



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:41 PM UTC

PDB ID : 1CVJ / pdb_00001cvj
Title : X-RAY CRYSTAL STRUCTURE OF THE POLY(A)-BINDING PROTEIN
IN COMPLEX WITH POLYADENYLATE RNA
Authors : Deo, R.C.; Bonanno, J.B.; Sonenberg, N.; Burley, S.K.
Deposited on : 1999-08-23
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

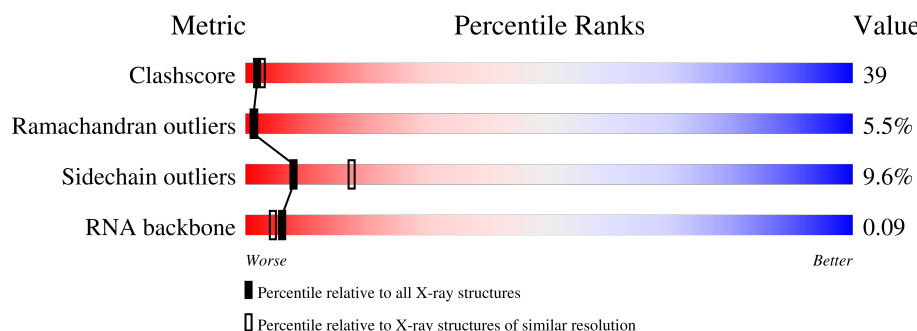
1 Overall quality at a glance

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	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RNA backbone	3983	1014 (2.84-2.36)

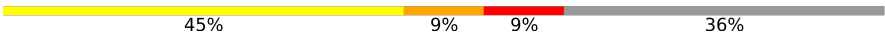
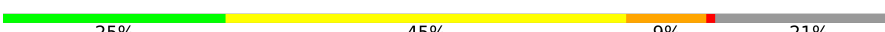
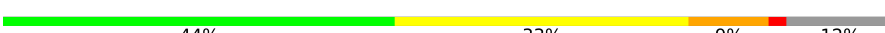
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	M	11	64% 9% 9% 18%
1	N	11	27% 36% 36%
1	O	11	27% 18% 9% 9% 36%
1	P	11	36% 27% 36%
1	Q	11	64% 9% 27%
1	R	11	9% 27% 18% 9% 36%

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Mol	Chain	Length	Quality of chain
1	S	11	
1	T	11	
2	A	190	
2	B	190	
2	C	190	
2	D	190	
2	E	190	
2	F	190	
2	G	190	
2	H	190	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11162 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 RNA chain called 5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	9	Total	C	N	O	P	36	0	0
			195	90	45	52	8			
1	N	7	Total	C	N	O	P	18	0	0
			151	70	35	40	6			
1	O	7	Total	C	N	O	P	18	0	0
			151	70	35	40	6			
1	P	7	Total	C	N	O	P	18	0	0
			151	70	35	40	6			
1	Q	8	Total	C	N	O	P	18	0	0
			173	80	40	46	7			
1	R	7	Total	C	N	O	P	36	0	0
			151	70	35	40	6			
1	S	7	Total	C	N	O	P	18	0	0
			151	70	35	40	6			
1	T	7	Total	C	N	O	P	18	0	0
			151	70	35	40	6			

- Molecule 2 is a protein called POLYADENYLATE BINDING PROTEIN 1.

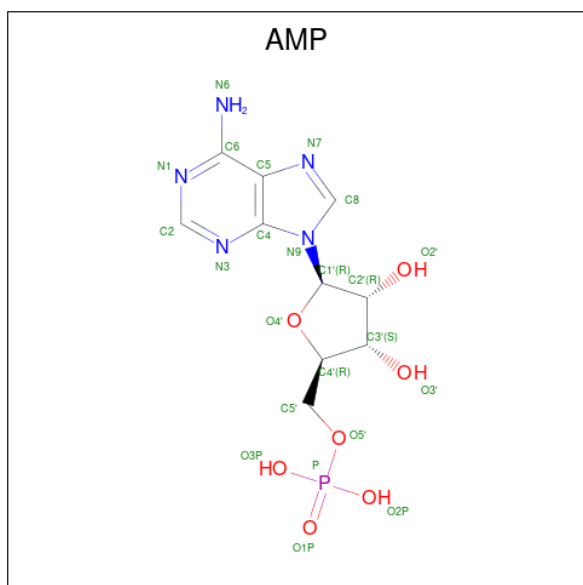
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	169	Total	C	N	O	S	0	0	0
			1298	821	232	236	9			
2	B	151	Total	C	N	O	S	0	0	0
			1178	749	206	215	8			
2	C	168	Total	C	N	O	S	0	0	0
			1291	821	228	233	9			
2	D	161	Total	C	N	O	S	0	0	0
			1253	797	219	228	9			
2	E	168	Total	C	N	O	S	0	0	0
			1315	834	233	239	9			
2	F	131	Total	C	N	O	S	0	0	0
			1028	658	178	185	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	165	Total	C	N	O	S	0	0	0
			1287	818	227	233	9			
2	H	132	Total	C	N	O	S	0	0	0
			1033	661	175	190	7			

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	N	1	Total	C	N	O	9	0
			19	10	5	4		
3	O	1	Total	C	N	O	9	0
			19	10	5	4		
3	Q	1	Total	C	N	O	9	0
			19	10	5	4		
3	S	1	Total	C	N	O	9	0
			19	10	5	4		
3	A	1	Total	C	N	O	9	0
			19	10	5	4		
3	D	1	Total	C	N	O	9	0
			19	10	5	4		
3	F	1	Total	C	N	O	9	0
			19	10	5	4		
3	H	1	Total	C	N	O	9	0
			19	10	5	4		

- Molecule 4 is water.

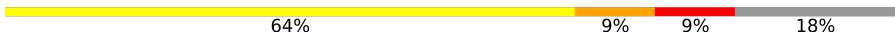
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	N	2	Total 2	O 2	0	0
4	O	2	Total 2	O 2	0	0
4	P	1	Total 1	O 1	0	0
4	Q	3	Total 3	O 3	0	0
4	T	2	Total 2	O 2	0	0
4	A	7	Total 7	O 7	0	0
4	B	5	Total 5	O 5	0	0
4	C	7	Total 7	O 7	0	0
4	D	3	Total 3	O 3	0	0
4	E	11	Total 11	O 11	0	0
4	F	3	Total 3	O 3	0	0
4	G	2	Total 2	O 2	0	0
4	H	5	Total 5	O 5	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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: 5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3'

Chain M: 

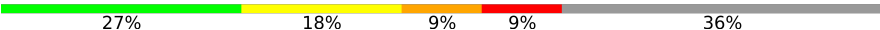


- Molecule 1: 5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3'

Chain N: 

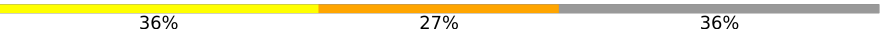


- Molecule 1: 5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3'

Chain O: 

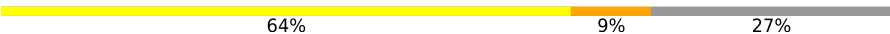


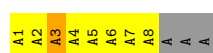
- Molecule 1: 5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3'

Chain P: 



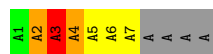
- Molecule 1: 5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3'

Chain Q: 



- Molecule 1: 5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3'

Chain R: 



- Molecule 1: 5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3'

Chain S: 

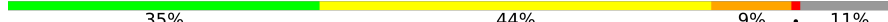


- Molecule 1: 5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3'

Chain T: 

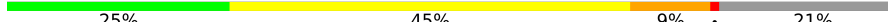


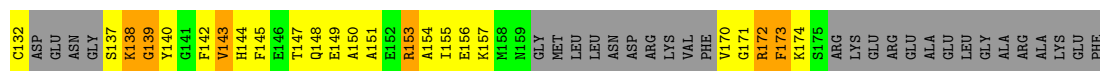
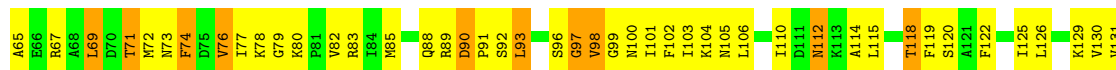
- Molecule 2: POLYADENYLATE BINDING PROTEIN 1

Chain A: 

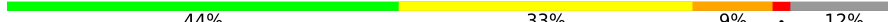


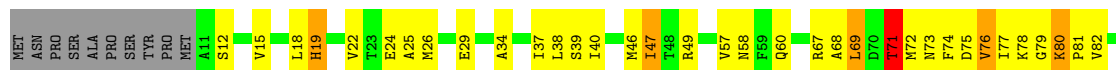
- Molecule 2: POLYADENYLATE BINDING PROTEIN 1

Chain B: 

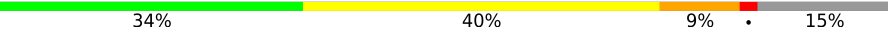


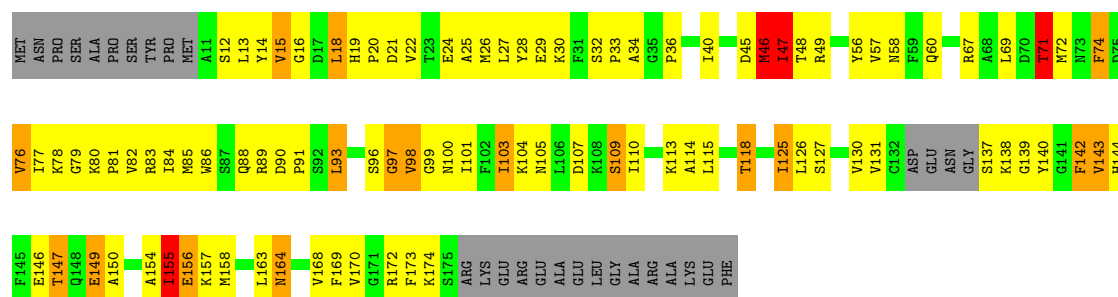
- Molecule 2: POLYADENYLATE BINDING PROTEIN 1

Chain C: 



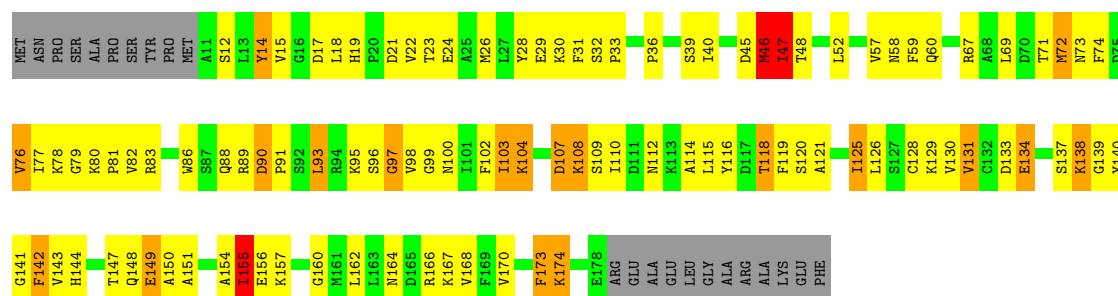
- Molecule 2: POLYADENYLATE BINDING PROTEIN 1

Chain D:  34% 40% 9% 15%

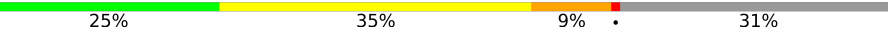


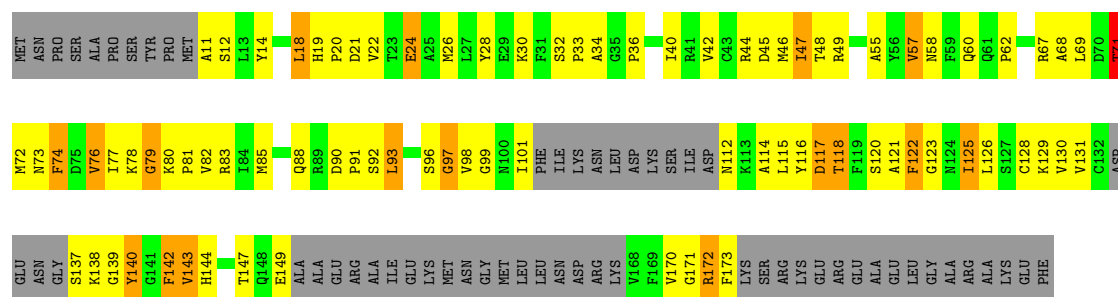
• Molecule 2: POLYADENYLATE BINDING PROTEIN 1

Chain E:  34% 43% 10% 12%

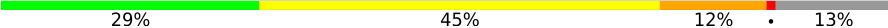


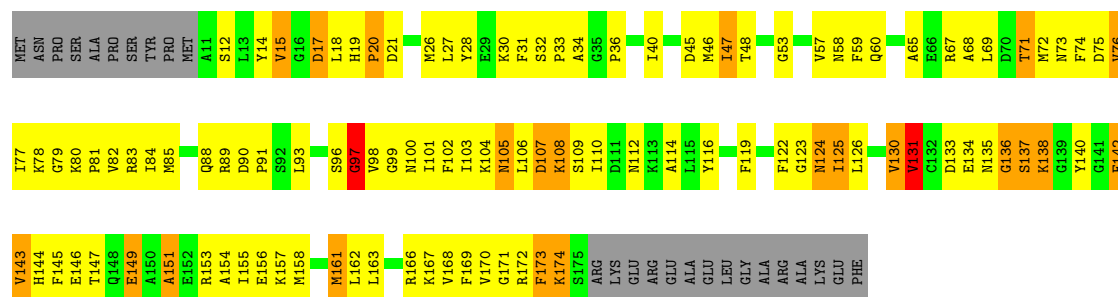
• Molecule 2: POLYADENYLATE BINDING PROTEIN 1

Chain F:  25% 35% 9% 31%

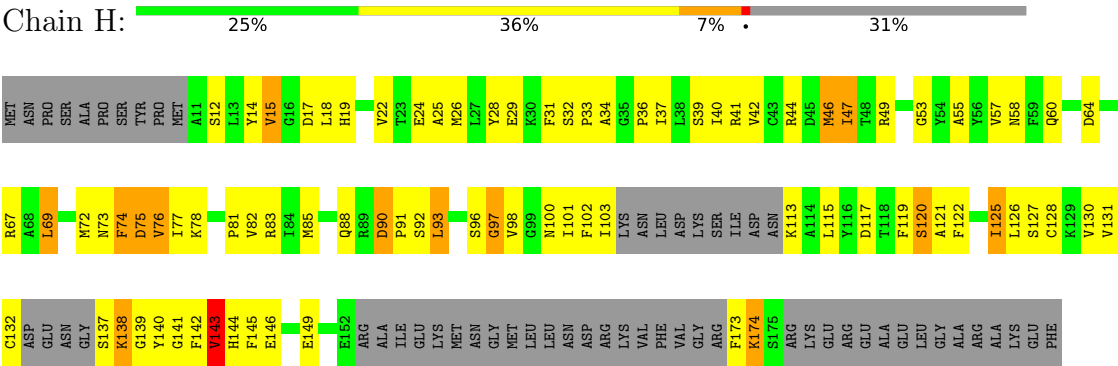


• Molecule 2: POLYADENYLATE BINDING PROTEIN 1

Chain G:  29% 45% 12% 13%



● Molecule 2: POLYADENYLATE BINDING PROTEIN 1



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.56Å 176.80Å 82.49Å 90.00° 117.67° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.60)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.230 , 0.304	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11162	wwPDB-VP
Average B, all atoms (Å ²)	56.0	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: AMP

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	M	0.55	0/221	1.35	7/343 (2.0%)
1	N	0.30	0/171	0.96	2/265 (0.8%)
1	O	0.38	0/171	0.64	0/265
1	P	0.31	0/171	0.91	1/265 (0.4%)
1	Q	0.32	0/196	1.00	2/304 (0.7%)
1	R	0.31	0/171	0.93	1/265 (0.4%)
1	S	0.34	0/171	0.96	1/265 (0.4%)
1	T	0.32	0/171	0.68	0/265
2	A	0.58	0/1323	1.10	13/1785 (0.7%)
2	B	0.55	0/1200	1.11	12/1615 (0.7%)
2	C	0.59	0/1316	1.13	11/1774 (0.6%)
2	D	0.54	0/1277	1.07	5/1721 (0.3%)
2	E	0.59	0/1340	1.11	13/1802 (0.7%)
2	F	0.54	0/1049	1.06	5/1413 (0.4%)
2	G	0.54	1/1312 (0.1%)	1.10	12/1766 (0.7%)
2	H	0.58	0/1054	1.05	8/1420 (0.6%)
All	All	0.54	1/11314 (0.0%)	1.08	93/15533 (0.6%)

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	O	0	1
1	P	0	1
1	S	0	1
1	T	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	97	GLY	CA-C	5.16	1.59	1.51

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	4	A	C2'-C3'-O3'	10.73	125.60	109.50
1	M	1	A	C4'-C3'-O3'	-10.60	97.11	113.00
1	R	3	A	C2'-C3'-O3'	10.13	124.70	109.50
2	B	112	ASN	N-CA-C	-9.20	100.64	112.23
2	D	47	ILE	N-CA-C	9.18	119.70	111.81
2	H	76	VAL	N-CA-C	9.07	122.06	109.55
1	S	3	A	C2'-C3'-O3'	9.00	123.00	109.50
2	G	136	GLY	N-CA-C	8.99	122.56	110.43
2	F	76	VAL	N-CA-C	8.94	120.31	110.21
1	N	3	A	C2'-C3'-O3'	8.48	122.22	109.50
2	A	47	ILE	N-CA-C	8.12	118.80	111.81
2	G	76	VAL	N-CA-C	7.94	120.36	109.80
2	C	155	ILE	N-CA-C	-7.94	99.34	109.58
1	M	5	A	C2'-C3'-O3'	7.80	121.20	109.50
2	G	173	PHE	N-CA-C	7.76	119.43	110.97
1	P	3	A	C2'-C3'-O3'	7.73	121.09	109.50
1	M	1	A	C2'-C3'-O3'	7.65	125.17	113.70
2	C	76	VAL	N-CA-C	7.62	118.82	110.21
2	D	109	SER	N-CA-C	-7.40	103.85	113.17
2	A	130	VAL	N-CA-C	-7.30	97.33	107.99
2	E	90	ASP	CA-C-N	7.25	128.49	120.45
2	E	90	ASP	C-N-CA	7.25	128.49	120.45
2	E	86	TRP	N-CA-C	-7.20	100.56	110.35
2	B	173	PHE	N-CA-C	7.17	120.49	111.24
2	A	38	LEU	N-CA-C	-7.00	104.37	113.12
2	G	48	THR	N-CA-C	-6.96	104.59	113.23
2	E	109	SER	N-CA-C	-6.94	104.89	113.15
2	C	46	MET	N-CA-C	6.93	119.43	111.11
2	B	76	VAL	N-CA-C	6.63	117.70	110.21
2	C	177	LYS	N-CA-C	-6.60	100.81	111.04
2	A	137	SER	N-CA-C	6.56	124.77	110.80
2	B	46	MET	N-CA-C	6.53	118.05	111.07
2	A	109	SER	N-CA-C	-6.48	105.48	113.19
1	M	1	A	O3'-P-O5'	-6.45	94.33	104.00
2	B	148	GLN	N-CA-C	-6.40	105.44	113.18
2	F	24	GLU	N-CA-C	-6.38	104.42	111.82
2	C	80	LYS	N-CA-C	6.34	117.64	109.72
2	A	149	GLU	N-CA-C	-6.27	103.98	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	4	A	C4'-C3'-O3'	6.19	118.68	109.40
2	C	139	GLY	N-CA-C	6.14	123.84	115.30
2	G	46	MET	N-CA-C	6.14	117.77	111.14
2	G	149	GLU	N-CA-C	-6.08	104.73	111.36
2	G	65	ALA	N-CA-C	-6.04	104.82	111.82
2	D	76	VAL	N-CA-C	6.03	121.87	109.34
2	B	139	GLY	N-CA-C	6.02	123.16	114.67
2	G	130	VAL	CB-CA-C	-6.00	106.49	113.22
2	A	14	TYR	N-CA-C	-5.99	99.52	109.46
1	M	1	A	C1'-C2'-O2'	5.97	117.36	108.40
2	C	109	SER	N-CA-C	-5.97	105.86	113.02
2	D	98	VAL	N-CA-C	5.96	116.15	110.42
2	F	140	TYR	N-CA-C	5.94	119.06	109.86
2	E	173	PHE	N-CA-C	5.88	117.38	110.97
2	A	17	ASP	N-CA-C	-5.82	105.48	112.58
2	A	100	ASN	N-CA-C	5.81	118.20	108.96
2	A	168	VAL	N-CA-C	5.69	117.79	108.97
2	E	14	TYR	N-CA-C	-5.66	100.02	109.24
2	B	98	VAL	N-CA-C	5.64	115.72	110.42
2	C	98	VAL	N-CA-C	5.63	116.09	110.23
2	E	162	LEU	N-CA-C	5.63	118.71	109.76
2	H	14	TYR	N-CA-C	-5.53	100.66	109.96
2	A	139	GLY	N-CA-C	5.51	126.25	113.18
2	B	90	ASP	CA-C-N	5.51	126.73	119.84
2	B	90	ASP	C-N-CA	5.51	126.73	119.84
1	M	1	A	N9-C1'-C2'	5.43	120.14	112.00
2	C	19	HIS	N-CA-C	-5.40	102.97	109.83
2	H	90	ASP	CA-C-N	5.33	125.41	119.87
2	H	90	ASP	C-N-CA	5.33	125.41	119.87
2	E	47	ILE	N-CA-C	5.30	116.19	111.90
2	H	64	ASP	N-CA-C	-5.29	104.94	111.40
2	G	14	TYR	N-CA-C	-5.29	100.62	109.24
2	G	17	ASP	N-CA-C	-5.27	104.63	111.74
2	B	19	HIS	N-CA-C	-5.24	102.99	109.64
1	M	1	A	C5'-C4'-C3'	-5.23	108.16	116.00
2	A	154	ALA	N-CA-C	-5.22	105.49	111.07
2	E	76	VAL	N-CA-C	5.22	120.19	109.34
2	G	45	ASP	N-CA-C	-5.22	103.46	110.24
2	H	138	LYS	N-CA-C	5.20	121.87	110.80
2	E	39	SER	N-CA-C	5.19	116.41	108.52
2	H	31	PHE	N-CA-C	5.18	118.76	112.23
2	D	149	GLU	N-CA-C	-5.17	105.77	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	52	LEU	N-CA-C	-5.16	106.66	113.17
2	H	53	GLY	N-CA-C	5.16	122.85	114.90
2	C	97	GLY	N-CA-C	5.13	125.35	113.18
2	B	14	TYR	N-CA-C	-5.13	100.88	109.24
2	G	151	ALA	N-CA-C	-5.11	105.89	111.82
2	F	79	GLY	N-CA-C	5.09	121.14	115.08
1	N	3	A	C4'-C3'-O3'	5.09	117.03	109.40
2	A	96	SER	CB-CA-C	-5.08	102.56	110.94
2	B	31	PHE	N-CA-C	5.05	118.60	112.23
2	F	57	VAL	N-CA-C	-5.05	100.37	107.75
2	C	107	ASP	N-CA-C	5.05	121.55	110.80
2	E	168	VAL	N-CA-C	5.04	117.01	109.20
2	E	155	ILE	N-CA-C	-5.01	98.92	109.34

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	O	2	A	Sidechain
1	P	2	A	Sidechain
1	S	2	A	Sidechain
1	T	2	A	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	195	0	101	8	0
1	N	151	0	79	12	0
1	O	151	0	79	5	0
1	P	151	0	79	6	0
1	Q	173	0	90	8	0
1	R	151	0	79	7	0
1	S	151	0	79	5	0
1	T	151	0	79	9	0
2	A	1298	0	1254	98	0
2	B	1178	0	1163	119	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1291	0	1266	91	0
2	D	1253	0	1232	115	0
2	E	1315	0	1307	106	0
2	F	1028	0	1009	90	0
2	G	1287	0	1279	133	0
2	H	1033	0	1007	89	0
3	A	19	0	12	0	0
3	D	19	0	12	0	0
3	F	19	0	12	0	0
3	H	19	0	12	0	0
3	N	19	0	12	0	0
3	O	19	0	12	0	0
3	Q	19	0	12	0	0
3	S	19	0	12	0	0
4	A	7	0	0	0	0
4	B	5	0	0	0	0
4	C	7	0	0	1	0
4	D	3	0	0	1	0
4	E	11	0	0	2	0
4	F	3	0	0	1	0
4	G	2	0	0	0	0
4	H	5	0	0	0	0
4	N	2	0	0	0	0
4	O	2	0	0	0	0
4	P	1	0	0	0	0
4	Q	3	0	0	0	0
4	T	2	0	0	1	0
All	All	11162	0	10278	822	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 39.

All (822) 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:B:153:ARG:HH11	2:B:153:ARG:HB3	1.10	1.14
2:D:47:ILE:HD13	2:D:47:ILE:H	1.18	1.06
2:H:47:ILE:HD13	2:H:47:ILE:H	1.18	1.06
2:A:113:LYS:H	2:A:113:LYS:HD2	1.19	1.05
2:D:88:GLN:HE21	2:D:90:ASP:H	1.05	1.03
2:C:47:ILE:H	2:C:47:ILE:HD13	1.25	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:40:ILE:HD12	2:E:57:VAL:HG22	1.40	1.02
2:A:47:ILE:HD13	2:A:47:ILE:H	1.19	1.02
2:C:155:ILE:O	2:C:156:GLU:HB3	1.62	1.00
2:E:88:GLN:NE2	2:E:90:ASP:H	1.60	0.99
2:F:88:GLN:HE21	2:F:90:ASP:H	1.11	0.98
2:D:147:THR:HG22	2:D:150:ALA:H	1.27	0.97
2:G:96:SER:O	2:G:98:VAL:N	1.97	0.97
2:F:60:GLN:NE2	2:G:88:GLN:HE22	1.63	0.96
2:G:155:ILE:HD13	2:G:170:VAL:HG12	1.45	0.96
2:F:60:GLN:HE22	2:G:88:GLN:NE2	1.63	0.96
2:C:88:GLN:HE21	2:C:90:ASP:H	0.98	0.95
2:F:96:SER:O	2:F:98:VAL:N	2.00	0.95
1:O:4:A:H62	2:C:85:MET:HE3	1.31	0.94
2:H:125:ILE:HD13	2:H:143:VAL:HG23	1.48	0.94
2:B:106:LEU:HB3	2:B:110:ILE:HD12	1.50	0.94
2:C:96:SER:O	2:C:98:VAL:N	2.01	0.94
2:F:47:ILE:HD13	2:F:47:ILE:H	1.32	0.94
2:A:88:GLN:HE21	2:A:90:ASP:H	1.01	0.93
2:E:88:GLN:HE21	2:E:90:ASP:H	1.02	0.92
2:D:96:SER:O	2:D:98:VAL:N	2.03	0.91
1:T:6:A:H61	2:H:58:ASN:HD21	0.92	0.90
2:C:88:GLN:HE22	2:H:60:GLN:HE22	1.20	0.90
1:S:6:A:H61	2:G:58:ASN:HD21	1.20	0.89
2:B:153:ARG:HB3	2:B:153:ARG:NH1	1.88	0.88
2:H:137:SER:O	2:H:139:GLY:N	2.06	0.88
2:D:88:GLN:NE2	2:D:90:ASP:H	1.72	0.87
2:B:47:ILE:HD13	2:B:47:ILE:H	1.38	0.87
2:E:96:SER:O	2:E:98:VAL:N	2.08	0.86
2:A:147:THR:HG22	2:A:149:GLU:H	1.38	0.86
2:D:47:ILE:H	2:D:47:ILE:CD1	1.89	0.85
2:A:113:LYS:H	2:A:113:LYS:CD	1.90	0.85
1:N:6:A:H61	2:B:58:ASN:HD21	1.21	0.85
2:C:88:GLN:NE2	2:C:90:ASP:H	1.74	0.85
2:H:88:GLN:HE21	2:H:90:ASP:H	1.24	0.84
1:Q:7:A:H61	2:E:58:ASN:HD21	1.26	0.83
1:P:6:A:H61	2:D:58:ASN:HD21	1.25	0.83
2:E:102:PHE:HE2	2:E:104:LYS:HG3	1.43	0.83
2:C:131:VAL:HG11	2:C:140:TYR:CZ	2.14	0.83
1:M:8:A:H61	2:A:58:ASN:HD21	1.22	0.82
2:G:88:GLN:HE21	2:G:90:ASP:H	1.28	0.82
2:E:98:VAL:HG23	2:E:99:GLY:H	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:40:ILE:HD11	2:F:57:VAL:HG13	1.62	0.81
2:B:88:GLN:HE21	2:B:90:ASP:H	1.27	0.81
2:G:34:ALA:HB2	2:G:72:MET:HE1	1.62	0.81
2:A:137:SER:O	2:A:139:GLY:N	2.14	0.80
2:A:88:GLN:NE2	2:A:90:ASP:H	1.78	0.80
2:A:88:GLN:HE22	2:C:60:GLN:HE22	1.28	0.80
2:A:107:ASP:O	2:A:109:SER:N	2.14	0.80
2:A:133:ASP:O	2:A:135:ASN:N	2.15	0.80
2:G:158:MET:HE1	2:G:163:LEU:HD21	1.64	0.80
2:A:47:ILE:HD13	2:A:47:ILE:N	1.96	0.80
2:E:102:PHE:CE2	2:E:104:LYS:HG3	2.17	0.79
2:E:131:VAL:HG22	2:E:138:LYS:HG3	1.63	0.79
2:C:131:VAL:HG12	2:C:140:TYR:O	1.82	0.79
2:C:158:MET:O	2:C:161:MET:HB2	1.81	0.79
2:E:23:THR:OG1	2:E:26:MET:HG3	1.83	0.79
2:F:88:GLN:NE2	2:F:90:ASP:H	1.80	0.79
2:F:60:GLN:HE22	2:G:88:GLN:HE22	0.86	0.79
1:T:6:A:H61	2:H:58:ASN:ND2	1.77	0.78
2:G:17:ASP:OD2	2:G:83:ARG:HB2	1.83	0.78
2:B:67:ARG:O	2:B:71:THR:HB	1.83	0.78
2:D:155:ILE:HG22	2:D:156:GLU:H	1.50	0.77
2:H:37:ILE:HD13	2:H:40:ILE:HD11	1.66	0.77
2:D:88:GLN:HE21	2:D:90:ASP:N	1.83	0.77
2:E:88:GLN:HE21	2:E:90:ASP:N	1.79	0.77
2:D:96:SER:O	2:D:97:GLY:C	2.28	0.76
2:A:96:SER:O	2:A:97:GLY:C	2.28	0.76
2:A:96:SER:O	2:A:98:VAL:N	2.19	0.76
2:H:47:ILE:H	2:H:47:ILE:CD1	1.97	0.76
2:D:76:VAL:HG12	2:D:77:ILE:N	2.00	0.75
2:A:147:THR:HG22	2:A:149:GLU:N	2.02	0.75
2:E:47:ILE:HD13	2:E:47:ILE:H	1.50	0.75
2:B:102:PHE:O	2:B:170:VAL:HA	1.87	0.74
2:H:96:SER:O	2:H:97:GLY:C	2.29	0.74
2:E:98:VAL:HG23	2:E:99:GLY:N	2.03	0.74
2:A:101:ILE:HG12	2:A:143:VAL:HG13	1.69	0.74
2:B:96:SER:O	2:B:98:VAL:N	2.21	0.74
2:D:163:LEU:HD12	2:D:168:VAL:HG21	1.68	0.74
2:F:96:SER:O	2:F:97:GLY:C	2.29	0.74
2:H:47:ILE:HD13	2:H:47:ILE:N	1.99	0.73
2:H:25:ALA:O	2:H:29:GLU:HG3	1.87	0.73
2:A:101:ILE:CG1	2:A:143:VAL:HG13	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:THR:HG22	2:B:72:MET:HG3	1.71	0.72
2:A:83:ARG:HH21	2:A:85:MET:HE2	1.54	0.72
2:G:133:ASP:O	2:G:135:ASN:N	2.23	0.72
2:G:155:ILE:HG23	2:G:170:VAL:O	1.88	0.72
2:F:137:SER:O	2:F:139:GLY:N	2.23	0.72
2:C:24:GLU:OE2	2:D:49:ARG:HD3	1.89	0.71
2:H:22:VAL:HG13	2:H:26:MET:HE2	1.69	0.71
2:F:19:HIS:CD2	2:F:20:PRO:HD2	2.25	0.71
2:F:12:SER:OG	2:F:58:ASN:ND2	2.23	0.71
2:E:107:ASP:OD2	2:E:164:ASN:HB3	1.90	0.71
1:N:3:A:O2'	1:N:4:A:H8	1.74	0.71
2:F:40:ILE:HD13	2:F:57:VAL:HA	1.73	0.71
2:A:83:ARG:NH2	2:A:85:MET:HE2	2.06	0.70
2:B:114:ALA:O	2:B:118:THR:HG22	1.91	0.70
2:B:60:GLN:HE22	2:D:88:GLN:HE22	1.38	0.70
2:G:100:ASN:HA	2:G:144:HIS:HA	1.73	0.70
2:F:88:GLN:HE21	2:F:90:ASP:N	1.87	0.70
2:B:151:ALA:O	2:B:155:ILE:HG12	1.91	0.70
2:B:40:ILE:CD1	2:B:57:VAL:HG13	2.21	0.70
2:G:107:ASP:C	2:G:109:SER:H	2.00	0.70
2:B:88:GLN:NE2	2:B:90:ASP:H	1.89	0.69
2:H:40:ILE:HD12	2:H:57:VAL:HG22	1.73	0.69
2:H:100:ASN:O	2:H:173:PHE:HB2	1.92	0.69
2:A:40:ILE:CD1	2:A:57:VAL:HG13	2.22	0.69
2:G:151:ALA:O	2:G:155:ILE:HG12	1.93	0.69
2:C:40:ILE:HD12	2:C:57:VAL:HG22	1.74	0.69
2:C:40:ILE:CD1	2:C:57:VAL:HG13	2.22	0.69
2:G:125:ILE:HG22	2:G:145:PHE:CE1	2.28	0.69
2:E:12:SER:OG	2:E:58:ASN:ND2	2.26	0.69
2:E:125:ILE:CD1	2:E:128:CYS:HB3	2.23	0.69
2:H:17:ASP:OD2	2:H:83:ARG:HB2	1.93	0.69
2:E:131:VAL:HG11	2:E:140:TYR:CE2	2.28	0.69
2:C:88:GLN:HE21	2:C:90:ASP:N	1.82	0.69
2:F:19:HIS:CG	2:F:20:PRO:HD2	2.29	0.68
2:F:80:LYS:HD2	2:F:80:LYS:N	2.08	0.68
2:E:47:ILE:H	2:E:47:ILE:CD1	2.05	0.68
2:F:79:GLY:C	2:F:80:LYS:HD2	2.19	0.68
2:E:114:ALA:O	2:E:118:THR:HG22	1.93	0.68
2:A:155:ILE:O	2:A:156:GLU:HB3	1.92	0.68
2:A:83:ARG:HH21	2:A:85:MET:CE	2.07	0.68
2:D:19:HIS:HB3	2:D:22:VAL:HG23	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:68:ALA:HA	2:C:71:THR:HG22	1.76	0.67
2:C:47:ILE:HD13	2:C:47:ILE:N	2.04	0.67
2:F:40:ILE:CD1	2:F:57:VAL:HG13	2.24	0.67
2:D:77:ILE:HD12	2:D:82:VAL:HG11	1.74	0.67
2:D:30:LYS:NZ	2:D:72:MET:HB3	2.09	0.67
2:F:73:ASN:O	2:F:74:PHE:HB2	1.94	0.67
2:B:88:GLN:HE21	2:B:90:ASP:N	1.94	0.66
2:A:151:ALA:O	2:A:155:ILE:HG12	1.95	0.66
2:E:103:ILE:HG23	2:E:170:VAL:HG22	1.77	0.66
2:F:40:ILE:CD1	2:F:57:VAL:HG22	2.25	0.66
2:B:98:VAL:HG23	2:B:99:GLY:N	2.10	0.66
2:D:104:LYS:HB3	2:D:169:PHE:HB3	1.78	0.66
2:C:125:ILE:HD12	2:C:127:SER:N	2.10	0.66
1:N:3:A:C2	2:B:85:MET:HE1	2.31	0.65
2:A:118:THR:HG23	2:A:119:PHE:CD1	2.31	0.65
2:C:118:THR:HG23	2:C:119:PHE:HD1	1.61	0.65
2:G:80:LYS:N	2:G:80:LYS:HD2	2.11	0.65
2:G:124:ASN:HD22	2:G:146:GLU:CD	2.03	0.65
2:H:101:ILE:HG12	2:H:143:VAL:HG13	1.78	0.65
2:E:155:ILE:HG22	2:E:156:GLU:H	1.61	0.65
2:D:155:ILE:O	2:D:157:LYS:N	2.28	0.65
2:D:155:ILE:HD13	2:D:170:VAL:HG12	1.78	0.65
2:G:107:ASP:O	2:G:109:SER:N	2.28	0.65
2:H:40:ILE:CD1	2:H:57:VAL:HG13	2.27	0.65
2:A:113:LYS:HD2	2:A:113:LYS:N	2.03	0.65
2:D:80:LYS:HD2	2:D:80:LYS:N	2.12	0.65
2:C:131:VAL:HG11	2:C:140:TYR:CE1	2.31	0.65
2:E:147:THR:HG22	2:E:150:ALA:H	1.62	0.64
2:G:100:ASN:HB2	2:G:144:HIS:ND1	2.13	0.64
2:F:101:ILE:CG1	2:F:143:VAL:HG13	2.28	0.64
2:C:175:SER:C	2:C:177:LYS:H	2.05	0.64
2:F:77:ILE:HD12	2:F:82:VAL:HG11	1.79	0.64
1:Q:1:A:H2	2:E:139:GLY:HA3	1.63	0.64
2:B:122:PHE:CD2	2:B:154:ALA:HA	2.33	0.64
2:C:96:SER:O	2:C:97:GLY:C	2.37	0.64
2:E:151:ALA:O	2:E:155:ILE:HG13	1.98	0.64
2:E:60:GLN:HE22	2:H:88:GLN:HE22	1.46	0.64
2:E:96:SER:O	2:E:97:GLY:C	2.38	0.64
2:H:26:MET:HE1	2:H:78:LYS:HG3	1.80	0.64
2:A:147:THR:CG2	2:A:149:GLU:H	2.11	0.63
2:C:101:ILE:CG1	2:C:143:VAL:HG13	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:107:ASP:C	2:D:109:SER:H	2.03	0.63
2:G:67:ARG:O	2:G:71:THR:HB	1.97	0.63
2:B:41:ARG:O	2:B:55:ALA:HB1	1.98	0.63
2:D:25:ALA:O	2:D:29:GLU:HG3	1.98	0.63
2:H:113:LYS:HD2	2:H:113:LYS:N	2.13	0.63
2:A:74:PHE:HB3	2:A:113:LYS:HE3	1.80	0.63
1:M:5:A:O2'	1:M:6:A:H8	1.81	0.63
2:D:47:ILE:HD13	2:D:47:ILE:N	2.02	0.63
1:T:6:A:N6	2:H:58:ASN:HD21	1.78	0.62
2:B:21:ASP:HB2	2:B:78:LYS:HE2	1.80	0.62
2:C:25:ALA:O	2:C:29:GLU:HG3	2.00	0.62
2:D:137:SER:O	2:D:139:GLY:N	2.29	0.62
2:B:47:ILE:H	2:B:47:ILE:CD1	2.11	0.62
2:B:28:TYR:O	2:B:32:SER:HB3	1.99	0.62
2:G:88:GLN:NE2	2:G:90:ASP:H	1.96	0.62
2:B:155:ILE:HG22	2:B:156:GLU:H	1.64	0.62
2:D:24:GLU:HG3	4:D:995:HOH:O	1.99	0.62
2:F:18:LEU:HD12	2:F:82:VAL:HG12	1.81	0.62
2:F:44:ARG:HD2	2:F:49:ARG:O	2.00	0.62
2:B:15:VAL:O	2:B:15:VAL:HG13	1.99	0.62
2:E:160:GLY:O	2:E:167:LYS:HG3	1.99	0.62
2:C:114:ALA:O	2:C:118:THR:HG22	2.00	0.62
2:D:22:VAL:HA	2:D:26:MET:CE	2.30	0.62
2:D:163:LEU:CD1	2:D:168:VAL:HG21	2.30	0.62
2:E:131:VAL:O	2:E:138:LYS:HB2	2.00	0.61
2:D:110:ILE:HD11	2:D:164:ASN:HD22	1.64	0.61
2:B:132:CYS:SG	2:B:137:SER:HA	2.41	0.61
2:E:107:ASP:O	2:E:108:LYS:CB	2.47	0.61
2:B:79:GLY:C	2:B:80:LYS:HD2	2.26	0.61
2:D:83:ARG:HH21	2:D:85:MET:CE	2.13	0.61
2:F:47:ILE:H	2:F:47:ILE:CD1	2.11	0.61
2:B:155:ILE:HD12	2:B:171:GLY:HA2	1.83	0.60
2:E:40:ILE:CD1	2:E:57:VAL:HG13	2.31	0.60
2:G:40:ILE:HD12	2:G:57:VAL:HG22	1.82	0.60
2:C:76:VAL:HG12	2:C:77:ILE:N	2.17	0.60
2:E:133:ASP:O	2:E:134:GLU:C	2.43	0.60
2:D:69:LEU:HD23	2:D:69:LEU:C	2.27	0.60
1:M:3:A:N3	2:A:173:PHE:O	2.34	0.60
2:E:131:VAL:HG11	2:E:140:TYR:CZ	2.36	0.60
1:Q:1:A:C2	2:E:139:GLY:HA3	2.36	0.60
2:F:98:VAL:HG23	2:F:99:GLY:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:12:SER:OG	2:C:58:ASN:ND2	2.34	0.59
2:C:176:ARG:O	2:C:176:ARG:HG2	2.00	0.59
2:D:131:VAL:HG12	2:D:140:TYR:O	2.01	0.59
2:H:131:VAL:HG11	2:H:140:TYR:CZ	2.37	0.59
1:S:1:A:N3	2:G:173:PHE:O	2.35	0.59
2:D:74:PHE:HB2	2:D:113:LYS:HE2	1.83	0.59
1:O:4:A:N6	2:C:85:MET:HE3	2.12	0.59
2:A:150:ALA:HA	2:A:153:ARG:NH2	2.17	0.59
2:B:61:GLN:HB2	2:B:64:ASP:OD2	2.01	0.59
2:C:98:VAL:HG23	2:C:99:GLY:N	2.16	0.59
2:G:163:LEU:HD12	2:G:168:VAL:HG11	1.85	0.59
2:B:96:SER:O	2:B:97:GLY:C	2.41	0.59
2:G:26:MET:HE1	2:G:78:LYS:HD2	1.84	0.59
2:G:71:THR:HG22	2:G:72:MET:HG3	1.84	0.59
2:F:115:LEU:O	2:F:118:THR:HG23	2.02	0.59
2:G:96:SER:O	2:G:97:GLY:C	2.43	0.59
2:H:125:ILE:HD11	2:H:128:CYS:N	2.17	0.59
2:A:69:LEU:O	2:A:69:LEU:HD23	2.03	0.59
2:B:40:ILE:HD12	2:B:57:VAL:HG22	1.84	0.59
2:D:114:ALA:O	2:D:118:THR:HG22	2.02	0.59
2:C:162:LEU:O	2:C:163:LEU:HD23	2.03	0.59
2:H:101:ILE:CG1	2:H:143:VAL:HG13	2.33	0.59
1:M:2:A:N7	2:A:104:LYS:HD3	2.17	0.58
2:B:106:LEU:HD22	2:B:110:ILE:HD13	1.85	0.58
2:B:155:ILE:HG23	2:B:170:VAL:O	2.03	0.58
2:D:125:ILE:HD12	2:D:127:SER:N	2.18	0.58
2:E:71:THR:HG22	2:E:72:MET:HG2	1.84	0.58
2:E:89:ARG:O	2:E:91:PRO:HD3	2.03	0.58
2:A:147:THR:HG22	2:A:150:ALA:H	1.68	0.58
2:F:101:ILE:HG13	2:F:143:VAL:HG13	1.85	0.58
2:H:119:PHE:O	2:H:122:PHE:HB2	2.03	0.58
2:A:22:VAL:HA	2:A:26:MET:HE1	1.86	0.58
2:F:122:PHE:HD1	2:F:122:PHE:H	1.49	0.58
2:D:76:VAL:CG1	2:D:77:ILE:N	2.66	0.58
2:G:101:ILE:CG1	2:G:143:VAL:HG13	2.33	0.58
1:P:3:A:O2'	1:P:4:A:H8	1.87	0.58
2:B:88:GLN:HE22	2:G:60:GLN:HE22	1.50	0.58
2:C:37:ILE:HD13	2:C:40:ILE:HD11	1.84	0.57
2:G:30:LYS:HG2	2:G:77:ILE:HD11	1.85	0.57
1:R:6:A:H61	2:F:58:ASN:HD21	1.51	0.57
2:C:80:LYS:HD2	2:C:80:LYS:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:114:ALA:O	2:F:118:THR:HG22	2.03	0.57
2:C:131:VAL:HG11	2:C:140:TYR:CE2	2.38	0.57
2:F:18:LEU:CD1	2:F:82:VAL:HG12	2.35	0.57
2:G:88:GLN:HE21	2:G:90:ASP:N	1.99	0.57
2:D:83:ARG:HH21	2:D:85:MET:HE2	1.69	0.57
2:G:98:VAL:HG23	2:G:99:GLY:N	2.20	0.57
2:H:143:VAL:HG22	2:H:145:PHE:CE2	2.39	0.57
2:A:22:VAL:HA	2:A:26:MET:CE	2.35	0.57
2:G:172:ARG:NH2	2:G:174:LYS:HG2	2.20	0.57
2:H:76:VAL:HG12	2:H:77:ILE:N	2.19	0.57
1:O:6:A:H61	2:C:58:ASN:HD21	1.53	0.56
2:A:108:LYS:HA	2:A:137:SER:CB	2.34	0.56
2:B:76:VAL:CG1	2:B:77:ILE:N	2.67	0.56
2:F:142:PHE:N	2:F:142:PHE:CD1	2.72	0.56
2:G:104:LYS:HB3	2:G:169:PHE:HB3	1.87	0.56
2:B:83:ARG:HH21	2:B:85:MET:CE	2.18	0.56
2:B:102:PHE:C	2:B:103:ILE:HD13	2.30	0.56
2:D:76:VAL:HG12	2:D:77:ILE:H	1.68	0.56
2:F:48:THR:HG22	2:H:28:TYR:CE2	2.41	0.56
2:H:34:ALA:O	2:H:67:ARG:NH2	2.37	0.56
2:A:88:GLN:HE21	2:A:90:ASP:N	1.86	0.56
2:C:26:MET:HE1	2:C:78:LYS:HD2	1.87	0.56
2:C:74:PHE:O	2:C:81:PRO:HB3	2.04	0.56
2:G:100:ASN:O	2:G:173:PHE:HB2	2.05	0.56
2:B:131:VAL:HG12	2:B:140:TYR:O	2.06	0.56
2:E:30:LYS:O	2:E:33:PRO:HD2	2.05	0.56
2:E:32:SER:HB3	2:E:33:PRO:HD3	1.88	0.56
2:H:46:MET:HB3	2:H:47:ILE:HD13	1.87	0.56
2:H:125:ILE:HD11	2:H:127:SER:C	2.30	0.56
2:B:149:GLU:O	2:B:153:ARG:HB2	2.06	0.56
2:G:125:ILE:HG13	2:G:125:ILE:O	2.06	0.55
2:E:102:PHE:C	2:E:103:ILE:HD13	2.31	0.55
2:D:40:ILE:CD1	2:D:57:VAL:HG22	2.37	0.55
2:D:147:THR:HG22	2:D:150:ALA:N	2.10	0.55
2:A:160:GLY:O	2:A:161:MET:C	2.50	0.55
2:B:76:VAL:HG12	2:B:77:ILE:N	2.22	0.55
2:H:74:PHE:HB3	2:H:113:LYS:HG3	1.89	0.55
2:A:22:VAL:HG13	2:A:26:MET:HE2	1.88	0.55
2:B:153:ARG:HH11	2:B:153:ARG:CB	2.02	0.55
2:G:147:THR:HG22	2:G:149:GLU:H	1.70	0.55
2:E:40:ILE:HD11	2:E:57:VAL:HG13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:133:ASP:O	2:A:136:GLY:N	2.40	0.55
2:B:60:GLN:HE22	2:D:88:GLN:NE2	2.02	0.55
2:B:101:ILE:CG1	2:B:143:VAL:HG13	2.36	0.55
2:H:88:GLN:NE2	2:H:90:ASP:H	2.01	0.55
2:A:12:SER:OG	2:A:58:ASN:ND2	2.39	0.55
2:A:103:ILE:O	2:A:140:TYR:HB2	2.07	0.54
2:G:172:ARG:HH21	2:G:174:LYS:HA	1.72	0.54
2:B:131:VAL:HG11	2:B:140:TYR:CZ	2.41	0.54
2:D:46:MET:HA	2:D:46:MET:HE2	1.90	0.54
2:G:18:LEU:HB2	2:G:53:GLY:O	2.07	0.54
2:A:150:ALA:HA	2:A:153:ARG:HH21	1.72	0.54
2:C:125:ILE:HD12	2:C:126:LEU:N	2.23	0.54
2:B:98:VAL:CG2	2:B:99:GLY:N	2.70	0.54
2:E:155:ILE:O	2:E:157:LYS:N	2.36	0.54
2:G:158:MET:CE	2:G:163:LEU:HD21	2.35	0.54
2:B:17:ASP:OD1	2:B:83:ARG:NH1	2.41	0.54
2:G:26:MET:HE1	2:G:78:LYS:HG3	1.89	0.54
2:C:47:ILE:H	2:C:47:ILE:CD1	2.06	0.54
2:E:47:ILE:HD13	2:E:47:ILE:N	2.21	0.54
2:A:126:LEU:CD1	2:A:146:GLU:HB2	2.38	0.54
2:B:101:ILE:CG2	2:B:155:ILE:HD11	2.37	0.54
2:F:49:ARG:HD3	2:H:24:GLU:OE2	2.06	0.54
2:G:122:PHE:CZ	2:G:158:MET:HG2	2.42	0.54
2:H:76:VAL:CG1	2:H:77:ILE:N	2.70	0.54
2:E:79:GLY:C	2:E:80:LYS:HD2	2.32	0.54
2:G:26:MET:HE1	2:G:78:LYS:CD	2.38	0.54
2:E:47:ILE:HD13	2:E:48:THR:H	1.73	0.54
2:C:12:SER:HA	2:C:58:ASN:HD22	1.73	0.53
2:D:101:ILE:CG1	2:D:143:VAL:HG13	2.38	0.53
2:F:76:VAL:CG1	2:F:77:ILE:N	2.70	0.53
2:G:79:GLY:C	2:G:80:LYS:HD2	2.33	0.53
2:H:15:VAL:HG23	2:H:18:LEU:HD11	1.90	0.53
2:G:105:ASN:HD21	2:G:166:ARG:HH11	1.55	0.53
2:G:162:LEU:HD12	2:G:166:ARG:C	2.33	0.53
2:C:67:ARG:O	2:C:71:THR:HB	2.08	0.53
2:D:101:ILE:HG12	2:D:143:VAL:HG13	1.90	0.53
2:G:68:ALA:HA	2:G:72:MET:HE3	1.90	0.53
2:G:12:SER:OG	2:G:58:ASN:ND2	2.36	0.53
1:N:3:A:H2	2:B:85:MET:HE1	1.72	0.53
1:Q:2:A:N3	2:E:173:PHE:O	2.41	0.53
1:S:1:A:C2	2:G:173:PHE:O	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:89:ARG:O	2:G:91:PRO:HD3	2.09	0.53
1:Q:6:A:N6	2:E:45:ASP:OD1	2.36	0.53
2:A:34:ALA:HB2	2:A:72:MET:HE3	1.91	0.53
2:B:101:ILE:HG13	2:B:143:VAL:HG13	1.90	0.53
2:B:137:SER:O	2:B:139:GLY:N	2.41	0.53
2:B:147:THR:HG22	2:B:149:GLU:H	1.73	0.53
2:E:76:VAL:HA	2:E:80:LYS:O	2.09	0.53
2:B:12:SER:OG	2:B:58:ASN:ND2	2.42	0.53
2:G:106:LEU:C	2:G:108:LYS:H	2.17	0.53
1:N:1:A:N3	2:B:173:PHE:O	2.41	0.52
1:N:2:A:C2	2:B:129:LYS:HE3	2.45	0.52
2:D:93:LEU:HD22	2:D:144:HIS:HE2	1.72	0.52
2:G:155:ILE:CD1	2:G:170:VAL:HG12	2.29	0.52
2:E:67:ARG:O	2:E:71:THR:HB	2.09	0.52
2:F:21:ASP:HB2	2:F:78:LYS:HE2	1.90	0.52
2:B:60:GLN:NE2	2:D:88:GLN:HE22	2.05	0.52
2:C:73:ASN:O	2:C:74:PHE:HB2	2.09	0.52
2:C:77:ILE:HD12	2:C:82:VAL:HG11	1.89	0.52
2:F:36:PRO:HB2	2:F:60:GLN:CD	2.35	0.52
2:G:158:MET:O	2:G:161:MET:HB2	2.08	0.52
2:B:115:LEU:O	2:B:118:THR:HG23	2.09	0.52
2:B:119:PHE:HB3	2:B:145:PHE:HZ	1.73	0.52
2:B:155:ILE:HG22	2:B:156:GLU:N	2.25	0.52
2:H:32:SER:HB3	2:H:33:PRO:HD3	1.91	0.52
2:C:107:ASP:C	2:C:109:SER:H	2.17	0.52
2:E:98:VAL:CG2	2:E:99:GLY:H	2.19	0.52
2:G:76:VAL:HG12	2:G:77:ILE:N	2.24	0.52
2:E:147:THR:HG22	2:E:149:GLU:N	2.24	0.52
2:F:142:PHE:CD2	2:F:173:PHE:HE1	2.27	0.52
2:D:158:MET:HE1	2:D:163:LEU:HD21	1.91	0.52
2:E:40:ILE:CD1	2:E:57:VAL:HG22	2.27	0.52
2:E:98:VAL:CG2	2:E:99:GLY:N	2.73	0.52
2:H:73:ASN:O	2:H:74:PHE:HB2	2.10	0.52
2:A:174:LYS:HA	2:A:178:GLU:OE2	2.10	0.52
2:C:158:MET:SD	2:C:161:MET:HG3	2.50	0.52
2:H:12:SER:OG	2:H:58:ASN:ND2	2.43	0.52
2:A:60:GLN:HE22	2:E:88:GLN:HE22	1.58	0.52
2:C:107:ASP:O	2:C:109:SER:N	2.43	0.52
2:E:107:ASP:HB3	2:E:110:ILE:HG13	1.92	0.52
2:H:72:MET:HA	2:H:75:ASP:OD2	2.09	0.52
1:N:6:A:H61	2:B:58:ASN:ND2	2.00	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:118:THR:HG23	2:A:119:PHE:HD1	1.73	0.51
2:D:26:MET:CE	2:D:78:LYS:HG3	2.40	0.51
2:G:28:TYR:O	2:G:32:SER:N	2.40	0.51
2:G:131:VAL:HG11	2:G:140:TYR:CE2	2.44	0.51
2:B:19:HIS:CE1	2:B:21:ASP:HB2	2.46	0.51
2:B:125:ILE:HG22	2:B:145:PHE:CE1	2.46	0.51
2:C:175:SER:O	2:C:177:LYS:N	2.43	0.51
2:D:26:MET:HE1	2:D:78:LYS:HD2	1.92	0.51
2:D:105:ASN:O	2:D:168:VAL:HG12	2.11	0.51
2:H:93:LEU:O	2:H:97:GLY:N	2.43	0.51
2:B:98:VAL:C	2:B:100:ASN:H	2.17	0.51
2:D:40:ILE:HD12	2:D:57:VAL:HG22	1.92	0.51
2:H:126:LEU:HD11	2:H:146:GLU:HB2	1.93	0.51
2:B:90:ASP:OD2	2:G:36:PRO:HA	2.11	0.51
2:A:25:ALA:O	2:A:29:GLU:HG3	2.11	0.51
2:G:47:ILE:HD11	2:H:91:PRO:HD3	1.92	0.51
2:C:152:GLU:O	2:C:155:ILE:O	2.29	0.51
2:H:42:VAL:HG22	2:H:55:ALA:HB2	1.90	0.51
2:E:30:LYS:HZ2	2:E:72:MET:HB3	1.76	0.51
2:E:100:ASN:HA	2:E:144:HIS:HA	1.93	0.51
2:C:175:SER:C	2:C:177:LYS:N	2.64	0.51
2:D:22:VAL:HA	2:D:26:MET:HE1	1.92	0.51
2:F:115:LEU:O	2:F:115:LEU:HD12	2.11	0.51
2:G:101:ILE:HD11	2:G:143:VAL:HG13	1.92	0.51
2:H:120:SER:O	2:H:122:PHE:N	2.44	0.51
2:F:121:ALA:O	2:F:123:GLY:N	2.43	0.51
2:H:41:ARG:O	2:H:55:ALA:HB1	2.11	0.51
2:D:30:LYS:HZ1	2:D:72:MET:HB3	1.74	0.50
2:E:71:THR:HG22	2:E:72:MET:CG	2.41	0.50
2:E:119:PHE:C	2:E:121:ALA:H	2.19	0.50
2:B:44:ARG:HA	2:B:52:LEU:HG	1.94	0.50
2:H:74:PHE:CB	2:H:113:LYS:HG3	2.42	0.50
1:T:4:A:H1'	4:T:118:HOH:O	2.10	0.50
2:G:153:ARG:O	2:G:157:LYS:HB2	2.11	0.50
2:B:102:PHE:CE2	2:B:104:LYS:HB2	2.47	0.50
2:D:12:SER:CB	2:D:58:ASN:HD22	2.24	0.50
2:E:74:PHE:O	2:E:81:PRO:HB3	2.12	0.50
2:D:107:ASP:C	2:D:109:SER:N	2.69	0.50
2:H:77:ILE:HD12	2:H:82:VAL:HG11	1.93	0.50
2:D:100:ASN:HA	2:D:144:HIS:HA	1.93	0.50
2:D:28:TYR:O	2:D:32:SER:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:125:ILE:HD12	2:D:125:ILE:C	2.37	0.50
2:H:15:VAL:HG22	2:H:15:VAL:O	2.12	0.50
2:F:28:TYR:O	2:F:32:SER:HB2	2.11	0.50
2:G:40:ILE:CD1	2:G:57:VAL:HG13	2.42	0.50
2:G:144:HIS:HD2	2:G:145:PHE:O	1.95	0.50
2:G:154:ALA:O	2:G:158:MET:HB2	2.12	0.50
1:M:3:A:C2	2:A:173:PHE:O	2.64	0.49
2:F:24:GLU:OE2	2:H:49:ARG:HD3	2.12	0.49
2:G:83:ARG:HH21	2:G:85:MET:CE	2.25	0.49
2:G:155:ILE:HG22	2:G:156:GLU:H	1.77	0.49
2:E:76:VAL:HG13	2:E:80:LYS:N	2.27	0.49
2:E:173:PHE:O	2:E:174:LYS:HB2	2.13	0.49
2:F:115:LEU:HD22	2:F:130:VAL:HG22	1.94	0.49
2:C:125:ILE:CD1	2:C:127:SER:N	2.75	0.49
2:D:32:SER:N	2:D:33:PRO:CD	2.76	0.49
2:G:93:LEU:HD21	2:G:98:VAL:HG22	1.93	0.49
2:H:128:CYS:HA	2:H:143:VAL:HA	1.93	0.49
1:R:3:A:C2	2:F:85:MET:HE1	2.48	0.49
1:S:2:A:O2'	1:S:3:A:H5'	2.12	0.49
2:G:47:ILE:HD13	2:G:47:ILE:H	1.76	0.49
2:H:88:GLN:HE21	2:H:90:ASP:N	2.02	0.49
2:G:142:PHE:N	2:G:142:PHE:CD1	2.81	0.49
2:A:36:PRO:HA	2:E:90:ASP:OD2	2.12	0.49
2:A:42:VAL:HA	2:A:55:ALA:HB2	1.95	0.49
2:A:47:ILE:N	2:A:47:ILE:CD1	2.65	0.49
2:B:40:ILE:HD11	2:B:57:VAL:HG13	1.94	0.49
2:G:19:HIS:C	2:G:21:ASP:H	2.21	0.49
2:A:137:SER:C	2:A:139:GLY:H	2.16	0.49
2:B:40:ILE:HD13	2:B:57:VAL:HA	1.94	0.49
2:B:122:PHE:O	2:B:150:ALA:HB1	2.13	0.49
2:C:125:ILE:HD12	2:C:125:ILE:C	2.38	0.49
2:D:76:VAL:CG1	2:D:77:ILE:H	2.23	0.49
2:F:137:SER:C	2:F:139:GLY:H	2.21	0.49
2:H:102:PHE:O	2:H:103:ILE:HD13	2.12	0.49
2:E:100:ASN:HB2	2:E:144:HIS:CE1	2.48	0.49
2:G:97:GLY:O	2:G:98:VAL:C	2.55	0.49
2:H:69:LEU:O	2:H:73:ASN:HB2	2.13	0.49
1:Q:2:A:C2	2:E:173:PHE:O	2.66	0.48
2:D:47:ILE:CD1	2:D:47:ILE:N	2.64	0.48
2:F:76:VAL:HG12	2:F:77:ILE:N	2.28	0.48
2:B:73:ASN:O	2:B:74:PHE:HB2	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:147:THR:CG2	2:E:149:GLU:HB3	2.42	0.48
2:H:131:VAL:HG11	2:H:140:TYR:CE1	2.48	0.48
2:H:91:PRO:O	2:H:92:SER:C	2.56	0.48
1:T:5:A:H2	2:H:46:MET:HE3	1.78	0.48
2:D:76:VAL:HA	2:D:81:PRO:HA	1.95	0.48
2:D:147:THR:CG2	2:D:149:GLU:HB3	2.44	0.48
2:E:36:PRO:HA	2:H:90:ASP:OD2	2.13	0.48
2:C:101:ILE:HG12	2:C:143:VAL:HG13	1.94	0.48
2:D:155:ILE:HG23	2:D:170:VAL:O	2.14	0.48
2:C:77:ILE:HD12	2:C:82:VAL:CG1	2.44	0.48
2:D:60:GLN:HE22	2:F:88:GLN:HE22	1.62	0.48
2:D:67:ARG:O	2:D:71:THR:HB	2.13	0.48
2:F:90:ASP:HB3	4:F:997:HOH:O	2.13	0.48
2:A:40:ILE:HD12	2:A:57:VAL:HG22	1.95	0.48
2:C:93:LEU:HD21	2:C:98:VAL:HG22	1.94	0.48
2:B:106:LEU:HD22	2:B:110:ILE:CD1	2.44	0.48
2:G:89:ARG:O	2:H:47:ILE:HG13	2.14	0.48
2:G:104:LYS:O	2:G:105:ASN:HB3	2.14	0.48
2:G:172:ARG:HH21	2:G:174:LYS:HG2	1.79	0.48
2:A:108:LYS:C	2:A:110:ILE:H	2.21	0.48
2:C:47:ILE:N	2:C:47:ILE:CD1	2.72	0.48
2:D:77:ILE:HD12	2:D:82:VAL:CG1	2.43	0.48
2:G:93:LEU:HD23	2:G:96:SER:OG	2.14	0.48
2:B:125:ILE:HG22	2:B:145:PHE:CD1	2.49	0.47
1:Q:7:A:H61	2:E:58:ASN:ND2	2.03	0.47
2:A:59:PHE:CD1	2:A:65:ALA:HA	2.49	0.47
2:C:115:LEU:HD22	2:C:130:VAL:HG22	1.95	0.47
2:E:103:ILE:HG12	2:E:141:GLY:O	2.14	0.47
2:A:140:TYR:N	2:A:140:TYR:CD1	2.82	0.47
2:F:98:VAL:CG2	2:F:99:GLY:N	2.77	0.47
2:G:73:ASN:O	2:G:74:PHE:HB2	2.15	0.47
2:A:89:ARG:O	2:D:47:ILE:HG13	2.13	0.47
2:C:76:VAL:HG13	2:C:79:GLY:C	2.40	0.47
2:C:131:VAL:O	2:C:137:SER:O	2.32	0.47
2:F:32:SER:N	2:F:33:PRO:CD	2.77	0.47
2:F:40:ILE:HD12	2:F:57:VAL:HG22	1.93	0.47
1:M:5:A:O2'	1:M:6:A:H2'	2.14	0.47
2:B:115:LEU:HA	2:B:118:THR:CG2	2.44	0.47
2:F:83:ARG:HH21	2:F:85:MET:CE	2.28	0.47
2:E:74:PHE:HA	2:E:82:VAL:O	2.15	0.47
2:F:22:VAL:HG13	2:F:26:MET:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:42:VAL:HG22	2:F:55:ALA:HB2	1.96	0.47
2:F:170:VAL:HG12	2:F:171:GLY:N	2.29	0.47
2:F:171:GLY:O	2:F:172:ARG:O	2.32	0.47
2:G:47:ILE:HG13	2:H:90:ASP:HA	1.97	0.47
2:A:40:ILE:HD11	2:A:57:VAL:HG13	1.97	0.47
2:A:69:LEU:HD23	2:A:69:LEU:C	2.39	0.47
2:C:69:LEU:C	2:C:69:LEU:CD2	2.87	0.47
2:C:177:LYS:O	2:C:178:GLU:C	2.57	0.47
2:E:137:SER:O	2:E:139:GLY:N	2.45	0.47
2:F:71:THR:HG22	2:F:72:MET:HG3	1.95	0.47
2:F:101:ILE:HG13	2:F:143:VAL:CG1	2.44	0.47
2:G:32:SER:N	2:G:33:PRO:CD	2.78	0.47
2:H:115:LEU:HD22	2:H:130:VAL:CG2	2.44	0.47
2:H:131:VAL:HG12	2:H:140:TYR:O	2.14	0.47
1:P:6:A:H61	2:D:58:ASN:ND2	2.02	0.47
2:B:147:THR:HG21	2:B:149:GLU:OE1	2.15	0.47
2:D:48:THR:O	2:D:49:ARG:HB2	2.14	0.47
2:F:116:TYR:HE1	2:F:125:ILE:HG12	1.80	0.47
2:B:155:ILE:C	2:B:157:LYS:N	2.72	0.47
2:C:22:VAL:HG22	2:C:77:ILE:HG22	1.97	0.47
2:D:34:ALA:O	2:D:67:ARG:NH2	2.48	0.47
2:D:98:VAL:HG23	2:D:99:GLY:N	2.30	0.47
2:F:131:VAL:HG12	2:F:140:TYR:O	2.14	0.47
2:G:125:ILE:HG22	2:G:145:PHE:CD1	2.50	0.47
2:H:83:ARG:HH21	2:H:85:MET:CE	2.28	0.47
2:A:108:LYS:HA	2:A:137:SER:HB3	1.96	0.46
2:A:177:LYS:O	2:A:178:GLU:C	2.59	0.46
2:B:16:GLY:O	2:B:17:ASP:HB2	2.15	0.46
2:D:26:MET:HE1	2:D:78:LYS:HG3	1.97	0.46
2:D:89:ARG:O	2:D:91:PRO:HD3	2.15	0.46
2:A:133:ASP:O	2:A:134:GLU:C	2.58	0.46
2:B:83:ARG:HE	2:B:85:MET:HE2	1.81	0.46
2:C:22:VAL:HA	2:C:26:MET:CE	2.45	0.46
2:E:137:SER:C	2:E:139:GLY:H	2.22	0.46
1:R:2:A:C2	2:F:129:LYS:HE3	2.51	0.46
2:B:22:VAL:HA	2:B:26:MET:HE1	1.97	0.46
2:B:24:GLU:HG2	2:B:42:VAL:HG23	1.97	0.46
2:D:46:MET:HA	2:D:46:MET:CE	2.45	0.46
2:G:77:ILE:HD12	2:G:82:VAL:HG11	1.95	0.46
2:A:143:VAL:O	2:A:143:VAL:HG22	2.14	0.46
2:A:155:ILE:HG23	2:A:170:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:34:ALA:HB2	2:C:72:MET:CE	2.46	0.46
2:C:80:LYS:HA	2:C:81:PRO:HD3	1.76	0.46
2:C:137:SER:C	2:C:139:GLY:H	2.24	0.46
2:D:18:LEU:HD21	2:D:27:LEU:HD11	1.98	0.46
2:G:124:ASN:ND2	2:G:146:GLU:CD	2.73	0.46
2:A:32:SER:HB3	2:A:33:PRO:HD3	1.97	0.46
2:E:47:ILE:CD1	2:E:47:ILE:N	2.73	0.46
2:F:67:ARG:O	2:F:71:THR:HB	2.15	0.46
2:A:24:GLU:OE2	2:B:49:ARG:HD3	2.15	0.46
2:B:50:ARG:HG3	2:B:50:ARG:HH11	1.80	0.46
2:B:122:PHE:CE2	2:B:154:ALA:HA	2.51	0.46
2:C:155:ILE:O	2:C:156:GLU:CB	2.46	0.46
2:E:93:LEU:HD21	2:E:98:VAL:HG22	1.97	0.46
2:G:93:LEU:CD2	2:G:98:VAL:HG22	2.45	0.46
1:T:1:A:N3	2:H:173:PHE:O	2.48	0.46
2:B:89:ARG:O	2:B:91:PRO:HD3	2.16	0.46
2:D:12:SER:OG	2:D:58:ASN:ND2	2.49	0.46
2:D:142:PHE:N	2:D:142:PHE:CD1	2.83	0.46
2:E:125:ILE:HD13	2:E:128:CYS:HB3	1.95	0.46
2:E:131:VAL:HG22	2:E:138:LYS:CG	2.42	0.46
2:F:117:ASP:HA	2:F:120:SER:OG	2.16	0.46
1:N:3:A:N6	2:B:144:HIS:ND1	2.50	0.46
1:R:2:A:O2'	1:R:3:A:H5'	2.16	0.45
2:B:18:LEU:HD22	2:B:54:TYR:HA	1.98	0.45
2:D:40:ILE:CD1	2:D:57:VAL:HG13	2.46	0.45
2:E:18:LEU:HA	4:E:197:HOH:O	2.15	0.45
2:G:155:ILE:HD12	2:G:171:GLY:CA	2.46	0.45
1:R:2:A:C2'	1:R:3:A:H5'	2.47	0.45
2:A:74:PHE:CB	2:A:113:LYS:HE3	2.47	0.45
2:B:98:VAL:CG2	2:B:99:GLY:H	2.29	0.45
2:B:143:VAL:O	2:B:143:VAL:HG22	2.16	0.45
2:C:91:PRO:HA	4:C:191:HOH:O	2.15	0.45
2:D:36:PRO:HB2	2:D:60:GLN:CD	2.40	0.45
2:H:125:ILE:HD12	2:H:127:SER:H	1.81	0.45
2:C:103:ILE:HD12	2:C:119:PHE:CZ	2.52	0.45
2:E:24:GLU:HG3	4:E:194:HOH:O	2.16	0.45
2:E:119:PHE:C	2:E:121:ALA:N	2.73	0.45
1:O:2:A:OP2	2:C:176:ARG:HB2	2.16	0.45
2:B:32:SER:N	2:B:33:PRO:CD	2.79	0.45
2:C:76:VAL:CG1	2:C:77:ILE:N	2.78	0.45
2:D:131:VAL:HG11	2:D:140:TYR:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:73:ASN:O	2:E:74:PHE:HB2	2.16	0.45
2:F:19:HIS:HE1	2:F:21:ASP:OD2	2.00	0.45
2:B:69:LEU:O	2:B:73:ASN:HB2	2.16	0.45
2:E:80:LYS:HA	2:E:81:PRO:HD3	1.87	0.45
2:B:32:SER:OG	2:B:33:PRO:HD3	2.16	0.45
2:D:154:ALA:C	2:D:155:ILE:O	2.57	0.45
2:G:102:PHE:O	2:G:103:ILE:HD13	2.17	0.45
2:A:96:SER:OG	2:A:98:VAL:HG13	2.16	0.45
2:C:122:PHE:O	2:C:153:ARG:NH1	2.42	0.45
2:E:95:LYS:C	2:E:97:GLY:H	2.25	0.45
2:E:107:ASP:O	2:E:108:LYS:HB3	2.16	0.45
2:F:11:ALA:HB2	2:F:62:PRO:HA	1.98	0.45
2:G:47:ILE:HD11	2:H:91:PRO:CD	2.47	0.45
2:A:40:ILE:HD13	2:A:57:VAL:HA	1.99	0.45
2:A:50:ARG:HG3	2:A:50:ARG:HH11	1.81	0.45
2:B:142:PHE:CD1	2:B:142:PHE:N	2.84	0.45
2:D:19:HIS:O	2:D:21:ASP:N	2.50	0.45
2:G:19:HIS:CE1	2:G:21:ASP:HB2	2.52	0.45
2:G:101:ILE:HG12	2:G:143:VAL:HG13	1.97	0.45
2:G:103:ILE:HA	2:G:169:PHE:O	2.16	0.45
2:H:15:VAL:CG2	2:H:18:LEU:HD11	2.46	0.45
2:H:173:PHE:O	2:H:174:LYS:O	2.35	0.45
2:C:98:VAL:CG2	2:C:99:GLY:N	2.80	0.45
2:G:119:PHE:N	2:G:119:PHE:CD1	2.84	0.45
2:B:77:ILE:HD12	2:B:82:VAL:HG11	1.97	0.44
2:B:93:LEU:HD23	2:B:93:LEU:HA	1.79	0.44
2:G:101:ILE:CG2	2:G:155:ILE:HD11	2.47	0.44
2:G:173:PHE:O	2:G:174:LYS:HB2	2.17	0.44
2:H:74:PHE:O	2:H:81:PRO:HB3	2.17	0.44
2:G:19:HIS:O	2:G:21:ASP:N	2.50	0.44
2:G:105:ASN:OD1	2:G:166:ARG:HD3	2.17	0.44
2:G:153:ARG:NH1	2:G:153:ARG:HB2	2.33	0.44
2:A:159:ASN:HA	2:A:170:VAL:HG23	1.99	0.44
2:E:19:HIS:HB3	2:E:22:VAL:HG23	1.98	0.44
2:F:32:SER:HB3	2:F:33:PRO:HD3	1.99	0.44
2:F:125:ILE:HD12	2:F:128:CYS:HB3	1.99	0.44
2:G:155:ILE:HD12	2:G:171:GLY:HA2	1.99	0.44
2:A:67:ARG:O	2:A:71:THR:HB	2.18	0.44
2:A:106:LEU:HB2	2:A:139:GLY:O	2.17	0.44
2:A:126:LEU:HD13	2:A:146:GLU:HB2	2.00	0.44
2:A:126:LEU:HD11	2:A:146:GLU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:PRO:O	2:B:92:SER:C	2.61	0.44
2:D:131:VAL:HG11	2:D:140:TYR:CZ	2.52	0.44
2:D:163:LEU:O	2:D:164:ASN:HB2	2.17	0.44
2:G:34:ALA:HB2	2:G:72:MET:CE	2.39	0.44
2:B:42:VAL:O	2:B:44:ARG:NH1	2.50	0.44
2:E:32:SER:N	2:E:33:PRO:CD	2.81	0.44
2:E:116:TYR:O	2:E:120:SER:HB3	2.18	0.44
1:N:1:A:C2	2:B:173:PHE:O	2.71	0.44
2:C:133:ASP:O	2:C:134:GLU:C	2.60	0.44
2:D:71:THR:O	2:D:71:THR:CG2	2.64	0.44
2:A:19:HIS:HB3	2:A:22:VAL:HG23	1.99	0.44
2:B:22:VAL:HA	2:B:26:MET:CE	2.47	0.44
2:C:89:ARG:O	2:C:91:PRO:HD3	2.18	0.44
2:C:98:VAL:HG23	2:C:99:GLY:H	1.83	0.44
2:C:125:ILE:HD12	2:C:127:SER:H	1.80	0.44
2:F:40:ILE:HD13	2:F:57:VAL:HG22	1.98	0.44
2:G:142:PHE:CE2	2:G:173:PHE:HE1	2.35	0.44
2:H:130:VAL:HA	2:H:141:GLY:HA3	2.00	0.44
1:P:5:A:H2	2:D:46:MET:HE3	1.83	0.44
2:B:131:VAL:HG11	2:B:140:TYR:CE2	2.53	0.44
2:E:154:ALA:C	2:E:155:ILE:O	2.54	0.44
2:F:140:TYR:H	2:F:140:TYR:HD1	1.64	0.44
2:G:138:LYS:O	2:G:138:LYS:HG3	2.18	0.44
2:A:17:ASP:OD2	2:A:83:ARG:HB2	2.17	0.43
2:F:112:ASN:C	2:F:114:ALA:N	2.75	0.43
2:G:108:LYS:HA	2:G:137:SER:HB3	1.99	0.43
2:G:130:VAL:O	2:G:131:VAL:C	2.59	0.43
2:D:69:LEU:HD23	2:D:69:LEU:O	2.18	0.43
2:D:93:LEU:CD2	2:D:98:VAL:HG22	2.48	0.43
2:D:115:LEU:HD22	2:D:130:VAL:HG22	1.99	0.43
1:Q:3:A:N6	2:E:144:HIS:HB2	2.33	0.43
2:F:93:LEU:HD21	2:F:98:VAL:HG22	2.00	0.43
2:G:100:ASN:HB2	2:G:144:HIS:CG	2.52	0.43
2:G:103:ILE:CD1	2:G:170:VAL:HG13	2.48	0.43
2:A:19:HIS:O	2:A:21:ASP:N	2.52	0.43
2:C:38:LEU:O	2:C:39:SER:HB3	2.17	0.43
2:C:103:ILE:CG2	2:C:106:LEU:HD21	2.48	0.43
2:D:15:VAL:HG22	2:D:18:LEU:CD1	2.49	0.43
2:D:79:GLY:C	2:D:80:LYS:HD2	2.43	0.43
2:E:17:ASP:OD2	2:E:83:ARG:HB2	2.17	0.43
2:F:73:ASN:O	2:F:74:PHE:CB	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:19:HIS:CG	2:G:20:PRO:HD2	2.53	0.43
2:G:74:PHE:O	2:G:81:PRO:HB3	2.19	0.43
2:B:44:ARG:HB3	2:B:49:ARG:O	2.18	0.43
2:E:133:ASP:CG	2:E:138:LYS:HE2	2.43	0.43
1:N:3:A:N3	2:B:85:MET:HE1	2.33	0.43
2:A:101:ILE:HD13	2:A:145:PHE:HE2	1.83	0.43
2:E:138:LYS:HA	2:E:138:LYS:HD3	1.82	0.43
2:F:142:PHE:HD2	2:F:173:PHE:HE1	1.65	0.43
2:G:84:ILE:HG22	2:G:85:MET:N	2.32	0.43
2:G:107:ASP:C	2:G:109:SER:N	2.67	0.43
2:H:22:VAL:HA	2:H:26:MET:CE	2.48	0.43
1:P:4:A:OP1	2:D:14:TYR:OH	2.35	0.43
2:A:42:VAL:HA	2:A:55:ALA:CB	2.49	0.43
2:B:155:ILE:O	2:B:156:GLU:C	2.61	0.43
2:C:118:THR:HG23	2:C:119:PHE:CD1	2.47	0.43
2:E:76:VAL:HG12	2:E:77:ILE:N	2.33	0.43
2:G:74:PHE:CD2	2:G:112:ASN:HB3	2.53	0.43
2:G:101:ILE:HD11	2:G:143:VAL:CG1	2.48	0.43
2:A:125:ILE:HD12	2:A:127:SER:N	2.33	0.43
2:B:37:ILE:HD13	2:B:40:ILE:HD11	2.01	0.43
2:G:91:PRO:HD3	2:H:47:ILE:HG13	2.01	0.43
2:A:125:ILE:HD13	2:A:128:CYS:HB3	2.00	0.43
2:G:106:LEU:O	2:G:108:LYS:N	2.52	0.43
2:B:155:ILE:O	2:B:157:LYS:N	2.52	0.43
2:C:49:ARG:HD3	2:D:24:GLU:OE2	2.18	0.43
2:D:13:LEU:O	2:D:56:TYR:HA	2.19	0.43
2:F:97:GLY:HA2	2:F:144:HIS:CE1	2.54	0.43
2:G:162:LEU:HD12	2:G:167:LYS:N	2.33	0.43
2:H:44:ARG:HB3	2:H:49:ARG:O	2.18	0.43
1:N:5:A:N6	2:B:45:ASP:OD1	2.48	0.42
2:B:101:ILE:HG21	2:B:155:ILE:HD11	1.99	0.42
2:C:155:ILE:HG23	2:C:170:VAL:O	2.18	0.42
2:C:156:GLU:HG2	2:C:157:LYS:N	2.33	0.42
2:F:22:VAL:HA	2:F:26:MET:CE	2.49	0.42
2:H:19:HIS:HB3	2:H:22:VAL:HG23	2.00	0.42
2:H:100:ASN:O	2:H:173:PHE:CB	2.66	0.42
1:S:5:A:H4'	2:H:46:MET:HB2	2.01	0.42
2:B:119:PHE:O	2:B:120:SER:C	2.61	0.42
2:D:36:PRO:HB2	2:D:60:GLN:OE1	2.19	0.42
2:G:123:GLY:O	2:G:124:ASN:C	2.62	0.42
2:A:108:LYS:C	2:A:110:ILE:N	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:LYS:HG2	2:B:140:TYR:HE1	1.83	0.42
2:E:116:TYR:CD2	2:E:116:TYR:C	2.97	0.42
2:E:125:ILE:CD1	2:E:128:CYS:CB	2.96	0.42
2:F:147:THR:C	2:F:149:GLU:N	2.76	0.42
2:G:76:VAL:CG1	2:G:77:ILE:N	2.82	0.42
2:G:136:GLY:O	2:G:138:LYS:N	2.51	0.42
2:H:115:LEU:HD22	2:H:130:VAL:HG22	2.01	0.42
2:A:73:ASN:O	2:A:74:PHE:HB2	2.20	0.42
2:A:161:MET:O	2:A:161:MET:HG3	2.19	0.42
2:B:41:ARG:HG2	2:B:42:VAL:N	2.34	0.42
2:F:44:ARG:HB3	2:F:49:ARG:O	2.19	0.42
2:G:73:ASN:O	2:G:74:PHE:CB	2.68	0.42
2:D:155:ILE:HG22	2:D:156:GLU:N	2.26	0.42
2:G:34:ALA:HB3	2:G:59:PHE:CE2	2.54	0.42
2:H:47:ILE:CD1	2:H:47:ILE:N	2.69	0.42
1:M:6:A:N7	2:A:85:MET:HE3	2.35	0.42
2:B:115:LEU:HD22	2:B:130:VAL:HG22	2.01	0.42
2:D:115:LEU:HA	2:D:118:THR:HG23	2.00	0.42
2:E:131:VAL:CG2	2:E:138:LYS:HG3	2.44	0.42
2:G:101:ILE:CD1	2:G:143:VAL:HG13	2.49	0.42
2:G:119:PHE:HB3	2:G:145:PHE:HZ	1.83	0.42
2:B:59:PHE:HB2	2:B:65:ALA:HB2	2.02	0.42
2:B:137:SER:C	2:B:139:GLY:H	2.27	0.42
2:B:29:GLU:O	2:B:33:PRO:HD3	2.19	0.42
2:C:157:LYS:O	2:C:157:LYS:HD3	2.20	0.42
2:D:110:ILE:HG23	2:D:114:ALA:HB3	2.01	0.42
2:E:21:ASP:HB2	2:E:78:LYS:HE2	2.01	0.42
2:H:28:TYR:O	2:H:32:SER:HB2	2.19	0.42
1:P:1:A:C2	2:D:173:PHE:O	2.73	0.42
2:B:42:VAL:HA	2:B:55:ALA:HB2	2.01	0.42
2:D:14:TYR:CE2	2:D:16:GLY:HA3	2.54	0.42
2:D:28:TYR:OH	2:F:90:ASP:OD1	2.29	0.42
2:D:126:LEU:HD11	2:D:146:GLU:HG3	2.01	0.42
2:E:28:TYR:O	2:E:32:SER:HB2	2.19	0.42
2:F:101:ILE:HG12	2:F:143:VAL:HG13	2.01	0.42
2:G:19:HIS:ND1	2:G:21:ASP:HB2	2.35	0.42
2:B:73:ASN:O	2:B:74:PHE:CB	2.68	0.42
2:B:76:VAL:HG13	2:B:80:LYS:N	2.35	0.42
2:D:80:LYS:N	2:D:80:LYS:CD	2.82	0.42
2:G:98:VAL:CG2	2:G:99:GLY:N	2.83	0.42
2:H:36:PRO:HB2	2:H:60:GLN:CD	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:68:ALA:HA	2:C:71:THR:CG2	2.49	0.41
2:C:101:ILE:HD11	2:C:143:VAL:HG13	2.01	0.41
2:D:93:LEU:HD21	2:D:98:VAL:HG22	2.02	0.41
2:D:101:ILE:HD11	2:D:143:VAL:HG13	2.02	0.41
2:D:103:ILE:HA	2:D:169:PHE:O	2.20	0.41
2:F:11:ALA:HB2	2:F:62:PRO:CA	2.50	0.41
2:F:11:ALA:CB	2:F:62:PRO:HA	2.49	0.41
2:G:116:TYR:CE1	2:G:125:ILE:HG12	2.55	0.41
2:H:113:LYS:O	2:H:117:ASP:OD2	2.38	0.41
2:H:93:LEU:HD21	2:H:98:VAL:HG22	2.02	0.41
1:M:7:A:H4'	2:D:46:MET:HB2	2.02	0.41
2:F:34:ALA:CB	2:F:68:ALA:HB2	2.50	0.41
2:F:137:SER:C	2:F:139:GLY:N	2.78	0.41
2:G:15:VAL:HG23	2:G:82:VAL:HB	2.02	0.41
2:A:115:LEU:O	2:A:118:THR:HG22	2.19	0.41
2:B:172:ARG:CG	2:B:173:PHE:N	2.83	0.41
2:D:140:TYR:CD1	2:D:140:TYR:N	2.88	0.41
2:E:129:LYS:HG2	2:E:130:VAL:N	2.35	0.41
2:F:14:TYR:HD2	2:F:85:MET:HG2	1.85	0.41
2:F:74:PHE:O	2:F:81:PRO:HB3	2.20	0.41
2:G:26:MET:HE1	2:G:78:LYS:CG	2.49	0.41
2:A:163:LEU:O	2:A:164:ASN:HB2	2.19	0.41
2:G:104:LYS:O	2:G:105:ASN:CB	2.68	0.41
2:G:130:VAL:O	2:G:130:VAL:HG12	2.19	0.41
2:A:155:ILE:HG12	2:A:155:ILE:H	1.64	0.41
2:B:98:VAL:C	2:B:100:ASN:N	2.79	0.41
2:C:97:GLY:O	2:C:98:VAL:C	2.64	0.41
2:E:46:MET:HE3	2:E:46:MET:HB2	1.79	0.41
2:A:48:THR:O	2:A:49:ARG:HB2	2.21	0.41
2:B:90:ASP:HA	2:B:91:PRO:HD2	1.93	0.41
2:H:15:VAL:O	2:H:15:VAL:CG2	2.69	0.41
2:A:77:ILE:O	2:A:78:LYS:C	2.64	0.41
2:D:45:ASP:O	2:D:46:MET:C	2.64	0.41
2:E:17:ASP:CG	2:E:83:ARG:NH1	2.79	0.41
2:G:105:ASN:ND2	2:G:166:ARG:HH11	2.18	0.41
1:N:6:A:N6	2:B:58:ASN:HD21	2.03	0.41
1:T:3:A:N6	2:H:144:HIS:ND1	2.60	0.41
2:A:125:ILE:HA	2:A:145:PHE:HA	2.03	0.41
2:A:164:ASN:C	2:A:166:ARG:H	2.28	0.41
2:C:75:ASP:O	2:C:82:VAL:HG22	2.20	0.41
2:D:84:ILE:HG22	2:D:85:MET:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:172:ARG:HG2	2:D:173:PHE:H	1.85	0.41
2:E:88:GLN:NE2	2:E:90:ASP:N	2.44	0.41
2:F:91:PRO:O	2:F:92:SER:C	2.63	0.41
2:G:101:ILE:HG12	2:G:143:VAL:O	2.21	0.41
2:H:39:SER:O	2:H:40:ILE:HD13	2.20	0.41
1:R:3:A:O2'	1:R:4:A:P	2.79	0.41
2:A:34:ALA:HB2	2:A:72:MET:CE	2.51	0.41
2:G:27:LEU:O	2:G:31:PHE:HD2	2.03	0.41
1:O:4:A:N7	2:C:85:MET:HE3	2.36	0.40
2:D:12:SER:CB	2:D:58:ASN:ND2	2.84	0.40
2:E:31:PHE:HB3	2:E:59:PHE:HZ	1.85	0.40
2:F:45:ASP:HB3	2:F:48:THR:OG1	2.21	0.40
1:T:5:A:C2	2:H:46:MET:HE3	2.56	0.40
2:C:19:HIS:HB3	2:C:22:VAL:HG23	2.02	0.40
2:C:40:ILE:HD11	2:C:57:VAL:HG13	2.01	0.40
2:D:15:VAL:HG23	2:D:82:VAL:HB	2.02	0.40
2:E:29:GLU:O	2:E:33:PRO:HD3	2.21	0.40
1:T:1:A:C2	2:H:173:PHE:O	2.75	0.40
2:E:107:ASP:HA	2:E:166:ARG:HD2	2.02	0.40
2:F:30:LYS:HZ1	2:F:72:MET:HG2	1.85	0.40
2:G:47:ILE:H	2:G:47:ILE:CD1	2.35	0.40
2:G:131:VAL:O	2:G:138:LYS:HB3	2.22	0.40
1:R:4:A:N6	2:F:85:MET:HG3	2.36	0.40
2:A:80:LYS:HA	2:A:81:PRO:HD3	1.84	0.40
2:B:74:PHE:CE2	2:B:112:ASN:HB3	2.57	0.40
2:C:161:MET:O	2:C:168:VAL:HG22	2.21	0.40
2:E:74:PHE:CD2	2:E:112:ASN:HB3	2.57	0.40
2:G:26:MET:CE	2:G:78:LYS:HG3	2.50	0.40
2:G:110:ILE:HG23	2:G:114:ALA:HB3	2.04	0.40
2:G:131:VAL:O	2:G:137:SER:O	2.39	0.40
2:H:131:VAL:HG22	2:H:132:CYS:N	2.36	0.40
2:A:79:GLY:C	2:A:80:LYS:HD2	2.47	0.40
2:A:107:ASP:C	2:A:109:SER:N	2.76	0.40
2:D:85:MET:O	2:D:86:TRP:C	2.64	0.40
2:E:115:LEU:O	2:E:118:THR:HG23	2.21	0.40
2:E:142:PHE:CD1	2:E:142:PHE:N	2.90	0.40
2:E:147:THR:HG21	2:E:149:GLU:HB3	2.03	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	
2	A	167/190 (88%)	140 (84%)	19 (11%)	8 (5%)	2	2
2	B	145/190 (76%)	123 (85%)	16 (11%)	6 (4%)	2	3
2	C	166/190 (87%)	145 (87%)	13 (8%)	8 (5%)	2	2
2	D	157/190 (83%)	129 (82%)	18 (12%)	10 (6%)	1	1
2	E	166/190 (87%)	140 (84%)	18 (11%)	8 (5%)	2	2
2	F	123/190 (65%)	105 (85%)	10 (8%)	8 (6%)	1	1
2	G	163/190 (86%)	135 (83%)	17 (10%)	11 (7%)	1	1
2	H	124/190 (65%)	103 (83%)	14 (11%)	7 (6%)	1	1
All	All	1211/1520 (80%)	1020 (84%)	125 (10%)	66 (6%)	1	1

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	108	LYS
2	A	134	GLU
2	A	137	SER
2	A	138	LYS
2	B	97	GLY
2	B	138	LYS
2	B	172	ARG
2	C	97	GLY
2	C	156	GLU
2	D	97	GLY
2	D	138	LYS
2	E	97	GLY
2	E	134	GLU
2	F	97	GLY
2	F	138	LYS
2	F	172	ARG
2	G	97	GLY

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Mol	Chain	Res	Type
2	G	108	LYS
2	G	134	GLU
2	G	137	SER
2	H	120	SER
2	H	138	LYS
2	H	174	LYS
2	A	97	GLY
2	A	161	MET
2	B	105	ASN
2	C	71	THR
2	C	107	ASP
2	C	108	LYS
2	C	176	ARG
2	E	108	LYS
2	F	122	PHE
2	G	107	ASP
2	H	97	GLY
2	H	121	ALA
2	B	174	LYS
2	C	135	ASN
2	D	71	THR
2	E	46	MET
2	E	107	ASP
2	E	138	LYS
2	G	124	ASN
2	A	20	PRO
2	A	78	LYS
2	D	155	ILE
2	D	156	GLU
2	D	164	ASN
2	E	174	LYS
2	F	74	PHE
2	G	174	LYS
2	B	74	PHE
2	C	134	GLU
2	D	20	PRO
2	D	46	MET
2	D	174	LYS
2	F	71	THR
2	F	117	ASP
2	G	20	PRO
2	G	105	ASN

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Mol	Chain	Res	Type
2	G	138	LYS
2	H	74	PHE
2	D	74	PHE
2	F	46	MET
2	G	131	VAL
2	E	155	ILE
2	H	143	VAL

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	
2	A	132/161 (82%)	118 (89%)	14 (11%)	6	14
2	B	125/161 (78%)	115 (92%)	10 (8%)	11	25
2	C	133/161 (83%)	120 (90%)	13 (10%)	7	17
2	D	132/161 (82%)	119 (90%)	13 (10%)	7	17
2	E	139/161 (86%)	122 (88%)	17 (12%)	5	10
2	F	110/161 (68%)	100 (91%)	10 (9%)	9	19
2	G	136/161 (84%)	125 (92%)	11 (8%)	11	24
2	H	110/161 (68%)	100 (91%)	10 (9%)	9	19
All	All	1017/1288 (79%)	919 (90%)	98 (10%)	8	17

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	12	SER
2	A	15	VAL
2	A	18	LEU
2	A	46	MET
2	A	47	ILE
2	A	71	THR
2	A	93	LEU
2	A	98	VAL

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Mol	Chain	Res	Type
2	A	125	ILE
2	A	126	LEU
2	A	131	VAL
2	A	142	PHE
2	A	143	VAL
2	A	155	ILE
2	B	18	LEU
2	B	19	HIS
2	B	47	ILE
2	B	69	LEU
2	B	71	THR
2	B	93	LEU
2	B	118	THR
2	B	126	LEU
2	B	143	VAL
2	B	153	ARG
2	C	15	VAL
2	C	18	LEU
2	C	47	ILE
2	C	69	LEU
2	C	71	THR
2	C	93	LEU
2	C	125	ILE
2	C	126	LEU
2	C	142	PHE
2	C	143	VAL
2	C	156	GLU
2	C	161	MET
2	C	162	LEU
2	D	15	VAL
2	D	18	LEU
2	D	46	MET
2	D	47	ILE
2	D	71	THR
2	D	93	LEU
2	D	103	ILE
2	D	118	THR
2	D	125	ILE
2	D	142	PHE
2	D	143	VAL
2	D	147	THR
2	D	155	ILE

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Mol	Chain	Res	Type
2	E	14	TYR
2	E	15	VAL
2	E	46	MET
2	E	47	ILE
2	E	69	LEU
2	E	72	MET
2	E	93	LEU
2	E	103	ILE
2	E	104	LYS
2	E	118	THR
2	E	125	ILE
2	E	126	LEU
2	E	131	VAL
2	E	142	PHE
2	E	143	VAL
2	E	148	GLN
2	E	149	GLU
2	F	18	LEU
2	F	47	ILE
2	F	69	LEU
2	F	71	THR
2	F	93	LEU
2	F	118	THR
2	F	125	ILE
2	F	126	LEU
2	F	142	PHE
2	F	143	VAL
2	G	15	VAL
2	G	47	ILE
2	G	69	LEU
2	G	71	THR
2	G	75	ASP
2	G	125	ILE
2	G	126	LEU
2	G	131	VAL
2	G	142	PHE
2	G	143	VAL
2	G	161	MET
2	H	15	VAL
2	H	46	MET
2	H	47	ILE
2	H	69	LEU

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Mol	Chain	Res	Type
2	H	75	ASP
2	H	93	LEU
2	H	125	ILE
2	H	142	PHE
2	H	143	VAL
2	H	149	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	58	ASN
2	A	88	GLN
2	A	124	ASN
2	B	58	ASN
2	B	88	GLN
2	B	124	ASN
2	C	58	ASN
2	C	61	GLN
2	C	88	GLN
2	C	124	ASN
2	C	164	ASN
2	D	58	ASN
2	D	88	GLN
2	D	164	ASN
2	E	58	ASN
2	E	88	GLN
2	E	164	ASN
2	F	58	ASN
2	F	88	GLN
2	G	58	ASN
2	G	88	GLN
2	G	105	ASN
2	G	124	ASN
2	H	58	ASN
2	H	88	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	M	8/11 (72%)	4 (50%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	N	6/11 (54%)	4 (66%)	0
1	O	6/11 (54%)	3 (50%)	0
1	P	6/11 (54%)	3 (50%)	0
1	Q	7/11 (63%)	3 (42%)	0
1	R	6/11 (54%)	5 (83%)	0
1	S	6/11 (54%)	3 (50%)	0
1	T	6/11 (54%)	4 (66%)	0
All	All	51/88 (57%)	29 (56%)	0

All (29) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	M	4	A
1	M	5	A
1	M	6	A
1	M	9	A
1	N	2	A
1	N	4	A
1	N	5	A
1	N	7	A
1	O	2	A
1	O	4	A
1	O	7	A
1	P	2	A
1	P	4	A
1	P	7	A
1	Q	3	A
1	Q	5	A
1	Q	8	A
1	R	2	A
1	R	3	A
1	R	4	A
1	R	5	A
1	R	7	A
1	S	2	A
1	S	4	A
1	S	7	A
1	T	2	A
1	T	4	A
1	T	5	A
1	T	7	A

There are no RNA pucker outliers to report.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
3	AMP	D	994	-	21,21,25	0.29	0	31,31,38	0.35	0
3	AMP	N	992	-	21,21,25	0.24	0	31,31,38	0.35	0
3	AMP	O	993	-	21,21,25	0.25	0	31,31,38	0.35	0
3	AMP	Q	995	-	21,21,25	0.22	0	31,31,38	0.37	0
3	AMP	H	998	-	21,21,25	0.27	0	31,31,38	0.35	0
3	AMP	S	997	-	21,21,25	0.27	0	31,31,38	0.37	0
3	AMP	F	996	-	21,21,25	0.26	0	31,31,38	0.36	0
3	AMP	A	991	-	21,21,25	0.27	0	31,31,38	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	D	994	-	-	0/6/22/26	0/3/3/3
3	AMP	N	992	-	-	0/6/22/26	0/3/3/3
3	AMP	O	993	-	-	0/6/22/26	0/3/3/3
3	AMP	Q	995	-	-	0/6/22/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	H	998	-	-	0/6/22/26	0/3/3/3
3	AMP	S	997	-	-	0/6/22/26	0/3/3/3
3	AMP	F	996	-	-	0/6/22/26	0/3/3/3
3	AMP	A	991	-	-	0/6/22/26	0/3/3/3

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

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.