



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:58 PM GMT

PDB ID : 6Q21  
Title : MOLECULAR SWITCH FOR SIGNAL TRANSDUCTION: STRUCTURAL DIFFERENCES BETWEEN ACTIVE AND INACTIVE FORMS OF PROTOONCOGENIC RAS PROTEINS  
Authors : Kim, S.-H.  
Deposited on : 1992-07-27  
Resolution : 1.95 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

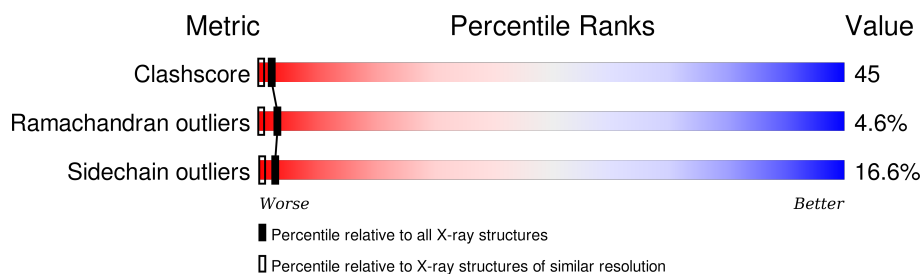
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	171	 27% 44% 23% 6%
1	B	171	 30% 47% 17% 6%
1	C	171	 43% 44% 9% •
1	D	171	 30% 47% 20% •

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6057 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

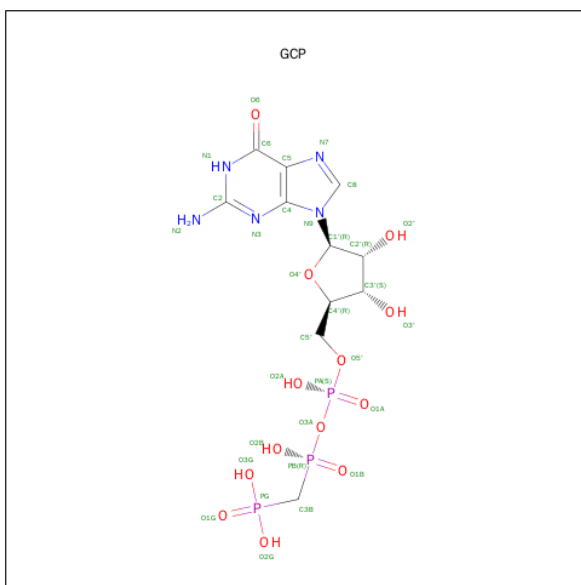
- Molecule 1 is a protein called C-H-RAS P21 PROTEIN CATALYTIC DOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	0	0
			1368	854	238	269	7			
1	B	171	Total	C	N	O	S	0	0	0
			1368	854	238	269	7			
1	C	171	Total	C	N	O	S	0	0	0
			1368	854	238	269	7			
1	D	171	Total	C	N	O	S	0	0	0
			1368	854	238	269	7			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula:  $C_{11}H_{18}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 32	C 11	N 5	O 13	P 3	0	0
3	B	1	Total 32	C 11	N 5	O 13	P 3	0	0
3	C	1	Total 32	C 11	N 5	O 13	P 3	0	0
3	D	1	Total 32	C 11	N 5	O 13	P 3	0	0

- Molecule 4 is water.

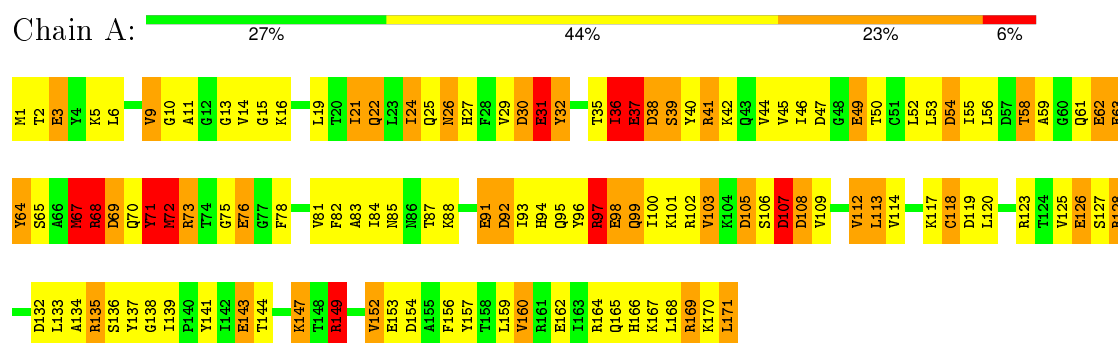
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	83	Total O 83 83	0	0
4	B	93	Total O 93 93	0	0
4	C	111	Total O 111 111	0	0
4	D	166	Total O 166 166	0	0

### 3 Residue-property plots

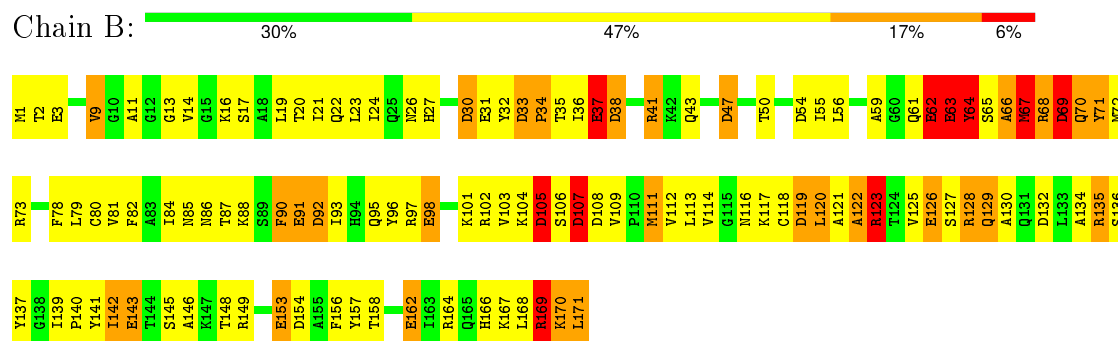
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

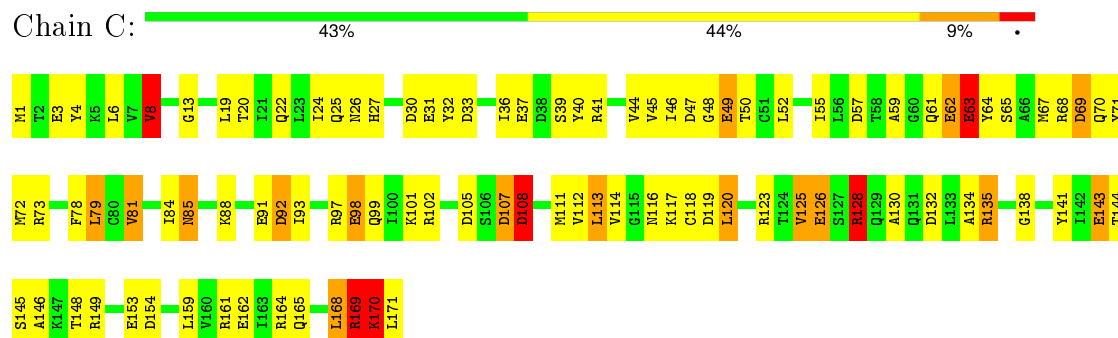
#### • Molecule 1: C-H-RAS P21 PROTEIN CATALYTIC DOMAIN



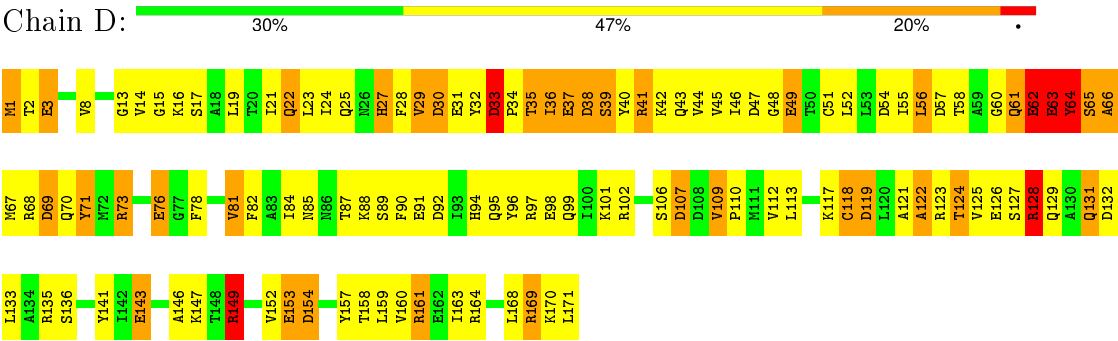
#### • Molecule 1: C-H-RAS P21 PROTEIN CATALYTIC DOMAIN



#### • Molecule 1: C-H-RAS P21 PROTEIN CATALYTIC DOMAIN



● Molecule 1: C-H-RAS P21 PROTEIN CATALYTIC DOMAIN



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 1 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	41.98Å 79.12Å 128.50Å 90.00° 90.00° 117.48°	Depositor
Resolution (Å)	(Not available) – 1.95	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.95)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6057	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	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: GCP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.06	13/1387 (0.9%)	1.69	30/1868 (1.6%)
1	B	1.06	11/1387 (0.8%)	1.63	33/1868 (1.8%)
1	C	1.11	11/1387 (0.8%)	1.62	27/1868 (1.4%)
1	D	1.11	13/1387 (0.9%)	1.67	31/1868 (1.7%)
All	All	1.08	48/5548 (0.9%)	1.65	121/7472 (1.6%)

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	A	2	0

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	3	GLU	CD-OE2	8.16	1.34	1.25
1	D	143	GLU	CD-OE2	8.05	1.34	1.25
1	C	126	GLU	CD-OE2	7.76	1.34	1.25
1	A	153	GLU	CD-OE2	7.70	1.34	1.25
1	B	126	GLU	CD-OE2	7.62	1.34	1.25
1	D	62	GLU	CD-OE2	7.55	1.33	1.25
1	B	98	GLU	CD-OE2	7.22	1.33	1.25
1	D	126	GLU	CD-OE2	7.20	1.33	1.25
1	D	76	GLU	CD-OE2	7.15	1.33	1.25
1	D	63	GLU	CD-OE2	6.90	1.33	1.25
1	A	98	GLU	CD-OE2	6.86	1.33	1.25
1	A	49	GLU	CD-OE2	6.76	1.33	1.25
1	A	63	GLU	CD-OE2	6.68	1.33	1.25
1	A	126	GLU	CD-OE2	6.68	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	62	GLU	CD-OE2	6.64	1.32	1.25
1	D	31	GLU	CD-OE2	6.43	1.32	1.25
1	C	91	GLU	CD-OE2	6.37	1.32	1.25
1	C	153	GLU	CD-OE2	6.35	1.32	1.25
1	D	118	CYS	CA-CB	6.35	1.68	1.53
1	A	62	GLU	CD-OE2	6.32	1.32	1.25
1	A	91	GLU	CD-OE2	6.23	1.32	1.25
1	C	63	GLU	CD-OE2	6.22	1.32	1.25
1	A	31	GLU	CD-OE2	6.21	1.32	1.25
1	A	37	GLU	CD-OE2	6.19	1.32	1.25
1	B	37	GLU	CD-OE2	6.18	1.32	1.25
1	B	62	GLU	CD-OE2	6.17	1.32	1.25
1	C	98	GLU	CD-OE2	6.15	1.32	1.25
1	D	98	GLU	CD-OE2	6.13	1.32	1.25
1	C	3	GLU	CD-OE2	6.10	1.32	1.25
1	B	91	GLU	CD-OE2	6.07	1.32	1.25
1	D	37	GLU	CD-OE2	6.04	1.32	1.25
1	B	31	GLU	CD-OE2	6.03	1.32	1.25
1	B	162	GLU	CD-OE2	6.02	1.32	1.25
1	A	162	GLU	CD-OE2	5.99	1.32	1.25
1	D	153	GLU	CD-OE2	5.97	1.32	1.25
1	C	49	GLU	CD-OE2	5.78	1.32	1.25
1	C	31	GLU	CD-OE2	5.76	1.31	1.25
1	A	3	GLU	CD-OE2	5.71	1.31	1.25
1	A	143	GLU	CD-OE2	5.63	1.31	1.25
1	D	3	GLU	CD-OE2	5.58	1.31	1.25
1	C	143	GLU	CD-OE2	5.57	1.31	1.25
1	B	153	GLU	CD-OE2	5.53	1.31	1.25
1	A	76	GLU	CD-OE2	5.42	1.31	1.25
1	D	49	GLU	CD-OE2	5.41	1.31	1.25
1	B	143	GLU	CD-OE2	5.23	1.31	1.25
1	B	63	GLU	CD-OE2	5.21	1.31	1.25
1	D	91	GLU	CD-OE2	5.18	1.31	1.25
1	C	162	GLU	CD-OE2	5.12	1.31	1.25

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	135	ARG	NE-CZ-NH1	11.51	126.06	120.30
1	A	132	ASP	CB-CG-OD2	-9.36	109.88	118.30
1	A	107	ASP	N-CA-CB	9.18	127.13	110.60
1	D	119	ASP	CB-CG-OD1	9.14	126.53	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	149	ARG	NE-CZ-NH1	8.93	124.77	120.30
1	B	47	ASP	CB-CG-OD2	-8.69	110.48	118.30
1	C	69	ASP	CB-CG-OD2	-8.68	110.49	118.30
1	A	105	ASP	CB-CG-OD2	-8.57	110.59	118.30
1	C	154	ASP	CB-CG-OD2	-8.30	110.83	118.30
1	A	149	ARG	N-CA-CB	8.22	125.41	110.60
1	C	135	ARG	NE-CZ-NH2	-8.15	116.23	120.30
1	B	169	ARG	CA-C-N	-8.14	99.30	117.20
1	D	149	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	A	69	ASP	CB-CG-OD1	7.92	125.43	118.30
1	D	64	TYR	CA-C-N	-7.88	99.87	117.20
1	A	105	ASP	CB-CG-OD1	7.86	125.37	118.30
1	D	30	ASP	CB-CG-OD2	-7.80	111.28	118.30
1	C	107	ASP	CB-CG-OD2	-7.77	111.30	118.30
1	C	108	ASP	CB-CG-OD2	-7.75	111.32	118.30
1	D	47	ASP	CB-CG-OD2	-7.66	111.41	118.30
1	A	119	ASP	CB-CG-OD2	-7.64	111.42	118.30
1	D	38	ASP	CB-CG-OD2	-7.57	111.49	118.30
1	D	128	ARG	NE-CZ-NH2	7.54	124.07	120.30
1	C	119	ASP	CB-CG-OD1	7.42	124.98	118.30
1	A	132	ASP	CB-CG-OD1	7.33	124.90	118.30
1	A	30	ASP	CB-CG-OD2	-7.32	111.71	118.30
1	A	97	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	D	73	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	A	54	ASP	CB-CG-OD2	-7.25	111.77	118.30
1	A	107	ASP	CA-CB-CG	-7.20	97.55	113.40
1	B	119	ASP	CB-CG-OD2	-7.14	111.88	118.30
1	B	92	ASP	CB-CG-OD1	7.10	124.69	118.30
1	A	119	ASP	CB-CG-OD1	7.00	124.60	118.30
1	A	69	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	D	33	ASP	CB-CG-OD1	6.96	124.56	118.30
1	A	97	ARG	NE-CZ-NH2	-6.95	116.82	120.30
1	B	169	ARG	N-CA-CB	6.80	122.83	110.60
1	C	154	ASP	CB-CG-OD1	6.73	124.36	118.30
1	D	33	ASP	CB-CA-C	6.68	123.75	110.40
1	D	119	ASP	CB-CG-OD2	-6.67	112.29	118.30
1	B	41	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	C	69	ASP	CB-CG-OD1	6.60	124.24	118.30
1	B	30	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	B	54	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	B	154	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	C	132	ASP	CB-CG-OD2	-6.48	112.46	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	33	ASP	CB-CG-OD2	-6.45	112.50	118.30
1	A	154	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	A	71	TYR	CB-CA-C	6.38	123.15	110.40
1	D	38	ASP	CB-CG-OD1	6.35	124.02	118.30
1	A	107	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	B	168	LEU	N-CA-CB	-6.30	97.79	110.40
1	C	27	HIS	N-CA-CB	6.30	121.94	110.60
1	B	169	ARG	C-N-CA	6.29	137.44	121.70
1	C	57	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	C	164	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	B	33	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	B	38	ASP	CB-CG-OD1	6.09	123.78	118.30
1	D	149	ARG	CD-NE-CZ	6.08	132.12	123.60
1	B	70	GLN	N-CA-CB	6.08	121.55	110.60
1	B	38	ASP	CB-CG-OD2	-6.05	112.85	118.30
1	D	54	ASP	CB-CG-OD2	-6.04	112.87	118.30
1	D	154	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	B	54	ASP	CB-CG-OD1	6.00	123.70	118.30
1	C	107	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	41	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	C	92	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	72	MET	N-CA-C	-5.85	95.21	111.00
1	A	135	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	B	64	TYR	CB-CA-C	5.79	121.97	110.40
1	A	54	ASP	CB-CG-OD1	5.78	123.51	118.30
1	A	64	TYR	N-CA-C	5.78	126.61	111.00
1	D	92	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	C	108	ASP	CB-CG-OD1	5.76	123.48	118.30
1	C	33	ASP	CB-CG-OD1	5.75	123.48	118.30
1	B	107	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	D	161	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	B	63	GLU	CA-C-N	-5.71	104.63	117.20
1	A	92	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	D	30	ASP	CB-CG-OD1	5.70	123.43	118.30
1	C	119	ASP	CB-CG-OD2	-5.68	113.18	118.30
1	C	169	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	69	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	C	8	VAL	CB-CA-C	5.66	122.16	111.40
1	B	108	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	B	33	ASP	CB-CG-OD1	5.63	123.37	118.30
1	C	132	ASP	CB-CG-OD1	5.63	123.37	118.30
1	B	111	MET	N-CA-CB	-5.62	100.47	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	92	ASP	CB-CG-OD2	-5.58	113.27	118.30
1	B	123	ARG	CB-CA-C	-5.58	99.25	110.40
1	C	164	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	B	169	ARG	O-C-N	5.52	131.53	122.70
1	D	47	ASP	CB-CG-OD1	5.52	123.27	118.30
1	D	41	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	D	54	ASP	CB-CG-OD1	5.51	123.26	118.30
1	D	64	TYR	O-C-N	5.49	131.48	122.70
1	B	105	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	A	30	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	102	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	A	154	ASP	CB-CG-OD1	5.35	123.11	118.30
1	B	108	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	63	GLU	O-C-N	5.31	131.20	122.70
1	D	66	ALA	N-CA-C	-5.29	96.70	111.00
1	A	71	TYR	N-CA-CB	5.28	120.10	110.60
1	A	103	VAL	CA-CB-CG1	-5.24	103.03	110.90
1	D	1	MET	CG-SD-CE	-5.24	91.82	100.20
1	C	92	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	B	92	ASP	CB-CA-C	5.20	120.81	110.40
1	C	40	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	C	128	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	71	TYR	N-CA-CB	5.18	119.92	110.60
1	D	154	ASP	CB-CG-OD1	5.16	122.94	118.30
1	C	30	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	D	128	ARG	CG-CD-NE	5.13	122.56	111.80
1	B	67	MET	N-CA-CB	5.08	119.75	110.60
1	D	107	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	D	132	ASP	CB-CG-OD1	5.06	122.85	118.30
1	C	125	VAL	CB-CA-C	5.02	120.94	111.40
1	D	118	CYS	CA-CB-SG	5.01	123.02	114.00
1	B	69	ASP	CB-CG-OD1	5.00	122.81	118.30
1	A	108	ASP	CB-CG-OD1	5.00	122.80	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	64	TYR	CA
1	A	107	ASP	CA

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1368	0	1357	132	0
1	B	1368	0	1355	151	0
1	C	1368	0	1355	70	0
1	D	1368	0	1356	160	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	32	0	14	6	0
3	B	32	0	14	2	0
3	C	32	0	14	4	0
3	D	32	0	14	5	0
4	A	83	0	0	18	0
4	B	93	0	0	14	0
4	C	111	0	0	16	0
4	D	166	0	0	58	0
All	All	6057	0	5479	502	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 45.

All (502) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:ASP:HB3	1:D:34:PRO:HD3	1.18	1.14
1:B:41:ARG:HD2	1:D:135:ARG:HD3	1.17	1.09
1:D:34:PRO:HB2	1:D:61:GLN:HG3	1.38	1.05
1:A:126:GLU:HB3	1:A:128:ARG:HE	1.24	1.02
1:D:13:GLY:H	3:D:180:GCP:H3B1	1.27	0.98
1:A:35:THR:HB	1:A:59:ALA:HB2	1.44	0.97
1:C:13:GLY:H	3:C:180:GCP:H3B1	1.31	0.94
1:D:127:SER:H	1:D:128:ARG:HH21	1.04	0.93
1:B:41:ARG:HD2	1:D:135:ARG:CD	1.98	0.92
1:D:157:TYR:O	4:D:1110:HOH:O	1.90	0.90
1:B:114:VAL:HA	4:B:1101:HOH:O	1.69	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:SER:H	1:D:128:ARG:NH2	1.70	0.88
1:A:127:SER:H	1:A:128:ARG:NH2	1.72	0.87
1:A:29:VAL:HG11	1:A:32:TYR:HB2	1.55	0.86
1:D:33:ASP:CB	1:D:34:PRO:HD3	2.05	0.85
1:D:68:ARG:HA	1:D:71:TYR:CZ	2.11	0.85
1:C:63:GLU:N	4:C:1055:HOH:O	2.09	0.84
1:D:82:PHE:HA	4:D:1174:HOH:O	1.76	0.84
1:C:128:ARG:HH11	1:C:128:ARG:HB2	1.42	0.84
1:A:108:ASP:HA	4:A:953:HOH:O	1.77	0.84
1:D:170:LYS:HD2	1:D:171:LEU:H	1.43	0.83
1:B:41:ARG:CD	1:D:135:ARG:HD3	2.06	0.83
1:D:160:VAL:HB	4:D:1110:HOH:O	1.79	0.82
1:B:13:GLY:H	3:B:180:GCP:H3B1	1.43	0.82
1:D:149:ARG:HA	4:D:1206:HOH:O	1.78	0.82
1:D:61:GLN:HB3	4:D:1021:HOH:O	1.79	0.82
1:D:128:ARG:H	1:D:128:ARG:HE	1.24	0.82
1:A:169:ARG:CZ	1:A:170:LYS:HE3	2.09	0.82
1:A:41:ARG:NH2	1:B:135:ARG:HG3	1.95	0.81
1:A:68:ARG:HG3	1:A:68:ARG:HH11	1.46	0.81
1:A:126:GLU:HB3	1:A:128:ARG:NE	1.96	0.80
1:B:130:ALA:HB1	1:B:141:TYR:CE1	2.18	0.79
1:B:117:LYS:HB3	1:B:120:LEU:HD22	1.63	0.79
1:A:149:ARG:HB2	1:A:152:VAL:CG1	2.14	0.78
1:B:126:GLU:HB2	1:B:129:GLN:HG2	1.65	0.77
4:A:1210:HOH:O	1:B:135:ARG:HD2	1.84	0.77
1:A:101:LYS:NZ	1:A:107:ASP:HB2	1.99	0.77
1:A:126:GLU:CB	1:A:128:ARG:HE	1.96	0.77
1:D:67:MET:HA	4:D:913:HOH:O	1.83	0.77
1:A:41:ARG:HD2	1:B:135:ARG:NH2	2.00	0.76
1:D:33:ASP:HB3	1:D:34:PRO:CD	2.08	0.76
1:D:62:GLU:HB2	4:D:1022:HOH:O	1.85	0.76
1:D:152:VAL:HG21	4:D:1206:HOH:O	1.86	0.76
1:D:97:ARG:HD3	4:D:865:HOH:O	1.86	0.75
1:A:108:ASP:HB3	1:A:166:HIS:NE2	2.02	0.75
1:C:118:CYS:SG	4:C:1053:HOH:O	2.44	0.75
1:A:2:THR:OG1	1:B:169:ARG:NH2	2.19	0.75
1:D:67:MET:HG3	4:D:1220:HOH:O	1.86	0.74
1:C:116:ASN:OD1	1:C:144:THR:HG23	1.87	0.74
1:D:13:GLY:N	3:D:180:GCP:H3B1	2.03	0.73
1:B:69:ASP:O	1:B:73:ARG:HG3	1.88	0.73
1:A:147:LYS:NZ	1:A:147:LYS:HB2	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:GLU:HG2	1:D:64:TYR:CD1	2.24	0.73
1:A:149:ARG:HB2	1:A:152:VAL:HG11	1.70	0.73
1:A:61:GLN:HG3	1:A:62:GLU:HG3	1.70	0.73
1:C:84:ILE:HG23	1:C:123:ARG:HB2	1.70	0.73
1:A:30:ASP:C	1:A:31:GLU:HG3	2.09	0.73
1:A:94:HIS:O	1:A:98:GLU:HG2	1.88	0.73
1:A:82:PHE:HB3	1:A:93:ILE:HD11	1.70	0.73
1:D:66:ALA:HB2	4:D:1237:HOH:O	1.88	0.72
1:A:147:LYS:HB2	1:A:147:LYS:HZ3	1.54	0.72
1:A:70:GLN:HG2	1:A:73:ARG:HE	1.54	0.72
1:B:90:PHE:HZ	1:B:130:ALA:HA	1.54	0.71
1:D:8:VAL:HG11	4:D:1016:HOH:O	1.90	0.71
1:D:95:GLN:O	1:D:99:GLN:HG3	1.89	0.71
1:B:64:TYR:O	1:B:67:MET:HG2	1.90	0.71
1:B:72:MET:CB	1:B:103:VAL:HG21	2.20	0.71
1:C:168:LEU:O	1:C:170:LYS:N	2.17	0.71
1:C:165:GLN:NE2	1:C:169:ARG:HH21	1.88	0.71
1:A:41:ARG:HD2	1:B:135:ARG:CZ	2.19	0.71
1:A:35:THR:HG23	1:A:38:ASP:OD1	1.89	0.71
1:C:39:SER:HB3	1:C:41:ARG:NH2	2.05	0.71
1:D:133:LEU:CB	4:D:1191:HOH:O	2.38	0.70
1:B:20:THR:O	1:B:24:ILE:HG12	1.90	0.70
1:C:6:LEU:HG	1:C:159:LEU:HD23	1.73	0.70
1:A:35:THR:HG22	1:A:36:ILE:N	2.07	0.70
1:B:67:MET:O	1:B:69:ASP:N	2.25	0.69
1:C:48:GLY:N	4:C:1149:HOH:O	2.16	0.69
1:B:43:GLN:HE22	1:D:141:TYR:H	1.39	0.69
1:D:68:ARG:HD2	1:D:71:TYR:OH	1.92	0.69
1:B:37:GLU:CG	1:B:56:LEU:HD11	2.22	0.69
1:B:37:GLU:HG2	1:B:56:LEU:HD11	1.75	0.69
1:A:24:ILE:HG22	1:A:25:GLN:N	2.08	0.68
1:B:113:LEU:O	4:B:1101:HOH:O	2.11	0.68
1:D:164:ARG:HD2	4:D:1065:HOH:O	1.93	0.68
1:B:142:ILE:HD12	1:B:143:GLU:N	2.08	0.68
1:A:30:ASP:HB2	4:A:1127:HOH:O	1.92	0.68
1:A:156:PHE:O	1:A:160:VAL:HG12	1.93	0.68
1:A:81:VAL:HG11	4:A:1141:HOH:O	1.93	0.68
1:B:134:ALA:HB1	1:B:139:ILE:O	1.94	0.68
1:B:166:HIS:HD2	1:B:170:LYS:NZ	1.91	0.67
1:D:128:ARG:NE	1:D:128:ARG:H	1.90	0.67
1:D:170:LYS:HD2	1:D:171:LEU:N	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:HIS:CD2	1:B:170:LYS:HG2	2.30	0.67
1:C:47:ASP:OD1	1:C:161:ARG:NH2	2.25	0.67
1:A:35:THR:CB	1:A:59:ALA:HB2	2.24	0.67
1:A:94:HIS:ND1	1:A:95:GLN:OE1	2.25	0.67
1:B:69:ASP:HB3	1:B:73:ARG:HH12	1.59	0.67
1:B:72:MET:CE	1:B:103:VAL:HG11	2.25	0.66
1:C:24:ILE:HD11	1:C:55:ILE:HD12	1.78	0.66
1:A:45:VAL:HA	1:A:49:GLU:O	1.95	0.66
1:D:127:SER:N	1:D:128:ARG:HH21	1.85	0.66
1:D:89:SER:HB2	4:D:1174:HOH:O	1.95	0.65
1:D:133:LEU:HB3	4:D:1191:HOH:O	1.94	0.65
1:B:72:MET:HB2	1:B:103:VAL:HG21	1.78	0.65
1:B:17:SER:O	1:B:21:ILE:HG12	1.97	0.65
1:D:49:GLU:OE1	1:D:164:ARG:NH2	2.27	0.65
1:A:16:LYS:NZ	3:A:180:GCP:O2B	2.30	0.64
1:A:118:CYS:SG	4:A:1061:HOH:O	2.55	0.64
1:D:67:MET:O	1:D:70:GLN:HG3	1.98	0.64
1:C:84:ILE:HG23	1:C:123:ARG:CB	2.27	0.64
1:D:61:GLN:HB2	4:D:813:HOH:O	1.98	0.64
1:D:37:GLU:HG3	1:D:58:THR:HA	1.79	0.64
1:D:17:SER:O	1:D:21:ILE:HD13	1.98	0.64
1:A:11:ALA:O	1:A:14:VAL:HG13	1.98	0.64
1:C:128:ARG:NH1	4:C:1140:HOH:O	2.30	0.64
1:D:147:LYS:N	4:D:1059:HOH:O	2.30	0.64
1:D:169:ARG:HD3	1:D:169:ARG:N	2.12	0.63
1:A:35:THR:HA	4:A:1242:HOH:O	1.98	0.63
1:D:61:GLN:NE2	4:D:1042:HOH:O	2.30	0.63
1:B:149:ARG:HH12	1:B:153:GLU:HG3	1.64	0.63
1:C:88:LYS:HE2	1:C:92:ASP:OD2	1.98	0.63
1:D:63:GLU:HG2	1:D:64:TYR:N	2.11	0.62
1:B:123:ARG:NE	1:B:125:VAL:O	2.24	0.62
1:D:24:ILE:HG22	1:D:25:GLN:N	2.14	0.62
1:C:20:THR:O	1:C:24:ILE:HG12	1.99	0.62
1:D:112:VAL:HG23	1:D:159:LEU:HD13	1.80	0.62
1:B:142:ILE:HD12	1:B:143:GLU:H	1.61	0.62
1:D:35:THR:HB	4:D:1015:HOH:O	1.99	0.62
1:A:45:VAL:HG23	1:A:49:GLU:O	1.99	0.62
1:B:145:SER:HB3	1:B:148:THR:OG1	1.99	0.62
1:A:169:ARG:NH2	1:A:170:LYS:HE3	2.15	0.62
1:A:44:VAL:HG22	1:A:45:VAL:N	2.15	0.62
1:C:134:ALA:O	1:C:138:GLY:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LYS:NZ	3:A:180:GCP:O2G	2.26	0.61
1:A:58:THR:HG23	1:A:59:ALA:N	2.15	0.61
1:A:168:LEU:HD12	4:A:1240:HOH:O	2.00	0.61
1:D:42:LYS:HE3	4:D:889:HOH:O	2.01	0.61
1:D:161:ARG:N	4:D:1110:HOH:O	2.10	0.61
1:B:72:MET:CE	1:B:103:VAL:HG21	2.31	0.60
1:B:72:MET:HB3	1:B:103:VAL:HG21	1.83	0.60
1:B:90:PHE:HD2	1:B:125:VAL:CG2	2.13	0.60
1:B:166:HIS:HA	1:B:170:LYS:HB2	1.83	0.60
1:A:61:GLN:OE1	1:A:61:GLN:HA	2.00	0.60
1:D:28:PHE:CD2	1:D:147:LYS:HA	2.36	0.60
1:B:171:LEU:HB3	4:B:1238:HOH:O	2.01	0.60
1:D:170:LYS:HB3	4:D:1160:HOH:O	2.02	0.60
1:D:48:GLY:N	4:D:916:HOH:O	2.32	0.60
1:C:69:ASP:OD1	1:C:73:ARG:NH2	2.34	0.60
1:D:101:LYS:HE3	1:D:107:ASP:OD1	2.01	0.60
1:C:1:MET:HB2	1:C:50:THR:O	2.02	0.60
1:D:90:PHE:CZ	4:D:1191:HOH:O	2.52	0.60
1:A:149:ARG:O	1:A:152:VAL:HG12	2.02	0.59
1:D:44:VAL:HG22	1:D:45:VAL:N	2.17	0.59
1:A:5:LYS:O	1:A:76:GLU:HB2	2.03	0.59
1:A:68:ARG:HE	1:A:96:TYR:HE1	1.50	0.59
1:A:26:ASN:O	1:A:26:ASN:ND2	2.35	0.59
1:A:2:THR:HG1	1:B:169:ARG:HH22	1.48	0.59
1:B:61:GLN:HA	4:B:1076:HOH:O	2.01	0.59
1:D:131:GLN:NE2	1:D:135:ARG:NH2	2.51	0.59
1:A:29:VAL:HG12	1:A:29:VAL:O	2.02	0.59
1:C:161:ARG:NH1	4:C:1092:HOH:O	2.27	0.59
1:B:72:MET:HE2	1:B:103:VAL:HG21	1.85	0.58
1:D:21:ILE:O	1:D:25:GLN:N	2.36	0.58
1:A:101:LYS:HZ2	1:A:107:ASP:HB2	1.67	0.58
1:D:15:GLY:O	1:D:19:LEU:HB2	2.03	0.58
1:D:34:PRO:HB2	1:D:61:GLN:CG	2.23	0.58
1:B:167:LYS:HE2	1:B:167:LYS:HA	1.86	0.58
1:B:13:GLY:N	3:B:180:GCP:H3B1	2.17	0.58
1:D:21:ILE:HG21	1:D:29:VAL:HG13	1.85	0.58
1:B:90:PHE:CZ	1:B:130:ALA:HA	2.38	0.58
1:D:2:THR:HB	1:D:49:GLU:OE2	2.04	0.57
1:D:94:HIS:HB2	4:D:837:HOH:O	2.03	0.57
1:B:97:ARG:HD3	1:B:137:TYR:CZ	2.40	0.57
1:A:41:ARG:CZ	1:B:135:ARG:HG3	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:ALA:HB1	1:C:141:TYR:CE1	2.39	0.57
1:D:22:GLN:NE2	1:D:149:ARG:HD3	2.19	0.57
1:D:62:GLU:HA	1:D:62:GLU:OE1	2.04	0.57
1:A:29:VAL:CG1	1:A:32:TYR:HB2	2.30	0.57
1:A:127:SER:H	1:A:128:ARG:HH21	1.51	0.57
1:B:116:ASN:O	1:B:117:LYS:HB2	2.04	0.57
1:D:3:GLU:HG2	1:D:52:LEU:HB3	1.85	0.57
4:A:971:HOH:O	1:C:45:VAL:HG21	2.05	0.57
1:C:59:ALA:HB1	4:C:808:HOH:O	2.04	0.56
1:D:85:ASN:HA	1:D:124:THR:HB	1.85	0.56
1:B:41:ARG:HB3	1:D:135:ARG:CZ	2.35	0.56
1:B:142:ILE:N	4:B:1101:HOH:O	2.14	0.56
1:A:70:GLN:HG2	1:A:73:ARG:NE	2.20	0.56
1:B:101:LYS:HE2	1:B:107:ASP:OD1	2.05	0.56
1:B:78:PHE:HB2	4:B:951:HOH:O	2.05	0.56
1:C:61:GLN:HB2	4:C:808:HOH:O	2.05	0.56
1:B:86:ASN:OD1	1:B:88:LYS:N	2.38	0.56
1:D:22:GLN:NE2	1:D:149:ARG:CD	2.69	0.56
1:B:81:VAL:HG12	1:B:82:PHE:N	2.21	0.56
1:D:22:GLN:HG3	1:D:146:ALA:O	2.06	0.56
1:D:34:PRO:CB	1:D:61:GLN:HG3	2.24	0.56
1:B:126:GLU:HB2	1:B:129:GLN:CG	2.34	0.56
1:A:171:LEU:HD23	4:A:1240:HOH:O	2.06	0.56
1:C:126:GLU:HA	1:C:126:GLU:OE1	2.06	0.56
1:A:123:ARG:NE	4:A:1201:HOH:O	2.28	0.56
1:A:169:ARG:NH1	4:A:1106:HOH:O	2.39	0.55
1:A:67:MET:HB2	4:A:1232:HOH:O	2.04	0.55
1:D:123:ARG:HH22	1:D:143:GLU:CD	2.09	0.55
1:C:13:GLY:O	4:C:1100:HOH:O	2.18	0.55
1:D:69:ASP:O	1:D:73:ARG:HB2	2.06	0.55
1:A:21:ILE:HD11	1:A:29:VAL:HG23	1.89	0.55
1:B:62:GLU:HG2	1:B:63:GLU:HG3	1.89	0.55
1:C:117:LYS:NZ	4:C:1100:HOH:O	2.18	0.55
1:D:128:ARG:N	1:D:128:ARG:HE	2.00	0.55
1:B:112:VAL:HG22	1:B:140:PRO:HG2	1.89	0.55
1:B:61:GLN:O	1:B:63:GLU:N	2.40	0.54
1:D:136:SER:HA	4:D:1108:HOH:O	2.05	0.54
1:D:22:GLN:CA	1:D:22:GLN:HE21	2.20	0.54
1:C:117:LYS:HG2	3:C:180:GCP:C6	2.37	0.54
1:A:72:MET:O	1:A:73:ARG:HB2	2.05	0.54
1:A:29:VAL:CG1	1:A:32:TYR:H	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:SER:OG	1:B:128:ARG:NH2	2.40	0.54
1:B:90:PHE:HD2	1:B:125:VAL:HG22	1.72	0.54
1:D:97:ARG:NH1	1:D:101:LYS:HD3	2.22	0.53
1:B:145:SER:O	1:B:149:ARG:N	2.40	0.53
1:B:81:VAL:HG12	1:B:82:PHE:H	1.74	0.53
1:C:149:ARG:NH2	4:C:1048:HOH:O	2.40	0.53
1:B:157:TYR:CD1	1:B:157:TYR:N	2.76	0.53
1:D:127:SER:N	1:D:128:ARG:HE	2.07	0.53
1:A:13:GLY:H	3:A:180:GCP:H3B1	1.73	0.53
1:C:13:GLY:N	3:C:180:GCP:H3B1	2.12	0.53
1:A:44:VAL:HG22	1:A:45:VAL:H	1.71	0.53
1:C:52:LEU:C	1:C:52:LEU:HD13	2.29	0.53
1:D:122:ALA:N	4:D:1073:HOH:O	2.24	0.53
1:D:146:ALA:HB3	4:D:1059:HOH:O	2.08	0.53
1:B:104:LYS:O	1:B:105:ASP:HB2	2.09	0.53
1:D:28:PHE:HA	4:D:901:HOH:O	2.09	0.53
1:A:9:VAL:HG13	1:A:10:GLY:N	2.23	0.53
1:C:36:ILE:O	1:C:37:GLU:HB2	2.08	0.53
1:D:25:GLN:HB2	1:D:27:HIS:CD2	2.44	0.53
1:D:43:GLN:HA	1:D:51:CYS:O	2.09	0.53
1:A:35:THR:CG2	1:A:36:ILE:N	2.72	0.53
1:B:61:GLN:NE2	1:B:64:TYR:CE2	2.77	0.52
1:C:128:ARG:HH11	1:C:128:ARG:CB	2.19	0.52
1:A:105:ASP:OD1	1:A:105:ASP:O	2.27	0.52
1:C:101:LYS:O	1:C:105:ASP:N	2.42	0.52
1:A:11:ALA:O	1:A:14:VAL:HG22	2.09	0.52
1:D:63:GLU:HA	4:D:1193:HOH:O	2.10	0.52
1:B:66:ALA:O	1:B:69:ASP:HB2	2.10	0.52
1:D:70:GLN:O	1:D:73:ARG:HB3	2.09	0.52
1:B:149:ARG:HH12	1:B:153:GLU:CG	2.23	0.52
1:C:145:SER:O	1:C:149:ARG:N	2.40	0.52
1:B:78:PHE:N	1:B:78:PHE:CD1	2.78	0.52
1:B:166:HIS:HD2	1:B:170:LYS:HZ3	1.57	0.51
1:B:85:ASN:ND2	1:B:120:LEU:HD23	2.25	0.51
1:D:121:ALA:HA	4:D:1073:HOH:O	2.09	0.51
1:B:33:ASP:O	1:B:34:PRO:O	2.28	0.51
1:B:111:MET:HG3	4:B:951:HOH:O	2.09	0.51
1:C:20:THR:OG1	4:C:1058:HOH:O	2.19	0.51
1:C:85:ASN:HD22	1:C:85:ASN:H	1.58	0.51
1:D:16:LYS:NZ	3:D:180:GCP:O1G	2.35	0.51
1:A:68:ARG:NH1	1:A:68:ARG:HG3	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:MET:O	1:B:112:VAL:HG23	2.10	0.51
1:D:27:HIS:CD2	1:D:27:HIS:N	2.78	0.51
1:B:47:ASP:OD2	1:B:164:ARG:NH1	2.41	0.51
1:A:103:VAL:HG12	1:A:103:VAL:O	2.10	0.51
1:C:72:MET:SD	1:C:99:GLN:HG2	2.51	0.51
1:B:126:GLU:O	1:B:129:GLN:HG3	2.11	0.51
1:D:90:PHE:CE1	4:D:1191:HOH:O	2.64	0.50
1:C:113:LEU:HB3	1:C:141:TYR:HD1	1.77	0.50
1:A:113:LEU:O	1:A:141:TYR:HA	2.11	0.50
1:D:127:SER:H	1:D:128:ARG:CZ	2.22	0.50
1:A:88:LYS:O	1:A:92:ASP:OD2	2.30	0.50
1:C:65:SER:HB3	4:C:1055:HOH:O	2.12	0.50
1:A:46:ILE:HD11	1:A:157:TYR:CD1	2.46	0.49
1:B:1:MET:HE1	4:D:941:HOH:O	2.12	0.49
1:A:137:TYR:HB2	1:A:139:ILE:HG12	1.93	0.49
1:D:170:LYS:O	1:D:171:LEU:HB2	2.11	0.49
1:B:102:ARG:HD2	4:B:1105:HOH:O	2.11	0.49
1:A:24:ILE:C	1:A:26:ASN:H	2.16	0.49
1:C:70:GLN:NE2	1:C:73:ARG:HH12	2.10	0.49
1:A:112:VAL:HG13	1:A:159:LEU:HB2	1.95	0.49
1:B:37:GLU:HG3	1:B:56:LEU:HD11	1.92	0.49
1:A:123:ARG:HD3	1:A:125:VAL:O	2.12	0.49
1:A:83:ALA:HB1	1:A:85:ASN:OD1	2.12	0.49
1:A:127:SER:N	1:A:128:ARG:NH2	2.52	0.49
1:B:69:ASP:O	1:B:73:ARG:NH1	2.46	0.49
1:D:102:ARG:HD2	4:D:843:HOH:O	2.12	0.49
1:A:36:ILE:HG23	1:A:64:TYR:HB3	1.93	0.49
1:A:35:THR:HG22	1:A:36:ILE:H	1.76	0.48
1:A:22:GLN:O	1:A:26:ASN:HA	2.12	0.48
1:A:108:ASP:HB3	1:A:166:HIS:CE1	2.48	0.48
1:B:117:LYS:O	1:B:119:ASP:N	2.46	0.48
1:A:46:ILE:O	1:A:47:ASP:HB2	2.13	0.48
1:A:30:ASP:OD1	1:A:31:GLU:OE2	2.31	0.48
1:B:126:GLU:HB2	1:B:129:GLN:OE1	2.13	0.48
1:B:84:ILE:HD12	1:B:84:ILE:C	2.33	0.48
1:B:85:ASN:ND2	1:B:120:LEU:CD2	2.76	0.48
1:A:24:ILE:HG22	1:A:25:GLN:CD	2.33	0.48
1:B:101:LYS:O	1:B:105:ASP:N	2.47	0.48
1:D:61:GLN:HB3	1:D:62:GLU:H	1.42	0.48
1:D:68:ARG:HA	1:D:71:TYR:CE1	2.47	0.48
1:B:2:THR:N	4:B:1085:HOH:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:LYS:CG	1:D:171:LEU:N	2.77	0.48
1:B:37:GLU:O	1:B:38:ASP:OD1	2.31	0.48
1:B:121:ALA:O	1:B:122:ALA:HB2	2.13	0.48
1:C:81:VAL:HB	1:C:114:VAL:HB	1.96	0.48
1:B:90:PHE:O	1:B:90:PHE:HD1	1.96	0.47
1:D:154:ASP:O	1:D:158:THR:N	2.45	0.47
1:A:97:ARG:NH2	4:A:974:HOH:O	2.47	0.47
1:A:47:ASP:OD2	1:A:164:ARG:NH1	2.36	0.47
1:A:167:LYS:NZ	4:A:995:HOH:O	2.47	0.47
1:D:129:GLN:HG2	4:D:842:HOH:O	2.14	0.47
1:D:66:ALA:HA	4:D:1083:HOH:O	2.13	0.47
1:D:123:ARG:NH2	1:D:143:GLU:OE2	2.42	0.47
1:C:145:SER:HB3	1:C:148:THR:OG1	2.13	0.47
1:D:64:TYR:HE2	1:D:96:TYR:CZ	2.33	0.47
1:B:72:MET:HB2	1:B:72:MET:HE2	1.53	0.47
1:D:41:ARG:CZ	1:D:41:ARG:HB2	2.44	0.47
1:D:109:VAL:HA	1:D:110:PRO:HD3	1.80	0.47
1:D:39:SER:HA	1:D:55:ILE:O	2.15	0.47
3:D:180:GCP:H3B2	4:D:872:HOH:O	2.14	0.47
1:B:130:ALA:HB1	1:B:141:TYR:CZ	2.49	0.47
1:A:37:GLU:HG2	1:A:56:LEU:HD11	1.96	0.47
1:D:60:GLY:HA2	4:D:949:HOH:O	2.15	0.47
1:B:170:LYS:O	1:B:171:LEU:HB2	2.15	0.47
1:C:111:MET:C	1:C:112:VAL:HG23	2.35	0.47
1:B:130:ALA:CB	1:B:141:TYR:CZ	2.98	0.47
1:D:89:SER:CB	4:D:1174:HOH:O	2.58	0.47
1:B:11:ALA:O	1:B:14:VAL:HG13	2.14	0.47
1:A:39:SER:C	1:A:40:TYR:CD1	2.88	0.47
1:D:44:VAL:CG2	1:D:45:VAL:N	2.78	0.46
1:B:157:TYR:HD1	1:B:157:TYR:N	2.13	0.46
1:C:4:TYR:OH	1:C:49:GLU:OE1	2.24	0.46
1:C:116:ASN:O	1:C:117:LYS:HB2	2.15	0.46
1:D:28:PHE:CD1	1:D:28:PHE:O	2.68	0.46
1:B:72:MET:HE2	1:B:103:VAL:HG11	1.98	0.46
1:B:166:HIS:HD2	1:B:170:LYS:HZ2	1.62	0.46
1:A:67:MET:HB3	1:A:71:TYR:HE2	1.80	0.46
1:B:79:LEU:HD13	1:B:114:VAL:HG21	1.97	0.46
1:B:149:ARG:NH1	1:B:153:GLU:OE2	2.48	0.46
1:D:36:ILE:HD12	4:D:1109:HOH:O	2.15	0.46
1:D:170:LYS:CD	1:D:171:LEU:N	2.77	0.46
1:B:149:ARG:NH1	1:B:153:GLU:HG3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:THR:CG2	1:A:59:ALA:N	2.78	0.46
1:C:78:PHE:O	1:C:111:MET:HA	2.15	0.46
1:C:41:ARG:NH2	4:C:863:HOH:O	2.49	0.46
1:D:133:LEU:CD2	4:D:1191:HOH:O	2.64	0.46
1:B:171:LEU:HD22	1:B:171:LEU:HA	1.44	0.46
1:D:102:ARG:HG2	4:D:843:HOH:O	2.15	0.46
1:B:128:ARG:NE	1:B:128:ARG:H	2.14	0.46
1:D:149:ARG:HD2	4:D:1206:HOH:O	2.16	0.46
1:C:108:ASP:OD2	1:C:169:ARG:NH1	2.47	0.46
1:B:97:ARG:NH1	1:B:98:GLU:OE1	2.49	0.46
1:C:46:ILE:O	1:C:49:GLU:N	2.44	0.46
1:A:21:ILE:HD12	1:A:27:HIS:O	2.16	0.45
1:D:160:VAL:N	4:D:1110:HOH:O	2.47	0.45
3:C:180:GCP:O4'	4:C:1100:HOH:O	2.21	0.45
1:D:22:GLN:HA	1:D:22:GLN:HE21	1.81	0.45
1:A:164:ARG:NH1	4:A:1064:HOH:O	2.47	0.45
1:C:85:ASN:OD1	1:C:120:LEU:HD23	2.17	0.45
1:B:36:ILE:HD13	1:B:36:ILE:N	2.31	0.45
1:B:68:ARG:HG3	1:B:71:TYR:OH	2.16	0.45
1:D:135:ARG:NH1	4:D:1094:HOH:O	2.28	0.45
1:B:69:ASP:HB3	1:B:73:ARG:NH1	2.30	0.45
1:A:81:VAL:HG12	1:A:82:PHE:N	2.31	0.45
1:B:33:ASP:HA	1:B:34:PRO:HD2	1.73	0.45
1:B:117:LYS:C	1:B:119:ASP:H	2.20	0.45
1:D:87:THR:OG1	1:D:124:THR:HG23	2.17	0.45
1:A:133:LEU:HG	1:A:137:TYR:CE2	2.51	0.45
1:A:117:LYS:N	1:A:144:THR:O	2.50	0.45
1:B:41:ARG:HD3	4:B:1175:HOH:O	2.16	0.45
1:A:24:ILE:HD11	1:A:55:ILE:HD12	1.99	0.45
1:B:87:THR:O	1:B:91:GLU:HG3	2.17	0.45
1:B:24:ILE:HD11	1:B:55:ILE:HD12	1.98	0.45
1:D:1:MET:CE	1:D:43:GLN:HG3	2.47	0.45
1:B:68:ARG:NH2	1:B:96:TYR:OH	2.50	0.45
1:C:64:TYR:HB3	1:C:67:MET:CE	2.47	0.45
1:C:116:ASN:HA	1:C:144:THR:HG22	1.99	0.44
1:B:158:THR:O	1:B:162:GLU:HG2	2.17	0.44
1:D:40:TYR:N	1:D:40:TYR:CD1	2.85	0.44
1:A:42:LYS:O	1:A:52:LEU:HD12	2.18	0.44
1:D:66:ALA:O	4:D:913:HOH:O	2.21	0.44
1:B:142:ILE:HD12	4:B:1208:HOH:O	2.16	0.44
1:B:35:THR:O	1:B:59:ALA:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:HIS:HD2	1:D:27:HIS:H	1.66	0.44
1:D:44:VAL:HG22	1:D:45:VAL:H	1.82	0.44
1:C:78:PHE:CD1	1:C:78:PHE:N	2.86	0.44
1:B:113:LEU:O	1:B:141:TYR:HA	2.17	0.44
1:B:64:TYR:HB3	1:B:67:MET:CE	2.47	0.44
1:D:109:VAL:HG13	4:D:1069:HOH:O	2.18	0.44
1:A:16:LYS:O	1:A:19:LEU:HB2	2.17	0.44
1:A:41:ARG:HA	1:A:53:LEU:O	2.17	0.44
1:B:170:LYS:HA	1:B:170:LYS:HD3	1.44	0.44
1:C:141:TYR:CE2	1:C:143:GLU:HG3	2.52	0.44
1:A:22:GLN:HE21	1:A:22:GLN:CA	2.30	0.44
1:D:23:LEU:HD12	1:D:153:GLU:HG3	2.00	0.44
1:A:78:PHE:CG	1:A:100:ILE:HD13	2.52	0.43
1:A:3:GLU:HA	1:A:52:LEU:O	2.18	0.43
1:B:61:GLN:C	1:B:63:GLU:N	2.72	0.43
1:B:169:ARG:HG2	4:B:1226:HOH:O	2.18	0.43
1:B:16:LYS:O	1:B:19:LEU:HB2	2.17	0.43
1:D:63:GLU:CG	1:D:64:TYR:N	2.72	0.43
1:B:141:TYR:CE2	1:B:143:GLU:CG	3.01	0.43
1:B:90:PHE:CE2	1:B:125:VAL:HG13	2.54	0.43
1:D:67:MET:HB3	1:D:70:GLN:HG3	2.00	0.43
1:B:166:HIS:HA	1:B:170:LYS:HG2	2.01	0.43
1:A:5:LYS:HD3	1:A:54:ASP:HB3	2.01	0.43
1:A:106:SER:OG	1:A:108:ASP:HB2	2.18	0.43
1:D:136:SER:HB2	4:D:1108:HOH:O	2.18	0.43
1:A:120:LEU:HD23	1:A:120:LEU:HA	1.76	0.43
1:B:92:ASP:O	1:B:95:GLN:HB2	2.19	0.43
1:B:120:LEU:HA	1:B:120:LEU:HD12	1.78	0.43
1:B:72:MET:HE3	1:B:103:VAL:CG2	2.49	0.43
1:A:6:LEU:CD1	1:A:6:LEU:N	2.81	0.43
1:D:78:PHE:CD1	1:D:78:PHE:N	2.87	0.43
1:C:171:LEU:O	1:C:171:LEU:HG	2.18	0.43
1:D:168:LEU:N	1:D:168:LEU:HD22	2.33	0.43
1:A:21:ILE:HD11	1:A:29:VAL:CG2	2.49	0.43
1:B:166:HIS:CD2	1:B:170:LYS:HZ2	2.37	0.43
1:D:161:ARG:NH1	4:D:1068:HOH:O	2.52	0.43
1:B:72:MET:CE	1:B:103:VAL:CG1	2.96	0.43
1:B:97:ARG:HD3	1:B:137:TYR:CE1	2.54	0.43
1:B:137:TYR:HA	1:B:137:TYR:HD1	1.70	0.43
1:A:134:ALA:O	1:A:138:GLY:N	2.52	0.43
1:B:23:LEU:HD22	1:B:156:PHE:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ARG:HG2	1:B:135:ARG:HH21	1.84	0.42
1:D:133:LEU:HB2	4:D:1191:HOH:O	2.12	0.42
1:B:24:ILE:HG22	1:B:24:ILE:O	2.19	0.42
1:A:165:GLN:NE2	4:A:828:HOH:O	2.51	0.42
1:D:19:LEU:HD13	1:D:146:ALA:HB2	2.01	0.42
1:B:61:GLN:HG3	1:B:63:GLU:OE1	2.19	0.42
1:C:85:ASN:HD22	1:C:85:ASN:N	2.15	0.42
1:A:68:ARG:HD3	1:A:99:GLN:OE1	2.19	0.42
1:A:68:ARG:NE	1:A:96:TYR:HE1	2.14	0.42
1:B:64:TYR:HB3	1:B:67:MET:HE2	2.01	0.42
1:A:6:LEU:HD12	1:A:6:LEU:N	2.34	0.42
1:C:135:ARG:HD2	4:D:992:HOH:O	2.19	0.42
1:A:35:THR:CG2	1:A:36:ILE:H	2.31	0.42
1:B:128:ARG:HG3	4:B:1209:HOH:O	2.18	0.42
1:D:67:MET:HA	4:D:1158:HOH:O	2.19	0.42
1:B:27:HIS:HD2	4:B:1192:HOH:O	2.03	0.42
1:D:63:GLU:CG	1:D:64:TYR:CD1	3.00	0.42
1:D:14:VAL:CG2	1:D:81:VAL:HG22	2.49	0.42
1:D:14:VAL:HG23	1:D:81:VAL:HG22	2.01	0.42
1:D:24:ILE:HG12	1:D:40:TYR:HB3	2.01	0.42
1:B:22:GLN:HG3	1:B:146:ALA:O	2.19	0.42
1:D:117:LYS:C	1:D:119:ASP:N	2.71	0.42
1:C:97:ARG:HG2	4:C:1087:HOH:O	2.19	0.42
1:A:45:VAL:HG23	1:A:49:GLU:N	2.35	0.42
1:A:14:VAL:HG23	1:A:15:GLY:N	2.35	0.42
1:B:13:GLY:O	1:B:117:LYS:NZ	2.50	0.42
1:A:107:ASP:O	1:A:107:ASP:OD2	2.37	0.42
1:B:70:GLN:HG3	1:B:73:ARG:HB2	2.02	0.42
1:D:68:ARG:HA	1:D:71:TYR:CE2	2.53	0.42
1:A:141:TYR:OH	1:A:143:GLU:OE2	2.35	0.42
1:D:170:LYS:HG3	1:D:171:LEU:N	2.35	0.41
1:B:70:GLN:CG	1:B:70:GLN:O	2.68	0.41
1:C:168:LEU:HD12	1:C:168:LEU:HA	1.60	0.41
1:D:17:SER:HB3	1:D:32:TYR:CD2	2.55	0.41
1:D:56:LEU:HD22	1:D:57:ASP:N	2.35	0.41
1:A:29:VAL:HG13	1:A:32:TYR:H	1.83	0.41
1:A:71:TYR:O	1:A:75:GLY:N	2.48	0.41
1:A:137:TYR:O	4:A:1037:HOH:O	2.22	0.41
1:B:97:ARG:O	1:B:101:LYS:HD3	2.21	0.41
1:B:41:ARG:CB	1:D:135:ARG:CZ	2.99	0.41
1:D:67:MET:HB3	4:D:1158:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:MET:O	1:D:71:TYR:CE1	2.74	0.41
1:D:14:VAL:HG11	4:D:1174:HOH:O	2.21	0.41
1:B:117:LYS:O	1:B:120:LEU:HB2	2.21	0.41
1:D:97:ARG:CG	1:D:97:ARG:O	2.66	0.41
1:A:123:ARG:NH2	4:A:1201:HOH:O	2.51	0.41
1:C:116:ASN:HA	1:C:144:THR:CG2	2.50	0.41
1:C:113:LEU:HD23	1:C:113:LEU:HA	1.82	0.41
1:A:30:ASP:HB3	3:A:180:GCP:O2'	2.21	0.41
1:A:35:THR:HB	3:A:180:GCP:O1G	2.21	0.41
1:B:166:HIS:CD2	1:B:170:LYS:NZ	2.80	0.41
1:D:27:HIS:CD2	1:D:27:HIS:H	2.39	0.41
1:D:160:VAL:O	1:D:163:ILE:HB	2.20	0.41
1:D:52:LEU:HD12	1:D:52:LEU:HA	1.83	0.41
1:C:98:GLU:OE1	1:C:101:LYS:NZ	2.53	0.41
1:C:101:LYS:HD3	1:C:107:ASP:HA	2.03	0.41
1:C:8:VAL:HB	1:C:79:LEU:HB2	2.03	0.41
1:B:9:VAL:HG12	1:B:80:CYS:HA	2.02	0.41
1:D:97:ARG:O	1:D:101:LYS:HG3	2.21	0.41
1:D:61:GLN:C	1:D:63:GLU:H	2.24	0.40
1:D:160:VAL:CA	4:D:1110:HOH:O	2.68	0.40
1:A:149:ARG:CB	1:A:152:VAL:HG11	2.46	0.40
1:B:166:HIS:HA	1:B:170:LYS:CB	2.49	0.40
1:D:136:SER:CA	4:D:1108:HOH:O	2.67	0.40
1:D:34:PRO:HB3	3:D:180:GCP:O2G	2.21	0.40
1:D:76:GLU:O	1:D:110:PRO:HG2	2.21	0.40
1:A:87:THR:HG22	1:A:91:GLU:OE2	2.21	0.40
1:B:127:SER:O	1:B:130:ALA:N	2.53	0.40
1:A:169:ARG:C	1:A:170:LYS:HG2	2.41	0.40
1:D:24:ILE:CG2	1:D:25:GLN:N	2.80	0.40
1:C:22:GLN:HG3	1:C:146:ALA:O	2.21	0.40
1:A:61:GLN:HB2	3:A:180:GCP:O3G	2.21	0.40
1:B:132:ASP:O	1:B:135:ARG:HB2	2.21	0.40
1:A:1:MET:HE2	1:A:50:THR:HG22	2.03	0.40
1:D:61:GLN:C	1:D:63:GLU:N	2.75	0.40
1:D:97:ARG:NH1	4:D:865:HOH:O	2.45	0.40
1:B:69:ASP:C	1:B:73:ARG:NH1	2.74	0.40
1:D:46:ILE:HG22	1:D:164:ARG:HH22	1.86	0.40
1:C:64:TYR:HB3	1:C:67:MET:HE2	2.04	0.40
1:C:25:GLN:NE2	4:C:1142:HOH:O	2.25	0.40
1:C:68:ARG:HA	1:C:71:TYR:CE2	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	169/171 (99%)	135 (80%)	25 (15%)	9 (5%)	2	0
1	B	169/171 (99%)	150 (89%)	8 (5%)	11 (6%)	1	0
1	C	169/171 (99%)	159 (94%)	7 (4%)	3 (2%)	11	2
1	D	169/171 (99%)	149 (88%)	12 (7%)	8 (5%)	3	0
All	All	676/684 (99%)	593 (88%)	52 (8%)	31 (5%)	3	0

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	GLU
1	A	67	MET
1	A	69	ASP
1	A	73	ARG
1	B	34	PRO
1	B	62	GLU
1	B	64	TYR
1	B	69	ASP
1	B	122	ALA
1	C	63	GLU
1	C	169	ARG
1	D	65	SER
1	D	122	ALA
1	A	26	ASN
1	A	68	ARG
1	B	66	ALA
1	B	106	SER
1	B	118	CYS
1	D	63	GLU
1	A	65	SER
1	B	169	ARG
1	C	170	LYS

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Mol	Chain	Res	Type
1	D	30	ASP
1	D	33	ASP
1	D	64	TYR
1	A	24	ILE
1	D	61	GLN
1	D	118	CYS
1	B	68	ARG
1	A	36	ILE
1	B	105	ASP

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	149/149 (100%)	117 (78%)	32 (22%)	1	0
1	B	149/149 (100%)	125 (84%)	24 (16%)	3	0
1	C	149/149 (100%)	131 (88%)	18 (12%)	6	1
1	D	149/149 (100%)	124 (83%)	25 (17%)	2	0
All	All	596/596 (100%)	497 (83%)	99 (17%)	3	0

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	21	ILE
1	A	22	GLN
1	A	31	GLU
1	A	32	TYR
1	A	36	ILE
1	A	37	GLU
1	A	38	ASP
1	A	39	SER
1	A	58	THR
1	A	67	MET
1	A	68	ARG

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Mol	Chain	Res	Type
1	A	71	TYR
1	A	72	MET
1	A	84	ILE
1	A	97	ARG
1	A	99	GLN
1	A	107	ASP
1	A	109	VAL
1	A	112	VAL
1	A	113	LEU
1	A	114	VAL
1	A	118	CYS
1	A	128	ARG
1	A	135	ARG
1	A	136	SER
1	A	147	LYS
1	A	149	ARG
1	A	152	VAL
1	A	160	VAL
1	A	169	ARG
1	A	171	LEU
1	B	9	VAL
1	B	26	ASN
1	B	30	ASP
1	B	32	TYR
1	B	37	GLU
1	B	50	THR
1	B	62	GLU
1	B	63	GLU
1	B	65	SER
1	B	67	MET
1	B	69	ASP
1	B	90	PHE
1	B	93	ILE
1	B	107	ASP
1	B	109	VAL
1	B	120	LEU
1	B	123	ARG
1	B	128	ARG
1	B	129	GLN
1	B	135	ARG
1	B	136	SER
1	B	142	ILE

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Mol	Chain	Res	Type
1	B	170	LYS
1	B	171	LEU
1	C	8	VAL
1	C	19	LEU
1	C	26	ASN
1	C	32	TYR
1	C	44	VAL
1	C	62	GLU
1	C	79	LEU
1	C	81	VAL
1	C	85	ASN
1	C	93	ILE
1	C	102	ARG
1	C	108	ASP
1	C	113	LEU
1	C	120	LEU
1	C	125	VAL
1	C	128	ARG
1	C	168	LEU
1	C	170	LYS
1	D	22	GLN
1	D	27	HIS
1	D	29	VAL
1	D	35	THR
1	D	36	ILE
1	D	38	ASP
1	D	39	SER
1	D	56	LEU
1	D	62	GLU
1	D	64	TYR
1	D	65	SER
1	D	69	ASP
1	D	71	TYR
1	D	81	VAL
1	D	84	ILE
1	D	88	LYS
1	D	106	SER
1	D	109	VAL
1	D	113	LEU
1	D	124	THR
1	D	125	VAL
1	D	128	ARG

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Mol	Chain	Res	Type
1	D	131	GLN
1	D	149	ARG
1	D	169	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	B	26	ASN
1	B	43	GLN
1	B	70	GLN
1	B	116	ASN
1	B	131	GLN
1	B	166	HIS
1	C	61	GLN
1	C	70	GLN
1	C	85	ASN
1	C	150	GLN
1	C	165	GLN
1	D	22	GLN
1	D	27	HIS
1	D	99	GLN
1	D	131	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GCP	A	180	2	26,34,34	1.53	2 (7%)	34,54,54	2.48	9 (26%)
3	GCP	B	180	2	26,34,34	1.36	3 (11%)	34,54,54	2.49	9 (26%)
3	GCP	C	180	2	26,34,34	1.50	5 (19%)	34,54,54	2.61	9 (26%)
3	GCP	D	180	2	26,34,34	1.88	7 (26%)	34,54,54	2.27	9 (26%)

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	GCP	A	180	2	-	0/15/38/38	0/3/3/3
3	GCP	B	180	2	-	0/15/38/38	0/3/3/3
3	GCP	C	180	2	-	0/15/38/38	0/3/3/3
3	GCP	D	180	2	-	0/15/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	180	GCP	PB-O2B	-2.74	1.49	1.56
3	B	180	GCP	PB-O3A	-2.13	1.56	1.58
3	C	180	GCP	C8-N7	-2.12	1.30	1.34
3	D	180	GCP	PB-O3A	-2.09	1.56	1.58
3	C	180	GCP	C4-N3	2.24	1.39	1.35
3	C	180	GCP	C2-N1	2.26	1.39	1.35
3	C	180	GCP	PG-O1G	2.45	1.55	1.50
3	D	180	GCP	C2-N1	2.58	1.40	1.35
3	D	180	GCP	O4'-C1'	2.68	1.44	1.41
3	A	180	GCP	C6-N1	2.70	1.38	1.33
3	B	180	GCP	C6-N1	3.04	1.38	1.33
3	D	180	GCP	C6-N1	3.82	1.40	1.33
3	D	180	GCP	PG-O1G	4.43	1.60	1.50
3	B	180	GCP	PG-O3G	4.74	1.66	1.54
3	D	180	GCP	PG-O3G	4.84	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	180	GCP	C6-N1	4.89	1.42	1.33
3	A	180	GCP	PG-O1G	5.64	1.63	1.50

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	180	GCP	C5-C6-N1	-8.49	111.98	123.59
3	A	180	GCP	C5-C6-N1	-8.47	112.01	123.59
3	B	180	GCP	C5-C6-N1	-8.47	112.02	123.59
3	C	180	GCP	C5-C6-N1	-7.75	113.00	123.59
3	B	180	GCP	O3G-PG-O1G	-4.88	99.93	112.40
3	A	180	GCP	O1B-PB-C3B	-4.31	98.18	109.02
3	C	180	GCP	O2G-PG-O1G	-4.22	101.60	112.40
3	C	180	GCP	O2B-PB-C3B	-4.06	89.20	106.88
3	B	180	GCP	O2B-PB-C3B	-3.28	92.59	106.88
3	D	180	GCP	O2G-PG-O1G	-2.61	105.72	112.40
3	A	180	GCP	PA-O3A-PB	-2.58	125.48	132.73
3	C	180	GCP	N3-C2-N1	-2.56	123.54	127.44
3	D	180	GCP	C4'-O4'-C1'	-2.45	107.03	109.72
3	B	180	GCP	PA-O3A-PB	-2.42	125.94	132.73
3	A	180	GCP	O3G-PG-O1G	-2.40	106.27	112.40
3	D	180	GCP	PA-O3A-PB	-2.35	126.13	132.73
3	D	180	GCP	N3-C2-N1	-2.26	124.00	127.44
3	B	180	GCP	N3-C2-N1	-2.12	124.21	127.44
3	D	180	GCP	O3G-PG-C3B	2.01	111.28	106.40
3	D	180	GCP	C4-C5-N7	2.19	111.49	109.48
3	C	180	GCP	O3G-PG-C3B	2.22	111.80	106.40
3	A	180	GCP	O2G-PG-C3B	2.26	111.89	106.40
3	B	180	GCP	O2B-PB-O1B	2.60	118.30	110.12
3	A	180	GCP	O3G-PG-C3B	2.79	113.16	106.40
3	C	180	GCP	C4'-O4'-C1'	2.85	112.86	109.72
3	A	180	GCP	O2B-PB-C3B	3.44	121.89	106.88
3	D	180	GCP	O2B-PB-O1B	3.73	121.85	110.12
3	A	180	GCP	O2B-PB-O1B	3.81	122.09	110.12
3	B	180	GCP	O3G-PG-C3B	3.84	115.70	106.40
3	C	180	GCP	O2B-PB-O1B	4.33	123.72	110.12
3	B	180	GCP	O1B-PB-C3B	4.44	120.20	109.02
3	C	180	GCP	C6-N1-C2	5.43	123.47	115.94
3	D	180	GCP	C6-N1-C2	6.05	124.33	115.94
3	C	180	GCP	O1B-PB-C3B	6.07	124.31	109.02
3	A	180	GCP	C6-N1-C2	6.13	124.44	115.94
3	B	180	GCP	C6-N1-C2	6.15	124.47	115.94



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	180	GCP	6	0
3	B	180	GCP	2	0
3	C	180	GCP	4	0
3	D	180	GCP	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.