



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:41 am GMT

PDB ID : 1QPN  
Title : Quinolinate Phosphoribosyl Transferase from Mycobacterium Tuberculosis in Complex with NCNN  
Authors : Sharma, V.; Grubmeyer, C.; Sacchettini, J.C.; TB Structural Genomics Consortium (TBSGC)  
Deposited on : 1998-11-20  
Resolution : 2.60 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

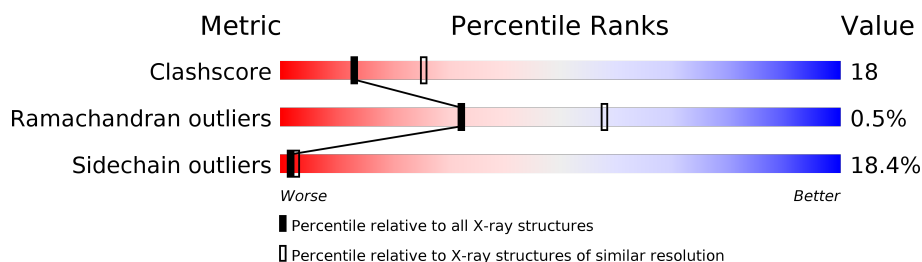
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	284	
1	B	284	
1	C	284	
1	D	284	
1	E	284	
1	F	284	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NCN	C	2905	-	-	X	-
2	NCN	F	2906	-	-	X	-

## 2 Entry composition [i](#)

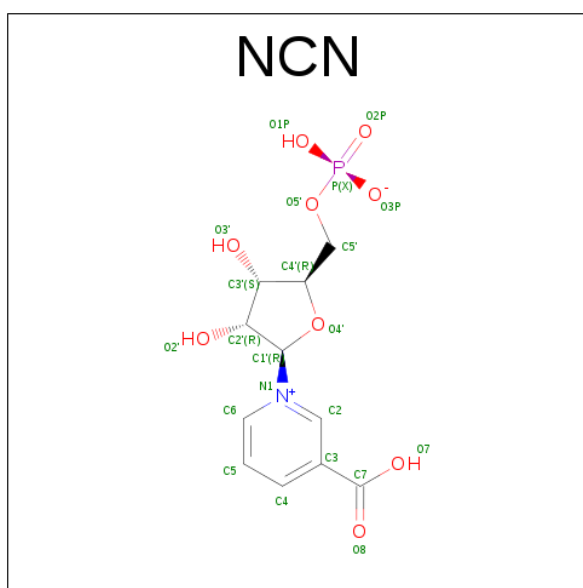
There are 3 unique types of molecules in this entry. The entry contains 12965 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (QUINOLINATE PHOSPHORIBOSYL TRANSFERASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2095	1301	378	411	5			
1	B	284	Total	C	N	O	S	0	0	0
			2095	1301	378	411	5			
1	C	284	Total	C	N	O	S	0	0	0
			2095	1301	378	411	5			
1	D	284	Total	C	N	O	S	0	0	0
			2095	1301	378	411	5			
1	E	284	Total	C	N	O	S	0	0	0
			2095	1301	378	411	5			
1	F	284	Total	C	N	O	S	0	0	0
			2095	1301	378	411	5			

- Molecule 2 is NICOTINATE MONONUCLEOTIDE (three-letter code: NCN) (formula:  $C_{11}H_{14}NO_9P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	11	1	9	1		
2	B	1	Total	C	N	O	P	0	0
			22	11	1	9	1		
2	E	1	Total	C	N	O	P	0	0
			22	11	1	9	1		
2	D	1	Total	C	N	O	P	0	0
			22	11	1	9	1		
2	C	1	Total	C	N	O	P	0	0
			22	11	1	9	1		
2	F	1	Total	C	N	O	P	0	0
			22	11	1	9	1		

- Molecule 3 is water.

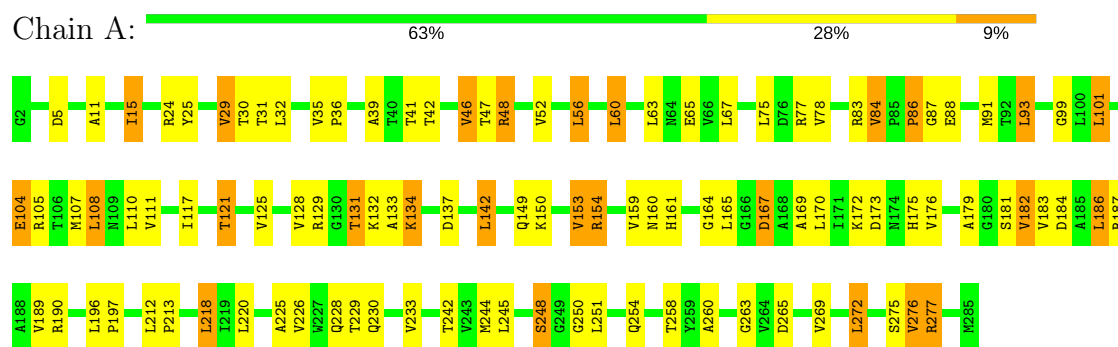
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	46	Total	O	0	0
			46	46		
3	B	48	Total	O	0	0
			48	48		
3	C	54	Total	O	0	0
			54	54		
3	D	40	Total	O	0	0
			40	40		
3	E	45	Total	O	0	0
			45	45		
3	F	30	Total	O	0	0
			30	30		

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

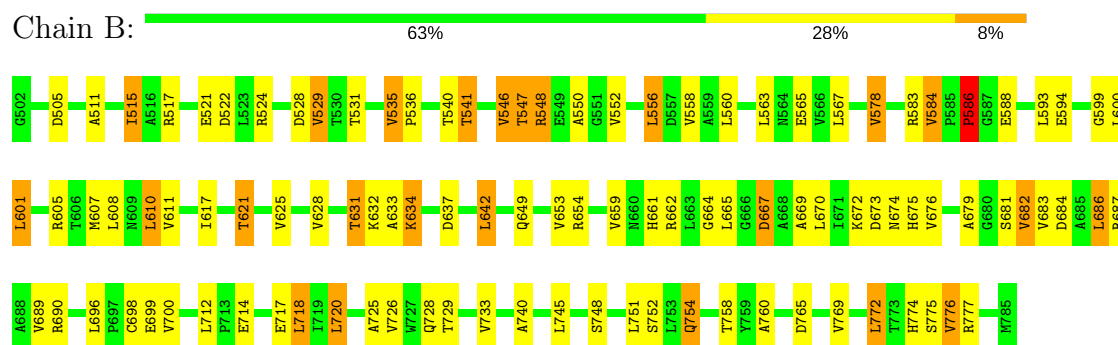
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

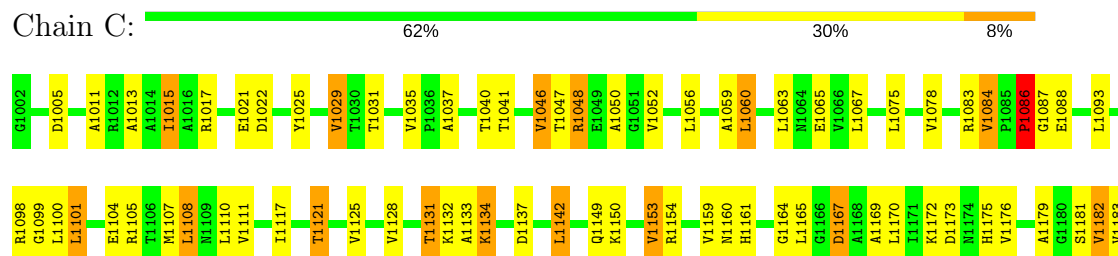
#### • Molecule 1: PROTEIN (QUINOLINATE PHOSPHORIBOSYL TRANSFERASE)



#### • Molecule 1: PROTEIN (QUINOLINATE PHOSPHORIBOSYL TRANSFERASE)



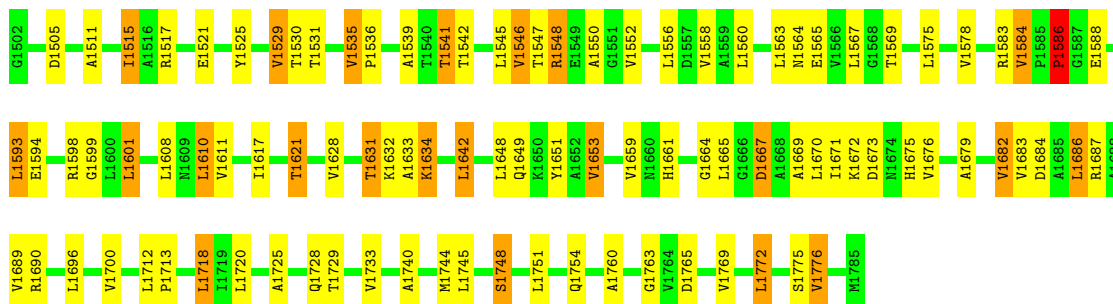
#### • Molecule 1: PROTEIN (QUINOLINATE PHOSPHORIBOSYL TRANSFERASE)





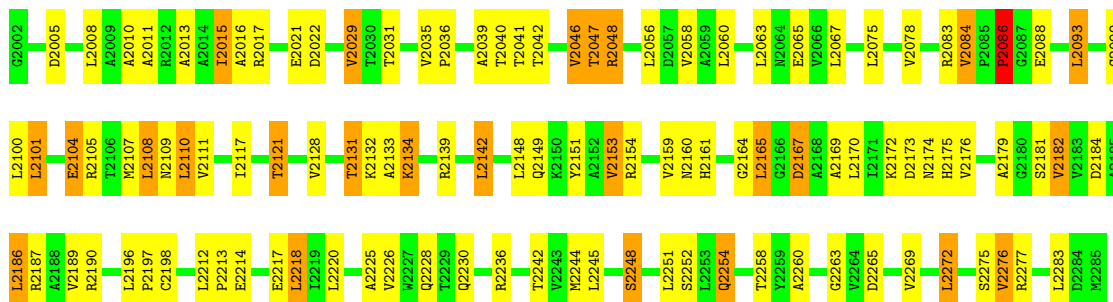
- Molecule 1: PROTEIN (QUINOLINATE PHOSPHORIBOSYL TRANSFERASE)

Chain D:  66% 26% 8%



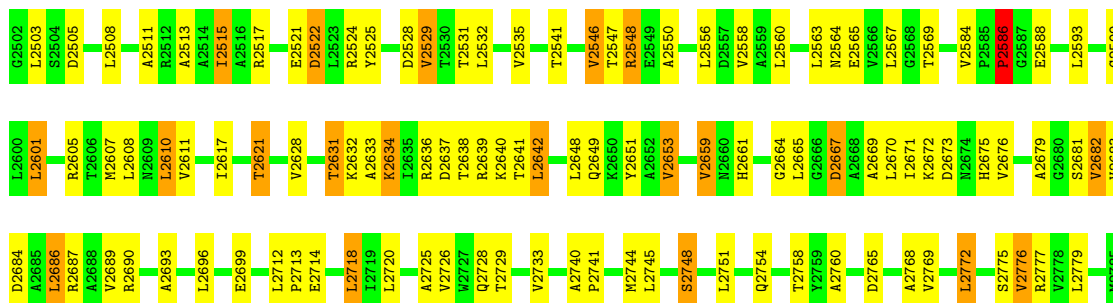
- Molecule 1: PROTEIN (QUINOLINATE PHOSPHORIBOSYL TRANSFERASE)

Chain E:  61% 30% 9%



- Molecule 1: PROTEIN (QUINOLINATE PHOSPHORIBOSYL TRANSFERASE)

Chain F:  62% 31% 7%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.38Å 100.38Å 144.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.60	Depositor
% Data completeness (in resolution range)	96.3 (8.00-2.60)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.185 , 0.269	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12965	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP



## 5 Model quality

### 5.1 Standard geometry

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

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	0.70	0/2120	0.89	2/2891 (0.1%)
1	B	0.71	0/2120	0.91	2/2891 (0.1%)
1	C	0.73	0/2120	0.88	1/2891 (0.0%)
1	D	0.69	0/2120	0.89	2/2891 (0.1%)
1	E	0.70	0/2120	0.89	1/2891 (0.0%)
1	F	0.69	0/2120	0.89	1/2891 (0.0%)
All	All	0.70	0/12720	0.89	9/17346 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1718	LEU	CA-CB-CG	7.92	133.51	115.30
1	F	2718	LEU	CA-CB-CG	7.90	133.47	115.30
1	B	718	LEU	CA-CB-CG	7.38	132.27	115.30
1	C	1218	LEU	CA-CB-CG	6.93	131.23	115.30
1	A	154	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	E	2218	LEU	CA-CB-CG	6.68	130.68	115.30
1	A	218	LEU	CA-CB-CG	5.59	128.17	115.30
1	D	1545	LEU	N-CA-C	-5.49	96.17	111.00
1	B	654	ARG	NE-CZ-NH2	-5.45	117.57	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	1525	TYR	Sidechain

## 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	2095	0	2135	81	0
1	B	2095	0	2135	79	0
1	C	2095	0	2135	87	0
1	D	2095	0	2135	70	0
1	E	2095	0	2135	87	0
1	F	2095	0	2135	84	0
2	A	22	0	12	5	0
2	B	22	0	12	6	0
2	C	22	0	12	8	0
2	D	22	0	12	6	0
2	E	22	0	12	6	0
2	F	22	0	12	7	0
3	A	46	0	0	5	0
3	B	48	0	0	2	0
3	C	54	0	0	5	0
3	D	40	0	0	1	0
3	E	45	0	0	3	0
3	F	30	0	0	2	0
All	All	12965	0	12882	465	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 18.

All (465) 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:E:2903:NCN:H2	3:E:3006:HOH:O	1.57	1.04
1:F:2661:HIS:ND1	2:F:2906:NCN:H4	1.75	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1748:SER:OG	2:D:2904:NCN:H3'	1.62	0.97
1:A:248:SER:OG	2:A:2901:NCN:H3'	1.65	0.96
1:E:2248:SER:OG	2:E:2903:NCN:H3'	1.66	0.94
1:A:67:LEU:HD21	1:A:99:GLY:HA3	1.50	0.93
1:A:131:THR:HG21	1:A:260:ALA:HB1	1.50	0.93
2:C:2905:NCN:H2	3:C:3005:HOH:O	1.68	0.92
1:E:2131:THR:HG21	1:E:2260:ALA:HB1	1.53	0.91
1:A:225:ALA:H	1:A:228:GLN:HE21	1.18	0.89
1:C:1248:SER:OG	2:C:2905:NCN:H3'	1.72	0.89
2:A:2901:NCN:H2	3:A:3014:HOH:O	1.71	0.89
1:D:1631:THR:HG21	1:D:1760:ALA:HB1	1.52	0.89
2:B:2902:NCN:H2	3:B:3031:HOH:O	1.72	0.89
1:D:1567:LEU:HD21	1:D:1599:GLY:HA3	1.51	0.88
1:B:725:ALA:H	1:B:728:GLN:HE21	1.17	0.88
1:B:631:THR:HG21	1:B:760:ALA:HB1	1.54	0.88
1:F:2748:SER:OG	2:F:2906:NCN:H3'	1.73	0.87
1:F:2725:ALA:H	1:F:2728:GLN:HE21	1.18	0.87
1:A:84:VAL:HG22	1:A:88:GLU:HG2	1.56	0.85
1:B:567:LEU:HD21	1:B:599:GLY:HA3	1.57	0.84
1:C:1225:ALA:H	1:C:1228:GLN:HE21	1.25	0.84
1:E:2067:LEU:HD21	1:E:2099:GLY:HA3	1.60	0.83
1:B:748:SER:OG	2:B:2902:NCN:H3'	1.78	0.83
1:D:1621:THR:HG21	1:D:1653:VAL:HA	1.61	0.83
1:B:584:VAL:HG22	1:B:588:GLU:HG2	1.62	0.82
1:B:725:ALA:H	1:B:728:GLN:NE2	1.77	0.82
1:C:1276:VAL:O	1:D:1775:SER:HA	1.79	0.82
1:D:1748:SER:HG	2:D:2904:NCN:H6	1.45	0.80
1:A:225:ALA:H	1:A:228:GLN:NE2	1.79	0.80
2:D:2904:NCN:H2	3:D:3008:HOH:O	1.83	0.79
1:F:2725:ALA:H	1:F:2728:GLN:NE2	1.80	0.78
1:E:2248:SER:OG	2:E:2903:NCN:H6	1.82	0.78
1:B:632:LYS:O	1:B:634:LYS:HE2	1.83	0.78
1:A:276:VAL:O	1:B:775:SER:HA	1.83	0.78
1:D:1725:ALA:H	1:D:1728:GLN:HE21	1.29	0.78
1:C:1132:LYS:O	1:C:1134:LYS:HE2	1.85	0.77
1:A:161:HIS:ND1	2:A:2901:NCN:H4	1.99	0.77
1:A:186:LEU:HD22	1:A:187:ARG:HH21	1.51	0.76
1:D:1661:HIS:ND1	2:D:2904:NCN:H4	2.02	0.75
1:F:2531:THR:HG22	1:F:2601:LEU:HD23	1.69	0.75
1:C:1161:HIS:ND1	2:C:2905:NCN:H4	2.03	0.74
1:F:2515:ILE:HD11	1:F:2565:GLU:HG2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:VAL:HB	1:A:272:LEU:HD22	1.68	0.74
1:B:686:LEU:HD22	1:B:687:ARG:HH21	1.53	0.74
1:C:1161:HIS:HD1	2:C:2905:NCN:H4	1.52	0.74
1:D:1672:LYS:H	1:D:1675:HIS:HD2	1.36	0.74
1:D:1515:ILE:HD11	1:D:1565:GLU:HG2	1.70	0.73
1:E:2225:ALA:H	1:E:2228:GLN:NE2	1.85	0.73
1:C:1186:LEU:HD22	1:C:1187:ARG:HH21	1.52	0.73
1:E:2121:THR:HG21	1:E:2153:VAL:HA	1.70	0.73
1:E:2275:SER:HA	1:F:2776:VAL:O	1.89	0.73
1:E:2132:LYS:O	1:E:2134:LYS:HE2	1.88	0.73
1:D:1748:SER:OG	2:D:2904:NCN:H6	1.89	0.72
1:C:1117:ILE:O	1:C:1121:THR:HG23	1.89	0.72
1:F:2503:LEU:HB2	1:F:2508:LEU:HD13	1.71	0.72
1:D:1725:ALA:H	1:D:1728:GLN:NE2	1.88	0.71
1:D:1634:LYS:HE3	1:D:1765:ASP:O	1.90	0.71
1:B:672:LYS:H	1:B:675:HIS:CD2	2.08	0.71
1:D:1632:LYS:O	1:D:1634:LYS:HE2	1.89	0.71
1:F:2632:LYS:O	1:F:2634:LYS:HE2	1.91	0.71
1:D:1672:LYS:H	1:D:1675:HIS:CD2	2.07	0.71
1:E:2128:VAL:O	1:E:2131:THR:HB	1.90	0.71
1:E:2134:LYS:HE3	1:E:2265:ASP:O	1.90	0.71
1:E:2225:ALA:H	1:E:2228:GLN:HE21	1.37	0.70
1:D:1661:HIS:CE1	2:D:2904:NCN:H4	2.26	0.70
1:A:186:LEU:HD22	1:A:187:ARG:NH2	2.05	0.70
1:E:2084:VAL:HG22	1:E:2088:GLU:HG2	1.74	0.70
1:E:2031:THR:HG22	1:E:2101:LEU:HD23	1.72	0.70
1:C:1218:LEU:HD23	1:C:1244:MET:HB2	1.74	0.70
1:C:1186:LEU:HD22	1:C:1187:ARG:NH2	2.06	0.70
1:F:2567:LEU:HD21	1:F:2599:GLY:HA3	1.74	0.70
1:C:1225:ALA:H	1:C:1228:GLN:NE2	1.90	0.69
1:D:1584:VAL:HG22	1:D:1588:GLU:HG2	1.74	0.69
1:C:1196:LEU:CD2	1:D:1529:VAL:HG11	2.22	0.69
1:F:2628:VAL:O	1:F:2631:THR:HB	1.93	0.68
1:E:2015:ILE:HD11	1:E:2065:GLU:HG2	1.74	0.68
1:B:672:LYS:H	1:B:675:HIS:HD2	1.39	0.68
1:F:2686:LEU:HD22	1:F:2687:ARG:NH2	2.09	0.68
1:D:1558:VAL:HG11	1:D:1610:LEU:HG	1.76	0.67
1:F:2686:LEU:HD22	1:F:2687:ARG:HH21	1.58	0.67
1:F:2631:THR:HG21	1:F:2760:ALA:HB1	1.76	0.67
1:B:686:LEU:HD22	1:B:687:ARG:NH2	2.10	0.67
1:E:2161:HIS:ND1	2:E:2903:NCN:H4	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:VAL:HG22	1:B:548:ARG:HH21	1.59	0.67
1:F:2676:VAL:HG22	1:F:2682:VAL:HA	1.76	0.67
1:A:132:LYS:O	1:A:134:LYS:HE2	1.94	0.67
1:C:1067:LEU:HD21	1:C:1099:GLY:HA3	1.77	0.66
1:B:676:VAL:HG13	1:B:682:VAL:N	2.10	0.66
1:A:31:THR:HG22	1:A:101:LEU:HD23	1.78	0.66
1:A:196:LEU:CD2	1:B:529:VAL:HG11	2.26	0.66
1:E:2196:LEU:CD2	1:F:2529:VAL:HG11	2.26	0.66
1:E:2029:VAL:HG11	1:F:2696:LEU:HD21	1.77	0.66
1:E:2276:VAL:O	1:F:2775:SER:HA	1.96	0.65
1:E:2029:VAL:HG11	1:F:2696:LEU:CD2	2.26	0.65
1:C:1186:LEU:O	1:C:1190:ARG:HG2	1.97	0.65
1:F:2621:THR:HG21	1:F:2653:VAL:HA	1.77	0.65
1:A:46:VAL:HG22	1:A:48:ARG:HH21	1.62	0.65
1:C:1187:ARG:HH22	1:C:1190:ARG:HE	1.44	0.64
1:A:83:ARG:HD3	3:A:3082:HOH:O	1.96	0.64
1:C:1084:VAL:HG22	1:C:1088:GLU:HG2	1.79	0.64
1:C:1029:VAL:HG11	1:D:1696:LEU:CD2	2.27	0.64
1:C:1050:ALA:HB2	1:C:1086:PRO:HD3	1.78	0.64
1:F:2661:HIS:CE1	2:F:2906:NCN:H4	2.33	0.64
1:B:531:THR:HG22	1:B:601:LEU:HD23	1.79	0.63
1:B:725:ALA:N	1:B:728:GLN:HE21	1.95	0.63
1:B:748:SER:OG	2:B:2902:NCN:H6	1.99	0.63
1:C:1011:ALA:O	1:C:1015:ILE:HG23	1.98	0.63
1:A:172:LYS:H	1:A:175:HIS:HD2	1.45	0.63
1:C:1015:ILE:HD11	1:C:1065:GLU:HG2	1.78	0.63
1:C:1121:THR:HG22	1:C:1272:LEU:HG	1.80	0.63
1:C:1275:SER:HA	1:D:1776:VAL:O	1.98	0.63
1:A:87:GLY:HA3	1:E:2230:GLN:HB3	1.81	0.63
1:C:1017:ARG:NH1	1:D:1517:ARG:HD3	2.14	0.63
1:D:1676:VAL:HG22	1:D:1682:VAL:HA	1.80	0.63
1:F:2676:VAL:HG13	1:F:2682:VAL:N	2.14	0.63
1:E:2161:HIS:HD1	2:E:2903:NCN:H4	1.63	0.62
1:E:2104:GLU:HG3	1:E:2283:LEU:HD23	1.81	0.62
1:C:1131:THR:HG23	1:C:1133:ALA:H	1.65	0.62
1:A:15:ILE:HD11	1:A:65:GLU:HG2	1.81	0.62
1:A:275:SER:HA	1:B:776:VAL:O	1.99	0.62
1:D:1686:LEU:HD22	1:D:1687:ARG:HH21	1.64	0.62
1:E:2132:LYS:HE2	1:E:2263:GLY:O	2.00	0.62
2:F:2906:NCN:H2	3:F:3101:HOH:O	1.97	0.62
1:C:1269:VAL:HB	1:C:1272:LEU:HD22	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:VAL:HG13	1:A:182:VAL:N	2.15	0.61
1:C:1134:LYS:HE3	1:C:1265:ASP:O	2.01	0.61
1:F:2617:ILE:O	1:F:2621:THR:HG23	2.00	0.61
1:B:621:THR:HG21	1:B:653:VAL:HA	1.82	0.61
1:B:515:ILE:HD11	1:B:565:GLU:HG2	1.82	0.61
1:B:634:LYS:HE3	1:B:765:ASP:O	2.01	0.60
1:A:172:LYS:H	1:A:175:HIS:CD2	2.18	0.60
1:C:1172:LYS:H	1:C:1175:HIS:CD2	2.19	0.60
1:E:2187:ARG:NH2	1:E:2214:GLU:HB3	2.17	0.60
1:C:1046:VAL:HG22	1:C:1048:ARG:HH21	1.66	0.60
1:C:1196:LEU:HD21	1:D:1529:VAL:HG11	1.83	0.60
1:D:1632:LYS:HE2	1:D:1763:GLY:O	2.01	0.60
1:E:2104:GLU:HG3	1:E:2283:LEU:CD2	2.32	0.60
1:A:67:LEU:CD2	1:A:99:GLY:HA3	2.30	0.59
1:E:2186:LEU:HD22	1:E:2187:ARG:HH21	1.67	0.59
1:F:2631:THR:HG23	1:F:2633:ALA:H	1.66	0.59
1:E:2036:PRO:HG2	1:E:2039:ALA:HB2	1.84	0.59
1:F:2584:VAL:HG22	1:F:2588:GLU:HG2	1.85	0.59
1:C:1176:VAL:HG13	1:C:1182:VAL:N	2.17	0.59
1:E:2046:VAL:HG22	1:E:2048:ARG:HH21	1.67	0.59
1:E:2172:LYS:H	1:E:2175:HIS:HD2	1.50	0.59
1:A:121:THR:HG21	1:A:153:VAL:HA	1.84	0.59
1:F:2607:MET:O	1:F:2611:VAL:HG13	2.01	0.59
1:F:2693:ALA:HB1	1:F:2696:LEU:HB2	1.84	0.59
1:C:1239:ARG:NH1	3:C:3047:HOH:O	2.35	0.59
1:A:161:HIS:CE1	2:A:2901:NCN:H4	2.37	0.59
1:C:1161:HIS:CE1	2:C:2905:NCN:H4	2.38	0.58
1:B:687:ARG:HH22	1:B:690:ARG:HE	1.49	0.58
1:F:2546:VAL:HG22	1:F:2548:ARG:HH21	1.67	0.58
1:E:2172:LYS:H	1:E:2175:HIS:CD2	2.20	0.58
1:B:769:VAL:HB	1:B:772:LEU:HD22	1.84	0.58
1:B:720:LEU:HD21	2:B:2902:NCN:C5	2.33	0.58
1:D:1686:LEU:HD22	1:D:1687:ARG:NH2	2.19	0.58
1:F:2558:VAL:HG11	1:F:2610:LEU:HG	1.83	0.58
1:F:2769:VAL:HB	1:F:2772:LEU:HD22	1.85	0.58
1:A:179:ALA:HB1	1:A:184:ASP:HB3	1.85	0.57
1:C:1052:VAL:HG22	1:C:1083:ARG:HD2	1.84	0.57
1:C:1172:LYS:H	1:C:1175:HIS:HD2	1.51	0.57
1:A:142:LEU:H	1:A:149:GLN:HE22	1.52	0.57
1:B:676:VAL:HG22	1:B:682:VAL:HA	1.86	0.57
1:C:1131:THR:HG21	1:C:1260:ALA:HB1	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2161:HIS:CE1	2:E:2903:NCN:H4	2.39	0.57
1:B:607:MET:O	1:B:611:VAL:HG13	2.03	0.57
1:C:1252:SER:OG	1:C:1254:GLN:HG2	2.05	0.57
1:C:1046:VAL:CG2	1:C:1048:ARG:HH21	2.18	0.57
1:D:1511:ALA:O	1:D:1515:ILE:HG23	2.04	0.57
1:E:2142:LEU:H	1:E:2149:GLN:HE22	1.51	0.57
1:F:2687:ARG:CZ	1:F:2690:ARG:HG3	2.36	0.56
1:D:1718:LEU:HD23	1:D:1744:MET:HB2	1.87	0.56
1:E:2225:ALA:N	1:E:2228:GLN:HE21	2.03	0.56
1:F:2725:ALA:N	1:F:2728:GLN:HE21	1.97	0.56
1:E:2187:ARG:HH22	1:E:2190:ARG:HE	1.52	0.56
1:E:2218:LEU:HD23	1:E:2244:MET:HB2	1.86	0.56
1:E:2186:LEU:HD22	1:E:2187:ARG:NH2	2.20	0.56
1:F:2672:LYS:H	1:F:2675:HIS:CD2	2.22	0.56
1:F:2511:ALA:O	1:F:2515:ILE:HG23	2.05	0.56
1:C:1031:THR:HG22	1:C:1101:LEU:HD23	1.88	0.55
1:C:1142:LEU:H	1:C:1149:GLN:HE22	1.52	0.55
1:F:2638:THR:OG1	1:F:2640:LYS:HG3	2.06	0.55
1:A:117:ILE:O	1:A:121:THR:HG23	2.06	0.55
1:A:169:ALA:HB1	1:A:189:VAL:HG11	1.88	0.55
1:B:712:LEU:HD22	1:B:740:ALA:HB3	1.87	0.55
1:D:1546:VAL:HG22	1:D:1548:ARG:HH21	1.71	0.55
1:C:1183:VAL:O	1:C:1187:ARG:HG2	2.07	0.55
1:C:1187:ARG:NH2	1:C:1190:ARG:HE	2.04	0.55
1:A:128:VAL:O	1:A:131:THR:HB	2.07	0.54
1:E:2187:ARG:CZ	1:E:2190:ARG:HG3	2.37	0.54
1:F:2687:ARG:HH22	1:F:2690:ARG:HE	1.55	0.54
1:F:2634:LYS:HE3	1:F:2765:ASP:O	2.07	0.54
1:A:11:ALA:O	1:A:15:ILE:HG23	2.07	0.54
1:C:1017:ARG:O	1:C:1021:GLU:HG3	2.08	0.54
1:E:2083:ARG:HB3	3:E:3033:HOH:O	2.07	0.54
1:A:134:LYS:HE3	1:A:265:ASP:O	2.07	0.54
1:D:1628:VAL:O	1:D:1631:THR:HB	2.07	0.54
1:D:1729:THR:O	1:D:1733:VAL:HG23	2.07	0.54
1:B:686:LEU:O	1:B:690:ARG:HG2	2.06	0.54
1:D:1676:VAL:HG13	1:D:1682:VAL:N	2.23	0.54
1:C:1121:THR:HG21	1:C:1153:VAL:HA	1.91	0.53
1:A:248:SER:OG	2:A:2901:NCN:H6	2.08	0.53
1:B:642:LEU:H	1:B:649:GLN:HE22	1.55	0.53
1:E:2107:MET:O	1:E:2111:VAL:HG13	2.08	0.53
1:D:1550:ALA:HB2	1:D:1586:PRO:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:THR:CG2	1:A:101:LEU:HD23	2.37	0.53
1:A:52:VAL:HG22	1:A:83:ARG:HD2	1.90	0.53
1:A:176:VAL:HG13	1:A:181:SER:C	2.28	0.53
1:E:2176:VAL:HG13	1:E:2182:VAL:N	2.23	0.53
1:C:1107:MET:O	1:C:1111:VAL:HG13	2.09	0.53
1:D:1536:PRO:HG2	1:D:1539:ALA:HB2	1.90	0.53
1:B:617:ILE:O	1:B:621:THR:HG23	2.09	0.53
1:B:669:ALA:HB1	1:B:689:VAL:HG11	1.90	0.53
1:B:670:LEU:HD13	1:B:672:LYS:HG3	1.90	0.53
1:C:1193:ALA:HB1	1:C:1196:LEU:HB2	1.91	0.53
1:D:1542:THR:HA	1:D:1593:LEU:O	2.09	0.53
1:B:687:ARG:NH2	1:B:690:ARG:HE	2.06	0.53
1:C:1187:ARG:CZ	1:C:1190:ARG:HG3	2.39	0.53
1:E:2169:ALA:HB1	1:E:2189:VAL:HG11	1.90	0.52
1:C:1176:VAL:HG22	1:C:1182:VAL:HA	1.92	0.52
1:A:131:THR:HG23	1:A:133:ALA:H	1.73	0.52
1:A:176:VAL:HG22	1:A:182:VAL:HA	1.92	0.52
1:A:187:ARG:HH22	1:A:190:ARG:HE	1.57	0.52
1:A:218:LEU:HD23	1:A:244:MET:HB2	1.92	0.52
1:D:1531:THR:HG22	1:D:1601:LEU:HD23	1.92	0.52
1:D:1683:VAL:O	1:D:1687:ARG:HG2	2.10	0.52
1:B:541:THR:O	1:B:594:GLU:HA	2.10	0.52
1:A:131:THR:CG2	1:A:133:ALA:H	2.23	0.52
1:B:631:THR:CG2	1:B:633:ALA:H	2.23	0.52
1:C:1029:VAL:HG11	1:D:1696:LEU:HD21	1.92	0.52
1:F:2664:GLY:N	1:F:2667:ASP:OD1	2.43	0.52
1:A:105:ARG:O	1:A:105:ARG:HD3	2.09	0.51
1:B:550:ALA:HB2	1:B:586:PRO:HD3	1.92	0.51
1:E:2269:VAL:HB	1:E:2272:LEU:HD22	1.90	0.51
1:F:2768:ALA:HB1	2:F:2906:NCN:H5	1.92	0.51
1:D:1712:LEU:N	1:D:1713:PRO:HD2	2.26	0.51
1:D:1687:ARG:HH22	1:D:1690:ARG:HE	1.58	0.51
1:F:2637:ASP:OD2	1:F:2653:VAL:HG21	2.09	0.51
1:F:2672:LYS:H	1:F:2675:HIS:HD2	1.59	0.51
1:E:2154:ARG:HE	1:E:2160:ASN:ND2	2.08	0.51
1:A:186:LEU:O	1:A:190:ARG:HG2	2.09	0.51
1:D:1642:LEU:H	1:D:1649:GLN:HE22	1.59	0.50
1:F:2712:LEU:N	1:F:2713:PRO:HD2	2.26	0.50
1:B:679:ALA:HB1	1:B:684:ASP:HB3	1.92	0.50
1:B:662:ARG:HG3	2:B:2902:NCN:O7	2.12	0.50
1:D:1769:VAL:HB	1:D:1772:LEU:HD22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2531:THR:CG2	1:F:2601:LEU:HD23	2.40	0.50
1:A:212:LEU:N	1:A:213:PRO:HD2	2.27	0.50
1:A:196:LEU:HD21	1:B:529:VAL:HG11	1.94	0.50
1:B:552:VAL:HG22	1:B:583:ARG:HD2	1.93	0.50
1:B:584:VAL:CG2	1:B:588:GLU:HG2	2.38	0.50
1:B:729:THR:O	1:B:733:VAL:HG23	2.12	0.50
1:C:1170:LEU:HD13	1:C:1172:LYS:HG3	1.94	0.50
1:D:1670:LEU:HD13	1:D:1672:LYS:HG3	1.94	0.50
1:E:2131:THR:HG23	1:E:2133:ALA:H	1.76	0.50
1:E:2179:ALA:HB1	1:E:2184:ASP:HB3	1.93	0.50
1:A:225:ALA:N	1:A:228:GLN:HE21	1.97	0.50
1:C:1229:THR:O	1:C:1233:VAL:HG23	2.11	0.50
1:D:1679:ALA:HB1	1:D:1684:ASP:HB3	1.94	0.49
1:E:2176:VAL:HG22	1:E:2182:VAL:HA	1.94	0.49
1:C:1161:HIS:ND1	3:C:3177:HOH:O	2.33	0.49
1:B:661:HIS:CE1	2:B:2902:NCN:H4	2.47	0.49
1:C:1037:ALA:HA	1:C:1098:ARG:HD2	1.94	0.49
1:A:132:LYS:HE2	1:A:263:GLY:O	2.12	0.49
1:C:1279:LEU:O	1:C:1281:ILE:HG13	2.13	0.49
1:C:1179:ALA:HB1	1:C:1184:ASP:HB3	1.95	0.49
1:D:1517:ARG:O	1:D:1521:GLU:HG3	2.13	0.49
1:E:2011:ALA:O	1:E:2015:ILE:HG23	2.12	0.49
1:E:2117:ILE:O	1:E:2121:THR:HG23	2.13	0.49
1:A:104:GLU:O	1:A:108:LEU:HD22	2.13	0.49
1:C:1142:LEU:H	1:C:1149:GLN:NE2	2.09	0.49
1:A:170:LEU:CD1	1:A:172:LYS:HG3	2.43	0.49
1:A:226:VAL:HG11	1:A:258:THR:HG22	1.95	0.49
1:D:1515:ILE:HD12	1:D:1515:ILE:C	2.32	0.49
1:A:170:LEU:HD13	1:A:172:LYS:HG3	1.94	0.48
1:B:605:ARG:O	1:B:605:ARG:HD3	2.13	0.48
1:F:2515:ILE:HD11	1:F:2565:GLU:CG	2.39	0.48
1:C:1226:VAL:HG11	1:C:1258:THR:HG22	1.95	0.48
1:E:2226:VAL:HG11	1:E:2258:THR:HG22	1.95	0.48
1:E:2047:THR:O	1:E:2086:PRO:O	2.32	0.48
1:E:2058:VAL:HG11	1:E:2110:LEU:HG	1.95	0.48
1:B:676:VAL:HG13	1:B:681:SER:C	2.33	0.48
1:D:1669:ALA:HB1	1:D:1689:VAL:HG11	1.95	0.48
1:F:2669:ALA:HB1	1:F:2689:VAL:HG11	1.96	0.48
1:F:2631:THR:CG2	1:F:2633:ALA:H	2.25	0.48
1:A:154:ARG:HH21	1:A:160:ASN:HD21	1.62	0.47
1:C:1154:ARG:HE	1:C:1160:ASN:ND2	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2905:NCN:C4	3:C:3177:HOH:O	2.61	0.47
1:F:2686:LEU:O	1:F:2690:ARG:HG2	2.14	0.47
1:A:137:ASP:OD1	1:A:150:LYS:NZ	2.47	0.47
1:E:2186:LEU:O	1:E:2190:ARG:HG2	2.13	0.47
1:A:24:ARG:HD2	1:A:25:TYR:CZ	2.50	0.47
1:B:628:VAL:O	1:B:631:THR:HB	2.15	0.47
1:E:2100:LEU:HA	1:E:2100:LEU:HD23	1.72	0.47
1:F:2524:ARG:HD2	1:F:2525:TYR:CZ	2.50	0.47
1:C:1219:ILE:HB	1:C:1245:LEU:HD12	1.97	0.47
1:E:2031:THR:CG2	1:E:2101:LEU:HD23	2.44	0.47
1:F:2687:ARG:NH2	1:F:2690:ARG:HE	2.12	0.47
1:B:556:LEU:HD23	1:B:578:VAL:O	2.14	0.47
1:B:718:LEU:CD1	1:B:720:LEU:HD12	2.45	0.47
1:C:1117:ILE:O	1:C:1121:THR:CG2	2.62	0.47
1:E:2164:GLY:N	1:E:2167:ASP:OD1	2.47	0.47
1:B:687:ARG:CZ	1:B:690:ARG:HG3	2.45	0.47
1:A:129:ARG:HA	3:A:3088:HOH:O	2.13	0.47
1:A:46:VAL:CG2	1:A:48:ARG:HH21	2.28	0.47
1:E:2187:ARG:NH2	1:E:2190:ARG:HE	2.11	0.47
1:D:1564:ASN:OD1	1:D:1569:THR:HA	2.15	0.47
1:D:1671:ILE:HG23	1:D:1675:HIS:HB2	1.96	0.47
1:E:2142:LEU:H	1:E:2149:GLN:NE2	2.11	0.46
1:F:2642:LEU:H	1:F:2649:GLN:HE22	1.63	0.46
1:A:229:THR:O	1:A:233:VAL:HG23	2.15	0.46
1:C:1013:ALA:O	1:C:1017:ARG:HG3	2.15	0.46
1:C:1181:SER:H	1:C:1184:ASP:HB2	1.81	0.46
1:F:2617:ILE:O	1:F:2621:THR:CG2	2.62	0.46
1:A:29:VAL:HG11	1:B:696:LEU:CD2	2.45	0.46
1:E:2154:ARG:HE	1:E:2160:ASN:HD21	1.63	0.46
1:A:121:THR:O	1:A:125:VAL:HG23	2.16	0.46
1:D:1617:ILE:O	1:D:1621:THR:HG23	2.15	0.46
1:A:36:PRO:HG2	1:A:39:ALA:HB2	1.96	0.46
1:C:1031:THR:HG22	1:D:1675:HIS:HE1	1.80	0.46
1:D:1712:LEU:HD22	1:D:1740:ALA:HB3	1.97	0.46
1:E:2046:VAL:CG2	1:E:2048:ARG:HH21	2.28	0.46
1:C:1031:THR:CG2	1:C:1101:LEU:HD23	2.46	0.46
1:C:1060:LEU:HD12	1:C:1060:LEU:HA	1.81	0.46
1:C:1198:CYS:O	1:C:1217:GLU:HB2	2.16	0.46
1:B:670:LEU:HA	1:B:699:GLU:O	2.16	0.46
1:F:2768:ALA:HB1	2:F:2906:NCN:C5	2.46	0.46
1:F:2633:ALA:HA	1:F:2765:ASP:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2768:ALA:CB	2:F:2906:NCN:H5	2.46	0.46
1:C:1128:VAL:O	1:C:1128:VAL:HG23	2.14	0.45
1:E:2017:ARG:O	1:E:2021:GLU:HG3	2.16	0.45
1:B:683:VAL:O	1:B:687:ARG:HG2	2.16	0.45
1:E:2170:LEU:CD1	1:E:2172:LYS:HG3	2.45	0.45
1:C:1225:ALA:N	1:C:1228:GLN:HE21	2.04	0.45
1:E:2196:LEU:HD21	1:F:2529:VAL:HG11	1.96	0.45
1:F:2564:ASN:OD1	1:F:2569:THR:HA	2.16	0.45
1:A:164:GLY:N	1:A:167:ASP:OD1	2.49	0.45
1:A:187:ARG:CZ	1:A:190:ARG:HG3	2.47	0.45
1:C:1176:VAL:HG13	1:C:1181:SER:C	2.37	0.45
1:B:621:THR:O	1:B:625:VAL:HG23	2.16	0.45
2:C:2905:NCN:C5	3:C:3177:HOH:O	2.64	0.45
1:F:2779:LEU:HD12	1:F:2779:LEU:HA	1.79	0.45
1:B:528:ASP:OD2	1:B:531:THR:HG23	2.17	0.45
1:B:547:THR:O	1:B:586:PRO:O	2.35	0.45
1:B:698:CYS:O	1:B:717:GLU:HB2	2.17	0.45
1:E:2117:ILE:O	1:E:2121:THR:CG2	2.65	0.45
1:F:2676:VAL:HG13	1:F:2681:SER:C	2.37	0.45
1:E:2017:ARG:NH1	1:F:2517:ARG:HD3	2.31	0.44
1:E:2131:THR:CG2	1:E:2133:ALA:H	2.29	0.44
1:F:2726:VAL:HG11	1:F:2758:THR:HG22	1.99	0.44
1:A:107:MET:O	1:A:111:VAL:HG13	2.17	0.44
1:B:670:LEU:CD1	1:B:672:LYS:HG3	2.47	0.44
1:A:183:VAL:O	1:A:187:ARG:HG2	2.17	0.44
1:D:1687:ARG:CZ	1:D:1690:ARG:HG3	2.47	0.44
1:D:1687:ARG:NH2	1:D:1690:ARG:HE	2.15	0.44
1:E:2236:ARG:C	1:E:2236:ARG:HD2	2.38	0.44
1:A:154:ARG:HE	1:A:160:ASN:ND2	2.16	0.44
1:C:1164:GLY:N	1:C:1167:ASP:OD1	2.50	0.44
1:D:1686:LEU:O	1:D:1690:ARG:HG2	2.17	0.43
1:E:2015:ILE:HG13	1:E:2016:ALA:N	2.33	0.43
1:E:2187:ARG:HH21	1:E:2214:GLU:HB3	1.82	0.43
1:E:2029:VAL:HG21	1:F:2693:ALA:HB2	2.00	0.43
1:A:154:ARG:NH2	3:A:3224:HOH:O	2.50	0.43
1:E:2010:ALA:HB1	3:E:3140:HOH:O	2.18	0.43
1:A:175:HIS:HE1	1:B:531:THR:CG2	2.31	0.43
1:B:642:LEU:H	1:B:649:GLN:NE2	2.15	0.43
1:E:2013:ALA:O	1:E:2017:ARG:HG3	2.17	0.43
1:F:2513:ALA:O	1:F:2517:ARG:HG3	2.17	0.43
1:A:77:ARG:HA	1:A:91:MET:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:VAL:CG2	1:B:548:ARG:HH21	2.29	0.43
1:D:1648:LEU:O	1:D:1651:TYR:HB3	2.17	0.43
1:F:2670:LEU:HD23	1:F:2699:GLU:HB2	2.00	0.43
1:F:2777:ARG:HH11	1:F:2777:ARG:CG	2.31	0.43
1:C:1105:ARG:O	1:C:1105:ARG:HD3	2.17	0.43
1:D:1535:VAL:HG22	1:D:1598:ARG:HG3	2.00	0.43
1:F:2671:ILE:HG23	1:F:2675:HIS:HB2	2.00	0.43
1:B:726:VAL:HG21	1:B:758:THR:CG2	2.48	0.43
1:D:1649:GLN:O	1:D:1653:VAL:HG13	2.19	0.43
1:D:1670:LEU:CD1	1:D:1672:LYS:HG3	2.48	0.43
1:E:2165:LEU:HG	1:F:2528:ASP:HB2	2.01	0.43
1:F:2639:ARG:NH2	3:F:3060:HOH:O	2.49	0.43
1:B:535:VAL:HA	1:B:536:PRO:HD2	1.79	0.43
1:B:726:VAL:HG21	1:B:758:THR:HG21	2.01	0.43
1:A:117:ILE:O	1:A:121:THR:CG2	2.66	0.43
1:B:631:THR:HG23	1:B:633:ALA:H	1.83	0.43
1:A:42:THR:HA	1:A:93:LEU:O	2.19	0.43
1:B:664:GLY:N	1:B:667:ASP:OD1	2.52	0.43
1:C:1031:THR:CG2	1:D:1675:HIS:HE1	2.31	0.43
1:D:1664:GLY:N	1:D:1667:ASP:OD1	2.51	0.43
1:E:2031:THR:HG22	1:F:2675:HIS:HE1	1.84	0.43
1:E:2212:LEU:N	1:E:2213:PRO:HD2	2.34	0.43
1:A:277:ARG:HH11	1:A:277:ARG:CG	2.32	0.42
1:B:752:SER:OG	1:B:754:GLN:HG2	2.19	0.42
1:D:1541:THR:O	1:D:1594:GLU:HA	2.19	0.42
1:E:2252:SER:OG	1:E:2254:GLN:HG2	2.18	0.42
1:B:600:LEU:HD23	1:B:600:LEU:HA	1.89	0.42
1:E:2017:ARG:HD3	1:F:2517:ARG:NH1	2.35	0.42
1:E:2104:GLU:O	1:E:2108:LEU:HD22	2.18	0.42
1:E:2196:LEU:HA	1:E:2197:PRO:HD3	1.87	0.42
1:F:2641:THR:HB	1:F:2649:GLN:NE2	2.33	0.42
1:F:2683:VAL:HG13	1:F:2714:GLU:HG3	2.01	0.42
1:A:56:LEU:HD12	1:A:56:LEU:HA	1.84	0.42
1:B:511:ALA:O	1:B:515:ILE:HG23	2.19	0.42
1:E:2139:ARG:NH1	1:F:2522:ASP:OD2	2.52	0.42
1:A:25:TYR:CD1	1:A:25:TYR:N	2.88	0.42
1:A:25:TYR:HE1	3:B:3093:HOH:O	2.01	0.42
1:F:2636:ARG:CD	1:F:2659:VAL:HG22	2.50	0.42
1:A:142:LEU:H	1:A:149:GLN:NE2	2.17	0.42
1:A:172:LYS:O	1:A:176:VAL:HG23	2.19	0.42
1:C:1196:LEU:HA	1:C:1197:PRO:HD3	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2031:THR:CG2	1:F:2675:HIS:HE1	2.32	0.42
1:F:2679:ALA:HB1	1:F:2684:ASP:HB3	2.02	0.42
1:C:1121:THR:O	1:C:1125:VAL:HG23	2.19	0.41
1:C:1142:LEU:HA	1:C:1142:LEU:HD13	1.88	0.41
1:E:2148:LEU:O	1:E:2151:TYR:HB3	2.20	0.41
1:F:2508:LEU:HD12	1:F:2508:LEU:HA	1.95	0.41
1:C:1025:TYR:CD1	1:C:1025:TYR:N	2.88	0.41
1:C:1059:ALA:HA	1:C:1107:MET:HG3	2.02	0.41
1:C:1220:LEU:HD21	2:C:2905:NCN:C5	2.50	0.41
1:E:2181:SER:H	1:E:2184:ASP:HB2	1.85	0.41
1:F:2517:ARG:O	1:F:2521:GLU:HG3	2.19	0.41
1:D:1676:VAL:CG2	1:D:1682:VAL:HG13	2.51	0.41
1:F:2729:THR:O	1:F:2733:VAL:HG23	2.20	0.41
1:C:1108:LEU:HD12	1:C:1108:LEU:HA	1.93	0.41
1:B:517:ARG:O	1:B:521:GLU:HG3	2.20	0.41
1:E:2105:ARG:HD3	1:E:2109:ASN:OD1	2.20	0.41
1:C:1181:SER:O	1:C:1184:ASP:HB2	2.20	0.41
1:D:1552:VAL:HG22	1:D:1583:ARG:HD2	2.01	0.41
1:B:601:LEU:HA	1:B:601:LEU:HD12	1.86	0.41
1:B:686:LEU:HD13	1:B:714:GLU:CB	2.50	0.41
1:A:60:LEU:HA	1:A:60:LEU:HD12	1.92	0.41
1:C:1137:ASP:OD1	1:C:1150:LYS:NZ	2.53	0.41
1:C:1170:LEU:CD1	1:C:1172:LYS:HG3	2.51	0.41
1:D:1515:ILE:HD11	1:D:1565:GLU:CG	2.45	0.41
1:B:558:VAL:HG11	1:B:610:LEU:HG	2.03	0.41
1:B:621:THR:HG22	1:B:772:LEU:HG	2.03	0.41
1:E:2131:THR:CG2	1:E:2260:ALA:HB1	2.36	0.41
1:C:1134:LYS:HD2	1:C:1266:TYR:HE1	1.86	0.41
1:D:1672:LYS:N	1:D:1675:HIS:HD2	2.13	0.41
1:A:230:GLN:HB3	1:C:1087:GLY:HA3	2.02	0.41
1:B:774:HIS:O	1:B:775:SER:C	2.59	0.41
1:C:1031:THR:HG22	1:D:1675:HIS:CE1	2.56	0.41
1:E:2008:LEU:HD12	1:E:2008:LEU:HA	1.89	0.41
1:F:2648:LEU:O	1:F:2651:TYR:HB3	2.20	0.41
1:F:2740:ALA:N	1:F:2741:PRO:HD3	2.36	0.40
1:B:681:SER:H	1:B:684:ASP:HB2	1.85	0.40
1:D:1631:THR:CG2	1:D:1633:ALA:H	2.34	0.40
1:A:187:ARG:NH2	1:A:190:ARG:HE	2.17	0.40
1:B:524:ARG:HG3	1:B:524:ARG:HH11	1.86	0.40
1:C:1169:ALA:HB1	1:C:1189:VAL:HG11	2.02	0.40
1:A:196:LEU:HA	1:A:197:PRO:HD3	1.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:GLY:N	3:A:3051:HOH:O	2.50	0.40
1:B:637:ASP:OD2	1:B:653:VAL:HG21	2.21	0.40
1:C:1100:LEU:HA	1:C:1100:LEU:HD23	1.73	0.40
1:D:1531:THR:HG21	1:D:1601:LEU:HB3	2.03	0.40
1:F:2515:ILE:HD11	1:F:2565:GLU:CB	2.50	0.40
1:F:2718:LEU:HD23	1:F:2744:MET:HB2	2.03	0.40
1:B:696:LEU:HA	1:B:696:LEU:HD12	1.90	0.40
1:C:1128:VAL:O	1:C:1131:THR:HB	2.22	0.40
1:E:2042:THR:HA	1:E:2093:LEU:O	2.21	0.40
1:E:2198:CYS:O	1:E:2217:GLU:HB2	2.21	0.40
1:F:2550:ALA:HB2	1:F:2586:PRO:HD3	2.02	0.40
1:F:2605:ARG:HD3	1:F:2605:ARG:O	2.21	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	282/284 (99%)	274 (97%)	6 (2%)	2 (1%)	25	49
1	B	282/284 (99%)	273 (97%)	8 (3%)	1 (0%)	38	63
1	C	282/284 (99%)	272 (96%)	8 (3%)	2 (1%)	25	49
1	D	282/284 (99%)	273 (97%)	8 (3%)	1 (0%)	38	63
1	E	282/284 (99%)	273 (97%)	7 (2%)	2 (1%)	25	49
1	F	282/284 (99%)	273 (97%)	8 (3%)	1 (0%)	38	63
All	All	1692/1704 (99%)	1638 (97%)	45 (3%)	9 (0%)	32	58

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	586	PRO

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Mol	Chain	Res	Type
1	A	86	PRO
1	C	1086	PRO
1	D	1586	PRO
1	F	2586	PRO
1	E	2086	PRO
1	E	2104	GLU
1	A	104	GLU
1	C	1104	GLU

### 5.3.2 Protein sidechains [i](#)

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	216/216 (100%)	175 (81%)	41 (19%)	2	2
1	B	216/216 (100%)	177 (82%)	39 (18%)	2	3
1	C	216/216 (100%)	176 (82%)	40 (18%)	2	3
1	D	216/216 (100%)	176 (82%)	40 (18%)	2	3
1	E	216/216 (100%)	174 (81%)	42 (19%)	1	2
1	F	216/216 (100%)	180 (83%)	36 (17%)	2	4
All	All	1296/1296 (100%)	1058 (82%)	238 (18%)	2	3

All (238) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
1	A	15	ILE
1	A	29	VAL
1	A	30	THR
1	A	32	LEU
1	A	35	VAL
1	A	41	THR
1	A	46	VAL
1	A	47	THR
1	A	48	ARG

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Mol	Chain	Res	Type
1	A	56	LEU
1	A	60	LEU
1	A	63	LEU
1	A	75	LEU
1	A	78	VAL
1	A	84	VAL
1	A	86	PRO
1	A	93	LEU
1	A	101	LEU
1	A	108	LEU
1	A	110	LEU
1	A	121	THR
1	A	131	THR
1	A	134	LYS
1	A	142	LEU
1	A	153	VAL
1	A	159	VAL
1	A	165	LEU
1	A	167	ASP
1	A	173	ASP
1	A	182	VAL
1	A	186	LEU
1	A	220	LEU
1	A	242	THR
1	A	245	LEU
1	A	248	SER
1	A	251	LEU
1	A	254	GLN
1	A	272	LEU
1	A	276	VAL
1	A	277	ARG
1	B	505	ASP
1	B	515	ILE
1	B	522	ASP
1	B	529	VAL
1	B	535	VAL
1	B	540	THR
1	B	541	THR
1	B	546	VAL
1	B	547	THR
1	B	548	ARG
1	B	556	LEU

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Mol	Chain	Res	Type
1	B	560	LEU
1	B	563	LEU
1	B	578	VAL
1	B	584	VAL
1	B	586	PRO
1	B	593	LEU
1	B	601	LEU
1	B	608	LEU
1	B	610	LEU
1	B	621	THR
1	B	631	THR
1	B	634	LYS
1	B	642	LEU
1	B	659	VAL
1	B	665	LEU
1	B	667	ASP
1	B	673	ASP
1	B	674	ASN
1	B	682	VAL
1	B	686	LEU
1	B	700	VAL
1	B	720	LEU
1	B	745	LEU
1	B	751	LEU
1	B	754	GLN
1	B	772	LEU
1	B	776	VAL
1	B	777	ARG
1	C	1005	ASP
1	C	1015	ILE
1	C	1022	ASP
1	C	1029	VAL
1	C	1035	VAL
1	C	1040	THR
1	C	1041	THR
1	C	1046	VAL
1	C	1047	THR
1	C	1048	ARG
1	C	1056	LEU
1	C	1060	LEU
1	C	1063	LEU
1	C	1075	LEU

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Mol	Chain	Res	Type
1	C	1078	VAL
1	C	1084	VAL
1	C	1086	PRO
1	C	1093	LEU
1	C	1101	LEU
1	C	1108	LEU
1	C	1110	LEU
1	C	1121	THR
1	C	1131	THR
1	C	1134	LYS
1	C	1142	LEU
1	C	1153	VAL
1	C	1159	VAL
1	C	1165	LEU
1	C	1167	ASP
1	C	1173	ASP
1	C	1182	VAL
1	C	1186	LEU
1	C	1220	LEU
1	C	1245	LEU
1	C	1248	SER
1	C	1251	LEU
1	C	1254	GLN
1	C	1272	LEU
1	C	1276	VAL
1	C	1277	ARG
1	D	1505	ASP
1	D	1515	ILE
1	D	1529	VAL
1	D	1530	THR
1	D	1535	VAL
1	D	1541	THR
1	D	1546	VAL
1	D	1547	THR
1	D	1548	ARG
1	D	1556	LEU
1	D	1560	LEU
1	D	1563	LEU
1	D	1575	LEU
1	D	1578	VAL
1	D	1584	VAL
1	D	1586	PRO

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Mol	Chain	Res	Type
1	D	1593	LEU
1	D	1601	LEU
1	D	1608	LEU
1	D	1610	LEU
1	D	1611	VAL
1	D	1621	THR
1	D	1631	THR
1	D	1634	LYS
1	D	1642	LEU
1	D	1653	VAL
1	D	1659	VAL
1	D	1665	LEU
1	D	1667	ASP
1	D	1673	ASP
1	D	1682	VAL
1	D	1686	LEU
1	D	1700	VAL
1	D	1720	LEU
1	D	1745	LEU
1	D	1748	SER
1	D	1751	LEU
1	D	1754	GLN
1	D	1772	LEU
1	D	1776	VAL
1	E	2005	ASP
1	E	2015	ILE
1	E	2022	ASP
1	E	2029	VAL
1	E	2035	VAL
1	E	2040	THR
1	E	2041	THR
1	E	2046	VAL
1	E	2047	THR
1	E	2048	ARG
1	E	2056	LEU
1	E	2060	LEU
1	E	2063	LEU
1	E	2075	LEU
1	E	2078	VAL
1	E	2084	VAL
1	E	2086	PRO
1	E	2093	LEU

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Mol	Chain	Res	Type
1	E	2101	LEU
1	E	2108	LEU
1	E	2110	LEU
1	E	2121	THR
1	E	2131	THR
1	E	2134	LYS
1	E	2142	LEU
1	E	2153	VAL
1	E	2159	VAL
1	E	2165	LEU
1	E	2167	ASP
1	E	2173	ASP
1	E	2174	ASN
1	E	2182	VAL
1	E	2186	LEU
1	E	2220	LEU
1	E	2242	THR
1	E	2245	LEU
1	E	2248	SER
1	E	2251	LEU
1	E	2254	GLN
1	E	2272	LEU
1	E	2276	VAL
1	E	2277	ARG
1	F	2505	ASP
1	F	2515	ILE
1	F	2522	ASP
1	F	2529	VAL
1	F	2532	LEU
1	F	2535	VAL
1	F	2541	THR
1	F	2546	VAL
1	F	2547	THR
1	F	2548	ARG
1	F	2556	LEU
1	F	2560	LEU
1	F	2563	LEU
1	F	2586	PRO
1	F	2593	LEU
1	F	2601	LEU
1	F	2608	LEU
1	F	2610	LEU

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Mol	Chain	Res	Type
1	F	2621	THR
1	F	2631	THR
1	F	2634	LYS
1	F	2642	LEU
1	F	2653	VAL
1	F	2659	VAL
1	F	2665	LEU
1	F	2667	ASP
1	F	2673	ASP
1	F	2682	VAL
1	F	2686	LEU
1	F	2720	LEU
1	F	2745	LEU
1	F	2748	SER
1	F	2751	LEU
1	F	2754	GLN
1	F	2772	LEU
1	F	2776	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	160	ASN
1	A	175	HIS
1	A	228	GLN
1	B	649	GLN
1	B	675	HIS
1	B	728	GLN
1	C	1149	GLN
1	C	1160	ASN
1	C	1174	ASN
1	C	1175	HIS
1	C	1228	GLN
1	D	1649	GLN
1	D	1660	ASN
1	D	1675	HIS
1	D	1728	GLN
1	E	2149	GLN
1	E	2160	ASN
1	E	2175	HIS
1	E	2228	GLN

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Mol	Chain	Res	Type
1	F	2649	GLN
1	F	2660	ASN
1	F	2675	HIS
1	F	2728	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NCN	A	2901	-	18,23,23	3.16	9 (50%)	24,34,34	1.96	6 (25%)
2	NCN	B	2902	-	18,23,23	3.30	9 (50%)	24,34,34	1.99	7 (29%)
2	NCN	C	2905	-	18,23,23	3.08	8 (44%)	24,34,34	2.01	6 (25%)
2	NCN	D	2904	-	18,23,23	3.29	10 (55%)	24,34,34	1.92	6 (25%)
2	NCN	E	2903	-	18,23,23	3.08	9 (50%)	24,34,34	2.00	6 (25%)
2	NCN	F	2906	-	18,23,23	3.06	8 (44%)	24,34,34	1.96	7 (29%)

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	NCN	A	2901	-	-	0/6/30/30	0/2/2/2
2	NCN	B	2902	-	-	0/6/30/30	0/2/2/2
2	NCN	C	2905	-	-	0/6/30/30	0/2/2/2
2	NCN	D	2904	-	-	0/6/30/30	0/2/2/2
2	NCN	E	2903	-	-	0/6/30/30	0/2/2/2
2	NCN	F	2906	-	-	0/6/30/30	0/2/2/2

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2902	NCN	P-O2P	2.04	1.57	1.50
2	A	2901	NCN	C4-C3	2.10	1.43	1.39
2	E	2903	NCN	C5'-C4'	2.17	1.58	1.51
2	B	2902	NCN	C6-C5	2.24	1.43	1.38
2	D	2904	NCN	C5'-C4'	2.36	1.59	1.51
2	E	2903	NCN	C6-C5	2.44	1.44	1.38
2	D	2904	NCN	P-O2P	2.47	1.59	1.50
2	F	2906	NCN	C5'-C4'	2.52	1.59	1.51
2	B	2902	NCN	P-O5'	2.54	1.68	1.60
2	C	2905	NCN	C3'-C4'	2.67	1.60	1.53
2	C	2905	NCN	P-O2P	2.71	1.60	1.50
2	A	2901	NCN	C6-C5	2.72	1.44	1.38
2	D	2904	NCN	O2'-C2'	2.80	1.49	1.43
2	F	2906	NCN	P-O5'	2.81	1.69	1.60
2	F	2906	NCN	O2'-C2'	2.83	1.49	1.43
2	D	2904	NCN	C6-C5	2.85	1.44	1.38
2	A	2901	NCN	P-O5'	2.88	1.69	1.60
2	F	2906	NCN	C3'-C4'	2.88	1.60	1.53
2	B	2902	NCN	C3'-C4'	2.93	1.60	1.53
2	E	2903	NCN	C3'-C4'	3.00	1.60	1.53
2	C	2905	NCN	O2'-C2'	3.04	1.49	1.43
2	D	2904	NCN	O3'-C3'	3.04	1.50	1.43
2	A	2901	NCN	C3'-C4'	3.06	1.61	1.53
2	C	2905	NCN	P-O5'	3.07	1.70	1.60
2	D	2904	NCN	C3'-C4'	3.18	1.61	1.53
2	B	2902	NCN	O2'-C2'	3.19	1.50	1.43
2	E	2903	NCN	P-O5'	3.25	1.70	1.60
2	A	2901	NCN	O2'-C2'	3.27	1.50	1.43
2	C	2905	NCN	C6-N1	3.27	1.43	1.35
2	E	2903	NCN	C6-N1	3.33	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2903	NCN	O2'-C2'	3.36	1.50	1.43
2	E	2903	NCN	O3'-C3'	3.46	1.50	1.43
2	F	2906	NCN	O3'-C3'	3.60	1.51	1.43
2	C	2905	NCN	O3'-C3'	3.67	1.51	1.43
2	A	2901	NCN	O3'-C3'	3.67	1.51	1.43
2	D	2904	NCN	C6-N1	3.74	1.45	1.35
2	D	2904	NCN	P-O5'	3.77	1.72	1.60
2	B	2902	NCN	O3'-C3'	3.78	1.51	1.43
2	B	2902	NCN	C6-N1	3.89	1.45	1.35
2	A	2901	NCN	C6-N1	3.90	1.45	1.35
2	F	2906	NCN	C6-N1	4.11	1.46	1.35
2	D	2904	NCN	C2'-C1'	4.80	1.61	1.53
2	F	2906	NCN	C2'-C1'	4.88	1.61	1.53
2	A	2901	NCN	C2'-C1'	5.00	1.61	1.53
2	E	2903	NCN	C2'-C1'	5.33	1.62	1.53
2	C	2905	NCN	C2'-C1'	5.71	1.62	1.53
2	B	2902	NCN	C2'-C1'	5.90	1.63	1.53
2	C	2905	NCN	O4'-C1'	8.54	1.53	1.41
2	E	2903	NCN	O4'-C1'	8.66	1.53	1.41
2	F	2906	NCN	O4'-C1'	8.70	1.53	1.41
2	A	2901	NCN	O4'-C1'	8.81	1.53	1.41
2	B	2902	NCN	O4'-C1'	9.46	1.54	1.41
2	D	2904	NCN	O4'-C1'	9.50	1.54	1.41

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2903	NCN	C4'-O4'-C1'	-4.81	104.65	109.77
2	C	2905	NCN	C4-C3-C7	-4.38	114.56	120.45
2	B	2902	NCN	C4'-O4'-C1'	-4.28	105.22	109.77
2	D	2904	NCN	C4'-O4'-C1'	-4.15	105.35	109.77
2	F	2906	NCN	C4-C3-C7	-4.10	114.93	120.45
2	A	2901	NCN	C4'-O4'-C1'	-4.02	105.49	109.77
2	C	2905	NCN	C4'-O4'-C1'	-3.88	105.64	109.77
2	D	2904	NCN	C4-C3-C7	-3.73	115.44	120.45
2	F	2906	NCN	C4'-O4'-C1'	-3.68	105.86	109.77
2	B	2902	NCN	C4-C3-C7	-3.66	115.53	120.45
2	E	2903	NCN	C4-C3-C7	-3.60	115.61	120.45
2	A	2901	NCN	C4-C3-C7	-3.53	115.71	120.45
2	B	2902	NCN	C5-C4-C3	2.23	123.39	120.57
2	C	2905	NCN	O5'-C5'-C4'	2.52	117.94	109.00
2	E	2903	NCN	O5'-C5'-C4'	2.59	118.19	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2902	NCN	O5'-C5'-C4'	2.66	118.44	109.00
2	F	2906	NCN	C5-C4-C3	2.74	124.03	120.57
2	B	2902	NCN	O3'-C3'-C4'	2.77	119.18	111.09
2	D	2904	NCN	O5'-C5'-C4'	2.86	119.13	109.00
2	F	2906	NCN	O3'-C3'-C4'	2.88	119.50	111.09
2	A	2901	NCN	O5'-C5'-C4'	2.96	119.49	109.00
2	C	2905	NCN	O3'-C3'-C4'	2.98	119.78	111.09
2	D	2904	NCN	O3'-C3'-C4'	2.99	119.82	111.09
2	F	2906	NCN	O5'-C5'-C4'	2.99	119.61	109.00
2	A	2901	NCN	O3'-C3'-C4'	3.03	119.92	111.09
2	E	2903	NCN	O3'-C3'-C4'	3.29	120.69	111.09
2	D	2904	NCN	C2-C3-C7	3.31	125.97	119.79
2	E	2903	NCN	O2'-C2'-C1'	3.37	122.16	111.61
2	E	2903	NCN	C2-C3-C7	3.38	126.10	119.79
2	A	2901	NCN	C2-C3-C7	3.39	126.13	119.79
2	D	2904	NCN	O2'-C2'-C1'	3.50	122.56	111.61
2	F	2906	NCN	C2-C3-C7	3.65	126.61	119.79
2	F	2906	NCN	O2'-C2'-C1'	3.74	123.33	111.61
2	A	2901	NCN	O2'-C2'-C1'	3.75	123.36	111.61
2	B	2902	NCN	O2'-C2'-C1'	3.80	123.50	111.61
2	B	2902	NCN	C2-C3-C7	3.84	126.97	119.79
2	C	2905	NCN	O2'-C2'-C1'	3.92	123.89	111.61
2	C	2905	NCN	C2-C3-C7	3.94	127.14	119.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2901	NCN	5	0
2	B	2902	NCN	6	0
2	C	2905	NCN	8	0
2	D	2904	NCN	6	0
2	E	2903	NCN	6	0
2	F	2906	NCN	7	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.