 93586 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15019	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.06% 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: NAP

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	0.51	0/3658	0.60	0/4933
1	B	0.53	0/3659	0.61	1/4934 (0.0%)
1	C	0.48	0/3639	0.59	0/4909
1	D	0.47	0/3629	0.58	0/4895
All	All	0.50	0/14585	0.59	1/19671 (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	B	228	LEU	CA-CB-CG	5.36	127.63	115.30

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	3579	0	3744	26	0
1	B	3580	0	3746	23	0
1	C	3566	0	3724	31	0
1	D	3560	0	3719	34	0
2	A	31	0	11	0	0
2	B	31	0	11	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	31	0	11	0	0
2	D	31	0	11	0	0
3	A	170	0	0	3	0
3	B	181	0	0	0	0
3	C	152	0	0	4	0
3	D	107	0	0	4	0
All	All	15019	0	14977	101	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 3.

All (101) 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:C:365:CYS:SG	1:C:377:ILE:HD11	2.30	0.72
1:D:97:ARG:HD2	1:D:430:ASP:OD2	1.91	0.70
1:A:114[A]:ASP:HB2	1:D:116:VAL:HB	1.74	0.70
1:B:116:VAL:HB	1:C:114[A]:ASP:HB2	1.73	0.69
1:B:107[A]:PHE:CD1	1:D:107[A]:PHE:HB3	2.29	0.67
1:B:360[B]:ARG:HH12	1:B:383:GLU:HG2	1.59	0.67
1:A:365:CYS:SG	1:A:377:ILE:HD11	2.36	0.66
1:C:165:PRO:HG3	1:C:196:LEU:HD11	1.78	0.65
1:A:116:VAL:HB	1:D:114:ASP:HB2	1.80	0.64
1:B:365:CYS:SG	1:B:377:ILE:HD11	2.41	0.60
1:B:107[A]:PHE:CE1	1:D:107[A]:PHE:HB3	2.37	0.60
1:C:448:LYS:O	1:C:452:GLU:HG3	2.02	0.59
1:D:121:ASP:HB2	3:D:527:HOH:O	2.04	0.58
1:B:107[A]:PHE:CD1	1:D:107[A]:PHE:CB	2.88	0.57
1:D:317:LEU:HD21	1:D:372:PRO:HD3	1.87	0.56
1:D:426:LEU:O	1:D:426:LEU:HG	2.06	0.55
1:A:241:GLU:HG2	3:A:731:HOH:O	2.08	0.54
1:C:120:ASP:HA	3:C:536:HOH:O	2.08	0.53
1:C:139:PRO:HA	3:C:753:HOH:O	2.08	0.53
1:D:130:PRO:HB3	1:D:157:THR:O	2.08	0.53
1:B:107[B]:PHE:HB3	1:D:107[B]:PHE:CE1	2.44	0.52
1:A:360[B]:ARG:HH12	1:A:383:GLU:HG2	1.75	0.52
1:B:181:GLU:HG3	1:B:191:LEU:HD22	1.92	0.52
1:D:55:ILE:HG23	1:D:109:VAL:HG12	1.91	0.52
1:A:112[A]:HIS:CE1	1:A:128:ARG:HD2	2.45	0.51
1:C:246:ASN:ND2	1:C:276:ILE:HA	2.26	0.50
1:C:93:VAL:O	1:C:97:ARG:HG3	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:HIS:CE1	1:D:128:ARG:HG3	2.45	0.50
1:D:43:ALA:HB1	1:D:160:VAL:HG11	1.93	0.50
1:C:19:PRO:HD2	1:C:82:ILE:O	2.12	0.49
1:D:464:LYS:C	3:D:487:HOH:O	2.51	0.49
1:C:55:ILE:HG23	1:C:109:VAL:HG12	1.93	0.49
1:B:399:ILE:HD12	1:B:410:PHE:CG	2.48	0.49
1:D:105:ALA:HA	1:D:447:VAL:HG11	1.95	0.49
1:D:365:CYS:SG	1:D:377:ILE:HD11	2.53	0.48
1:D:322:HIS:O	1:D:326:VAL:HG23	2.14	0.48
1:A:55:ILE:HG23	1:A:109:VAL:HG12	1.95	0.48
1:C:122:ARG:HD3	1:D:427:PHE:CZ	2.49	0.48
1:B:403:ASP:CG	1:C:402[B]:ASN:HD21	2.18	0.47
1:C:421:ILE:HD12	1:D:462:ILE:HD13	1.97	0.47
1:C:398:ALA:HA	1:C:420:VAL:O	2.14	0.47
1:A:321:GLU:CD	1:A:321:GLU:H	2.18	0.47
1:A:429:GLN:O	1:A:432:MET:HG2	2.15	0.47
1:C:426:LEU:O	1:C:426:LEU:HG	2.14	0.47
1:A:112[A]:HIS:CE1	3:A:543:HOH:O	2.68	0.47
1:A:60:ASN:HB3	1:A:187:TYR:CZ	2.50	0.46
1:C:140:PHE:N	3:C:753:HOH:O	2.45	0.46
1:B:123:LEU:HD23	1:B:462:ILE:HD12	1.98	0.46
1:C:207:GLU:O	1:C:211:ASN:HB2	2.16	0.46
1:A:276:ILE:HG13	1:A:426:LEU:HD12	1.98	0.46
1:C:445:GLU:OE1	3:C:519:HOH:O	2.20	0.46
1:D:105:ALA:O	1:D:109:VAL:HG23	2.16	0.46
1:A:429:GLN:HG2	1:A:431:ASN:OD1	2.16	0.46
1:D:342:LEU:HG	1:D:343:GLY:N	2.32	0.45
1:B:165:PRO:HG3	1:B:196:LEU:HD11	1.99	0.45
1:D:49:VAL:HG23	3:D:503:HOH:O	2.17	0.44
1:D:60:ASN:HB3	1:D:187:TYR:CZ	2.52	0.44
1:C:112[A]:HIS:CE1	1:C:128:ARG:HD2	2.51	0.44
1:D:399:ILE:HG23	1:D:421:ILE:HG12	1.99	0.44
1:D:50:MET:HG2	1:D:193:VAL:HB	1.98	0.44
1:A:105:ALA:O	1:A:109:VAL:HG23	2.17	0.44
1:C:63:MET:HE2	1:C:103:LYS:HG2	2.00	0.44
1:B:317:LEU:HD21	1:B:372:PRO:HD3	2.00	0.44
1:C:429:GLN:O	1:C:432:MET:HG2	2.18	0.44
1:B:140:PHE:O	1:B:143:PRO:HD3	2.17	0.44
1:B:108:TYR:O	1:B:112[B]:HIS:HB3	2.18	0.44
1:A:49:VAL:HG23	3:A:494:HOH:O	2.18	0.43
1:B:256:LEU:HD21	1:B:287:ILE:HD12	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:PRO:HG3	1:D:196:LEU:HD11	2.00	0.43
1:C:9:ILE:HD13	1:C:9:ILE:N	2.33	0.43
1:D:43:ALA:HB1	1:D:160:VAL:CG1	2.49	0.43
1:A:464:LYS:HG2	1:C:408:LEU:HD13	2.01	0.43
1:B:246:ASN:ND2	1:B:276:ILE:HA	2.34	0.43
1:D:61:ILE:HD11	1:D:189:VAL:HG21	2.01	0.43
1:C:128:ARG:HH12	1:C:452:GLU:CG	2.31	0.42
1:B:364:LEU:HB3	1:B:375:PRO:HG3	2.00	0.42
1:B:207:GLU:O	1:B:211:ASN:HB2	2.19	0.42
1:B:107[B]:PHE:HB3	1:D:107[B]:PHE:CD1	2.54	0.42
1:C:317:LEU:HD21	1:C:372:PRO:HD3	2.00	0.42
1:C:399:ILE:HG23	1:C:421:ILE:HG12	2.02	0.42
1:D:152:ALA:N	1:D:153:PRO:HD2	2.35	0.42
1:C:63:MET:CE	1:C:103:LYS:HG2	2.49	0.42
1:A:385:ILE:HG13	1:A:410:PHE:CE2	2.55	0.42
1:A:185:LYS:HG3	1:A:191:LEU:HD21	2.00	0.42
1:A:93:VAL:O	1:A:97:ARG:HG3	2.19	0.42
1:A:165:PRO:HG3	1:A:196:LEU:HD11	2.02	0.41
1:D:206:ASP:O	1:D:210:VAL:HB	2.20	0.41
1:C:265:LYS:O	1:C:269:ILE:HG12	2.21	0.41
1:A:399:ILE:HD13	1:A:410:PHE:CG	2.56	0.41
1:C:306:ASN:HA	1:C:307:PRO:HD3	1.92	0.41
1:B:322:HIS:O	1:B:326:VAL:HG23	2.21	0.41
1:D:214:VAL:O	1:D:236:LYS:HE3	2.21	0.41
1:B:105:ALA:HA	1:B:447:VAL:HG11	2.02	0.41
1:D:9:ILE:N	3:D:545:HOH:O	2.54	0.41
1:A:43:ALA:HB1	1:A:160:VAL:CG1	2.51	0.41
1:A:381:GLU:HA	1:A:384:MET:SD	2.61	0.40
1:B:114[A]:ASP:HB2	1:C:116:VAL:HB	2.02	0.40
1:A:136:ALA:O	1:A:163:HIS:HA	2.22	0.40
1:A:164:HIS:HE1	1:A:199:GLY:O	2.03	0.40
1:A:150:LYS:NZ	1:A:445:GLU:OE2	2.51	0.40
1:C:256:LEU:HD21	1:C:287:ILE:HD12	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	462/486 (95%)	447 (97%)	15 (3%)	0	100	100
1	B	462/486 (95%)	449 (97%)	13 (3%)	0	100	100
1	C	460/486 (95%)	448 (97%)	12 (3%)	0	100	100
1	D	459/486 (94%)	442 (96%)	16 (4%)	1 (0%)	52	59
All	All	1843/1944 (95%)	1786 (97%)	56 (3%)	1 (0%)	56	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	395	LEU

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	397/417 (95%)	382 (96%)	15 (4%)	40	49
1	B	397/417 (95%)	392 (99%)	5 (1%)	76	87
1	C	395/417 (95%)	390 (99%)	5 (1%)	76	87
1	D	394/417 (94%)	390 (99%)	4 (1%)	82	91
All	All	1583/1668 (95%)	1554 (98%)	29 (2%)	66	79

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	10	ASN
1	A	26	LYS
1	A	107[A]	PHE
1	A	107[B]	PHE
1	A	121	ASP
1	A	210	VAL
1	A	224	LYS
1	A	228	LEU
1	A	235	PHE
1	A	241	GLU
1	A	257	ASN
1	A	311	LYS
1	A	370	PHE
1	A	383	GLU
1	B	9	ILE
1	B	117	ILE
1	B	228	LEU
1	B	335	ASP
1	B	370	PHE
1	C	9	ILE
1	C	26	LYS
1	C	290	LYS
1	C	370	PHE
1	C	383	GLU
1	D	9	ILE
1	D	210	VAL
1	D	235	PHE
1	D	370	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	112	HIS

5.3.3 RNA

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	NAP	A	500	-	27,33,52	1.35	3 (11%)	34,52,80	2.52	4 (11%)
2	NAP	B	500	-	27,33,52	1.33	3 (11%)	34,52,80	2.34	5 (14%)
2	NAP	C	500	-	27,33,52	1.34	3 (11%)	34,52,80	2.19	2 (5%)
2	NAP	D	500	-	27,33,52	1.36	3 (11%)	34,52,80	2.23	3 (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	NAP	A	500	-	-	0/17/37/67	0/3/3/5
2	NAP	B	500	-	-	0/17/37/67	0/3/3/5
2	NAP	C	500	-	-	0/17/37/67	0/3/3/5
2	NAP	D	500	-	-	0/17/37/67	0/3/3/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	NAP	C2A-N1A	2.26	1.38	1.33
2	C	500	NAP	C2A-N1A	2.31	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	NAP	C2A-N1A	2.64	1.38	1.33
2	A	500	NAP	C2A-N1A	2.94	1.39	1.33
2	A	500	NAP	C2A-N3A	3.28	1.38	1.32
2	C	500	NAP	C2A-N3A	3.32	1.38	1.32
2	D	500	NAP	C2A-N3A	3.56	1.38	1.32
2	A	500	NAP	PN-O1N	3.64	1.61	1.50
2	B	500	NAP	C2A-N3A	3.71	1.38	1.32
2	B	500	NAP	PN-O1N	3.82	1.62	1.50
2	C	500	NAP	PN-O1N	3.99	1.62	1.50
2	D	500	NAP	PN-O1N	4.03	1.62	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	NAP	N3A-C2A-N1A	-13.32	118.69	128.89
2	B	500	NAP	N3A-C2A-N1A	-11.95	119.75	128.89
2	C	500	NAP	N3A-C2A-N1A	-11.63	119.99	128.89
2	D	500	NAP	N3A-C2A-N1A	-11.55	120.05	128.89
2	D	500	NAP	C4A-C5A-N7A	-2.67	107.02	109.48
2	A	500	NAP	C1B-N9A-C4A	-2.53	123.12	126.94
2	B	500	NAP	O5D-PN-O1N	-2.41	101.99	110.85
2	B	500	NAP	C4A-C5A-N7A	-2.36	107.31	109.48
2	A	500	NAP	O3-PN-O1N	-2.35	100.36	107.70
2	B	500	NAP	C1B-N9A-C4A	-2.01	123.91	126.94
2	D	500	NAP	O5D-PN-O2N	2.72	121.60	110.61
2	A	500	NAP	O5D-PN-O2N	2.89	122.30	110.61
2	C	500	NAP	O5D-PN-O2N	3.12	123.22	110.61
2	B	500	NAP	O5D-PN-O2N	3.67	125.44	110.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	456/486 (93%)	-0.42	3 (0%) 89 88	24, 38, 55, 69	0
1	B	456/486 (93%)	-0.50	0 100 100	20, 34, 50, 71	0
1	C	456/486 (93%)	-0.38	2 (0%) 93 93	23, 41, 59, 86	0
1	D	456/486 (93%)	-0.29	3 (0%) 89 88	26, 44, 67, 80	0
All	All	1824/1944 (93%)	-0.40	8 (0%) 93 93	20, 39, 60, 86	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	9	ILE	3.3
1	A	10	ASN	2.6
1	C	10	ASN	2.6
1	A	85	GLY	2.5
1	D	10	ASN	2.5
1	A	335	ASP	2.4
1	D	121	ASP	2.2
1	D	335	ASP	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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	NAP	C	500	31/48	0.92	0.11	0.12	43,46,52,57	0
2	NAP	D	500	31/48	0.94	0.09	-0.34	42,44,49,56	0
2	NAP	A	500	31/48	0.96	0.08	-0.43	32,35,43,47	0
2	NAP	B	500	31/48	0.94	0.10	-0.52	35,36,43,47	0

6.5 Other polymers (i)

There are no such residues in this entry.