



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 05:53 AM GMT

PDB ID : 1NXG  
Title : The F383A variant of type II Citrate Synthase complexed with NADH  
Authors : Maurus, R.; Nguyen, N.T.; Stokell, D.J.; Ayed, A.; Hultin, P.G.; Duckworth, H.W.; Brayer, G.D.  
Deposited on : 2003-02-10  
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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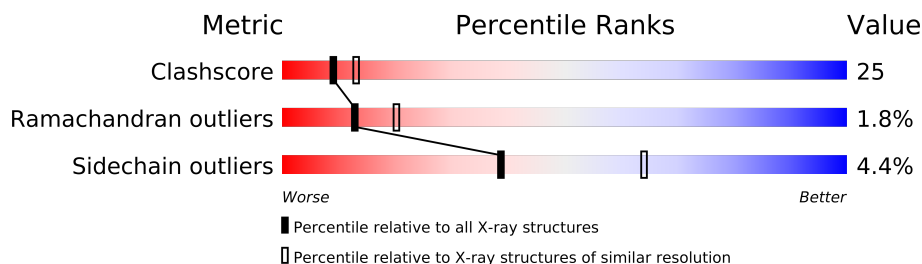
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : NOT EXECUTED  
EDS : NOT EXECUTED  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.50 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))
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	427	
1	B	427	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7409 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

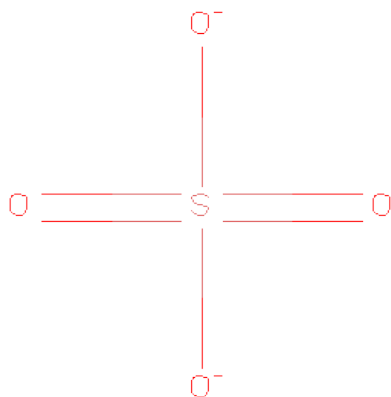
- Molecule 1 is a protein called Citrate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	0	0
			3359	2129	579	626	25			
1	B	426	Total	C	N	O	S	0	0	0
			3360	2129	579	627	25			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	383	ALA	PHE	ENGINEERED	UNP P0ABH7
B	1383	ALA	PHE	ENGINEERED	UNP P0ABH7

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



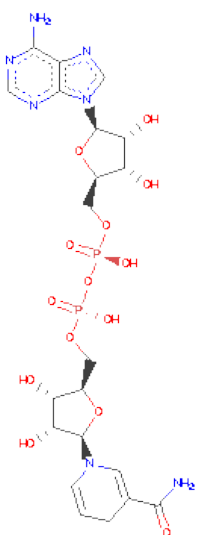
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDEADENINE 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
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	293	Total	O	0	0
			293	293		
4	B	289	Total	O	0	0
			289	289		

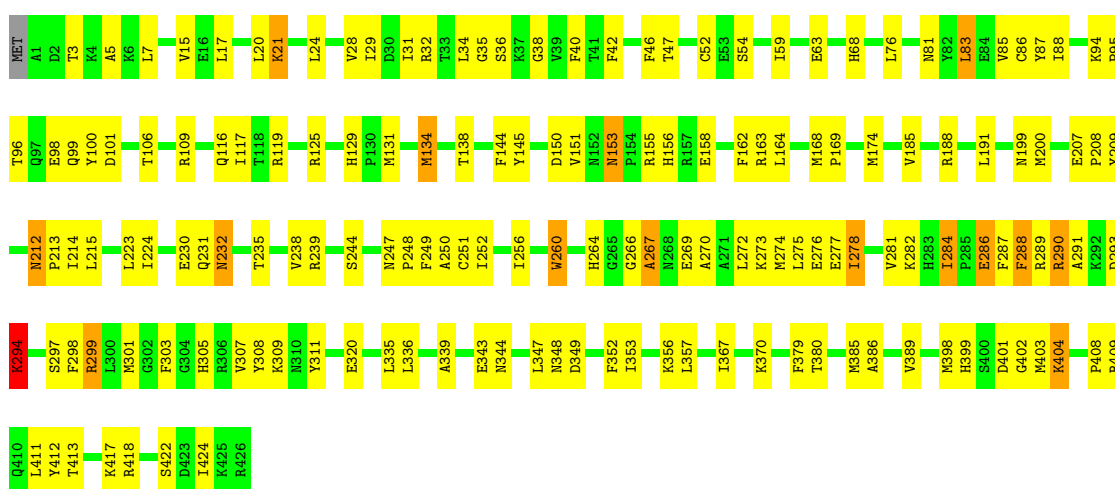
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

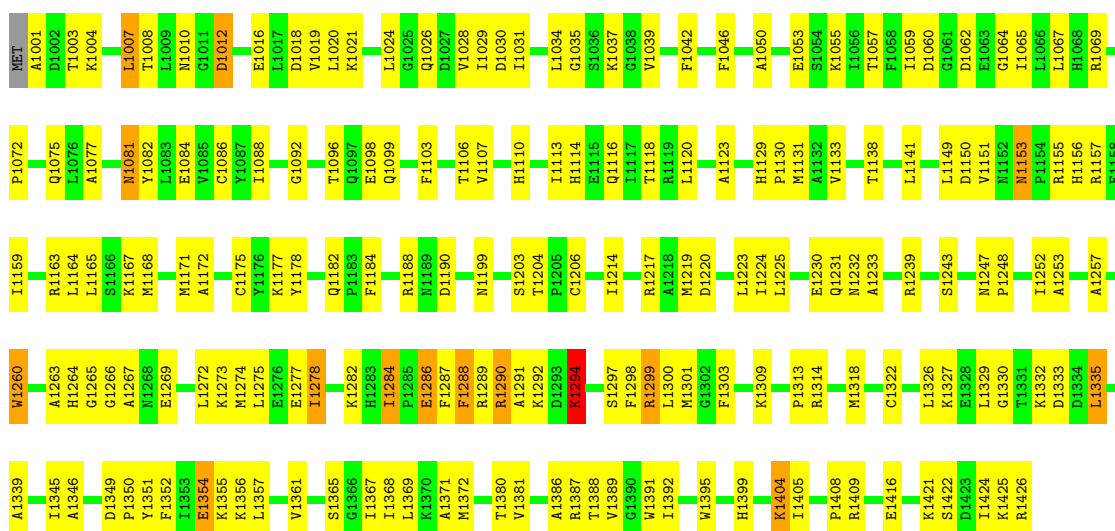
#### • Molecule 1: Citrate synthase

Chain A:



#### • Molecule 1: Citrate synthase

Chain B:



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	164.89Å 164.89Å 158.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.187 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7409	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAI, SO4

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	0.38	0/3436	0.67	0/4645
1	B	0.37	0/3437	0.67	1/4645 (0.0%)
All	All	0.37	0/6873	0.67	1/9290 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1165	LEU	CB-CG-CD1	-6.45	100.03	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3359	0	3309	172	0
1	B	3360	0	3306	189	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	A	44	0	27	6	0
3	B	44	0	27	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	293	0	0	19	0
4	B	289	0	0	17	0
All	All	7409	0	6669	339	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 25.

All (339) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:404:LYS:HD3	1:A:404:LYS:H	1.16	1.06
1:B:1081:ASN:ND2	1:B:1084:GLU:H	1.67	0.91
1:B:1272:LEU:HA	1:B:1275:LEU:HG	1.55	0.88
1:B:1287:PHE:HA	1:B:1291:ALA:HB3	1.58	0.86
1:A:275:LEU:HD22	1:A:289:ARG:HE	1.39	0.85
1:A:96:THR:H	1:A:99:GLN:HE21	1.24	0.85
1:A:287:PHE:HA	1:A:291:ALA:HB3	1.61	0.82
1:A:282:LYS:HA	1:A:288:PHE:HD2	1.45	0.81
1:B:1129:HIS:CD2	1:B:1131:MET:H	1.99	0.81
1:A:309:LYS:NZ	1:A:356:LYS:HE3	1.96	0.80
1:B:1275:LEU:HD22	1:B:1289:ARG:HE	1.46	0.80
3:A:3000:NAI:H3B	3:A:3000:NAI:O3	1.83	0.79
1:A:404:LYS:N	1:A:404:LYS:HD3	1.96	0.79
1:B:1335:LEU:HD23	1:B:1335:LEU:H	1.49	0.77
1:A:305:HIS:HD2	1:A:307:VAL:H	1.31	0.76
1:A:294:LYS:HB3	1:A:301:MET:HE3	1.68	0.76
1:A:158:GLU:HG2	4:A:3008:HOH:O	1.85	0.76
1:B:1282:LYS:HA	1:B:1288:PHE:HD2	1.51	0.76
1:A:274:MET:HG3	1:A:293:ASP:HA	1.67	0.75
1:A:52:CYS:SG	4:A:3233:HOH:O	2.43	0.75
1:A:269:GLU:HA	1:A:272:LEU:HB2	1.70	0.74
1:A:101:ASP:HA	1:B:1426:ARG:HH21	1.52	0.74
1:B:1129:HIS:HD2	1:B:1131:MET:H	1.32	0.73
1:B:1113:ILE:HA	4:B:49:HOH:O	1.87	0.73
1:B:1230:GLU:HG2	1:B:1231:GLN:H	1.55	0.72
1:A:85:VAL:HG21	1:A:224:ILE:HG23	1.70	0.72
1:B:1339:ALA:HB1	1:B:1367:ILE:HD13	1.71	0.71
1:B:1081:ASN:HD21	1:B:1084:GLU:H	1.34	0.71
1:B:1004:LYS:HB3	1:B:1021:LYS:HD3	1.71	0.71
1:A:129:HIS:CD2	1:A:131:MET:H	2.09	0.71
1:B:1077:ALA:HA	1:B:1224:ILE:HG21	1.71	0.71
1:A:188:ARG:HB2	1:A:191:LEU:HD12	1.72	0.70
1:A:129:HIS:HD2	1:A:131:MET:H	1.37	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1123:ALA:HB3	4:B:187:HOH:O	1.92	0.70
1:A:272:LEU:HA	1:A:275:LEU:HG	1.74	0.70
1:A:305:HIS:CD2	1:A:307:VAL:H	2.10	0.69
1:A:404:LYS:CD	1:A:404:LYS:H	2.00	0.68
1:A:117:ILE:HG13	4:A:3062:HOH:O	1.93	0.68
1:A:100:TYR:HE1	1:B:1426:ARG:HB3	1.58	0.68
1:A:145:TYR:HE1	3:A:3000:NAI:O2A	1.76	0.68
1:A:252:ILE:O	1:A:256:ILE:HG13	1.94	0.67
1:A:249:PHE:HE2	4:A:3292:HOH:O	1.77	0.67
1:A:163:ARG:HB2	4:A:3292:HOH:O	1.93	0.67
1:B:1290:ARG:HB2	4:B:24:HOH:O	1.95	0.66
1:B:1188:ARG:HG2	4:B:165:HOH:O	1.95	0.66
1:B:1230:GLU:CG	1:B:1231:GLN:H	2.09	0.65
1:B:1388:THR:O	1:B:1392:ILE:HG13	1.96	0.65
1:A:47:THR:HG22	1:B:1409:ARG:HH11	1.62	0.64
1:B:1289:ARG:HA	4:B:324:HOH:O	1.96	0.64
1:A:100:TYR:CE1	1:B:1426:ARG:HB3	2.33	0.64
1:A:129:HIS:HD2	1:A:131:MET:N	1.97	0.63
1:A:7:LEU:HB2	1:B:1010:ASN:O	1.98	0.63
1:B:1303:PHE:HB3	1:B:1357:LEU:HB3	1.80	0.63
1:A:116:GLN:HB3	4:A:3062:HOH:O	1.99	0.63
1:A:244:SER:HB3	1:B:1233:ALA:HB1	1.80	0.63
1:B:1007:LEU:HD21	1:B:1029:ILE:HG23	1.81	0.62
1:B:1008:THR:HG22	1:B:1016:GLU:HG2	1.81	0.62
1:A:282:LYS:HA	1:A:288:PHE:CD2	2.33	0.62
1:B:1020:LEU:HD22	1:B:1020:LEU:H	1.65	0.62
1:B:1248:PRO:HG3	1:B:1395:TRP:CH2	2.35	0.61
1:B:1284:ILE:HD12	1:B:1287:PHE:H	1.65	0.61
1:A:232:ASN:ND2	1:A:235:THR:H	1.99	0.61
1:B:1288:PHE:O	1:B:1288:PHE:HD1	1.84	0.61
1:A:298:PHE:HB2	1:A:301:MET:HG3	1.82	0.60
1:B:1062:ASP:HA	1:B:1309:LYS:HB2	1.83	0.60
1:A:164:LEU:HG	4:A:3292:HOH:O	2.01	0.60
1:A:269:GLU:O	1:A:273:LYS:HB2	2.02	0.60
1:B:1272:LEU:HA	1:B:1275:LEU:CG	2.31	0.59
1:B:1352:PHE:HA	1:B:1357:LEU:HD12	1.83	0.59
1:B:1103:PHE:O	1:B:1107:VAL:HG23	2.03	0.59
1:B:1081:ASN:C	1:B:1081:ASN:HD22	2.05	0.59
1:A:309:LYS:HZ3	1:A:356:LYS:HE3	1.67	0.59
1:A:418:ARG:O	1:B:1072:PRO:HD3	2.02	0.59
1:B:1269:GLU:O	1:B:1273:LYS:HB2	2.03	0.58
1:B:1082:TYR:CD1	1:B:1223:LEU:HB3	2.39	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1220:ASP:O	1:B:1224:ILE:HG13	2.01	0.58
1:B:1248:PRO:HG3	1:B:1395:TRP:CZ2	2.38	0.58
1:A:169:PRO:HG2	4:A:3124:HOH:O	2.03	0.58
1:A:398:MET:SD	1:A:403:MET:HG3	2.42	0.58
1:B:1368:ILE:O	1:B:1372:MET:HG3	2.03	0.58
1:A:199:ASN:HD22	1:A:209:TYR:HD1	1.50	0.58
1:A:153:ASN:HD22	1:A:155:ARG:H	1.52	0.58
1:A:284:ILE:HD12	1:A:287:PHE:H	1.69	0.57
1:B:1164:LEU:HD13	1:B:1252:ILE:HG13	1.86	0.57
1:B:1269:GLU:HA	1:B:1272:LEU:HB2	1.86	0.57
1:B:1120:LEU:HD12	4:B:187:HOH:O	2.05	0.57
1:B:1278:ILE:O	1:B:1278:ILE:HD13	2.05	0.57
1:A:54:SER:HB2	4:A:3233:HOH:O	2.05	0.57
1:A:101:ASP:HA	1:B:1426:ARG:NH2	2.19	0.57
1:B:1072:PRO:HG2	1:B:1075:GLN:HE21	1.69	0.57
1:B:1069:ARG:CD	1:B:1092:GLY:HA2	2.35	0.57
1:B:1069:ARG:HD2	1:B:1092:GLY:HA2	1.85	0.57
1:A:370:LYS:HG3	1:A:379:PHE:HZ	1.69	0.57
1:A:7:LEU:HD21	1:A:29:ILE:HG12	1.87	0.56
1:A:275:LEU:HD22	1:A:289:ARG:NE	2.16	0.56
1:A:298:PHE:HD2	1:A:301:MET:HE1	1.70	0.56
1:B:1177:LYS:NZ	1:B:1182:GLN:HE21	2.04	0.56
1:A:267:ALA:HB3	1:A:270:ALA:HB2	1.88	0.56
1:A:212:ASN:HD22	1:A:213:PRO:N	2.03	0.56
1:A:305:HIS:CD2	1:A:307:VAL:HB	2.41	0.56
1:A:96:THR:HG23	1:A:99:GLN:NE2	2.21	0.55
1:A:21:LYS:H	1:A:21:LYS:HE2	1.72	0.55
1:B:1294:LYS:HB2	1:B:1297:SER:HA	1.87	0.55
1:A:289:ARG:HG2	1:A:290:ARG:H	1.71	0.55
1:A:230:GLU:CG	1:A:231:GLN:H	2.19	0.55
1:A:281:VAL:HG11	4:A:3270:HOH:O	2.05	0.55
1:A:408:PRO:HA	1:B:1046:PHE:O	2.07	0.55
1:B:1062:ASP:HA	1:B:1309:LYS:CB	2.37	0.55
1:A:278:ILE:HD13	1:A:278:ILE:O	2.07	0.55
1:A:131:MET:HG2	1:A:260:TRP:CD2	2.43	0.54
1:A:352:PHE:HA	1:A:357:LEU:HD23	1.89	0.54
1:A:153:ASN:ND2	1:A:155:ARG:H	2.05	0.54
1:A:299:ARG:HA	1:A:303:PHE:O	2.07	0.54
1:B:1219:MET:O	1:B:1223:LEU:HD13	2.07	0.54
1:B:1012:ASP:HA	4:B:78:HOH:O	2.07	0.54
1:B:1020:LEU:CD2	1:B:1030:ASP:HB2	2.39	0.53
1:B:1204:THR:HG22	1:B:1206:CYS:H	1.73	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:289:ARG:HG2	1:A:290:ARG:N	2.24	0.53
1:B:1303:PHE:CE1	1:B:1346:ALA:HB2	2.44	0.53
1:A:20:LEU:HB2	1:A:28:VAL:HG23	1.90	0.53
1:B:1019:VAL:HA	1:B:1028:VAL:O	2.08	0.53
1:B:1289:ARG:HG2	1:B:1290:ARG:H	1.73	0.53
1:A:153:ASN:HD21	1:A:155:ARG:HD3	1.73	0.53
1:A:47:THR:O	1:B:1409:ARG:NE	2.42	0.52
1:B:1151:VAL:HB	1:B:1399:HIS:CE1	2.45	0.52
1:B:1057:THR:HG23	1:B:1067:LEU:O	2.08	0.52
1:A:223:LEU:CD2	1:A:386:ALA:HB2	2.40	0.52
1:A:278:ILE:O	1:A:282:LYS:HB3	2.10	0.52
1:A:212:ASN:ND2	1:A:214:ILE:H	2.07	0.52
1:A:145:TYR:CE1	3:A:3000:NAI:O2A	2.61	0.52
1:B:1177:LYS:NZ	1:B:1182:GLN:NE2	2.58	0.52
3:A:3000:NAI:H42N	4:A:3008:HOH:O	2.10	0.52
1:B:1230:GLU:HG2	1:B:1231:GLN:N	2.24	0.52
1:B:1035:GLY:C	1:B:1037:LYS:H	2.13	0.52
1:B:1034:LEU:HD22	1:B:1039:VAL:CG1	2.40	0.51
1:B:1243:SER:HB2	1:B:1405:ILE:HA	1.92	0.51
1:B:1345:ILE:HG23	1:B:1349:ASP:HB2	1.92	0.51
3:A:3000:NAI:H8A	3:A:3000:NAI:H51A	1.93	0.51
1:A:169:PRO:HA	1:A:385:MET:SD	2.50	0.51
1:A:275:LEU:HA	1:A:289:ARG:HG3	1.93	0.51
1:B:1069:ARG:NE	1:B:1092:GLY:HA2	2.26	0.51
1:B:1275:LEU:HD22	4:B:24:HOH:O	2.09	0.51
1:A:212:ASN:HB3	1:A:215:LEU:HG	1.91	0.51
1:A:68:HIS:HB2	1:A:76:LEU:HD11	1.91	0.51
1:A:232:ASN:C	1:A:232:ASN:HD22	2.13	0.51
1:B:1020:LEU:HD21	1:B:1030:ASP:HB2	1.92	0.51
1:B:1422:SER:OG	1:B:1424:ILE:HG12	2.11	0.51
1:B:1081:ASN:HD22	1:B:1084:GLU:H	1.57	0.50
1:A:36:SER:C	1:A:38:GLY:H	2.14	0.50
1:B:1351:TYR:O	1:B:1355:LYS:HD3	2.11	0.50
1:B:1204:THR:CG2	1:B:1206:CYS:SG	3.00	0.50
1:A:223:LEU:HD22	1:A:386:ALA:HB2	1.94	0.50
1:B:1096:THR:H	1:B:1099:GLN:HB2	1.76	0.50
1:A:335:LEU:H	1:A:335:LEU:HD23	1.76	0.50
1:B:1081:ASN:HD21	1:B:1084:GLU:N	2.04	0.50
1:A:288:PHE:CD1	1:A:288:PHE:O	2.64	0.50
1:A:134:MET:HA	1:A:134:MET:HE2	1.93	0.50
1:B:1327:LYS:HG2	1:B:1327:LYS:O	2.11	0.50
1:A:153:ASN:HD22	1:A:155:ARG:N	2.10	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1289:ARG:HG2	1:B:1290:ARG:N	2.27	0.50
1:B:1287:PHE:HA	1:B:1291:ALA:CB	2.37	0.50
1:B:1288:PHE:O	1:B:1288:PHE:CD1	2.65	0.50
1:B:1133:VAL:HG21	4:B:96:HOH:O	2.12	0.50
1:A:288:PHE:HD1	1:A:288:PHE:O	1.94	0.50
1:B:1365:SER:O	1:B:1369:LEU:HG	2.12	0.50
1:B:1167:LYS:HE3	3:B:3001:NAI:O2N	2.11	0.50
1:A:343:GLU:O	1:A:347:LEU:HG	2.13	0.49
1:A:46:PHE:O	1:B:1408:PRO:HA	2.12	0.49
1:B:1060:ASP:HB3	1:B:1065:ILE:HB	1.95	0.49
1:A:131:MET:HE2	1:A:380:THR:HB	1.95	0.49
1:B:1287:PHE:O	1:B:1292:LYS:HB2	2.12	0.49
1:B:1007:LEU:HD22	1:B:1029:ILE:HG12	1.95	0.49
1:A:277:GLU:O	1:A:281:VAL:HG22	2.12	0.49
1:B:1354:GLU:HB3	1:B:1355:LYS:HD2	1.95	0.49
1:B:1387:ARG:HG3	1:B:1391:TRP:CE2	2.48	0.49
1:B:1086:CYS:SG	1:B:1389:VAL:HG21	2.52	0.49
1:B:1260:TRP:HA	4:B:321:HOH:O	2.13	0.49
1:A:336:LEU:HG	4:A:3151:HOH:O	2.12	0.48
1:A:409:ARG:HB2	1:B:1050:ALA:HA	1.94	0.48
1:A:174:MET:HG3	4:A:3030:HOH:O	2.12	0.48
1:A:272:LEU:HA	1:A:275:LEU:CG	2.42	0.48
1:B:1164:LEU:O	1:B:1168:MET:HG2	2.13	0.48
1:A:349:ASP:HB3	1:A:352:PHE:CD1	2.48	0.48
1:A:207:GLU:HB2	1:A:208:PRO:HD2	1.96	0.48
1:A:88:ILE:HG12	1:A:94:LYS:HA	1.95	0.48
1:A:150:ASP:HB3	1:A:156:HIS:CD2	2.48	0.48
1:B:1322:CYS:O	1:B:1326:LEU:HD13	2.14	0.48
1:A:151:VAL:HB	1:A:399:HIS:CE1	2.48	0.48
1:A:230:GLU:HG2	1:A:231:GLN:H	1.78	0.48
1:B:1204:THR:HG22	1:B:1206:CYS:SG	2.54	0.48
1:A:81:ASN:HA	1:A:224:ILE:HD11	1.94	0.47
1:A:29:ILE:O	1:A:31:ILE:HG23	2.14	0.47
1:B:1294:LYS:NZ	1:B:1298:PHE:H	2.12	0.47
1:A:35:GLY:HA2	1:A:40:PHE:CE2	2.49	0.47
1:B:1243:SER:O	1:B:1405:ILE:HG12	2.14	0.47
1:A:15:VAL:HA	4:A:3205:HOH:O	2.13	0.47
1:A:290:ARG:O	1:A:290:ARG:HG2	2.14	0.47
1:B:1326:LEU:HG	1:B:1333:ASP:OD1	2.15	0.47
1:A:164:LEU:HD22	1:A:168:MET:HE3	1.97	0.47
1:B:1303:PHE:HE1	1:B:1346:ALA:HB2	1.79	0.47
1:B:1269:GLU:HB2	1:B:1273:LYS:CA	2.44	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1300:LEU:HD13	1:B:1300:LEU:O	2.15	0.47
1:B:1214:ILE:HG12	1:B:1217:ARG:NH1	2.29	0.47
1:A:153:ASN:C	1:A:153:ASN:HD22	2.19	0.47
1:B:1264:HIS:ND1	1:B:1265:GLY:N	2.63	0.47
1:B:1277:GLU:HA	4:B:246:HOH:O	2.14	0.47
1:A:399:HIS:NE2	1:A:403:MET:SD	2.88	0.47
1:A:212:ASN:HD22	1:A:212:ASN:C	2.17	0.47
1:A:7:LEU:HD12	1:A:17:LEU:HB2	1.97	0.46
1:A:266:GLY:O	1:A:267:ALA:HB2	2.16	0.46
1:A:413:THR:HB	1:B:1055:LYS:NZ	2.31	0.46
1:B:1113:ILE:HD13	1:B:1118:THR:OG1	2.15	0.46
1:B:1149:LEU:HD22	1:B:1247:ASN:HB2	1.96	0.46
1:B:1275:LEU:HA	1:B:1289:ARG:HG3	1.98	0.46
1:B:1069:ARG:HG3	1:B:1088:ILE:HG22	1.98	0.46
1:A:239:ARG:HD3	4:A:3022:HOH:O	2.15	0.46
1:B:1153:ASN:C	1:B:1153:ASN:HD22	2.19	0.46
1:B:1272:LEU:CA	1:B:1275:LEU:HG	2.36	0.46
1:B:1290:ARG:HG2	1:B:1290:ARG:O	2.15	0.46
1:A:212:ASN:HD22	1:A:213:PRO:CD	2.29	0.46
1:A:96:THR:OG1	1:A:99:GLN:HG3	2.16	0.46
1:A:370:LYS:HG3	1:A:379:PHE:CZ	2.49	0.46
1:B:1355:LYS:N	1:B:1355:LYS:HD2	2.31	0.46
1:A:185:VAL:HB	1:A:200:MET:HA	1.98	0.46
1:A:289:ARG:CG	1:A:290:ARG:H	2.28	0.46
1:B:1404:LYS:HE3	4:B:154:HOH:O	2.15	0.46
1:A:344:ASN:OD1	1:A:348:ASN:ND2	2.49	0.46
1:A:24:LEU:HD11	1:B:1416:GLU:HA	1.99	0.45
1:A:162:PHE:HB3	4:A:3144:HOH:O	2.15	0.45
1:A:94:LYS:NZ	1:B:1421:LYS:O	2.41	0.45
1:B:1188:ARG:HB3	1:B:1190:ASP:OD1	2.15	0.45
1:B:1141:LEU:HD21	1:B:1171:MET:HE2	1.98	0.45
1:A:3:THR:C	1:A:5:ALA:H	2.20	0.45
1:B:1157:ARG:NH2	4:B:337:HOH:O	2.49	0.45
1:A:290:ARG:HA	1:A:293:ASP:CB	2.47	0.45
1:A:411:LEU:HD23	1:B:1028:VAL:HG22	1.98	0.45
1:A:59:ILE:HG21	1:A:307:VAL:CG1	2.46	0.45
1:B:1282:LYS:HA	1:B:1288:PHE:CD2	2.41	0.45
1:B:1266:GLY:O	1:B:1267:ALA:HB2	2.17	0.44
1:B:1269:GLU:HB2	1:B:1273:LYS:HB2	1.98	0.44
1:B:1064:GLY:O	1:B:1313:PRO:HB3	2.18	0.44
1:A:247:ASN:HB2	1:A:248:PRO:HD2	2.00	0.44
1:B:1225:LEU:HD12	1:B:1318:MET:SD	2.58	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1159:ILE:O	1:B:1163:ARG:HG3	2.17	0.44
1:A:138:THR:HG21	1:A:252:ILE:HG22	1.99	0.44
1:B:1167:LYS:O	1:B:1171:MET:HB2	2.17	0.44
1:A:308:TYR:HB3	1:A:311:TYR:O	2.17	0.44
1:B:1231:GLN:HE22	1:B:1239:ARG:NE	2.15	0.44
1:A:370:LYS:HE3	1:A:379:PHE:HE1	1.82	0.44
1:A:42:PHE:HB2	1:B:1028:VAL:CG2	2.47	0.44
1:A:298:PHE:CD2	1:A:301:MET:HE1	2.53	0.44
1:A:412:TYR:HD1	1:B:1024:LEU:HB2	1.83	0.44
1:A:32:ARG:HD2	1:B:1042:PHE:CD1	2.53	0.44
1:A:286:GLU:OE1	1:A:291:ALA:HB2	2.18	0.44
1:A:117:ILE:HG12	1:A:144:PHE:CD1	2.53	0.44
1:A:411:LEU:O	1:B:1053:GLU:HG3	2.18	0.43
1:A:272:LEU:N	1:A:272:LEU:HD12	2.33	0.43
1:A:288:PHE:H	1:A:288:PHE:HD1	1.66	0.43
1:B:1230:GLU:CG	1:B:1231:GLN:N	2.79	0.43
1:B:1034:LEU:HD22	1:B:1039:VAL:HG11	2.00	0.43
1:A:275:LEU:CD2	1:A:289:ARG:HE	2.21	0.43
1:B:1069:ARG:HG3	1:B:1088:ILE:CG2	2.49	0.43
1:B:1106:THR:O	1:B:1110:HIS:HD2	2.02	0.43
1:A:290:ARG:HA	1:A:293:ASP:HB2	2.00	0.43
1:A:287:PHE:HA	1:A:291:ALA:CB	2.41	0.43
1:B:1298:PHE:HD2	1:B:1301:MET:HE2	1.83	0.43
1:B:1386:ALA:O	1:B:1389:VAL:HG12	2.18	0.43
1:B:1003:THR:O	1:B:1019:VAL:HG11	2.18	0.43
1:A:150:ASP:H	1:A:156:HIS:HD2	1.64	0.43
1:A:412:TYR:CE1	1:B:1024:LEU:HD12	2.52	0.43
1:B:1129:HIS:CD2	1:B:1130:PRO:HD2	2.54	0.43
1:B:1149:LEU:HD22	1:B:1247:ASN:CB	2.49	0.43
1:A:320:GLU:HB3	4:A:3165:HOH:O	2.19	0.43
1:B:1273:LYS:HB3	1:B:1273:LYS:NZ	2.33	0.43
1:B:1082:TYR:CE2	1:B:1086:CYS:SG	3.12	0.43
1:A:418:ARG:HH11	1:B:1069:ARG:HB3	1.84	0.42
1:B:1318:MET:HA	1:B:1318:MET:CE	2.49	0.42
1:B:1114:HIS:CE1	1:B:1116:GLN:HB2	2.54	0.42
1:A:286:GLU:O	1:A:291:ALA:HB3	2.20	0.42
1:A:17:LEU:HD21	1:A:34:LEU:HD21	2.01	0.42
1:B:1001:ALA:N	1:B:1004:LYS:HZ2	2.17	0.42
1:B:1059:ILE:HG22	1:B:1060:ASP:N	2.34	0.42
1:A:273:LYS:O	1:A:276:GLU:HB3	2.20	0.42
1:A:32:ARG:HD2	1:B:1042:PHE:CE1	2.54	0.42
1:A:106:THR:HG23	1:A:109:ARG:HH21	1.83	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:250:ALA:HB1	1:B:1257:ALA:HB1	2.02	0.42
1:B:1294:LYS:HE2	1:B:1357:LEU:HD13	2.01	0.42
1:B:1007:LEU:HD11	1:B:1029:ILE:HG21	2.01	0.42
1:B:1059:ILE:HA	1:B:1065:ILE:O	2.19	0.42
1:B:1153:ASN:ND2	1:B:1155:ARG:H	2.17	0.42
1:B:1138:THR:HG22	1:B:1253:ALA:HB2	2.01	0.42
1:B:1356:LYS:HD3	4:B:558:HOH:O	2.19	0.42
1:A:86:CYS:HA	1:A:389:VAL:HG21	2.02	0.42
1:B:1329:LEU:HD13	1:B:1371:ALA:O	2.19	0.42
1:B:1314:ARG:HB2	1:B:1361:VAL:HB	2.02	0.42
1:B:1286:GLU:OE1	1:B:1291:ALA:HB2	2.20	0.42
1:A:305:HIS:HD2	1:A:307:VAL:N	2.06	0.42
1:A:21:LYS:H	1:A:21:LYS:CE	2.31	0.42
1:B:1034:LEU:HD22	1:B:1039:VAL:HG13	2.02	0.42
1:B:1274:MET:CB	4:B:324:HOH:O	2.68	0.41
1:A:7:LEU:CD1	1:A:17:LEU:HB2	2.50	0.41
1:A:20:LEU:HB2	1:A:28:VAL:CG2	2.50	0.41
1:B:1199:ASN:O	1:B:1203:SER:HB3	2.20	0.41
1:A:87:TYR:CD1	1:A:95:PRO:HB3	2.54	0.41
1:B:1288:PHE:C	1:B:1288:PHE:CD1	2.93	0.41
1:B:1018:ASP:HB2	1:B:1030:ASP:HB3	2.01	0.41
1:A:339:ALA:HB1	1:A:367:ILE:HD13	2.03	0.41
1:B:1029:ILE:O	1:B:1031:ILE:HG23	2.21	0.41
1:B:1178:TYR:HB2	1:B:1184:PHE:CE1	2.55	0.41
1:A:212:ASN:HD22	1:A:214:ILE:H	1.66	0.41
1:B:1172:ALA:O	1:B:1175:CYS:HB2	2.20	0.41
1:B:1072:PRO:HB2	1:B:1075:GLN:HG3	2.03	0.41
1:B:1272:LEU:N	1:B:1272:LEU:HD12	2.35	0.41
1:A:303:PHE:HB3	1:A:357:LEU:HB3	2.03	0.41
1:B:1269:GLU:HB2	1:B:1273:LYS:HA	2.02	0.41
1:B:1426:ARG:NH1	4:B:53:HOH:O	2.53	0.41
1:B:1113:ILE:HD12	1:B:1113:ILE:O	2.21	0.41
1:A:250:ALA:CB	1:B:1257:ALA:HB1	2.51	0.41
1:B:1231:GLN:HE22	1:B:1239:ARG:CD	2.34	0.41
1:B:1001:ALA:HA	1:B:1004:LYS:CG	2.51	0.41
1:A:83:LEU:O	1:A:86:CYS:HB2	2.21	0.41
1:A:98:GLU:HB2	4:A:3166:HOH:O	2.20	0.41
1:B:1274:MET:SD	1:B:1277:GLU:OE2	2.79	0.41
1:A:412:TYR:CD1	1:B:1024:LEU:HB2	2.56	0.41
1:A:417:LYS:HD3	1:A:417:LYS:C	2.41	0.41
1:B:1231:GLN:HE22	1:B:1239:ARG:HD2	1.86	0.40
1:B:1299:ARG:HA	1:B:1303:PHE:O	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1263:ALA:HB2	4:B:321:HOH:O	2.20	0.40
1:A:35:GLY:HA2	1:A:40:PHE:CD2	2.55	0.40
1:B:1131:MET:SD	1:B:1381:VAL:HG22	2.61	0.40
1:A:294:LYS:HB2	1:A:297:SER:HA	2.02	0.40
1:A:274:MET:HB2	1:A:293:ASP:OD2	2.21	0.40
3:A:3000:NAI:H3B	3:A:3000:NAI:PA	2.60	0.40
1:A:260:TRP:CE2	1:A:264:HIS:HD2	2.40	0.40
1:A:125:ARG:NH2	4:A:3083:HOH:O	2.54	0.40
1:B:1131:MET:HE2	1:B:1380:THR:CG2	2.52	0.40
1:B:1349:ASP:HA	1:B:1350:PRO:HD3	1.98	0.40
1:A:348:ASN:HA	1:A:353:ILE:HD11	2.04	0.40
1:A:238:VAL:HG13	1:A:251:CYS:HB3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	424/427 (99%)	373 (88%)	43 (10%)	8 (2%)	12	19
1	B	424/427 (99%)	369 (87%)	48 (11%)	7 (2%)	14	22
All	All	848/854 (99%)	742 (88%)	91 (11%)	15 (2%)	13	20

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	ALA
1	A	294	LYS
1	A	422	SER
1	B	1294	LYS
1	B	1330	GLY
1	A	290	ARG
1	A	401	ASP
1	B	1150	ASP

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Mol	Chain	Res	Type
1	B	1286	GLU
1	B	1290	ARG
1	A	286	GLU
1	A	402	GLY
1	B	1012	ASP
1	B	1332	LYS
1	A	424	ILE

### 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	360/361 (100%)	345 (96%)	15 (4%)	40	66
1	B	360/361 (100%)	343 (95%)	17 (5%)	36	61
All	All	720/722 (100%)	688 (96%)	32 (4%)	39	64

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	63	GLU
1	A	83	LEU
1	A	119	ARG
1	A	134	MET
1	A	153	ASN
1	A	212	ASN
1	A	232	ASN
1	A	260	TRP
1	A	278	ILE
1	A	284	ILE
1	A	288	PHE
1	A	294	LYS
1	A	299	ARG
1	A	404	LYS
1	B	1007	LEU
1	B	1026	GLN
1	B	1081	ASN

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Mol	Chain	Res	Type
1	B	1098	GLU
1	B	1153	ASN
1	B	1156	HIS
1	B	1232	ASN
1	B	1260	TRP
1	B	1278	ILE
1	B	1284	ILE
1	B	1288	PHE
1	B	1294	LYS
1	B	1299	ARG
1	B	1335	LEU
1	B	1354	GLU
1	B	1404	LYS
1	B	1425	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	129	HIS
1	A	146	HIS
1	A	153	ASN
1	A	156	HIS
1	A	199	ASN
1	A	212	ASN
1	A	231	GLN
1	A	232	ASN
1	A	264	HIS
1	A	305	HIS
1	A	348	ASN
1	B	1026	GLN
1	B	1081	ASN
1	B	1097	GLN
1	B	1110	HIS
1	B	1129	HIS
1	B	1153	ASN
1	B	1182	GLN
1	B	1231	GLN
1	B	1232	ASN
1	B	1264	HIS
1	B	1305	HIS
1	B	1323	HIS

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Mol	Chain	Res	Type
1	B	1399	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

6 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	SO4	A	2004	-	4,4,4	0.91	0	6,6,6	0.23	0
2	SO4	A	2006	-	4,4,4	0.92	0	6,6,6	0.45	0
3	NAI	A	3000	-	48,48,48	1.67	8 (16%)	73,73,73	2.09	15 (20%)
2	SO4	B	2001	-	4,4,4	1.01	0	6,6,6	3.59	3 (50%)
2	SO4	B	2003	-	4,4,4	1.14	0	6,6,6	3.53	4 (66%)
3	NAI	B	3001	-	48,48,48	1.79	9 (18%)	73,73,73	1.74	10 (13%)

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	SO4	A	2004	-	-	0/0/0/0	0/0/0/0
2	SO4	A	2006	-	-	0/0/0/0	0/0/0/0
3	NAI	A	3000	-	-	1/30/72/72	0/3/5/5
2	SO4	B	2001	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2003	-	-	0/0/0/0	0/0/0/0
3	NAI	B	3001	-	-	0/30/72/72	0/3/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3001	NAI	PN-O3	6.29	1.71	1.59
3	A	3000	NAI	PN-O3	5.56	1.69	1.59
3	B	3001	NAI	C2N-C3N	-5.38	1.24	1.34
3	A	3000	NAI	C2N-C3N	-5.18	1.24	1.34
3	A	3000	NAI	C4N-C5N	-3.79	1.40	1.49
3	A	3000	NAI	PN-O2N	-3.56	1.37	1.51
3	B	3001	NAI	PN-O2N	-3.20	1.39	1.51
3	B	3001	NAI	C4N-C5N	-2.94	1.42	1.49
3	A	3000	NAI	C7N-C3N	-2.74	1.40	1.47
3	B	3001	NAI	C1D-N1N	-2.53	1.40	1.46
3	A	3000	NAI	C2A-N1A	2.42	1.38	1.33
3	B	3001	NAI	C6N-C5N	2.38	1.38	1.33
3	B	3001	NAI	C4A-N3A	-2.32	1.32	1.35
3	B	3001	NAI	C6N-N1N	2.18	1.44	1.37
3	A	3000	NAI	C6N-N1N	2.09	1.43	1.37
3	A	3000	NAI	C6N-C5N	2.07	1.37	1.33
3	B	3001	NAI	C2A-N1A	2.01	1.37	1.33

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3000	NAI	C1D-N1N-C2N	-8.51	106.52	121.02
2	B	2001	SO4	O2-S-O1	-7.31	85.33	109.53
3	B	3001	NAI	C6N-N1N-C2N	6.53	127.98	119.44
3	A	3000	NAI	C6N-N1N-C2N	6.32	127.71	119.44
2	B	2003	SO4	O4-S-O3	-5.30	86.70	109.08
3	B	3001	NAI	C1D-N1N-C2N	-5.25	112.08	121.02
2	B	2003	SO4	O2-S-O1	5.23	126.83	109.53
3	B	3001	NAI	C5N-C6N-N1N	-5.19	112.43	123.03
3	A	3000	NAI	O4B-C1B-N9A	-4.92	103.87	108.44
3	A	3000	NAI	C5N-C6N-N1N	-4.86	113.11	123.03
3	A	3000	NAI	C3N-C2N-N1N	-4.64	116.46	123.05
3	B	3001	NAI	O7N-C7N-C3N	-4.61	111.86	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3000	NAI	O7N-C7N-C3N	-4.28	112.47	120.51
3	A	3000	NAI	C4N-C3N-C2N	4.20	126.80	121.68
3	B	3001	NAI	C3N-C2N-N1N	-3.77	117.70	123.05
3	B	3001	NAI	C4N-C3N-C2N	3.56	126.03	121.68
3	B	3001	NAI	C3N-C7N-N7N	3.47	124.16	117.48
2	B	2003	SO4	O4-S-O1	-3.46	78.70	110.12
2	B	2001	SO4	O4-S-O1	-3.30	80.16	110.12
3	A	3000	NAI	C4B-O4B-C1B	3.24	113.27	109.75
3	A	3000	NAI	C4N-C3N-C7N	-3.17	109.73	118.38
3	A	3000	NAI	O5B-C5B-C4B	2.98	119.88	108.94
3	B	3001	NAI	O4B-C1B-N9A	-2.91	105.73	108.44
2	B	2001	SO4	O3-S-O1	-2.67	85.86	110.12
2	B	2003	SO4	O4-S-O2	-2.64	86.15	110.12
3	A	3000	NAI	C3N-C7N-N7N	2.60	122.49	117.48
3	A	3000	NAI	O4B-C4B-C5B	-2.60	100.07	109.36
3	A	3000	NAI	C3B-C2B-C1B	2.43	104.70	100.91
3	A	3000	NAI	O3-PN-O5D	-2.26	93.30	103.41
3	B	3001	NAI	C4N-C3N-C7N	-2.25	112.25	118.38
3	A	3000	NAI	C1D-N1N-C6N	2.25	125.77	120.79
3	B	3001	NAI	O3-PN-O5D	-2.24	93.38	103.41

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3000	NAI	PA-O5B-C5B-C4B

There are no ring outliers.

## 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.