



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:05 am GMT

PDB ID : 4FW8  
Title : Crystal structure of FABG4 complexed with Coenzyme NADH  
Authors : Dutta, D.; Bhattacharyya, S.; Das, A.K.  
Deposited on : 2012-06-30  
Resolution : 2.79 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

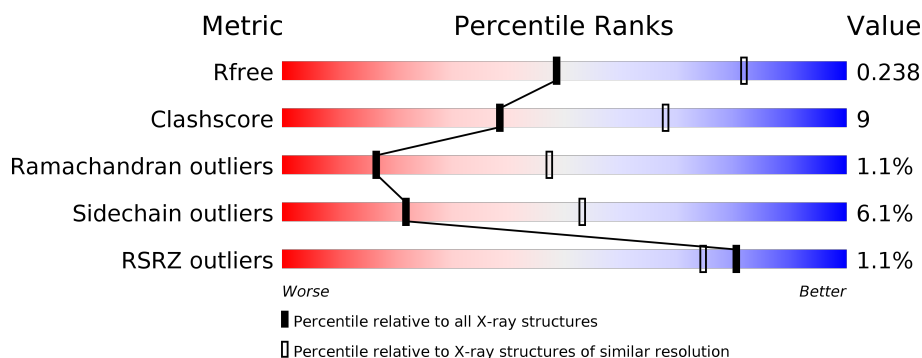
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.79 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))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (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  $\geq 3$ , 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  $\leq 5\%$ . 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	454	 73% 19% • 6%
1	B	454	 76% 16% • 6%
1	C	454	 75% 16% • 8%
1	D	454	 65% 24% • 10%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZPG	A	502	-	-	-	X

## 2 Entry composition [i](#)

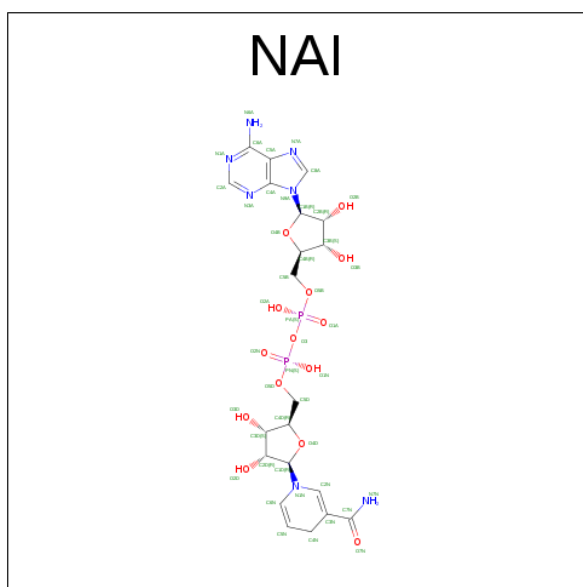
There are 4 unique types of molecules in this entry. The entry contains 12462 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-oxoacyl-(Acyl-carrier-protein) reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3080	1925	553	595	7			
1	B	425	Total	C	N	O	S	0	0	0
			3059	1916	543	593	7			
1	C	418	Total	C	N	O	S	0	0	0
			2991	1871	530	584	6			
1	D	409	Total	C	N	O	S	0	0	0
			2927	1836	514	571	6			

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C<sub>21</sub>H<sub>29</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



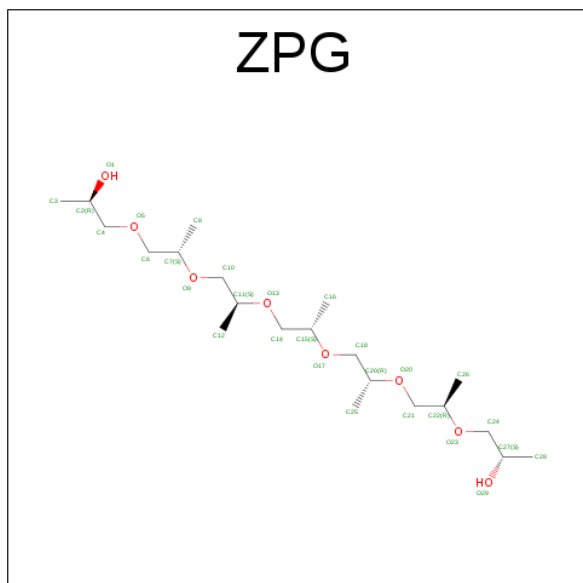
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0
			44	21	7	14	2	
2	D	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 3 is (2S,5R,8R,11S,14S,17S,21R)-5,8,11,14,17-PENTAMETHYL-4,7,10,13,16,19-H EXAOXADOCOSANE-2,21-DIOL (three-letter code: ZPG) (formula: C<sub>21</sub>H<sub>44</sub>O<sub>8</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	9	4		

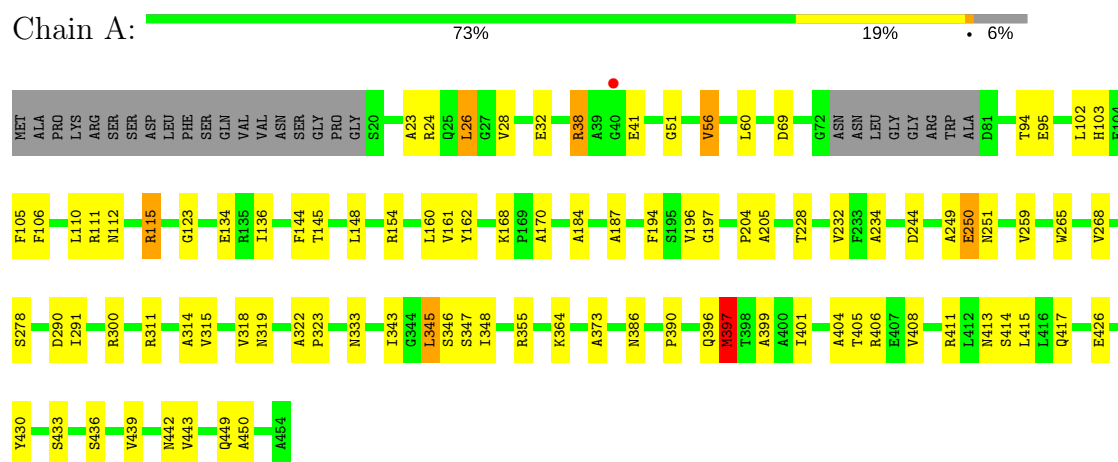
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	79	Total	O	0	0
			79	79		
4	B	68	Total	O	0	0
			68	68		
4	C	38	Total	O	0	0
			38	38		
4	D	31	Total	O	0	0
			31	31		

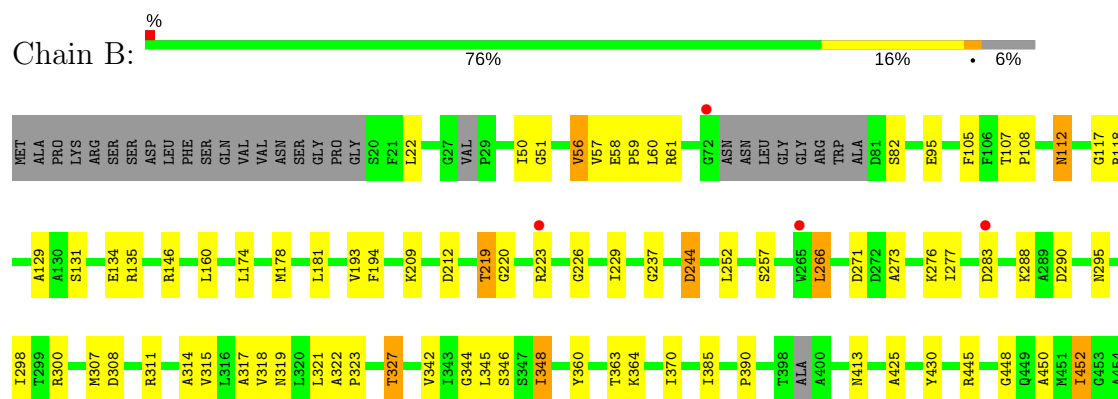
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

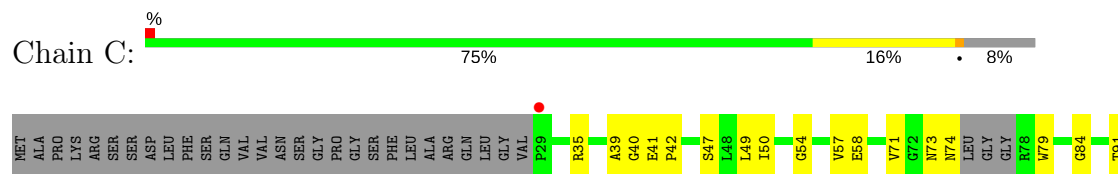
#### • Molecule 1: 3-oxoacyl-(Acyl-carrier-protein) reductase

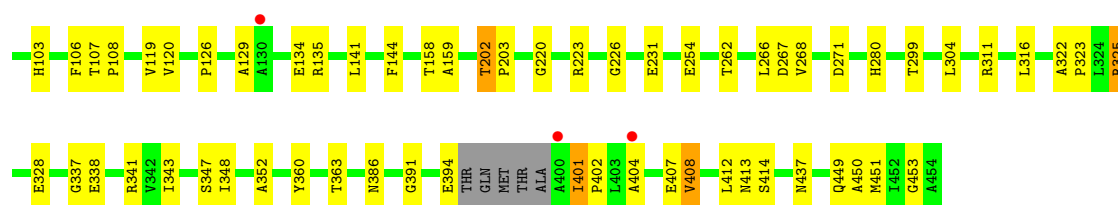


#### • Molecule 1: 3-oxoacyl-(Acyl-carrier-protein) reductase

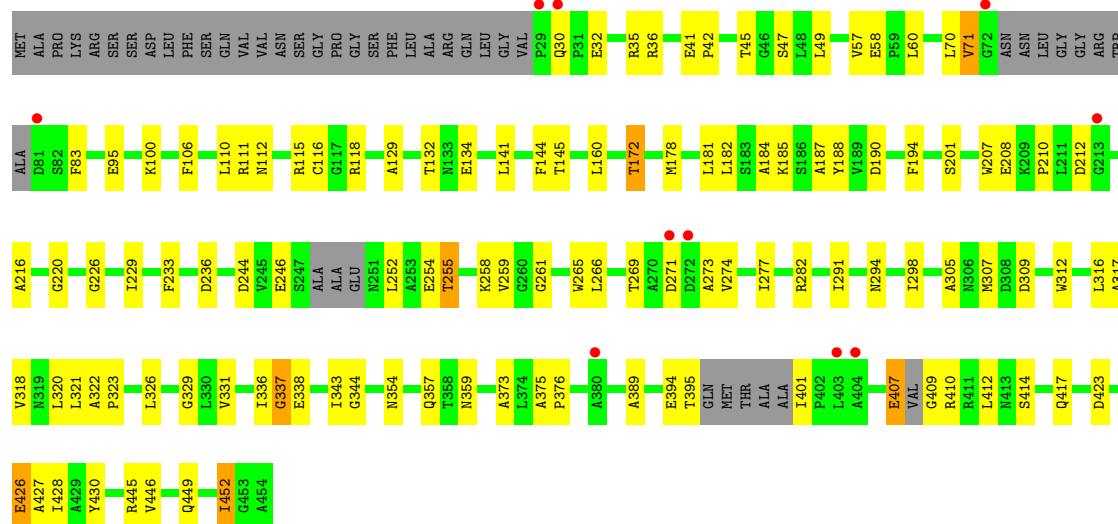


#### • Molecule 1: 3-oxoacyl-(Acyl-carrier-protein) reductase





● Molecule 1: 3-oxoacyl-(Acyl-carrier-protein) reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.33Å 71.30Å 93.29Å 104.99° 97.08° 93.66°	Depositor
Resolution (Å)	19.86 – 2.79 19.86 – 2.79	Depositor EDS
% Data completeness (in resolution range)	96.2 (19.86-2.79) 88.5 (19.86-2.79)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.162 , 0.238 0.166 , 0.238	Depositor DCC
$R_{free}$ test set	1887 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.7	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 40.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12462	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: NAI, ZPG

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	0/3125	0.79	1/4248 (0.0%)
1	B	0.66	0/3102	0.78	3/4212 (0.1%)
1	C	0.65	0/3036	0.74	0/4132
1	D	0.60	0/2968	0.70	0/4032
All	All	0.65	0/12231	0.75	4/16624 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	LEU	CA-CB-CG	-6.17	101.12	115.30
1	B	146	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	B	146	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	345	LEU	CA-CB-CG	5.22	127.30	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	3080	0	3100	61	0
1	B	3059	0	3073	51	0
1	C	2991	0	2963	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2927	0	2916	60	0
2	A	44	0	27	3	0
2	B	44	0	27	1	0
2	C	44	0	27	1	0
2	D	44	0	27	1	0
3	A	13	0	19	1	0
4	A	79	0	0	2	0
4	B	68	0	0	3	0
4	C	38	0	0	2	0
4	D	31	0	0	3	0
All	All	12462	0	12179	209	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 9.

All (209) 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:337:GLY:HA2	1:D:338:GLU:HB2	1.38	1.03
1:A:38:ARG:HH11	1:A:38:ARG:HG2	1.33	0.93
1:B:323:PRO:O	1:B:327:THR:HG22	1.78	0.82
1:B:322:ALA:HB3	1:B:323:PRO:HD3	1.60	0.82
1:A:115:ARG:NH2	1:A:154:ARG:HD2	1.99	0.78
1:A:249:ALA:O	1:A:250:GLU:HB2	1.84	0.78
1:D:41:GLU:HG3	1:D:42:PRO:HD2	1.68	0.74
1:C:316:LEU:HD13	1:C:363:THR:HG22	1.71	0.72
1:D:407:GLU:O	1:D:409:GLY:N	2.23	0.72
1:D:57:VAL:HG13	1:D:58:GLU:HG2	1.73	0.71
1:B:413:ASN:HB3	1:B:450:ALA:HA	1.76	0.66
1:A:426:GLU:OE1	1:A:426:GLU:HA	1.96	0.66
1:C:103:HIS:HE1	1:D:307:MET:O	1.79	0.66
1:C:311:ARG:NE	4:C:624:HOH:O	2.28	0.66
1:D:337:GLY:CA	1:D:338:GLU:HB2	2.19	0.65
1:A:404:ALA:O	1:A:408:VAL:HG23	1.97	0.65
1:A:315:VAL:O	1:A:319:ASN:HB2	1.98	0.64
1:D:181:LEU:HD21	1:D:194:PHE:CZ	2.32	0.64
1:C:129:ALA:HB1	1:C:134:GLU:HB3	1.79	0.64
1:A:38:ARG:CG	1:A:38:ARG:HH11	2.09	0.64
1:B:244:ASP:HB2	1:B:252:LEU:HD13	1.80	0.63
1:B:319:ASN:HB2	1:B:363:THR:HG21	1.80	0.63
1:C:49:LEU:HD13	1:C:71:VAL:HG22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:SER:OG	1:A:333:ASN:ND2	2.32	0.63
1:B:129:ALA:HB1	1:B:134:GLU:HB3	1.81	0.63
1:C:135:ARG:HD3	1:D:373:ALA:CB	2.29	0.63
1:C:107:THR:HB	1:C:108:PRO:HD3	1.81	0.62
1:B:308:ASP:OD1	1:B:311:ARG:HD2	2.01	0.61
1:C:325:ARG:HH12	1:C:328:GLU:HB2	1.64	0.61
1:A:401:ILE:O	1:A:406:ARG:NH1	2.34	0.61
1:C:220:GLY:O	1:C:226:GLY:HA3	2.00	0.60
1:A:414:SER:HB2	1:A:449:GLN:HB3	1.81	0.60
1:D:132:THR:HG21	4:D:615:HOH:O	2.00	0.60
1:C:103:HIS:CE1	1:D:307:MET:O	2.54	0.60
1:B:311:ARG:O	1:B:315:VAL:HG23	2.01	0.60
1:C:41:GLU:HB2	1:C:42:PRO:HD2	1.83	0.60
1:A:249:ALA:O	1:A:250:GLU:CB	2.49	0.59
1:A:103:HIS:HE1	1:B:307:MET:O	1.85	0.59
1:D:244:ASP:HB2	1:D:252:LEU:HD13	1.84	0.59
1:D:318:VAL:O	1:D:323:PRO:HD3	2.03	0.59
1:B:226:GLY:HA2	1:B:229:ILE:HD12	1.84	0.59
1:B:360:TYR:O	1:B:363:THR:OG1	2.21	0.59
1:B:60:LEU:HD11	1:B:178:MET:HG3	1.84	0.58
1:C:135:ARG:HD3	1:D:373:ALA:HB2	1.84	0.58
1:A:322:ALA:HB3	1:A:323:PRO:HD3	1.85	0.58
1:A:38:ARG:HG2	1:A:38:ARG:NH1	2.10	0.58
1:C:126:PRO:O	1:C:135:ARG:HG3	2.04	0.57
1:A:268:VAL:HG22	2:A:501:NAI:N1A	2.19	0.57
1:D:273:ALA:O	1:D:277:ILE:HG13	2.03	0.57
1:A:145:THR:HG21	1:A:160:LEU:HB2	1.85	0.57
1:A:343:ILE:HD12	1:A:343:ILE:N	2.20	0.57
1:D:32:GLU:OE2	1:D:115:ARG:HD2	2.04	0.57
1:B:344:GLY:HA3	4:B:666:HOH:O	2.05	0.57
1:D:190:ASP:HB3	1:D:449:GLN:HB2	1.87	0.57
1:C:343:ILE:HA	1:C:386:ASN:O	2.04	0.57
1:B:266:LEU:CD1	1:B:273:ALA:HA	2.35	0.55
1:D:410:ARG:CB	4:D:629:HOH:O	2.54	0.55
1:C:401:ILE:H	1:C:401:ILE:HD13	1.71	0.55
1:C:413:ASN:HB3	1:C:450:ALA:HA	1.88	0.55
1:C:268:VAL:HG22	2:C:501:NAI:N1A	2.22	0.55
1:D:210:PRO:HD2	1:D:236:ASP:HB3	1.89	0.54
1:D:36:ARG:NH2	1:D:423:ASP:OD2	2.36	0.54
1:B:220:GLY:O	1:B:226:GLY:HA3	2.08	0.54
1:D:41:GLU:CG	1:D:42:PRO:HD2	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:427:ALA:O	1:D:430:TYR:HB3	2.08	0.54
1:C:120:VAL:HG22	1:C:159:ALA:HB3	1.90	0.54
1:D:118:ARG:NH2	1:D:187:ALA:HA	2.22	0.54
1:C:322:ALA:HB3	1:C:323:PRO:HD3	1.90	0.54
1:D:172:THR:HB	1:D:201:SER:H	1.73	0.54
1:B:342:VAL:O	1:B:385:ILE:HA	2.07	0.53
1:B:107:THR:HB	1:B:108:PRO:HD3	1.89	0.53
1:A:23:ALA:O	1:A:26:LEU:O	2.25	0.53
1:D:294:ASN:HB2	1:D:344:GLY:HA2	1.89	0.53
1:A:433:SER:HB3	1:A:436:SER:OG	2.09	0.53
1:B:413:ASN:HB2	1:B:448:GLY:O	2.09	0.53
1:D:188:TYR:HD2	1:D:446:VAL:HG12	1.74	0.53
1:A:115:ARG:CZ	1:A:154:ARG:HD2	2.39	0.53
1:D:259:VAL:HG23	1:D:261:GLY:H	1.74	0.53
1:B:266:LEU:HD11	1:B:273:ALA:HA	1.91	0.52
1:D:322:ALA:O	1:D:326:LEU:HG	2.09	0.52
1:D:266:LEU:HD21	1:D:273:ALA:HB1	1.92	0.52
1:D:229:ILE:HD11	1:D:428:ILE:HD13	1.90	0.52
1:B:219:THR:O	1:B:295:ASN:HB3	2.10	0.52
1:C:49:LEU:HD13	1:C:71:VAL:CG2	2.41	0.51
1:D:317:ALA:HA	1:D:321:LEU:HB2	1.92	0.51
1:A:38:ARG:CG	1:A:38:ARG:NH1	2.70	0.50
1:A:413:ASN:HB3	1:A:450:ALA:HA	1.94	0.49
1:D:110:LEU:C	1:D:112:ASN:H	2.15	0.49
1:B:322:ALA:HB3	1:B:323:PRO:CD	2.39	0.49
1:D:244:ASP:OD1	2:D:501:NAI:H1B	2.13	0.49
1:C:408:VAL:O	1:C:412:LEU:HB2	2.13	0.49
1:A:249:ALA:HB2	1:A:265:TRP:HE1	1.76	0.49
1:C:50:ILE:HG22	1:C:57:VAL:HG23	1.94	0.49
1:D:207:TRP:O	1:D:210:PRO:HG3	2.12	0.49
1:C:141:LEU:O	1:C:144:PHE:HB3	2.13	0.49
1:B:229:ILE:HA	1:B:425:ALA:HB1	1.95	0.48
1:B:58:GLU:HB3	1:B:59:PRO:CD	2.42	0.48
1:C:394:GLU:HB3	4:C:634:HOH:O	2.13	0.48
1:D:337:GLY:HA2	1:D:338:GLU:CB	2.15	0.48
1:A:56:VAL:O	1:A:60:LEU:HB2	2.12	0.48
1:B:50:ILE:HD12	1:B:61:ARG:HG2	1.95	0.48
1:D:220:GLY:O	1:D:226:GLY:HA3	2.13	0.48
1:A:396:GLN:O	1:A:397:MET:HB3	2.12	0.48
1:D:255:THR:O	1:D:259:VAL:HG22	2.13	0.48
1:A:234:ALA:HB2	1:A:259:VAL:HB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:VAL:O	1:B:60:LEU:HB2	2.13	0.48
1:C:57:VAL:HG13	1:C:58:GLU:H	1.79	0.48
1:D:452:ILE:HG22	4:D:623:HOH:O	2.13	0.48
1:A:290:ASP:C	1:A:291:ILE:HG13	2.32	0.48
1:B:314:ALA:O	1:B:318:VAL:HG23	2.14	0.48
1:B:445:ARG:NH2	1:B:450:ALA:HB3	2.29	0.47
1:C:35:ARG:NH2	1:C:42:PRO:O	2.42	0.47
1:A:249:ALA:HB2	1:A:265:TRP:NE1	2.30	0.47
1:A:249:ALA:CB	1:A:265:TRP:HE1	2.28	0.47
1:B:82:SER:HA	1:B:112:ASN:ND2	2.29	0.47
1:B:131:SER:HB2	4:B:640:HOH:O	2.15	0.47
1:A:390:PRO:HB2	2:A:501:NAI:C5N	2.45	0.47
1:A:373:ALA:HA	1:B:135:ARG:HD3	1.97	0.47
1:B:390:PRO:HB2	2:B:501:NAI:C5N	2.45	0.47
1:A:228:THR:O	1:A:232:VAL:HG23	2.15	0.46
1:B:58:GLU:HB3	1:B:59:PRO:HD3	1.97	0.46
1:D:49:LEU:HB2	1:D:71:VAL:HG23	1.97	0.46
1:B:212:ASP:HA	1:B:237:GLY:HA3	1.96	0.46
1:D:216:ALA:HB2	1:D:291:ILE:HD12	1.98	0.46
1:A:346:SER:OG	1:A:347:SER:N	2.48	0.46
1:C:262:THR:HG1	1:C:280:HIS:CE1	2.32	0.46
1:D:375:ALA:N	1:D:376:PRO:HD2	2.31	0.46
1:B:58:GLU:N	1:B:59:PRO:HD2	2.31	0.45
1:D:274:VAL:HG11	1:D:329:GLY:HA3	1.98	0.45
1:A:110:LEU:C	1:A:112:ASN:H	2.20	0.45
1:B:174:LEU:HG	1:B:178:MET:HG2	1.98	0.45
1:A:415:LEU:O	1:A:417:GLN:HG2	2.17	0.45
1:C:262:THR:OG1	1:C:280:HIS:NE2	2.39	0.45
1:C:413:ASN:CB	1:C:450:ALA:HA	2.46	0.45
1:C:54:GLY:HA3	1:C:91:THR:OG1	2.16	0.45
1:A:123:GLY:O	1:A:162:TYR:HA	2.16	0.45
1:D:178:MET:O	1:D:182:LEU:HB2	2.17	0.45
1:A:314:ALA:O	1:A:318:VAL:HG23	2.17	0.45
1:B:117:GLY:C	1:B:118:ARG:HG2	2.37	0.45
1:B:298:ILE:HG13	1:B:300:ARG:NH1	2.32	0.45
1:A:161:VAL:HG22	1:A:194:PHE:HB2	1.99	0.44
3:A:502:ZPG:H212	4:B:602:HOH:O	2.17	0.44
1:A:26:LEU:HD23	1:B:22:LEU:CD1	2.47	0.44
1:B:82:SER:HA	1:B:112:ASN:HD22	1.82	0.44
1:D:47:SER:O	1:D:83:PHE:HA	2.18	0.44
1:A:300:ARG:HB3	1:A:311:ARG:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:ASP:HB3	1:D:449:GLN:CB	2.47	0.44
1:D:35:ARG:NH1	1:D:184:ALA:HB2	2.33	0.44
1:A:443:VAL:HG23	4:A:622:HOH:O	2.17	0.44
1:C:57:VAL:HG13	1:C:58:GLU:N	2.33	0.44
1:A:204:PRO:O	1:A:205:ALA:C	2.56	0.44
1:B:348:ILE:HA	1:B:348:ILE:HD12	1.83	0.43
1:C:106:PHE:O	1:C:107:THR:C	2.57	0.43
1:D:343:ILE:N	1:D:343:ILE:HD12	2.33	0.43
1:C:119:VAL:O	1:C:158:THR:HA	2.18	0.43
1:C:47:SER:N	1:C:84:GLY:H	2.16	0.43
1:A:106:PHE:O	1:A:110:LEU:HG	2.18	0.43
1:A:110:LEU:O	1:A:112:ASN:N	2.51	0.43
1:A:115:ARG:NH2	1:A:154:ARG:CD	2.77	0.43
1:A:396:GLN:O	1:A:397:MET:CB	2.67	0.43
1:C:348:ILE:HG12	1:C:391:GLY:HA2	2.00	0.43
1:D:320:LEU:C	1:D:323:PRO:HD2	2.38	0.43
1:B:452:ILE:HD13	1:B:452:ILE:HG21	1.77	0.43
1:B:160:LEU:O	1:B:193:VAL:HA	2.18	0.43
1:B:209:LYS:HG2	1:B:212:ASP:HB2	2.01	0.43
1:A:32:GLU:OE2	1:A:115:ARG:HG2	2.20	0.42
1:B:57:VAL:O	1:B:61:ARG:HG3	2.19	0.42
1:D:185:LYS:HB3	1:D:426:GLU:HG2	2.00	0.42
1:B:364:LYS:HA	1:B:364:LYS:HD3	1.80	0.42
1:A:170:ALA:HB3	4:A:671:HOH:O	2.19	0.42
1:B:317:ALA:HA	1:B:321:LEU:HB2	2.00	0.42
1:C:299:THR:HG22	1:C:360:TYR:CD1	2.54	0.42
1:D:129:ALA:HB1	1:D:134:GLU:HB3	2.00	0.42
1:A:196:VAL:HG22	1:A:439:VAL:HG22	2.01	0.42
1:D:312:TRP:CE3	1:D:359:ASN:HB3	2.55	0.42
1:A:184:ALA:O	1:A:187:ALA:HB2	2.20	0.41
1:A:386:ASN:OD1	1:A:442:ASN:HB2	2.20	0.41
1:C:337:GLY:O	1:C:338:GLU:C	2.59	0.41
1:D:354:ASN:O	1:D:357:GLN:HB2	2.20	0.41
1:A:102:LEU:HD13	1:A:144:PHE:CD1	2.55	0.41
1:A:397:MET:O	1:A:397:MET:SD	2.78	0.41
1:D:145:THR:HG21	1:D:160:LEU:HB2	2.02	0.41
1:A:94:THR:O	1:A:134:GLU:HA	2.20	0.41
1:D:389:ALA:O	1:D:445:ARG:HA	2.20	0.41
1:C:41:GLU:CB	1:C:42:PRO:HD2	2.49	0.41
1:D:60:LEU:HD12	1:D:60:LEU:HA	1.86	0.41
1:A:51:GLY:HA3	1:A:105:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:401:ILE:HA	1:C:402:PRO:HD2	1.76	0.41
1:C:414:SER:HB2	1:C:449:GLN:HB3	2.02	0.41
1:C:202:THR:HA	1:C:203:PRO:HD2	1.85	0.41
1:A:110:LEU:C	1:A:112:ASN:N	2.73	0.41
1:A:102:LEU:HD13	1:A:144:PHE:CG	2.55	0.41
1:A:364:LYS:NZ	2:A:501:NAI:O3D	2.51	0.41
1:D:414:SER:HB2	1:D:449:GLN:HB3	2.01	0.41
1:A:148:LEU:HA	1:A:148:LEU:HD12	1.87	0.41
1:D:210:PRO:HD2	1:D:236:ASP:CB	2.50	0.41
1:B:244:ASP:O	1:B:266:LEU:N	2.46	0.41
1:C:352:ALA:HB2	1:C:453:GLY:HA2	2.02	0.41
1:C:341:ARG:HH22	1:C:437:ASN:HB3	1.85	0.41
1:D:190:ASP:HB3	1:D:449:GLN:N	2.36	0.41
1:B:181:LEU:HD21	1:B:194:PHE:CZ	2.56	0.41
1:C:304:LEU:HD21	1:D:106:PHE:HB2	2.03	0.41
1:B:51:GLY:HA3	1:B:105:PHE:CE1	2.57	0.40
1:D:141:LEU:O	1:D:144:PHE:HB3	2.20	0.40
1:A:404:ALA:O	1:A:405:THR:C	2.59	0.40
1:B:273:ALA:O	1:B:277:ILE:HG13	2.22	0.40
1:A:136:ILE:HG12	1:B:370:ILE:HA	2.02	0.40
1:D:331:VAL:HG23	1:D:336:ILE:HD12	2.02	0.40
1:C:266:LEU:HG	1:C:267:ASP:N	2.36	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	423/454 (93%)	392 (93%)	26 (6%)	5 (1%)	15	44
1	B	417/454 (92%)	390 (94%)	25 (6%)	2 (0%)	32	67
1	C	412/454 (91%)	384 (93%)	22 (5%)	6 (2%)	12	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	399/454 (88%)	360 (90%)	34 (8%)	5 (1%)	14	41
All	All	1651/1816 (91%)	1526 (92%)	107 (6%)	18 (1%)	17	47

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	GLU
1	C	347	SER
1	D	100	LYS
1	D	337	GLY
1	A	111	ARG
1	A	197	GLY
1	A	397	MET
1	C	39	ALA
1	C	79	TRP
1	D	111	ARG
1	B	283	ASP
1	C	404	ALA
1	D	116	CYS
1	A	399	ALA
1	B	346	SER
1	C	73	ASN
1	D	305	ALA
1	C	40	GLY

### 5.3.2 Protein sidechains ⓘ

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	306/331 (92%)	288 (94%)	18 (6%)	23	54
1	B	303/331 (92%)	287 (95%)	16 (5%)	26	59
1	C	292/331 (88%)	281 (96%)	11 (4%)	38	72
1	D	287/331 (87%)	259 (90%)	28 (10%)	9	27
All	All	1188/1324 (90%)	1115 (94%)	73 (6%)	22	53



All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	26	LEU
1	A	28	VAL
1	A	38	ARG
1	A	41	GLU
1	A	56	VAL
1	A	69	ASP
1	A	95	GLU
1	A	115	ARG
1	A	168	LYS
1	A	244	ASP
1	A	251	ASN
1	A	345	LEU
1	A	348	ILE
1	A	355	ARG
1	A	397	MET
1	A	411	ARG
1	A	430	TYR
1	B	56	VAL
1	B	95	GLU
1	B	112	ASN
1	B	219	THR
1	B	223	ARG
1	B	244	ASP
1	B	257	SER
1	B	266	LEU
1	B	271	ASP
1	B	276	LYS
1	B	288	LYS
1	B	290	ASP
1	B	327	THR
1	B	348	ILE
1	B	430	TYR
1	B	452	ILE
1	C	74	ASN
1	C	202	THR
1	C	223	ARG
1	C	231	GLU
1	C	254	GLU
1	C	271	ASP
1	C	325	ARG
1	C	401	ILE

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Mol	Chain	Res	Type
1	C	407	GLU
1	C	408	VAL
1	C	451	MET
1	D	30	GLN
1	D	45	THR
1	D	70	LEU
1	D	71	VAL
1	D	95	GLU
1	D	172	THR
1	D	208	GLU
1	D	212	ASP
1	D	233	PHE
1	D	246	GLU
1	D	254	GLU
1	D	255	THR
1	D	258	LYS
1	D	265	TRP
1	D	269	THR
1	D	271	ASP
1	D	282	ARG
1	D	298	ILE
1	D	309	ASP
1	D	316	LEU
1	D	394	GLU
1	D	395	THR
1	D	401	ILE
1	D	407	GLU
1	D	412	LEU
1	D	417	GLN
1	D	426	GLU
1	D	452	ILE

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

Mol	Chain	Res	Type
1	A	30	GLN
1	A	103	HIS
1	A	251	ASN
1	B	112	ASN
1	B	280	HIS
1	B	294	ASN
1	C	74	ASN

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Mol	Chain	Res	Type
1	C	103	HIS
1	C	192	GLN
1	C	251	ASN
1	C	284	HIS
1	C	285	HIS
1	C	420	GLN
1	D	192	GLN
1	D	417	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](#)

5 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	NAI	A	501	-	40,48,48	1.67	7 (17%)	41,73,73	2.48	5 (12%)
3	ZPG	A	502	-	12,12,28	0.86	1 (8%)	9,14,34	1.07	0
2	NAI	B	501	-	40,48,48	1.80	9 (22%)	41,73,73	2.72	8 (19%)
2	NAI	C	501	-	40,48,48	1.78	8 (20%)	41,73,73	2.50	8 (19%)
2	NAI	D	501	-	40,48,48	1.91	10 (25%)	41,73,73	2.13	6 (14%)

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	NAI	A	501	-	-	0/25/72/72	0/4/5/5
3	ZPG	A	502	-	-	0/12/12/31	0/0/0/0
2	NAI	B	501	-	-	0/25/72/72	0/4/5/5
2	NAI	C	501	-	-	0/25/72/72	0/4/5/5
2	NAI	D	501	-	-	0/25/72/72	0/4/5/5

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	NAI	C4N-C5N	-4.26	1.39	1.49
2	B	501	NAI	C4N-C5N	-3.99	1.40	1.49
2	A	501	NAI	C4N-C5N	-3.30	1.41	1.49
2	C	501	NAI	C4N-C5N	-3.06	1.42	1.49
2	C	501	NAI	C5A-C4A	-3.01	1.33	1.40
2	B	501	NAI	C5A-C4A	-2.71	1.34	1.40
2	A	501	NAI	C5A-C4A	-2.63	1.34	1.40
2	D	501	NAI	C5A-C4A	-2.46	1.35	1.40
2	D	501	NAI	O2B-C2B	2.03	1.47	1.43
2	D	501	NAI	O4D-C1D	2.04	1.47	1.42
2	C	501	NAI	O4D-C1D	2.04	1.47	1.42
2	B	501	NAI	PN-O1N	2.07	1.65	1.55
3	A	502	ZPG	C18-C20	2.09	1.54	1.51
2	B	501	NAI	C2N-C3N	2.37	1.41	1.34
2	D	501	NAI	C2N-C3N	2.51	1.42	1.34
2	C	501	NAI	C2N-C3N	2.54	1.42	1.34
2	A	501	NAI	C2N-C3N	2.71	1.42	1.34
2	D	501	NAI	O4B-C1B	2.98	1.45	1.41
2	C	501	NAI	C2A-N1A	3.17	1.39	1.33
2	C	501	NAI	PA-O1A	3.39	1.63	1.50
2	B	501	NAI	C2A-N1A	3.54	1.40	1.33
2	B	501	NAI	PA-O1A	3.62	1.64	1.50
2	A	501	NAI	C2A-N1A	3.69	1.40	1.33
2	B	501	NAI	O4B-C1B	3.74	1.46	1.41
2	D	501	NAI	C2A-N1A	3.76	1.41	1.33
2	B	501	NAI	C6N-C5N	3.91	1.40	1.33
2	D	501	NAI	PA-O1A	3.92	1.65	1.50
2	D	501	NAI	C6N-C5N	4.03	1.40	1.33
2	A	501	NAI	PA-O1A	4.11	1.66	1.50
2	C	501	NAI	C6N-C5N	4.11	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NAI	C2A-N3A	4.14	1.39	1.32
2	A	501	NAI	C6N-C5N	4.31	1.41	1.33
2	C	501	NAI	C2A-N3A	4.65	1.39	1.32
2	B	501	NAI	C2A-N3A	5.11	1.40	1.32
2	D	501	NAI	C2A-N3A	5.33	1.41	1.32

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NAI	N3A-C2A-N1A	-13.48	117.11	128.86
2	C	501	NAI	N3A-C2A-N1A	-12.92	117.60	128.86
2	A	501	NAI	N3A-C2A-N1A	-12.81	117.70	128.86
2	D	501	NAI	N3A-C2A-N1A	-10.40	119.80	128.86
2	B	501	NAI	C4B-O4B-C1B	-6.66	102.68	109.77
2	A	501	NAI	C1D-N1N-C6N	-4.50	111.01	120.77
2	D	501	NAI	C1D-N1N-C6N	-4.09	111.89	120.77
2	A	501	NAI	C4B-O4B-C1B	-4.07	105.43	109.77
2	C	501	NAI	C3N-C2N-N1N	-3.91	117.40	123.08
2	A	501	NAI	C1B-N9A-C4A	-3.59	120.43	126.64
2	B	501	NAI	C1D-N1N-C6N	-3.56	113.05	120.77
2	C	501	NAI	C4B-O4B-C1B	-3.53	106.01	109.77
2	C	501	NAI	O4B-C4B-C5B	-3.50	97.58	109.40
2	B	501	NAI	C5B-C4B-C3B	-3.22	103.03	115.29
2	B	501	NAI	C3N-C2N-N1N	-2.88	118.90	123.08
2	C	501	NAI	C1B-N9A-C4A	-2.70	121.97	126.64
2	B	501	NAI	C1B-N9A-C4A	-2.61	122.12	126.64
2	D	501	NAI	C3N-C2N-N1N	-2.21	119.87	123.08
2	D	501	NAI	C4A-C5A-N7A	-2.11	107.37	109.41
2	B	501	NAI	C4A-C5A-N7A	-2.11	107.37	109.41
2	C	501	NAI	C1D-N1N-C6N	-2.10	116.21	120.77
2	C	501	NAI	C5A-C6A-N6A	-2.03	116.34	120.47
2	D	501	NAI	C2B-C3B-C4B	2.07	106.65	102.62
2	C	501	NAI	O4D-C1D-N1N	2.34	112.78	108.07
2	B	501	NAI	O4D-C1D-N1N	2.70	113.50	108.07
2	A	501	NAI	O4D-C1D-N1N	3.15	114.42	108.07
2	D	501	NAI	O4D-C1D-N1N	4.30	116.73	108.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAI	3	0
3	A	502	ZPG	1	0
2	B	501	NAI	1	0
2	C	501	NAI	1	0
2	D	501	NAI	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	427/454 (94%)	-0.61	1 (0%) 94 94	13, 31, 51, 62	0
1	B	425/454 (93%)	-0.49	4 (0%) 84 79	11, 35, 66, 79	0
1	C	418/454 (92%)	-0.45	4 (0%) 82 77	21, 39, 61, 76	0
1	D	409/454 (90%)	-0.20	10 (2%) 59 49	26, 52, 82, 93	0
All	All	1679/1816 (92%)	-0.44	19 (1%) 80 74	11, 39, 71, 93	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	72	GLY	3.7
1	C	400	ALA	3.3
1	D	81	ASP	3.2
1	D	29	PRO	3.0
1	B	72	GLY	2.9
1	D	403	LEU	2.6
1	C	130	ALA	2.5
1	D	30	GLN	2.5
1	D	272	ASP	2.5
1	D	404	ALA	2.4
1	C	404	ALA	2.3
1	A	40	GLY	2.3
1	C	29	PRO	2.2
1	D	380	ALA	2.2
1	D	271	ASP	2.1
1	B	223	ARG	2.1
1	B	265	TRP	2.1
1	B	283	ASP	2.1
1	D	213	GLY	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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	ZPG	A	502	13/29	0.86	0.20	2.36	65,67,69,70	0
2	NAI	B	501	44/44	0.93	0.16	0.15	63,67,72,73	0
2	NAI	C	501	44/44	0.96	0.14	0.14	34,45,56,58	0
2	NAI	D	501	44/44	0.95	0.14	-0.43	54,64,74,77	0
2	NAI	A	501	44/44	0.97	0.11	-0.72	29,37,43,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.