



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:53 am GMT

PDB ID : 4B7X  
Title : Crystal structure of hypothetical protein PA1648 from *Pseudomonas aeruginosa*.  
Authors : Alphey, M.S.; McMahon, S.A.; Duthie, F.; Naismith, J.H.  
Deposited on : 2012-08-24  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

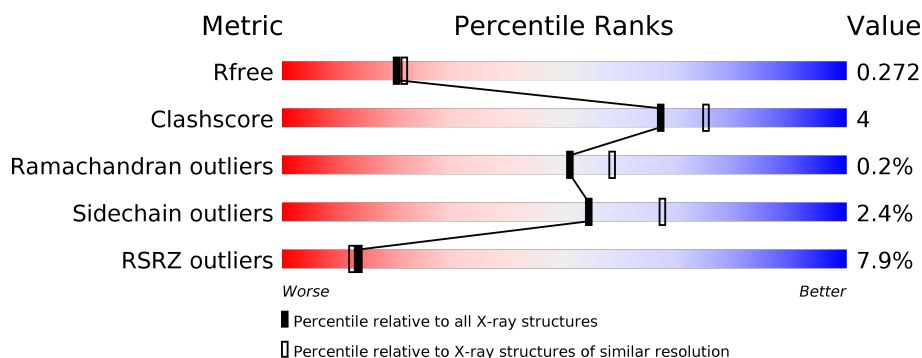
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	336	<div> <div>90%</div> <div>7% ..</div> </div>
1	B	336	<div> <div>90%</div> <div>9% .</div> </div>
1	C	336	<div> <div>7%</div> <div>85%</div> <div>11% .</div> </div>
1	D	336	<div> <div>7%</div> <div>87%</div> <div>10% ..</div> </div>
1	E	336	<div> <div>3%</div> <div>91%</div> <div>7% .</div> </div>
1	F	336	<div> <div>5%</div> <div>88%</div> <div>10% .</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	336	<div><div></div><div>11%</div><div>84%</div><div>11%</div><div></div><div></div></div>
1	H	336	<div><div></div><div>4%</div><div>84%</div><div>13%</div><div></div><div></div></div>
1	I	336	<div><div></div><div>22%</div><div>60%</div><div>9%</div><div></div><div>30%</div></div>
1	J	336	<div><div></div><div>7%</div><div>84%</div><div>13%</div><div></div><div></div></div>
1	K	336	<div><div></div><div>16%</div><div>71%</div><div>18%</div><div></div><div>10%</div></div>
1	L	336	<div><div></div><div>8%</div><div>79%</div><div>15%</div><div></div><div>5%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30208 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 PROBABLE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2504	1597	431	463	13			
1	B	331	Total	C	N	O	S	0	0	0
			2521	1608	434	466	13			
1	C	325	Total	C	N	O	S	0	0	0
			2473	1581	423	456	13			
1	D	327	Total	C	N	O	S	0	0	0
			2490	1590	428	459	13			
1	E	331	Total	C	N	O	S	0	0	0
			2521	1608	434	466	13			
1	F	331	Total	C	N	O	S	0	0	0
			2521	1608	434	466	13			
1	G	321	Total	C	N	O	S	0	0	0
			2446	1564	417	452	13			
1	H	327	Total	C	N	O	S	0	0	0
			2489	1591	426	459	13			
1	I	234	Total	C	N	O	S	0	0	0
			1768	1129	303	324	12			
1	J	327	Total	C	N	O	S	0	0	0
			2486	1586	428	459	13			
1	K	302	Total	C	N	O	S	0	0	0
			2316	1484	399	421	12			
1	L	320	Total	C	N	O	S	0	0	0
			2443	1563	417	450	13			

There are 24 discrepancies between the modelled and reference sequences:

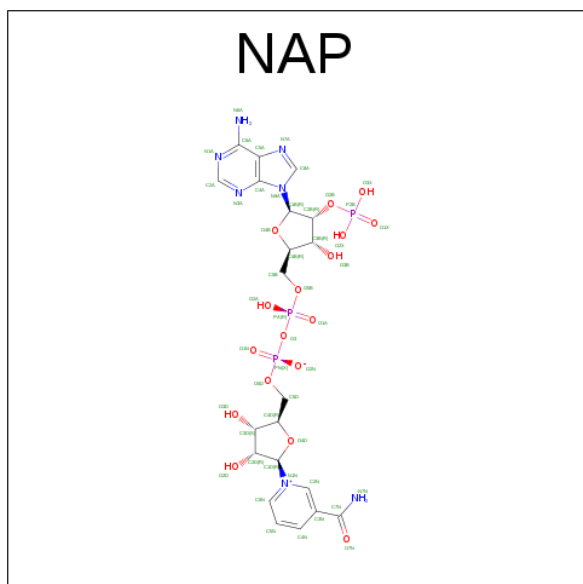
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q9I377
A	0	ALA	-	EXPRESSION TAG	UNP Q9I377
B	-1	GLY	-	EXPRESSION TAG	UNP Q9I377
B	0	ALA	-	EXPRESSION TAG	UNP Q9I377
C	-1	GLY	-	EXPRESSION TAG	UNP Q9I377

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	ALA	-	EXPRESSION TAG	UNP Q9I377
D	-1	GLY	-	EXPRESSION TAG	UNP Q9I377
D	0	ALA	-	EXPRESSION TAG	UNP Q9I377
E	-1	GLY	-	EXPRESSION TAG	UNP Q9I377
E	0	ALA	-	EXPRESSION TAG	UNP Q9I377
F	-1	GLY	-	EXPRESSION TAG	UNP Q9I377
F	0	ALA	-	EXPRESSION TAG	UNP Q9I377
G	-1	GLY	-	EXPRESSION TAG	UNP Q9I377
G	0	ALA	-	EXPRESSION TAG	UNP Q9I377
H	-1	GLY	-	EXPRESSION TAG	UNP Q9I377
H	0	ALA	-	EXPRESSION TAG	UNP Q9I377
I	-1	GLY	-	EXPRESSION TAG	UNP Q9I377
I	0	ALA	-	EXPRESSION TAG	UNP Q9I377
J	-1	GLY	-	EXPRESSION TAG	UNP Q9I377
J	0	ALA	-	EXPRESSION TAG	UNP Q9I377
K	-1	GLY	-	EXPRESSION TAG	UNP Q9I377
K	0	ALA	-	EXPRESSION TAG	UNP Q9I377
L	-1	GLY	-	EXPRESSION TAG	UNP Q9I377
L	0	ALA	-	EXPRESSION TAG	UNP Q9I377

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



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		
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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	118	Total	O	0	0
			118	118		
3	B	68	Total	O	0	0
			68	68		
3	C	46	Total	O	0	0
			46	46		
3	D	60	Total	O	0	0
			60	60		
3	E	81	Total	O	0	0
			81	81		
3	F	67	Total	O	0	0
			67	67		
3	G	43	Total	O	0	0
			43	43		
3	H	41	Total	O	0	0
			41	41		

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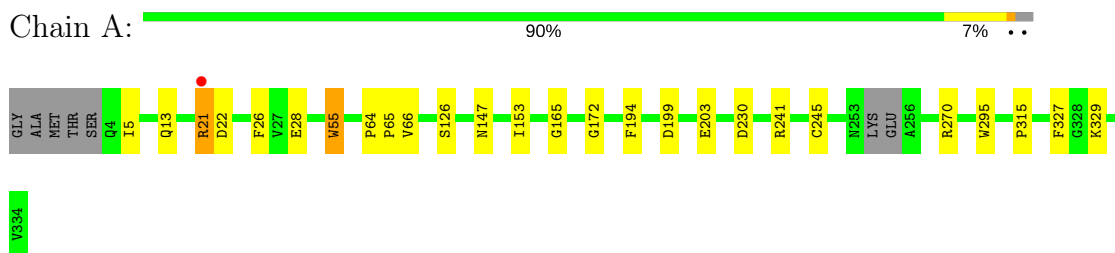
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	20	Total 20	O 20	0	0
3	J	37	Total 37	O 37	0	0
3	K	30	Total 30	O 30	0	0
3	L	43	Total 43	O 43	0	0

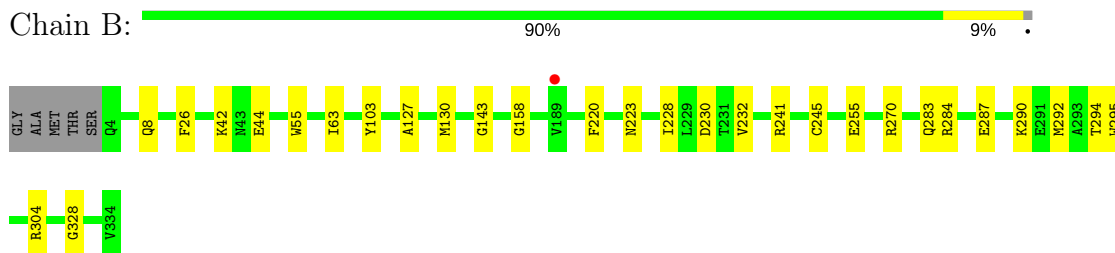
### 3 Residue-property plots [i](#)

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

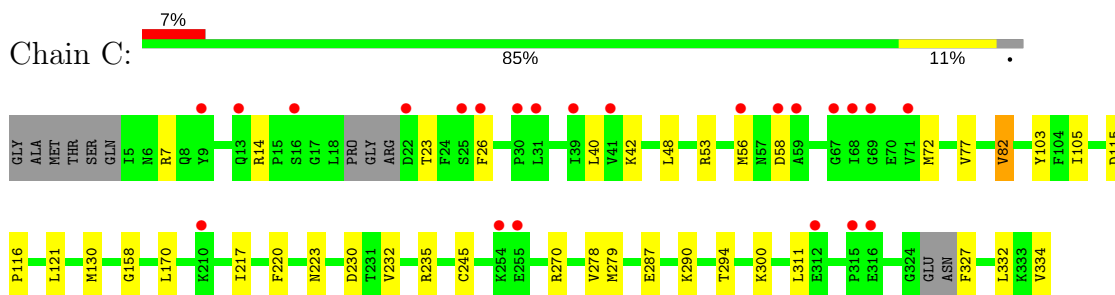
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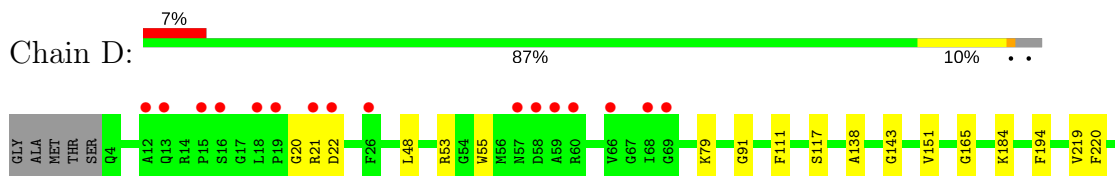
#### • Molecule 1: PROBABLE OXIDOREDUCTASE



#### • Molecule 1: PROBABLE OXIDOREDUCTASE



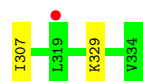
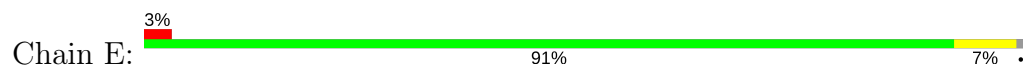
#### • Molecule 1: PROBABLE OXIDOREDUCTASE



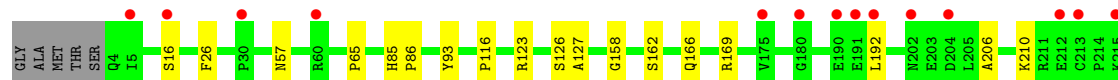
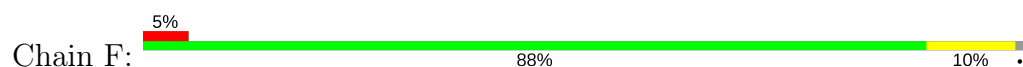




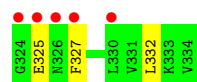
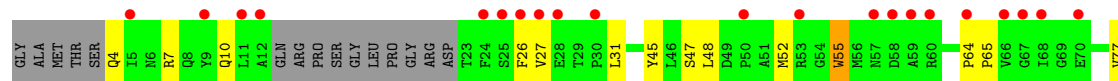
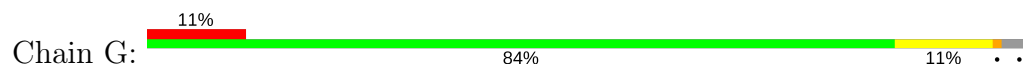
• Molecule 1: PROBABLE OXIDOREDUCTASE



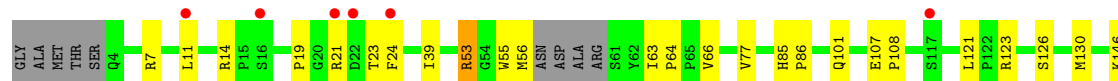
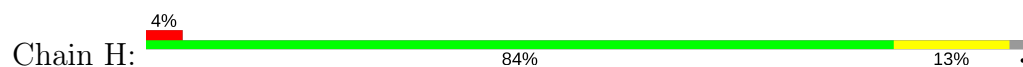
• Molecule 1: PROBABLE OXIDOREDUCTASE



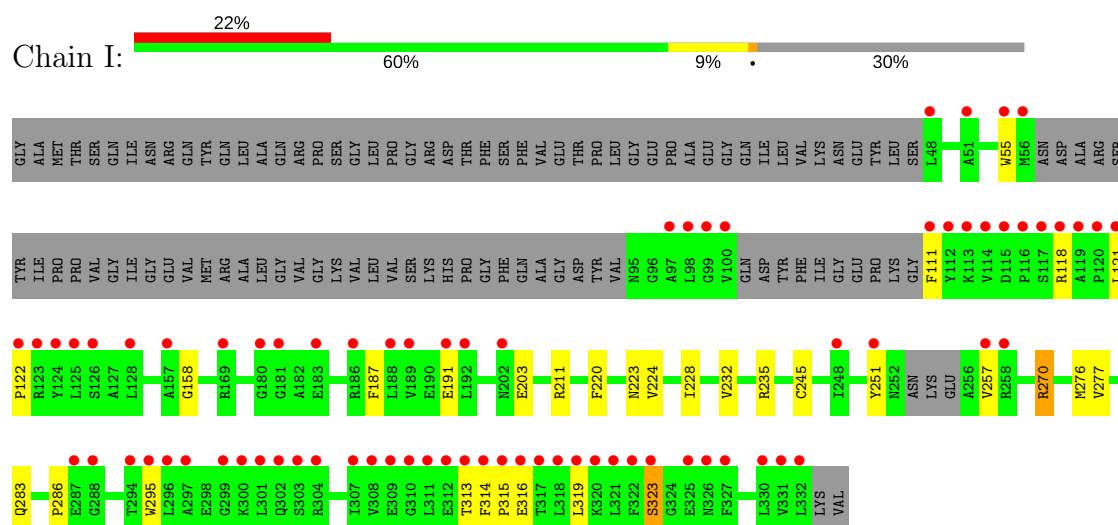
• Molecule 1: PROBABLE OXIDOREDUCTASE



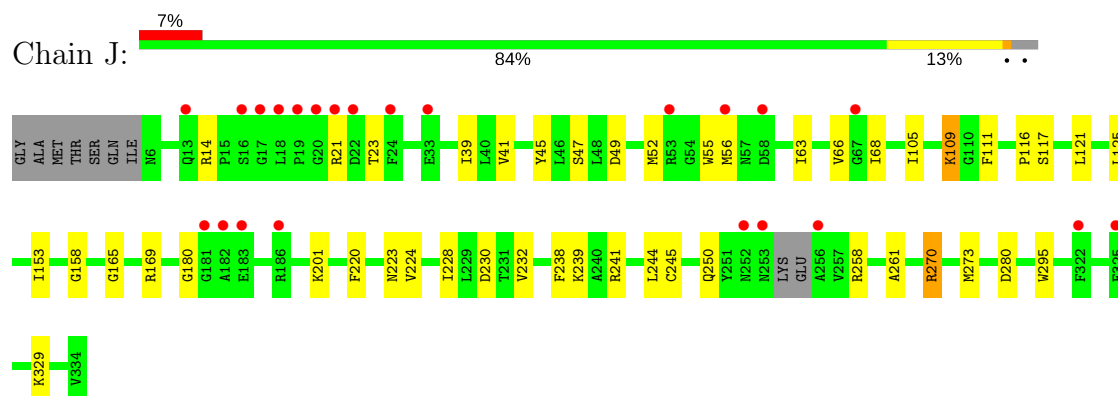
• Molecule 1: PROBABLE OXIDOREDUCTASE



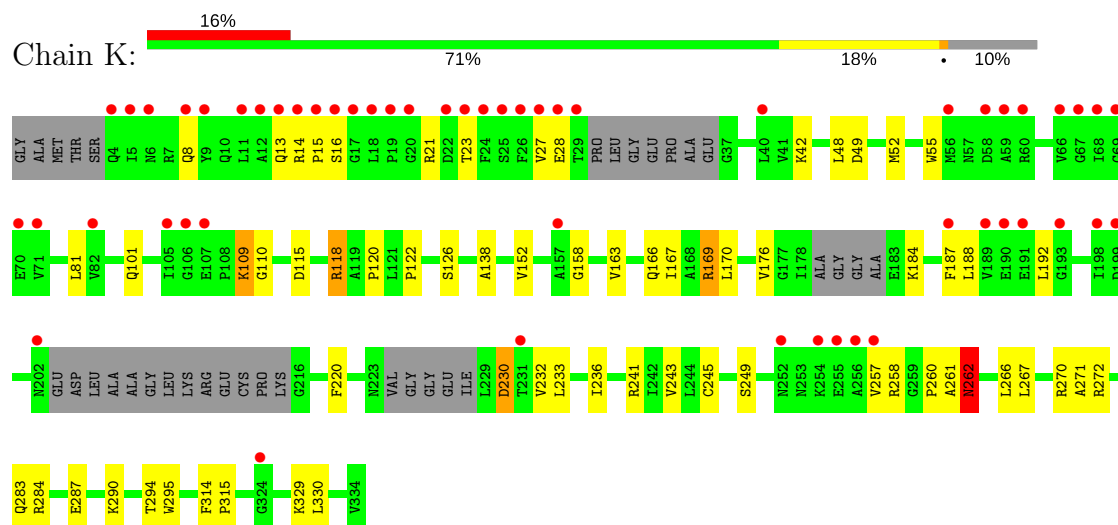
• Molecule 1: PROBABLE OXIDOREDUCTASE



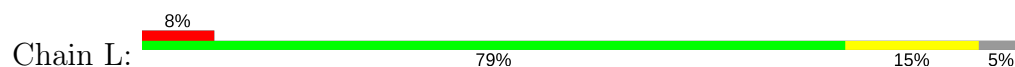
• Molecule 1: PROBABLE OXIDOREDUCTASE

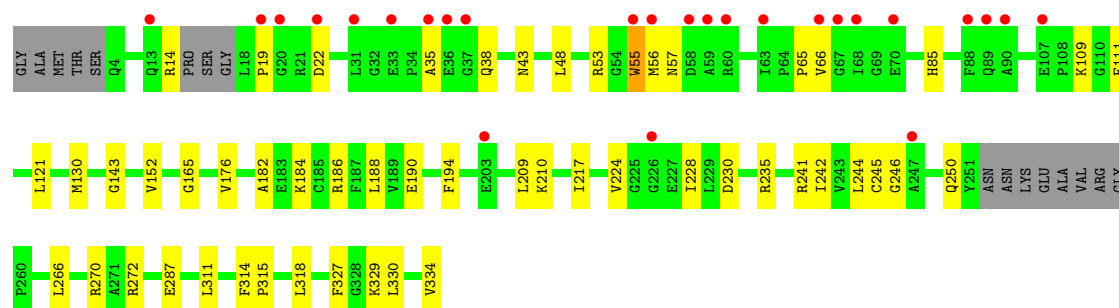


● Molecule 1: PROBABLE OXIDOREDUCTASE



● Molecule 1: PROBABLE OXIDOREDUCTASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.26Å 175.97Å 182.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.42 – 2.20 55.83 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (56.42-2.20) 99.8 (55.83-2.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.79 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.237 , 0.276 0.234 , 0.272	Depositor DCC
$R_{free}$ test set	13809 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.8	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 44.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	30208	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.56	2/2551 (0.1%)	0.67	0/3443
1	B	0.50	1/2569 (0.0%)	0.63	0/3469
1	C	0.44	0/2518	0.59	0/3397
1	D	0.48	1/2537 (0.0%)	0.61	0/3425
1	E	0.53	1/2569 (0.0%)	0.67	0/3469
1	F	0.49	0/2569	0.60	0/3469
1	G	0.44	2/2491 (0.1%)	0.58	0/3362
1	H	0.42	1/2536 (0.0%)	0.56	0/3423
1	I	0.42	2/1795 (0.1%)	0.53	0/2416
1	J	0.43	1/2533 (0.0%)	0.58	0/3420
1	K	0.44	2/2357 (0.1%)	0.56	0/3177
1	L	0.44	1/2488 (0.0%)	0.58	0/3356
All	All	0.47	14/29513 (0.0%)	0.60	0/39826

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	295	TRP	CD2-CE2	5.67	1.48	1.41
1	K	295	TRP	CD2-CE2	5.32	1.47	1.41
1	E	55	TRP	CD2-CE2	5.20	1.47	1.41
1	B	295	TRP	CD2-CE2	5.18	1.47	1.41
1	A	55	TRP	CD2-CE2	5.18	1.47	1.41
1	D	55	TRP	CD2-CE2	5.17	1.47	1.41
1	G	295	TRP	CD2-CE2	5.16	1.47	1.41
1	H	55	TRP	CD2-CE2	5.16	1.47	1.41
1	I	55	TRP	CD2-CE2	5.13	1.47	1.41
1	I	295	TRP	CD2-CE2	5.10	1.47	1.41
1	K	55	TRP	CD2-CE2	5.08	1.47	1.41
1	J	295	TRP	CD2-CE2	5.04	1.47	1.41
1	L	55	TRP	CD2-CE2	5.02	1.47	1.41
1	G	55	TRP	CD2-CE2	5.01	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2504	0	2524	16	0
1	B	2521	0	2544	14	0
1	C	2473	0	2499	24	0
1	D	2490	0	2513	22	0
1	E	2521	0	2544	18	0
1	F	2521	0	2544	25	0
1	G	2446	0	2469	24	0
1	H	2489	0	2515	29	0
1	I	1768	0	1794	18	0
1	J	2486	0	2505	35	0
1	K	2316	0	2334	33	0
1	L	2443	0	2467	28	0
2	A	48	0	25	1	0
2	B	48	0	25	4	0
2	C	48	0	25	4	0
2	D	48	0	25	3	0
2	E	48	0	25	2	0
2	F	48	0	25	3	0
2	G	48	0	25	4	0
2	H	48	0	25	2	0
2	I	48	0	25	4	0
2	J	48	0	25	3	0
2	K	48	0	25	2	0
2	L	48	0	25	2	0
3	A	118	0	0	0	0
3	B	68	0	0	0	0
3	C	46	0	0	1	0
3	D	60	0	0	0	0
3	E	81	0	0	0	0
3	F	67	0	0	0	0
3	G	43	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	41	0	0	0	0
3	I	20	0	0	0	0
3	J	37	0	0	1	0
3	K	30	0	0	0	0
3	L	43	0	0	0	0
All	All	30208	0	29552	264	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 4.

All (264) 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)
2:D:400:NAP:H4B	2:D:400:NAP:O2A	1.26	1.02
1:F:16:SER:O	1:F:254:LYS:HG3	1.65	0.96
1:C:48:LEU:HD11	1:C:332:LEU:HB2	1.51	0.91
2:D:400:NAP:C4B	2:D:400:NAP:O2A	2.19	0.84
1:F:206:ALA:O	1:F:210:LYS:HG3	1.80	0.81
1:I:319:LEU:O	1:I:323:SER:HB2	1.79	0.81
1:E:126:SER:HB3	1:E:329:LYS:HG2	1.69	0.72
1:L:224:VAL:HG11	1:L:228:ILE:HD12	1.71	0.70
1:L:182:ALA:O	1:L:186:ARG:HG2	1.93	0.69
1:I:283:GLN:NE2	1:L:111:PHE:O	2.27	0.67
1:F:57:ASN:O	1:F:65:PRO:HB3	1.96	0.66
1:D:53:ARG:HB2	1:D:322:PHE:CZ	2.30	0.66
1:I:224:VAL:HG11	1:I:228:ILE:HD12	1.78	0.66
1:F:16:SER:O	1:F:254:LYS:CG	2.41	0.65
1:J:244:LEU:HD21	1:J:273:MET:CE	2.28	0.64
1:H:227:GLU:HG2	1:H:258:ARG:HH21	1.62	0.64
1:J:245:CYS:O	2:J:400:NAP:H2N	1.98	0.62
1:H:24:PHE:CZ	1:H:56:MET:HE3	2.35	0.62
1:J:153:ILE:CD1	1:J:165:GLY:HA2	2.30	0.62
1:K:230:ASP:OD1	1:K:262:ASN:HB2	2.00	0.61
1:C:270:ARG:HD3	1:D:277:VAL:HB	1.82	0.61
1:A:153:ILE:HD11	1:A:165:GLY:HA2	1.82	0.60
1:A:126:SER:HB3	1:A:329:LYS:HG2	1.84	0.60
3:J:2014:HOH:O	1:L:287:GLU:HG3	2.01	0.59
1:K:27:VAL:HG12	1:K:28:GLU:H	1.68	0.59
1:J:111:PHE:O	1:K:283:GLN:NE2	2.36	0.59
1:K:284:ARG:O	1:K:287:GLU:HG2	2.03	0.59
1:H:24:PHE:CZ	1:H:56:MET:CE	2.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:266:LEU:HA	1:K:271:ALA:HB3	1.84	0.58
1:J:244:LEU:HD21	1:J:273:MET:HE2	1.85	0.58
1:H:210:LYS:HA	1:H:235:ARG:HH21	1.68	0.58
1:K:109:LYS:HG3	1:K:110:GLY:H	1.67	0.58
1:K:48:LEU:HD12	1:K:330:LEU:HG	1.86	0.58
1:D:250:GLN:HE21	1:D:258:ARG:H	1.51	0.57
1:E:272:ARG:CZ	1:F:272:ARG:HH21	2.16	0.57
1:H:165:GLY:HA3	1:H:194:PHE:CZ	2.39	0.57
1:K:314:PHE:HB3	1:K:315:PRO:HD3	1.85	0.57
1:F:313:THR:CG2	1:F:317:THR:OG1	2.53	0.57
1:H:153:ILE:CD1	1:H:165:GLY:HA2	2.35	0.57
1:J:47:SER:HB2	1:J:125:LEU:HD22	1.85	0.57
1:L:130:MET:SD	2:L:400:NAP:H5N	2.45	0.57
1:L:210:LYS:HA	1:L:235:ARG:HH21	1.69	0.57
1:A:21:ARG:O	1:A:21:ARG:HD2	2.04	0.57
1:J:14:ARG:NH1	1:J:66:VAL:O	2.37	0.57
1:L:329:LYS:HD2	1:L:330:LEU:N	2.20	0.57
1:G:45:TYR:OH	1:J:116:PRO:HG2	2.04	0.57
1:H:227:GLU:HG2	1:H:258:ARG:NH2	2.19	0.56
1:B:55:TRP:NE1	1:B:63:ILE:HD11	2.20	0.56
2:E:400:NAP:H4B	2:E:400:NAP:O2A	2.06	0.56
1:K:245:CYS:O	2:K:400:NAP:H2N	2.06	0.56
1:E:57:ASN:O	1:E:65:PRO:HB3	2.06	0.56
1:F:158:GLY:HA3	2:F:400:NAP:O2A	2.06	0.56
1:I:314:PHE:HB3	1:I:315:PRO:HD3	1.88	0.55
1:K:267:LEU:HD11	1:L:246:GLY:HA2	1.88	0.55
1:H:63:ILE:HG13	1:H:64:PRO:HD2	1.87	0.55
1:A:245:CYS:O	2:A:400:NAP:H2N	2.07	0.55
1:J:55:TRP:NE1	1:J:63:ILE:HD11	2.22	0.55
1:E:53:ARG:NH2	1:E:57:ASN:OD1	2.39	0.54
1:G:116:PRO:HG2	1:J:45:TYR:OH	2.06	0.54
1:H:126:SER:HB3	1:H:329:LYS:HG2	1.90	0.54
1:E:214:PRO:HB3	1:L:186:ARG:HH21	1.72	0.54
2:G:400:NAP:H4B	2:G:400:NAP:O2A	2.06	0.54
1:E:52:MET:O	1:E:56:MET:HG3	2.08	0.54
1:G:52:MET:HA	1:G:55:TRP:CE3	2.42	0.53
1:J:250:GLN:NE2	1:J:258:ARG:H	2.05	0.53
1:A:13:GLN:NE2	1:A:22:ASP:HB3	2.23	0.53
1:J:153:ILE:HD13	1:J:165:GLY:CA	2.39	0.53
1:H:39:ILE:HG12	1:H:108:PRO:HG3	1.90	0.53
1:C:245:CYS:O	2:C:400:NAP:H2N	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:228:ILE:O	1:G:232:VAL:HG23	2.09	0.53
1:C:14:ARG:HD2	1:C:58:ASP:HB2	1.92	0.52
1:A:153:ILE:CD1	1:A:165:GLY:HA2	2.39	0.52
1:D:117:SER:CB	1:E:307:ILE:HD12	2.40	0.52
1:F:313:THR:HG22	1:F:317:THR:OG1	2.10	0.52
1:D:151:VAL:HG22	1:D:219:VAL:HB	1.93	0.51
1:I:121:LEU:HB3	1:I:122:PRO:HD3	1.92	0.51
1:B:223:ASN:HB3	2:B:400:NAP:H4D	1.93	0.51
1:K:158:GLY:HA3	2:K:400:NAP:O2A	2.11	0.51
1:F:233:LEU:HD21	1:F:242:ILE:CD1	2.41	0.50
1:H:233:LEU:HD21	1:H:242:ILE:HD13	1.92	0.50
1:L:143:GLY:O	1:L:241:ARG:HD2	2.10	0.50
1:G:47:SER:HB2	1:G:125:LEU:HD22	1.92	0.50
1:D:138:ALA:HB1	1:D:243:VAL:HG11	1.92	0.50
1:E:257:VAL:HG21	1:F:264:LEU:HD12	1.94	0.50
1:G:77:VAL:CG1	1:G:121:LEU:HD13	2.42	0.50
1:L:165:GLY:HA3	1:L:194:PHE:CZ	2.45	0.50
1:K:169:ARG:NH2	1:K:192:LEU:O	2.45	0.50
1:D:250:GLN:NE2	1:D:258:ARG:H	2.08	0.50
1:I:203:GLU:OE2	1:I:211:ARG:NH1	2.42	0.50
1:L:35:ALA:O	1:L:38:GLN:HB2	2.12	0.50
1:J:158:GLY:HA3	2:J:400:NAP:O2A	2.12	0.49
1:D:184:LYS:NZ	2:D:400:NAP:O2X	2.41	0.49
1:I:286:PRO:HG2	1:L:85:HIS:NE2	2.27	0.49
1:F:233:LEU:HD23	1:F:242:ILE:HD11	1.94	0.49
1:I:245:CYS:O	2:I:400:NAP:H2N	2.13	0.49
1:C:40:LEU:HD13	1:C:105:ILE:HG12	1.94	0.49
1:E:58:ASP:N	1:E:58:ASP:OD1	2.44	0.49
1:G:77:VAL:HG12	1:G:121:LEU:HD13	1.94	0.48
1:K:42:LYS:HB2	1:K:81:LEU:HD11	1.95	0.48
1:K:188:LEU:HD23	1:K:192:LEU:HD12	1.94	0.48
1:D:48:LEU:HD11	1:D:332:LEU:HB2	1.95	0.48
1:G:158:GLY:HA3	2:G:400:NAP:O2A	2.14	0.48
1:J:238:PHE:CE2	1:J:239:LYS:HD2	2.48	0.48
1:B:283:GLN:NE2	1:E:111:PHE:O	2.47	0.48
1:E:199:ASP:O	1:E:203:GLU:HG2	2.13	0.48
1:G:248:ILE:HD13	2:G:400:NAP:H52A	1.96	0.48
1:A:55:TRP:HB3	1:A:66:VAL:HG23	1.95	0.47
1:H:53:ARG:CD	1:H:252:ASN:OD1	2.63	0.47
1:I:276:MET:HA	1:J:270:ARG:HG3	1.96	0.47
1:J:39:ILE:HD12	1:J:41:VAL:CG2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:ARG:CD	1:D:280:ASP:OD2	2.63	0.47
1:H:77:VAL:HG11	1:H:121:LEU:HD22	1.96	0.47
1:I:187:PHE:O	1:I:191:GLU:HB2	2.14	0.47
1:D:321:LEU:O	1:D:322:PHE:HB2	2.14	0.47
1:F:233:LEU:HD21	1:F:242:ILE:HD12	1.97	0.47
1:F:310:GLY:O	1:F:313:THR:HB	2.14	0.47
1:H:233:LEU:CD2	1:H:242:ILE:CD1	2.93	0.47
1:L:242:ILE:HD12	1:L:266:LEU:HD21	1.95	0.47
1:E:14:ARG:HG2	1:E:68:ILE:HD11	1.97	0.47
1:A:199:ASP:O	1:A:203:GLU:HG2	2.16	0.46
1:D:224:VAL:HG11	1:D:228:ILE:HD12	1.96	0.46
1:J:153:ILE:HD13	1:J:165:GLY:HA2	1.96	0.46
1:K:260:PRO:O	1:K:262:ASN:N	2.48	0.46
1:E:186:ARG:NH2	1:G:211:ARG:O	2.48	0.46
1:A:13:GLN:HE21	1:A:22:ASP:HB3	1.80	0.46
1:F:223:ASN:HB3	2:F:400:NAP:H4D	1.97	0.46
1:G:64:PRO:HA	1:G:65:PRO:HD3	1.83	0.46
1:B:228:ILE:O	1:B:232:VAL:HG23	2.15	0.46
1:K:241:ARG:HD3	1:K:241:ARG:N	2.31	0.46
1:L:57:ASN:O	1:L:65:PRO:HB3	2.15	0.46
1:J:244:LEU:HD21	1:J:273:MET:HE1	1.98	0.46
1:B:245:CYS:O	2:B:400:NAP:H2N	2.16	0.46
1:C:42:LYS:HG2	1:C:103:TYR:CE2	2.51	0.46
1:C:48:LEU:CD1	1:C:332:LEU:HB2	2.36	0.46
1:I:220:PHE:CG	1:I:232:VAL:HG11	2.50	0.46
1:C:217:ILE:HD12	1:C:235:ARG:HB3	1.97	0.45
1:G:220:PHE:CG	1:G:232:VAL:HG11	2.50	0.45
1:E:245:CYS:O	2:E:400:NAP:H2N	2.16	0.45
1:E:190:GLU:OE1	1:G:174:ARG:NH1	2.49	0.45
1:G:310:GLY:O	1:G:332:LEU:HD11	2.17	0.45
1:J:223:ASN:HB3	2:J:400:NAP:H4D	1.99	0.45
1:J:49:ASP:OD1	1:J:329:LYS:NZ	2.49	0.45
1:K:120:PRO:HB2	1:K:122:PRO:HD2	1.98	0.45
1:F:224:VAL:HG11	1:F:228:ILE:HD12	1.98	0.45
1:G:307:ILE:HD13	1:J:117:SER:HB2	1.99	0.45
1:D:117:SER:HB2	1:E:307:ILE:HD12	1.99	0.45
1:G:272:ARG:HG3	1:H:272:ARG:HG3	1.99	0.45
1:C:158:GLY:HA3	2:C:400:NAP:O2A	2.17	0.45
1:L:184:LYS:O	1:L:188:LEU:HG	2.17	0.45
1:C:220:PHE:CG	1:C:232:VAL:HG11	2.52	0.44
1:B:127:ALA:O	1:B:292:MET:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:LEU:HD23	1:C:82:VAL:HG23	1.99	0.44
1:D:165:GLY:HA3	1:D:194:PHE:CZ	2.52	0.44
1:G:4:GLN:HG2	1:G:31:LEU:HD22	1.99	0.44
1:L:14:ARG:HD2	1:L:56:MET:O	2.17	0.44
1:F:126:SER:HB3	1:F:329:LYS:HG2	1.98	0.44
1:G:318:LEU:O	1:G:321:LEU:HD12	2.17	0.44
1:G:7:ARG:HD2	1:G:26:PHE:HZ	1.83	0.44
1:H:245:CYS:O	2:H:400:NAP:H2N	2.17	0.44
1:D:220:PHE:CG	1:D:232:VAL:HG11	2.53	0.44
1:J:220:PHE:CG	1:J:232:VAL:HG11	2.52	0.44
1:A:147:ASN:OD1	1:A:172:GLY:HA3	2.18	0.44
1:C:7:ARG:HD2	1:C:26:PHE:HZ	1.83	0.44
1:D:79:LYS:HE2	1:D:91:GLY:HA2	2.00	0.44
1:H:7:ARG:O	1:H:101:GLN:HA	2.18	0.44
1:B:158:GLY:HA3	2:B:400:NAP:O2A	2.17	0.44
1:C:130:MET:SD	2:C:400:NAP:H5N	2.58	0.44
1:K:272:ARG:HD3	1:L:272:ARG:HD3	1.99	0.44
1:F:127:ALA:O	1:F:292:MET:HG2	2.18	0.44
1:I:277:VAL:HG13	1:J:270:ARG:HD2	2.00	0.44
1:J:270:ARG:N	1:J:270:ARG:HD3	2.33	0.44
1:A:5:ILE:CG2	1:A:28:GLU:HB3	2.48	0.43
1:B:220:PHE:CG	1:B:232:VAL:HG11	2.53	0.43
1:D:20:GLY:O	1:D:22:ASP:N	2.51	0.43
1:I:257:VAL:HG22	1:J:261:ALA:O	2.18	0.43
1:B:284:ARG:O	1:B:287:GLU:HG2	2.18	0.43
1:K:152:VAL:HA	1:K:176:VAL:O	2.18	0.43
1:K:138:ALA:HB1	1:K:243:VAL:HG11	2.00	0.43
1:L:314:PHE:N	1:L:315:PRO:HD2	2.33	0.43
1:K:233:LEU:O	1:K:236:ILE:HG12	2.19	0.43
1:A:165:GLY:HA3	1:A:194:PHE:CZ	2.53	0.43
1:D:117:SER:HB2	1:E:307:ILE:CD1	2.49	0.43
1:F:162:SER:HB2	1:F:192:LEU:HD21	2.00	0.43
1:F:233:LEU:CD2	1:F:242:ILE:CD1	2.96	0.43
1:J:14:ARG:HG2	1:J:68:ILE:HD11	2.01	0.43
1:K:115:ASP:HB3	1:K:118:ARG:HG3	2.00	0.43
1:C:115:ASP:HA	1:C:116:PRO:HD2	1.90	0.43
1:G:10:GLN:HE21	1:G:27:VAL:HG21	1.84	0.43
1:C:130:MET:HG2	1:C:278:VAL:HG11	2.00	0.43
1:D:111:PHE:O	1:H:283:GLN:NE2	2.48	0.43
1:H:130:MET:SD	2:H:400:NAP:H5N	2.59	0.43
1:H:19:PRO:HG3	1:H:53:ARG:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:163:VAL:O	1:K:167:ILE:HG13	2.19	0.43
1:K:220:PHE:CG	1:K:232:VAL:HG11	2.54	0.43
1:B:143:GLY:O	1:B:241:ARG:HD2	2.19	0.42
1:E:53:ARG:HD3	1:E:252:ASN:OD1	2.19	0.42
1:H:85:HIS:HA	1:H:86:PRO:HD3	1.91	0.42
1:G:93:TYR:CD1	1:G:116:PRO:HG3	2.54	0.42
1:J:14:ARG:HD2	1:J:56:MET:O	2.19	0.42
1:J:224:VAL:HG11	1:J:228:ILE:HD12	2.00	0.42
1:F:245:CYS:O	2:F:400:NAP:H2N	2.18	0.42
1:A:21:ARG:HD3	1:A:315:PRO:HG2	2.00	0.42
1:H:233:LEU:HD21	1:H:242:ILE:CD1	2.50	0.42
1:H:24:PHE:HZ	1:H:56:MET:CE	2.32	0.42
1:K:290:LYS:O	1:K:294:THR:HG23	2.19	0.42
1:K:8:GLN:HG2	1:K:101:GLN:HB3	2.01	0.42
1:L:43:ASN:O	1:L:334:VAL:HG23	2.19	0.42
1:G:165:GLY:HA3	1:G:194:PHE:CZ	2.54	0.42
1:I:158:GLY:HA3	2:I:400:NAP:O2A	2.20	0.42
1:C:311:LEU:HB2	1:C:334:VAL:HG13	2.01	0.42
1:L:245:CYS:O	2:L:400:NAP:H2N	2.20	0.42
1:B:130:MET:SD	2:B:400:NAP:H5N	2.60	0.42
1:J:250:GLN:HE22	1:J:258:ARG:H	1.67	0.42
1:K:257:VAL:HG12	1:K:258:ARG:N	2.35	0.42
1:L:329:LYS:C	1:L:329:LYS:HD2	2.40	0.41
1:L:48:LEU:HD23	1:L:318:LEU:HA	2.02	0.41
1:C:270:ARG:HD3	1:D:280:ASP:OD2	2.20	0.41
1:J:116:PRO:HB3	1:J:121:LEU:HD21	2.02	0.41
1:A:64:PRO:HA	1:A:65:PRO:HD3	1.94	0.41
1:G:245:CYS:O	2:G:400:NAP:H2N	2.19	0.41
1:I:223:ASN:HB3	2:I:400:NAP:H4D	2.03	0.41
1:H:14:ARG:NH1	1:H:66:VAL:O	2.53	0.41
1:H:224:VAL:HA	1:H:248:ILE:HG22	2.03	0.41
1:L:209:LEU:HD22	1:L:217:ILE:HD11	2.03	0.41
1:K:184:LYS:O	1:K:187:PHE:HB3	2.21	0.41
1:L:152:VAL:HA	1:L:176:VAL:O	2.20	0.41
1:B:42:LYS:HD2	1:B:103:TYR:CE1	2.56	0.41
1:F:93:TYR:CD1	1:F:116:PRO:HG3	2.55	0.41
1:H:242:ILE:HD12	1:H:266:LEU:HD21	2.03	0.41
1:L:55:TRP:HB3	1:L:66:VAL:HG23	2.02	0.41
1:K:13:GLN:HB3	1:K:23:THR:HA	2.02	0.41
1:C:170:LEU:HD21	1:C:300:LYS:HB3	2.02	0.41
1:J:109:LYS:HD3	1:J:109:LYS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ILE:CD1	1:A:165:GLY:CA	2.98	0.41
1:F:233:LEU:CD2	1:F:242:ILE:HD11	2.50	0.41
1:G:48:LEU:HD11	1:G:332:LEU:HB2	2.03	0.41
1:H:21:ARG:C	1:H:23:THR:H	2.24	0.41
1:J:55:TRP:HE1	1:J:63:ILE:HD11	1.85	0.41
1:K:126:SER:HB3	1:K:329:LYS:HG2	2.03	0.41
1:K:14:ARG:HA	1:K:15:PRO:HD3	1.83	0.41
1:K:49:ASP:O	1:K:52:MET:HB2	2.21	0.41
1:B:290:LYS:O	1:B:294:THR:HG23	2.21	0.41
1:F:220:PHE:CG	1:F:232:VAL:HG11	2.56	0.41
1:F:85:HIS:HA	1:F:86:PRO:HD3	1.90	0.41
1:I:251:TYR:HH	2:I:400:NAP:HO2N	1.69	0.41
1:J:180:GLY:HA3	1:J:201:LYS:HE3	2.03	0.41
1:A:241:ARG:N	1:A:241:ARG:HD3	2.35	0.40
1:B:304:ARG:HG2	1:B:328:GLY:HA3	2.03	0.40
1:C:223:ASN:HB3	2:C:400:NAP:H4D	2.03	0.40
1:C:77:VAL:HG11	1:C:121:LEU:HD22	2.03	0.40
1:F:166:GLN:HG2	1:F:169:ARG:HH21	1.86	0.40
1:K:166:GLN:O	1:K:170:LEU:HG	2.21	0.40
1:L:19:PRO:HG3	1:L:53:ARG:HG3	2.03	0.40
1:C:290:LYS:O	1:C:294:THR:HG23	2.21	0.40
1:C:53:ARG:O	1:C:56:MET:HG2	2.22	0.40
1:I:313:THR:HA	1:I:316:GLU:OE2	2.20	0.40
1:J:52:MET:HA	1:J:55:TRP:CE3	2.55	0.40
1:D:143:GLY:O	1:D:241:ARG:HD2	2.21	0.40
1:L:311:LEU:HB2	1:L:334:VAL:HG12	2.03	0.40
1:C:287:GLU:HG3	3:C:2040:HOH:O	2.20	0.40
1:H:53:ARG:HD3	1:H:252:ASN:OD1	2.21	0.40
1:I:270:ARG:HG2	1:J:280:ASP:OD2	2.21	0.40
1:D:323:SER:HB2	1:D:325:GLU:HG3	2.04	0.40
1:H:107:GLU:HA	1:H:108:PRO:HD3	1.93	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	325/336 (97%)	322 (99%)	3 (1%)	0	100	100
1	B	329/336 (98%)	324 (98%)	5 (2%)	0	100	100
1	C	319/336 (95%)	310 (97%)	9 (3%)	0	100	100
1	D	323/336 (96%)	316 (98%)	6 (2%)	1 (0%)	44	49
1	E	329/336 (98%)	323 (98%)	6 (2%)	0	100	100
1	F	329/336 (98%)	323 (98%)	6 (2%)	0	100	100
1	G	317/336 (94%)	307 (97%)	9 (3%)	1 (0%)	44	49
1	H	323/336 (96%)	313 (97%)	10 (3%)	0	100	100
1	I	226/336 (67%)	216 (96%)	10 (4%)	0	100	100
1	J	323/336 (96%)	314 (97%)	8 (2%)	1 (0%)	44	49
1	K	292/336 (87%)	277 (95%)	12 (4%)	3 (1%)	18	16
1	L	314/336 (94%)	308 (98%)	6 (2%)	0	100	100
All	All	3749/4032 (93%)	3653 (97%)	90 (2%)	6 (0%)	51	58

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	21	ARG
1	K	262	ASN
1	K	261	ALA
1	G	258	ARG
1	K	109	LYS
1	J	21	ARG

### 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	258/263 (98%)	253 (98%)	5 (2%)	62	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	260/263 (99%)	254 (98%)	6 (2%)	56	69
1	C	255/263 (97%)	249 (98%)	6 (2%)	54	67
1	D	257/263 (98%)	251 (98%)	6 (2%)	56	69
1	E	260/263 (99%)	255 (98%)	5 (2%)	62	76
1	F	260/263 (99%)	257 (99%)	3 (1%)	75	86
1	G	252/263 (96%)	247 (98%)	5 (2%)	60	74
1	H	257/263 (98%)	250 (97%)	7 (3%)	50	62
1	I	180/263 (68%)	175 (97%)	5 (3%)	49	61
1	J	256/263 (97%)	249 (97%)	7 (3%)	50	62
1	K	239/263 (91%)	231 (97%)	8 (3%)	43	54
1	L	252/263 (96%)	243 (96%)	9 (4%)	40	50
All	All	2986/3156 (95%)	2914 (98%)	72 (2%)	54	67

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	26	PHE
1	A	230	ASP
1	A	270	ARG
1	A	327	PHE
1	B	8	GLN
1	B	26	PHE
1	B	44	GLU
1	B	230	ASP
1	B	255	GLU
1	B	270	ARG
1	C	23	THR
1	C	72	MET
1	C	82	VAL
1	C	230	ASP
1	C	279	MET
1	C	327	PHE
1	D	230	ASP
1	D	270	ARG
1	D	287	GLU
1	D	304	ARG
1	D	321	LEU

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Mol	Chain	Res	Type
1	D	323	SER
1	E	26	PHE
1	E	53	ARG
1	E	230	ASP
1	E	241	ARG
1	E	270	ARG
1	F	26	PHE
1	F	123	ARG
1	F	230	ASP
1	G	121	LEU
1	G	270	ARG
1	G	323	SER
1	G	325	GLU
1	G	327	PHE
1	H	11	LEU
1	H	53	ARG
1	H	123	ARG
1	H	146	LYS
1	H	190	GLU
1	H	241	ARG
1	H	270	ARG
1	I	111	PHE
1	I	118	ARG
1	I	235	ARG
1	I	270	ARG
1	I	323	SER
1	J	23	THR
1	J	105	ILE
1	J	109	LYS
1	J	169	ARG
1	J	230	ASP
1	J	241	ARG
1	J	270	ARG
1	K	16	SER
1	K	21	ARG
1	K	118	ARG
1	K	169	ARG
1	K	230	ASP
1	K	249	SER
1	K	262	ASN
1	K	270	ARG
1	L	22	ASP

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Mol	Chain	Res	Type
1	L	109	LYS
1	L	121	LEU
1	L	190	GLU
1	L	230	ASP
1	L	244	LEU
1	L	250	GLN
1	L	270	ARG
1	L	327	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	C	13	GLN
1	D	250	GLN
1	E	8	GLN
1	G	8	GLN
1	G	10	GLN
1	I	283	GLN
1	J	8	GLN
1	J	250	GLN
1	K	8	GLN
1	L	326	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 ⓘ

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAP	A	400	-	44,52,52	1.38	6 (13%)	51,80,80	1.52	5 (9%)
2	NAP	B	400	-	44,52,52	1.38	6 (13%)	51,80,80	1.69	6 (11%)
2	NAP	C	400	-	44,52,52	1.26	6 (13%)	51,80,80	1.60	4 (7%)
2	NAP	D	400	-	44,52,52	1.73	7 (15%)	51,80,80	1.66	4 (7%)
2	NAP	E	400	-	44,52,52	1.43	4 (9%)	51,80,80	1.72	7 (13%)
2	NAP	F	400	-	44,52,52	1.41	6 (13%)	51,80,80	1.60	5 (9%)
2	NAP	G	400	-	44,52,52	1.29	5 (11%)	51,80,80	1.47	2 (3%)
2	NAP	H	400	-	44,52,52	1.43	6 (13%)	51,80,80	1.50	4 (7%)
2	NAP	I	400	-	44,52,52	1.29	8 (18%)	51,80,80	1.64	5 (9%)
2	NAP	J	400	-	44,52,52	1.28	7 (15%)	51,80,80	1.58	4 (7%)
2	NAP	K	400	-	44,52,52	1.38	7 (15%)	51,80,80	1.56	4 (7%)
2	NAP	L	400	-	44,52,52	1.22	4 (9%)	51,80,80	1.75	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	400	-	-	0/27/67/67	0/5/5/5
2	NAP	B	400	-	-	0/27/67/67	0/5/5/5
2	NAP	C	400	-	-	0/27/67/67	0/5/5/5
2	NAP	D	400	-	-	1/27/67/67	0/5/5/5
2	NAP	E	400	-	-	0/27/67/67	0/5/5/5
2	NAP	F	400	-	-	0/27/67/67	0/5/5/5
2	NAP	G	400	-	-	0/27/67/67	0/5/5/5
2	NAP	H	400	-	-	0/27/67/67	0/5/5/5
2	NAP	I	400	-	-	0/27/67/67	0/5/5/5
2	NAP	J	400	-	-	0/27/67/67	0/5/5/5
2	NAP	K	400	-	-	0/27/67/67	0/5/5/5
2	NAP	L	400	-	-	0/27/67/67	0/5/5/5

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	NAP	C2D-C1D	-2.53	1.49	1.53
2	J	400	NAP	C2D-C1D	-2.16	1.50	1.53
2	F	400	NAP	C2D-C1D	-2.12	1.50	1.53
2	A	400	NAP	P2B-O2B	2.01	1.63	1.59
2	B	400	NAP	C3N-C7N	2.04	1.53	1.50
2	I	400	NAP	P2B-O2B	2.08	1.63	1.59
2	B	400	NAP	P2B-O1X	2.09	1.57	1.50
2	D	400	NAP	O5B-C5B	2.09	1.53	1.44
2	A	400	NAP	C6N-N1N	2.13	1.41	1.35
2	I	400	NAP	C6N-N1N	2.15	1.41	1.35
2	H	400	NAP	C6N-N1N	2.17	1.41	1.35
2	J	400	NAP	C6N-N1N	2.17	1.41	1.35
2	K	400	NAP	C3N-C7N	2.26	1.54	1.50
2	L	400	NAP	C6N-N1N	2.28	1.41	1.35
2	C	400	NAP	O4B-C1B	2.35	1.44	1.41
2	F	400	NAP	C6N-N1N	2.36	1.41	1.35
2	K	400	NAP	C6N-N1N	2.36	1.41	1.35
2	H	400	NAP	C3N-C7N	2.38	1.54	1.50
2	D	400	NAP	C6N-N1N	2.40	1.41	1.35
2	C	400	NAP	PA-O1A	2.41	1.59	1.50
2	J	400	NAP	PA-O1A	2.42	1.60	1.50
2	J	400	NAP	P2B-O2B	2.43	1.63	1.59
2	C	400	NAP	C6N-N1N	2.44	1.41	1.35
2	B	400	NAP	C6N-N1N	2.45	1.41	1.35
2	L	400	NAP	PA-O1A	2.47	1.60	1.50
2	I	400	NAP	O4D-C1D	2.52	1.44	1.41
2	I	400	NAP	O4B-C1B	2.53	1.44	1.41
2	G	400	NAP	C6N-N1N	2.56	1.42	1.35
2	I	400	NAP	P2B-O2X	2.57	1.65	1.54
2	I	400	NAP	C3N-C7N	2.61	1.54	1.50
2	C	400	NAP	P2B-O1X	2.65	1.59	1.50
2	H	400	NAP	PA-O1A	2.65	1.60	1.50
2	J	400	NAP	O4D-C1D	2.75	1.45	1.41
2	E	400	NAP	O4D-C1D	2.75	1.45	1.41
2	J	400	NAP	P2B-O1X	2.75	1.60	1.50
2	C	400	NAP	P2B-O2X	2.76	1.66	1.54
2	B	400	NAP	P2B-O2B	2.76	1.64	1.59
2	A	400	NAP	P2B-O1X	2.78	1.60	1.50
2	K	400	NAP	P2B-O2B	2.78	1.64	1.59
2	K	400	NAP	O4B-C1B	2.80	1.45	1.41
2	I	400	NAP	PA-O1A	2.88	1.61	1.50
2	K	400	NAP	PA-O1A	2.92	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	400	NAP	PA-O1A	2.93	1.61	1.50
2	K	400	NAP	P2B-O1X	2.99	1.60	1.50
2	A	400	NAP	O4B-C1B	3.00	1.45	1.41
2	H	400	NAP	P2B-O1X	3.06	1.61	1.50
2	G	400	NAP	PA-O1A	3.06	1.62	1.50
2	G	400	NAP	O4B-C1B	3.11	1.45	1.41
2	G	400	NAP	P2B-O1X	3.17	1.61	1.50
2	B	400	NAP	O4B-C1B	3.22	1.45	1.41
2	F	400	NAP	PA-O1A	3.35	1.63	1.50
2	D	400	NAP	O4D-C1D	3.36	1.45	1.41
2	L	400	NAP	P2B-O1X	3.38	1.62	1.50
2	F	400	NAP	O4D-C1D	3.44	1.46	1.41
2	I	400	NAP	P2B-O1X	3.59	1.63	1.50
2	F	400	NAP	P2B-O1X	3.61	1.63	1.50
2	G	400	NAP	O4D-C1D	3.62	1.46	1.41
2	K	400	NAP	O4D-C1D	3.65	1.46	1.41
2	C	400	NAP	O4D-C1D	3.67	1.46	1.41
2	D	400	NAP	P2B-O1X	3.68	1.63	1.50
2	E	400	NAP	P2B-O2B	3.69	1.66	1.59
2	L	400	NAP	O4B-C1B	3.70	1.46	1.41
2	E	400	NAP	P2B-O1X	3.77	1.63	1.50
2	F	400	NAP	O4B-C1B	3.81	1.46	1.41
2	H	400	NAP	O4B-C1B	3.83	1.46	1.41
2	D	400	NAP	C5B-C4B	4.12	1.64	1.51
2	J	400	NAP	O4B-C1B	4.12	1.47	1.41
2	H	400	NAP	O4D-C1D	4.76	1.47	1.41
2	E	400	NAP	O4B-C1B	4.83	1.47	1.41
2	A	400	NAP	O4D-C1D	4.86	1.48	1.41
2	B	400	NAP	O4D-C1D	5.03	1.48	1.41
2	D	400	NAP	O4B-C1B	6.27	1.49	1.41

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	NAP	N3A-C2A-N1A	-9.36	120.70	128.86
2	C	400	NAP	N3A-C2A-N1A	-8.73	121.25	128.86
2	K	400	NAP	N3A-C2A-N1A	-8.69	121.29	128.86
2	I	400	NAP	N3A-C2A-N1A	-8.37	121.57	128.86
2	D	400	NAP	N3A-C2A-N1A	-8.34	121.59	128.86
2	J	400	NAP	N3A-C2A-N1A	-8.32	121.61	128.86
2	G	400	NAP	N3A-C2A-N1A	-8.15	121.76	128.86
2	H	400	NAP	N3A-C2A-N1A	-8.14	121.77	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	400	NAP	N3A-C2A-N1A	-8.14	121.77	128.86
2	A	400	NAP	N3A-C2A-N1A	-8.01	121.88	128.86
2	L	400	NAP	N3A-C2A-N1A	-7.97	121.91	128.86
2	F	400	NAP	N3A-C2A-N1A	-7.88	122.00	128.86
2	L	400	NAP	C4B-O4B-C1B	-5.57	103.84	109.77
2	I	400	NAP	C4B-O4B-C1B	-4.75	104.71	109.77
2	F	400	NAP	C4B-O4B-C1B	-3.82	105.70	109.77
2	J	400	NAP	C3N-C7N-N7N	-3.78	113.46	117.77
2	L	400	NAP	C3N-C7N-N7N	-3.75	113.49	117.77
2	E	400	NAP	C3N-C7N-N7N	-3.57	113.70	117.77
2	E	400	NAP	C4D-O4D-C1D	-2.92	106.66	109.77
2	H	400	NAP	C4B-O4B-C1B	-2.86	106.73	109.77
2	K	400	NAP	C3N-C7N-N7N	-2.80	114.57	117.77
2	B	400	NAP	C4B-O4B-C1B	-2.77	106.82	109.77
2	E	400	NAP	O3D-C3D-C4D	-2.72	103.14	111.09
2	I	400	NAP	C4D-O4D-C1D	-2.71	106.88	109.77
2	A	400	NAP	C3N-C7N-N7N	-2.66	114.74	117.77
2	A	400	NAP	C4A-C5A-N7A	-2.63	106.87	109.41
2	B	400	NAP	C1B-N9A-C4A	-2.61	122.12	126.64
2	C	400	NAP	C4B-O4B-C1B	-2.53	107.07	109.77
2	I	400	NAP	O4B-C4B-C3B	-2.45	100.29	105.17
2	B	400	NAP	O2X-P2B-O1X	-2.43	101.01	110.50
2	H	400	NAP	C4D-O4D-C1D	-2.30	107.32	109.77
2	L	400	NAP	C4D-O4D-C1D	-2.30	107.33	109.77
2	A	400	NAP	O4B-C4B-C3B	-2.26	100.67	105.17
2	F	400	NAP	C3N-C7N-N7N	-2.26	115.19	117.77
2	G	400	NAP	C3N-C7N-N7N	-2.24	115.22	117.77
2	C	400	NAP	C3N-C7N-N7N	-2.19	115.27	117.77
2	J	400	NAP	C4D-O4D-C1D	-2.17	107.46	109.77
2	I	400	NAP	C3N-C7N-N7N	-2.16	115.31	117.77
2	A	400	NAP	O3D-C3D-C4D	-2.13	104.87	111.09
2	E	400	NAP	C3N-C2N-N1N	-2.12	118.29	120.43
2	L	400	NAP	C4A-C5A-N7A	-2.09	107.39	109.41
2	B	400	NAP	C4D-O4D-C1D	-2.07	107.56	109.77
2	F	400	NAP	C4D-O4D-C1D	-2.06	107.57	109.77
2	H	400	NAP	C3N-C7N-N7N	-2.06	115.42	117.77
2	D	400	NAP	O2B-P2B-O1X	-2.05	101.22	109.26
2	J	400	NAP	C2N-C3N-C4N	2.00	120.55	118.26
2	L	400	NAP	O7N-C7N-C3N	2.05	122.03	119.62
2	B	400	NAP	C2A-N1A-C6A	2.24	122.69	118.77
2	K	400	NAP	O7N-C7N-C3N	2.28	122.29	119.62
2	K	400	NAP	O3X-P2B-O2B	2.28	116.39	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	400	NAP	C2N-C3N-C4N	2.29	120.88	118.26
2	E	400	NAP	C2N-C3N-C4N	2.36	120.95	118.26
2	E	400	NAP	O3X-P2B-O2B	2.57	117.70	106.00
2	D	400	NAP	O5B-C5B-C4B	2.59	118.19	109.00
2	C	400	NAP	C2N-C3N-C4N	2.63	121.27	118.26
2	D	400	NAP	O5B-PA-O1A	2.67	120.00	109.25

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	400	NAP	PA-O5B-C5B-C4B

There are no ring outliers.

12 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	NAP	1	0
2	B	400	NAP	4	0
2	C	400	NAP	4	0
2	D	400	NAP	3	0
2	E	400	NAP	2	0
2	F	400	NAP	3	0
2	G	400	NAP	4	0
2	H	400	NAP	2	0
2	I	400	NAP	4	0
2	J	400	NAP	3	0
2	K	400	NAP	2	0
2	L	400	NAP	2	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	329/336 (97%)	-0.14	1 (0%) 93 93	14, 23, 42, 62	0
1	B	331/336 (98%)	-0.10	1 (0%) 93 93	20, 33, 51, 61	0
1	C	325/336 (96%)	0.47	23 (7%) 17 16	23, 45, 79, 98	0
1	D	327/336 (97%)	0.25	22 (6%) 19 17	20, 33, 83, 109	0
1	E	331/336 (98%)	0.00	9 (2%) 55 52	14, 26, 55, 87	0
1	F	331/336 (98%)	0.07	16 (4%) 31 30	25, 37, 59, 77	0
1	G	321/336 (95%)	0.52	38 (11%) 5 4	23, 43, 96, 120	0
1	H	327/336 (97%)	0.34	14 (4%) 36 34	27, 49, 69, 92	0
1	I	234/336 (69%)	1.49	75 (32%) 0 0	31, 63, 122, 140	0
1	J	327/336 (97%)	0.36	23 (7%) 17 16	25, 47, 81, 109	0
1	K	302/336 (89%)	0.93	54 (17%) 2 1	27, 55, 91, 112	0
1	L	320/336 (95%)	0.54	26 (8%) 13 12	27, 47, 77, 105	0
All	All	3805/4032 (94%)	0.36	302 (7%) 13 12	14, 40, 84, 140	0

All (302) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	315	PRO	12.0
1	K	5	ILE	9.1
1	I	312	GLU	7.8
1	D	16	SER	7.5
1	J	21	ARG	7.3
1	G	321	LEU	7.3
1	J	182	ALA	7.1
1	I	318	LEU	7.1
1	I	307	ILE	6.9
1	K	256	ALA	6.8
1	I	117	SER	6.8

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Mol	Chain	Res	Type	RSRZ
1	I	319	LEU	6.5
1	I	327	PHE	6.4
1	I	114	VAL	6.3
1	I	310	GLY	6.3
1	G	24	PHE	6.2
1	I	116	PRO	6.2
1	I	308	VAL	6.0
1	G	57	ASN	5.9
1	K	22	ASP	5.9
1	K	67	GLY	5.7
1	I	118	ARG	5.7
1	G	26	PHE	5.7
1	I	313	THR	5.6
1	G	254	LYS	5.6
1	D	58	ASP	5.5
1	G	58	ASP	5.4
1	G	319	LEU	5.4
1	G	64	PRO	5.3
1	I	122	PRO	5.2
1	G	59	ALA	5.2
1	I	316	GLU	5.1
1	K	16	SER	5.1
1	G	322	PHE	5.1
1	D	319	LEU	5.0
1	G	12	ALA	5.0
1	I	331	VAL	5.0
1	I	111	PHE	5.0
1	I	317	THR	5.0
1	K	68	ILE	4.9
1	K	18	LEU	4.8
1	L	68	ILE	4.8
1	K	26	PHE	4.8
1	I	325	GLU	4.8
1	K	66	VAL	4.8
1	J	19	PRO	4.7
1	C	67	GLY	4.7
1	C	58	ASP	4.7
1	H	16	SER	4.7
1	I	330	LEU	4.6
1	J	181	GLY	4.6
1	K	105	ILE	4.6
1	J	16	SER	4.6

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Mol	Chain	Res	Type	RSRZ
1	K	11	LEU	4.6
1	G	255	GLU	4.6
1	I	320	LYS	4.5
1	I	295	TRP	4.5
1	J	18	LEU	4.5
1	G	327	PHE	4.4
1	C	31	LEU	4.4
1	I	124	TYR	4.4
1	I	300	LYS	4.3
1	C	39	ILE	4.3
1	I	180	GLY	4.3
1	I	332	LEU	4.3
1	I	186	ARG	4.2
1	I	297	ALA	4.2
1	J	24	PHE	4.2
1	C	254	LYS	4.2
1	I	123	ARG	4.2
1	I	191	GLU	4.2
1	I	121	LEU	4.2
1	I	314	PHE	4.1
1	L	66	VAL	4.1
1	K	17	GLY	4.1
1	C	68	ILE	4.1
1	K	27	VAL	4.0
1	D	59	ALA	4.0
1	D	22	ASP	4.0
1	I	120	PRO	4.0
1	E	58	ASP	3.9
1	H	297	ALA	3.9
1	I	257	VAL	3.9
1	I	309	GLU	3.9
1	I	301	LEU	3.9
1	J	252	ASN	3.9
1	K	58	ASP	3.9
1	C	25	SER	3.9
1	J	256	ALA	3.8
1	K	24	PHE	3.8
1	I	311	LEU	3.8
1	L	37	GLY	3.8
1	K	13	GLN	3.8
1	G	60	ARG	3.8
1	D	66	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	I	113	LYS	3.7
1	E	16	SER	3.7
1	D	13	GLN	3.7
1	L	59	ALA	3.7
1	C	30	PRO	3.6
1	I	157	ALA	3.6
1	D	57	ASN	3.6
1	J	253	ASN	3.6
1	D	324	GLY	3.5
1	G	67	GLY	3.5
1	G	66	VAL	3.5
1	I	192	LEU	3.5
1	K	193	GLY	3.4
1	L	33	GLU	3.4
1	C	56	MET	3.4
1	G	11	LEU	3.4
1	I	202	ASN	3.4
1	K	69	GLY	3.4
1	L	22	ASP	3.4
1	F	180	GLY	3.3
1	K	324	GLY	3.3
1	L	67	GLY	3.3
1	C	71	VAL	3.3
1	I	55	TRP	3.3
1	I	119	ALA	3.3
1	G	316	GLU	3.3
1	C	9	TYR	3.2
1	C	16	SER	3.2
1	I	288	GLY	3.2
1	K	19	PRO	3.2
1	I	304	ARG	3.2
1	K	6	ASN	3.2
1	K	14	ARG	3.2
1	K	29	THR	3.2
1	G	186	ARG	3.2
1	K	12	ALA	3.2
1	C	255	GLU	3.2
1	H	298	GLU	3.2
1	D	60	ARG	3.2
1	D	325	GLU	3.2
1	K	190	GLU	3.2
1	D	21	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	300	LYS	3.1
1	C	13	GLN	3.1
1	G	53	ARG	3.1
1	L	13	GLN	3.1
1	F	212	GLU	3.1
1	J	22	ASP	3.0
1	I	98	LEU	3.0
1	D	15	PRO	3.0
1	K	56	MET	3.0
1	K	231	THR	3.0
1	L	58	ASP	3.0
1	K	71	VAL	3.0
1	I	188	LEU	3.0
1	H	256	ALA	3.0
1	L	247	ALA	3.0
1	K	20	GLY	3.0
1	F	60	ARG	3.0
1	J	20	GLY	3.0
1	E	253	ASN	3.0
1	G	326	ASN	3.0
1	I	56	MET	3.0
1	D	18	LEU	2.9
1	I	321	LEU	2.9
1	E	254	LYS	2.9
1	H	24	PHE	2.9
1	C	41	VAL	2.9
1	J	58	ASP	2.9
1	F	202	ASN	2.9
1	K	202	ASN	2.9
1	F	215	LYS	2.9
1	I	99	GLY	2.9
1	I	287	GLU	2.9
1	C	26	PHE	2.9
1	I	294	THR	2.8
1	I	183	GLU	2.8
1	K	9	TYR	2.8
1	C	22	ASP	2.8
1	G	70	GLU	2.8
1	H	187	PHE	2.8
1	K	4	GLN	2.8
1	F	235	ARG	2.8
1	K	254	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	K	59	ALA	2.7
1	C	69	GLY	2.7
1	I	251	TYR	2.7
1	K	82	VAL	2.7
1	L	60	ARG	2.7
1	I	115	ASP	2.7
1	I	299	GLY	2.7
1	I	302	GLN	2.7
1	L	36	GLU	2.7
1	L	63	ILE	2.7
1	E	60	ARG	2.7
1	I	326	ASN	2.7
1	F	190	GLU	2.7
1	I	303	SER	2.6
1	K	157	ALA	2.6
1	K	23	THR	2.6
1	C	210	LYS	2.6
1	K	198	ILE	2.6
1	I	323	SER	2.6
1	H	294	THR	2.6
1	I	48	LEU	2.6
1	H	308	VAL	2.6
1	K	15	PRO	2.6
1	G	308	VAL	2.6
1	K	187	PHE	2.6
1	D	68	ILE	2.6
1	J	186	ARG	2.5
1	K	60	ARG	2.5
1	K	191	GLU	2.5
1	K	255	GLU	2.5
1	G	27	VAL	2.5
1	I	100	VAL	2.5
1	G	9	TYR	2.5
1	E	63	ILE	2.5
1	I	125	LEU	2.5
1	J	322	PHE	2.5
1	E	64	PRO	2.5
1	G	5	ILE	2.5
1	H	11	LEU	2.5
1	D	322	PHE	2.5
1	G	68	ILE	2.5
1	L	89	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	70	GLU	2.4
1	L	56	MET	2.4
1	I	169	ARG	2.4
1	F	30	PRO	2.4
1	E	319	LEU	2.4
1	G	325	GLU	2.4
1	H	21	ARG	2.3
1	L	107	GLU	2.3
1	G	252	ASN	2.3
1	G	50	PRO	2.3
1	G	330	LEU	2.3
1	F	191	GLU	2.3
1	F	5	ILE	2.3
1	D	12	ALA	2.3
1	L	35	ALA	2.3
1	J	56	MET	2.3
1	J	183	GLU	2.3
1	J	17	GLY	2.3
1	I	322	PHE	2.3
1	K	257	VAL	2.3
1	D	19	PRO	2.3
1	D	251	TYR	2.3
1	I	112	TYR	2.3
1	K	8	GLN	2.3
1	J	67	GLY	2.3
1	L	19	PRO	2.3
1	G	25	SER	2.3
1	G	317	THR	2.2
1	I	181	GLY	2.2
1	F	213	CYS	2.2
1	G	315	PRO	2.2
1	J	13	GLN	2.2
1	I	258	ARG	2.2
1	L	90	ALA	2.2
1	K	40	LEU	2.2
1	L	20	GLY	2.2
1	F	16	SER	2.2
1	H	117	SER	2.2
1	F	192	LEU	2.2
1	I	128	LEU	2.2
1	F	175	VAL	2.2
1	L	55	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	203	GLU	2.2
1	L	31	LEU	2.2
1	A	21	ARG	2.2
1	K	189	VAL	2.2
1	C	59	ALA	2.2
1	I	97	ALA	2.2
1	I	248	ILE	2.2
1	J	33	GLU	2.2
1	I	189	VAL	2.2
1	F	204	ASP	2.2
1	H	255	GLU	2.1
1	I	296	LEU	2.1
1	G	201	LYS	2.1
1	K	25	SER	2.1
1	C	312	GLU	2.1
1	J	53	ARG	2.1
1	J	325	GLU	2.1
1	K	107	GLU	2.1
1	B	189	VAL	2.1
1	F	327	PHE	2.1
1	I	51	ALA	2.1
1	K	199	ASP	2.1
1	K	252	ASN	2.1
1	D	323	SER	2.1
1	I	126	SER	2.1
1	L	226	GLY	2.1
1	G	30	PRO	2.1
1	G	324	GLY	2.0
1	L	88	PHE	2.0
1	G	28	GLU	2.0
1	K	28	GLU	2.0
1	D	69	GLY	2.0
1	C	315	PRO	2.0
1	H	22	ASP	2.0
1	D	26	PHE	2.0
1	E	251	TYR	2.0
1	C	316	GLU	2.0
1	L	70	GLU	2.0
1	K	106	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAP	L	400	48/48	0.90	0.18	0.16	35,48,63,65	0
2	NAP	D	400	48/48	0.95	0.13	-0.08	28,35,51,53	0
2	NAP	G	400	48/48	0.95	0.15	-0.31	30,48,64,71	0
2	NAP	E	400	48/48	0.96	0.13	-0.31	19,32,38,40	0
2	NAP	F	400	48/48	0.95	0.12	-0.38	26,31,38,40	0
2	NAP	C	400	48/48	0.95	0.12	-0.51	25,36,40,44	0
2	NAP	K	400	48/48	0.92	0.14	-0.55	38,49,60,61	0
2	NAP	J	400	48/48	0.95	0.13	-0.61	30,48,58,61	0
2	NAP	A	400	48/48	0.97	0.11	-0.62	15,21,26,26	0
2	NAP	B	400	48/48	0.96	0.12	-0.73	25,30,33,34	0
2	NAP	I	400	48/48	0.92	0.14	-0.74	47,59,65,70	0
2	NAP	H	400	48/48	0.96	0.11	-1.02	33,40,43,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.