



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:39 AM GMT

PDB ID : 2RIR  
Title : Crystal structure of dipicolinate synthase, A chain, from *Bacillus subtilis*  
Authors : Osipiuk, J.; Quartey, P.; Moy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2007-10-12  
Resolution : 2.79 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

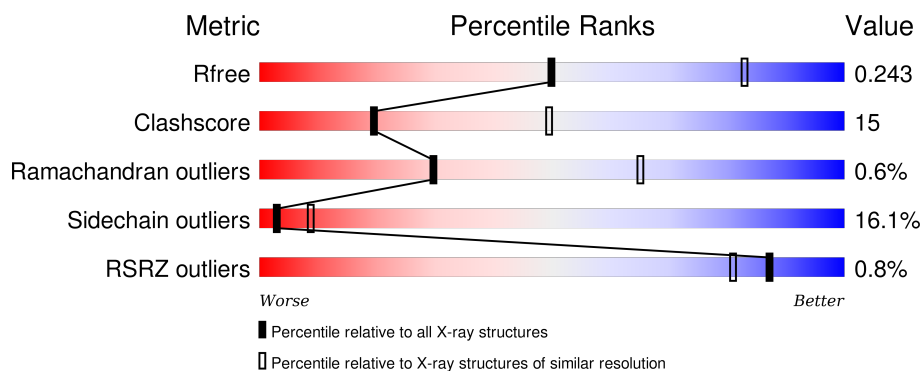
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.79 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	300	<div> <div>67%</div> <div>25%</div> <div>6%</div> <div>..</div> </div>
1	B	300	<div> <div>67%</div> <div>26%</div> <div>5%</div> <div>.</div> </div>
1	C	300	<div> <div>69%</div> <div>23%</div> <div>7%</div> <div>.</div> </div>
1	D	300	<div> <div>2%</div> <div>66%</div> <div>26%</div> <div>7%</div> <div>.</div> </div>
1	E	300	<div> <div>2%</div> <div>66%</div> <div>27%</div> <div>7%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	300	<div><div>%</div><div><div></div></div><div>69%24%6%</div><div></div></div>
1	G	300	<div><div></div><div>65%28%6%</div><div></div></div>
1	H	300	<div><div>%</div><div><div></div></div><div>63%27%9%</div><div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18495 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 Dipicolinate synthase, A chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	Se	0	1	0
			2248	1428	383	427	3	7			
1	B	296	Total	C	N	O	S	Se	0	1	0
			2240	1424	381	425	3	7			
1	C	297	Total	C	N	O	S	Se	0	1	0
			2248	1428	383	427	3	7			
1	D	297	Total	C	N	O	S	Se	0	1	0
			2248	1428	383	427	3	7			
1	E	298	Total	C	N	O	S	Se	0	1	0
			2254	1431	384	429	3	7			
1	F	297	Total	C	N	O	S	Se	0	1	0
			2248	1428	383	427	3	7			
1	G	297	Total	C	N	O	S	Se	0	1	0
			2248	1428	383	427	3	7			
1	H	297	Total	C	N	O	S	Se	0	1	0
			2248	1428	383	427	3	7			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q04809
A	-1	ASN	-	EXPRESSION TAG	UNP Q04809
A	0	ALA	-	EXPRESSION TAG	UNP Q04809
A	1	MSE	-	EXPRESSION TAG	UNP Q04809
A	297	LEU	-	EXPRESSION TAG	UNP Q04809
B	-2	SER	-	EXPRESSION TAG	UNP Q04809
B	-1	ASN	-	EXPRESSION TAG	UNP Q04809
B	0	ALA	-	EXPRESSION TAG	UNP Q04809
B	1	MSE	-	EXPRESSION TAG	UNP Q04809
B	297	LEU	-	EXPRESSION TAG	UNP Q04809
C	-2	SER	-	EXPRESSION TAG	UNP Q04809
C	-1	ASN	-	EXPRESSION TAG	UNP Q04809
C	0	ALA	-	EXPRESSION TAG	UNP Q04809

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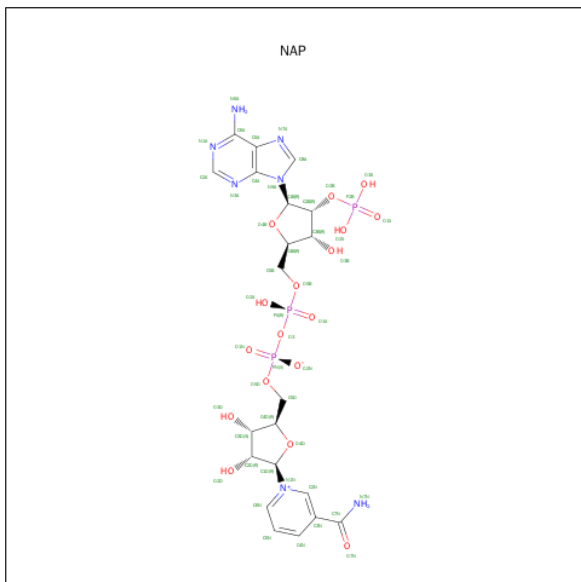
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MSE	-	EXPRESSION TAG	UNP Q04809
C	297	LEU	-	EXPRESSION TAG	UNP Q04809
D	-2	SER	-	EXPRESSION TAG	UNP Q04809
D	-1	ASN	-	EXPRESSION TAG	UNP Q04809
D	0	ALA	-	EXPRESSION TAG	UNP Q04809
D	1	MSE	-	EXPRESSION TAG	UNP Q04809
D	297	LEU	-	EXPRESSION TAG	UNP Q04809
E	-2	SER	-	EXPRESSION TAG	UNP Q04809
E	-1	ASN	-	EXPRESSION TAG	UNP Q04809
E	0	ALA	-	EXPRESSION TAG	UNP Q04809
E	1	MSE	-	EXPRESSION TAG	UNP Q04809
E	297	LEU	-	EXPRESSION TAG	UNP Q04809
F	-2	SER	-	EXPRESSION TAG	UNP Q04809
F	-1	ASN	-	EXPRESSION TAG	UNP Q04809
F	0	ALA	-	EXPRESSION TAG	UNP Q04809
F	1	MSE	-	EXPRESSION TAG	UNP Q04809
F	297	LEU	-	EXPRESSION TAG	UNP Q04809
G	-2	SER	-	EXPRESSION TAG	UNP Q04809
G	-1	ASN	-	EXPRESSION TAG	UNP Q04809
G	0	ALA	-	EXPRESSION TAG	UNP Q04809
G	1	MSE	-	EXPRESSION TAG	UNP Q04809
G	297	LEU	-	EXPRESSION TAG	UNP Q04809
H	-2	SER	-	EXPRESSION TAG	UNP Q04809
H	-1	ASN	-	EXPRESSION TAG	UNP Q04809
H	0	ALA	-	EXPRESSION TAG	UNP Q04809
H	1	MSE	-	EXPRESSION TAG	UNP Q04809
H	297	LEU	-	EXPRESSION TAG	UNP Q04809

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0
2	H	2	Total Cl 2 2	0	0
2	B	1	Total Cl 1 1	0	0
2	A	1	Total Cl 1 1	0	0

- Molecule 3 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
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	17	Total	O	0	0
			17	17		
4	B	25	Total	O	0	1
			26	26		

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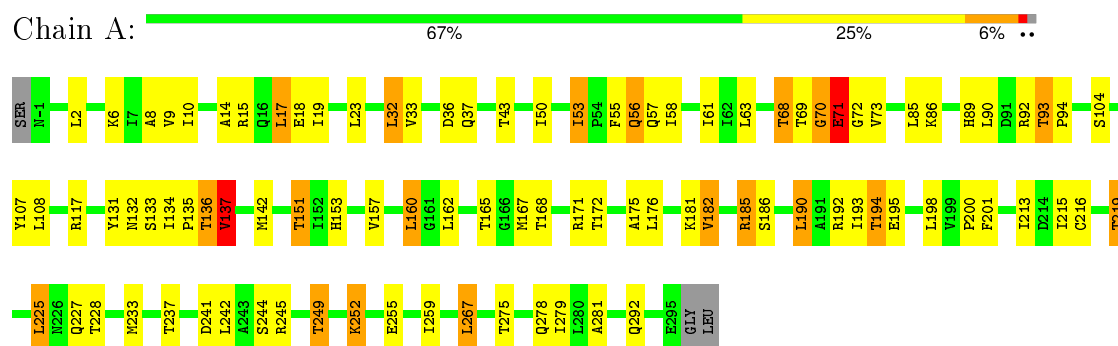
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	23	Total 23	O 23	0	0
4	D	15	Total 15	O 15	0	0
4	E	6	Total 6	O 6	0	0
4	F	5	Total 5	O 5	0	0
4	G	20	Total 20	O 20	0	0
4	H	10	Total 10	O 10	0	0

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

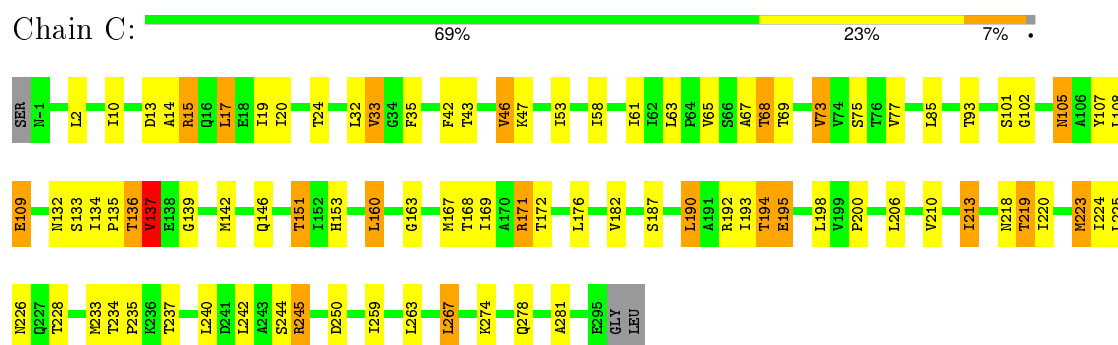
- Molecule 1: Dipicolinate synthase, A chain



- Molecule 1: Dipicolinate synthase, A chain

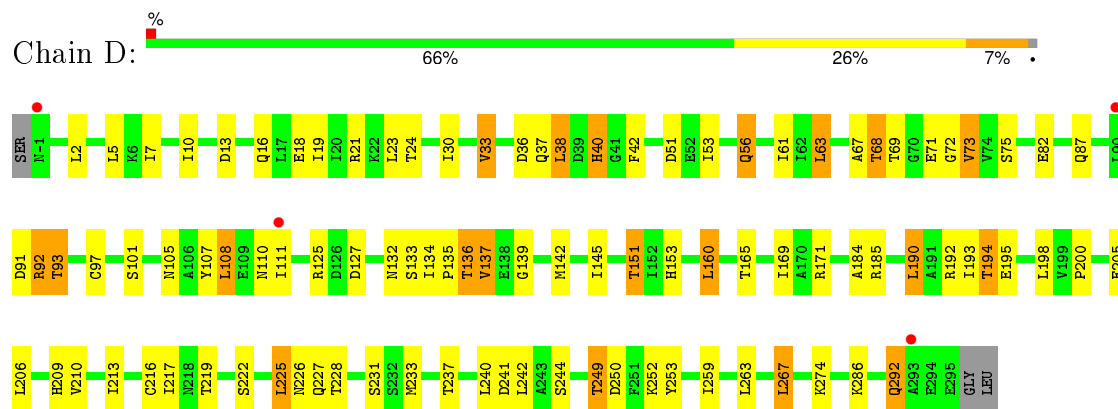


- Molecule 1: Dipicolinate synthase, A chain

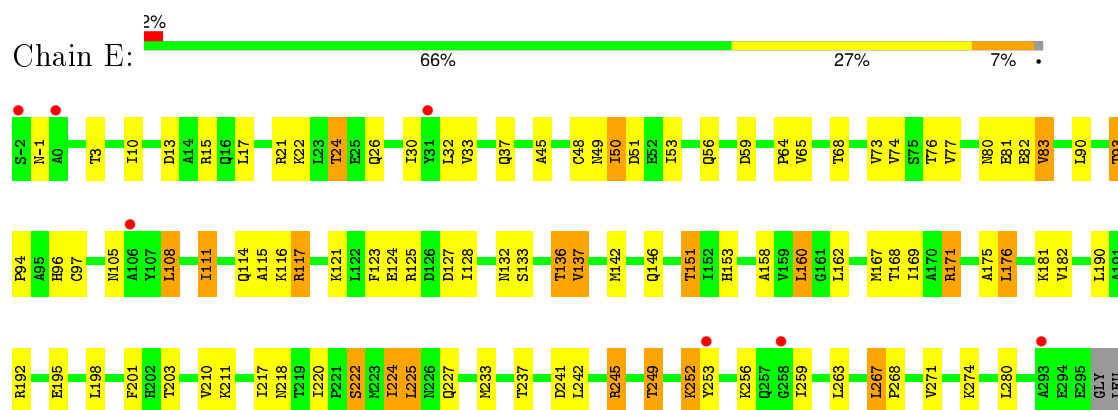




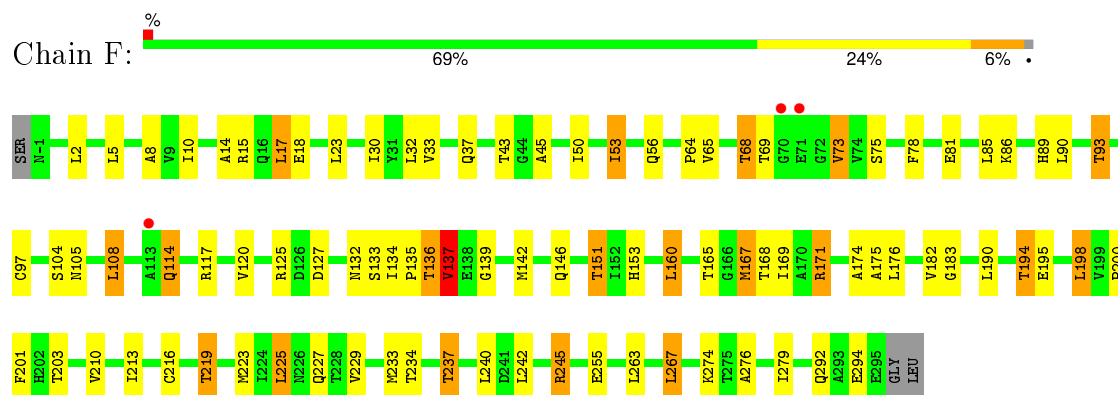
- Molecule 1: Dipicolinate synthase, A chain



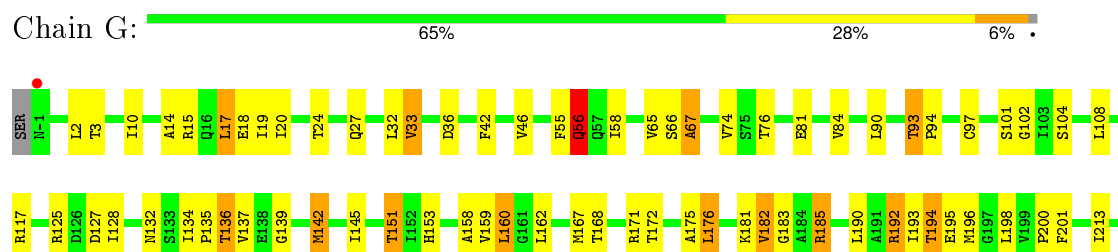
- Molecule 1: Dipicolinate synthase, A chain

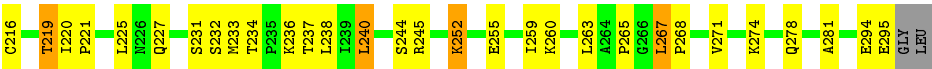


- Molecule 1: Dipicolinate synthase, A chain

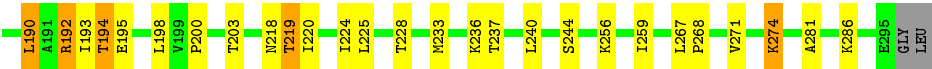
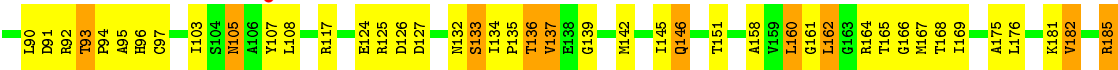


- Molecule 1: Dipicolinate synthase, A chain





• Molecule 1: Dipicolinate synthase, A chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	261.58Å 75.11Å 200.46Å 90.00° 119.74° 90.00°	Depositor
Resolution (Å)	40.00 – 2.79 40.02 – 2.79	Depositor EDS
% Data completeness (in resolution range)	96.4 (40.00-2.79) 96.3 (40.02-2.79)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.199 , 0.249 0.193 , 0.243	Depositor DCC
$R_{free}$ test set	4079 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.8	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 45.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 81350 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18495	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.65	0/2277	0.75	2/3078 (0.1%)
1	B	0.60	0/2269	0.74	1/3067 (0.0%)
1	C	0.62	0/2277	0.77	2/3078 (0.1%)
1	D	0.59	0/2277	0.72	0/3078
1	E	0.54	0/2283	0.69	0/3086
1	F	0.54	0/2277	0.70	1/3078 (0.0%)
1	G	0.62	0/2277	0.76	2/3078 (0.1%)
1	H	0.62	0/2277	0.73	1/3078 (0.0%)
All	All	0.60	0/18214	0.73	9/24621 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	137	VAL	CB-CA-C	-5.72	100.52	111.40
1	C	137	VAL	CB-CA-C	-5.62	100.71	111.40
1	G	192	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	F	137	VAL	CB-CA-C	-5.53	100.89	111.40
1	C	46	VAL	CB-CA-C	-5.45	101.05	111.40
1	H	32	LEU	CA-CB-CG	5.43	127.79	115.30
1	G	192	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	137	VAL	CB-CA-C	-5.27	101.39	111.40
1	A	176	LEU	CA-CB-CG	5.21	127.28	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2248	0	2328	73	0
1	B	2240	0	2322	78	0
1	C	2248	0	2328	76	0
1	D	2248	0	2328	78	0
1	E	2254	0	2333	68	0
1	F	2248	0	2328	63	0
1	G	2248	0	2328	73	0
1	H	2248	0	2328	81	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	G	1	0	0	0	0
2	H	2	0	0	0	0
3	A	48	0	25	5	0
3	B	48	0	25	4	0
3	C	48	0	25	3	0
3	D	48	0	25	4	0
3	E	48	0	25	1	0
3	F	48	0	25	4	0
3	G	48	0	25	3	0
3	H	48	0	25	5	0
4	A	17	0	0	1	0
4	B	26	0	0	1	0
4	C	23	0	0	6	0
4	D	15	0	0	2	0
4	E	6	0	0	1	0
4	F	5	0	0	1	0
4	G	20	0	0	2	0
4	H	10	0	0	2	0
All	All	18495	0	18823	557	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 15.

All (557) 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:C:171:ARG:HG3	1:C:171:ARG:HH11	1.08	1.17
4:E:511:HOH:O	1:F:194:THR:HG21	1.40	1.16
1:E:245:ARG:HB2	1:E:245:ARG:HH21	0.99	1.09
1:C:142[B]:MSE:HE1	1:D:142[B]:MSE:HA	1.27	1.06
1:H:68:THR:HG22	1:H:105:ASN:HD21	1.16	1.05
1:H:219:THR:HG21	4:H:511:HOH:O	1.59	1.02
1:E:245:ARG:HB2	1:E:245:ARG:NH2	1.78	0.97
1:B:171:ARG:HH11	1:B:171:ARG:HG3	1.30	0.95
1:D:194:THR:HG22	1:D:200:PRO:HG3	1.47	0.94
1:C:68:THR:HG22	1:C:105:ASN:HD21	1.32	0.94
1:B:40:HIS:HB3	4:B:505:HOH:O	1.68	0.92
1:G:233:MSE:HE3	1:G:237:THR:HB	1.51	0.91
1:E:245:ARG:CB	1:E:245:ARG:HH21	1.84	0.91
1:C:233:MSE:HE3	1:C:237:THR:HB	1.52	0.90
1:H:95:ALA:HA	1:H:117:ARG:NH2	1.89	0.86
1:H:194:THR:HG22	1:H:200:PRO:HG3	1.57	0.86
1:G:93:THR:HG22	1:G:117:ARG:HE	1.40	0.85
1:D:233:MSE:HE3	1:D:237:THR:HB	1.58	0.84
1:B:86:LYS:H	1:B:89:HIS:CD2	1.94	0.83
1:E:133:SER:HA	1:E:136:THR:HG23	1.60	0.83
1:D:24:THR:HG22	1:D:30:ILE:HD12	1.60	0.82
1:E:33:VAL:HG11	1:E:53:ILE:HD11	1.60	0.82
1:C:223:MSE:HE2	1:C:226:ASN:HA	1.60	0.82
1:G:185:ARG:HD3	3:G:407:NAP:O1X	1.79	0.82
1:E:132:ASN:O	1:E:136:THR:HG22	1.79	0.82
1:B:196:MSE:HG2	1:C:171:ARG:HH21	1.45	0.81
1:C:171:ARG:CG	1:C:171:ARG:HH11	1.90	0.81
1:B:93:THR:HG22	1:B:117:ARG:HE	1.45	0.80
1:A:93:THR:HG22	1:A:117:ARG:HE	1.46	0.79
1:B:171:ARG:HH11	1:B:171:ARG:CG	1.95	0.79
1:H:40:HIS:HE2	1:H:47:LYS:HD3	1.46	0.79
1:B:53:ILE:HD11	1:B:58:ILE:HG12	1.64	0.79
1:H:11:GLY:HA2	1:H:76:THR:HG22	1.62	0.79
1:D:92:ARG:HG2	1:D:92:ARG:HH11	1.48	0.78
1:C:142[B]:MSE:HE3	1:D:145:ILE:HB	1.66	0.77
1:D:24:THR:CG2	1:D:30:ILE:HD12	2.14	0.77
1:D:38:LEU:HD21	1:D:40:HIS:HB3	1.67	0.77
1:C:151:THR:HG22	1:C:153:HIS:O	1.83	0.77
1:G:93:THR:HG23	1:G:97:CYS:HB3	1.66	0.76
1:F:171:ARG:HG3	1:F:171:ARG:HH11	1.50	0.76
1:B:86:LYS:H	1:B:89:HIS:HD2	1.31	0.76
1:C:68:THR:HG22	1:C:105:ASN:ND2	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:MSE:HE3	1:A:237:THR:HB	1.67	0.75
1:D:5:LEU:HD11	1:D:292:GLN:HB2	1.66	0.75
1:F:2:LEU:HA	1:F:292:GLN:HE22	1.52	0.75
1:H:0:ALA:O	1:H:1:MSE:HE2	1.86	0.75
1:G:245:ARG:HH11	1:G:265:PRO:HG2	1.51	0.75
1:H:68:THR:HG22	1:H:105:ASN:ND2	1.97	0.75
1:H:160:LEU:O	1:H:219:THR:HB	1.87	0.74
1:D:40:HIS:CD2	1:D:42:PHE:HB2	2.22	0.74
1:A:90:LEU:O	1:A:93:THR:HB	1.88	0.74
1:H:18:GLU:OE1	1:H:21:ARG:NH1	2.21	0.73
1:A:160:LEU:O	1:A:219:THR:HB	1.87	0.73
1:H:68:THR:HG23	1:H:69:THR:N	2.03	0.73
1:C:142[B]:MSE:CE	1:D:142[B]:MSE:HA	2.14	0.73
1:H:185:ARG:HD2	3:H:408:NAP:C2A	2.19	0.73
1:G:132:ASN:O	1:G:136:THR:HG23	1.89	0.73
1:C:233:MSE:HE3	1:C:237:THR:CB	2.19	0.72
1:C:233:MSE:CE	1:C:237:THR:HB	2.18	0.72
1:G:132:ASN:O	1:G:136:THR:CG2	2.36	0.72
1:B:196:MSE:HG2	1:C:171:ARG:NH2	2.04	0.72
1:E:245:ARG:CB	1:E:245:ARG:NH2	2.48	0.72
1:E:220:ILE:HB	1:E:224:ILE:HD11	1.71	0.72
1:A:133:SER:HA	1:A:136:THR:HG23	1.72	0.72
1:G:252:LYS:O	1:G:255:GLU:HB3	1.89	0.72
1:E:59:ASP:O	1:E:97:CYS:HA	1.89	0.71
1:A:132:ASN:O	1:A:136:THR:HG22	1.90	0.71
1:F:133:SER:HA	1:F:136:THR:HG23	1.71	0.71
1:G:136:THR:HG22	1:G:268:PRO:HG3	1.73	0.71
1:A:171:ARG:HG3	1:A:171:ARG:HH11	1.55	0.71
1:B:142[A]:MSE:HE2	1:B:146:GLN:NE2	2.05	0.70
1:H:233:MSE:HE3	1:H:237:THR:HB	1.73	0.70
1:F:69:THR:OG1	1:F:73:VAL:HG13	1.92	0.69
1:C:245:ARG:CD	1:C:245:ARG:H	2.04	0.69
1:H:219:THR:CG2	4:H:511:HOH:O	2.28	0.69
1:F:132:ASN:O	1:F:135:PRO:HD2	1.92	0.69
1:F:146:GLN:HE21	1:H:142[B]:MSE:HE1	1.57	0.69
1:E:171:ARG:HB3	1:E:171:ARG:HH11	1.58	0.68
1:C:132:ASN:O	1:C:136:THR:HG22	1.94	0.68
1:B:171:ARG:NH2	1:C:195:GLU:OE2	2.23	0.68
1:B:213:ILE:HD11	1:B:216:CYS:HB2	1.75	0.68
1:H:68:THR:HG23	1:H:69:THR:H	1.58	0.68
1:F:242:LEU:O	3:F:406:NAP:H2N	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:194:THR:HG22	1:F:200:PRO:HG3	1.76	0.68
1:H:68:THR:HG21	1:H:107:TYR:HD1	1.59	0.68
1:G:194:THR:HG22	1:G:200:PRO:HG3	1.76	0.67
1:E:24:THR:HG23	1:E:30:ILE:HD12	1.76	0.67
1:E:252:LYS:HD3	1:E:252:LYS:H	1.58	0.67
1:F:132:ASN:O	1:F:136:THR:HG22	1.93	0.67
1:F:105:ASN:OD1	1:F:108:LEU:HB2	1.94	0.67
1:C:192:ARG:HD2	4:C:424:HOH:O	1.95	0.67
1:G:294:GLU:O	1:G:295:GLU:HG2	1.94	0.67
1:G:255:GLU:HA	1:G:255:GLU:OE1	1.94	0.66
1:B:160:LEU:HB3	1:B:220:ILE:HD12	1.77	0.66
1:E:146:GLN:HB3	1:G:142[A]:MSE:CE	2.24	0.66
1:C:132:ASN:O	1:C:136:THR:CG2	2.43	0.66
1:C:75:SER:HB3	4:C:425:HOH:O	1.95	0.66
1:B:233:MSE:HE3	1:B:237:THR:HB	1.77	0.66
1:C:171:ARG:NH1	1:C:171:ARG:HG3	1.90	0.66
1:B:171:ARG:NH1	1:B:171:ARG:CG	2.56	0.66
1:A:233:MSE:CE	1:A:237:THR:HB	2.26	0.66
1:E:142[B]:MSE:HE1	1:G:142[B]:MSE:HA	1.77	0.66
1:B:160:LEU:O	1:B:219:THR:HB	1.96	0.65
1:F:93:THR:HG22	1:F:117:ARG:HE	1.61	0.65
1:C:219:THR:HG21	4:C:404:HOH:O	1.96	0.65
1:A:142[A]:MSE:HG3	1:B:142[A]:MSE:HE1	1.78	0.65
1:B:24:THR:HG21	1:B:42:PHE:HB3	1.79	0.65
1:G:171:ARG:NH2	1:H:195:GLU:OE2	2.23	0.64
1:A:194:THR:HG22	1:A:200:PRO:HG3	1.77	0.64
1:D:213:ILE:HD11	1:D:216:CYS:HB2	1.78	0.64
1:E:252:LYS:H	1:E:252:LYS:CD	2.07	0.64
1:B:265:PRO:HA	3:B:402:NAP:H72N	1.62	0.64
1:H:68:THR:HG21	1:H:107:TYR:CD1	2.33	0.64
1:F:86:LYS:H	1:F:89:HIS:CD2	2.15	0.64
1:C:218:ASN:OD1	1:C:224:ILE:HD11	1.98	0.64
1:A:69:THR:OG1	1:A:73:VAL:HG12	1.97	0.63
1:H:66:SER:O	1:H:67:ALA:HB3	1.97	0.63
1:F:213:ILE:O	1:F:237:THR:HG23	1.99	0.63
1:A:132:ASN:O	1:A:136:THR:CG2	2.47	0.63
1:H:70:GLY:HA2	1:H:107:TYR:CB	2.28	0.63
1:A:69:THR:HG1	1:A:73:VAL:HG12	1.63	0.63
1:A:241:ASP:OD2	1:A:249:THR:CG2	2.47	0.63
1:H:133:SER:HA	1:H:136:THR:HG23	1.80	0.63
1:A:162:LEU:HD22	1:A:193:ILE:HG13	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ASP:O	1:B:97:CYS:HA	1.99	0.62
1:H:70:GLY:HA2	1:H:107:TYR:HB3	1.82	0.62
1:E:146:GLN:HE21	1:G:142[A]:MSE:HE1	1.64	0.62
1:D:16:GLN:HA	1:D:19:ILE:HD12	1.81	0.61
1:E:10:ILE:HG22	1:E:74:VAL:HG11	1.80	0.61
1:A:134:ILE:O	1:A:137:VAL:HG23	2.00	0.61
1:G:233:MSE:HE3	1:G:237:THR:CB	2.29	0.61
1:H:66:SER:O	1:H:67:ALA:CB	2.49	0.61
1:H:132:ASN:O	1:H:135:PRO:HD2	2.01	0.61
1:H:48:CYS:SG	1:H:53:ILE:HG22	2.40	0.61
1:B:68:THR:HG23	1:B:105:ASN:HD21	1.66	0.61
1:E:132:ASN:O	1:E:136:THR:CG2	2.49	0.61
1:D:38:LEU:CD2	1:D:40:HIS:HB3	2.30	0.61
1:C:133:SER:HA	1:C:136:THR:HG23	1.82	0.61
1:B:220:ILE:HD13	1:B:224:ILE:HD11	1.84	0.60
1:F:93:THR:HG23	1:F:97:CYS:HB3	1.83	0.60
1:D:233:MSE:HE3	1:D:237:THR:CB	2.29	0.60
1:E:142[B]:MSE:CE	1:G:145:ILE:HB	2.32	0.60
1:A:157:VAL:HG22	1:A:215:ILE:HB	1.83	0.60
1:C:142[B]:MSE:HE1	1:D:142[B]:MSE:CA	2.18	0.60
1:F:160:LEU:O	1:F:219:THR:HB	2.01	0.60
1:B:132:ASN:O	1:B:136:THR:CG2	2.49	0.60
1:D:68:THR:HG23	1:D:72:GLY:HA2	1.84	0.60
1:E:76:THR:HG21	1:E:83:VAL:CG1	2.32	0.59
1:H:190:LEU:HA	1:H:193:ILE:HD12	1.83	0.59
1:B:133:SER:HA	1:B:136:THR:HG23	1.85	0.59
1:B:192:ARG:HH21	1:B:195:GLU:HG2	1.66	0.59
1:D:10:ILE:HD12	1:D:61:ILE:HG23	1.83	0.59
1:A:131:TYR:HB3	1:A:279:ILE:HD13	1.84	0.59
1:C:192:ARG:HH21	1:C:195:GLU:HG2	1.67	0.58
1:A:93:THR:HG22	1:A:117:ARG:NE	2.18	0.58
1:F:132:ASN:O	1:F:136:THR:CG2	2.51	0.58
1:E:252:LYS:N	1:E:252:LYS:HD3	2.18	0.58
1:A:168:THR:OG1	1:D:192:ARG:NH2	2.36	0.58
1:C:242:LEU:O	3:C:403:NAP:H2N	2.03	0.58
1:D:184:ALA:HB3	1:D:190:LEU:HD13	1.85	0.58
1:D:33:VAL:CG1	1:D:53:ILE:HD11	2.32	0.58
1:H:136:THR:HG22	1:H:268:PRO:HG3	1.83	0.58
1:G:234:THR:HG23	1:G:236:LYS:HB2	1.86	0.58
1:H:23:LEU:HB2	1:H:30:ILE:HD11	1.86	0.58
1:H:14:ALA:HA	1:H:17:LEU:HD22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ASP:OD2	1:A:249:THR:HG22	2.04	0.57
1:F:90:LEU:O	1:F:93:THR:HB	2.04	0.57
1:A:134:ILE:HB	1:A:135:PRO:HD3	1.85	0.57
1:G:183:GLY:HA2	1:G:201:PHE:O	2.05	0.57
1:G:93:THR:CG2	1:G:97:CYS:HB3	2.33	0.57
1:C:105:ASN:O	1:C:109:GLU:HB2	2.05	0.57
1:A:9:VAL:HB	1:A:32:LEU:HD12	1.86	0.57
1:B:168:THR:OG1	1:C:192:ARG:NH2	2.38	0.57
1:B:225:LEU:HB3	1:B:249:THR:HG23	1.86	0.57
1:E:121:LYS:O	1:E:124:GLU:HB2	2.04	0.57
1:A:133:SER:HB3	1:A:165:THR:HG22	1.87	0.57
1:D:132:ASN:O	1:D:136:THR:CG2	2.52	0.57
1:D:68:THR:HG21	1:D:107:TYR:HD1	1.70	0.56
1:H:94:PRO:HB2	1:H:96:HIS:ND1	2.20	0.56
1:F:213:ILE:CD1	1:F:216:CYS:HB2	2.35	0.56
1:A:56:GLN:OE1	1:A:57:GLN:HG2	2.04	0.56
1:B:68:THR:HG22	1:B:105:ASN:ND2	2.19	0.56
1:A:86:LYS:H	1:A:89:HIS:CD2	2.24	0.56
1:E:267:LEU:O	1:E:271:VAL:HG23	2.05	0.56
1:B:234:THR:OG1	1:B:235:PRO:HD2	2.05	0.56
1:H:203:THR:HG21	3:H:408:NAP:H2A	1.87	0.56
1:C:151:THR:CG2	1:C:153:HIS:HB3	2.36	0.56
1:C:146:GLN:HB3	1:D:142[A]:MSE:HE1	1.88	0.56
1:C:223:MSE:HE2	1:C:226:ASN:CA	2.32	0.56
1:D:160:LEU:O	1:D:219:THR:HB	2.06	0.56
1:G:192:ARG:HH21	1:G:195:GLU:HG2	1.70	0.56
1:H:37:GLN:HB2	1:H:78:PHE:O	2.06	0.56
1:F:137:VAL:HG13	1:F:169:ILE:HA	1.88	0.56
1:G:90:LEU:O	1:G:93:THR:HB	2.05	0.55
1:B:233:MSE:HE2	1:B:259:ILE:HD13	1.88	0.55
1:G:24:THR:HG21	1:G:42:PHE:HB3	1.88	0.55
1:F:171:ARG:CG	1:F:171:ARG:HH11	2.20	0.55
1:D:225:LEU:CB	1:D:249:THR:HB	2.36	0.55
1:H:15:ARG:NH1	1:H:65:VAL:HG21	2.21	0.55
1:A:171:ARG:NH1	1:A:171:ARG:HG3	2.21	0.55
1:B:122:LEU:O	1:B:125:ARG:HG3	2.07	0.55
1:D:67:ALA:HB2	1:D:101:SER:OG	2.06	0.55
1:G:67:ALA:HB2	1:G:101:SER:OG	2.07	0.55
1:C:142[B]:MSE:HE2	1:D:145:ILE:HD12	1.88	0.55
1:H:69:THR:C	1:H:71:GLU:H	2.10	0.55
1:H:68:THR:CG2	1:H:69:THR:N	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:GLN:HG2	4:D:509:HOH:O	2.07	0.55
1:E:137:VAL:HG21	1:E:168:THR:HG22	1.87	0.55
1:G:192:ARG:NH2	1:H:168:THR:OG1	2.40	0.55
1:C:160:LEU:HB2	1:C:218:ASN:HA	1.89	0.55
1:H:134:ILE:O	1:H:137:VAL:HG23	2.07	0.55
1:H:10:ILE:HG12	1:H:33:VAL:HG13	1.90	0.54
1:F:183:GLY:HA2	1:F:201:PHE:O	2.07	0.54
1:F:134:ILE:HB	1:F:135:PRO:HD3	1.88	0.54
1:H:125:ARG:NH1	1:H:127:ASP:OD2	2.40	0.54
1:B:68:THR:CG2	1:B:105:ASN:HD21	2.21	0.54
1:D:134:ILE:HB	1:D:135:PRO:HD3	1.89	0.54
1:H:95:ALA:HA	1:H:117:ARG:HH21	1.71	0.54
1:B:192:ARG:NH2	1:B:195:GLU:HG2	2.22	0.54
1:G:213:ILE:HD11	1:G:216:CYS:HB2	1.90	0.54
1:E:48:CYS:SG	1:E:49:ASN:N	2.81	0.54
1:C:233:MSE:HE2	1:C:259:ILE:HD13	1.90	0.54
1:H:94:PRO:HB2	1:H:96:HIS:CE1	2.43	0.54
1:C:75:SER:CB	4:C:425:HOH:O	2.53	0.54
1:H:95:ALA:HA	1:H:117:ARG:HH22	1.72	0.53
1:C:219:THR:CG2	4:C:404:HOH:O	2.53	0.53
1:A:175:ALA:HB1	1:B:175:ALA:HB1	1.90	0.53
1:D:63:LEU:HD23	1:D:108:LEU:HD11	1.89	0.53
1:E:233:MSE:HE3	1:E:237:THR:HB	1.90	0.53
1:G:151:THR:HG23	1:G:153:HIS:O	2.08	0.53
1:D:190:LEU:HA	1:D:193:ILE:HD12	1.91	0.53
1:C:19:ILE:HA	1:C:281:ALA:HB2	1.90	0.53
1:H:233:MSE:HE2	1:H:259:ILE:HD13	1.90	0.53
1:D:213:ILE:CD1	1:D:216:CYS:HB2	2.38	0.53
1:E:133:SER:CA	1:E:136:THR:HG23	2.37	0.53
1:E:192:ARG:NH2	1:F:168:THR:OG1	2.42	0.53
1:D:33:VAL:HG11	1:D:53:ILE:HD11	1.91	0.53
1:A:56:GLN:HA	1:A:92:ARG:O	2.08	0.53
1:E:222:SER:O	1:E:224:ILE:HG12	2.09	0.53
1:F:125:ARG:NH1	1:F:127:ASP:OD1	2.41	0.53
1:C:210:VAL:HA	1:C:213:ILE:HG12	1.90	0.53
1:A:185:ARG:HD3	3:A:401:NAP:O1X	2.08	0.53
1:B:68:THR:CG2	1:B:105:ASN:ND2	2.71	0.53
1:D:132:ASN:O	1:D:136:THR:HG23	2.09	0.53
1:B:137:VAL:HG11	1:B:172:THR:HB	1.89	0.53
1:G:233:MSE:HE2	1:G:259:ILE:HD13	1.91	0.52
1:D:5:LEU:HD11	1:D:292:GLN:OE1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:LEU:HB3	1:E:220:ILE:HD12	1.92	0.52
1:B:213:ILE:CD1	1:B:216:CYS:HB2	2.38	0.52
1:C:206:LEU:O	1:C:210:VAL:HG22	2.10	0.52
1:H:69:THR:O	1:H:71:GLU:N	2.32	0.52
1:C:67:ALA:HB2	1:C:101:SER:OG	2.10	0.52
1:G:14:ALA:HA	1:G:17:LEU:HD22	1.92	0.52
1:A:70:GLY:O	1:A:72:GLY:N	2.42	0.52
1:G:65:VAL:HA	1:G:102:GLY:HA3	1.92	0.52
1:C:134:ILE:HB	1:C:135:PRO:CD	2.40	0.52
1:F:50:ILE:HD11	1:F:85:LEU:HD12	1.91	0.52
1:F:233:MSE:HE2	1:F:237:THR:HB	1.92	0.51
1:B:5:LEU:HD23	1:B:7:ILE:HD11	1.91	0.51
1:B:220:ILE:HD13	1:B:224:ILE:CD1	2.40	0.51
1:F:165:THR:HG23	3:F:406:NAP:O1N	2.10	0.51
1:B:233:MSE:HE1	1:B:259:ILE:HG21	1.91	0.51
1:E:175:ALA:HB1	1:G:175:ALA:HB1	1.92	0.51
1:G:167:MSE:CE	1:G:171:ARG:HH22	2.24	0.51
1:C:43:THR:HG22	4:C:419:HOH:O	2.11	0.51
1:A:233:MSE:HE3	1:A:237:THR:CB	2.38	0.51
1:G:245:ARG:HH11	1:G:265:PRO:CG	2.23	0.51
1:F:68:THR:HG23	1:F:105:ASN:OD1	2.10	0.51
1:D:136:THR:HG21	3:D:404:NAP:H4N	1.91	0.51
1:H:90:LEU:O	1:H:93:THR:HB	2.10	0.51
1:A:167:MSE:CE	1:A:171:ARG:NH2	2.74	0.51
1:B:132:ASN:O	1:B:136:THR:HG23	2.09	0.51
1:G:93:THR:HG23	1:G:97:CYS:CB	2.37	0.51
1:B:265:PRO:HA	3:B:402:NAP:N7N	2.26	0.51
1:B:93:THR:HG23	1:B:97:CYS:HB3	1.93	0.50
1:G:132:ASN:O	1:G:136:THR:HG22	2.11	0.50
1:B:132:ASN:O	1:B:136:THR:HG22	2.10	0.50
1:B:181:LYS:HG3	1:B:201:PHE:CE2	2.47	0.50
1:A:151:THR:CG2	1:A:153:HIS:O	2.60	0.50
1:D:133:SER:HA	1:D:136:THR:HG23	1.93	0.50
1:G:55:PHE:HA	1:G:58:ILE:HD13	1.93	0.50
1:D:225:LEU:HB3	1:D:249:THR:HB	1.94	0.50
1:D:139:GLY:HA3	1:D:267:LEU:HG	1.92	0.50
1:B:12:GLY:HA2	1:B:64:PRO:HB3	1.93	0.50
1:C:69:THR:HG23	1:C:73:VAL:HG12	1.94	0.50
1:D:233:MSE:HE2	1:D:259:ILE:HD13	1.93	0.50
1:H:94:PRO:CB	1:H:96:HIS:CE1	2.94	0.50
1:G:20:ILE:CD1	1:G:32:LEU:HD11	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:8:ALA:HB2	1:F:53:ILE:CD1	2.42	0.50
1:B:182:VAL:HG22	1:B:193:ILE:CD1	2.42	0.49
1:E:146:GLN:HE21	1:G:142[A]:MSE:CE	2.25	0.49
1:F:233:MSE:CE	1:F:237:THR:HB	2.42	0.49
1:D:56:GLN:H	1:D:56:GLN:CD	2.16	0.49
1:G:10:ILE:HA	1:G:33:VAL:HG13	1.94	0.49
1:E:90:LEU:O	1:E:93:THR:HG22	2.12	0.49
1:D:226:ASN:OD1	1:D:226:ASN:C	2.50	0.49
1:F:146:GLN:HB3	1:H:142[B]:MSE:CE	2.42	0.49
1:E:32:LEU:HD22	1:E:45:ALA:HB1	1.95	0.49
1:A:14:ALA:O	1:A:17:LEU:HB2	2.13	0.49
1:E:158:ALA:HA	1:E:181:LYS:O	2.13	0.49
1:A:55:PHE:HA	1:A:58:ILE:HD13	1.95	0.49
1:G:219:THR:HG21	4:G:508:HOH:O	2.12	0.49
1:D:2:LEU:HA	1:D:292:GLN:HE22	1.78	0.49
1:D:5:LEU:CD1	1:D:292:GLN:OE1	2.61	0.49
1:D:219:THR:O	3:D:404:NAP:H52N	2.11	0.49
1:A:151:THR:HG23	1:A:153:HIS:O	2.12	0.49
1:G:3:THR:HA	1:G:27:GLN:O	2.13	0.49
1:G:219:THR:O	3:G:407:NAP:H52N	2.13	0.49
1:C:142[B]:MSE:CE	1:D:145:ILE:HD12	2.43	0.48
1:E:160:LEU:HB2	1:E:218:ASN:HA	1.95	0.48
1:B:192:ARG:NH2	1:C:168:THR:OG1	2.46	0.48
1:C:194:THR:HG22	1:C:200:PRO:HG3	1.94	0.48
1:E:80:ASN:O	1:E:81:GLU:HG2	2.13	0.48
1:D:24:THR:HG23	1:D:30:ILE:HD12	1.94	0.48
1:F:142[A]:MSE:HE2	1:H:145:ILE:HG22	1.94	0.48
1:B:171:ARG:HG3	1:B:171:ARG:NH1	2.11	0.48
1:A:242:LEU:O	3:A:401:NAP:H2N	2.14	0.48
1:C:146:GLN:HB3	1:D:142[A]:MSE:CE	2.42	0.48
1:C:134:ILE:O	1:C:137:VAL:HG23	2.14	0.48
1:D:91:ASP:C	1:D:93:THR:H	2.17	0.48
1:B:220:ILE:CD1	1:B:224:ILE:HD11	2.43	0.48
1:E:137:VAL:CG2	1:E:168:THR:HG22	2.43	0.48
1:D:93:THR:HG23	1:D:97:CYS:HB3	1.95	0.48
1:F:23:LEU:HB3	1:F:30:ILE:HD11	1.96	0.48
1:A:68:THR:HG21	1:A:107:TYR:CD1	2.48	0.48
1:D:227:GLN:HG3	1:D:253:TYR:CD1	2.49	0.48
1:C:15:ARG:NH1	1:C:65:VAL:HG21	2.29	0.48
1:C:14:ALA:HA	1:C:17:LEU:HD22	1.94	0.48
1:C:245:ARG:HD2	1:C:245:ARG:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:158:ALA:HA	1:H:181:LYS:HG2	1.95	0.48
1:G:185:ARG:NH1	3:G:407:NAP:O3X	2.47	0.47
1:D:40:HIS:HD2	1:D:42:PHE:HB2	1.78	0.47
1:D:185:ARG:HD2	3:D:404:NAP:C2A	2.44	0.47
1:C:137:VAL:HG13	1:C:169:ILE:HA	1.95	0.47
1:C:33:VAL:CG1	1:C:53:ILE:HD11	2.43	0.47
1:F:276:ALA:HA	1:F:279:ILE:HD12	1.95	0.47
1:D:125:ARG:NH1	1:D:127:ASP:OD2	2.47	0.47
1:A:233:MSE:HE2	1:A:259:ILE:HD13	1.95	0.47
1:B:136:THR:HG22	1:B:268:PRO:HG3	1.95	0.47
1:A:56:GLN:O	1:A:94:PRO:HG3	2.14	0.47
1:F:133:SER:CA	1:F:136:THR:HG23	2.40	0.47
1:H:233:MSE:HE3	1:H:237:THR:CB	2.41	0.47
4:F:410:HOH:O	1:H:274:LYS:HE2	2.13	0.47
1:E:10:ILE:O	1:E:64:PRO:HD3	2.14	0.47
1:F:225:LEU:HD12	1:F:229:VAL:HG11	1.97	0.47
1:B:171:ARG:NH1	1:B:171:ARG:CB	2.78	0.47
1:A:267:LEU:HD12	1:A:267:LEU:HA	1.66	0.47
1:F:30:ILE:O	1:F:45:ALA:HA	2.15	0.47
1:F:151:THR:CG2	1:F:153:HIS:O	2.63	0.47
1:F:151:THR:HG22	1:F:153:HIS:O	2.15	0.47
1:C:151:THR:CG2	1:C:153:HIS:O	2.58	0.47
1:F:137:VAL:CG1	1:F:169:ILE:HA	2.45	0.47
1:G:139:GLY:HA3	1:G:267:LEU:HG	1.97	0.47
1:H:162:LEU:HG	1:H:167:MSE:HG3	1.97	0.47
1:G:134:ILE:O	1:G:137:VAL:HG12	2.13	0.47
1:D:206:LEU:O	1:D:210:VAL:HG22	2.15	0.47
1:A:190:LEU:HA	1:A:190:LEU:HD12	1.72	0.47
1:B:93:THR:HG23	1:B:97:CYS:CB	2.44	0.47
1:C:132:ASN:O	1:C:136:THR:HG23	2.14	0.47
1:E:50:ILE:O	1:E:50:ILE:CG1	2.63	0.47
1:F:219:THR:O	3:F:406:NAP:H52N	2.15	0.47
1:H:93:THR:HG23	1:H:97:CYS:HB3	1.97	0.47
1:A:61:ILE:HG22	1:A:63:LEU:HD22	1.97	0.47
1:D:40:HIS:ND1	1:D:40:HIS:N	2.63	0.47
1:G:219:THR:CG2	4:G:508:HOH:O	2.63	0.46
1:D:105:ASN:OD1	1:D:108:LEU:HB2	2.16	0.46
1:A:19:ILE:HA	1:A:281:ALA:HB2	1.97	0.46
1:E:242:LEU:O	3:E:405:NAP:H2N	2.14	0.46
1:G:220:ILE:HA	1:G:221:PRO:HD3	1.76	0.46
1:C:10:ILE:HD12	1:C:61:ILE:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:14:ALA:HA	1:F:17:LEU:HD22	1.97	0.46
1:F:175:ALA:HB1	1:H:175:ALA:HB1	1.97	0.46
1:A:137:VAL:HG11	1:A:172:THR:HB	1.96	0.46
1:B:234:THR:HG23	1:B:236:LYS:HG2	1.98	0.46
1:B:171:ARG:HB2	1:B:171:ARG:NH1	2.31	0.46
1:B:134:ILE:O	1:B:137:VAL:HG23	2.16	0.46
1:E:108:LEU:HA	1:E:111:ILE:HD13	1.97	0.46
1:G:213:ILE:CD1	1:G:216:CYS:HB2	2.46	0.46
1:D:217:ILE:HG22	1:D:242:LEU:HD12	1.98	0.46
1:E:94:PRO:HB2	1:E:96:HIS:CE1	2.50	0.46
1:H:70:GLY:HA2	1:H:107:TYR:HB2	1.97	0.46
1:D:5:LEU:HD11	1:D:292:GLN:CD	2.35	0.46
1:G:134:ILE:HB	1:G:135:PRO:HD3	1.97	0.46
1:H:11:GLY:CA	1:H:76:THR:HG22	2.38	0.46
1:B:10:ILE:HG23	1:B:33:VAL:HG22	1.98	0.46
1:B:196:MSE:CG	1:C:171:ARG:HH21	2.22	0.46
1:B:101:SER:OG	1:B:102:GLY:N	2.46	0.46
1:B:167:MSE:HB3	1:B:167:MSE:HE2	1.88	0.46
1:F:142[A]:MSE:CE	1:H:146:GLN:HE21	2.28	0.46
1:A:252:LYS:H	1:A:252:LYS:HG2	1.45	0.46
1:G:19:ILE:HA	1:G:281:ALA:HB2	1.98	0.46
1:A:244:SER:O	1:A:245:ARG:C	2.54	0.46
1:F:32:LEU:HD13	1:F:45:ALA:HB1	1.98	0.46
1:C:137:VAL:HG11	1:C:172:THR:HB	1.97	0.45
1:H:19:ILE:HA	1:H:281:ALA:HB2	1.96	0.45
1:E:233:MSE:HE2	1:E:259:ILE:HD13	1.99	0.45
1:G:162:LEU:HD22	1:G:193:ILE:HG13	1.97	0.45
1:D:171:ARG:HH11	1:D:171:ARG:HG2	1.80	0.45
1:D:21:ARG:HH11	1:D:42:PHE:HZ	1.64	0.45
1:E:105:ASN:HB3	1:E:108:LEU:HB2	1.98	0.45
1:E:225:LEU:CB	1:E:249:THR:HB	2.47	0.45
1:D:68:THR:HG22	1:D:105:ASN:OD1	2.16	0.45
1:A:71:GLU:HG2	1:A:71:GLU:H	1.33	0.45
1:C:101:SER:OG	1:C:102:GLY:N	2.49	0.45
1:C:223:MSE:HE1	1:C:250:ASP:N	2.32	0.45
1:G:127:ASP:OD1	1:G:128:ILE:N	2.49	0.45
1:B:167:MSE:HE2	1:C:192:ARG:CZ	2.47	0.45
1:H:219:THR:O	3:H:408:NAP:H52N	2.16	0.45
1:D:132:ASN:O	1:D:136:THR:HG22	2.16	0.45
1:A:86:LYS:H	1:A:89:HIS:HD2	1.64	0.45
1:F:167:MSE:HB3	1:F:167:MSE:HE2	1.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:THR:HG21	1:D:107:TYR:CD1	2.50	0.44
1:A:85:LEU:HD12	1:A:89:HIS:HD2	1.81	0.44
1:C:13:ASP:HB2	1:C:15:ARG:HB2	1.99	0.44
1:C:24:THR:HG21	1:C:42:PHE:HB3	1.99	0.44
1:F:245:ARG:H	1:F:245:ARG:CD	2.30	0.44
1:F:203:THR:HG21	3:F:406:NAP:H2A	1.98	0.44
1:E:22:LYS:O	1:E:26:GLN:HG3	2.17	0.44
1:G:20:ILE:HD13	1:G:32:LEU:HD11	1.99	0.44
1:A:181:LYS:HG3	1:A:201:PHE:HE2	1.82	0.44
1:G:158:ALA:HA	1:G:181:LYS:O	2.17	0.44
1:E:128:ILE:O	1:E:132:ASN:HB2	2.17	0.44
1:C:223:MSE:HE1	1:C:250:ASP:H	1.83	0.44
1:H:233:MSE:HE3	1:H:237:THR:CG2	2.48	0.44
1:F:86:LYS:H	1:F:89:HIS:HD2	1.64	0.44
1:C:20:ILE:CD1	1:C:32:LEU:HD11	2.48	0.44
1:G:74:VAL:O	1:G:76:THR:HG23	2.17	0.44
1:F:114:GLN:HE21	1:F:114:GLN:HB2	1.65	0.44
1:G:238:LEU:HG	1:G:240:LEU:HD13	1.99	0.44
1:F:213:ILE:HD11	1:F:216:CYS:HB2	2.00	0.44
1:E:176:LEU:HD13	1:G:176:LEU:HD13	2.00	0.44
1:A:267:LEU:HB2	3:A:401:NAP:O7N	2.17	0.44
1:A:241:ASP:OD2	1:A:249:THR:HG23	2.18	0.44
1:G:125:ARG:NH1	1:G:127:ASP:OD2	2.51	0.44
1:A:8:ALA:HB2	1:A:53:ILE:CD1	2.48	0.44
1:F:171:ARG:CG	1:F:171:ARG:NH1	2.79	0.44
1:H:69:THR:HG23	1:H:73:VAL:O	2.17	0.43
1:B:90:LEU:O	1:B:93:THR:HB	2.17	0.43
1:B:94:PRO:HD2	1:B:97:CYS:HB2	2.00	0.43
1:D:92:ARG:CG	1:D:92:ARG:HH11	2.25	0.43
1:C:171:ARG:CG	1:C:171:ARG:NH1	2.59	0.43
3:A:401:NAP:H1B	4:A:504:HOH:O	2.17	0.43
1:B:264:ALA:O	3:B:402:NAP:N7N	2.51	0.43
1:D:205:GLU:HB2	1:D:209:HIS:HD2	1.82	0.43
1:D:137:VAL:CG1	1:D:169:ILE:HA	2.48	0.43
1:G:93:THR:HG22	1:G:117:ARG:NE	2.20	0.43
1:F:210:VAL:HA	1:F:213:ILE:HG12	2.01	0.43
1:A:225:LEU:HB2	1:A:249:THR:HB	2.00	0.43
1:H:126:ASP:HA	1:H:164:ARG:HH21	1.84	0.43
1:G:233:MSE:CE	1:G:237:THR:HB	2.36	0.43
1:E:10:ILE:HG12	1:E:33:VAL:HG22	2.01	0.43
1:F:68:THR:OG1	1:F:69:THR:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:171:ARG:HG3	1:G:171:ARG:HH11	1.81	0.43
1:C:242:LEU:O	3:C:403:NAP:C2N	2.66	0.43
1:H:24:THR:HG23	1:H:30:ILE:HD12	2.01	0.43
1:F:137:VAL:HG21	1:F:168:THR:HG22	2.01	0.43
1:E:181:LYS:HG3	1:E:201:PHE:CE2	2.53	0.43
1:A:185:ARG:HG2	1:A:186:SER:N	2.33	0.43
1:D:267:LEU:HA	1:D:267:LEU:HD12	1.86	0.43
1:H:161:GLY:O	1:H:166:GLY:HA3	2.18	0.43
1:F:37:GLN:HB2	1:F:78:PHE:C	2.39	0.43
1:E:151:THR:CG2	1:E:153:HIS:O	2.67	0.43
1:G:219:THR:HG23	1:G:219:THR:O	2.17	0.43
1:A:275:THR:O	1:A:279:ILE:HG13	2.19	0.43
1:G:192:ARG:HH21	1:G:195:GLU:CG	2.30	0.43
1:G:101:SER:OG	1:G:102:GLY:N	2.52	0.43
1:H:69:THR:C	1:H:71:GLU:N	2.72	0.43
1:G:160:LEU:O	1:G:219:THR:HG22	2.19	0.43
1:A:165:THR:HG23	3:A:401:NAP:O1N	2.19	0.43
1:A:10:ILE:HD12	1:A:61:ILE:HG23	2.01	0.43
1:A:50:ILE:O	1:A:53:ILE:HG23	2.19	0.43
1:A:213:ILE:HD11	1:A:216:CYS:HB2	2.00	0.43
1:E:142[B]:MSE:HE3	1:G:145:ILE:HB	2.01	0.43
1:B:242:LEU:O	3:B:402:NAP:H2N	2.19	0.43
1:E:210:VAL:O	1:E:211:LYS:C	2.56	0.43
1:E:136:THR:HG22	1:E:268:PRO:HG3	2.00	0.43
1:H:182:VAL:HG13	1:H:193:ILE:CG2	2.49	0.43
1:E:241:ASP:OD2	1:E:249:THR:HG22	2.18	0.43
1:C:139:GLY:HA3	1:C:267:LEU:HG	2.00	0.43
1:F:10:ILE:O	1:F:64:PRO:HD3	2.19	0.43
1:B:93:THR:HG22	1:B:117:ARG:NE	2.25	0.43
1:C:85:LEU:O	1:C:107:TYR:OH	2.33	0.43
1:B:3:THR:HG22	1:B:4:GLY:N	2.34	0.43
1:B:63:LEU:CD2	1:B:99:ILE:HG23	2.49	0.43
1:D:18:GLU:OE1	1:D:21:ARG:NH2	2.51	0.42
1:A:14:ALA:HA	1:A:17:LEU:HD22	2.01	0.42
1:H:133:SER:HB2	1:H:165:THR:HA	2.02	0.42
1:G:151:THR:CG2	1:G:153:HIS:O	2.67	0.42
1:E:15:ARG:NH1	1:E:65:VAL:HG21	2.34	0.42
1:A:132:ASN:O	1:A:135:PRO:HD2	2.19	0.42
1:D:87:GLN:HE22	1:D:111:ILE:HA	1.85	0.42
1:G:168:THR:OG1	1:H:192:ARG:NH2	2.52	0.42
1:H:203:THR:CG2	3:H:408:NAP:H2A	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:VAL:HG22	1:A:193:ILE:CD1	2.50	0.42
1:D:133:SER:HB3	1:D:165:THR:HG22	2.01	0.42
1:G:137:VAL:HG21	1:G:172:THR:HB	2.01	0.42
1:C:190:LEU:HA	1:C:193:ILE:HD12	2.01	0.42
1:F:93:THR:HG22	1:F:117:ARG:NE	2.32	0.42
1:E:49:ASN:C	1:E:51:ASP:H	2.22	0.42
1:C:234:THR:OG1	1:C:235:PRO:HD2	2.19	0.42
1:E:169:ILE:HG21	1:E:217:ILE:HG21	2.00	0.42
1:B:181:LYS:HG3	1:B:201:PHE:HE2	1.83	0.42
1:H:139:GLY:HA2	1:H:271:VAL:HG21	2.01	0.42
1:E:162:LEU:HG	1:E:167:MSE:HG3	2.02	0.42
1:E:123:PHE:HE1	1:E:280:LEU:HD21	1.85	0.42
1:E:50:ILE:HG13	1:E:50:ILE:O	2.19	0.42
1:C:35:PHE:O	1:C:47:LYS:HE2	2.19	0.42
1:A:181:LYS:HG3	1:A:201:PHE:CE2	2.55	0.42
1:E:227:GLN:HG3	1:E:253:TYR:CD1	2.55	0.42
1:H:10:ILE:HG23	1:H:33:VAL:HG22	2.01	0.41
1:F:174:ALA:HB2	1:F:198:LEU:HD11	2.01	0.41
1:C:160:LEU:HB3	1:C:220:ILE:HD12	2.01	0.41
1:H:137:VAL:HG13	1:H:169:ILE:HA	2.03	0.41
1:H:219:THR:HG23	3:H:408:NAP:H52N	2.02	0.41
1:A:85:LEU:HD12	1:A:89:HIS:CD2	2.55	0.41
3:D:404:NAP:H5N	4:D:506:HOH:O	2.19	0.41
1:G:56:GLN:H	1:G:56:GLN:HG3	1.51	0.41
1:B:184:ALA:HB3	1:B:190:LEU:HD13	2.03	0.41
1:D:2:LEU:HA	1:D:292:GLN:NE2	2.36	0.41
1:B:220:ILE:HA	1:B:221:PRO:HD3	1.94	0.41
1:A:2:LEU:HA	1:A:292:GLN:HE22	1.86	0.41
1:H:63:LEU:HB3	1:H:64:PRO:CD	2.50	0.41
1:E:133:SER:HA	1:E:136:THR:CG2	2.39	0.41
1:H:134:ILE:HB	1:H:135:PRO:HD3	2.02	0.41
1:H:15:ARG:HH11	1:H:65:VAL:HG21	1.85	0.41
1:B:56:GLN:HA	1:B:92:ARG:O	2.20	0.41
1:H:160:LEU:HB2	1:H:218:ASN:HA	2.02	0.41
1:C:163:GLY:HA3	3:C:403:NAP:H4B	2.03	0.41
1:E:267:LEU:HD12	1:E:267:LEU:HA	1.90	0.41
1:D:69:THR:OG1	1:D:73:VAL:HG13	2.21	0.41
1:F:139:GLY:HA3	1:F:267:LEU:HG	2.03	0.41
1:H:220:ILE:HD12	1:H:224:ILE:HD13	2.02	0.41
1:C:245:ARG:NE	1:C:245:ARG:H	2.18	0.41
1:A:225:LEU:CB	1:A:249:THR:HB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:ARG:HH21	1:B:195:GLU:CG	2.30	0.41
1:D:93:THR:HG23	1:D:97:CYS:CB	2.51	0.41
1:G:56:GLN:O	1:G:94:PRO:HG3	2.21	0.41
1:F:15:ARG:NH1	1:F:65:VAL:HG21	2.36	0.41
1:B:88:ASP:O	1:B:92:ARG:HG3	2.21	0.41
1:H:133:SER:O	1:H:137:VAL:HG22	2.21	0.40
1:E:125:ARG:NH1	1:E:127:ASP:OD2	2.54	0.40
1:B:287:LEU:HD23	1:B:287:LEU:HA	1.86	0.40
1:D:7:ILE:HD13	1:D:23:LEU:HD13	2.02	0.40
1:F:213:ILE:HD12	1:F:216:CYS:HB2	2.02	0.40
1:B:5:LEU:HD13	1:B:292:GLN:HG3	2.03	0.40
1:E:115:ALA:O	1:E:117:ARG:NH2	2.54	0.40
1:A:171:ARG:NH1	1:A:171:ARG:CG	2.80	0.40
1:E:76:THR:HG21	1:E:83:VAL:HG11	2.02	0.40
1:A:56:GLN:HG3	1:A:56:GLN:H	1.52	0.40
1:A:61:ILE:HG22	1:A:63:LEU:CD2	2.52	0.40
1:B:10:ILE:HG12	1:B:33:VAL:HG13	2.03	0.40
1:D:151:THR:HG23	1:D:153:HIS:HB3	2.02	0.40
1:D:241:ASP:OD2	1:D:249:THR:CG2	2.70	0.40
1:G:159:VAL:HB	1:G:182:VAL:HB	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	296/300 (99%)	282 (95%)	12 (4%)	2 (1%)	26	62
1	B	295/300 (98%)	281 (95%)	14 (5%)	0	100	100
1	C	296/300 (99%)	280 (95%)	15 (5%)	1 (0%)	46	79
1	D	296/300 (99%)	277 (94%)	16 (5%)	3 (1%)	19	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	297/300 (99%)	278 (94%)	17 (6%)	2 (1%)	26	62
1	F	296/300 (99%)	274 (93%)	21 (7%)	1 (0%)	46	79
1	G	296/300 (99%)	277 (94%)	16 (5%)	3 (1%)	19	52
1	H	296/300 (99%)	270 (91%)	24 (8%)	2 (1%)	26	62
All	All	2368/2400 (99%)	2219 (94%)	135 (6%)	14 (1%)	30	65

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	H	67	ALA
1	A	70	GLY
1	C	223	MSE
1	D	110	ASN
1	G	56	GLN
1	G	196	MSE
1	D	71	GLU
1	D	250	ASP
1	E	-1	ASN
1	E	50	ILE
1	G	67	ALA
1	F	223	MSE
1	H	70	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	245/240 (102%)	208 (85%)	37 (15%)	3	10
1	B	244/240 (102%)	205 (84%)	39 (16%)	3	9
1	C	245/240 (102%)	207 (84%)	38 (16%)	3	10
1	D	245/240 (102%)	208 (85%)	37 (15%)	3	10
1	E	246/240 (102%)	207 (84%)	39 (16%)	3	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	245/240 (102%)	205 (84%)	40 (16%)	3	8
1	G	245/240 (102%)	206 (84%)	39 (16%)	3	9
1	H	245/240 (102%)	198 (81%)	47 (19%)	2	5
All	All	1960/1920 (102%)	1644 (84%)	316 (16%)	3	9

All (316) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	15	ARG
1	A	17	LEU
1	A	18	GLU
1	A	23	LEU
1	A	32	LEU
1	A	33	VAL
1	A	36	ASP
1	A	37	GLN
1	A	43	THR
1	A	53	ILE
1	A	56	GLN
1	A	68	THR
1	A	71	GLU
1	A	93	THR
1	A	104	SER
1	A	108	LEU
1	A	136	THR
1	A	137	VAL
1	A	151	THR
1	A	160	LEU
1	A	182	VAL
1	A	185	ARG
1	A	190	LEU
1	A	192	ARG
1	A	194	THR
1	A	195	GLU
1	A	198	LEU
1	A	219	THR
1	A	225	LEU
1	A	227	GLN
1	A	228	THR
1	A	249	THR

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Mol	Chain	Res	Type
1	A	252	LYS
1	A	255	GLU
1	A	267	LEU
1	A	278	GLN
1	B	2	LEU
1	B	3	THR
1	B	6	LYS
1	B	13	ASP
1	B	17	LEU
1	B	25	GLU
1	B	33	VAL
1	B	37	GLN
1	B	38	LEU
1	B	39	ASP
1	B	46	VAL
1	B	53	ILE
1	B	56	GLN
1	B	58	ILE
1	B	93	THR
1	B	104	SER
1	B	108	LEU
1	B	114	GLN
1	B	116	LYS
1	B	136	THR
1	B	137	VAL
1	B	151	THR
1	B	160	LEU
1	B	167	MSE
1	B	171	ARG
1	B	176	LEU
1	B	182	VAL
1	B	190	LEU
1	B	195	GLU
1	B	198	LEU
1	B	222	SER
1	B	224	ILE
1	B	225	LEU
1	B	228	THR
1	B	236	LYS
1	B	263	LEU
1	B	267	LEU
1	B	271	VAL

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Mol	Chain	Res	Type
1	B	274	LYS
1	C	2	LEU
1	C	15	ARG
1	C	17	LEU
1	C	33	VAL
1	C	46	VAL
1	C	58	ILE
1	C	63	LEU
1	C	68	THR
1	C	73	VAL
1	C	77	VAL
1	C	93	THR
1	C	105	ASN
1	C	108	LEU
1	C	109	GLU
1	C	136	THR
1	C	137	VAL
1	C	151	THR
1	C	160	LEU
1	C	167	MSE
1	C	171	ARG
1	C	176	LEU
1	C	182	VAL
1	C	187	SER
1	C	190	LEU
1	C	194	THR
1	C	195	GLU
1	C	198	LEU
1	C	213	ILE
1	C	219	THR
1	C	225	LEU
1	C	228	THR
1	C	240	LEU
1	C	244	SER
1	C	245	ARG
1	C	263	LEU
1	C	267	LEU
1	C	274	LYS
1	C	278	GLN
1	D	13	ASP
1	D	33	VAL
1	D	36	ASP

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Mol	Chain	Res	Type
1	D	37	GLN
1	D	38	LEU
1	D	40	HIS
1	D	51	ASP
1	D	56	GLN
1	D	63	LEU
1	D	68	THR
1	D	73	VAL
1	D	75	SER
1	D	82	GLU
1	D	92	ARG
1	D	93	THR
1	D	108	LEU
1	D	136	THR
1	D	137	VAL
1	D	151	THR
1	D	160	LEU
1	D	190	LEU
1	D	194	THR
1	D	195	GLU
1	D	198	LEU
1	D	222	SER
1	D	225	LEU
1	D	228	THR
1	D	231	SER
1	D	240	LEU
1	D	244	SER
1	D	249	THR
1	D	252	LYS
1	D	263	LEU
1	D	267	LEU
1	D	274	LYS
1	D	286	LYS
1	D	292	GLN
1	E	3	THR
1	E	13	ASP
1	E	17	LEU
1	E	21	ARG
1	E	24	THR
1	E	37	GLN
1	E	56	GLN
1	E	68	THR

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Mol	Chain	Res	Type
1	E	73	VAL
1	E	77	VAL
1	E	82	GLU
1	E	83	VAL
1	E	93	THR
1	E	108	LEU
1	E	111	ILE
1	E	114	GLN
1	E	116	LYS
1	E	117	ARG
1	E	136	THR
1	E	137	VAL
1	E	151	THR
1	E	160	LEU
1	E	171	ARG
1	E	176	LEU
1	E	182	VAL
1	E	190	LEU
1	E	195	GLU
1	E	198	LEU
1	E	203	THR
1	E	222	SER
1	E	224	ILE
1	E	225	LEU
1	E	245	ARG
1	E	249	THR
1	E	252	LYS
1	E	256	LYS
1	E	263	LEU
1	E	267	LEU
1	E	274	LYS
1	F	5	LEU
1	F	17	LEU
1	F	18	GLU
1	F	33	VAL
1	F	43	THR
1	F	53	ILE
1	F	56	GLN
1	F	68	THR
1	F	73	VAL
1	F	75	SER
1	F	81	GLU

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Mol	Chain	Res	Type
1	F	93	THR
1	F	104	SER
1	F	108	LEU
1	F	114	GLN
1	F	120	VAL
1	F	136	THR
1	F	137	VAL
1	F	151	THR
1	F	160	LEU
1	F	167	MSE
1	F	171	ARG
1	F	176	LEU
1	F	182	VAL
1	F	190	LEU
1	F	194	THR
1	F	195	GLU
1	F	198	LEU
1	F	219	THR
1	F	225	LEU
1	F	227	GLN
1	F	234	THR
1	F	237	THR
1	F	240	LEU
1	F	245	ARG
1	F	255	GLU
1	F	263	LEU
1	F	267	LEU
1	F	274	LYS
1	F	294	GLU
1	G	2	LEU
1	G	15	ARG
1	G	17	LEU
1	G	18	GLU
1	G	33	VAL
1	G	36	ASP
1	G	46	VAL
1	G	56	GLN
1	G	66	SER
1	G	81	GLU
1	G	84	VAL
1	G	93	THR
1	G	104	SER

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Mol	Chain	Res	Type
1	G	108	LEU
1	G	136	THR
1	G	142[A]	MSE
1	G	142[B]	MSE
1	G	151	THR
1	G	160	LEU
1	G	176	LEU
1	G	182	VAL
1	G	185	ARG
1	G	190	LEU
1	G	194	THR
1	G	198	LEU
1	G	219	THR
1	G	225	LEU
1	G	227	GLN
1	G	231	SER
1	G	232	SER
1	G	240	LEU
1	G	244	SER
1	G	252	LYS
1	G	260	LYS
1	G	263	LEU
1	G	267	LEU
1	G	271	VAL
1	G	274	LYS
1	G	278	GLN
1	H	2	LEU
1	H	6	LYS
1	H	15	ARG
1	H	17	LEU
1	H	18	GLU
1	H	33	VAL
1	H	37	GLN
1	H	47	LYS
1	H	51	ASP
1	H	53	ILE
1	H	56	GLN
1	H	58	ILE
1	H	60	SER
1	H	66	SER
1	H	68	THR
1	H	71	GLU

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Mol	Chain	Res	Type
1	H	91	ASP
1	H	92	ARG
1	H	93	THR
1	H	103	ILE
1	H	105	ASN
1	H	108	LEU
1	H	124	GLU
1	H	133	SER
1	H	136	THR
1	H	137	VAL
1	H	146	GLN
1	H	151	THR
1	H	160	LEU
1	H	162	LEU
1	H	176	LEU
1	H	182	VAL
1	H	185	ARG
1	H	190	LEU
1	H	192	ARG
1	H	194	THR
1	H	198	LEU
1	H	219	THR
1	H	225	LEU
1	H	228	THR
1	H	236	LYS
1	H	240	LEU
1	H	244	SER
1	H	256	LYS
1	H	267	LEU
1	H	274	LYS
1	H	286	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	89	HIS
1	A	114	GLN
1	A	132	ASN
1	A	227	GLN
1	A	292	GLN
1	B	49	ASN

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Mol	Chain	Res	Type
1	B	57	GLN
1	B	89	HIS
1	B	105	ASN
1	B	114	GLN
1	B	146	GLN
1	B	189	HIS
1	C	37	GLN
1	C	49	ASN
1	C	105	ASN
1	C	146	GLN
1	C	209	HIS
1	C	227	GLN
1	D	37	GLN
1	D	57	GLN
1	D	87	GLN
1	D	209	HIS
1	D	292	GLN
1	E	26	GLN
1	E	87	GLN
1	E	96	HIS
1	E	146	GLN
1	E	209	HIS
1	E	278	GLN
1	E	292	GLN
1	F	37	GLN
1	F	49	ASN
1	F	89	HIS
1	F	114	GLN
1	F	146	GLN
1	F	227	GLN
1	F	257	GLN
1	F	292	GLN
1	G	80	ASN
1	G	227	GLN
1	H	27	GLN
1	H	37	GLN
1	H	56	GLN
1	H	105	ASN
1	H	146	GLN

### 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 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 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$
3	NAP	A	401	-	42,52,52	1.63	3 (7%)	54,80,80	1.80	4 (7%)
3	NAP	B	402	-	42,52,52	1.68	4 (9%)	54,80,80	1.92	8 (14%)
3	NAP	C	403	-	42,52,52	1.62	4 (9%)	54,80,80	2.04	2 (3%)
3	NAP	D	404	-	42,52,52	1.69	3 (7%)	54,80,80	1.80	3 (5%)
3	NAP	E	405	-	42,52,52	1.60	4 (9%)	54,80,80	2.01	4 (7%)
3	NAP	F	406	-	42,52,52	1.60	3 (7%)	54,80,80	1.99	5 (9%)
3	NAP	G	407	-	42,52,52	1.63	3 (7%)	54,80,80	1.95	7 (12%)
3	NAP	H	408	-	42,52,52	1.67	3 (7%)	54,80,80	1.87	7 (12%)

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
3	NAP	A	401	-	-	0/27/67/67	0/5/5/5
3	NAP	B	402	-	-	0/27/67/67	0/5/5/5
3	NAP	C	403	-	-	0/27/67/67	0/5/5/5
3	NAP	D	404	-	-	0/27/67/67	0/5/5/5
3	NAP	E	405	-	-	0/27/67/67	0/5/5/5
3	NAP	F	406	-	-	0/27/67/67	0/5/5/5
3	NAP	G	407	-	-	0/27/67/67	0/5/5/5
3	NAP	H	408	-	-	0/27/67/67	0/5/5/5

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	403	NAP	O4B-C4B	-2.03	1.40	1.45
3	B	402	NAP	O4B-C4B	-2.02	1.40	1.45
3	E	405	NAP	O4D-C1D	2.17	1.43	1.41
3	H	408	NAP	C2A-N1A	2.62	1.38	1.33
3	A	401	NAP	C2A-N1A	2.78	1.39	1.33
3	B	402	NAP	C2A-N1A	2.91	1.39	1.33
3	F	406	NAP	C2A-N1A	2.93	1.39	1.33
3	E	405	NAP	C2A-N1A	2.95	1.39	1.33
3	C	403	NAP	C2A-N1A	2.99	1.39	1.33
3	G	407	NAP	C2A-N1A	3.08	1.39	1.33
3	D	404	NAP	C2A-N1A	3.16	1.39	1.33
3	E	405	NAP	C2A-N3A	3.48	1.38	1.32
3	H	408	NAP	C2A-N3A	3.82	1.39	1.32
3	D	404	NAP	C2A-N3A	3.95	1.39	1.32
3	A	401	NAP	C2A-N3A	3.95	1.39	1.32
3	C	403	NAP	C2A-N3A	4.04	1.39	1.32
3	B	402	NAP	C2A-N3A	4.11	1.39	1.32
3	G	407	NAP	C2A-N3A	4.15	1.39	1.32
3	F	406	NAP	C2A-N3A	4.28	1.39	1.32
3	F	406	NAP	O7N-C7N	7.51	1.40	1.24
3	E	405	NAP	O7N-C7N	7.58	1.40	1.24
3	A	401	NAP	O7N-C7N	7.62	1.40	1.24
3	G	407	NAP	O7N-C7N	7.66	1.40	1.24
3	C	403	NAP	O7N-C7N	7.70	1.40	1.24
3	B	402	NAP	O7N-C7N	8.09	1.41	1.24
3	H	408	NAP	O7N-C7N	8.10	1.41	1.24
3	D	404	NAP	O7N-C7N	8.41	1.42	1.24

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	403	NAP	N3A-C2A-N1A	-13.11	118.86	128.89
3	F	406	NAP	N3A-C2A-N1A	-12.22	119.53	128.89
3	G	407	NAP	N3A-C2A-N1A	-11.36	120.19	128.89
3	B	402	NAP	N3A-C2A-N1A	-11.35	120.20	128.89
3	D	404	NAP	N3A-C2A-N1A	-11.34	120.21	128.89
3	E	405	NAP	N3A-C2A-N1A	-11.23	120.29	128.89
3	A	401	NAP	N3A-C2A-N1A	-10.90	120.55	128.89
3	H	408	NAP	N3A-C2A-N1A	-10.39	120.94	128.89
3	H	408	NAP	O7N-C7N-N7N	-3.02	118.34	122.59
3	G	407	NAP	C1B-N9A-C4A	-2.83	122.67	126.94
3	G	407	NAP	C4N-C3N-C7N	-2.74	113.85	121.09
3	B	402	NAP	C1B-N9A-C4A	-2.57	123.06	126.94
3	A	401	NAP	PN-O3-PA	-2.45	125.85	132.73
3	D	404	NAP	C1B-N9A-C4A	-2.44	123.26	126.94
3	B	402	NAP	PN-O3-PA	-2.42	125.94	132.73
3	G	407	NAP	O2B-C2B-C1B	-2.21	101.41	110.02
3	A	401	NAP	O7N-C7N-N7N	-2.16	119.55	122.59
3	H	408	NAP	O3D-C3D-C2D	-2.13	104.89	111.83
3	F	406	NAP	C1B-N9A-C4A	-2.10	123.78	126.94
3	F	406	NAP	C3N-C7N-N7N	2.01	120.02	117.82
3	B	402	NAP	O2N-PN-O1N	2.02	123.46	112.53
3	G	407	NAP	O2N-PN-O1N	2.04	123.57	112.53
3	H	408	NAP	C2D-C3D-C4D	2.04	106.81	102.61
3	B	402	NAP	C2B-C3B-C4B	2.06	106.72	101.85
3	B	402	NAP	C4D-O4D-C1D	2.07	111.99	109.72
3	F	406	NAP	O3X-P2B-O2X	2.16	115.59	107.38
3	E	405	NAP	C3N-C7N-N7N	2.17	120.19	117.82
3	D	404	NAP	C2B-C3B-C4B	2.19	107.03	101.85
3	G	407	NAP	O3-PA-O5B	2.35	109.17	102.94
3	E	405	NAP	O3-PA-O5B	2.41	109.33	102.94
3	B	402	NAP	O3-PN-O5D	2.43	109.38	102.94
3	C	403	NAP	O2A-PA-O3	2.46	116.27	105.09
3	F	406	NAP	O5D-C5D-C4D	2.47	118.24	109.12
3	H	408	NAP	O5D-C5D-C4D	2.48	118.27	109.12
3	B	402	NAP	O4D-C1D-N1N	2.86	111.28	108.13
3	A	401	NAP	C3N-C7N-N7N	3.19	121.30	117.82
3	H	408	NAP	O4D-C1D-N1N	3.28	111.74	108.13
3	H	408	NAP	O7N-C7N-C3N	3.60	123.52	119.59
3	G	407	NAP	O4D-C1D-N1N	4.15	112.69	108.13
3	E	405	NAP	O4D-C1D-N1N	5.75	114.45	108.13

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

8 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	NAP	5	0
3	B	402	NAP	4	0
3	C	403	NAP	3	0
3	D	404	NAP	4	0
3	E	405	NAP	1	0
3	F	406	NAP	4	0
3	G	407	NAP	3	0
3	H	408	NAP	5	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	291/300 (97%)	-0.33	0 100 100	19, 32, 50, 59	0
1	B	290/300 (96%)	-0.12	1 (0%) 94 92	22, 39, 57, 65	0
1	C	291/300 (97%)	-0.30	0 100 100	18, 28, 42, 50	0
1	D	291/300 (97%)	0.05	4 (1%) 78 69	19, 41, 60, 63	0
1	E	292/300 (97%)	0.10	7 (2%) 62 50	20, 42, 59, 64	0
1	F	291/300 (97%)	-0.14	3 (1%) 84 77	17, 33, 46, 50	0
1	G	291/300 (97%)	-0.32	1 (0%) 94 92	18, 28, 43, 50	0
1	H	291/300 (97%)	-0.26	2 (0%) 89 84	15, 30, 45, 56	0
All	All	2328/2400 (97%)	-0.17	18 (0%) 87 81	15, 34, 55, 65	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	90	LEU	4.4
1	E	0	ALA	3.2
1	G	-1	ASN	3.2
1	B	0	ALA	3.1
1	E	106	ALA	3.0
1	F	70	GLY	3.0
1	D	293	ALA	3.0
1	H	-1	ASN	2.8
1	E	-2	SER	2.8
1	E	258	GLY	2.7
1	E	293	ALA	2.6
1	D	111	ILE	2.6
1	D	-1	ASN	2.4
1	F	71	GLU	2.2
1	E	31	TYR	2.2
1	F	113	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	107	TYR	2.2
1	E	253	TYR	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	NAP	H	408	48/48	0.96	0.18	1.31	43,51,66,67	0
3	NAP	E	405	48/48	0.91	0.20	1.25	65,71,80,81	0
3	NAP	A	401	48/48	0.95	0.16	0.86	53,59,61,62	0
3	NAP	D	404	48/48	0.96	0.15	0.33	48,58,65,67	0
3	NAP	F	406	48/48	0.94	0.15	0.10	62,67,71,72	0
3	NAP	B	402	48/48	0.95	0.15	-0.00	52,60,67,67	0
3	NAP	C	403	48/48	0.96	0.13	-0.46	44,50,55,55	0
3	NAP	G	407	48/48	0.97	0.12	-0.91	42,54,58,59	0
2	CL	H	509	1/1	0.96	0.08	-4.20	42,42,42,42	0
2	CL	E	505	1/1	0.96	0.12	-	44,44,44,44	0
2	CL	D	504	1/1	0.95	0.13	-	39,39,39,39	0
2	CL	G	507	1/1	0.97	0.14	-	51,51,51,51	0
2	CL	A	501	1/1	0.94	0.09	-	44,44,44,44	0
2	CL	H	508	1/1	0.98	0.14	-	37,37,37,37	0
2	CL	B	502	1/1	0.90	0.12	-	46,46,46,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.