



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:00 am GMT

PDB ID : 1H5Q  
Title : MANNITOL DEHYDROGENASE FROM AGARICUS BISPORUS  
Authors : Horer, S.; Stoop, J.; Mooibroek, H.; Baumann, U.; Sassoon, J.  
Deposited on : 2001-05-24  
Resolution : 1.50 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	:	1.7.2 (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

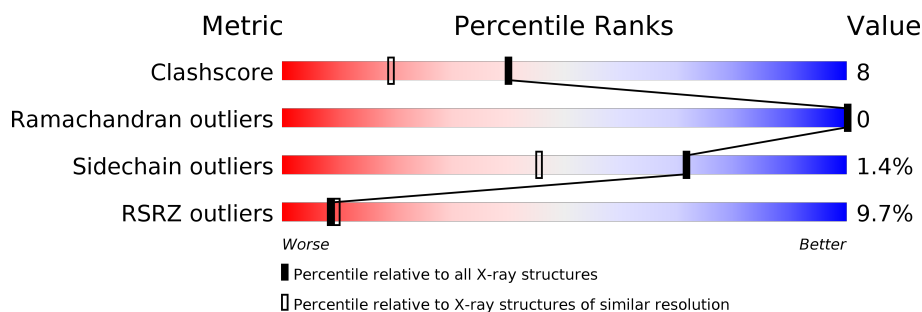
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	112137	2503 (1.50-1.50)
Ramachandran outliers	110173	2445 (1.50-1.50)
Sidechain outliers	110143	2443 (1.50-1.50)
RSRZ outliers	101464	2305 (1.50-1.50)

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. 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	265	<div> <div>37%</div> <div>65%</div> <div>31%</div> <div>..</div> </div>
1	B	265	<div> <div>12%</div> <div>79%</div> <div>17%</div> <div>..</div> </div>
1	C	265	<div> <div>8%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>
1	D	265	<div> <div>13%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>
1	E	265	<div> <div>5%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
1	F	265	<div> <div>5%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>
1	G	265	<div> <div>9%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	H	265	
1	I	265	
1	J	265	
1	K	265	
1	L	265	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NI	B	2263	-	-	-	X
3	NI	J	3263	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27197 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 NADP-DEPENDENT MANNITOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			1952	1232	335	378	7			
1	B	260	Total	C	N	O	S	0	0	0
			1952	1232	335	378	7			
1	C	260	Total	C	N	O	S	0	0	0
			1952	1232	335	378	7			
1	D	260	Total	C	N	O	S	0	0	0
			1952	1232	335	378	7			
1	E	260	Total	C	N	O	S	0	0	0
			1952	1232	335	378	7			
1	F	260	Total	C	N	O	S	0	0	0
			1952	1232	335	378	7			
1	G	260	Total	C	N	O	S	0	0	0
			1952	1232	335	378	7			
1	H	260	Total	C	N	O	S	0	0	0
			1952	1232	335	378	7			
1	I	260	Total	C	N	O	S	0	0	0
			1952	1232	335	378	7			
1	J	260	Total	C	N	O	S	0	0	0
			1952	1232	335	378	7			
1	K	260	Total	C	N	O	S	0	0	0
			1952	1232	335	378	7			
1	L	260	Total	C	N	O	S	0	0	0
			1952	1232	335	378	7			

There are 12 discrepancies between the modelled and reference sequences:

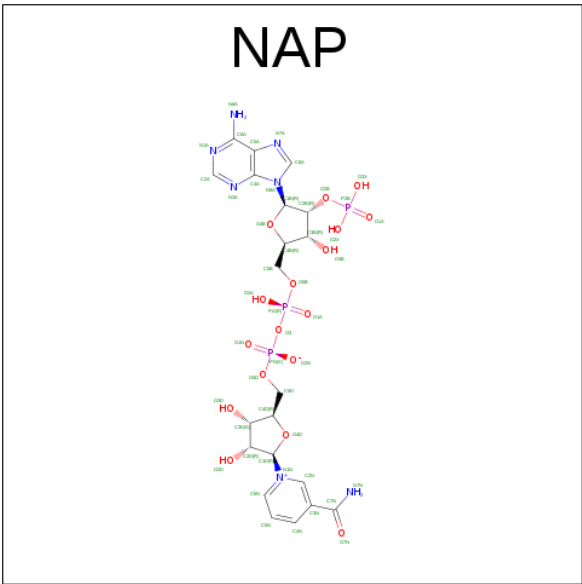
Chain	Residue	Modelled	Actual	Comment	Reference
A	89	PRO	ALA	CONFLICT	UNP O93868
B	89	PRO	ALA	CONFLICT	UNP O93868
C	89	PRO	ALA	CONFLICT	UNP O93868
D	89	PRO	ALA	CONFLICT	UNP O93868
E	89	PRO	ALA	CONFLICT	UNP O93868

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	89	PRO	ALA	CONFLICT	UNP O93868
G	89	PRO	ALA	CONFLICT	UNP O93868
H	89	PRO	ALA	CONFLICT	UNP O93868
I	89	PRO	ALA	CONFLICT	UNP O93868
J	89	PRO	ALA	CONFLICT	UNP O93868
K	89	PRO	ALA	CONFLICT	UNP O93868
L	89	PRO	ALA	CONFLICT	UNP O93868

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	J	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	K	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	L	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	1	Total	Ni	0	0
			1	1		
3	E	1	Total	Ni	0	0
			1	1		
3	B	1	Total	Ni	0	0
			1	1		
3	I	1	Total	Ni	0	0
			1	1		
3	A	1	Total	Ni	0	0
			1	1		
3	F	1	Total	Ni	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	130	Total	O	0	0
			130	130		
4	B	202	Total	O	0	0
			202	202		
4	C	251	Total	O	0	0
			251	251		
4	D	190	Total	O	0	0
			190	190		
4	E	342	Total	O	0	0
			342	342		
4	F	313	Total	O	0	0
			313	313		

*Continued on next page...*

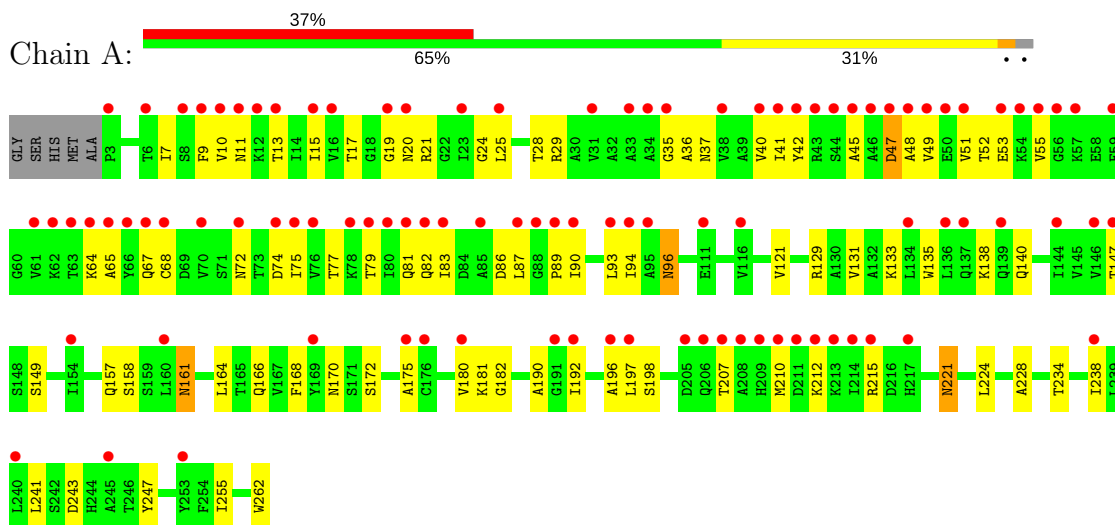
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	291	Total 291	O 291	0	0
4	H	302	Total 302	O 302	0	0
4	I	311	Total 311	O 311	0	0
4	J	268	Total 268	O 268	0	0
4	K	284	Total 284	O 284	0	0
4	L	307	Total 307	O 307	0	0

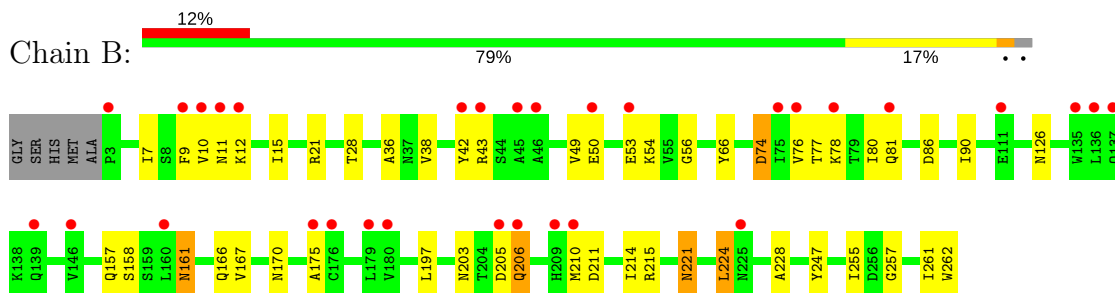
### 3 Residue-property plots

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.

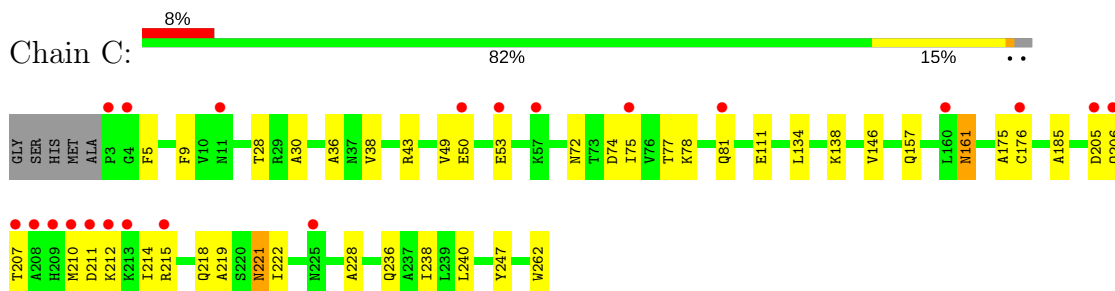
#### • Molecule 1: NADP-DEPENDENT MANNITOL DEHYDROGENASE



#### • Molecule 1: NADP-DEPENDENT MANNITOL DEHYDROGENASE

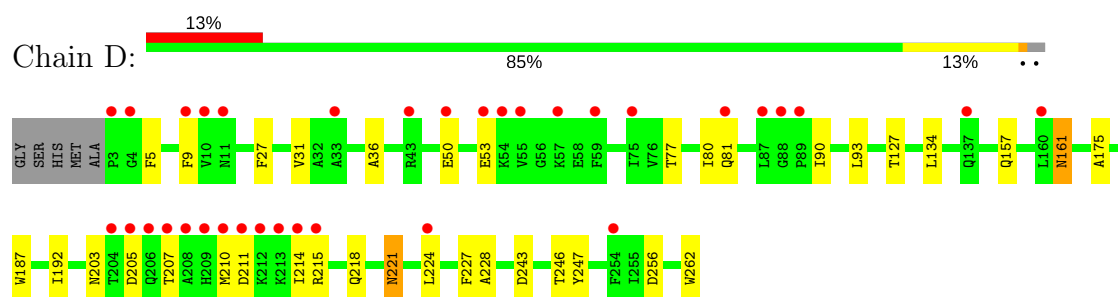


#### • Molecule 1: NADP-DEPENDENT MANNITOL DEHYDROGENASE

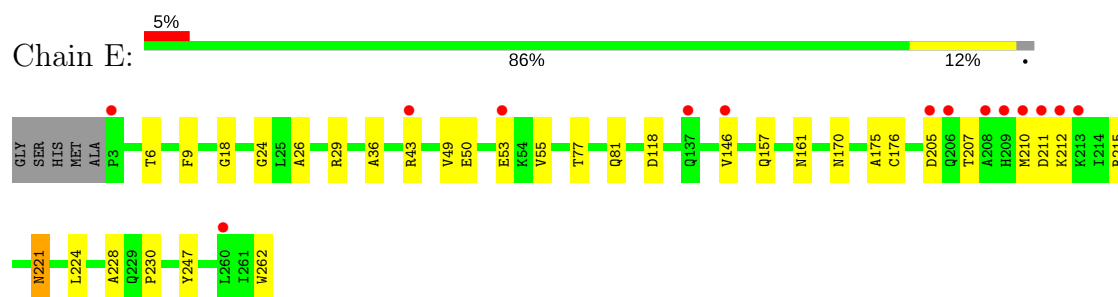


#### • Molecule 1: NADP-DEPENDENT MANNITOL DEHYDROGENASE

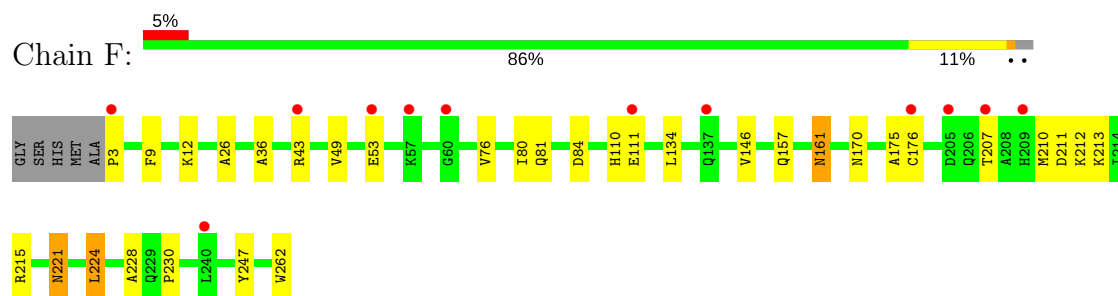




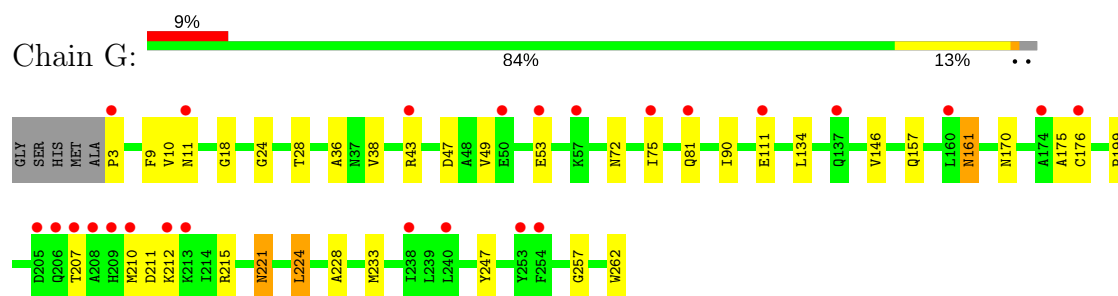
• Molecule 1: NADP-DEPENDENT MANNITOL DEHYDROGENASE



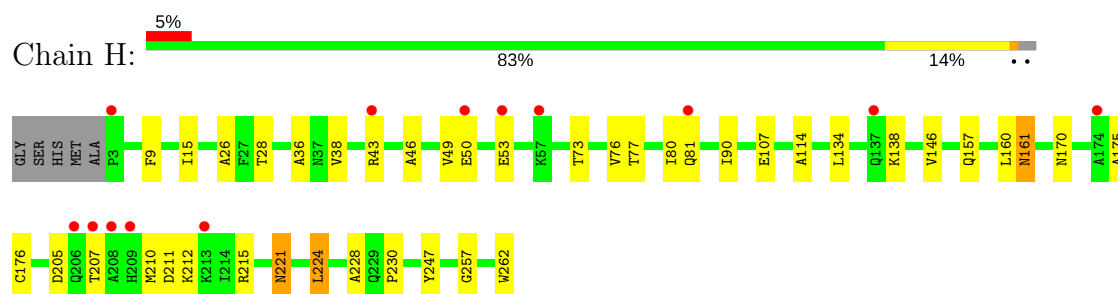
• Molecule 1: NADP-DEPENDENT MANNITOL DEHYDROGENASE



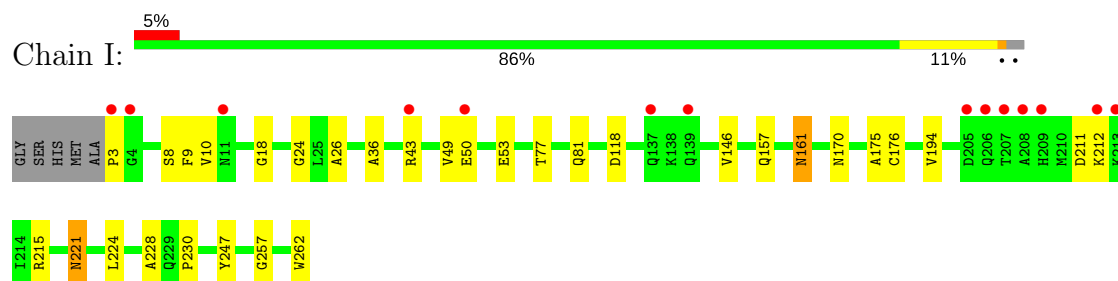
• Molecule 1: NADP-DEPENDENT MANNITOL DEHYDROGENASE



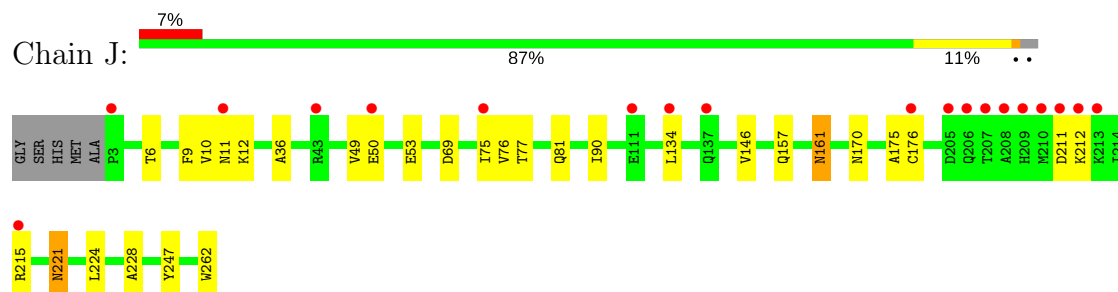
• Molecule 1: NADP-DEPENDENT MANNITOL DEHYDROGENASE



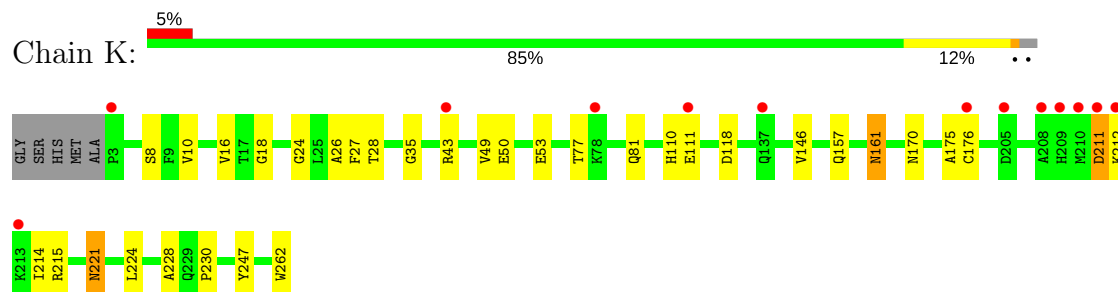
- Molecule 1: NADP-DEPENDENT MANNITOL DEHYDROGENASE



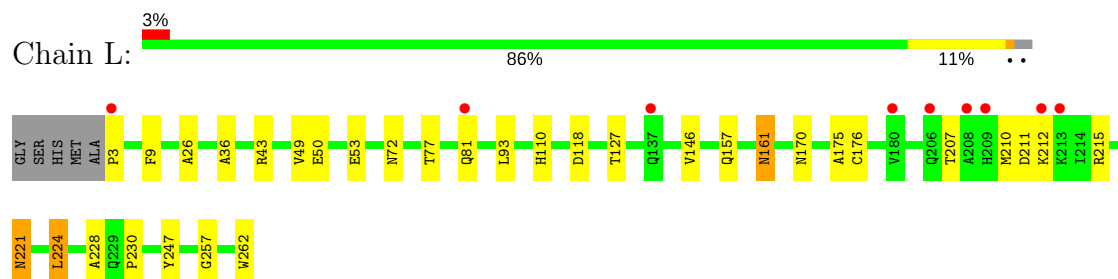
- Molecule 1: NADP-DEPENDENT MANNITOL DEHYDROGENASE



- Molecule 1: NADP-DEPENDENT MANNITOL DEHYDROGENASE



- Molecule 1: NADP-DEPENDENT MANNITOL DEHYDROGENASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	227.25Å 124.85Å 132.69Å 90.00° 118.54° 90.00°	Depositor
Resolution (Å)	20.00 – 1.50 39.89 – 1.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.50) 98.3 (39.89-1.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.92 (at 1.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.193 , 0.209 (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
Wilson B-factor (Å <sup>2</sup> )	15.0	Xtriage
Anisotropy	0.695	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	27197	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 7.94% 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 [i](#)

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

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.30	0/1985	0.70	3/2693 (0.1%)
1	B	0.30	0/1985	0.68	2/2693 (0.1%)
1	C	0.32	0/1985	0.68	2/2693 (0.1%)
1	D	0.31	0/1985	0.67	3/2693 (0.1%)
1	E	0.36	0/1985	0.68	2/2693 (0.1%)
1	F	0.36	0/1985	0.68	1/2693 (0.0%)
1	G	0.34	0/1985	0.67	2/2693 (0.1%)
1	H	0.35	0/1985	0.69	2/2693 (0.1%)
1	I	0.35	0/1985	0.68	2/2693 (0.1%)
1	J	0.35	0/1985	0.67	1/2693 (0.0%)
1	K	0.35	0/1985	0.68	1/2693 (0.0%)
1	L	0.35	0/1985	0.69	1/2693 (0.0%)
All	All	0.34	0/23820	0.68	22/32316 (0.1%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	211	ASP	CB-CG-OD2	6.40	124.06	118.30
1	H	211	ASP	CB-CG-OD2	6.28	123.96	118.30
1	K	211	ASP	CB-CG-OD2	6.09	123.78	118.30
1	B	211	ASP	CB-CG-OD2	6.06	123.75	118.30
1	E	211	ASP	CB-CG-OD2	6.04	123.74	118.30
1	C	211	ASP	CB-CG-OD2	5.68	123.42	118.30
1	L	211	ASP	CB-CG-OD2	5.58	123.32	118.30
1	D	211	ASP	CB-CG-OD2	5.44	123.19	118.30
1	A	47	ASP	CB-CG-OD2	5.34	123.10	118.30
1	A	74	ASP	CB-CG-OD2	5.33	123.09	118.30
1	I	211	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	243	ASP	CB-CG-OD2	5.29	123.06	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	256	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	74	ASP	CB-CG-OD2	5.28	123.05	118.30
1	E	205	ASP	CB-CG-OD2	5.27	123.04	118.30
1	G	211	ASP	CB-CG-OD2	5.25	123.02	118.30
1	J	211	ASP	CB-CG-OD2	5.13	122.92	118.30
1	G	47	ASP	CB-CG-OD2	5.12	122.91	118.30
1	C	205	ASP	CB-CG-OD2	5.08	122.88	118.30
1	H	205	ASP	CB-CG-OD2	5.07	122.86	118.30
1	I	118	ASP	CB-CG-OD2	5.07	122.86	118.30
1	D	205	ASP	CB-CG-OD2	5.07	122.86	118.30

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	1952	0	1949	88	0
1	B	1952	0	1949	52	1
1	C	1952	0	1949	35	0
1	D	1952	0	1949	28	0
1	E	1952	0	1949	34	0
1	F	1952	0	1949	36	0
1	G	1952	0	1949	40	0
1	H	1952	0	1949	36	0
1	I	1952	0	1949	32	0
1	J	1952	0	1949	31	1
1	K	1952	0	1949	39	0
1	L	1952	0	1949	31	0
2	A	48	0	25	1	0
2	B	48	0	25	1	0
2	C	48	0	25	0	0
2	D	48	0	25	0	0
2	E	48	0	24	0	0
2	F	48	0	25	0	0
2	G	48	0	24	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	48	0	25	0	0
2	I	48	0	25	0	0
2	J	48	0	25	0	0
2	K	48	0	24	0	0
2	L	48	0	25	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
4	A	130	0	0	14	0
4	B	202	0	0	17	0
4	C	251	0	0	5	0
4	D	190	0	0	3	0
4	E	342	0	0	9	1
4	F	313	0	0	9	1
4	G	291	0	0	11	0
4	H	302	0	0	7	0
4	I	311	0	0	6	0
4	J	268	0	0	7	0
4	K	284	0	0	11	0
4	L	307	0	0	4	0
All	All	27197	0	23685	397	2

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 8.

All (397) 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:K:16:VAL:HG11	4:K:2029:HOH:O	1.60	1.01
1:C:50:GLU:HG3	4:C:2061:HOH:O	1.66	0.95
1:F:157:GLN:HE22	1:H:221:ASN:HD21	1.11	0.95
1:L:50:GLU:HG3	4:L:2074:HOH:O	1.64	0.94
1:A:212:LYS:HD2	1:F:3:PRO:HD2	1.46	0.93
1:F:221:ASN:HD21	1:H:157:GLN:HE22	1.15	0.92
1:A:15:ILE:HD11	1:A:90:ILE:HD13	1.50	0.92
1:E:157:GLN:HE22	1:G:221:ASN:HD21	1.17	0.92
1:I:221:ASN:HD21	1:K:157:GLN:HE22	1.20	0.89
1:A:10:VAL:HA	1:A:35:GLY:O	1.75	0.87

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:GLN:HE22	1:C:221:ASN:HD21	1.19	0.86
1:E:221:ASN:HD21	1:G:157:GLN:HE22	1.23	0.86
1:A:215:ARG:CZ	1:G:10:VAL:HG11	2.06	0.86
1:C:134:LEU:HD11	1:C:138:LYS:HE3	1.58	0.85
1:B:157:GLN:HE22	1:D:221:ASN:HD21	1.25	0.85
1:D:50:GLU:HG3	4:D:2040:HOH:O	1.76	0.84
1:D:9:PHE:HB3	1:D:36:ALA:HB2	1.57	0.83
1:A:215:ARG:HD2	1:G:11:ASN:HD21	1.43	0.82
1:B:221:ASN:HD21	1:D:157:GLN:HE22	1.24	0.81
1:J:221:ASN:HD21	1:L:157:GLN:HE22	1.27	0.81
1:A:82:GLN:HG3	4:A:2028:HOH:O	1.83	0.79
1:H:50:GLU:HG3	4:H:2074:HOH:O	1.83	0.79
1:E:50:GLU:HG3	4:E:2090:HOH:O	1.84	0.77
1:A:215:ARG:NH2	1:G:10:VAL:HG11	2.01	0.76
1:A:49:VAL:O	1:A:53:GLU:HG3	1.87	0.74
1:I:157:GLN:HE22	1:K:221:ASN:HD21	1.35	0.74
1:G:111:GLU:OE2	1:L:72:ASN:HA	1.88	0.74
1:G:111:GLU:OE2	4:G:2161:HOH:O	2.06	0.73
1:J:75:ILE:HB	4:J:2103:HOH:O	1.89	0.72
1:G:212:LYS:HG2	1:G:215:ARG:NH2	2.05	0.71
1:E:212:LYS:HG2	1:E:215:ARG:NH2	2.06	0.71
1:A:215:ARG:HD2	1:G:11:ASN:ND2	2.07	0.70
1:F:81:GLN:HG3	4:F:2124:HOH:O	1.92	0.70
1:B:11:ASN:HB3	4:B:2008:HOH:O	1.91	0.70
1:J:49:VAL:O	1:J:53:GLU:HG3	1.92	0.69
1:H:107:GLU:HG3	4:H:2026:HOH:O	1.92	0.68
1:G:146:VAL:HG11	1:G:176:CYS:SG	2.33	0.68
1:K:49:VAL:O	1:K:53:GLU:HG3	1.94	0.68
1:I:49:VAL:O	1:I:53:GLU:HG3	1.93	0.67
1:F:146:VAL:HG11	1:F:176:CYS:SG	2.34	0.67
1:A:212:LYS:CD	1:F:3:PRO:HD2	2.24	0.67
1:H:134:LEU:HD11	1:H:138:LYS:HE3	1.77	0.67
1:B:215:ARG:NH2	4:B:2149:HOH:O	2.08	0.67
1:J:6:THR:HB	4:J:2007:HOH:O	1.95	0.67
1:A:20:ASN:HB3	1:A:40:VAL:HG11	1.77	0.66
1:D:210:MET:SD	1:D:215:ARG:HB2	2.35	0.66
1:K:28:THR:N	4:K:2029:HOH:O	2.28	0.66
1:D:9:PHE:CB	1:D:36:ALA:HB2	2.26	0.65
1:A:45:ALA:HB3	1:A:48:ALA:HB2	1.79	0.64
1:I:146:VAL:HG11	1:I:176:CYS:SG	2.38	0.64
1:C:146:VAL:HG11	1:C:176:CYS:SG	2.36	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:194:VAL:HG23	4:I:2233:HOH:O	1.97	0.64
1:A:47:ASP:O	1:A:51:VAL:HG23	1.97	0.64
1:C:212:LYS:HG2	1:C:215:ARG:NH2	2.13	0.64
1:D:53:GLU:HG3	4:D:2038:HOH:O	1.99	0.64
1:H:73:THR:N	1:K:111:GLU:OE2	2.31	0.63
1:K:146:VAL:HG11	1:K:176:CYS:SG	2.38	0.63
1:A:42:TYR:CE2	1:A:65:ALA:HB1	2.33	0.62
1:A:210:MET:SD	1:A:215:ARG:HB2	2.39	0.62
1:B:50:GLU:HG3	4:B:2042:HOH:O	1.98	0.62
1:J:76:VAL:HG23	4:J:2103:HOH:O	2.00	0.62
1:J:9:PHE:HB3	1:J:36:ALA:HB2	1.82	0.61
1:F:49:VAL:O	1:F:53:GLU:HG3	2.01	0.61
1:A:51:VAL:O	1:A:55:VAL:HG23	2.01	0.61
1:J:10:VAL:HG12	1:J:11:ASN:ND2	2.15	0.61
1:A:19:GLY:HA2	1:A:24:GLY:HA3	1.83	0.61
1:A:42:TYR:HE2	1:A:65:ALA:HB1	1.65	0.60
1:B:21:ARG:HH22	1:B:206:GLN:NE2	1.99	0.60
1:D:243:ASP:O	1:D:246:THR:HG23	2.01	0.60
1:F:157:GLN:HE22	1:H:221:ASN:ND2	1.92	0.60
1:E:6:THR:HB	4:E:2006:HOH:O	2.01	0.60
1:A:135:TRP:HB3	1:A:140:GLN:O	2.02	0.60
1:C:49:VAL:O	1:C:53:GLU:HG3	2.01	0.59
1:B:10:VAL:HG12	1:B:11:ASN:OD1	2.02	0.59
1:J:146:VAL:HG11	1:J:176:CYS:SG	2.42	0.59
1:A:77:THR:O	1:A:81:GLN:HG3	2.02	0.59
1:B:66:TYR:O	4:B:2059:HOH:O	2.17	0.58
1:H:46:ALA:HB2	4:K:2043:HOH:O	2.04	0.58
1:A:180:VAL:HG21	1:A:196:ALA:HB2	1.86	0.58
1:K:10:VAL:HA	1:K:35:GLY:O	2.04	0.58
1:A:7:ILE:HB	1:D:5:PHE:HB3	1.86	0.57
1:F:213:LYS:HE3	4:F:2254:HOH:O	2.02	0.57
1:L:212:LYS:HG2	1:L:215:ARG:NH2	2.20	0.57
1:A:17:THR:HG22	1:A:41:ILE:HD12	1.87	0.57
1:A:93:LEU:HD22	1:A:131:VAL:HG21	1.86	0.57
1:B:53:GLU:HG3	4:B:2038:HOH:O	2.05	0.57
1:G:81:GLN:HG3	4:G:2128:HOH:O	2.04	0.57
1:A:221:ASN:HD21	1:C:157:GLN:HE22	1.52	0.57
1:F:9:PHE:HB3	1:F:36:ALA:HB2	1.86	0.57
1:G:212:LYS:HG2	1:G:215:ARG:HH22	1.67	0.57
1:G:49:VAL:O	1:G:53:GLU:HG3	2.04	0.57
1:I:221:ASN:ND2	1:K:157:GLN:HE22	1.95	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:VAL:HG11	1:E:176:CYS:SG	2.45	0.56
1:K:50:GLU:HG3	4:K:2058:HOH:O	2.05	0.56
1:F:212:LYS:HG2	1:F:215:ARG:NH2	2.20	0.56
1:H:43:ARG:CZ	4:H:2059:HOH:O	2.53	0.56
1:A:9:PHE:HB3	1:A:36:ALA:HB2	1.88	0.56
1:B:42:TYR:CD2	4:B:2059:HOH:O	2.52	0.56
1:A:129:ARG:O	1:A:133:LYS:HG3	2.06	0.56
1:B:74:ASP:O	1:B:78:LYS:HG3	2.06	0.56
1:B:15:ILE:HD11	1:B:90:ILE:HD13	1.89	0.55
1:F:43:ARG:NE	4:F:2057:HOH:O	2.38	0.55
1:A:212:LYS:HG2	1:A:215:ARG:NH2	2.22	0.55
1:E:49:VAL:O	1:E:53:GLU:HG3	2.06	0.55
1:E:55:VAL:HA	4:E:2051:HOH:O	2.06	0.55
1:E:77:THR:O	1:E:81:GLN:HG3	2.06	0.55
1:J:77:THR:O	1:J:81:GLN:HG3	2.07	0.55
1:A:72:ASN:HB2	4:A:2030:HOH:O	2.06	0.55
1:L:207:THR:O	1:L:210:MET:HG2	2.06	0.54
1:A:90:ILE:HB	1:A:135:TRP:HE1	1.73	0.54
1:G:175:ALA:HB2	1:H:175:ALA:HB2	1.90	0.54
1:G:43:ARG:CZ	4:G:2062:HOH:O	2.55	0.54
1:B:224:LEU:HD22	1:B:257:GLY:HA2	1.89	0.54
1:G:146:VAL:CG1	1:G:176:CYS:SG	2.95	0.54
1:B:50:GLU:HG2	4:B:2043:HOH:O	2.08	0.53
1:J:157:GLN:HE22	1:L:221:ASN:HD21	1.53	0.53
1:L:9:PHE:CB	1:L:36:ALA:HB2	2.38	0.53
1:D:50:GLU:HB3	4:D:2039:HOH:O	2.07	0.53
1:G:3:PRO:HA	4:G:2002:HOH:O	2.09	0.53
1:C:77:THR:O	1:C:81:GLN:HG3	2.08	0.53
1:I:50:GLU:HG3	4:I:2083:HOH:O	2.09	0.53
1:L:43:ARG:CZ	4:L:2061:HOH:O	2.56	0.53
1:C:212:LYS:HG2	1:C:215:ARG:HH22	1.72	0.53
1:J:69:ASP:HB3	4:J:2102:HOH:O	2.07	0.53
1:L:77:THR:O	1:L:81:GLN:HG3	2.09	0.53
1:A:79:THR:O	1:A:83:ILE:HG13	2.09	0.53
1:B:21:ARG:HH22	1:B:206:GLN:HE22	1.57	0.53
1:D:207:THR:O	1:D:210:MET:HG2	2.09	0.53
1:K:175:ALA:HB2	1:L:175:ALA:HB2	1.91	0.53
1:C:207:THR:O	1:C:210:MET:HG2	2.09	0.53
1:I:157:GLN:HE22	1:K:221:ASN:ND2	2.06	0.53
1:A:19:GLY:HA2	1:A:24:GLY:C	2.30	0.53
1:A:64:LYS:HA	4:A:2025:HOH:O	2.09	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:THR:HG21	4:A:2024:HOH:O	2.09	0.53
1:B:49:VAL:O	1:B:53:GLU:HG3	2.10	0.53
1:C:28:THR:HG23	1:C:38:VAL:HG11	1.91	0.53
1:E:29:ARG:NH1	4:E:2051:HOH:O	2.42	0.53
1:A:68:CYS:HA	4:A:2031:HOH:O	2.09	0.52
1:C:175:ALA:HB2	1:D:175:ALA:HB2	1.89	0.52
1:I:3:PRO:O	4:I:2002:HOH:O	2.19	0.52
1:F:146:VAL:CG1	1:F:176:CYS:SG	2.98	0.52
1:L:146:VAL:HG11	1:L:176:CYS:SG	2.50	0.52
1:L:212:LYS:HG2	1:L:215:ARG:HH22	1.74	0.52
1:H:53:GLU:HG3	4:H:2073:HOH:O	2.10	0.52
1:A:138:LYS:HB2	1:A:140:GLN:HG3	1.91	0.52
1:A:149:SER:C	1:A:198:SER:HB3	2.30	0.52
1:B:203:ASN:HB2	4:B:2133:HOH:O	2.09	0.52
1:C:111:GLU:HB2	4:C:2132:HOH:O	2.10	0.51
1:A:20:ASN:HB3	1:A:40:VAL:CG1	2.39	0.51
1:E:53:GLU:HB3	4:E:2039:HOH:O	2.10	0.51
1:G:43:ARG:NH1	4:G:2058:HOH:O	2.44	0.51
1:H:114:ALA:HB1	4:H:2170:HOH:O	2.09	0.51
1:J:212:LYS:HG2	1:J:215:ARG:NH2	2.26	0.51
1:G:207:THR:O	1:G:210:MET:HG2	2.11	0.51
1:I:43:ARG:CZ	4:I:2063:HOH:O	2.57	0.51
1:B:9:PHE:HA	1:B:12:LYS:HD2	1.91	0.51
1:A:89:PRO:HB3	1:A:140:GLN:HE22	1.75	0.51
1:E:175:ALA:HB2	1:F:175:ALA:HB2	1.91	0.51
1:B:43:ARG:NH1	4:B:2030:HOH:O	2.36	0.51
1:G:111:GLU:HG3	4:G:2163:HOH:O	2.10	0.51
1:J:10:VAL:HG12	1:J:11:ASN:CG	2.32	0.51
1:L:49:VAL:O	1:L:53:GLU:HG3	2.11	0.51
1:H:77:THR:O	1:H:81:GLN:HG3	2.11	0.50
1:B:56:GLY:HA3	4:B:2046:HOH:O	2.11	0.50
1:A:10:VAL:HG12	1:A:11:ASN:ND2	2.26	0.50
1:A:247:TYR:CD2	1:D:228:ALA:HB2	2.46	0.50
1:I:228:ALA:HB2	1:L:247:TYR:CD2	2.46	0.50
1:B:210:MET:HE1	4:B:2154:HOH:O	2.11	0.50
1:A:161:ASN:ND2	1:C:262:TRP:HE1	2.08	0.50
1:A:82:GLN:NE2	1:A:86:ASP:OD1	2.45	0.50
1:A:83:ILE:HA	4:A:2028:HOH:O	2.11	0.50
1:I:8:SER:OG	1:I:10:VAL:HG23	2.11	0.50
1:J:9:PHE:HA	1:J:12:LYS:HD2	1.93	0.50
1:A:10:VAL:CA	1:A:35:GLY:O	2.55	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:212:LYS:HG2	1:K:215:ARG:HH22	1.77	0.50
1:K:146:VAL:CG1	1:K:176:CYS:SG	3.00	0.49
1:A:133:LYS:HD3	4:A:2037:HOH:O	2.12	0.49
1:C:43:ARG:NE	4:C:2039:HOH:O	2.44	0.49
1:C:72:ASN:OD1	1:C:75:ILE:HG13	2.13	0.49
1:A:19:GLY:HA2	1:A:24:GLY:CA	2.41	0.49
1:C:146:VAL:CG1	1:C:176:CYS:SG	3.01	0.49
1:E:247:TYR:CD2	1:H:228:ALA:HB2	2.47	0.49
1:G:53:GLU:HG2	4:G:2097:HOH:O	2.12	0.49
1:K:212:LYS:HG2	1:K:215:ARG:NH2	2.27	0.49
1:A:175:ALA:HB2	1:B:175:ALA:HB2	1.94	0.49
1:A:221:ASN:ND2	1:C:157:GLN:HE22	2.09	0.49
1:A:228:ALA:HB2	1:D:247:TYR:CE2	2.48	0.49
1:A:75:ILE:HG21	4:A:2031:HOH:O	2.13	0.49
1:H:76:VAL:O	1:H:80:ILE:HG12	2.11	0.49
1:J:212:LYS:NZ	1:J:215:ARG:HH22	2.11	0.49
1:B:167:VAL:HG22	4:B:2091:HOH:O	2.13	0.49
1:I:161:ASN:ND2	1:K:262:TRP:HE1	2.10	0.49
1:E:157:GLN:HE22	1:G:221:ASN:ND2	1.99	0.49
1:C:214:ILE:O	1:C:218:GLN:HG3	2.13	0.49
1:F:247:TYR:CD2	1:G:228:ALA:HB2	2.47	0.49
1:G:9:PHE:HB3	1:G:36:ALA:HB2	1.95	0.49
1:G:212:LYS:NZ	1:G:215:ARG:HH22	2.11	0.49
1:I:247:TYR:CD2	1:L:228:ALA:HB2	2.47	0.49
1:J:212:LYS:HZ2	1:J:215:ARG:HH22	1.61	0.48
1:K:43:ARG:NE	4:K:2044:HOH:O	2.46	0.48
1:A:182:GLY:HA3	1:B:167:VAL:HG12	1.94	0.48
1:A:29:ARG:HG2	1:A:29:ARG:HH11	1.78	0.48
1:A:40:VAL:HB	4:A:2024:HOH:O	2.13	0.48
1:B:9:PHE:HD1	1:B:12:LYS:HD2	1.78	0.48
1:B:262:TRP:HE1	1:D:161:ASN:ND2	2.11	0.48
1:I:175:ALA:HB2	1:J:175:ALA:HB2	1.95	0.48
1:B:205:ASP:HB2	4:B:2141:HOH:O	2.13	0.48
1:H:49:VAL:O	1:H:53:GLU:HG3	2.13	0.48
1:I:224:LEU:HD22	1:I:257:GLY:HA2	1.94	0.48
1:D:27:PHE:O	1:D:31:VAL:HG22	2.13	0.48
1:F:111:GLU:OE2	4:F:2169:HOH:O	2.20	0.48
1:H:81:GLN:HG3	4:H:2123:HOH:O	2.14	0.48
1:F:12:LYS:HA	4:F:2146:HOH:O	2.12	0.48
1:I:77:THR:O	1:I:81:GLN:HG3	2.14	0.48
1:A:17:THR:HA	1:A:41:ILE:HB	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:GLU:HA	4:B:2046:HOH:O	2.15	0.47
1:D:203:ASN:ND2	1:D:227:PHE:HB2	2.29	0.47
1:J:228:ALA:HB2	1:K:247:TYR:CD2	2.49	0.47
1:I:161:ASN:HD22	1:K:262:TRP:HE1	1.63	0.47
1:A:94:ILE:HD11	1:A:241:LEU:HD11	1.95	0.47
1:A:161:ASN:HD22	1:C:262:TRP:HE1	1.61	0.47
1:I:9:PHE:HB3	1:I:36:ALA:HB2	1.96	0.47
1:I:212:LYS:HG3	4:I:2245:HOH:O	2.14	0.47
1:A:221:ASN:HD22	1:A:221:ASN:HA	1.57	0.47
1:E:228:ALA:HB2	1:H:247:TYR:CD2	2.49	0.47
1:E:212:LYS:HG2	1:E:215:ARG:HH22	1.79	0.47
1:I:146:VAL:CG1	1:I:176:CYS:SG	3.02	0.47
1:J:170:ASN:H	1:J:170:ASN:HD22	1.63	0.47
4:G:2161:HOH:O	1:K:110:HIS:HD2	1.97	0.47
1:J:247:TYR:CD2	1:K:228:ALA:HB2	2.50	0.47
1:E:81:GLN:HG3	4:E:2153:HOH:O	2.13	0.47
1:D:93:LEU:HD21	1:D:127:THR:HG22	1.97	0.47
1:F:43:ARG:NH2	4:F:2059:HOH:O	2.47	0.47
1:A:21:ARG:NE	2:A:263:NAP:O3X	2.30	0.46
1:B:228:ALA:HB2	1:C:247:TYR:CD2	2.49	0.46
1:G:28:THR:HG23	1:G:38:VAL:HG11	1.96	0.46
1:B:247:TYR:CD2	1:C:228:ALA:HB2	2.50	0.46
1:E:212:LYS:NZ	1:E:215:ARG:HH22	2.13	0.46
1:I:43:ARG:NH2	4:I:2063:HOH:O	2.49	0.46
1:A:207:THR:O	1:A:210:MET:HG2	2.15	0.46
1:L:9:PHE:HB3	1:L:36:ALA:HB2	1.97	0.46
1:B:7:ILE:HB	1:C:5:PHE:HB3	1.98	0.46
1:H:28:THR:HG23	1:H:38:VAL:HG11	1.96	0.46
1:F:84:ASP:HB2	1:F:134:LEU:HD21	1.98	0.46
4:F:2268:HOH:O	1:H:160:LEU:HD11	2.16	0.46
1:J:146:VAL:CG1	1:J:176:CYS:SG	3.03	0.46
1:K:77:THR:O	1:K:81:GLN:HG3	2.16	0.46
1:G:224:LEU:HD22	1:G:257:GLY:HA2	1.97	0.46
1:E:170:ASN:HD22	1:E:170:ASN:H	1.62	0.46
1:G:90:ILE:HD12	1:G:134:LEU:HD23	1.98	0.46
1:B:158:SER:HA	1:B:214:ILE:HG23	1.98	0.45
1:B:43:ARG:NE	4:B:2031:HOH:O	2.49	0.45
1:D:77:THR:O	1:D:81:GLN:HG3	2.16	0.45
1:G:170:ASN:H	1:G:170:ASN:HD22	1.63	0.45
1:H:207:THR:O	1:H:210:MET:HG2	2.16	0.45
1:A:212:LYS:HB3	4:A:2091:HOH:O	2.16	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:PHE:CB	1:A:36:ALA:HB2	2.45	0.45
1:B:10:VAL:O	1:B:11:ASN:CB	2.62	0.45
1:B:21:ARG:NH1	2:B:263:NAP:H3B	2.31	0.45
1:I:212:LYS:HG2	1:I:215:ARG:NH2	2.32	0.45
1:K:27:PHE:HB2	4:K:2029:HOH:O	2.16	0.45
1:E:53:GLU:HG2	4:E:2118:HOH:O	2.16	0.45
1:A:9:PHE:O	1:A:35:GLY:O	2.35	0.45
1:F:161:ASN:HD22	1:H:262:TRP:HE1	1.63	0.45
1:A:212:LYS:CG	1:A:215:ARG:NH2	2.80	0.45
1:K:81:GLN:HG3	4:K:2119:HOH:O	2.17	0.45
1:L:53:GLU:HG2	4:L:2094:HOH:O	2.17	0.45
1:B:10:VAL:HG13	4:B:2010:HOH:O	2.16	0.45
1:H:224:LEU:HD22	1:H:257:GLY:HA2	1.98	0.45
1:L:224:LEU:HD22	1:L:257:GLY:HA2	1.99	0.45
1:C:219:ALA:HA	1:C:222:ILE:HD12	1.98	0.45
1:E:118:ASP:OD1	1:F:110:HIS:HE1	2.00	0.45
1:H:26:ALA:HB2	1:H:230:PRO:HB2	1.98	0.45
1:J:157:GLN:HE22	1:L:221:ASN:ND2	2.15	0.45
1:J:50:GLU:HB3	4:J:2062:HOH:O	2.17	0.45
1:F:170:ASN:HD22	1:F:170:ASN:H	1.63	0.45
1:H:15:ILE:HD11	1:H:90:ILE:HD13	1.99	0.45
1:J:81:GLN:HG3	4:J:2109:HOH:O	2.16	0.45
1:F:221:ASN:ND2	1:H:157:GLN:HE22	1.98	0.44
1:J:75:ILE:HB	4:J:2102:HOH:O	2.16	0.44
1:F:228:ALA:HB2	1:G:247:TYR:CD2	2.52	0.44
1:A:212:LYS:HE3	1:F:3:PRO:HG2	1.99	0.44
1:H:212:LYS:HG2	1:H:215:ARG:NH2	2.32	0.44
1:I:262:TRP:HE1	1:K:161:ASN:ND2	2.16	0.44
1:F:161:ASN:ND2	1:H:262:TRP:HE1	2.16	0.44
1:A:168:PHE:HB2	4:A:2074:HOH:O	2.17	0.44
1:C:30:ALA:HB1	1:C:238:ILE:HD11	2.00	0.44
1:C:81:GLN:HG3	4:C:2094:HOH:O	2.16	0.44
1:G:18:GLY:O	1:G:24:GLY:HA3	2.17	0.44
1:K:18:GLY:O	1:K:24:GLY:HA3	2.17	0.44
1:K:110:HIS:HE1	1:L:118:ASP:OD1	2.01	0.44
1:B:166:GLN:HE21	1:B:170:ASN:HD21	1.66	0.44
1:A:247:TYR:CE2	1:D:228:ALA:HB2	2.52	0.44
1:F:262:TRP:HE1	1:H:161:ASN:ND2	2.16	0.44
1:E:221:ASN:ND2	1:G:157:GLN:HE22	2.02	0.44
1:G:212:LYS:HG3	4:G:2233:HOH:O	2.17	0.44
1:G:221:ASN:HD22	1:G:221:ASN:HA	1.65	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:212:LYS:NZ	1:I:215:ARG:HH22	2.15	0.44
1:A:10:VAL:HG23	4:A:2004:HOH:O	2.16	0.44
1:B:9:PHE:HB3	1:B:36:ALA:HB2	1.99	0.44
1:B:262:TRP:HE1	1:D:161:ASN:HD22	1.66	0.44
1:B:161:ASN:ND2	1:D:262:TRP:HE1	2.16	0.44
1:H:146:VAL:HG11	1:H:176:CYS:SG	2.57	0.44
1:K:16:VAL:HG21	4:K:2029:HOH:O	2.18	0.44
1:L:93:LEU:HD21	1:L:127:THR:HG22	1.99	0.44
1:B:170:ASN:H	1:B:170:ASN:HD22	1.66	0.44
1:E:207:THR:O	1:E:210:MET:HG2	2.18	0.44
1:H:134:LEU:CD1	1:H:138:LYS:HE3	2.47	0.44
1:K:43:ARG:HA	4:K:2103:HOH:O	2.16	0.44
1:A:158:SER:HB3	1:A:164:LEU:CD1	2.48	0.43
1:E:228:ALA:HB2	1:H:247:TYR:CE2	2.53	0.43
1:I:170:ASN:HD22	1:I:170:ASN:H	1.66	0.43
1:A:121:VAL:HG23	1:A:172:SER:HB2	2.01	0.43
1:A:262:TRP:HE1	1:C:161:ASN:HD22	1.67	0.43
1:A:96:ASN:HA	1:A:147:THR:HB	2.00	0.43
1:A:197:LEU:HD21	1:A:255:ILE:HD12	2.01	0.43
1:D:90:ILE:HD12	1:D:134:LEU:HD23	2.00	0.43
1:D:187:TRP:HB3	1:D:192:ILE:HB	2.00	0.43
1:J:161:ASN:HD22	1:L:262:TRP:HE1	1.67	0.43
1:F:221:ASN:HB2	4:F:2268:HOH:O	2.17	0.43
1:A:13:THR:OG1	1:A:37:ASN:HB2	2.19	0.43
1:E:18:GLY:O	1:E:24:GLY:HA3	2.19	0.43
1:G:72:ASN:OD1	1:G:75:ILE:HG13	2.18	0.43
1:J:221:ASN:ND2	1:L:157:GLN:HE22	2.07	0.43
1:F:207:THR:O	1:F:210:MET:HG2	2.19	0.42
1:I:18:GLY:O	1:I:24:GLY:HA3	2.19	0.42
1:I:221:ASN:HD21	1:K:157:GLN:NE2	2.02	0.42
1:I:247:TYR:CE2	1:L:228:ALA:HB2	2.53	0.42
1:C:53:GLU:HG2	4:C:2070:HOH:O	2.18	0.42
1:E:262:TRP:HE1	1:G:161:ASN:ND2	2.17	0.42
1:B:76:VAL:O	1:B:80:ILE:HG12	2.19	0.42
1:K:50:GLU:HG3	4:K:2068:HOH:O	2.18	0.42
1:J:161:ASN:ND2	1:L:262:TRP:HE1	2.16	0.42
1:A:234:THR:O	1:A:238:ILE:HG13	2.20	0.42
1:A:181:LYS:NZ	4:A:2080:HOH:O	2.49	0.42
1:B:50:GLU:O	1:B:54:LYS:HG3	2.19	0.42
1:B:28:THR:HG23	1:B:38:VAL:HG11	2.02	0.42
1:A:212:LYS:HZ2	1:A:215:ARG:HH22	1.67	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3:PRO:HB3	4:G:2049:HOH:O	2.19	0.42
1:E:161:ASN:ND2	1:G:262:TRP:HE1	2.18	0.42
1:K:211:ASP:HB3	1:K:214:ILE:HD12	2.00	0.42
1:L:3:PRO:N	4:L:2001:HOH:O	2.53	0.42
1:C:206:GLN:N	1:C:206:GLN:OE1	2.44	0.42
1:E:212:LYS:HZ2	1:E:215:ARG:HH22	1.65	0.42
1:F:247:TYR:CE2	1:G:228:ALA:HB2	2.54	0.42
1:H:9:PHE:HB3	1:H:36:ALA:HB2	2.01	0.42
1:K:26:ALA:HB2	1:K:230:PRO:HB2	2.01	0.42
1:B:261:ILE:HG21	1:C:185:ALA:HB2	2.02	0.41
1:E:146:VAL:CG1	1:E:176:CYS:SG	3.08	0.41
1:E:26:ALA:HB2	1:E:230:PRO:HB2	2.02	0.41
1:A:166:GLN:HG3	1:A:170:ASN:ND2	2.35	0.41
1:D:214:ILE:O	1:D:218:GLN:HG3	2.20	0.41
1:F:9:PHE:CB	1:F:36:ALA:HB2	2.50	0.41
1:K:170:ASN:H	1:K:170:ASN:HD22	1.66	0.41
1:J:262:TRP:HE1	1:L:161:ASN:ND2	2.18	0.41
1:A:41:ILE:HG13	4:A:2017:HOH:O	2.19	0.41
1:I:262:TRP:HE1	1:K:161:ASN:HD22	1.68	0.41
1:K:118:ASP:OD1	1:L:110:HIS:HE1	2.03	0.41
1:F:26:ALA:HB2	1:F:230:PRO:HB2	2.03	0.41
1:J:90:ILE:HD12	1:J:134:LEU:HD23	2.03	0.41
1:A:190:ALA:O	1:A:192:ILE:HG13	2.21	0.41
1:A:25:LEU:O	1:A:28:THR:HB	2.20	0.41
1:E:247:TYR:CE2	1:H:228:ALA:HB2	2.55	0.41
1:I:26:ALA:HB2	1:I:230:PRO:HB2	2.01	0.41
1:L:26:ALA:HB2	1:L:230:PRO:HB2	2.01	0.41
1:A:86:ASP:C	1:A:87:LEU:HG	2.41	0.41
1:B:247:TYR:CE2	1:C:228:ALA:HB2	2.56	0.41
1:A:228:ALA:HB2	1:D:247:TYR:CD2	2.56	0.41
1:B:10:VAL:HG12	1:B:11:ASN:CG	2.41	0.41
1:B:161:ASN:HD22	1:D:262:TRP:HE1	1.67	0.41
1:C:9:PHE:HB3	1:C:36:ALA:HB2	2.02	0.41
1:A:42:TYR:CE1	1:A:67:GLN:HA	2.56	0.41
1:B:197:LEU:HD21	1:B:255:ILE:HD12	2.02	0.41
1:I:228:ALA:HB2	1:L:247:TYR:CE2	2.56	0.41
1:B:76:VAL:HG21	1:B:126:ASN:ND2	2.36	0.41
1:A:9:PHE:C	1:A:35:GLY:O	2.59	0.41
1:B:77:THR:O	1:B:81:GLN:HG3	2.20	0.41
1:G:215:ARG:HD2	4:G:2228:HOH:O	2.20	0.41
1:G:199:PRO:HB3	1:G:233:MET:SD	2.61	0.41

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:43:ARG:NH2	4:K:2046:HOH:O	2.53	0.41
1:A:29:ARG:HG2	1:A:29:ARG:NH1	2.35	0.40
1:B:81:GLN:HG3	4:B:2070:HOH:O	2.20	0.40
1:C:236:GLN:HE21	1:C:240:LEU:HG	1.86	0.40
1:E:43:ARG:CZ	4:E:2341:HOH:O	2.69	0.40
1:F:224:LEU:HD12	1:F:224:LEU:HA	1.89	0.40
1:J:228:ALA:HB2	1:K:247:TYR:CE2	2.55	0.40
1:H:170:ASN:HD22	1:H:170:ASN:H	1.70	0.40
1:K:8:SER:OG	1:K:10:VAL:HG23	2.21	0.40
1:L:170:ASN:H	1:L:170:ASN:HD22	1.69	0.40
1:A:157:GLN:HE22	1:C:221:ASN:ND2	2.01	0.40
1:C:74:ASP:O	1:C:78:LYS:HG3	2.21	0.40
1:E:53:GLU:HG3	4:E:2089:HOH:O	2.20	0.40
1:H:212:LYS:HG3	4:H:2241:HOH:O	2.20	0.40
1:D:80:ILE:HA	1:D:80:ILE:HD13	1.94	0.40
1:E:9:PHE:HB3	1:E:36:ALA:HB2	2.04	0.40
1:F:12:LYS:HE3	4:F:2013:HOH:O	2.22	0.40
1:F:76:VAL:O	1:F:80:ILE:HG12	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:ASP:O	1:J:11:ASN:OD1[3_546]	1.88	0.32
4:E:2145:HOH:O	4:F:2169:HOH:O[2_656]	2.17	0.03

## 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	258/265 (97%)	239 (93%)	19 (7%)	0	<b>100</b> <b>100</b>

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	258/265 (97%)	245 (95%)	13 (5%)	0	100	100
1	C	258/265 (97%)	251 (97%)	7 (3%)	0	100	100
1	D	258/265 (97%)	250 (97%)	8 (3%)	0	100	100
1	E	258/265 (97%)	253 (98%)	5 (2%)	0	100	100
1	F	258/265 (97%)	253 (98%)	5 (2%)	0	100	100
1	G	258/265 (97%)	252 (98%)	6 (2%)	0	100	100
1	H	258/265 (97%)	253 (98%)	5 (2%)	0	100	100
1	I	258/265 (97%)	253 (98%)	5 (2%)	0	100	100
1	J	258/265 (97%)	253 (98%)	5 (2%)	0	100	100
1	K	258/265 (97%)	252 (98%)	6 (2%)	0	100	100
1	L	258/265 (97%)	252 (98%)	6 (2%)	0	100	100
All	All	3096/3180 (97%)	3006 (97%)	90 (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	208/211 (99%)	204 (98%)	4 (2%)	62	30
1	B	208/211 (99%)	204 (98%)	4 (2%)	62	30
1	C	208/211 (99%)	206 (99%)	2 (1%)	80	60
1	D	208/211 (99%)	205 (99%)	3 (1%)	71	45
1	E	208/211 (99%)	206 (99%)	2 (1%)	80	60
1	F	208/211 (99%)	205 (99%)	3 (1%)	71	45
1	G	208/211 (99%)	205 (99%)	3 (1%)	71	45
1	H	208/211 (99%)	205 (99%)	3 (1%)	71	45
1	I	208/211 (99%)	206 (99%)	2 (1%)	80	60
1	J	208/211 (99%)	205 (99%)	3 (1%)	71	45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	208/211 (99%)	205 (99%)	3 (1%)	71	45
1	L	208/211 (99%)	205 (99%)	3 (1%)	71	45
All	All	2496/2532 (99%)	2461 (99%)	35 (1%)	71	45

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	161	ASN
1	A	221	ASN
1	A	224	LEU
1	B	161	ASN
1	B	206	GLN
1	B	221	ASN
1	B	224	LEU
1	C	161	ASN
1	C	221	ASN
1	D	161	ASN
1	D	221	ASN
1	D	224	LEU
1	E	221	ASN
1	E	224	LEU
1	F	161	ASN
1	F	221	ASN
1	F	224	LEU
1	G	161	ASN
1	G	221	ASN
1	G	224	LEU
1	H	161	ASN
1	H	221	ASN
1	H	224	LEU
1	I	161	ASN
1	I	221	ASN
1	J	161	ASN
1	J	221	ASN
1	J	224	LEU
1	K	161	ASN
1	K	221	ASN
1	K	224	LEU
1	L	161	ASN
1	L	221	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	L	224	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	110	HIS
1	A	140	GLN
1	A	161	ASN
1	A	170	ASN
1	A	178	ASN
1	A	221	ASN
1	B	140	GLN
1	B	161	ASN
1	B	170	ASN
1	B	178	ASN
1	B	203	ASN
1	B	209	HIS
1	B	221	ASN
1	C	110	HIS
1	C	153	GLN
1	C	161	ASN
1	C	170	ASN
1	C	178	ASN
1	C	221	ASN
1	D	161	ASN
1	D	170	ASN
1	D	178	ASN
1	D	221	ASN
1	E	110	HIS
1	E	161	ASN
1	E	170	ASN
1	E	178	ASN
1	E	221	ASN
1	F	110	HIS
1	F	161	ASN
1	F	170	ASN
1	F	178	ASN
1	F	221	ASN
1	G	11	ASN
1	G	153	GLN
1	G	161	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	170	ASN
1	G	178	ASN
1	G	221	ASN
1	H	82	GLN
1	H	161	ASN
1	H	170	ASN
1	H	178	ASN
1	H	221	ASN
1	I	161	ASN
1	I	170	ASN
1	I	178	ASN
1	I	221	ASN
1	J	110	HIS
1	J	140	GLN
1	J	161	ASN
1	J	170	ASN
1	J	178	ASN
1	J	221	ASN
1	K	110	HIS
1	K	161	ASN
1	K	170	ASN
1	K	178	ASN
1	K	221	ASN
1	L	110	HIS
1	L	161	ASN
1	L	170	ASN
1	L	178	ASN
1	L	221	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	NAP	A	263	-	44,52,52	1.61	3 (6%)	51,80,80	1.93	6 (11%)
2	NAP	B	263	-	44,52,52	1.49	3 (6%)	51,80,80	1.88	6 (11%)
2	NAP	C	263	-	44,52,52	1.54	4 (9%)	51,80,80	2.03	6 (11%)
2	NAP	D	263	-	44,52,52	1.54	4 (9%)	51,80,80	2.08	6 (11%)
2	NAP	E	263	-	44,52,52	1.56	4 (9%)	51,80,80	2.11	6 (11%)
2	NAP	F	263	-	44,52,52	1.53	4 (9%)	51,80,80	2.03	8 (15%)
2	NAP	G	263	-	44,52,52	1.53	4 (9%)	51,80,80	2.18	6 (11%)
2	NAP	H	263	-	44,52,52	1.53	4 (9%)	51,80,80	2.10	7 (13%)
2	NAP	I	263	-	44,52,52	1.57	4 (9%)	51,80,80	1.87	6 (11%)
2	NAP	J	263	-	44,52,52	1.47	5 (11%)	51,80,80	2.02	7 (13%)
2	NAP	K	263	-	44,52,52	1.54	4 (9%)	51,80,80	2.02	7 (13%)
2	NAP	L	263	-	44,52,52	1.52	4 (9%)	51,80,80	2.16	6 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	A	263	-	-	0/27/67/67	0/5/5/5
2	NAP	B	263	-	-	0/27/67/67	0/5/5/5
2	NAP	C	263	-	-	0/27/67/67	0/5/5/5
2	NAP	D	263	-	-	0/27/67/67	0/5/5/5
2	NAP	E	263	-	-	0/27/67/67	0/5/5/5
2	NAP	F	263	-	-	0/27/67/67	0/5/5/5
2	NAP	G	263	-	-	0/27/67/67	0/5/5/5
2	NAP	H	263	-	-	0/27/67/67	0/5/5/5
2	NAP	I	263	-	-	0/27/67/67	0/5/5/5
2	NAP	J	263	-	-	0/27/67/67	0/5/5/5

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	K	263	-	-	0/27/67/67	0/5/5/5
2	NAP	L	263	-	-	0/27/67/67	0/5/5/5

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	263	NAP	O3B-C3B	-3.02	1.36	1.43
2	E	263	NAP	O3B-C3B	-2.88	1.36	1.43
2	G	263	NAP	O3B-C3B	-2.70	1.36	1.43
2	F	263	NAP	O3B-C3B	-2.63	1.36	1.43
2	C	263	NAP	O3B-C3B	-2.56	1.37	1.43
2	H	263	NAP	O3B-C3B	-2.51	1.37	1.43
2	I	263	NAP	O3B-C3B	-2.48	1.37	1.43
2	L	263	NAP	O3B-C3B	-2.44	1.37	1.43
2	D	263	NAP	O3B-C3B	-2.31	1.37	1.43
2	J	263	NAP	O3B-C3B	-2.23	1.37	1.43
2	E	263	NAP	O4B-C4B	-2.10	1.40	1.45
2	J	263	NAP	O4B-C4B	-2.06	1.40	1.45
2	K	263	NAP	C2A-N1A	2.17	1.38	1.33
2	J	263	NAP	C2A-N1A	2.19	1.38	1.33
2	D	263	NAP	C2A-N1A	2.21	1.38	1.33
2	C	263	NAP	C2A-N1A	2.25	1.38	1.33
2	L	263	NAP	C2A-N1A	2.25	1.38	1.33
2	G	263	NAP	C2A-N1A	2.26	1.38	1.33
2	H	263	NAP	C2A-N1A	2.27	1.38	1.33
2	B	263	NAP	C2A-N1A	2.41	1.38	1.33
2	A	263	NAP	C2A-N1A	2.51	1.38	1.33
2	I	263	NAP	C2A-N1A	2.64	1.38	1.33
2	F	263	NAP	C2A-N1A	2.65	1.38	1.33
2	K	263	NAP	C2A-N3A	2.92	1.37	1.32
2	C	263	NAP	C2A-N3A	3.07	1.37	1.32
2	J	263	NAP	C2A-N3A	3.08	1.37	1.32
2	B	263	NAP	C2A-N3A	3.14	1.37	1.32
2	E	263	NAP	C2A-N3A	3.16	1.37	1.32
2	G	263	NAP	C2A-N3A	3.25	1.37	1.32
2	F	263	NAP	C2A-N3A	3.27	1.37	1.32
2	H	263	NAP	C2A-N3A	3.32	1.37	1.32
2	D	263	NAP	C2A-N3A	3.37	1.37	1.32
2	L	263	NAP	C2A-N3A	3.46	1.37	1.32
2	I	263	NAP	C2A-N3A	3.51	1.38	1.32
2	A	263	NAP	C2A-N3A	3.67	1.38	1.32
2	L	263	NAP	O7N-C7N	7.37	1.39	1.24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	263	NAP	O7N-C7N	7.49	1.39	1.24
2	H	263	NAP	O7N-C7N	7.59	1.39	1.24
2	B	263	NAP	O7N-C7N	7.64	1.39	1.24
2	G	263	NAP	O7N-C7N	7.71	1.40	1.24
2	K	263	NAP	O7N-C7N	7.74	1.40	1.24
2	F	263	NAP	O7N-C7N	7.75	1.40	1.24
2	E	263	NAP	O7N-C7N	7.79	1.40	1.24
2	D	263	NAP	O7N-C7N	7.89	1.40	1.24
2	I	263	NAP	O7N-C7N	7.95	1.40	1.24
2	C	263	NAP	O7N-C7N	8.10	1.40	1.24
2	A	263	NAP	O7N-C7N	8.43	1.41	1.24

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	263	NAP	N3A-C2A-N1A	-11.01	119.27	128.86
2	L	263	NAP	N3A-C2A-N1A	-10.83	119.43	128.86
2	A	263	NAP	N3A-C2A-N1A	-10.64	119.59	128.86
2	G	263	NAP	N3A-C2A-N1A	-10.30	119.89	128.86
2	B	263	NAP	N3A-C2A-N1A	-10.22	119.96	128.86
2	C	263	NAP	N3A-C2A-N1A	-10.17	120.00	128.86
2	F	263	NAP	N3A-C2A-N1A	-10.11	120.05	128.86
2	H	263	NAP	N3A-C2A-N1A	-9.92	120.22	128.86
2	E	263	NAP	N3A-C2A-N1A	-9.86	120.27	128.86
2	J	263	NAP	N3A-C2A-N1A	-9.80	120.32	128.86
2	K	263	NAP	N3A-C2A-N1A	-9.51	120.58	128.86
2	I	263	NAP	N3A-C2A-N1A	-8.24	121.68	128.86
2	G	263	NAP	O3B-C3B-C4B	-7.25	89.92	111.09
2	E	263	NAP	O3B-C3B-C4B	-7.24	89.94	111.09
2	L	263	NAP	O3B-C3B-C4B	-6.57	91.89	111.09
2	H	263	NAP	O3B-C3B-C4B	-6.47	92.18	111.09
2	J	263	NAP	O3B-C3B-C4B	-6.11	93.23	111.09
2	I	263	NAP	O3B-C3B-C4B	-5.70	94.43	111.09
2	C	263	NAP	O3B-C3B-C4B	-5.52	94.95	111.09
2	K	263	NAP	O3B-C3B-C4B	-5.46	95.13	111.09
2	F	263	NAP	O3B-C3B-C4B	-5.20	95.89	111.09
2	D	263	NAP	O3B-C3B-C4B	-4.84	96.95	111.09
2	A	263	NAP	O3B-C3B-C4B	-3.96	99.53	111.09
2	B	263	NAP	O3B-C3B-C4B	-3.49	100.88	111.09
2	I	263	NAP	C1B-N9A-C4A	-3.30	120.93	126.64
2	E	263	NAP	C1B-N9A-C4A	-3.14	121.22	126.64
2	A	263	NAP	C1B-N9A-C4A	-3.13	121.23	126.64

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	263	NAP	C1B-N9A-C4A	-3.06	121.34	126.64
2	J	263	NAP	C1B-N9A-C4A	-2.91	121.61	126.64
2	C	263	NAP	C1B-N9A-C4A	-2.83	121.74	126.64
2	G	263	NAP	C1B-N9A-C4A	-2.82	121.75	126.64
2	K	263	NAP	C1B-N9A-C4A	-2.81	121.77	126.64
2	L	263	NAP	C1B-N9A-C4A	-2.78	121.84	126.64
2	H	263	NAP	C1B-N9A-C4A	-2.72	121.93	126.64
2	D	263	NAP	C1B-N9A-C4A	-2.62	122.11	126.64
2	K	263	NAP	O7N-C7N-C3N	-2.59	116.60	119.62
2	B	263	NAP	C1B-N9A-C4A	-2.56	122.21	126.64
2	H	263	NAP	O7N-C7N-C3N	-2.46	116.74	119.62
2	B	263	NAP	C4A-C5A-N7A	-2.23	107.26	109.41
2	H	263	NAP	C4A-C5A-N7A	-2.23	107.26	109.41
2	J	263	NAP	O7N-C7N-C3N	-2.20	117.05	119.62
2	F	263	NAP	O7N-C7N-C3N	-2.17	117.09	119.62
2	F	263	NAP	C4A-C5A-N7A	-2.13	107.35	109.41
2	E	263	NAP	O7N-C7N-C3N	-2.08	117.19	119.62
2	D	263	NAP	C4A-C5A-N7A	-2.08	107.40	109.41
2	I	263	NAP	O7N-C7N-C3N	-2.03	117.25	119.62
2	C	263	NAP	C4A-C5A-N7A	-2.02	107.46	109.41
2	A	263	NAP	C3N-C7N-N7N	2.00	120.06	117.77
2	G	263	NAP	C2N-C3N-C4N	2.01	120.56	118.26
2	K	263	NAP	O2B-C2B-C3B	2.02	119.12	111.63
2	A	263	NAP	O2X-P2B-O2B	2.07	115.42	106.00
2	J	263	NAP	C3N-C7N-N7N	2.10	120.18	117.77
2	L	263	NAP	C2N-C3N-C4N	2.26	120.84	118.26
2	F	263	NAP	C2N-C3N-C4N	2.27	120.85	118.26
2	J	263	NAP	C2N-C3N-C4N	2.38	120.98	118.26
2	L	263	NAP	C3N-C7N-N7N	2.58	120.72	117.77
2	B	263	NAP	C3N-C7N-N7N	2.61	120.76	117.77
2	A	263	NAP	C2B-C3B-C4B	2.66	108.00	101.95
2	E	263	NAP	C3N-C7N-N7N	2.80	120.97	117.77
2	F	263	NAP	C3N-C7N-N7N	2.84	121.02	117.77
2	B	263	NAP	C2B-C3B-C4B	2.85	108.42	101.95
2	C	263	NAP	C3N-C7N-N7N	2.87	121.05	117.77
2	D	263	NAP	C2B-C3B-C4B	3.06	108.91	101.95
2	H	263	NAP	C3N-C7N-N7N	3.17	121.40	117.77
2	I	263	NAP	C3N-C7N-N7N	3.19	121.42	117.77
2	G	263	NAP	C3N-C7N-N7N	3.23	121.46	117.77
2	F	263	NAP	C2B-C3B-C4B	3.27	109.38	101.95
2	J	263	NAP	C2B-C3B-C4B	3.41	109.70	101.95
2	D	263	NAP	C3N-C7N-N7N	3.49	121.76	117.77

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	263	NAP	C2B-C3B-C4B	3.52	109.95	101.95
2	H	263	NAP	C2B-C3B-C4B	3.62	110.18	101.95
2	I	263	NAP	C2B-C3B-C4B	3.64	110.23	101.95
2	L	263	NAP	C2B-C3B-C4B	3.65	110.25	101.95
2	K	263	NAP	C2B-C3B-C4B	3.72	110.42	101.95
2	C	263	NAP	C2B-C3B-C4B	3.82	110.62	101.95
2	E	263	NAP	C2B-C3B-C4B	4.06	111.18	101.95
2	K	263	NAP	C3N-C7N-N7N	4.21	122.58	117.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	263	NAP	1	0
2	B	263	NAP	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	260/265 (98%)	1.90	99 (38%) 0 0	26, 49, 74, 82	0
1	B	260/265 (98%)	0.87	31 (11%) 5 5	21, 29, 38, 45	0
1	C	260/265 (98%)	0.39	21 (8%) 13 14	17, 23, 33, 41	0
1	D	260/265 (98%)	0.81	34 (13%) 4 4	18, 29, 41, 55	0
1	E	260/265 (98%)	0.16	14 (5%) 26 30	14, 18, 25, 30	0
1	F	260/265 (98%)	0.30	12 (4%) 33 37	14, 19, 28, 34	0
1	G	260/265 (98%)	0.39	25 (9%) 9 10	14, 21, 31, 36	0
1	H	260/265 (98%)	0.28	13 (5%) 30 33	14, 18, 27, 30	0
1	I	260/265 (98%)	0.24	14 (5%) 26 30	14, 19, 27, 32	0
1	J	260/265 (98%)	0.37	19 (7%) 16 18	15, 21, 31, 36	0
1	K	260/265 (98%)	0.30	13 (5%) 30 33	14, 20, 29, 37	0
1	L	260/265 (98%)	0.24	9 (3%) 44 50	14, 19, 27, 31	0
All	All	3120/3180 (98%)	0.52	304 (9%) 8 10	14, 21, 45, 82	0

All (304) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3	PRO	11.7
1	D	208	ALA	9.4
1	A	208	ALA	8.4
1	B	11	ASN	8.3
1	I	3	PRO	8.0
1	D	209	HIS	8.0
1	H	3	PRO	7.7
1	B	10	VAL	7.7
1	D	207	THR	7.3
1	A	57	LYS	6.9
1	A	65	ALA	6.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	11	ASN	6.8
1	A	209	HIS	6.7
1	B	3	PRO	6.6
1	J	3	PRO	6.5
1	A	50	GLU	6.4
1	A	45	ALA	6.3
1	A	3	PRO	6.2
1	C	3	PRO	6.1
1	A	46	ALA	5.8
1	A	61	VAL	5.7
1	L	3	PRO	5.6
1	A	63	THR	5.6
1	D	206	GLN	5.3
1	D	210	MET	5.2
1	L	209	HIS	5.0
1	G	3	PRO	5.0
1	D	205	ASP	5.0
1	K	209	HIS	4.8
1	A	78	LYS	4.8
1	B	137	GLN	4.7
1	J	208	ALA	4.7
1	D	215	ARG	4.7
1	J	209	HIS	4.7
1	J	212	LYS	4.6
1	A	55	VAL	4.6
1	A	81	GLN	4.6
1	K	137	GLN	4.6
1	G	209	HIS	4.5
1	F	3	PRO	4.5
1	A	66	TYR	4.5
1	A	83	ILE	4.4
1	K	3	PRO	4.4
1	L	208	ALA	4.4
1	H	208	ALA	4.4
1	I	209	HIS	4.4
1	J	11	ASN	4.3
1	A	42	TYR	4.3
1	A	88	GLY	4.2
1	D	11	ASN	4.2
1	A	43	ARG	4.1
1	A	54	LYS	4.1
1	I	208	ALA	4.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	137	GLN	4.0
1	C	210	MET	4.0
1	A	48	ALA	4.0
1	B	139	GLN	3.9
1	A	10	VAL	3.9
1	A	44	SER	3.9
1	C	208	ALA	3.9
1	A	87	LEU	3.9
1	G	210	MET	3.9
1	E	209	HIS	3.8
1	C	206	GLN	3.8
1	D	212	LYS	3.8
1	A	213	LYS	3.8
1	L	212	LYS	3.8
1	B	78	LYS	3.7
1	A	9	PHE	3.7
1	A	212	LYS	3.7
1	A	38	VAL	3.7
1	A	211	ASP	3.7
1	C	213	LYS	3.7
1	A	51	VAL	3.6
1	C	209	HIS	3.6
1	B	12	LYS	3.6
1	C	11	ASN	3.6
1	A	67	GLN	3.6
1	A	34	ALA	3.6
1	A	176	CYS	3.6
1	A	75	ILE	3.6
1	D	213	LYS	3.5
1	A	59	PHE	3.5
1	A	56	GLY	3.5
1	C	4	GLY	3.5
1	A	136	LEU	3.5
1	H	209	HIS	3.4
1	J	210	MET	3.4
1	E	3	PRO	3.4
1	A	240	LEU	3.4
1	A	214	ILE	3.4
1	J	137	GLN	3.4
1	D	53	GLU	3.4
1	A	74	ASP	3.3
1	G	212	LYS	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	9	PHE	3.3
1	B	81	GLN	3.3
1	D	211	ASP	3.3
1	K	211	ASP	3.3
1	G	176	CYS	3.3
1	D	57	LYS	3.3
1	A	85	ALA	3.3
1	B	146	VAL	3.3
1	A	35	GLY	3.2
1	A	89	PRO	3.2
1	K	212	LYS	3.2
1	A	196	ALA	3.2
1	A	210	MET	3.2
1	A	205	ASP	3.2
1	A	139	GLN	3.2
1	A	13	THR	3.1
1	A	79	THR	3.1
1	I	212	LYS	3.1
1	I	206	GLN	3.1
1	B	43	ARG	3.1
1	A	169	TYR	3.1
1	K	205	ASP	3.1
1	D	59	PHE	3.1
1	G	81	GLN	3.1
1	G	205	ASP	3.1
1	A	8	SER	3.1
1	A	41	ILE	3.1
1	A	206	GLN	3.0
1	F	53	GLU	3.0
1	J	134	LEU	3.0
1	L	206	GLN	3.0
1	D	4	GLY	3.0
1	J	211	ASP	3.0
1	D	81	GLN	3.0
1	E	208	ALA	3.0
1	A	64	LYS	2.9
1	E	212	LYS	2.9
1	D	55	VAL	2.9
1	B	111	GLU	2.9
1	K	176	CYS	2.9
1	J	111	GLU	2.9
1	J	213	LYS	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	147	THR	2.9
1	A	16	VAL	2.9
1	D	10	VAL	2.9
1	A	47	ASP	2.9
1	B	210	MET	2.9
1	B	160	LEU	2.9
1	L	213	LYS	2.9
1	B	209	HIS	2.8
1	B	76	VAL	2.8
1	F	209	HIS	2.8
1	D	254	PHE	2.8
1	G	254	PHE	2.8
1	A	94	ILE	2.8
1	D	224	LEU	2.8
1	A	160	LEU	2.7
1	D	87	LEU	2.7
1	D	43	ARG	2.7
1	G	213	LYS	2.7
1	B	75	ILE	2.7
1	G	137	GLN	2.7
1	F	111	GLU	2.7
1	G	206	GLN	2.7
1	A	90	ILE	2.7
1	A	180	VAL	2.7
1	D	50	GLU	2.7
1	I	139	GLN	2.7
1	A	25	LEU	2.7
1	A	49	VAL	2.6
1	A	146	VAL	2.6
1	G	208	ALA	2.6
1	A	53	GLU	2.6
1	C	53	GLU	2.6
1	F	176	CYS	2.6
1	A	70	VAL	2.6
1	C	212	LYS	2.6
1	G	111	GLU	2.6
1	A	62	LYS	2.6
1	A	82	GLN	2.6
1	I	4	GLY	2.6
1	A	76	VAL	2.6
1	A	40	VAL	2.6
1	A	80	ILE	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	215	ARG	2.5
1	K	43	ARG	2.5
1	A	20	ASN	2.5
1	A	111	GLU	2.5
1	D	160	LEU	2.5
1	B	53	GLU	2.5
1	D	137	GLN	2.5
1	I	137	GLN	2.5
1	L	137	GLN	2.5
1	A	144	ILE	2.5
1	G	174	ALA	2.5
1	G	57	LYS	2.5
1	K	213	LYS	2.5
1	J	206	GLN	2.5
1	B	179	LEU	2.5
1	A	12	LYS	2.5
1	E	206	GLN	2.5
1	G	11	ASN	2.5
1	B	42	TYR	2.5
1	H	174	ALA	2.5
1	I	11	ASN	2.5
1	D	214	ILE	2.5
1	B	206	GLN	2.5
1	B	45	ALA	2.4
1	D	88	GLY	2.4
1	J	205	ASP	2.4
1	A	175	ALA	2.4
1	L	180	VAL	2.4
1	B	50	GLU	2.4
1	G	238	ILE	2.4
1	H	137	GLN	2.4
1	F	57	LYS	2.4
1	B	176	CYS	2.4
1	B	225	ASN	2.4
1	C	207	THR	2.4
1	D	204	THR	2.4
1	D	89	PRO	2.4
1	H	213	LYS	2.4
1	C	160	LEU	2.4
1	I	213	LYS	2.3
1	G	207	THR	2.3
1	I	207	THR	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	50	GLU	2.3
1	G	160	LEU	2.3
1	B	46	ALA	2.3
1	B	180	VAL	2.3
1	C	176	CYS	2.3
1	J	176	CYS	2.3
1	I	43	ARG	2.3
1	E	137	GLN	2.3
1	E	213	LYS	2.3
1	H	207	THR	2.3
1	A	15	ILE	2.3
1	D	75	ILE	2.3
1	C	50	GLU	2.3
1	D	54	LYS	2.3
1	C	205	ASP	2.3
1	A	68	CYS	2.2
1	A	238	ILE	2.2
1	F	240	LEU	2.2
1	G	240	LEU	2.2
1	G	253	TYR	2.2
1	D	33	ALA	2.2
1	C	211	ASP	2.2
1	E	205	ASP	2.2
1	F	205	ASP	2.2
1	G	50	GLU	2.2
1	A	23	ILE	2.2
1	J	215	ARG	2.2
1	A	253	TYR	2.2
1	E	211	ASP	2.2
1	I	205	ASP	2.2
1	E	146	VAL	2.2
1	A	191	GLY	2.2
1	E	43	ARG	2.2
1	A	95	ALA	2.2
1	A	154	ILE	2.2
1	J	75	ILE	2.2
1	I	50	GLU	2.2
1	K	111	GLU	2.2
1	C	215	ARG	2.2
1	B	205	ASP	2.2
1	A	192	ILE	2.1
1	A	72	ASN	2.1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	81	GLN	2.1
1	F	43	ARG	2.1
1	A	207	THR	2.1
1	E	53	GLU	2.1
1	G	53	GLU	2.1
1	F	137	GLN	2.1
1	L	81	GLN	2.1
1	E	210	MET	2.1
1	G	43	ARG	2.1
1	A	93	LEU	2.1
1	J	50	GLU	2.1
1	C	225	ASN	2.1
1	E	260	LEU	2.1
1	A	6	THR	2.1
1	J	43	ARG	2.1
1	C	57	LYS	2.1
1	A	116	VAL	2.1
1	H	53	GLU	2.1
1	B	9	PHE	2.1
1	F	207	THR	2.1
1	J	207	THR	2.1
1	B	175	ALA	2.1
1	A	217	HIS	2.0
1	C	75	ILE	2.0
1	G	75	ILE	2.0
1	H	43	ARG	2.0
1	A	31	VAL	2.0
1	K	210	MET	2.0
1	H	57	LYS	2.0
1	A	134	LEU	2.0
1	A	197	LEU	2.0
1	B	135	TRP	2.0
1	B	136	LEU	2.0
1	A	19	GLY	2.0
1	F	60	GLY	2.0
1	H	81	GLN	2.0
1	H	206	GLN	2.0
1	K	78	LYS	2.0
1	A	33	ALA	2.0
1	A	245	ALA	2.0
1	K	208	ALA	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(Å <sup>2</sup> )	Q<0.9
3	NI	B	2263	1/1	0.88	0.41	11.81	78,78,78,78	0
3	NI	J	3263	1/1	0.98	0.17	2.94	16,16,16,16	0
2	NAP	J	263	48/48	0.95	0.09	-0.09	18,20,24,28	0
2	NAP	A	263	48/48	0.86	0.17	-0.09	40,54,62,68	0
2	NAP	K	263	48/48	0.95	0.09	-0.18	16,18,22,27	0
3	NI	A	2263	1/1	0.96	0.11	-0.22	32,32,32,32	0
2	NAP	H	263	48/48	0.95	0.09	-0.23	15,18,21,28	0
2	NAP	D	263	48/48	0.94	0.09	-0.26	22,25,30,32	0
2	NAP	C	263	48/48	0.95	0.09	-0.27	17,21,25,30	0
2	NAP	I	263	48/48	0.96	0.08	-0.31	16,18,22,28	0
2	NAP	B	263	48/48	0.91	0.10	-0.38	22,28,31,34	0
2	NAP	G	263	48/48	0.95	0.09	-0.39	16,20,23,26	0
2	NAP	E	263	48/48	0.96	0.08	-0.40	15,17,20,25	0
3	NI	I	3263	1/1	1.00	0.10	-0.42	21,21,21,21	0
2	NAP	L	263	48/48	0.96	0.08	-0.45	15,18,22,27	0
3	NI	F	3263	1/1	0.99	0.10	-0.52	20,20,20,20	0
2	NAP	F	263	48/48	0.96	0.08	-0.53	15,17,21,27	0
3	NI	E	3263	1/1	1.00	0.09	-1.11	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.