



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:54 PM GMT

PDB ID : 4Q9N  
Title : Crystal structure of Chlamydia trachomatis enoyl-ACP reductase (FabI) in complex with NADH and AFN-1252  
Authors : Yao, J.; Abdelrahman, Y.; Robertson, R.M.; Cox, J.V.; Belland, R.J.; White, S.W.; Rock, C.O.  
Deposited on : 2014-05-01  
Resolution : 1.79 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.

---

The following versions of software and data (see [references ⓘ](#)) 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

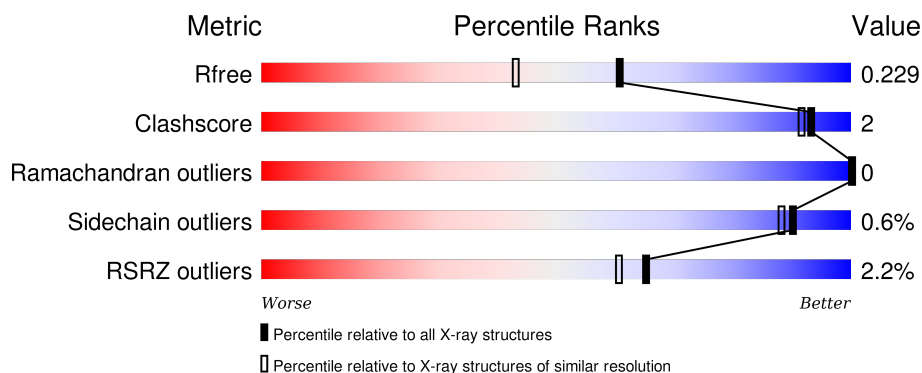
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.79 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))
$R_{free}$	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	298	<div> <div style="width: 96%;"></div> <div>96%</div> </div>
1	B	298	<div> <div style="width: 95%;"></div> <div>95%</div> </div>
1	C	298	<div> <div style="width: 93%;"></div> <div>93%</div> </div>
1	D	298	<div> <div style="width: 92%;"></div> <div>92%</div> </div>
1	E	298	<div> <div style="width: 95%;"></div> <div>95%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	298	<div><div>%</div><div><div></div></div><div>95%</div><div><div></div><div></div></div></div>
1	G	298	<div><div>%</div><div><div></div></div><div>93%</div><div>6%</div><div><div></div><div></div></div></div>
1	H	298	<div><div>%</div><div><div></div></div><div>95%</div><div><div></div><div></div></div></div>

## 2 Entry composition

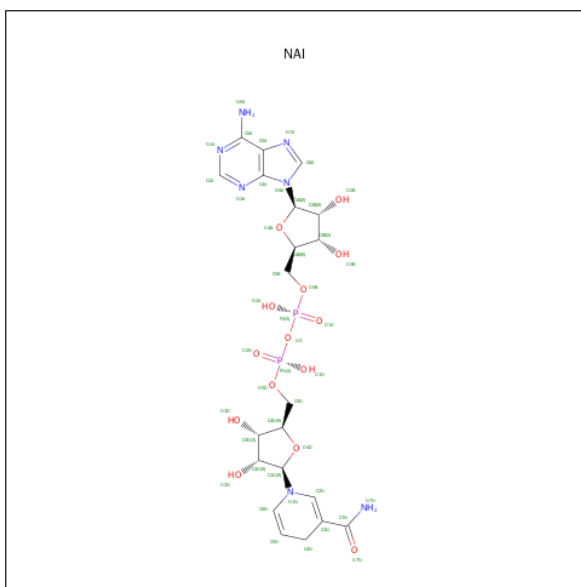
There are 4 unique types of molecules in this entry. The entry contains 19232 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Enoyl-[acyl-carrier-protein] reductase [NADH].

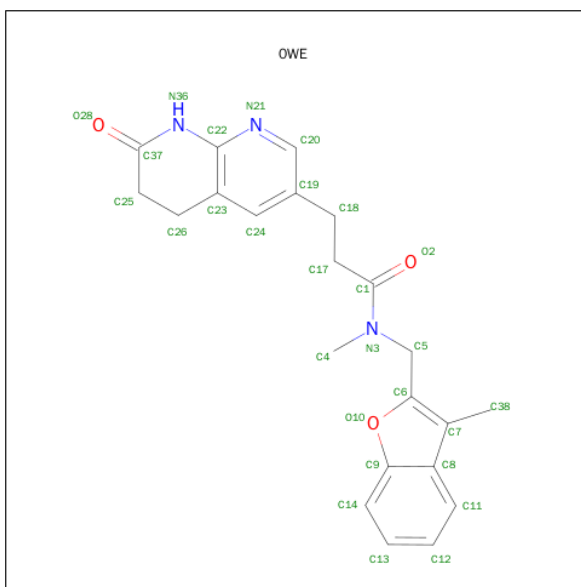
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	0	0
			2212	1421	364	418	9			
1	B	295	Total	C	N	O	S	0	0	0
			2206	1420	362	415	9			
1	C	295	Total	C	N	O	S	0	0	0
			2220	1427	366	418	9			
1	D	295	Total	C	N	O	S	0	0	0
			2216	1425	366	416	9			
1	E	295	Total	C	N	O	S	0	0	0
			2202	1418	362	413	9			
1	F	295	Total	C	N	O	S	0	0	0
			2220	1427	366	418	9			
1	G	295	Total	C	N	O	S	0	0	0
			2210	1422	363	416	9			
1	H	295	Total	C	N	O	S	0	0	0
			2214	1424	363	418	9			

- 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		
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 N-METHYL-N-[(3-METHYL-1-BENZOFURAN-2-YL)METHYL]-3-(7-OXO-5,6,7,8-TETRAHYDRO-1,8-NAPHTHYRIDIN-3-YL)PROPANAMIDE (three-letter code: 0WE) (formula: C<sub>22</sub>H<sub>23</sub>N<sub>3</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	22	3	3		
3	B	1	Total	C	N	O	0	0
			28	22	3	3		
3	C	1	Total	C	N	O	0	0
			28	22	3	3		
3	D	1	Total	C	N	O	0	0
			28	22	3	3		
3	E	1	Total	C	N	O	0	0
			28	22	3	3		
3	F	1	Total	C	N	O	0	0
			28	22	3	3		
3	G	1	Total	C	N	O	0	0
			28	22	3	3		
3	H	1	Total	C	N	O	0	0
			28	22	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	120	Total	O	0	0
			120	120		
4	B	106	Total	O	0	0
			106	106		
4	C	110	Total	O	0	0
			110	110		
4	D	99	Total	O	0	0
			99	99		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	119	Total 119	O 119	0	0
4	F	129	Total 129	O 129	0	0
4	G	132	Total 132	O 132	0	0
4	H	141	Total 141	O 141	0	0

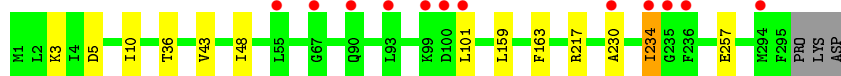
### 3 Residue-property plots [i](#)

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: Enoyl-[acyl-carrier-protein] reductase [NADH]



- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



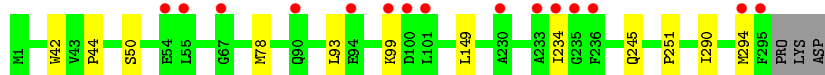
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



Chain F:  95%



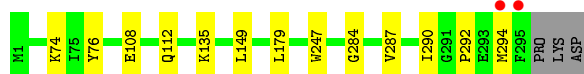
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain G:  93% 6%



- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain H:  95%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.15Å 96.15Å 263.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.61 – 1.79 48.07 – 1.79	Depositor EDS
% Data completeness (in resolution range)	98.6 (38.61-1.79) 98.7 (48.07-1.79)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 1.79Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.186 , 0.229 0.186 , 0.229	Depositor DCC
$R_{free}$ test set	10940 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.5	Xtriage
Anisotropy	0.669	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.3	EDS
Estimated twinning fraction	0.470 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	1 of 218478 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	19232	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.33	0/2263	0.50	0/3075
1	B	0.33	0/2257	0.51	0/3066
1	C	0.34	0/2271	0.52	0/3083
1	D	0.34	0/2267	0.51	0/3078
1	E	0.34	0/2253	0.52	0/3061
1	F	0.33	0/2271	0.50	0/3083
1	G	0.35	0/2261	0.52	0/3071
1	H	0.35	0/2265	0.52	0/3076
All	All	0.34	0/18108	0.51	0/24593

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2212	0	2193	6	0
1	B	2206	0	2194	12	0
1	C	2220	0	2215	13	0
1	D	2216	0	2211	11	0
1	E	2202	0	2190	6	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2220	0	2215	8	0
1	G	2210	0	2200	11	0
1	H	2214	0	2204	6	0
2	A	44	0	27	0	0
2	B	44	0	27	0	0
2	C	44	0	27	0	0
2	D	44	0	27	0	0
2	E	44	0	27	0	0
2	F	44	0	27	0	0
2	G	44	0	27	0	0
2	H	44	0	27	0	0
3	A	28	0	23	1	0
3	B	28	0	23	1	0
3	C	28	0	23	1	0
3	D	28	0	23	1	0
3	E	28	0	23	1	0
3	F	28	0	23	0	0
3	G	28	0	23	0	0
3	H	28	0	23	1	0
4	A	120	0	0	0	0
4	B	106	0	0	1	0
4	C	110	0	0	1	0
4	D	99	0	0	0	0
4	E	119	0	0	0	0
4	F	129	0	0	2	0
4	G	132	0	0	0	0
4	H	141	0	0	0	0
All	All	19232	0	18022	68	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 2.

All (68) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:LYS:HE3	1:B:5:ASP:HA	1.77	0.66
1:B:3:LYS:NZ	1:C:2:LEU:H	1.94	0.66
1:G:149:LEU:HD13	1:H:149:LEU:HD13	1.79	0.63
1:H:74:LYS:HG2	1:H:76:TYR:CZ	2.34	0.62
1:D:245:GLN:HG3	1:D:251:PRO:O	2.01	0.61
1:F:250:LEU:HD11	1:G:217:ARG:HG2	1.83	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ARG:HG2	1:C:250:LEU:HD11	1.84	0.60
1:H:290:ILE:HD12	1:H:294:MET:HB2	1.81	0.60
1:C:74:LYS:HG2	1:C:76:TYR:CZ	2.40	0.56
3:E:302:0WE:H12	3:E:302:0WE:H19	1.87	0.56
3:C:302:0WE:H12	3:C:302:0WE:H19	1.88	0.54
1:C:290:ILE:HD12	1:C:294:MET:HB2	1.90	0.54
1:G:86:GLU:OE1	1:G:86:GLU:N	2.37	0.53
1:G:133:ILE:HD13	1:G:234:ILE:HD11	1.91	0.52
1:B:3:LYS:HZ2	1:C:2:LEU:H	1.56	0.51
1:C:231:GLY:O	1:C:234:ILE:HG12	2.11	0.51
1:G:43:VAL:HG13	1:G:101:LEU:HD12	1.92	0.51
3:H:302:0WE:H19	3:H:302:0WE:H12	1.91	0.51
1:F:217:ARG:HG2	1:G:250:LEU:HD11	1.93	0.50
1:C:149:LEU:HD13	1:D:149:LEU:HD13	1.93	0.50
1:B:257:GLU:OE1	1:B:257:GLU:N	2.43	0.50
1:F:231:GLY:O	1:F:234:ILE:HG12	2.13	0.49
1:D:68:GLU:HG2	1:D:69:LEU:N	2.28	0.48
1:A:89:PRO:HG2	1:A:92:ILE:HG12	1.95	0.48
1:C:135:LYS:HD3	4:C:424:HOH:O	2.14	0.48
1:G:74:LYS:HG2	1:G:76:TYR:CZ	2.49	0.48
1:E:93:LEU:O	1:E:99:LYS:HD3	2.14	0.48
1:F:28:LYS:HG3	1:F:70:LEU:HD22	1.96	0.47
1:A:132:GLU:HB3	1:A:135:LYS:HD2	1.96	0.47
1:C:135:LYS:N	1:C:135:LYS:HD2	2.30	0.47
1:B:43:VAL:HG13	1:B:101:LEU:HD12	1.96	0.47
1:F:42:TRP:HA	1:F:78:MET:O	2.15	0.47
3:D:302:0WE:H19	3:D:302:0WE:H12	1.98	0.46
1:F:183:ARG:NH2	4:F:463:HOH:O	2.49	0.46
1:C:52:SER:HA	1:C:57:LYS:HD2	1.98	0.46
3:B:302:0WE:H19	3:B:302:0WE:H12	1.96	0.46
1:E:290:ILE:HD12	1:E:294:MET:HB2	1.97	0.46
1:G:108:GLU:O	1:G:111:GLU:HG2	2.17	0.45
1:B:3:LYS:HZ3	1:C:2:LEU:H	1.63	0.45
1:H:284:GLY:O	1:H:287:VAL:HG22	2.17	0.45
1:B:10:ILE:HD13	1:B:36:THR:HB	1.98	0.45
1:E:42:TRP:CG	1:E:44:PRO:HD2	2.52	0.44
1:H:247:TRP:CD1	1:H:292:PRO:HD3	2.53	0.44
1:D:234:ILE:HD12	1:D:236:PHE:H	1.83	0.43
1:G:123:LEU:HB3	1:G:173:THR:HG22	2.01	0.43
1:A:231:GLY:O	1:A:234:ILE:HG12	2.20	0.42
1:H:108:GLU:O	1:H:112:GLN:HG3	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:LEU:HD11	1:D:217:ARG:HG2	2.01	0.42
1:B:3:LYS:HG3	1:B:5:ASP:HB2	2.01	0.42
1:D:231:GLY:O	1:D:234:ILE:HG13	2.20	0.42
1:G:4:ILE:HG23	1:G:268:SER:HB3	2.01	0.42
1:C:42:TRP:CG	1:C:44:PRO:HD2	2.54	0.42
1:E:149:LEU:HD13	1:F:149:LEU:HD13	2.01	0.42
1:F:86:GLU:OE1	4:F:481:HOH:O	2.22	0.42
1:D:52:SER:HB3	1:D:57:LYS:HG2	2.03	0.41
1:B:48:ILE:HG12	4:B:425:HOH:O	2.21	0.41
1:E:245:GLN:HG2	1:E:251:PRO:O	2.20	0.41
1:E:42:TRP:HA	1:E:78:MET:O	2.21	0.41
1:C:24:TRP:HE1	1:C:28:LYS:HD2	1.85	0.41
1:A:47:LYS:O	1:A:51:GLN:HB2	2.20	0.41
1:A:217:ARG:HG2	1:D:250:LEU:HD11	2.01	0.41
1:D:4:ILE:HG23	1:D:268:SER:HB3	2.02	0.41
1:B:159:LEU:O	1:B:163:PHE:HB2	2.21	0.41
1:B:230:ALA:O	1:B:234:ILE:HD12	2.20	0.41
3:A:302:0WE:H19	3:A:302:0WE:H12	2.03	0.41
1:G:42:TRP:CD2	1:G:44:PRO:HD2	2.56	0.40
1:D:74:LYS:HG2	1:D:76:TYR:CZ	2.57	0.40
1:D:42:TRP:CD2	1:D:44:PRO:HD2	2.56	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	293/298 (98%)	283 (97%)	10 (3%)	0	100	100
1	B	293/298 (98%)	285 (97%)	8 (3%)	0	100	100
1	C	293/298 (98%)	285 (97%)	8 (3%)	0	100	100
1	D	293/298 (98%)	285 (97%)	8 (3%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	293/298 (98%)	284 (97%)	9 (3%)	0	100	100
1	F	293/298 (98%)	282 (96%)	11 (4%)	0	100	100
1	G	293/298 (98%)	287 (98%)	6 (2%)	0	100	100
1	H	293/298 (98%)	286 (98%)	7 (2%)	0	100	100
All	All	2344/2384 (98%)	2277 (97%)	67 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	226/233 (97%)	226 (100%)	0	100	100
1	B	225/233 (97%)	224 (100%)	1 (0%)	93	92
1	C	228/233 (98%)	226 (99%)	2 (1%)	84	80
1	D	227/233 (97%)	225 (99%)	2 (1%)	84	80
1	E	224/233 (96%)	222 (99%)	2 (1%)	84	80
1	F	228/233 (98%)	227 (100%)	1 (0%)	93	92
1	G	226/233 (97%)	225 (100%)	1 (0%)	93	92
1	H	227/233 (97%)	225 (99%)	2 (1%)	84	80
All	All	1811/1864 (97%)	1800 (99%)	11 (1%)	90	88

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	234	ILE
1	C	153	SER
1	C	179	LEU
1	D	127	LEU
1	D	179	LEU
1	E	50	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	234	ILE
1	F	179	LEU
1	G	179	LEU
1	H	135	LYS
1	H	179	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

16 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	301	-	38,48,48	3.62	14 (36%)	48,73,73	2.73	11 (22%)
3	0WE	A	302	-	27,31,31	3.21	10 (37%)	26,44,44	2.03	11 (42%)
2	NAI	B	301	-	38,48,48	3.66	15 (39%)	48,73,73	2.76	10 (20%)
3	0WE	B	302	-	27,31,31	3.16	9 (33%)	26,44,44	2.10	11 (42%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAI	C	301	-	38,48,48	3.68	15 (39%)	48,73,73	2.70	11 (22%)
3	0WE	C	302	-	27,31,31	3.02	9 (33%)	26,44,44	2.14	12 (46%)
2	NAI	D	301	-	38,48,48	3.69	14 (36%)	48,73,73	2.64	10 (20%)
3	0WE	D	302	-	27,31,31	3.21	9 (33%)	26,44,44	2.07	10 (38%)
2	NAI	E	301	-	38,48,48	3.68	14 (36%)	48,73,73	2.70	9 (18%)
3	0WE	E	302	-	27,31,31	3.06	9 (33%)	26,44,44	2.13	9 (34%)
2	NAI	F	301	-	38,48,48	3.66	15 (39%)	48,73,73	2.74	10 (20%)
3	0WE	F	302	-	27,31,31	3.15	10 (37%)	26,44,44	2.04	10 (38%)
2	NAI	G	301	-	38,48,48	3.68	13 (34%)	48,73,73	2.84	12 (25%)
3	0WE	G	302	-	27,31,31	3.20	10 (37%)	26,44,44	2.07	9 (34%)
2	NAI	H	301	-	38,48,48	3.64	13 (34%)	48,73,73	2.69	11 (22%)
3	0WE	H	302	-	27,31,31	2.98	9 (33%)	26,44,44	2.10	11 (42%)

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	301	-	-	0/25/72/72	0/5/5/5
3	0WE	A	302	-	-	0/11/22/22	0/3/4/4
2	NAI	B	301	-	-	0/25/72/72	0/5/5/5
3	0WE	B	302	-	-	0/11/22/22	0/3/4/4
2	NAI	C	301	-	-	0/25/72/72	0/5/5/5
3	0WE	C	302	-	-	0/11/22/22	0/3/4/4
2	NAI	D	301	-	-	0/25/72/72	0/5/5/5
3	0WE	D	302	-	-	0/11/22/22	0/3/4/4
2	NAI	E	301	-	-	0/25/72/72	0/5/5/5
3	0WE	E	302	-	-	0/11/22/22	0/3/4/4
2	NAI	F	301	-	-	0/25/72/72	0/5/5/5
3	0WE	F	302	-	-	0/11/22/22	0/3/4/4
2	NAI	G	301	-	-	0/25/72/72	0/5/5/5
3	0WE	G	302	-	-	0/11/22/22	0/3/4/4
2	NAI	H	301	-	-	0/25/72/72	0/5/5/5
3	0WE	H	302	-	-	0/11/22/22	0/3/4/4

All (188) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	NAI	C4N-C5N	-9.00	1.29	1.49

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	301	NAI	C4N-C5N	-8.91	1.29	1.49
2	D	301	NAI	C4N-C5N	-8.88	1.30	1.49
2	E	301	NAI	C4N-C5N	-8.86	1.30	1.49
2	C	301	NAI	C4N-C5N	-8.85	1.30	1.49
2	B	301	NAI	C4N-C5N	-8.83	1.30	1.49
2	F	301	NAI	C4N-C5N	-8.64	1.30	1.49
2	A	301	NAI	C4N-C5N	-8.31	1.31	1.49
2	C	301	NAI	C6N-C5N	-5.09	1.23	1.33
2	G	301	NAI	C6N-C5N	-4.84	1.23	1.33
2	H	301	NAI	C6N-C5N	-4.84	1.23	1.33
2	E	301	NAI	C6N-C5N	-4.79	1.23	1.33
2	A	301	NAI	C6N-C5N	-4.79	1.23	1.33
2	F	301	NAI	C6N-C5N	-4.75	1.23	1.33
2	D	301	NAI	C6N-C5N	-4.68	1.24	1.33
2	B	301	NAI	C6N-C5N	-4.50	1.24	1.33
2	A	301	NAI	C5A-C4A	-4.47	1.30	1.40
2	F	301	NAI	C5A-C4A	-4.45	1.30	1.40
2	G	301	NAI	C5A-C4A	-4.20	1.31	1.40
2	D	301	NAI	C5A-C4A	-4.16	1.31	1.40
2	B	301	NAI	C5A-C4A	-4.14	1.31	1.40
2	E	301	NAI	C5A-C4A	-4.07	1.31	1.40
2	H	301	NAI	C5A-C4A	-3.88	1.31	1.40
2	C	301	NAI	C5A-C4A	-3.81	1.31	1.40
2	G	301	NAI	C6N-N1N	-3.64	1.27	1.37
2	D	301	NAI	C6N-N1N	-3.53	1.27	1.37
2	C	301	NAI	C6N-N1N	-3.41	1.27	1.37
2	H	301	NAI	C6N-N1N	-3.40	1.27	1.37
2	F	301	NAI	C6N-N1N	-3.37	1.27	1.37
2	E	301	NAI	C6N-N1N	-3.27	1.28	1.37
2	B	301	NAI	C6N-N1N	-3.23	1.28	1.37
2	A	301	NAI	C6N-N1N	-3.15	1.28	1.37
2	B	301	NAI	C2B-C3B	-3.03	1.45	1.53
2	G	301	NAI	C2B-C3B	-3.02	1.45	1.53
2	F	301	NAI	C2B-C3B	-3.01	1.45	1.53
2	D	301	NAI	C2B-C3B	-2.98	1.45	1.53
2	C	301	NAI	C2B-C3B	-2.97	1.45	1.53
2	H	301	NAI	C2B-C3B	-2.94	1.45	1.53
3	E	302	0WE	C18-C17	-2.91	1.37	1.52
2	E	301	NAI	C2B-C3B	-2.90	1.45	1.53
3	H	302	0WE	C18-C17	-2.89	1.37	1.52
3	A	302	0WE	C18-C17	-2.88	1.37	1.52
3	F	302	0WE	C18-C17	-2.85	1.38	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NAI	C2B-C3B	-2.83	1.45	1.53
3	C	302	0WE	C18-C17	-2.80	1.38	1.52
3	G	302	0WE	C18-C17	-2.74	1.38	1.52
3	B	302	0WE	C18-C17	-2.72	1.38	1.52
3	D	302	0WE	C18-C17	-2.68	1.38	1.52
2	G	301	NAI	O3B-C3B	-2.41	1.37	1.43
2	E	301	NAI	O3B-C3B	-2.37	1.37	1.43
2	D	301	NAI	O3B-C3B	-2.31	1.37	1.43
2	B	301	NAI	O3B-C3B	-2.30	1.37	1.43
2	H	301	NAI	O3B-C3B	-2.22	1.37	1.43
2	A	301	NAI	C2D-C3D	-2.20	1.47	1.53
2	C	301	NAI	O3B-C3B	-2.17	1.37	1.43
2	A	301	NAI	O3B-C3B	-2.17	1.37	1.43
2	B	301	NAI	O4D-C4D	-2.09	1.40	1.45
2	C	301	NAI	C2D-C1D	-2.07	1.46	1.53
2	F	301	NAI	C2D-C1D	-2.04	1.46	1.53
2	F	301	NAI	O3B-C3B	-2.02	1.38	1.43
2	F	301	NAI	C5A-N7A	2.00	1.46	1.39
2	B	301	NAI	C5A-N7A	2.01	1.46	1.39
2	D	301	NAI	C5A-N7A	2.03	1.46	1.39
2	E	301	NAI	C5A-N7A	2.04	1.46	1.39
3	G	302	0WE	C12-C11	2.04	1.41	1.36
3	A	302	0WE	C12-C11	2.04	1.41	1.36
3	F	302	0WE	C12-C11	2.05	1.41	1.36
2	C	301	NAI	C5A-N7A	2.06	1.46	1.39
3	E	302	0WE	C14-C9	2.47	1.43	1.38
3	F	302	0WE	C22-N36	2.48	1.41	1.38
3	E	302	0WE	C24-C19	2.51	1.43	1.39
3	C	302	0WE	C14-C9	2.57	1.43	1.38
3	H	302	0WE	C14-C9	2.63	1.43	1.38
3	D	302	0WE	C14-C9	2.63	1.43	1.38
3	F	302	0WE	C14-C9	2.64	1.43	1.38
3	B	302	0WE	C14-C9	2.65	1.43	1.38
3	B	302	0WE	C24-C19	2.66	1.44	1.39
3	A	302	0WE	C37-N36	2.66	1.38	1.35
3	G	302	0WE	C14-C9	2.66	1.43	1.38
3	D	302	0WE	C24-C19	2.67	1.44	1.39
3	G	302	0WE	C24-C19	2.67	1.44	1.39
3	A	302	0WE	C14-C9	2.75	1.43	1.38
3	F	302	0WE	C37-N36	2.83	1.38	1.35
3	A	302	0WE	C22-N36	2.84	1.41	1.38
3	A	302	0WE	C24-C19	2.87	1.44	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	0WE	C22-N36	2.88	1.42	1.38
2	F	301	NAI	C6A-N6A	2.92	1.44	1.34
3	F	302	0WE	C24-C19	2.94	1.44	1.39
3	E	302	0WE	C22-N36	2.97	1.42	1.38
3	C	302	0WE	C24-C19	3.00	1.44	1.39
3	H	302	0WE	C24-C19	3.05	1.44	1.39
2	G	301	NAI	O7N-C7N	3.06	1.32	1.24
3	H	302	0WE	C22-N36	3.07	1.42	1.38
2	A	301	NAI	C6A-N6A	3.10	1.44	1.34
3	C	302	0WE	C22-N36	3.11	1.42	1.38
2	F	301	NAI	O7N-C7N	3.14	1.32	1.24
2	A	301	NAI	O7N-C7N	3.16	1.32	1.24
3	G	302	0WE	C22-N36	3.18	1.42	1.38
2	E	301	NAI	C6A-N6A	3.25	1.45	1.34
3	B	302	0WE	C37-N36	3.26	1.39	1.35
2	B	301	NAI	C6A-N6A	3.26	1.45	1.34
2	D	301	NAI	O7N-C7N	3.31	1.32	1.24
2	D	301	NAI	C6A-N6A	3.33	1.45	1.34
2	C	301	NAI	O7N-C7N	3.33	1.32	1.24
2	B	301	NAI	O7N-C7N	3.38	1.32	1.24
2	C	301	NAI	C6A-N6A	3.40	1.45	1.34
3	C	302	0WE	C37-N36	3.40	1.39	1.35
2	H	301	NAI	C6A-N6A	3.42	1.45	1.34
2	H	301	NAI	O7N-C7N	3.45	1.33	1.24
2	E	301	NAI	O7N-C7N	3.45	1.33	1.24
2	G	301	NAI	C6A-N6A	3.47	1.45	1.34
3	D	302	0WE	C22-N36	3.48	1.42	1.38
3	E	302	0WE	C37-N36	3.52	1.39	1.35
3	H	302	0WE	C37-N36	3.57	1.39	1.35
3	G	302	0WE	C37-N36	3.63	1.39	1.35
3	D	302	0WE	C37-N36	3.68	1.39	1.35
3	E	302	0WE	C20-C19	4.33	1.45	1.38
3	C	302	0WE	C7-C8	4.39	1.45	1.40
3	F	302	0WE	C20-C19	4.59	1.46	1.38
3	H	302	0WE	C20-C19	4.63	1.46	1.38
3	A	302	0WE	C20-C19	4.69	1.46	1.38
3	C	302	0WE	C20-C19	4.69	1.46	1.38
3	E	302	0WE	C7-C8	4.75	1.45	1.40
3	B	302	0WE	C20-C19	4.77	1.46	1.38
3	H	302	0WE	C7-C8	4.86	1.45	1.40
3	D	302	0WE	C20-C19	4.86	1.46	1.38
3	G	302	0WE	C20-C19	4.96	1.46	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	302	0WE	C7-C8	5.14	1.46	1.40
3	G	302	0WE	C7-C8	5.16	1.46	1.40
3	D	302	0WE	C7-C8	5.22	1.46	1.40
3	B	302	0WE	C7-C8	5.30	1.46	1.40
2	H	301	NAI	C4A-N3A	5.40	1.43	1.35
3	A	302	0WE	C7-C8	5.42	1.46	1.40
2	G	301	NAI	C4A-N3A	5.56	1.43	1.35
2	B	301	NAI	C4A-N3A	5.57	1.43	1.35
2	E	301	NAI	C4A-N3A	5.74	1.44	1.35
2	A	301	NAI	C4A-N3A	5.97	1.44	1.35
2	D	301	NAI	C4A-N3A	6.04	1.44	1.35
2	C	301	NAI	C4A-N3A	6.05	1.44	1.35
2	F	301	NAI	C4A-N3A	6.13	1.44	1.35
2	D	301	NAI	C8A-N7A	6.13	1.46	1.34
2	G	301	NAI	C8A-N7A	6.24	1.46	1.34
2	A	301	NAI	C8A-N7A	6.27	1.46	1.34
2	F	301	NAI	C8A-N7A	6.35	1.46	1.34
2	H	301	NAI	C8A-N7A	6.41	1.46	1.34
2	B	301	NAI	C8A-N7A	6.41	1.46	1.34
2	C	301	NAI	C8A-N7A	6.42	1.46	1.34
2	E	301	NAI	C8A-N7A	6.48	1.47	1.34
3	A	302	0WE	C23-C22	6.90	1.48	1.41
3	H	302	0WE	C23-C22	6.99	1.48	1.41
3	C	302	0WE	C23-C22	7.05	1.48	1.41
3	B	302	0WE	C23-C22	7.06	1.48	1.41
3	D	302	0WE	C23-C22	7.10	1.48	1.41
3	E	302	0WE	C23-C22	7.14	1.48	1.41
2	F	301	NAI	C2A-N1A	7.33	1.47	1.33
2	C	301	NAI	C2A-N1A	7.37	1.47	1.33
2	A	301	NAI	C2A-N1A	7.39	1.47	1.33
3	G	302	0WE	C23-C22	7.39	1.48	1.41
2	H	301	NAI	C2A-N1A	7.45	1.48	1.33
3	F	302	0WE	C23-C22	7.48	1.48	1.41
2	B	301	NAI	C2A-N1A	7.50	1.48	1.33
2	D	301	NAI	C2A-N1A	7.65	1.48	1.33
2	G	301	NAI	C2A-N1A	7.65	1.48	1.33
2	E	301	NAI	C2A-N1A	7.66	1.48	1.33
2	B	301	NAI	C2A-N3A	8.48	1.47	1.32
2	E	301	NAI	C2A-N3A	8.48	1.47	1.32
2	G	301	NAI	C2A-N3A	8.57	1.47	1.32
2	A	301	NAI	C2A-N3A	8.77	1.47	1.32
2	H	301	NAI	C2A-N3A	8.78	1.47	1.32

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	NAI	C2A-N3A	8.81	1.47	1.32
2	D	301	NAI	C2A-N3A	8.84	1.47	1.32
2	C	301	NAI	C2A-N3A	8.87	1.47	1.32
3	H	302	0WE	C1-N3	9.05	1.45	1.34
3	C	302	0WE	C1-N3	9.80	1.46	1.34
3	E	302	0WE	C1-N3	10.15	1.47	1.34
2	H	301	NAI	C2N-C3N	10.21	1.59	1.34
2	A	301	NAI	C2N-C3N	10.23	1.59	1.34
2	C	301	NAI	C2N-C3N	10.28	1.60	1.34
3	G	302	0WE	C1-N3	10.36	1.47	1.34
3	F	302	0WE	C1-N3	10.40	1.47	1.34
2	D	301	NAI	C2N-C3N	10.42	1.60	1.34
2	F	301	NAI	C2N-C3N	10.44	1.60	1.34
2	E	301	NAI	C2N-C3N	10.48	1.60	1.34
3	D	302	0WE	C1-N3	10.54	1.47	1.34
2	G	301	NAI	C2N-C3N	10.56	1.60	1.34
2	B	301	NAI	C2N-C3N	10.58	1.60	1.34
3	B	302	0WE	C1-N3	10.61	1.47	1.34
3	A	302	0WE	C1-N3	11.05	1.48	1.34

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	NAI	N3A-C2A-N1A	-15.45	117.07	128.89
2	B	301	NAI	N3A-C2A-N1A	-14.74	117.61	128.89
2	F	301	NAI	N3A-C2A-N1A	-14.74	117.61	128.89
2	E	301	NAI	N3A-C2A-N1A	-14.59	117.72	128.89
2	C	301	NAI	N3A-C2A-N1A	-14.53	117.77	128.89
2	H	301	NAI	N3A-C2A-N1A	-14.52	117.78	128.89
2	A	301	NAI	N3A-C2A-N1A	-14.42	117.86	128.89
2	D	301	NAI	N3A-C2A-N1A	-14.14	118.06	128.89
2	A	301	NAI	C4B-O4B-C1B	-4.93	104.31	109.72
2	F	301	NAI	C4B-O4B-C1B	-4.88	104.36	109.72
2	B	301	NAI	C4B-O4B-C1B	-4.72	104.53	109.72
3	E	302	0WE	O28-C37-N36	-4.46	117.37	121.53
3	A	302	0WE	O28-C37-N36	-4.36	117.46	121.53
2	E	301	NAI	C4B-O4B-C1B	-4.28	105.01	109.72
2	B	301	NAI	C1B-N9A-C4A	-4.26	120.52	126.94
3	B	302	0WE	O28-C37-N36	-4.17	117.64	121.53
2	G	301	NAI	C4B-O4B-C1B	-4.16	105.15	109.72
2	C	301	NAI	C3N-C2N-N1N	-4.12	117.23	123.14
2	A	301	NAI	C1B-N9A-C4A	-4.11	120.74	126.94

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301	NAI	C1B-N9A-C4A	-3.90	121.06	126.94
2	F	301	NAI	C1B-N9A-C4A	-3.86	121.11	126.94
3	F	302	0WE	O28-C37-N36	-3.78	118.01	121.53
2	C	301	NAI	C4B-O4B-C1B	-3.77	105.58	109.72
2	E	301	NAI	C1B-N9A-C4A	-3.75	121.29	126.94
3	C	302	0WE	O28-C37-N36	-3.72	118.06	121.53
2	D	301	NAI	C4B-O4B-C1B	-3.69	105.66	109.72
2	D	301	NAI	C1B-N9A-C4A	-3.68	121.39	126.94
2	H	301	NAI	C4B-O4B-C1B	-3.66	105.70	109.72
2	G	301	NAI	C1B-N9A-C4A	-3.64	121.45	126.94
3	D	302	0WE	C6-C5-N3	-3.53	106.24	113.84
2	B	301	NAI	C3N-C2N-N1N	-3.42	118.25	123.14
2	G	301	NAI	C3N-C2N-N1N	-3.39	118.29	123.14
2	H	301	NAI	C3N-C2N-N1N	-3.29	118.43	123.14
3	H	302	0WE	C23-C24-C19	-3.29	116.45	121.80
2	E	301	NAI	C3N-C2N-N1N	-3.26	118.48	123.14
2	C	301	NAI	C1B-N9A-C4A	-3.16	122.18	126.94
3	E	302	0WE	C18-C19-C20	-3.09	116.59	121.85
2	F	301	NAI	C3N-C2N-N1N	-3.06	118.76	123.14
3	C	302	0WE	C6-C5-N3	-3.05	107.28	113.84
3	F	302	0WE	C18-C19-C20	-3.02	116.71	121.85
3	D	302	0WE	C23-C24-C19	-2.99	116.94	121.80
3	G	302	0WE	C6-C5-N3	-2.95	107.49	113.84
3	C	302	0WE	C18-C19-C20	-2.94	116.85	121.85
3	H	302	0WE	O2-C1-N3	-2.94	117.79	122.18
3	F	302	0WE	C23-C24-C19	-2.94	117.02	121.80
3	C	302	0WE	C23-C24-C19	-2.93	117.04	121.80
3	B	302	0WE	C18-C19-C20	-2.91	116.91	121.85
3	H	302	0WE	C6-C5-N3	-2.90	107.59	113.84
3	D	302	0WE	O28-C37-N36	-2.90	118.82	121.53
3	C	302	0WE	O2-C1-N3	-2.89	117.86	122.18
3	H	302	0WE	O28-C37-N36	-2.82	118.90	121.53
3	H	302	0WE	C18-C19-C20	-2.80	117.09	121.85
3	D	302	0WE	C18-C19-C20	-2.75	117.18	121.85
2	B	301	NAI	C4A-C5A-N7A	-2.73	106.97	109.48
3	G	302	0WE	C23-C24-C19	-2.73	117.37	121.80
3	A	302	0WE	C18-C19-C20	-2.69	117.28	121.85
3	A	302	0WE	C19-C20-N21	-2.67	119.27	123.80
3	E	302	0WE	C6-C5-N3	-2.67	108.09	113.84
3	G	302	0WE	O28-C37-N36	-2.58	119.12	121.53
2	H	301	NAI	C4A-C5A-N7A	-2.57	107.12	109.48
3	E	302	0WE	C23-C24-C19	-2.54	117.67	121.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	0WE	C23-C24-C19	-2.51	117.72	121.80
2	A	301	NAI	C1D-N1N-C2N	-2.50	116.55	120.91
3	C	302	0WE	C19-C20-N21	-2.50	119.56	123.80
2	D	301	NAI	C3N-C2N-N1N	-2.48	119.59	123.14
3	B	302	0WE	C6-C5-N3	-2.45	108.55	113.84
2	F	301	NAI	C4A-C5A-N7A	-2.45	107.23	109.48
3	B	302	0WE	O2-C1-N3	-2.44	118.53	122.18
3	H	302	0WE	C19-C20-N21	-2.42	119.68	123.80
3	G	302	0WE	C18-C19-C20	-2.36	117.85	121.85
2	A	301	NAI	C3N-C2N-N1N	-2.35	119.78	123.14
3	E	302	0WE	C19-C20-N21	-2.33	119.83	123.80
2	A	301	NAI	C4A-C5A-N7A	-2.31	107.35	109.48
3	F	302	0WE	O2-C1-N3	-2.30	118.75	122.18
2	C	301	NAI	C4A-C5A-N7A	-2.29	107.37	109.48
2	A	301	NAI	O4D-C1D-C2D	-2.29	101.27	106.58
3	B	302	0WE	C19-C20-N21	-2.27	119.93	123.80
2	D	301	NAI	O4D-C1D-C2D	-2.27	101.32	106.58
2	G	301	NAI	C4A-C5A-N7A	-2.27	107.39	109.48
2	G	301	NAI	O4D-C1D-C2D	-2.24	101.38	106.58
2	E	301	NAI	C4A-C5A-N7A	-2.23	107.43	109.48
3	B	302	0WE	C23-C24-C19	-2.21	118.21	121.80
3	D	302	0WE	O2-C1-N3	-2.19	118.91	122.18
3	A	302	0WE	O2-C1-N3	-2.18	118.92	122.18
3	A	302	0WE	C6-C5-N3	-2.17	109.16	113.84
2	D	301	NAI	C4A-C5A-N7A	-2.15	107.50	109.48
2	D	301	NAI	O4D-C1D-N1N	-2.13	103.57	108.07
2	B	301	NAI	O4D-C1D-C2D	-2.11	101.68	106.58
2	H	301	NAI	PN-O3-PA	-2.09	126.87	132.73
3	D	302	0WE	C19-C20-N21	-2.08	120.25	123.80
3	G	302	0WE	O2-C1-N3	-2.08	119.08	122.18
2	G	301	NAI	O4D-C1D-N1N	-2.06	103.71	108.07
2	C	301	NAI	PN-O3-PA	-2.06	126.94	132.73
2	G	301	NAI	C1D-N1N-C2N	-2.03	117.37	120.91
2	F	301	NAI	O4D-C1D-C2D	-2.01	101.91	106.58
3	F	302	0WE	C19-C20-N21	-2.01	120.39	123.80
2	H	301	NAI	O3-PN-O5D	2.06	108.41	102.94
3	H	302	0WE	C17-C1-N3	2.07	122.07	118.03
3	F	302	0WE	C20-N21-C22	2.11	120.46	116.30
3	B	302	0WE	C17-C1-N3	2.18	122.30	118.03
3	C	302	0WE	C26-C23-C24	2.19	124.17	119.84
3	H	302	0WE	C26-C23-C24	2.20	124.20	119.84
3	C	302	0WE	C17-C18-C19	2.21	121.65	112.75

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	NAI	O3-PN-O5D	2.24	108.88	102.94
3	C	302	0WE	C17-C1-N3	2.25	122.43	118.03
2	H	301	NAI	O3-PA-O5B	2.26	108.93	102.94
3	E	302	0WE	C17-C18-C19	2.27	121.86	112.75
3	E	302	0WE	C20-N21-C22	2.30	120.84	116.30
3	H	302	0WE	C20-N21-C22	2.34	120.92	116.30
3	B	302	0WE	C20-N21-C22	2.40	121.05	116.30
3	A	302	0WE	C17-C18-C19	2.45	122.58	112.75
2	B	301	NAI	C4N-C5N-C6N	2.46	126.64	122.58
3	D	302	0WE	C17-C1-N3	2.48	122.88	118.03
3	C	302	0WE	C20-N21-C22	2.53	121.29	116.30
2	C	301	NAI	C4N-C5N-C6N	2.53	126.75	122.58
3	F	302	0WE	C17-C18-C19	2.58	123.12	112.75
3	G	302	0WE	C17-C1-N3	2.59	123.09	118.03
3	D	302	0WE	C17-C18-C19	2.60	123.19	112.75
3	B	302	0WE	C17-C18-C19	2.66	123.46	112.75
3	A	302	0WE	C17-C1-N3	2.67	123.25	118.03
2	C	301	NAI	O3-PA-O5B	2.70	110.09	102.94
3	F	302	0WE	C17-C1-N3	2.74	123.39	118.03
2	B	301	NAI	O3-PA-O5B	2.76	110.25	102.94
3	A	302	0WE	C20-N21-C22	2.78	121.80	116.30
2	F	301	NAI	O3-PA-O5B	2.79	110.33	102.94
3	G	302	0WE	C17-C18-C19	2.82	124.10	112.75
2	C	301	NAI	C1D-N1N-C6N	2.88	127.26	120.81
2	G	301	NAI	O3-PA-O5B	2.92	110.69	102.94
2	E	301	NAI	C4N-C5N-C6N	3.04	127.60	122.58
2	H	301	NAI	C4N-C5N-C6N	3.05	127.61	122.58
2	E	301	NAI	O3-PA-O5B	3.06	111.06	102.94
2	F	301	NAI	C4N-C5N-C6N	3.07	127.65	122.58
2	F	301	NAI	C1D-N1N-C6N	3.10	127.75	120.81
2	E	301	NAI	C1D-N1N-C6N	3.11	127.78	120.81
2	G	301	NAI	C4N-C5N-C6N	3.14	127.76	122.58
2	H	301	NAI	C1D-N1N-C6N	3.18	127.93	120.81
2	A	301	NAI	O3-PA-O5B	3.24	111.53	102.94
3	A	302	0WE	C25-C37-N36	3.28	118.66	116.00
2	B	301	NAI	C1D-N1N-C6N	3.43	128.49	120.81
3	B	302	0WE	C24-C19-C20	3.45	120.33	116.57
2	D	301	NAI	C4N-C5N-C6N	3.52	128.38	122.58
2	G	301	NAI	C1D-N1N-C6N	3.53	128.72	120.81
2	A	301	NAI	C4N-C5N-C6N	3.58	128.48	122.58
2	A	301	NAI	C1D-N1N-C6N	3.65	128.96	120.81
2	D	301	NAI	C1D-N1N-C6N	3.71	129.11	120.81

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	0WE	C24-C19-C20	3.78	120.70	116.57
3	G	302	0WE	C24-C19-C20	3.79	120.71	116.57
3	F	302	0WE	C24-C19-C20	3.95	120.88	116.57
3	C	302	0WE	C25-C37-N36	3.95	119.21	116.00
3	E	302	0WE	C24-C19-C20	4.13	121.08	116.57
3	D	302	0WE	C24-C19-C20	4.16	121.11	116.57
3	D	302	0WE	C25-C37-N36	4.17	119.38	116.00
3	F	302	0WE	C25-C37-N36	4.19	119.40	116.00
3	C	302	0WE	C24-C19-C20	4.27	121.23	116.57
3	H	302	0WE	C25-C37-N36	4.43	119.59	116.00
3	H	302	0WE	C24-C19-C20	4.54	121.52	116.57
2	D	301	NAI	O7N-C7N-N7N	4.59	134.17	122.76
3	E	302	0WE	C25-C37-N36	4.61	119.73	116.00
2	A	301	NAI	O7N-C7N-N7N	4.80	134.70	122.76
2	F	301	NAI	O7N-C7N-N7N	4.94	135.05	122.76
3	B	302	0WE	C25-C37-N36	5.01	120.06	116.00
2	B	301	NAI	O7N-C7N-N7N	5.09	135.40	122.76
2	G	301	NAI	O7N-C7N-N7N	5.16	135.59	122.76
2	E	301	NAI	O7N-C7N-N7N	5.23	135.77	122.76
2	H	301	NAI	O7N-C7N-N7N	5.31	135.97	122.76
2	C	301	NAI	O7N-C7N-N7N	5.34	136.03	122.76
3	G	302	0WE	C25-C37-N36	5.45	120.42	116.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	0WE	1	0
3	B	302	0WE	1	0
3	C	302	0WE	1	0
3	D	302	0WE	1	0
3	E	302	0WE	1	0
3	H	302	0WE	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<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	295/298 (98%)	0.18	4 (1%) 78 74	13, 22, 41, 53	0
1	B	295/298 (98%)	0.36	12 (4%) 41 35	12, 24, 47, 64	0
1	C	295/298 (98%)	0.12	3 (1%) 84 82	12, 22, 42, 56	0
1	D	295/298 (98%)	0.18	8 (2%) 58 53	12, 22, 43, 58	0
1	E	295/298 (98%)	0.35	15 (5%) 32 26	11, 23, 46, 60	0
1	F	295/298 (98%)	0.19	4 (1%) 78 74	12, 22, 43, 57	0
1	G	295/298 (98%)	0.16	4 (1%) 78 74	13, 21, 43, 71	0
1	H	295/298 (98%)	0.08	2 (0%) 89 87	12, 22, 42, 55	0
All	All	2360/2384 (98%)	0.20	52 (2%) 65 60	11, 22, 44, 71	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	235	GLY	6.4
1	B	235	GLY	3.9
1	C	295	PHE	3.8
1	E	234	ILE	3.5
1	A	295	PHE	3.4
1	B	234	ILE	3.4
1	F	234	ILE	3.3
1	B	294	MET	3.2
1	H	295	PHE	3.2
1	B	101	LEU	3.1
1	A	234	ILE	3.1
1	B	55	LEU	3.1
1	C	294	MET	3.0
1	E	101	LEU	3.0
1	E	236	PHE	3.0
1	E	90	GLN	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	54	GLU	2.9
1	H	294	MET	2.9
1	B	236	PHE	2.9
1	A	233	ALA	2.8
1	F	236	PHE	2.7
1	G	101	LEU	2.7
1	G	100	ASP	2.7
1	B	100	ASP	2.6
1	E	230	ALA	2.6
1	D	48	ILE	2.6
1	E	100	ASP	2.6
1	E	233	ALA	2.5
1	E	55	LEU	2.5
1	B	230	ALA	2.5
1	G	234	ILE	2.5
1	A	235	GLY	2.5
1	E	295	PHE	2.5
1	E	99	LYS	2.4
1	D	1	MET	2.4
1	D	101	LEU	2.4
1	F	233	ALA	2.4
1	B	93	LEU	2.3
1	B	99	LYS	2.3
1	B	90	GLN	2.3
1	E	294	MET	2.3
1	F	100	ASP	2.2
1	D	100	ASP	2.2
1	E	67	GLY	2.1
1	G	48	ILE	2.1
1	E	94	GLU	2.1
1	D	55	LEU	2.1
1	D	51	GLN	2.0
1	D	50	SER	2.0
1	B	67	GLY	2.0
1	D	54	GLU	2.0
1	C	1	MET	2.0

## 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 [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
2	NAI	A	301	44/44	0.95	0.11	0.84	13,19,27,35	0
2	NAI	F	301	44/44	0.95	0.11	0.83	11,20,29,32	0
3	0WE	H	302	28/28	0.95	0.10	0.29	14,23,30,36	0
3	0WE	C	302	28/28	0.94	0.10	0.15	16,22,31,34	0
2	NAI	H	301	44/44	0.95	0.09	-0.11	10,20,27,29	0
2	NAI	C	301	44/44	0.95	0.09	-0.13	13,20,30,31	0
2	NAI	G	301	44/44	0.96	0.10	-0.22	11,21,29,31	0
2	NAI	D	301	44/44	0.96	0.09	-0.36	14,22,28,32	0
2	NAI	B	301	44/44	0.95	0.10	-0.45	14,24,31,37	0
3	0WE	A	302	28/28	0.95	0.09	-0.50	17,23,30,34	0
3	0WE	F	302	28/28	0.95	0.09	-0.55	14,21,34,38	0
2	NAI	E	301	44/44	0.95	0.09	-0.57	14,23,28,35	0
3	0WE	D	302	28/28	0.95	0.09	-0.58	16,22,28,40	0
3	0WE	E	302	28/28	0.95	0.10	-0.67	16,23,28,34	0
3	0WE	G	302	28/28	0.95	0.09	-0.83	17,21,26,39	0
3	0WE	B	302	28/28	0.95	0.09	-0.97	14,23,29,33	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.