



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:37 PM GMT

PDB ID : 1U8R  
Title : Crystal Structure of an IdeR-DNA Complex Reveals a Conformational Change  
in Activated IdeR for Base-specific Interactions  
Authors : Wisedchaisri, G.; Holmes, R.K.; Hol, W.G.J.  
Deposited on : 2004-08-06  
Resolution : 2.75 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

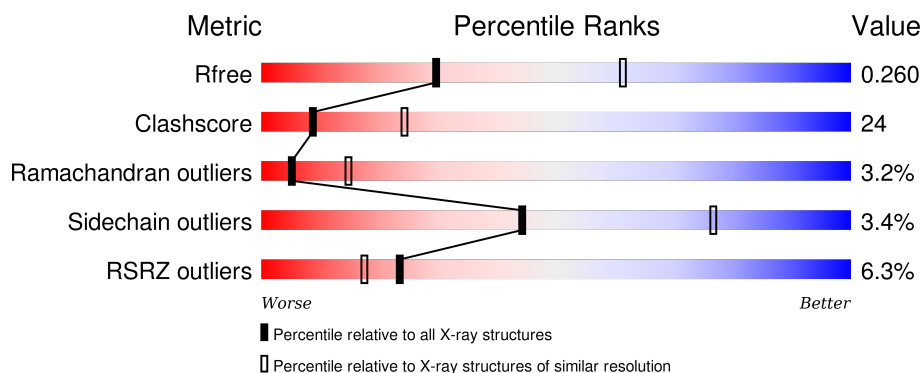
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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	E	33	<div> <div>15%</div> <div>67%</div> <div>18%</div> </div>
1	K	33	<div> <div>9%</div> <div>73%</div> <div>18%</div> </div>
2	F	33	<div> <div>24%</div> <div>64%</div> <div>12%</div> </div>
2	L	33	<div> <div>3%</div> <div>18%</div> <div>73%</div> <div>9%</div> </div>
3	A	230	<div> <div>3%</div> <div>57%</div> <div>35%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
3	B	230	
3	C	230	
3	D	230	
3	G	230	
3	H	230	
3	I	230	
3	J	230	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CO	B	2002	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16481 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 DNA chain called mbtA operator DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	33	Total	C	N	O	P	0	0	0
			670	321	117	200	32			
1	K	33	Total	C	N	O	P	0	0	0
			670	321	117	200	32			

- Molecule 2 is a DNA chain called mbtB operator DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	33	Total	C	N	O	P	0	0	0
			677	322	131	192	32			
2	L	33	Total	C	N	O	P	0	0	0
			677	322	131	192	32			

- Molecule 3 is a protein called Iron-dependent repressor ideR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	221	Total	C	N	O	S	0	0	0
			1711	1067	312	325	7			
3	B	221	Total	C	N	O	S	0	0	0
			1711	1067	312	325	7			
3	C	221	Total	C	N	O	S	0	0	0
			1711	1067	312	325	7			
3	D	221	Total	C	N	O	S	0	0	0
			1711	1067	312	325	7			
3	G	221	Total	C	N	O	S	0	0	0
			1711	1067	312	325	7			
3	H	222	Total	C	N	O	S	0	0	0
			1719	1071	314	327	7			
3	I	221	Total	C	N	O	S	0	0	0
			1711	1067	312	325	7			
3	J	222	Total	C	N	O	S	0	0	0
			1719	1071	314	327	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	136	ASP	VAL	SEE REMARK 999	UNP P0A672
B	136	ASP	VAL	SEE REMARK 999	UNP P0A672
C	136	ASP	VAL	SEE REMARK 999	UNP P0A672
D	136	ASP	VAL	SEE REMARK 999	UNP P0A672
G	136	ASP	VAL	SEE REMARK 999	UNP P0A672
H	136	ASP	VAL	SEE REMARK 999	UNP P0A672
I	136	ASP	VAL	SEE REMARK 999	UNP P0A672
J	136	ASP	VAL	SEE REMARK 999	UNP P0A672

- Molecule 4 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	3	Total Co 3 3	0	0
4	J	3	Total Co 3 3	0	0
4	D	3	Total Co 3 3	0	0
4	H	3	Total Co 3 3	0	0
4	B	3	Total Co 3 3	0	0
4	I	3	Total Co 3 3	0	0
4	C	3	Total Co 3 3	0	0
4	A	3	Total Co 3 3	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total Na 1 1	0	0
5	J	1	Total Na 1 1	0	0
5	D	1	Total Na 1 1	0	0
5	H	1	Total Na 1 1	0	0
5	B	1	Total Na 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	1	Total 1	Na 1	0	0
5	C	1	Total 1	Na 1	0	0
5	A	1	Total 1	Na 1	0	0

- Molecule 6 is water.

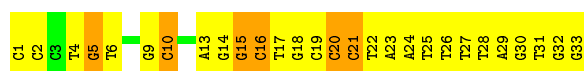
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total 2	O 2	0	0
6	B	3	Total 3	O 3	0	0
6	C	6	Total 6	O 6	0	0
6	D	7	Total 7	O 7	0	0
6	E	1	Total 1	O 1	0	0
6	F	7	Total 7	O 7	0	0
6	G	3	Total 3	O 3	0	0
6	H	5	Total 5	O 5	0	0
6	I	4	Total 4	O 4	0	0
6	J	2	Total 2	O 2	0	0
6	K	2	Total 2	O 2	0	0
6	L	9	Total 9	O 9	0	0

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

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

- Molecule 1: mbtA operator DNA

Chain E: 



- Molecule 1: mbtA operator DNA

Chain K: 



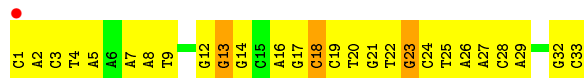
- Molecule 2: mbtB operator DNA

Chain F: 



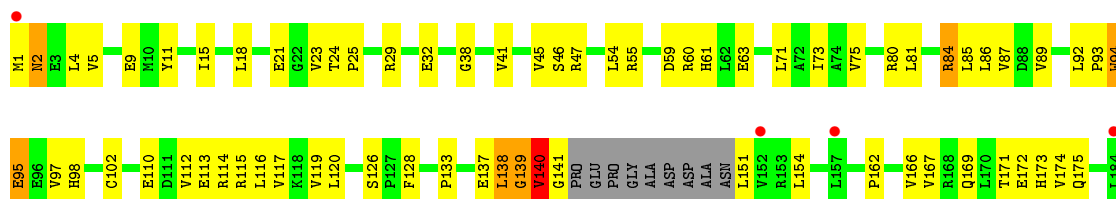
- Molecule 2: mbtB operator DNA

Chain L: 



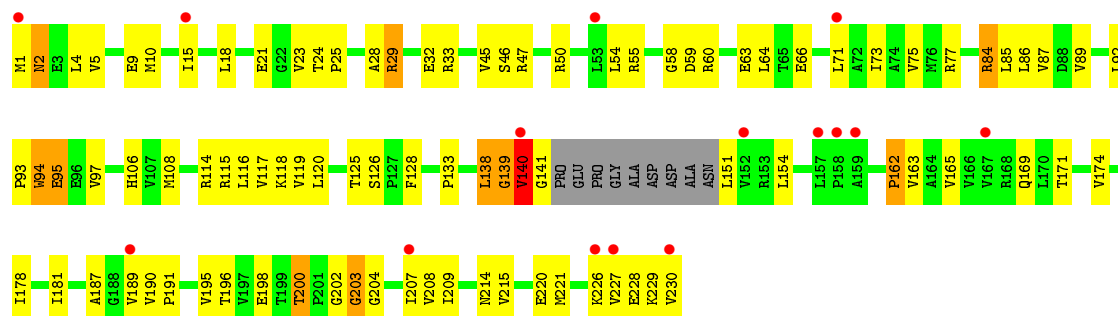
- Molecule 3: Iron-dependent repressor ideR

Chain A: 

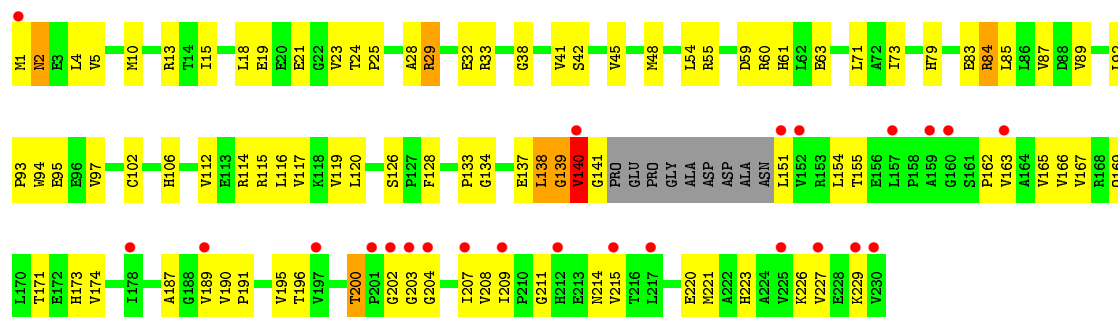




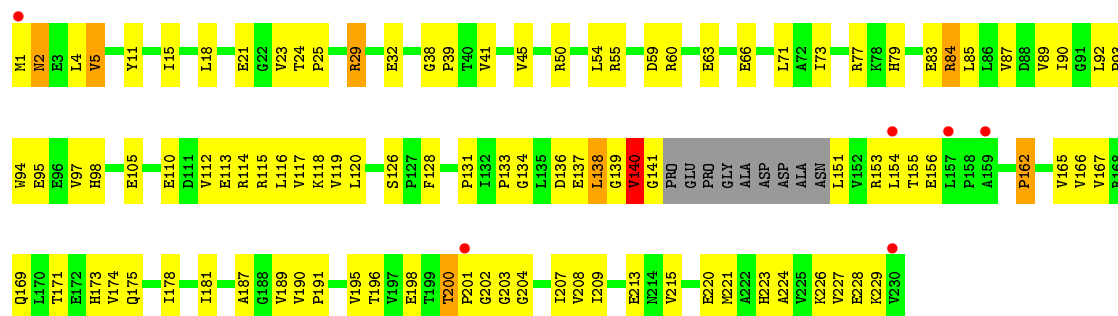
• Molecule 3: Iron-dependent repressor ideR



• Molecule 3: Iron-dependent repressor ideR



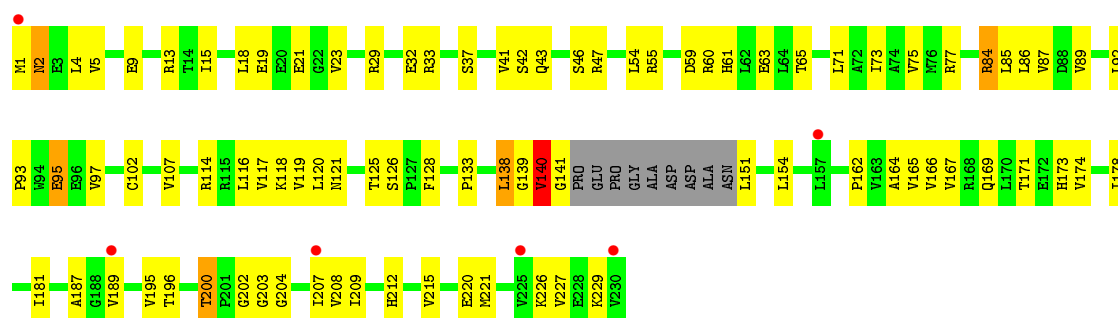
• Molecule 3: Iron-dependent repressor ideR



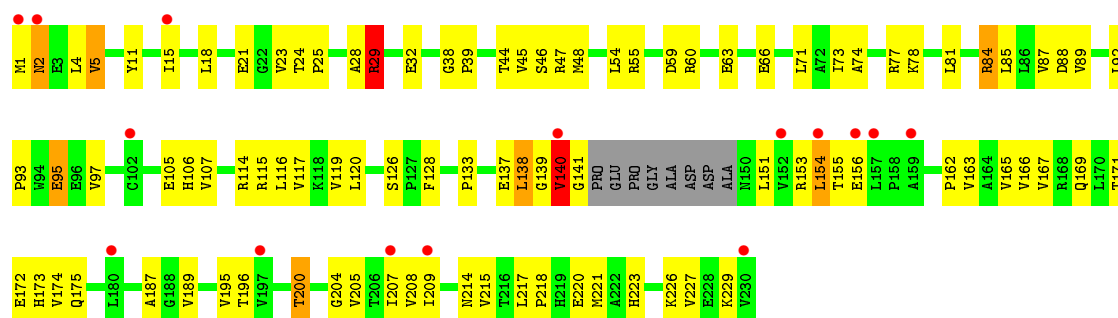
• Molecule 3: Iron-dependent repressor ideR



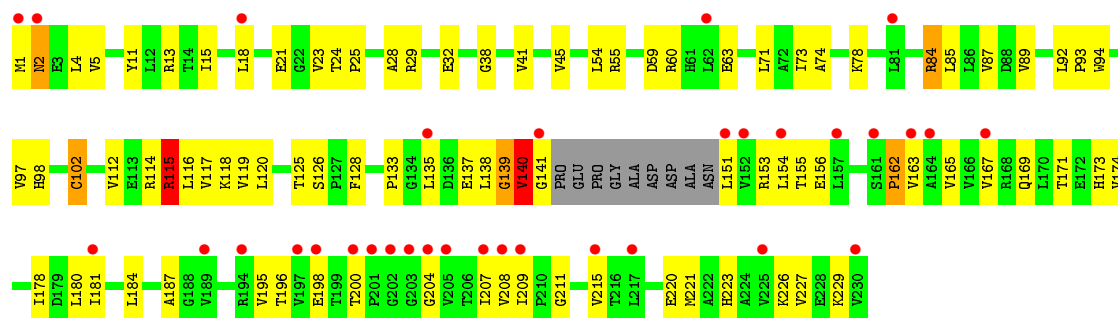




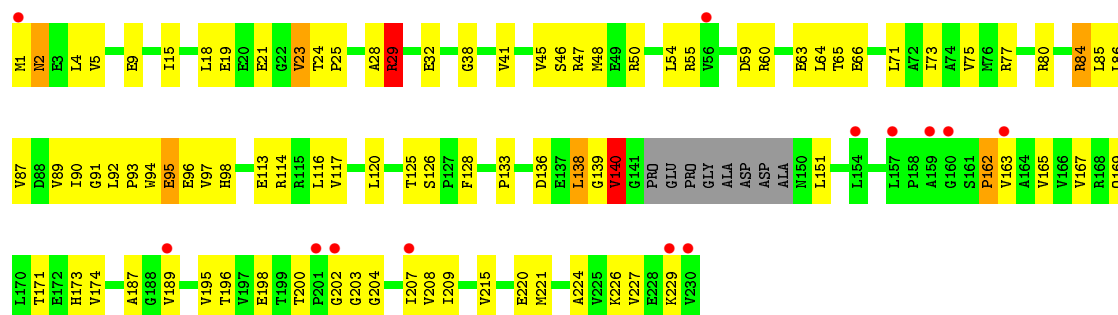
• Molecule 3: Iron-dependent repressor ideR



• Molecule 3: Iron-dependent repressor ideR



• Molecule 3: Iron-dependent repressor ideR



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.96Å 107.96Å 215.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.75 – 2.75 46.75 – 2.75	Depositor EDS
% Data completeness (in resolution range)	86.6 (46.75-2.75) 86.8 (46.75-2.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.81	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.74 (at 2.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.230 , 0.265 0.231 , 0.260	Depositor DCC
$R_{free}$ test set	3193 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.5	Xtriage
Anisotropy	0.886	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 69.0	EDS
Estimated twinning fraction	0.046 for -h,-k,l 0.106 for h,-h-k,-l 0.049 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 63213 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16481	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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: NA, CO

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	E	0.59	0/749	0.83	0/1154
1	K	0.56	0/749	0.83	0/1154
2	F	0.59	0/761	0.86	0/1173
2	L	0.55	0/761	0.86	0/1173
3	A	0.40	0/1737	0.69	2/2361 (0.1%)
3	B	0.35	0/1737	0.65	0/2361
3	C	0.35	0/1737	0.65	1/2361 (0.0%)
3	D	0.36	0/1737	0.64	0/2361
3	G	0.36	0/1737	0.64	0/2361
3	H	0.35	0/1745	0.68	3/2372 (0.1%)
3	I	0.35	0/1737	0.68	2/2361 (0.1%)
3	J	0.36	0/1745	0.65	1/2372 (0.0%)
All	All	0.41	0/16932	0.70	9/23564 (0.0%)

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	E	0	6
1	K	0	6
2	F	0	5
2	L	0	3
All	All	0	20

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	84	ARG	NE-CZ-NH1	-7.21	116.69	120.30
3	A	194	ARG	NE-CZ-NH1	-7.13	116.74	120.30
3	A	194	ARG	NE-CZ-NH2	6.93	123.77	120.30
3	I	115	ARG	NE-CZ-NH1	-6.82	116.89	120.30
3	I	115	ARG	NE-CZ-NH2	6.77	123.69	120.30
3	H	84	ARG	NE-CZ-NH2	6.16	123.38	120.30
3	J	29	ARG	NE-CZ-NH2	-5.13	117.74	120.30
3	C	29	ARG	NE-CZ-NH2	5.08	122.84	120.30
3	H	29	ARG	NE-CZ-NH2	-5.08	117.76	120.30

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	10	DC	Sidechain
1	E	15	DG	Sidechain
1	E	16	DC	Sidechain
1	E	20	DC	Sidechain
1	E	21	DC	Sidechain
1	E	5	DG	Sidechain
2	F	13	DG	Sidechain
2	F	14	DG	Sidechain
2	F	18	DC	Sidechain
2	F	23	DG	Sidechain
2	F	24	DC	Sidechain
1	K	10	DC	Sidechain
1	K	11	DA	Sidechain
1	K	15	DG	Sidechain
1	K	16	DC	Sidechain
1	K	20	DC	Sidechain
1	K	21	DC	Sidechain
2	L	13	DG	Sidechain
2	L	18	DC	Sidechain
2	L	23	DG	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	E	670	0	375	42	0
1	K	670	0	375	40	0
2	F	677	0	371	32	0
2	L	677	0	371	33	0
3	A	1711	0	1748	66	0
3	B	1711	0	1748	81	0
3	C	1711	0	1748	79	0
3	D	1711	0	1748	88	0
3	G	1711	0	1748	70	0
3	H	1719	0	1754	83	0
3	I	1711	0	1748	76	0
3	J	1719	0	1754	84	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
4	G	3	0	0	0	0
4	H	3	0	0	0	0
4	I	3	0	0	0	0
4	J	3	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
6	A	2	0	0	1	0
6	B	3	0	0	1	0
6	C	6	0	0	1	0
6	D	7	0	0	0	0
6	E	1	0	0	0	0
6	F	7	0	0	0	0
6	G	3	0	0	1	0
6	H	5	0	0	0	0
6	I	4	0	0	1	0
6	J	2	0	0	0	0
6	K	2	0	0	0	0
6	L	9	0	0	0	0
All	All	16481	0	15488	753	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 24.

All (753) 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)
3:H:84:ARG:HG3	3:H:120:LEU:HD13	1.33	1.06
1:E:28:DT:H2"	1:E:29:DA:H5"	1.39	1.05
1:K:28:DT:H2"	1:K:29:DA:H5"	1.36	1.03
2:F:2:DA:H2"	2:F:3:DC:H5'	1.45	0.98
1:K:23:DA:H2"	1:K:24:DA:H5"	1.48	0.93
2:L:2:DA:H2"	2:L:3:DC:H5'	1.49	0.92
1:K:4:DT:H2"	1:K:5:DG:H5"	1.49	0.92
1:E:4:DT:H2"	1:E:5:DG:H5"	1.52	0.91
3:A:92:LEU:HD12	3:A:93:PRO:HD2	1.52	0.91
1:E:23:DA:H2"	1:E:24:DA:H5"	1.53	0.91
3:D:92:LEU:HD12	3:D:93:PRO:HD2	1.52	0.90
3:I:92:LEU:HD12	3:I:93:PRO:HD2	1.54	0.90
3:B:92:LEU:HD12	3:B:93:PRO:HD2	1.53	0.89
3:G:174:VAL:HA	3:G:221:MET:HE1	1.56	0.87
1:E:24:DA:H2"	1:E:25:DT:C5'	2.05	0.87
1:K:24:DA:H2"	1:K:25:DT:H5"	1.56	0.86
3:A:171:THR:HB	6:A:1102:HOH:O	1.74	0.86
3:J:92:LEU:HD12	3:J:93:PRO:HD2	1.59	0.85
3:J:87:VAL:HG23	3:J:97:VAL:HG11	1.57	0.85
1:K:24:DA:H2"	1:K:25:DT:C5'	2.05	0.85
2:F:26:DA:H1'	2:F:27:DA:H5'	1.59	0.85
3:G:92:LEU:HD12	3:G:93:PRO:HD2	1.60	0.84
2:L:16:DA:H2"	2:L:17:DG:H5'	1.58	0.83
1:E:24:DA:H2"	1:E:25:DT:H5"	1.60	0.83
3:D:174:VAL:HA	3:D:221:MET:HE1	1.61	0.83
2:L:26:DA:H1'	2:L:27:DA:H5'	1.60	0.82
3:A:174:VAL:HA	3:A:221:MET:HE1	1.59	0.82
3:C:87:VAL:HG23	3:C:97:VAL:HG11	1.62	0.82
3:B:85:LEU:HD22	3:B:116:LEU:HD21	1.61	0.81
3:C:1:MET:HG3	3:C:2:ASN:H	1.43	0.81
3:D:1:MET:HG3	3:D:2:ASN:H	1.45	0.81
3:C:92:LEU:HD12	3:C:93:PRO:HD2	1.62	0.81
2:F:12:DG:H1'	2:F:13:DG:H5"	1.61	0.81
1:K:23:DA:C2'	1:K:24:DA:H5"	2.12	0.80
3:A:85:LEU:HD22	3:A:116:LEU:HD21	1.62	0.80
2:F:19:DC:H2'	2:F:20:DT:H72	1.64	0.80
3:A:18:LEU:HD22	3:A:23:VAL:CG2	2.11	0.80
3:G:1:MET:HG3	3:G:2:ASN:H	1.46	0.79
1:E:23:DA:C2'	1:E:24:DA:H5"	2.14	0.77
3:D:85:LEU:HD22	3:D:116:LEU:HD21	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1:MET:HG3	3:A:2:ASN:H	1.49	0.77
3:B:1:MET:HG3	3:B:2:ASN:H	1.49	0.77
3:C:85:LEU:HD22	3:C:116:LEU:HD21	1.65	0.77
3:H:87:VAL:HG23	3:H:97:VAL:HG11	1.66	0.77
2:L:12:DG:H1'	2:L:13:DG:H5''	1.67	0.77
3:J:85:LEU:HD22	3:J:116:LEU:HD21	1.67	0.76
1:K:4:DT:C2'	1:K:5:DG:H5''	2.15	0.76
3:B:174:VAL:HA	3:B:221:MET:HE1	1.67	0.76
3:C:1:MET:HG3	3:C:2:ASN:N	1.98	0.76
2:F:4:DT:H2''	2:F:5:DA:C8	2.21	0.76
3:B:203:GLY:HA2	6:B:2103:HOH:O	1.85	0.76
3:H:1:MET:HG3	3:H:2:ASN:H	1.51	0.76
3:I:171:THR:O	3:I:174:VAL:HG12	1.86	0.75
3:J:1:MET:HG3	3:J:2:ASN:H	1.51	0.75
1:K:28:DT:C2'	1:K:29:DA:H5''	2.15	0.74
2:F:16:DA:H2''	2:F:17:DG:H5'	1.68	0.74
3:C:171:THR:O	3:C:174:VAL:HG12	1.88	0.74
2:F:19:DC:H5'	2:F:19:DC:H6	1.53	0.74
1:K:4:DT:H2''	1:K:5:DG:C5'	2.16	0.74
3:I:1:MET:HG3	3:I:2:ASN:H	1.53	0.74
3:J:174:VAL:HA	3:J:221:MET:HE1	1.70	0.73
3:D:171:THR:O	3:D:174:VAL:HG12	1.89	0.73
2:L:19:DC:H5'	2:L:19:DC:H6	1.53	0.73
3:H:85:LEU:HD22	3:H:116:LEU:HD21	1.70	0.73
2:L:4:DT:H2''	2:L:5:DA:C8	2.24	0.73
1:K:19:DC:H2''	1:K:20:DC:H5'	1.70	0.73
3:D:1:MET:HG3	3:D:2:ASN:N	2.03	0.73
3:I:174:VAL:HA	3:I:221:MET:HE1	1.72	0.72
1:E:13:DA:H2''	1:E:14:DG:H5'	1.70	0.72
3:J:171:THR:O	3:J:174:VAL:HG12	1.90	0.72
1:E:30:DG:H2''	1:E:31:DT:H5'	1.71	0.72
3:A:1:MET:HG3	3:A:2:ASN:N	2.05	0.71
3:B:209:ILE:N	3:B:209:ILE:HD12	2.05	0.71
1:E:4:DT:C2'	1:E:5:DG:H5''	2.20	0.71
3:I:1:MET:HG3	3:I:2:ASN:N	2.05	0.71
3:D:220:GLU:HG3	3:D:221:MET:N	2.06	0.71
3:C:89:VAL:HG11	3:D:89:VAL:HG11	1.73	0.71
1:E:28:DT:C2'	1:E:29:DA:H5''	2.18	0.70
1:K:24:DA:H2'	1:K:25:DT:H71	1.73	0.70
3:D:87:VAL:HG23	3:D:97:VAL:HG11	1.71	0.70
3:B:84:ARG:HB3	3:B:120:LEU:HD13	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:171:THR:HB	6:I:7108:HOH:O	1.92	0.70
3:B:171:THR:O	3:B:174:VAL:HG12	1.92	0.70
3:A:171:THR:O	3:A:174:VAL:HG12	1.91	0.70
3:C:174:VAL:HA	3:C:221:MET:HE1	1.74	0.69
3:J:1:MET:HG3	3:J:2:ASN:N	2.06	0.69
3:G:220:GLU:HG3	3:G:221:MET:N	2.08	0.69
3:C:220:GLU:HG3	3:C:221:MET:N	2.08	0.69
3:A:87:VAL:HG23	3:A:97:VAL:HG11	1.74	0.69
3:H:174:VAL:HA	3:H:221:MET:HE1	1.72	0.69
3:J:220:GLU:HG3	3:J:221:MET:N	2.08	0.69
3:G:1:MET:HG3	3:G:2:ASN:N	2.07	0.69
3:I:87:VAL:HG23	3:I:97:VAL:HG11	1.75	0.69
3:B:87:VAL:HG23	3:B:97:VAL:HG11	1.73	0.69
1:E:9:DG:H1'	1:E:10:DC:H5''	1.74	0.69
3:H:171:THR:O	3:H:174:VAL:HG12	1.93	0.69
1:E:4:DT:H2''	1:E:5:DG:C5'	2.23	0.68
2:L:19:DC:H2'	2:L:20:DT:H72	1.73	0.68
3:G:87:VAL:HG23	3:G:97:VAL:HG11	1.75	0.68
3:B:220:GLU:HG3	3:B:221:MET:N	2.09	0.68
1:K:24:DA:C2'	1:K:25:DT:H5''	2.22	0.68
3:H:1:MET:HG3	3:H:2:ASN:N	2.08	0.68
1:K:30:DG:H2''	1:K:31:DT:H5'	1.74	0.68
3:D:55:ARG:HH22	3:D:63:GLU:HG2	1.58	0.68
3:B:1:MET:HG3	3:B:2:ASN:N	2.08	0.68
3:I:85:LEU:HD22	3:I:116:LEU:HD21	1.76	0.67
1:E:24:DA:H2''	1:E:25:DT:H5'	1.75	0.67
3:B:73:ILE:HG23	3:B:133:PRO:HB2	1.77	0.67
1:E:24:DA:C2'	1:E:25:DT:H5''	2.23	0.67
2:F:1:DC:H2''	2:F:2:DA:C8	2.29	0.67
3:H:55:ARG:HH22	3:H:63:GLU:HG2	1.60	0.67
2:F:7:DA:H1'	2:F:8:DA:H5''	1.77	0.67
3:H:84:ARG:CG	3:H:120:LEU:HD13	2.20	0.66
3:C:1:MET:HE1	3:C:5:VAL:HG13	1.77	0.66
3:G:212:HIS:NE2	6:G:5108:HOH:O	2.24	0.66
3:D:209:ILE:N	3:D:209:ILE:HD12	2.10	0.66
3:J:18:LEU:HD22	3:J:23:VAL:CG2	2.25	0.66
3:C:220:GLU:HG3	3:C:221:MET:H	1.61	0.66
1:K:18:DG:H2''	1:K:19:DC:H5''	1.77	0.66
3:G:55:ARG:HH22	3:G:63:GLU:HG2	1.60	0.66
3:J:209:ILE:N	3:J:209:ILE:HD12	2.11	0.66
2:L:1:DC:H2''	2:L:2:DA:C8	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:220:GLU:HG3	3:I:221:MET:N	2.10	0.65
3:B:18:LEU:HD22	3:B:23:VAL:CG2	2.27	0.65
3:I:84:ARG:HB3	3:I:120:LEU:HD13	1.78	0.64
3:A:151:LEU:HD12	3:A:227:VAL:O	1.97	0.64
1:K:24:DA:H2''	1:K:25:DT:H5'	1.79	0.64
3:A:209:ILE:N	3:A:209:ILE:HD12	2.11	0.64
3:C:55:ARG:HH22	3:C:63:GLU:HG2	1.63	0.64
3:D:220:GLU:HG3	3:D:221:MET:H	1.61	0.63
1:E:25:DT:H1'	1:E:26:DT:H5'	1.80	0.63
3:G:220:GLU:HG3	3:G:221:MET:H	1.63	0.63
3:I:209:ILE:HD12	3:I:209:ILE:N	2.12	0.63
3:C:1:MET:HE2	3:C:5:VAL:HA	1.80	0.63
3:B:45:VAL:HG13	3:B:54:LEU:HD11	1.81	0.63
3:D:55:ARG:NH2	3:D:63:GLU:HG2	2.14	0.63
3:I:139:GLY:O	3:I:140:VAL:HG13	1.99	0.63
3:G:85:LEU:HD22	3:G:116:LEU:HD21	1.81	0.62
3:I:55:ARG:HH22	3:I:63:GLU:HG2	1.65	0.62
3:C:211:GLY:HA2	3:J:66:GLU:OE2	1.98	0.62
3:H:209:ILE:HD12	3:H:209:ILE:N	2.14	0.62
3:C:209:ILE:N	3:C:209:ILE:HD12	2.13	0.62
3:G:84:ARG:HB3	3:G:120:LEU:HD13	1.81	0.62
3:A:18:LEU:HD22	3:A:23:VAL:HG21	1.81	0.62
3:H:139:GLY:O	3:H:140:VAL:HG13	1.99	0.62
3:H:18:LEU:HD22	3:H:23:VAL:CG2	2.30	0.61
3:A:220:GLU:HG3	3:A:221:MET:N	2.14	0.61
3:H:92:LEU:HD12	3:H:93:PRO:HD2	1.82	0.61
3:H:169:GLN:HB2	3:H:226:LYS:HB2	1.82	0.61
3:A:84:ARG:HB3	3:A:120:LEU:HD13	1.82	0.61
3:H:151:LEU:HD12	3:H:227:VAL:O	2.00	0.61
3:G:171:THR:O	3:G:174:VAL:HG12	2.00	0.61
2:L:22:DT:H2''	2:L:23:DG:H5'	1.83	0.61
3:D:151:LEU:HD12	3:D:227:VAL:O	2.00	0.61
2:F:21:DG:H2''	2:F:22:DT:H5'	1.83	0.61
1:K:9:DG:H1'	1:K:10:DC:H5''	1.81	0.61
2:L:7:DA:H1'	2:L:8:DA:H5''	1.83	0.61
3:H:220:GLU:HG3	3:H:221:MET:N	2.15	0.61
3:D:66:GLU:CD	3:I:211:GLY:HA2	2.21	0.61
3:G:18:LEU:HD22	3:G:23:VAL:CG2	2.31	0.61
3:D:84:ARG:HB3	3:D:120:LEU:HD13	1.82	0.61
2:F:19:DC:H2'	2:F:20:DT:C7	2.29	0.61
3:C:38:GLY:O	3:C:41:VAL:HG22	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:13:ARG:NH2	3:I:102:CYS:SG	2.74	0.60
3:B:58:GLY:HA3	3:H:66:GLU:HG2	1.83	0.60
3:A:114:ARG:O	3:A:117:VAL:HB	2.01	0.60
3:J:220:GLU:HG3	3:J:221:MET:H	1.66	0.60
1:K:23:DA:H2"	1:K:24:DA:C5'	2.25	0.60
1:E:19:DC:H2"	1:E:20:DC:H5'	1.84	0.60
2:L:3:DC:H2"	2:L:4:DT:H5'	1.82	0.60
3:C:45:VAL:HG13	3:C:54:LEU:HD11	1.84	0.60
2:F:22:DT:H2"	2:F:23:DG:H5'	1.84	0.60
3:D:114:ARG:HG3	3:D:138:LEU:HD21	1.84	0.59
3:C:29:ARG:HH11	3:C:32:GLU:CD	2.05	0.59
2:F:3:DC:H2"	2:F:4:DT:H5'	1.82	0.59
3:C:55:ARG:NH2	3:C:63:GLU:HG2	2.16	0.59
1:E:23:DA:H2"	1:E:24:DA:C5'	2.29	0.59
3:I:187:ALA:O	3:I:209:ILE:HG21	2.03	0.59
3:A:200:THR:HG22	3:A:204:GLY:N	2.17	0.59
1:E:5:DG:C8	1:E:6:DT:H72	2.38	0.59
3:H:200:THR:HG22	3:H:204:GLY:N	2.17	0.59
3:G:207:ILE:HB	3:G:215:VAL:CG1	2.32	0.59
3:J:55:ARG:HH22	3:J:63:GLU:HG2	1.68	0.59
3:D:195:VAL:HG21	3:D:207:ILE:HG22	1.84	0.59
3:D:187:ALA:O	3:D:209:ILE:HG21	2.03	0.59
3:G:55:ARG:NH2	3:G:63:GLU:HG2	2.17	0.59
3:J:139:GLY:O	3:J:140:VAL:HG13	2.03	0.59
3:C:18:LEU:HD22	3:C:23:VAL:CG2	2.32	0.59
2:L:2:DA:H2"	2:L:3:DC:C5'	2.30	0.59
1:K:18:DG:C2'	1:K:19:DC:H5"	2.33	0.59
3:J:209:ILE:H	3:J:209:ILE:HD12	1.67	0.59
3:C:187:ALA:O	3:C:209:ILE:HG21	2.03	0.58
3:I:115:ARG:HD3	3:J:91:GLY:C	2.23	0.58
3:H:187:ALA:O	3:H:209:ILE:HG21	2.04	0.58
1:E:18:DG:H2"	1:E:19:DC:H5"	1.86	0.58
3:A:21:GLU:OE2	3:A:173:HIS:HB2	2.03	0.58
3:H:73:ILE:HG23	3:H:133:PRO:HB2	1.85	0.58
2:F:19:DC:C2'	2:F:20:DT:H72	2.34	0.58
3:H:1:MET:CE	3:H:5:VAL:HG13	2.35	0.57
3:A:55:ARG:HH22	3:A:63:GLU:HG2	1.67	0.57
1:K:18:DG:H2"	1:K:19:DC:C5'	2.34	0.57
1:K:19:DC:H2"	1:K:20:DC:C5'	2.34	0.57
3:B:187:ALA:O	3:B:209:ILE:HG21	2.04	0.57
3:G:200:THR:HG22	3:G:204:GLY:N	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:45:VAL:HG13	3:I:54:LEU:HD11	1.87	0.57
3:B:18:LEU:HD22	3:B:23:VAL:HG21	1.86	0.57
3:C:84:ARG:HB3	3:C:120:LEU:HD13	1.85	0.57
3:A:73:ILE:HG23	3:A:133:PRO:HB2	1.86	0.57
3:J:84:ARG:HB3	3:J:120:LEU:HD13	1.85	0.57
3:A:115:ARG:O	3:A:119:VAL:HG23	2.05	0.57
3:J:187:ALA:O	3:J:209:ILE:HG21	2.04	0.57
2:F:32:DG:H2"	2:F:33:DC:OP2	2.04	0.57
3:C:73:ILE:HG23	3:C:133:PRO:HB2	1.85	0.57
3:J:9:GLU:HG2	3:J:75:VAL:HG21	1.86	0.57
3:A:200:THR:HG22	3:A:204:GLY:H	1.70	0.57
3:G:209:ILE:HD12	3:G:209:ILE:N	2.20	0.57
3:I:18:LEU:HD22	3:I:23:VAL:CG2	2.35	0.57
3:J:84:ARG:NH1	3:J:125:THR:O	2.37	0.56
3:C:200:THR:HG22	3:C:204:GLY:N	2.19	0.56
1:K:13:DA:H2"	1:K:14:DG:C5'	2.34	0.56
3:B:200:THR:HG22	3:B:204:GLY:N	2.20	0.56
3:B:174:VAL:HA	3:B:221:MET:CE	2.32	0.56
1:E:14:DG:H2"	1:E:15:DG:H5'	1.87	0.56
3:B:220:GLU:HG3	3:B:221:MET:H	1.69	0.56
3:A:9:GLU:HG2	3:A:75:VAL:HG21	1.88	0.56
3:D:4:LEU:O	3:D:5:VAL:HB	2.05	0.56
3:I:114:ARG:O	3:I:117:VAL:HB	2.06	0.56
3:B:209:ILE:HD12	3:B:209:ILE:H	1.71	0.56
3:C:151:LEU:HD12	3:C:227:VAL:O	2.06	0.56
3:C:139:GLY:O	3:C:140:VAL:HG13	2.05	0.56
3:A:29:ARG:HH11	3:A:32:GLU:CD	2.08	0.56
3:A:1:MET:HE2	3:A:5:VAL:HA	1.88	0.56
3:A:55:ARG:NH2	3:A:63:GLU:HG2	2.21	0.56
3:H:114:ARG:HG3	3:H:138:LEU:CD2	2.36	0.56
3:H:77:ARG:HD2	3:H:138:LEU:HD12	1.88	0.56
3:B:139:GLY:O	3:B:140:VAL:HG13	2.05	0.56
2:L:32:DG:H2"	2:L:33:DC:OP2	2.05	0.56
3:J:38:GLY:O	3:J:41:VAL:HG22	2.06	0.56
3:A:4:LEU:O	3:A:5:VAL:HB	2.06	0.55
3:H:4:LEU:O	3:H:5:VAL:HB	2.06	0.55
3:A:220:GLU:HG3	3:A:221:MET:H	1.70	0.55
1:K:25:DT:H1'	1:K:26:DT:H5'	1.88	0.55
3:A:167:VAL:HA	3:A:227:VAL:HG12	1.87	0.55
3:D:29:ARG:NH1	3:D:32:GLU:OE1	2.39	0.55
3:B:200:THR:HG22	3:B:204:GLY:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:4:LEU:O	3:I:5:VAL:HB	2.06	0.55
3:H:200:THR:HG22	3:H:204:GLY:H	1.70	0.55
3:G:200:THR:HG22	3:G:204:GLY:H	1.71	0.55
2:L:21:DG:H2''	2:L:22:DT:H5'	1.88	0.55
3:D:114:ARG:HG3	3:D:138:LEU:CD2	2.37	0.55
3:B:55:ARG:HH22	3:B:63:GLU:HG2	1.71	0.55
3:J:21:GLU:OE2	3:J:173:HIS:HB2	2.07	0.55
3:A:94:TRP:O	3:A:97:VAL:HG22	2.07	0.55
3:G:207:ILE:HB	3:G:215:VAL:HG13	1.89	0.55
3:J:18:LEU:HD22	3:J:23:VAL:HG21	1.88	0.55
3:I:55:ARG:NH2	3:I:63:GLU:HG2	2.22	0.55
2:F:2:DA:H2''	2:F:3:DC:C5'	2.26	0.54
3:B:29:ARG:NH1	3:B:32:GLU:OE1	2.40	0.54
3:J:85:LEU:HD12	3:J:89:VAL:HB	1.89	0.54
2:L:19:DC:H2'	2:L:20:DT:C7	2.37	0.54
3:C:209:ILE:H	3:C:209:ILE:HD12	1.72	0.54
3:H:167:VAL:HA	3:H:227:VAL:HG12	1.89	0.54
3:A:11:TYR:O	3:A:15:ILE:HG12	2.08	0.54
3:B:9:GLU:HG2	3:B:75:VAL:HG21	1.90	0.54
3:B:4:LEU:O	3:B:5:VAL:HB	2.08	0.54
3:G:200:THR:HG22	3:G:204:GLY:CA	2.38	0.54
3:I:18:LEU:HD22	3:I:23:VAL:HG21	1.89	0.54
3:D:38:GLY:O	3:D:41:VAL:HG22	2.07	0.54
2:L:16:DA:C2'	2:L:17:DG:H5'	2.34	0.54
3:B:84:ARG:NH1	3:B:125:THR:O	2.41	0.54
3:H:105:GLU:HG2	3:H:106:HIS:CD2	2.42	0.54
3:G:187:ALA:O	3:G:209:ILE:HG21	2.08	0.54
3:G:151:LEU:HD12	3:G:227:VAL:O	2.08	0.54
1:E:18:DG:H2''	1:E:19:DC:C5'	2.38	0.54
3:J:55:ARG:NH2	3:J:63:GLU:HG2	2.23	0.54
3:C:200:THR:HG22	3:C:204:GLY:H	1.72	0.54
3:J:207:ILE:HB	3:J:215:VAL:CG1	2.38	0.54
3:D:200:THR:HG22	3:D:204:GLY:N	2.23	0.54
3:D:139:GLY:O	3:D:140:VAL:HG13	2.08	0.54
3:H:55:ARG:NH2	3:H:63:GLU:HG2	2.22	0.53
3:C:167:VAL:HA	3:C:227:VAL:HG12	1.90	0.53
2:L:1:DC:H2''	2:L:2:DA:N7	2.24	0.53
3:I:21:GLU:OE2	3:I:173:HIS:HB2	2.08	0.53
3:H:45:VAL:O	3:H:48:MET:HB2	2.09	0.53
3:G:59:ASP:O	3:G:60:ARG:HB2	2.07	0.53
1:E:5:DG:H2'	1:E:6:DT:C7	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:4:LEU:O	3:G:5:VAL:HB	2.08	0.53
3:A:1:MET:HE1	3:A:5:VAL:HG13	1.91	0.53
3:J:1:MET:HE1	3:J:5:VAL:HA	1.91	0.53
3:B:55:ARG:NH2	3:B:63:GLU:HG2	2.24	0.53
3:J:200:THR:HG22	3:J:204:GLY:N	2.24	0.53
3:H:59:ASP:O	3:H:60:ARG:HB2	2.09	0.53
3:J:45:VAL:HG13	3:J:54:LEU:HD11	1.91	0.53
3:A:86:LEU:HB3	3:A:97:VAL:HG12	1.89	0.53
1:E:1:DC:H5'	1:E:1:DC:H6	1.72	0.53
3:C:21:GLU:OE2	3:C:173:HIS:HB2	2.09	0.53
3:G:9:GLU:HG2	3:G:75:VAL:HG21	1.91	0.53
3:B:95:GLU:OE2	3:B:95:GLU:N	2.37	0.53
3:I:220:GLU:HG3	3:I:221:MET:H	1.73	0.53
3:D:59:ASP:O	3:D:60:ARG:HB2	2.08	0.53
3:B:169:GLN:HB2	3:B:226:LYS:HB2	1.91	0.53
2:F:1:DC:H2''	2:F:2:DA:N7	2.23	0.53
3:C:4:LEU:O	3:C:5:VAL:HB	2.08	0.53
3:A:209:ILE:HD12	3:A:209:ILE:H	1.73	0.53
3:I:151:LEU:HD12	3:I:227:VAL:O	2.09	0.53
3:G:139:GLY:O	3:G:140:VAL:HG13	2.09	0.53
3:I:115:ARG:HG2	3:J:90:ILE:HG22	1.90	0.52
1:K:14:DG:H2''	1:K:15:DG:H5'	1.91	0.52
1:K:11:DA:H2''	1:K:12:DC:C6	2.43	0.52
3:H:44:THR:O	3:H:48:MET:HG3	2.09	0.52
3:A:139:GLY:O	3:A:140:VAL:HG13	2.09	0.52
2:L:3:DC:H2''	2:L:4:DT:C5'	2.40	0.52
1:E:5:DG:H2'	1:E:6:DT:H72	1.91	0.52
3:A:195:VAL:HG21	3:A:207:ILE:HG22	1.91	0.52
2:F:4:DT:H2''	2:F:5:DA:N7	2.25	0.52
3:I:89:VAL:HG11	3:J:89:VAL:HG11	1.91	0.52
3:A:187:ALA:O	3:A:209:ILE:HG21	2.10	0.52
3:H:196:THR:OG1	3:H:208:VAL:HB	2.10	0.52
2:L:4:DT:H2''	2:L:5:DA:N7	2.24	0.52
3:J:86:LEU:HB3	3:J:97:VAL:HG12	1.91	0.52
3:C:169:GLN:NE2	3:C:226:LYS:HD2	2.25	0.52
3:I:200:THR:HG22	3:I:204:GLY:N	2.24	0.52
3:D:209:ILE:H	3:D:209:ILE:HD12	1.74	0.52
3:I:209:ILE:HD12	3:I:209:ILE:H	1.74	0.52
3:H:18:LEU:HD22	3:H:23:VAL:HG21	1.90	0.52
3:J:73:ILE:HG23	3:J:133:PRO:HB2	1.91	0.52
3:A:110:GLU:O	3:A:113:GLU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:119:VAL:O	3:I:119:VAL:HG12	2.08	0.52
3:C:28:ALA:O	3:C:32:GLU:HG3	2.10	0.52
3:I:162:PRO:HD3	3:I:198:GLU:OE2	2.09	0.52
3:B:114:ARG:O	3:B:117:VAL:HB	2.08	0.52
3:H:74:ALA:O	3:H:78:LYS:HG3	2.08	0.52
3:H:1:MET:HE1	3:H:5:VAL:HG22	1.92	0.52
1:K:13:DA:H2''	1:K:14:DG:H5'	1.90	0.52
1:K:15:DG:H1'	1:K:16:DC:H5'	1.91	0.52
3:B:200:THR:HG22	3:B:204:GLY:CA	2.40	0.52
3:C:55:ARG:NH2	6:C:3108:HOH:O	2.43	0.51
3:I:73:ILE:HG23	3:I:133:PRO:HB2	1.91	0.51
3:G:95:GLU:OE2	3:G:95:GLU:N	2.41	0.51
3:I:126:SER:C	3:I:128:PHE:H	2.13	0.51
2:F:3:DC:H2''	2:F:4:DT:C5'	2.40	0.51
1:E:13:DA:H2''	1:E:14:DG:C5'	2.37	0.51
1:E:18:DG:C2'	1:E:19:DC:H5''	2.39	0.51
3:B:207:ILE:HB	3:B:215:VAL:HG13	1.92	0.51
3:G:209:ILE:HD12	3:G:209:ILE:H	1.74	0.51
3:B:10:MET:SD	3:B:106:HIS:CE1	3.04	0.51
3:I:28:ALA:O	3:I:32:GLU:HG3	2.11	0.51
3:J:151:LEU:HD12	3:J:227:VAL:O	2.11	0.51
3:D:200:THR:HG22	3:D:204:GLY:H	1.75	0.51
3:G:89:VAL:HG11	3:H:89:VAL:HG11	1.92	0.51
2:F:19:DC:C2'	2:F:20:DT:C7	2.89	0.51
3:H:195:VAL:HG21	3:H:207:ILE:HG22	1.92	0.51
2:L:18:DC:H2''	2:L:19:DC:H5'	1.93	0.51
3:B:207:ILE:HB	3:B:215:VAL:CG1	2.40	0.51
3:H:84:ARG:HD3	3:H:88:ASP:OD2	2.11	0.51
3:C:200:THR:HG22	3:C:204:GLY:CA	2.41	0.51
3:D:115:ARG:O	3:D:119:VAL:HG23	2.11	0.51
3:J:95:GLU:N	3:J:95:GLU:OE2	2.39	0.51
1:K:27:DT:H1'	1:K:28:DT:H5''	1.91	0.51
2:L:8:DA:C8	2:L:9:DT:H72	2.45	0.51
3:D:21:GLU:OE2	3:D:173:HIS:HB2	2.10	0.51
1:E:27:DT:H1'	1:E:28:DT:H5''	1.93	0.50
3:I:1:MET:HE1	3:I:5:VAL:HG22	1.92	0.50
3:G:46:SER:O	3:G:47:ARG:C	2.49	0.50
3:C:211:GLY:HA2	3:J:66:GLU:CD	2.32	0.50
1:K:11:DA:H2''	1:K:12:DC:H6	1.76	0.50
3:B:59:ASP:O	3:B:60:ARG:HB2	2.11	0.50
3:C:112:VAL:HG22	3:D:92:LEU:HD22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:13:DG:H2"	2:F:14:DG:H8	1.77	0.50
3:J:15:ILE:HG21	3:J:64:LEU:HD21	1.93	0.50
3:H:220:GLU:HG3	3:H:221:MET:H	1.77	0.50
3:J:28:ALA:O	3:J:32:GLU:HG3	2.11	0.50
3:J:77:ARG:HD2	3:J:138:LEU:HD12	1.94	0.50
3:H:29:ARG:NH1	3:H:32:GLU:OE1	2.45	0.50
2:F:16:DA:H1'	2:F:17:DG:H5"	1.92	0.50
2:F:19:DC:H5'	2:F:19:DC:C6	2.42	0.50
3:I:174:VAL:HA	3:I:221:MET:CE	2.41	0.50
3:J:114:ARG:O	3:J:117:VAL:HB	2.12	0.50
3:H:1:MET:HE1	3:H:5:VAL:HG13	1.93	0.49
1:E:15:DG:H1'	1:E:16:DC:H5'	1.94	0.49
3:C:114:ARG:HG3	3:C:138:LEU:CD2	2.42	0.49
3:J:114:ARG:HG3	3:J:138:LEU:CD2	2.43	0.49
1:E:9:DG:H2"	1:E:10:DC:C5'	2.43	0.49
3:J:215:VAL:HG13	3:J:215:VAL:O	2.12	0.49
3:H:200:THR:HG22	3:H:204:GLY:CA	2.42	0.49
3:J:200:THR:HG22	3:J:204:GLY:CA	2.43	0.49
3:B:15:ILE:HG21	3:B:64:LEU:CD2	2.42	0.49
3:B:50:ARG:HG2	3:B:50:ARG:O	2.12	0.49
3:J:18:LEU:HD11	3:J:29:ARG:CB	2.42	0.49
3:B:15:ILE:HG21	3:B:64:LEU:HD21	1.93	0.49
2:L:22:DT:H73	3:J:47:ARG:NH1	2.28	0.49
1:K:1:DC:H2"	1:K:2:DC:C6	2.48	0.49
3:H:215:VAL:HG13	3:H:215:VAL:O	2.12	0.49
3:G:18:LEU:HD22	3:G:23:VAL:HG21	1.95	0.49
3:A:200:THR:HG22	3:A:204:GLY:CA	2.43	0.49
3:I:200:THR:HG22	3:I:204:GLY:CA	2.43	0.49
3:A:207:ILE:HB	3:A:215:VAL:CG1	2.43	0.49
3:I:74:ALA:O	3:I:78:LYS:HG3	2.13	0.49
2:L:19:DC:H2"	2:L:20:DT:C6	2.48	0.49
2:F:21:DG:H2"	2:F:22:DT:C5'	2.43	0.49
3:H:114:ARG:HG3	3:H:138:LEU:HD21	1.95	0.49
3:C:195:VAL:HG23	3:C:209:ILE:HA	1.95	0.48
3:G:54:LEU:HA	3:G:65:THR:HG23	1.95	0.48
1:E:9:DG:C1'	1:E:10:DC:H5"	2.43	0.48
3:G:29:ARG:HH11	3:G:32:GLU:CD	2.16	0.48
3:I:38:GLY:O	3:I:41:VAL:HG22	2.13	0.48
3:C:87:VAL:CG2	3:C:97:VAL:HG11	2.40	0.48
3:H:209:ILE:HD12	3:H:209:ILE:H	1.78	0.48
3:J:59:ASP:O	3:J:60:ARG:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:166:VAL:HG13	3:D:166:VAL:O	2.14	0.48
3:C:10:MET:SD	3:C:106:HIS:CE1	3.06	0.48
3:C:92:LEU:HD22	3:D:112:VAL:HG22	1.93	0.48
3:J:174:VAL:HA	3:J:221:MET:CE	2.41	0.48
3:B:151:LEU:HD12	3:B:227:VAL:O	2.13	0.48
1:K:32:DG:H2''	1:K:33:DG:C8	2.48	0.48
3:H:207:ILE:HB	3:H:215:VAL:CG1	2.44	0.48
3:I:200:THR:HG22	3:I:204:GLY:H	1.77	0.48
3:J:169:GLN:HB2	3:J:226:LYS:HB2	1.96	0.48
3:A:126:SER:C	3:A:128:PHE:H	2.17	0.48
3:A:112:VAL:HG22	3:B:92:LEU:HD22	1.96	0.48
3:B:108:MET:HE1	3:B:116:LEU:HD12	1.96	0.48
2:F:12:DG:C1'	2:F:13:DG:H5''	2.38	0.48
3:J:46:SER:O	3:J:47:ARG:C	2.51	0.48
3:A:215:VAL:HG13	3:A:215:VAL:O	2.14	0.48
3:D:1:MET:HE1	3:D:5:VAL:HG22	1.96	0.48
1:E:16:DC:C2'	1:E:17:DT:H72	2.44	0.48
3:I:115:ARG:HD3	3:J:91:GLY:O	2.14	0.48
3:C:169:GLN:HB2	3:C:226:LYS:HB2	1.96	0.48
3:H:174:VAL:HA	3:H:221:MET:CE	2.43	0.47
3:G:114:ARG:O	3:G:117:VAL:HB	2.14	0.47
3:H:4:LEU:O	3:H:5:VAL:CB	2.62	0.47
3:H:1:MET:HE1	3:H:5:VAL:HA	1.96	0.47
3:B:209:ILE:HD11	3:B:215:VAL:HG12	1.95	0.47
3:I:163:VAL:O	3:I:196:THR:HA	2.14	0.47
3:D:202:GLY:O	3:D:204:GLY:N	2.48	0.47
3:D:73:ILE:HG23	3:D:133:PRO:HB2	1.96	0.47
3:B:215:VAL:HG13	3:B:215:VAL:O	2.15	0.47
3:I:207:ILE:HB	3:I:215:VAL:CG1	2.44	0.47
2:L:28:DC:H2''	2:L:29:DA:OP2	2.14	0.47
3:D:174:VAL:HA	3:D:221:MET:CE	2.39	0.47
2:L:19:DC:C6	2:L:19:DC:H5'	2.41	0.47
3:G:73:ILE:HG23	3:G:133:PRO:HB2	1.95	0.47
3:G:77:ARG:HD2	3:G:138:LEU:HD12	1.96	0.47
3:I:196:THR:OG1	3:I:208:VAL:HB	2.14	0.47
3:A:95:GLU:N	3:A:95:GLU:OE2	2.42	0.47
3:I:59:ASP:O	3:I:60:ARG:HB2	2.14	0.47
3:D:169:GLN:CD	3:D:226:LYS:HD2	2.34	0.47
3:C:59:ASP:O	3:C:60:ARG:HB2	2.15	0.47
3:A:38:GLY:O	3:A:41:VAL:HG22	2.15	0.47
3:C:163:VAL:O	3:C:196:THR:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:89:VAL:HG11	3:B:89:VAL:HG11	1.96	0.47
3:C:134:GLY:HA2	3:C:137:GLU:OE1	2.14	0.47
3:D:1:MET:HE1	3:D:5:VAL:HG13	1.96	0.47
3:D:200:THR:HG22	3:D:204:GLY:CA	2.44	0.47
1:K:1:DC:H5'	1:K:1:DC:H6	1.80	0.47
3:H:155:THR:HG21	3:H:223:HIS:CD2	2.50	0.47
1:E:32:DG:H2''	1:E:33:DG:C8	2.48	0.47
3:H:126:SER:C	3:H:128:PHE:H	2.18	0.47
3:J:1:MET:CE	3:J:5:VAL:HG13	2.45	0.46
3:G:84:ARG:NH1	3:G:125:THR:O	2.47	0.46
3:D:169:GLN:HB2	3:D:226:LYS:HB2	1.97	0.46
3:I:221:MET:HB3	3:I:221:MET:HE2	1.79	0.46
3:C:215:VAL:HG13	3:C:215:VAL:O	2.15	0.46
3:B:66:GLU:OE1	3:H:59:ASP:OD2	2.33	0.46
3:H:165:VAL:HG12	3:H:229:LYS:HA	1.97	0.46
3:A:174:VAL:HA	3:A:221:MET:CE	2.39	0.46
3:B:202:GLY:O	3:B:204:GLY:N	2.48	0.46
3:C:114:ARG:O	3:C:117:VAL:HB	2.15	0.46
3:G:21:GLU:OE2	3:G:173:HIS:HB2	2.14	0.46
3:D:155:THR:HG21	3:D:223:HIS:CD2	2.50	0.46
3:I:1:MET:HE1	3:I:5:VAL:HA	1.97	0.46
3:J:77:ARG:NE	3:J:113:GLU:OE1	2.48	0.46
3:G:114:ARG:HG3	3:G:138:LEU:CD2	2.46	0.46
3:C:59:ASP:OD1	3:C:61:HIS:ND1	2.46	0.46
1:K:9:DG:H2''	1:K:10:DC:C5'	2.45	0.46
3:A:140:VAL:HB	3:A:141:GLY:H	1.51	0.46
3:A:59:ASP:O	3:A:60:ARG:HB2	2.16	0.46
3:J:200:THR:HG22	3:J:204:GLY:H	1.78	0.46
3:H:208:VAL:HA	3:H:214:ASN:OD1	2.15	0.46
3:D:79:HIS:O	3:D:83:GLU:HG3	2.16	0.46
3:C:24:THR:HA	3:C:25:PRO:HD3	1.79	0.46
3:D:162:PRO:HD3	3:D:198:GLU:OE2	2.15	0.46
3:A:1:MET:O	3:A:2:ASN:HB2	2.15	0.46
3:B:221:MET:HE2	3:B:221:MET:HB3	1.85	0.46
3:J:202:GLY:O	3:J:204:GLY:N	2.49	0.46
3:H:28:ALA:O	3:H:32:GLU:HG3	2.16	0.46
3:H:153:ARG:O	3:H:156:GLU:N	2.48	0.46
3:J:195:VAL:HG21	3:J:207:ILE:HG22	1.97	0.46
1:K:13:DA:H2''	1:K:14:DG:H5''	1.98	0.46
3:J:45:VAL:O	3:J:48:MET:HB2	2.16	0.46
3:I:153:ARG:O	3:I:156:GLU:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:86:LEU:HB3	3:G:97:VAL:HG12	1.96	0.46
3:D:165:VAL:HG12	3:D:229:LYS:HA	1.97	0.46
3:J:94:TRP:O	3:J:97:VAL:HG22	2.16	0.46
3:J:1:MET:O	3:J:2:ASN:HB2	2.16	0.46
3:C:174:VAL:HA	3:C:221:MET:CE	2.44	0.46
3:H:166:VAL:HG13	3:H:166:VAL:O	2.15	0.46
3:B:195:VAL:HG23	3:B:209:ILE:HA	1.97	0.45
3:G:215:VAL:O	3:G:215:VAL:HG13	2.15	0.45
3:D:202:GLY:C	3:D:204:GLY:H	2.19	0.45
3:H:209:ILE:HD11	3:H:215:VAL:HG12	1.99	0.45
3:B:140:VAL:HB	3:B:141:GLY:H	1.51	0.45
3:I:29:ARG:HH11	3:I:32:GLU:CD	2.19	0.45
3:J:171:THR:OG1	3:J:224:ALA:HB1	2.16	0.45
3:A:45:VAL:HG13	3:A:54:LEU:HD11	1.98	0.45
3:D:1:MET:O	3:D:2:ASN:HB2	2.16	0.45
3:H:1:MET:O	3:H:2:ASN:HB2	2.17	0.45
3:A:81:LEU:O	3:A:84:ARG:HB2	2.16	0.45
2:F:21:DG:H1'	2:F:22:DT:H5''	1.98	0.45
3:I:24:THR:HA	3:I:25:PRO:HD3	1.79	0.45
3:I:118:LYS:HD3	3:I:118:LYS:HA	1.85	0.45
2:F:19:DC:H2''	2:F:20:DT:C6	2.51	0.45
3:J:221:MET:HB3	3:J:221:MET:HE2	1.82	0.45
3:D:171:THR:OG1	3:D:224:ALA:HB1	2.16	0.45
2:L:13:DG:OP2	3:I:28:ALA:HB2	2.16	0.45
3:B:4:LEU:O	3:B:5:VAL:CB	2.64	0.45
3:D:195:VAL:HG23	3:D:208:VAL:O	2.17	0.45
3:G:169:GLN:HB2	3:G:226:LYS:HB2	1.98	0.45
3:I:11:TYR:O	3:I:15:ILE:HG12	2.17	0.45
3:A:98:HIS:CG	3:A:175:GLN:HB3	2.52	0.45
3:C:209:ILE:HD11	3:C:215:VAL:HG12	1.99	0.45
3:D:29:ARG:NH1	3:D:32:GLU:CD	2.69	0.45
3:B:118:LYS:HD3	3:B:118:LYS:HA	1.84	0.45
3:H:95:GLU:OE2	3:H:95:GLU:N	2.41	0.45
3:G:119:VAL:HG12	3:G:119:VAL:O	2.17	0.45
3:G:1:MET:HE1	3:G:5:VAL:HG22	1.98	0.45
3:C:207:ILE:HB	3:C:215:VAL:CG1	2.47	0.45
1:K:13:DA:C2'	1:K:14:DG:H5''	2.47	0.45
3:D:134:GLY:HA2	3:D:137:GLU:OE1	2.17	0.45
3:D:59:ASP:O	3:D:60:ARG:CB	2.65	0.45
3:J:15:ILE:HG21	3:J:64:LEU:CD2	2.47	0.45
3:A:46:SER:O	3:A:47:ARG:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:46:SER:O	3:B:47:ARG:C	2.55	0.45
1:E:21:DC:C2'	1:E:22:DT:H72	2.47	0.45
2:L:13:DG:H2''	2:L:14:DG:H8	1.81	0.44
3:H:163:VAL:O	3:H:196:THR:HA	2.17	0.44
3:J:15:ILE:O	3:J:19:GLU:HG3	2.17	0.44
3:H:11:TYR:O	3:H:15:ILE:HG12	2.17	0.44
3:G:165:VAL:HG12	3:G:229:LYS:HA	1.98	0.44
3:J:126:SER:C	3:J:128:PHE:H	2.19	0.44
3:H:172:GLU:O	3:H:175:GLN:HB2	2.16	0.44
3:D:190:VAL:HB	3:D:191:PRO:CD	2.47	0.44
3:H:1:MET:HE3	3:H:5:VAL:HG13	2.00	0.44
3:D:195:VAL:HG21	3:D:207:ILE:CG2	2.48	0.44
3:C:195:VAL:HG21	3:C:207:ILE:HG22	1.99	0.44
3:G:120:LEU:O	3:G:121:ASN:HB2	2.17	0.44
3:C:202:GLY:O	3:C:204:GLY:N	2.50	0.44
3:D:38:GLY:N	3:D:39:PRO:CD	2.79	0.44
3:G:21:GLU:OE2	3:G:33:ARG:NH1	2.40	0.44
3:C:165:VAL:HG12	3:C:229:LYS:HA	1.99	0.44
3:C:95:GLU:OE2	3:C:95:GLU:N	2.37	0.44
2:F:18:DC:H2''	2:F:19:DC:H5'	1.98	0.44
3:H:140:VAL:HB	3:H:141:GLY:H	1.54	0.44
3:H:154:LEU:HD13	3:H:205:VAL:HG11	1.99	0.44
3:I:215:VAL:O	3:I:215:VAL:HG13	2.17	0.44
1:K:9:DG:OP1	3:G:29:ARG:NH2	2.48	0.44
3:A:59:ASP:OD1	3:A:61:HIS:ND1	2.50	0.44
3:J:196:THR:OG1	3:J:208:VAL:HB	2.17	0.44
2:L:22:DT:H2''	2:L:23:DG:C5'	2.48	0.44
3:A:204:GLY:O	3:A:205:VAL:HG23	2.18	0.44
1:E:1:DC:H2''	1:E:2:DC:C6	2.53	0.44
3:I:140:VAL:HB	3:I:141:GLY:H	1.56	0.44
3:C:18:LEU:HD23	3:C:33:ARG:NH1	2.33	0.44
3:J:114:ARG:HG3	3:J:138:LEU:HD21	2.00	0.44
3:D:196:THR:OG1	3:D:208:VAL:HB	2.17	0.44
1:K:16:DC:C2'	1:K:17:DT:H72	2.48	0.44
3:H:45:VAL:HG13	3:H:54:LEU:HD11	1.99	0.44
2:L:24:DC:C2'	2:L:25:DT:H72	2.48	0.44
3:C:155:THR:HG21	3:C:223:HIS:CD2	2.53	0.44
3:H:24:THR:HA	3:H:25:PRO:HD3	1.78	0.44
3:A:166:VAL:HG13	3:A:166:VAL:O	2.18	0.44
3:B:208:VAL:HA	3:B:214:ASN:OD1	2.17	0.44
3:I:112:VAL:HG22	3:J:92:LEU:HD22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4:LEU:O	3:D:5:VAL:CB	2.65	0.43
3:H:114:ARG:O	3:H:117:VAL:HB	2.17	0.43
3:H:46:SER:O	3:H:47:ARG:C	2.56	0.43
2:F:12:DG:C2'	2:F:13:DG:H5''	2.48	0.43
3:B:195:VAL:HG21	3:B:207:ILE:HG22	1.99	0.43
3:A:195:VAL:HG22	3:A:196:THR:N	2.33	0.43
3:D:98:HIS:CG	3:D:175:GLN:HB3	2.53	0.43
3:I:169:GLN:HB2	3:I:226:LYS:HB2	2.00	0.43
3:B:126:SER:C	3:B:128:PHE:H	2.22	0.43
2:L:12:DG:C1'	2:L:13:DG:H5''	2.43	0.43
3:D:167:VAL:HA	3:D:227:VAL:HG12	2.00	0.43
3:D:77:ARG:HD2	3:D:138:LEU:HD12	1.98	0.43
3:C:202:GLY:C	3:C:204:GLY:H	2.21	0.43
3:H:59:ASP:O	3:H:60:ARG:CB	2.66	0.43
3:G:1:MET:HE1	3:G:5:VAL:HA	2.00	0.43
3:D:195:VAL:HG22	3:D:196:THR:N	2.33	0.43
3:J:209:ILE:HD11	3:J:215:VAL:HG12	2.00	0.43
3:A:207:ILE:HB	3:A:215:VAL:HG13	1.99	0.43
3:J:80:ARG:HG2	3:J:126:SER:HB3	2.00	0.43
3:D:178:ILE:HA	3:D:181:ILE:HG22	2.01	0.43
3:A:171:THR:OG1	3:A:224:ALA:HB1	2.19	0.43
3:D:110:GLU:O	3:D:113:GLU:HB2	2.18	0.43
1:E:5:DG:H2''	1:E:6:DT:H6	1.84	0.43
3:J:97:VAL:HG23	3:J:98:HIS:N	2.33	0.43
3:J:195:VAL:HG23	3:J:209:ILE:HA	2.00	0.43
3:J:202:GLY:C	3:J:204:GLY:H	2.22	0.43
3:C:169:GLN:CD	3:C:226:LYS:HD2	2.39	0.43
3:D:79:HIS:HB2	3:D:105:GLU:OE1	2.18	0.43
3:D:24:THR:HA	3:D:25:PRO:HD3	1.78	0.43
3:G:118:LYS:HA	3:G:118:LYS:HD3	1.83	0.43
3:B:77:ARG:HD2	3:B:138:LEU:HD12	1.99	0.43
3:I:1:MET:O	3:I:2:ASN:HB2	2.18	0.43
1:E:14:DG:H2''	1:E:15:DG:C5'	2.48	0.43
3:H:218:PRO:HD2	3:H:221:MET:HB2	2.00	0.43
3:C:196:THR:OG1	3:C:208:VAL:HB	2.18	0.43
3:D:126:SER:C	3:D:128:PHE:H	2.21	0.43
3:D:209:ILE:HD11	3:D:215:VAL:HG12	2.00	0.43
3:C:140:VAL:HB	3:C:141:GLY:H	1.53	0.43
3:G:54:LEU:CA	3:G:65:THR:HG23	2.49	0.43
3:D:136:ASP:OD1	3:D:137:GLU:OE1	2.36	0.43
3:B:196:THR:OG1	3:B:208:VAL:HB	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:178:ILE:O	3:D:181:ILE:HG22	2.18	0.43
3:G:15:ILE:O	3:G:19:GLU:HG3	2.19	0.43
3:B:85:LEU:HD12	3:B:89:VAL:HB	2.00	0.43
3:J:4:LEU:O	3:J:5:VAL:HB	2.18	0.43
3:G:202:GLY:O	3:G:204:GLY:N	2.51	0.43
3:I:155:THR:HG21	3:I:223:HIS:CD2	2.53	0.43
3:G:126:SER:C	3:G:128:PHE:H	2.22	0.43
3:C:190:VAL:HB	3:C:191:PRO:CD	2.49	0.43
3:D:45:VAL:HG13	3:D:54:LEU:HD11	2.00	0.43
3:G:59:ASP:O	3:G:60:ARG:CB	2.66	0.42
1:E:9:DG:C2'	1:E:10:DC:H5''	2.49	0.42
3:I:84:ARG:NH1	3:I:125:THR:O	2.52	0.42
3:J:163:VAL:O	3:J:196:THR:HA	2.19	0.42
2:F:28:DC:H2''	2:F:29:DA:OP2	2.19	0.42
3:A:169:GLN:HB2	3:A:226:LYS:HB2	2.00	0.42
3:B:178:ILE:HA	3:B:181:ILE:HG22	2.02	0.42
3:J:162:PRO:HD3	3:J:198:GLU:OE2	2.19	0.42
3:C:166:VAL:O	3:C:166:VAL:HG13	2.19	0.42
3:B:1:MET:HE1	3:B:5:VAL:HA	2.01	0.42
3:I:126:SER:C	3:I:128:PHE:N	2.73	0.42
3:C:115:ARG:O	3:C:119:VAL:HG23	2.19	0.42
3:H:217:LEU:HA	3:H:218:PRO:HD3	1.92	0.42
3:C:45:VAL:O	3:C:48:MET:HB2	2.20	0.42
3:I:165:VAL:HG12	3:I:229:LYS:HA	2.00	0.42
3:D:118:LYS:HD3	3:D:118:LYS:HA	1.84	0.42
1:K:5:DG:H2'	1:K:6:DT:H72	2.01	0.42
3:C:1:MET:O	3:C:2:ASN:HB2	2.20	0.42
3:D:207:ILE:HB	3:D:215:VAL:CG1	2.49	0.42
3:D:77:ARG:NH1	3:D:138:LEU:HB2	2.34	0.42
3:D:153:ARG:O	3:D:156:GLU:N	2.50	0.42
3:D:50:ARG:O	3:D:50:ARG:HG2	2.20	0.42
3:C:207:ILE:HB	3:C:215:VAL:HG13	2.01	0.42
3:B:169:GLN:CD	3:B:226:LYS:HD2	2.40	0.42
3:D:134:GLY:HA2	3:D:137:GLU:CD	2.39	0.42
3:C:190:VAL:HB	3:C:191:PRO:HD2	2.02	0.42
3:A:24:THR:HA	3:A:25:PRO:HD3	1.79	0.42
3:C:15:ILE:O	3:C:19:GLU:HG3	2.20	0.42
3:G:166:VAL:HG13	3:G:166:VAL:O	2.20	0.42
2:F:21:DG:C8	2:F:22:DT:H72	2.54	0.42
3:G:209:ILE:HD11	3:G:215:VAL:HG12	2.01	0.42
3:C:13:ARG:NH2	3:C:102:CYS:SG	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:167:VAL:HA	3:G:227:VAL:HG12	2.01	0.42
3:C:79:HIS:O	3:C:83:GLU:HG3	2.19	0.42
3:C:1:MET:CE	3:C:5:VAL:HA	2.49	0.42
3:C:85:LEU:HD21	3:D:90:ILE:HD11	2.02	0.42
3:B:94:TRP:O	3:B:97:VAL:HG22	2.19	0.42
3:I:207:ILE:HB	3:I:215:VAL:HG13	2.01	0.42
1:K:13:DA:H1'	1:K:14:DG:H5''	2.02	0.42
3:G:140:VAL:HB	3:G:141:GLY:H	1.53	0.42
3:I:209:ILE:HD11	3:I:215:VAL:HG12	2.02	0.42
3:H:207:ILE:HB	3:H:215:VAL:HG13	2.00	0.42
3:G:195:VAL:HG23	3:G:209:ILE:HA	2.02	0.42
3:H:84:ARG:CD	3:H:88:ASP:OD2	2.68	0.41
3:H:174:VAL:HG23	3:H:221:MET:HE1	2.01	0.41
3:H:81:LEU:O	3:H:84:ARG:HB3	2.20	0.41
3:J:94:TRP:C	3:J:96:GLU:H	2.23	0.41
3:I:94:TRP:O	3:I:97:VAL:HG22	2.20	0.41
3:B:15:ILE:HG21	3:B:64:LEU:HG	2.02	0.41
3:I:181:ILE:HD12	3:I:181:ILE:HA	1.97	0.41
3:J:50:ARG:O	3:J:50:ARG:HG2	2.20	0.41
1:K:21:DC:H2''	1:K:22:DT:H71	2.02	0.41
3:I:4:LEU:O	3:I:5:VAL:CB	2.69	0.41
3:D:207:ILE:HB	3:D:215:VAL:HG13	2.01	0.41
3:J:165:VAL:HG12	3:J:229:LYS:HA	2.02	0.41
3:I:135:LEU:HD23	3:I:135:LEU:HA	1.87	0.41
3:C:85:LEU:HD12	3:C:89:VAL:HB	2.01	0.41
2:L:21:DG:H2''	2:L:22:DT:C5'	2.50	0.41
3:B:163:VAL:O	3:B:196:THR:HA	2.20	0.41
3:G:13:ARG:NH2	3:G:102:CYS:SG	2.93	0.41
3:D:11:TYR:O	3:D:15:ILE:HG12	2.20	0.41
3:G:4:LEU:O	3:G:5:VAL:CB	2.68	0.41
3:B:1:MET:O	3:B:2:ASN:HB2	2.20	0.41
1:E:9:DG:H2''	1:E:10:DC:H5'	2.03	0.41
3:I:167:VAL:HA	3:I:227:VAL:HG12	2.00	0.41
3:J:136:ASP:C	3:J:138:LEU:H	2.23	0.41
3:D:131:PRO:O	3:D:133:PRO:HD3	2.21	0.41
3:A:190:VAL:HB	3:A:191:PRO:CD	2.50	0.41
3:H:38:GLY:N	3:H:39:PRO:CD	2.83	0.41
3:D:18:LEU:HD22	3:D:23:VAL:CG2	2.50	0.41
1:K:29:DA:H2''	1:K:30:DG:O5'	2.20	0.41
3:B:202:GLY:C	3:B:204:GLY:H	2.24	0.41
3:G:59:ASP:OD1	3:G:61:HIS:ND1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:208:VAL:HA	3:C:214:ASN:OD1	2.20	0.41
3:B:165:VAL:HG12	3:B:229:LYS:HA	2.03	0.41
3:B:21:GLU:OE2	3:B:33:ARG:NH1	2.44	0.41
3:B:18:LEU:HD11	3:B:29:ARG:CB	2.51	0.41
3:I:195:VAL:HG23	3:I:209:ILE:HA	2.03	0.41
2:L:21:DG:H1'	2:L:22:DT:H5''	2.01	0.41
1:E:21:DC:H2'	1:E:22:DT:H72	2.02	0.41
3:H:21:GLU:OE2	3:H:173:HIS:HB2	2.20	0.41
3:G:42:SER:O	3:G:43:GLN:C	2.59	0.41
3:B:24:THR:HA	3:B:25:PRO:HD3	1.77	0.41
3:H:87:VAL:CG2	3:H:97:VAL:HG11	2.44	0.41
3:B:86:LEU:HB3	3:B:97:VAL:HG12	2.03	0.41
3:C:41:VAL:HG23	3:C:42:SER:N	2.35	0.41
3:H:29:ARG:NH1	3:H:32:GLU:CD	2.74	0.41
3:J:24:THR:HA	3:J:25:PRO:HD3	1.82	0.41
3:B:115:ARG:O	3:B:119:VAL:HG23	2.20	0.41
2:L:2:DA:H1'	2:L:3:DC:H5''	2.02	0.41
2:F:18:DC:H2''	2:F:19:DC:OP2	2.21	0.41
3:I:1:MET:CE	3:I:5:VAL:HA	2.50	0.41
3:J:207:ILE:HB	3:J:215:VAL:HG13	2.02	0.41
3:B:28:ALA:O	3:B:32:GLU:HG3	2.21	0.41
3:D:202:GLY:C	3:D:204:GLY:N	2.74	0.41
3:A:196:THR:OG1	3:A:208:VAL:HB	2.21	0.41
3:J:167:VAL:HA	3:J:227:VAL:HG12	2.02	0.41
3:G:178:ILE:O	3:G:181:ILE:HG22	2.20	0.41
3:B:162:PRO:HD3	3:B:198:GLU:OE2	2.21	0.41
3:H:115:ARG:O	3:H:119:VAL:HG23	2.21	0.41
3:G:164:ALA:HA	3:G:196:THR:HG22	2.02	0.41
1:E:5:DG:C2'	1:E:6:DT:C7	2.99	0.41
3:D:221:MET:HE2	3:D:221:MET:HB3	1.82	0.41
3:D:114:ARG:O	3:D:117:VAL:HB	2.21	0.41
3:B:9:GLU:HG2	3:B:75:VAL:CG2	2.51	0.41
3:I:178:ILE:O	3:I:181:ILE:HG22	2.21	0.41
3:I:180:LEU:O	3:I:184:LEU:HG	2.21	0.41
3:J:29:ARG:HA	3:J:29:ARG:HD3	1.80	0.40
3:B:29:ARG:NH1	3:B:32:GLU:CD	2.75	0.40
3:A:195:VAL:HG23	3:A:208:VAL:O	2.21	0.40
3:B:228:GLU:HG2	3:B:230:VAL:HG23	2.04	0.40
3:G:107:VAL:HG21	3:H:107:VAL:HG21	2.03	0.40
3:B:190:VAL:HB	3:B:191:PRO:CD	2.50	0.40
3:C:126:SER:C	3:C:128:PHE:H	2.23	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:DT:H2"	1:E:27:DT:OP2	2.21	0.40
3:D:94:TRP:O	3:D:97:VAL:HG22	2.21	0.40
3:A:114:ARG:HG3	3:A:138:LEU:CD2	2.52	0.40
3:G:37:SER:O	3:G:41:VAL:HG13	2.22	0.40
3:I:97:VAL:HG23	3:I:98:HIS:N	2.37	0.40
3:G:202:GLY:C	3:G:204:GLY:H	2.25	0.40
3:D:200:THR:OG1	3:D:201:PRO:HD2	2.21	0.40
3:J:54:LEU:HA	3:J:65:THR:HG23	2.04	0.40
3:I:119:VAL:O	3:I:119:VAL:CG1	2.69	0.40
3:D:166:VAL:CG1	3:D:228:GLU:HB3	2.51	0.40
3:B:229:LYS:O	3:B:230:VAL:HG23	2.21	0.40
3:G:196:THR:OG1	3:G:208:VAL:HB	2.22	0.40
1:E:30:DG:C8	1:E:31:DT:H72	2.56	0.40
3:D:140:VAL:HB	3:D:141:GLY:H	1.49	0.40
3:J:15:ILE:HG21	3:J:64:LEU:HG	2.02	0.40
3:A:80:ARG:HH21	3:A:172:GLU:HG2	1.86	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	
3	A	217/230 (94%)	186 (86%)	24 (11%)	7 (3%)	5	15
3	B	217/230 (94%)	186 (86%)	23 (11%)	8 (4%)	4	12
3	C	217/230 (94%)	192 (88%)	18 (8%)	7 (3%)	5	15
3	D	217/230 (94%)	190 (88%)	18 (8%)	9 (4%)	3	10
3	G	217/230 (94%)	189 (87%)	21 (10%)	7 (3%)	5	15
3	H	218/230 (95%)	190 (87%)	21 (10%)	7 (3%)	5	15
3	I	217/230 (94%)	191 (88%)	21 (10%)	5 (2%)	8	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	J	218/230 (95%)	193 (88%)	19 (9%)	6 (3%)	6	18
All	All	1738/1840 (94%)	1517 (87%)	165 (10%)	56 (3%)	5	15

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	140	VAL
3	B	140	VAL
3	C	140	VAL
3	D	140	VAL
3	G	140	VAL
3	H	140	VAL
3	I	140	VAL
3	J	140	VAL
3	A	2	ASN
3	B	2	ASN
3	B	95	GLU
3	C	2	ASN
3	D	2	ASN
3	H	2	ASN
3	H	154	LEU
3	I	2	ASN
3	I	154	LEU
3	J	2	ASN
3	B	154	LEU
3	B	203	GLY
3	C	154	LEU
3	C	162	PRO
3	D	154	LEU
3	G	154	LEU
3	J	95	GLU
3	J	162	PRO
3	J	203	GLY
3	A	95	GLU
3	A	154	LEU
3	B	162	PRO
3	C	203	GLY
3	D	95	GLU
3	D	162	PRO
3	D	203	GLY
3	H	162	PRO
3	I	162	PRO

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Mol	Chain	Res	Type
3	D	189	VAL
3	D	213	GLU
3	G	2	ASN
3	G	95	GLU
3	G	203	GLY
3	H	95	GLU
3	H	189	VAL
3	A	162	PRO
3	B	189	VAL
3	G	189	VAL
3	J	189	VAL
3	A	189	VAL
3	C	189	VAL
3	D	5	VAL
3	G	162	PRO
3	H	5	VAL
3	I	139	GLY
3	A	139	GLY
3	B	139	GLY
3	C	139	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	
3	A	189/195 (97%)	181 (96%)	8 (4%)	36	68
3	B	189/195 (97%)	182 (96%)	7 (4%)	41	74
3	C	189/195 (97%)	183 (97%)	6 (3%)	46	78
3	D	189/195 (97%)	183 (97%)	6 (3%)	46	78
3	G	189/195 (97%)	184 (97%)	5 (3%)	54	84
3	H	190/195 (97%)	184 (97%)	6 (3%)	46	78
3	I	189/195 (97%)	182 (96%)	7 (4%)	41	74
3	J	190/195 (97%)	184 (97%)	6 (3%)	46	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1514/1560 (97%)	1463 (97%)	51 (3%)	44 76

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	71	LEU
3	A	84	ARG
3	A	94	TRP
3	A	102	CYS
3	A	137	GLU
3	A	138	LEU
3	A	140	VAL
3	A	200	THR
3	B	29	ARG
3	B	71	LEU
3	B	84	ARG
3	B	94	TRP
3	B	138	LEU
3	B	140	VAL
3	B	200	THR
3	C	71	LEU
3	C	84	ARG
3	C	94	TRP
3	C	138	LEU
3	C	140	VAL
3	C	200	THR
3	D	29	ARG
3	D	71	LEU
3	D	84	ARG
3	D	138	LEU
3	D	140	VAL
3	D	200	THR
3	G	71	LEU
3	G	84	ARG
3	G	138	LEU
3	G	140	VAL
3	G	200	THR
3	H	29	ARG
3	H	71	LEU
3	H	137	GLU
3	H	138	LEU
3	H	140	VAL

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Mol	Chain	Res	Type
3	H	200	THR
3	I	71	LEU
3	I	84	ARG
3	I	102	CYS
3	I	115	ARG
3	I	137	GLU
3	I	138	LEU
3	I	140	VAL
3	J	23	VAL
3	J	29	ARG
3	J	71	LEU
3	J	84	ARG
3	J	138	LEU
3	J	140	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	121	ASN
3	A	130	ASN
3	A	169	GLN
3	B	121	ASN
3	B	130	ASN
3	C	121	ASN
3	C	130	ASN
3	C	169	GLN
3	D	121	ASN
3	G	121	ASN
3	G	130	ASN
3	G	169	GLN
3	H	121	ASN
3	H	130	ASN
3	H	169	GLN
3	I	121	ASN
3	I	130	ASN
3	I	169	GLN
3	J	121	ASN
3	J	130	ASN
3	J	169	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](#)

Of 32 ligands modelled in this entry, 32 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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	E	33/33 (100%)	-0.36	0 100 100	46, 69, 122, 126	0
1	K	33/33 (100%)	-0.27	0 100 100	46, 75, 164, 173	0
2	F	33/33 (100%)	-0.35	0 100 100	43, 74, 106, 109	0
2	L	33/33 (100%)	-0.14	1 (3%) 54 47	50, 78, 151, 160	0
3	A	221/230 (96%)	0.19	7 (3%) 51 44	40, 73, 124, 170	3 (1%)
3	B	221/230 (96%)	0.35	15 (6%) 20 15	46, 82, 132, 152	3 (1%)
3	C	221/230 (96%)	0.54	24 (10%) 7 4	44, 83, 142, 199	3 (1%)
3	D	221/230 (96%)	0.25	6 (2%) 58 51	40, 74, 122, 166	3 (1%)
3	G	221/230 (96%)	0.25	6 (2%) 58 51	39, 73, 122, 171	3 (1%)
3	H	222/230 (96%)	0.40	15 (6%) 20 15	48, 82, 133, 176	3 (1%)
3	I	221/230 (96%)	0.67	33 (14%) 3 2	39, 85, 155, 200	3 (1%)
3	J	222/230 (96%)	0.28	13 (5%) 26 19	46, 74, 127, 146	3 (1%)
All	All	1902/1972 (96%)	0.32	120 (6%) 23 17	39, 79, 137, 200	24 (1%)

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	230	VAL	6.9
3	I	230	VAL	6.4
3	I	204	GLY	5.9
3	D	230	VAL	5.9
3	I	200	THR	5.9
3	I	197	VAL	5.7
3	I	205	VAL	5.5
3	B	230	VAL	5.4
3	C	201	PRO	5.1
3	C	207	ILE	5.1
3	I	163	VAL	4.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	C	157	LEU	4.8
3	C	160	GLY	4.4
3	H	152	VAL	4.4
3	I	201	PRO	4.3
3	B	189	VAL	4.3
3	B	1	MET	4.1
3	I	194	ARG	4.1
3	I	181	ILE	4.1
3	I	203	GLY	4.1
3	G	230	VAL	4.0
3	I	202	GLY	4.0
3	H	1	MET	3.9
3	C	159	ALA	3.9
3	H	230	VAL	3.9
3	I	157	LEU	3.9
3	I	207	ILE	3.7
3	B	207	ILE	3.7
3	I	209	ILE	3.7
3	B	15	ILE	3.7
3	H	197	VAL	3.7
3	G	157	LEU	3.6
3	J	202	GLY	3.6
3	B	226	LYS	3.4
3	A	230	VAL	3.4
3	J	1	MET	3.3
3	D	1	MET	3.3
3	I	1	MET	3.3
3	A	229	LYS	3.1
3	J	159	ALA	3.1
3	I	215	VAL	3.1
3	I	189	VAL	3.1
3	A	157	LEU	3.0
3	I	225	VAL	3.0
2	L	1	DC	3.0
3	B	157	LEU	3.0
3	A	152	VAL	3.0
3	C	225	VAL	3.0
3	H	159	ALA	2.9
3	B	227	VAL	2.9
3	I	217	LEU	2.9
3	C	202	GLY	2.9
3	G	207	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
3	J	207	ILE	2.9
3	J	229	LYS	2.9
3	H	140	VAL	2.8
3	D	201	PRO	2.8
3	C	197	VAL	2.8
3	B	71	LEU	2.7
3	G	225	VAL	2.7
3	H	2	ASN	2.7
3	J	230	VAL	2.7
3	I	154	LEU	2.7
3	C	152	VAL	2.7
3	C	227	VAL	2.7
3	C	163	VAL	2.6
3	I	208	VAL	2.6
3	D	159	ALA	2.6
3	H	154	LEU	2.6
3	I	62	LEU	2.6
3	C	140	VAL	2.6
3	A	184	LEU	2.6
3	J	157	LEU	2.6
3	J	163	VAL	2.6
3	J	201	PRO	2.5
3	B	159	ALA	2.5
3	I	141	GLY	2.5
3	J	56	VAL	2.5
3	H	157	LEU	2.4
3	C	1	MET	2.4
3	C	217	LEU	2.4
3	H	180	LEU	2.4
3	I	152	VAL	2.4
3	C	215	VAL	2.4
3	C	178	ILE	2.4
3	I	135	LEU	2.4
3	H	209	ILE	2.4
3	I	198	GLU	2.4
3	H	156	GLU	2.3
3	H	15	ILE	2.3
3	B	53	LEU	2.3
3	B	140	VAL	2.3
3	H	207	ILE	2.3
3	D	157	LEU	2.3
3	I	81	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
3	B	158	PRO	2.3
3	A	225	VAL	2.3
3	C	189	VAL	2.3
3	C	209	ILE	2.3
3	B	167	VAL	2.2
3	I	18	LEU	2.2
3	G	189	VAL	2.2
3	J	189	VAL	2.2
3	D	154	LEU	2.2
3	I	151	LEU	2.2
3	C	203	GLY	2.2
3	C	212	HIS	2.2
3	C	204	GLY	2.1
3	J	160	GLY	2.1
3	G	1	MET	2.1
3	I	2	ASN	2.1
3	I	161	SER	2.1
3	H	102	CYS	2.1
3	J	154	LEU	2.1
3	A	1	MET	2.0
3	C	229	LYS	2.0
3	I	167	VAL	2.0
3	B	152	VAL	2.0
3	C	151	LEU	2.0
3	I	164	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CO	B	2002	1/1	0.96	0.22	2.20	70,70,70,70	0
4	CO	I	7002	1/1	0.97	0.20	1.18	66,66,66,66	0
4	CO	H	6002	1/1	1.00	0.21	0.46	53,53,53,53	0
4	CO	A	1002	1/1	0.95	0.18	-0.27	60,60,60,60	0
4	CO	C	3002	1/1	0.98	0.18	-0.41	61,61,61,61	0
4	CO	J	8002	1/1	0.99	0.17	-1.35	55,55,55,55	0
4	CO	G	5002	1/1	0.98	0.13	-1.41	45,45,45,45	0
4	CO	D	4002	1/1	0.99	0.17	-1.47	48,48,48,48	0
5	NA	H	6106	1/1	0.88	0.53	-	59,59,59,59	0
4	CO	C	3001	1/1	0.99	0.14	-	67,67,67,67	0
4	CO	I	7003	1/1	0.96	0.13	-	90,90,90,90	0
4	CO	A	1003	1/1	0.96	0.15	-	73,73,73,73	0
5	NA	I	7107	1/1	0.88	0.22	-	50,50,50,50	0
5	NA	G	5105	1/1	0.94	0.10	-	51,51,51,51	0
5	NA	A	1101	1/1	0.91	0.07	-	65,65,65,65	0
5	NA	J	8108	1/1	0.96	0.30	-	50,50,50,50	0
4	CO	H	6003	1/1	0.95	0.19	-	85,85,85,85	0
4	CO	B	2003	1/1	0.96	0.13	-	85,85,85,85	0
4	CO	I	7001	1/1	0.97	0.13	-	73,73,73,73	0
4	CO	J	8003	1/1	0.97	0.17	-	78,78,78,78	0
4	CO	D	4003	1/1	0.99	0.18	-	73,73,73,73	0
5	NA	C	3103	1/1	0.81	0.21	-	58,58,58,58	0
4	CO	D	4001	1/1	0.99	0.15	-	56,56,56,56	0
5	NA	B	2102	1/1	0.91	0.32	-	41,41,41,41	0
4	CO	B	2001	1/1	0.98	0.14	-	67,67,67,67	0
4	CO	G	5003	1/1	0.99	0.16	-	76,76,76,76	0
4	CO	C	3003	1/1	0.98	0.14	-	73,73,73,73	0
4	CO	A	1001	1/1	0.98	0.13	-	65,65,65,65	0
5	NA	D	4104	1/1	0.92	0.39	-	50,50,50,50	0
4	CO	G	5001	1/1	0.99	0.11	-	52,52,52,52	0
4	CO	H	6001	1/1	0.97	0.17	-	66,66,66,66	0
4	CO	J	8001	1/1	0.99	0.16	-	56,56,56,56	0

## 6.5 Other polymers

There are no such residues in this entry.