



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 06:33 pm BST

PDB ID : 2HWB  
Title : A comparison of the anti-rhinoviral drug binding pocket in hrv14 and hrv1a  
Authors : Kim, K.H.; Rossmann, M.G.  
Deposited on : 1994-01-25  
Resolution : 3.00 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

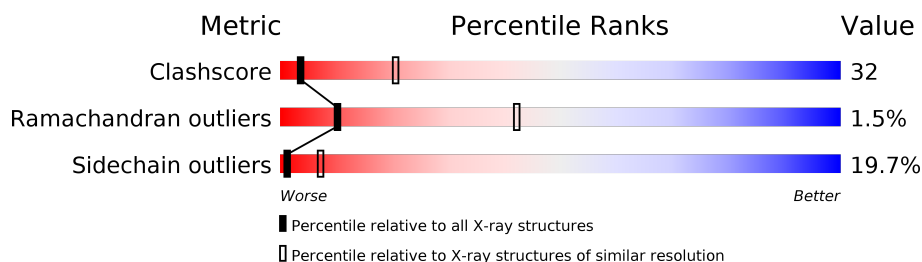
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 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	1	289	
2	2	262	
3	3	236	
4	4	68	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6290 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 HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	273	Total	C	N	O	S	0	0	0
			2170	1373	375	414	8			

- Molecule 2 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	255	Total	C	N	O	S	0	0	0
			1951	1237	330	372	12			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	170	VAL	ILE	CONFLICT	UNP P03303

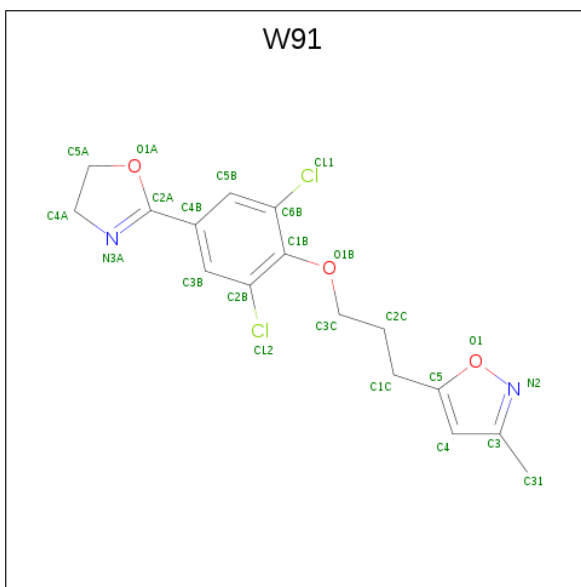
- Molecule 3 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	236	Total	C	N	O	S	0	0	0
			1849	1184	305	353	7			

- Molecule 4 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP4).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	40	Total	C	N	O	S	0	0	0
			297	186	47	62	2			

- Molecule 5 is 5-(3-(2,6-DICHLORO-4-(4,5-DIHYDRO-2-OXAZOLYL)PHENOXY)PROPYL)-3-METHYL ISOXAZOLE (three-letter code: W91) (formula: C<sub>16</sub>H<sub>16</sub>Cl<sub>2</sub>N<sub>2</sub>O<sub>3</sub>).



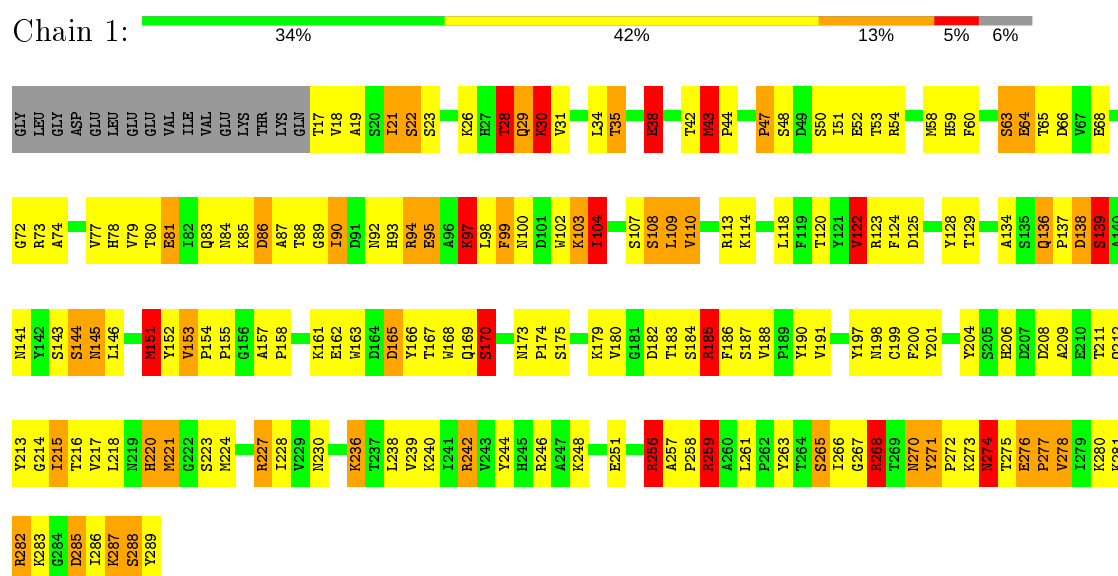
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	1	1	Total	C	Cl	N	O	0	0
			23	16	2	2	3		

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

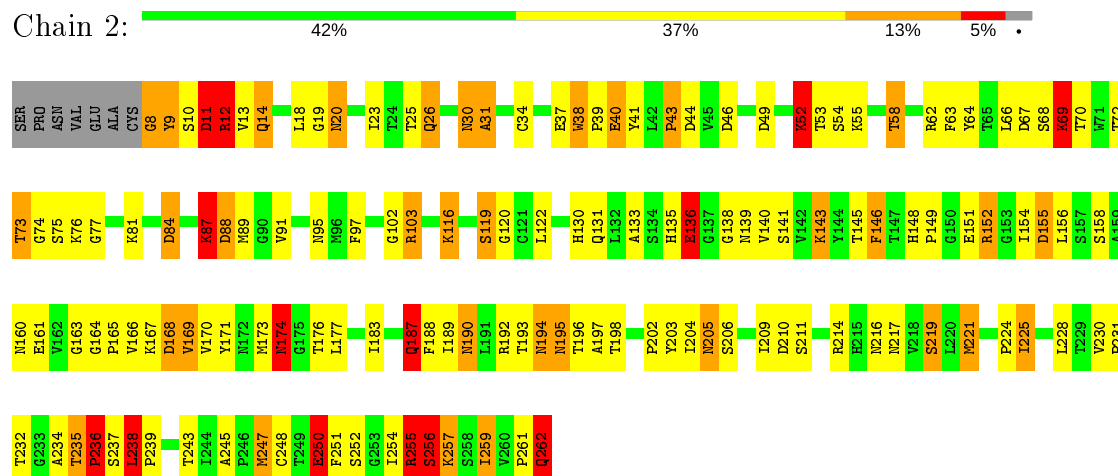
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP1)

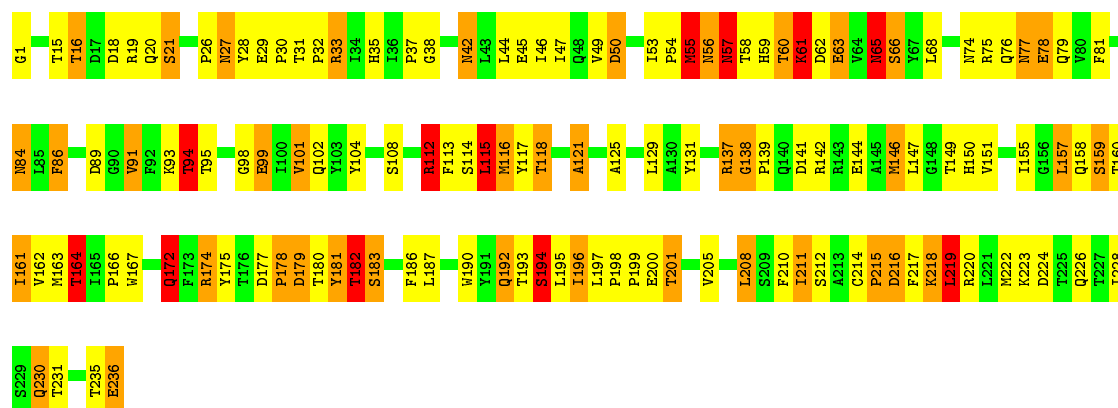


#### • Molecule 2: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP2)




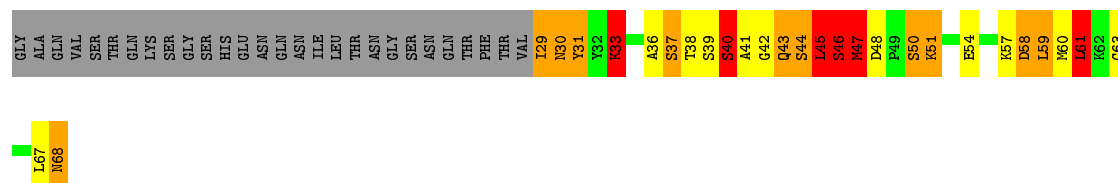
#### • Molecule 3: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP3)

Chain 3: 



• Molecule 4: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP4)

Chain 4: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	445.10Å 445.10Å 445.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	unknown	Depositor
R, $R_{free}$	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6290	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	0.0	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: W91

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	1	1.67	32/2228 (1.4%)	2.13	93/3031 (3.1%)
2	2	1.86	33/2000 (1.6%)	2.16	76/2734 (2.8%)
3	3	1.77	21/1898 (1.1%)	2.16	72/2597 (2.8%)
4	4	2.30	13/302 (4.3%)	2.46	21/406 (5.2%)
All	All	1.80	99/6428 (1.5%)	2.16	262/8768 (3.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	2
2	2	0	2
All	All	0	4

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	285	ASP	CA-CB	11.82	1.79	1.53
4	4	42	GLY	N-CA	11.70	1.63	1.46
4	4	40	SER	CB-OG	10.74	1.56	1.42
2	2	256	SER	CB-OG	10.20	1.55	1.42
1	1	95	GLU	CB-CG	10.13	1.71	1.52
4	4	44	SER	CB-OG	9.94	1.55	1.42
2	2	169	VAL	C-N	-9.75	1.11	1.34
1	1	188	VAL	C-N	9.73	1.52	1.34
4	4	41	ALA	C-O	9.37	1.41	1.23
1	1	38	GLU	CB-CG	-9.07	1.34	1.52
1	1	63	SER	CB-OG	-8.78	1.30	1.42
3	3	21	SER	CA-CB	8.71	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	248	CYS	CB-SG	-8.67	1.67	1.82
3	3	57	ASN	CA-CB	8.44	1.75	1.53
2	2	40	GLU	CD-OE1	8.22	1.34	1.25
1	1	288	SER	CA-CB	8.05	1.65	1.52
2	2	52	LYS	CE-NZ	7.91	1.68	1.49
3	3	1	GLY	N-CA	7.85	1.57	1.46
2	2	219	SER	CA-CB	-7.69	1.41	1.52
3	3	63	GLU	CD-OE1	7.69	1.34	1.25
1	1	283	LYS	N-CA	7.66	1.61	1.46
2	2	136	GLU	CB-CG	7.53	1.66	1.52
3	3	108	SER	CB-OG	7.45	1.51	1.42
4	4	33	LYS	CE-NZ	7.42	1.67	1.49
1	1	282	ARG	CD-NE	7.28	1.58	1.46
1	1	139	SER	CB-OG	7.26	1.51	1.42
2	2	152	ARG	CD-NE	7.20	1.58	1.46
2	2	152	ARG	CZ-NH2	7.04	1.42	1.33
2	2	194	ASN	CA-CB	6.97	1.71	1.53
4	4	46	SER	CB-OG	6.93	1.51	1.42
3	3	164	THR	C-O	6.89	1.36	1.23
4	4	51	LYS	CE-NZ	6.78	1.66	1.49
1	1	143	SER	CB-OG	6.75	1.51	1.42
3	3	61	LYS	CE-NZ	6.70	1.65	1.49
2	2	256	SER	C-O	6.69	1.36	1.23
1	1	72	GLY	C-O	6.55	1.34	1.23
1	1	30	LYS	CE-NZ	6.49	1.65	1.49
1	1	81	GLU	CD-OE1	6.42	1.32	1.25
2	2	8	GLY	N-CA	6.41	1.55	1.46
2	2	12	ARG	NE-CZ	6.37	1.41	1.33
1	1	283	LYS	CE-NZ	6.36	1.65	1.49
1	1	52	GLU	C-O	6.32	1.35	1.23
3	3	138	GLY	N-CA	6.32	1.55	1.46
2	2	87	LYS	CB-CG	-6.31	1.35	1.52
1	1	30	LYS	CD-CE	6.28	1.67	1.51
3	3	194	SER	CB-OG	-6.26	1.34	1.42
4	4	33	LYS	CD-CE	6.18	1.66	1.51
3	3	50	ASP	CA-CB	-6.08	1.40	1.53
1	1	144	SER	N-CA	6.03	1.58	1.46
1	1	94	ARG	CD-NE	6.02	1.56	1.46
3	3	108	SER	CA-CB	-6.02	1.44	1.52
4	4	54	GLU	CD-OE1	5.97	1.32	1.25
2	2	102	GLY	N-CA	5.93	1.54	1.46
3	3	99	GLU	CB-CG	-5.90	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	285	ASP	N-CA	-5.83	1.34	1.46
2	2	11	ASP	CA-CB	5.69	1.66	1.53
2	2	168	ASP	C-O	5.66	1.34	1.23
4	4	37	SER	CB-OG	-5.64	1.34	1.42
3	3	45	GLU	CD-OE1	5.64	1.31	1.25
3	3	172	GLN	CG-CD	-5.62	1.38	1.51
2	2	235	THR	C-N	-5.62	1.23	1.34
1	1	97	LYS	CD-CE	5.60	1.65	1.51
4	4	63	GLY	N-CA	5.60	1.54	1.46
2	2	187	GLN	N-CA	5.59	1.57	1.46
3	3	222	MET	CG-SD	5.56	1.95	1.81
1	1	139	SER	CA-CB	5.56	1.61	1.52
4	4	45	LEU	C-N	5.54	1.46	1.34
4	4	50	SER	CB-OG	5.52	1.49	1.42
2	2	219	SER	CB-OG	-5.49	1.35	1.42
2	2	236	PRO	C-O	5.43	1.34	1.23
1	1	276	GLU	CD-OE1	5.41	1.31	1.25
2	2	262	GLN	CD-OE1	5.41	1.35	1.24
2	2	187	GLN	CB-CG	-5.38	1.38	1.52
1	1	73	ARG	C-O	5.38	1.33	1.23
2	2	54	SER	CA-CB	-5.37	1.44	1.52
1	1	267	GLY	C-O	5.36	1.32	1.23
1	1	94	ARG	NE-CZ	5.31	1.40	1.33
2	2	40	GLU	CB-CG	5.29	1.62	1.52
1	1	246	ARG	CZ-NH2	5.28	1.40	1.33
1	1	251	GLU	CA-CB	-5.26	1.42	1.53
2	2	68	SER	CB-OG	-5.23	1.35	1.42
3	3	33	ARG	CZ-NH2	5.22	1.39	1.33
2	2	120	GLY	N-CA	5.21	1.53	1.46
3	3	118	THR	CB-OG1	5.19	1.53	1.43
2	2	161	GLU	CA-CB	-5.17	1.42	1.53
2	2	74	GLY	C-O	5.17	1.31	1.23
2	2	12	ARG	CZ-NH2	5.13	1.39	1.33
1	1	143	SER	C-O	5.12	1.33	1.23
1	1	68	GLU	CD-OE2	-5.12	1.20	1.25
1	1	283	LYS	CD-CE	5.11	1.64	1.51
3	3	38	GLY	CA-C	-5.11	1.43	1.51
3	3	77	ASN	C-O	5.09	1.33	1.23
2	2	136	GLU	CD-OE1	5.09	1.31	1.25
1	1	26	LYS	CB-CG	-5.08	1.38	1.52
2	2	38	TRP	CG-CD1	5.05	1.43	1.36
2	2	58	THR	C-O	5.05	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	86	PHE	CA-CB	-5.04	1.42	1.53
1	1	288	SER	C-O	5.04	1.32	1.23
3	3	30	PRO	N-CD	-5.02	1.40	1.47

All (262) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	246	ARG	NE-CZ-NH1	22.45	131.52	120.30
1	1	256	ARG	NE-CZ-NH2	20.38	130.49	120.30
1	1	123	ARG	NE-CZ-NH1	19.14	129.87	120.30
2	2	255	ARG	NE-CZ-NH2	-18.74	110.93	120.30
2	2	87	LYS	CA-CB-CG	17.62	152.17	113.40
1	1	285	ASP	CB-CG-OD1	-17.61	102.45	118.30
3	3	137	ARG	NE-CZ-NH1	-16.95	111.83	120.30
1	1	256	ARG	NE-CZ-NH1	-16.89	111.86	120.30
1	1	94	ARG	NE-CZ-NH2	-16.57	112.01	120.30
3	3	216	ASP	CB-CG-OD2	16.11	132.80	118.30
2	2	255	ARG	NE-CZ-NH1	14.18	127.39	120.30
1	1	282	ARG	NE-CZ-NH2	-14.11	113.25	120.30
2	2	168	ASP	CB-CG-OD1	-12.82	106.76	118.30
3	3	50	ASP	CA-CB-CG	12.24	140.32	113.40
1	1	94	ARG	CD-NE-CZ	-12.06	106.72	123.60
2	2	11	ASP	CB-CG-OD1	-11.72	107.75	118.30
2	2	194	ASN	N-CA-CB	-11.55	89.81	110.60
2	2	193	THR	C-N-CA	11.38	150.16	121.70
3	3	215	PRO	C-N-CA	11.00	149.19	121.70
2	2	152	ARG	NE-CZ-NH2	-11.00	114.80	120.30
4	4	41	ALA	CA-C-N	10.88	137.96	116.20
4	4	48	ASP	CB-CG-OD1	-10.86	108.52	118.30
3	3	19	ARG	NE-CZ-NH2	10.82	125.71	120.30
3	3	33	ARG	NE-CZ-NH2	-10.66	114.97	120.30
1	1	285	ASP	CB-CG-OD2	10.59	127.83	118.30
1	1	285	ASP	CA-CB-CG	-10.46	90.38	113.40
3	3	50	ASP	CB-CG-OD1	10.43	127.68	118.30
2	2	151	GLU	CA-CB-CG	10.39	136.26	113.40
1	1	246	ARG	NE-CZ-NH2	-10.04	115.28	120.30
1	1	246	ARG	CD-NE-CZ	10.03	137.65	123.60
1	1	282	ARG	CD-NE-CZ	-9.97	109.64	123.60
3	3	57	ASN	N-CA-CB	-9.83	92.91	110.60
3	3	146	MET	CG-SD-CE	9.80	115.88	100.20
3	3	216	ASP	CB-CG-OD1	-9.73	109.55	118.30
2	2	88	ASP	CB-CG-OD1	-9.68	109.59	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	242	ARG	NE-CZ-NH2	-9.39	115.61	120.30
1	1	54	ARG	CD-NE-CZ	-9.38	110.48	123.60
1	1	66	ASP	CB-CG-OD2	-9.17	110.05	118.30
3	3	57	ASN	CB-CA-C	-9.04	92.32	110.40
2	2	11	ASP	CA-CB-CG	-8.99	93.62	113.40
1	1	38	GLU	CA-CB-CG	8.89	132.97	113.40
3	3	137	ARG	NE-CZ-NH2	8.88	124.74	120.30
3	3	112	ARG	NE-CZ-NH2	-8.81	115.89	120.30
3	3	182	THR	CA-CB-CG2	8.56	124.39	112.40
1	1	285	ASP	N-CA-CB	-8.52	95.27	110.60
1	1	268	ARG	CD-NE-CZ	-8.44	111.78	123.60
1	1	123	ARG	CD-NE-CZ	8.38	135.34	123.60
1	1	63	SER	CB-CA-C	-8.36	94.22	110.10
2	2	250	GLU	CA-CB-CG	8.33	131.73	113.40
1	1	285	ASP	CB-CA-C	-8.31	93.79	110.40
3	3	172	GLN	CB-CG-CD	8.23	133.01	111.60
1	1	251	GLU	CA-CB-CG	8.19	131.41	113.40
2	2	152	ARG	NE-CZ-NH1	8.17	124.39	120.30
4	4	45	LEU	N-CA-CB	-8.16	94.08	110.40
3	3	224	ASP	CB-CG-OD1	-8.09	111.02	118.30
2	2	255	ARG	CA-CB-CG	8.04	131.08	113.40
2	2	11	ASP	OD1-CG-OD2	8.02	138.54	123.30
4	4	48	ASP	OD1-CG-OD2	8.02	138.53	123.30
3	3	181	TYR	CB-CG-CD2	-8.00	116.20	121.00
1	1	38	GLU	CB-CG-CD	7.98	135.74	114.20
1	1	95	GLU	OE1-CD-OE2	7.98	132.87	123.30
2	2	219	SER	CA-CB-OG	7.83	132.35	111.20
4	4	47	MET	CA-CB-CG	-7.83	99.99	113.30
1	1	145	ASN	OD1-CG-ND2	7.79	139.83	121.90
3	3	21	SER	CB-CA-C	-7.68	95.50	110.10
2	2	155	ASP	CB-CG-OD1	-7.64	111.43	118.30
2	2	187	GLN	CA-CB-CG	7.59	130.09	113.40
3	3	78	GLU	OE1-CD-OE2	7.58	132.40	123.30
2	2	11	ASP	C-N-CA	7.54	140.56	121.70
1	1	277	PRO	N-CD-CG	-7.54	91.90	103.20
2	2	187	GLN	CB-CA-C	7.49	125.39	110.40
1	1	123	ARG	NE-CZ-NH2	-7.47	116.56	120.30
3	3	236	GLU	CA-CB-CG	7.43	129.76	113.40
1	1	259	ARG	CA-CB-CG	-7.35	97.23	113.40
2	2	214	ARG	NE-CZ-NH1	7.33	123.96	120.30
3	3	112	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	1	227	ARG	NE-CZ-NH2	7.29	123.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	282	ARG	NH1-CZ-NH2	7.27	127.39	119.40
1	1	113	ARG	NE-CZ-NH2	7.26	123.93	120.30
3	3	142	ARG	CA-CB-CG	7.21	129.27	113.40
2	2	194	ASN	CA-CB-CG	-7.15	97.68	113.40
2	2	190	ASN	CA-CB-CG	7.09	129.00	113.40
2	2	168	ASP	N-CA-CB	-7.03	97.95	110.60
3	3	121	ALA	CB-CA-C	-7.02	99.56	110.10
3	3	137	ARG	CD-NE-CZ	-7.02	113.78	123.60
2	2	256	SER	CA-C-O	-7.01	105.38	120.10
1	1	68	GLU	CG-CD-OE2	7.00	132.29	118.30
3	3	28	TYR	CB-CG-CD1	-6.99	116.81	121.00
4	4	41	ALA	CA-C-O	-6.97	105.47	120.10
1	1	28	THR	CB-CA-C	-6.91	92.95	111.60
1	1	42	THR	CA-CB-CG2	6.91	122.07	112.40
1	1	125	ASP	CB-CG-OD1	-6.90	112.09	118.30
1	1	26	LYS	CA-CB-CG	6.86	128.50	113.40
2	2	136	GLU	CG-CD-OE1	-6.78	104.74	118.30
4	4	37	SER	CB-CA-C	6.76	122.95	110.10
3	3	194	SER	N-CA-CB	-6.75	100.38	110.50
3	3	163	MET	CA-CB-CG	-6.73	101.87	113.30
3	3	216	ASP	N-CA-CB	-6.67	98.60	110.60
2	2	103	ARG	CD-NE-CZ	-6.64	114.31	123.60
2	2	146	PHE	CB-CG-CD1	-6.63	116.16	120.80
1	1	265	SER	N-CA-CB	-6.63	100.56	110.50
3	3	57	ASN	CA-CB-CG	-6.63	98.82	113.40
2	2	87	LYS	CB-CG-CD	6.59	128.74	111.60
3	3	27	ASN	CB-CA-C	-6.57	97.25	110.40
3	3	45	GLU	CG-CD-OE2	6.57	131.43	118.30
1	1	94	ARG	NH1-CZ-NH2	6.56	126.62	119.40
1	1	276	GLU	OE1-CD-OE2	6.56	131.17	123.30
1	1	68	GLU	CG-CD-OE1	-6.56	105.19	118.30
1	1	288	SER	CB-CA-C	-6.54	97.67	110.10
1	1	53	THR	CA-CB-OG1	-6.52	95.31	109.00
2	2	203	TYR	CB-CG-CD2	6.52	124.91	121.00
4	4	45	LEU	CB-CA-C	6.49	122.53	110.20
1	1	288	SER	N-CA-CB	-6.48	100.78	110.50
3	3	74	ASN	CA-CB-CG	-6.48	99.15	113.40
1	1	22	SER	N-CA-CB	-6.46	100.80	110.50
1	1	144	SER	N-CA-CB	-6.46	100.81	110.50
3	3	183	SER	N-CA-CB	-6.45	100.82	110.50
3	3	55	MET	CA-CB-CG	-6.43	102.37	113.30
2	2	168	ASP	OD1-CG-OD2	6.42	135.50	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	29	GLU	CB-CG-CD	6.42	131.52	114.20
1	1	274	ASN	O-C-N	6.35	132.85	122.70
2	2	97	PHE	CB-CG-CD1	-6.34	116.36	120.80
1	1	187	SER	C-N-CA	-6.31	105.93	121.70
3	3	16	THR	N-CA-CB	-6.30	98.32	110.30
3	3	65	ASN	CA-CB-CG	-6.30	99.54	113.40
1	1	138	ASP	CB-CG-OD1	6.30	123.97	118.30
1	1	95	GLU	CB-CG-CD	-6.28	97.25	114.20
4	4	44	SER	CA-C-N	-6.25	103.44	117.20
2	2	38	TRP	N-CA-CB	-6.25	99.35	110.60
1	1	271	TYR	CB-CG-CD1	6.25	124.75	121.00
3	3	19	ARG	CA-CB-CG	6.23	127.11	113.40
3	3	63	GLU	CG-CD-OE1	-6.23	105.84	118.30
3	3	27	ASN	CA-CB-CG	-6.23	99.70	113.40
1	1	145	ASN	CA-CB-CG	-6.22	99.71	113.40
1	1	151	MET	CG-SD-CE	6.21	110.14	100.20
1	1	122	VAL	N-CA-CB	-6.17	97.92	111.50
1	1	224	MET	CG-SD-CE	6.15	110.04	100.20
2	2	69	LYS	CA-CB-CG	6.14	126.92	113.40
2	2	136	GLU	CB-CG-CD	-6.14	97.62	114.20
2	2	203	TYR	CB-CG-CD1	-6.14	117.32	121.00
1	1	221	MET	CG-SD-CE	6.12	109.99	100.20
1	1	97	LYS	CD-CE-NZ	-6.11	97.66	111.70
3	3	222	MET	CG-SD-CE	-6.09	90.45	100.20
2	2	219	SER	CB-CA-C	6.09	121.66	110.10
3	3	66	SER	CB-CA-C	6.06	121.62	110.10
3	3	219	LEU	CA-CB-CG	6.06	129.24	115.30
1	1	86	ASP	CB-CG-OD1	6.05	123.74	118.30
2	2	235	THR	CA-CB-CG2	-6.04	103.94	112.40
2	2	119	SER	N-CA-CB	6.04	119.56	110.50
2	2	67	ASP	CA-CB-CG	-6.02	100.15	113.40
2	2	247	MET	CB-CA-C	6.01	122.41	110.40
2	2	103	ARG	CA-CB-CG	6.00	126.60	113.40
4	4	61	LEU	CB-CG-CD2	-5.99	100.82	111.00
2	2	169	VAL	CA-C-N	5.99	130.37	117.20
4	4	48	ASP	CB-CG-OD2	-5.97	112.93	118.30
3	3	1	GLY	N-CA-C	5.96	128.01	113.10
2	2	12	ARG	NE-CZ-NH2	-5.92	117.34	120.30
3	3	58	THR	CA-CB-CG2	-5.92	104.11	112.40
1	1	257	ALA	N-CA-CB	-5.91	101.83	110.10
1	1	256	ARG	CD-NE-CZ	-5.90	115.34	123.60
1	1	35	THR	N-CA-CB	-5.90	99.10	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	94	ARG	CG-CD-NE	-5.87	99.47	111.80
2	2	256	SER	CA-C-N	5.87	130.11	117.20
4	4	30	ASN	CA-CB-CG	-5.87	100.49	113.40
3	3	45	GLU	CG-CD-OE1	-5.85	106.60	118.30
4	4	33	LYS	CD-CE-NZ	-5.85	98.24	111.70
1	1	236	LYS	CD-CE-NZ	-5.84	98.27	111.70
1	1	268	ARG	NE-CZ-NH2	-5.84	117.38	120.30
2	2	238	LEU	N-CA-CB	-5.83	98.75	110.40
2	2	214	ARG	NE-CZ-NH2	-5.82	117.39	120.30
2	2	31	ALA	N-CA-CB	5.82	118.24	110.10
3	3	27	ASN	O-C-N	5.80	131.97	122.70
1	1	28	THR	OG1-CB-CG2	5.78	123.29	110.00
2	2	255	ARG	CB-CG-CD	5.75	126.56	111.60
2	2	73	THR	CA-CB-OG1	-5.75	96.93	109.00
3	3	77	ASN	CA-C-N	5.74	129.84	117.20
2	2	68	SER	N-CA-CB	-5.74	101.89	110.50
1	1	95	GLU	CA-CB-CG	-5.72	100.81	113.40
1	1	274	ASN	N-CA-CB	5.72	120.90	110.60
3	3	147	LEU	CA-CB-CG	5.71	128.44	115.30
1	1	246	ARG	NH1-CZ-NH2	-5.70	113.13	119.40
3	3	1	GLY	O-C-N	-5.70	113.59	122.70
1	1	48	SER	CA-C-O	-5.69	108.15	120.10
2	2	52	LYS	CD-CE-NZ	-5.69	98.61	111.70
2	2	161	GLU	CA-CB-CG	5.69	125.91	113.40
2	2	75	SER	N-CA-CB	-5.68	101.98	110.50
1	1	244	TYR	CB-CG-CD2	-5.65	117.61	121.00
3	3	164	THR	N-CA-CB	-5.63	99.60	110.30
3	3	177	ASP	CB-CG-OD1	-5.62	113.24	118.30
4	4	44	SER	O-C-N	5.61	131.67	122.70
2	2	210	ASP	N-CA-CB	-5.57	100.58	110.60
3	3	94	THR	O-C-N	5.56	131.60	122.70
2	2	84	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	1	122	VAL	CB-CA-C	5.53	121.91	111.40
2	2	9	TYR	CB-CA-C	5.50	121.40	110.40
4	4	44	SER	C-N-CA	-5.49	107.97	121.70
3	3	186	PHE	CB-CG-CD1	-5.48	116.96	120.80
2	2	12	ARG	CD-NE-CZ	-5.48	115.93	123.60
3	3	112	ARG	CA-CB-CG	5.47	125.44	113.40
1	1	43	MET	CG-SD-CE	5.47	108.95	100.20
2	2	43	PRO	N-CD-CG	-5.47	95.00	103.20
1	1	26	LYS	CD-CE-NZ	-5.47	99.13	111.70
1	1	81	GLU	CG-CD-OE1	-5.46	107.38	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	270	ASN	O-C-N	5.43	131.39	122.70
3	3	60	THR	CA-CB-OG1	-5.42	97.61	109.00
2	2	174	ASN	CA-C-N	5.42	127.03	116.20
3	3	161	ILE	CA-CB-CG1	-5.40	100.74	111.00
4	4	44	SER	N-CA-CB	5.39	118.59	110.50
2	2	44	ASP	CA-CB-CG	5.39	125.26	113.40
3	3	115	LEU	CA-CB-CG	5.39	127.69	115.30
1	1	123	ARG	NH1-CZ-NH2	-5.38	113.48	119.40
2	2	169	VAL	CB-CA-C	-5.36	101.21	111.40
2	2	262	GLN	CA-C-O	-5.36	108.84	120.10
3	3	231	THR	CA-CB-OG1	-5.36	97.74	109.00
3	3	65	ASN	N-CA-CB	-5.35	100.96	110.60
1	1	64	GLU	CA-CB-CG	5.35	125.16	113.40
2	2	259	ILE	CB-CG1-CD1	-5.31	99.03	113.90
3	3	42	ASN	CB-CG-OD1	-5.31	110.99	121.60
2	2	88	ASP	CA-CB-CG	-5.29	101.76	113.40
1	1	187	SER	O-C-N	5.28	131.15	122.70
2	2	143	LYS	CD-CE-NZ	-5.28	99.56	111.70
3	3	116	MET	CB-CG-SD	-5.26	96.61	112.40
3	3	33	ARG	CB-CG-CD	-5.25	97.94	111.60
3	3	74	ASN	OD1-CG-ND2	5.24	133.94	121.90
2	2	38	TRP	CA-CB-CG	-5.22	103.78	113.70
1	1	242	ARG	CD-NE-CZ	-5.22	116.29	123.60
1	1	275	THR	CA-C-O	-5.22	109.14	120.10
1	1	275	THR	CA-C-N	5.21	128.66	117.20
3	3	78	GLU	CA-CB-CG	5.21	124.85	113.40
4	4	48	ASP	CA-CB-CG	-5.20	101.96	113.40
1	1	271	TYR	CB-CG-CD2	-5.20	117.88	121.00
3	3	222	MET	CB-CG-SD	-5.19	96.82	112.40
2	2	219	SER	N-CA-CB	5.19	118.29	110.50
2	2	203	TYR	CZ-CE2-CD2	-5.18	115.14	119.80
4	4	36	ALA	C-N-CA	-5.17	108.77	121.70
1	1	21	ILE	CA-CB-CG1	-5.17	101.18	111.00
1	1	187	SER	CB-CA-C	5.17	119.92	110.10
2	2	14	GLN	OE1-CD-NE2	5.16	133.77	121.90
4	4	31	TYR	CG-CD2-CE2	-5.16	117.17	121.30
2	2	11	ASP	CB-CG-OD2	-5.16	113.66	118.30
2	2	52	LYS	CA-C-N	5.15	128.52	117.20
1	1	50	SER	CA-C-N	5.14	128.50	117.20
1	1	282	ARG	CG-CD-NE	-5.12	101.05	111.80
2	2	203	TYR	CG-CD2-CE2	5.12	125.39	121.30
2	2	221	MET	CA-CB-CG	-5.11	104.61	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	141	ASN	CA-CB-CG	-5.11	102.17	113.40
2	2	14	GLN	CA-CB-CG	-5.10	102.17	113.40
3	3	144	GLU	CA-CB-CG	5.09	124.59	113.40
4	4	58	ASP	O-C-N	5.08	130.84	122.70
3	3	141	ASP	CB-CG-OD1	5.08	122.88	118.30
2	2	18	LEU	CB-CA-C	5.08	119.85	110.20
1	1	17	THR	CA-CB-CG2	-5.06	105.31	112.40
4	4	39	SER	O-C-N	5.06	130.80	122.70
3	3	86	PHE	CB-CA-C	5.05	120.49	110.40
1	1	270	ASN	CB-CA-C	-5.04	100.31	110.40
3	3	172	GLN	CG-CD-NE2	5.04	128.80	116.70
1	1	282	ARG	CB-CA-C	-5.04	100.32	110.40
1	1	185	ARG	NE-CZ-NH2	5.04	122.82	120.30
3	3	178	PRO	O-C-N	5.02	130.73	122.70
1	1	274	ASN	CA-C-N	-5.01	106.17	117.20
3	3	187	LEU	N-CA-CB	-5.01	100.39	110.40
1	1	22	SER	CA-C-O	-5.00	109.60	120.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	259	ARG	Sidechain
1	1	268	ARG	Sidechain
2	2	12	ARG	Sidechain
2	2	255	ARG	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	1	2170	0	2106	166	0
2	2	1951	0	1923	128	0
3	3	1849	0	1831	138	0
4	4	297	0	294	35	0
5	1	23	0	16	2	0
All	All	6290	0	6170	393	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 32.

All (393) 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)
4:4:33:LYS:NZ	4:4:33:LYS:CE	1.67	1.57
3:3:57:ASN:CA	3:3:57:ASN:CB	1.75	1.55
1:1:285:ASP:CB	1:1:285:ASP:CA	1.80	1.54
2:2:52:LYS:NZ	2:2:52:LYS:CE	1.68	1.53
3:3:179:ASP:OD2	3:3:182:THR:HB	1.41	1.19
2:2:158:SER:OG	2:2:167:LYS:HE2	1.46	1.13
1:1:285:ASP:CA	1:1:285:ASP:OD1	2.00	1.08
1:1:47:PRO:HA	3:3:164:THR:HG21	1.34	1.07
1:1:258:PRO:HG2	3:3:99:GLU:HG2	1.36	1.07
3:3:21:SER:O	4:4:37:SER:HB2	1.54	1.06
2:2:12:ARG:HG3	2:2:12:ARG:NH1	1.69	1.04
2:2:255:ARG:HG2	2:2:256:SER:H	1.24	1.00
1:1:282:ARG:HG3	3:3:57:ASN:HB3	1.41	0.99
2:2:136:GLU:HB3	2:2:140:VAL:HG21	1.44	0.96
3:3:57:ASN:N	3:3:57:ASN:CB	2.28	0.95
1:1:83:GLN:HG3	1:1:85:LYS:HE2	1.47	0.94
3:3:57:ASN:C	3:3:57:ASN:CB	2.37	0.94
1:1:191:VAL:O	1:1:191:VAL:HG23	1.66	0.93
2:2:12:ARG:HH11	2:2:12:ARG:HG3	1.27	0.93
1:1:152:TYR:O	1:1:154:PRO:HD3	1.69	0.93
1:1:285:ASP:CG	1:1:285:ASP:CA	2.37	0.93
1:1:58:MET:HE1	3:3:216:ASP:HA	1.48	0.92
2:2:41:TYR:CE2	2:2:55:LYS:HD3	2.05	0.92
2:2:235:THR:HG23	2:2:236:PRO:HD2	1.53	0.91
1:1:28:THR:HB	1:1:30:LYS:H	1.35	0.91
2:2:11:ASP:HB2	4:4:68:ASN:OD1	1.71	0.90
1:1:285:ASP:CB	1:1:285:ASP:C	2.40	0.90
1:1:285:ASP:CB	1:1:285:ASP:N	2.34	0.90
1:1:47:PRO:HA	3:3:164:THR:CG2	2.03	0.88
3:3:198:PRO:HD2	3:3:201:THR:HG21	1.55	0.88
2:2:20:ASN:ND2	2:2:62:ARG:HE	1.72	0.87
1:1:285:ASP:HA	1:1:285:ASP:OD1	1.73	0.87
1:1:162:GLU:HB2	1:1:165:ASP:OD1	1.75	0.85
2:2:9:TYR:CD1	2:2:9:TYR:N	2.43	0.85
1:1:90:ILE:HD13	1:1:90:ILE:N	1.92	0.84
3:3:57:ASN:CA	3:3:57:ASN:CG	2.45	0.84
2:2:195:ASN:ND2	2:2:196:THR:HG23	1.91	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:282:ARG:HD2	1:1:285:ASP:O	1.78	0.83
2:2:116:LYS:HB3	3:3:121:ALA:HB3	1.58	0.83
2:2:10:SER:OG	2:2:12:ARG:HB2	1.78	0.83
2:2:9:TYR:N	2:2:9:TYR:HD1	1.77	0.83
2:2:136:GLU:CB	2:2:140:VAL:HG21	2.09	0.83
2:2:52:LYS:NZ	2:2:52:LYS:CD	2.43	0.82
4:4:68:ASN:OD1	4:4:68:ASN:N	2.11	0.82
1:1:102:TRP:O	1:1:104:ILE:N	2.12	0.81
2:2:12:ARG:HH11	2:2:12:ARG:CG	1.89	0.81
1:1:191:VAL:O	1:1:191:VAL:CG2	2.27	0.81
1:1:58:MET:CE	3:3:216:ASP:HA	2.11	0.81
4:4:59:LEU:HD21	4:4:61:LEU:HD13	1.61	0.81
1:1:248:LYS:HE3	4:4:38:THR:O	1.80	0.79
2:2:158:SER:OG	2:2:167:LYS:CE	2.27	0.79
2:2:195:ASN:HD22	2:2:196:THR:HG23	1.48	0.78
2:2:30:ASN:HD22	2:2:31:ALA:H	1.27	0.77
1:1:58:MET:HE1	3:3:216:ASP:CA	2.13	0.77
2:2:12:ARG:CG	2:2:12:ARG:NH1	2.44	0.77
1:1:47:PRO:CA	3:3:164:THR:HG21	2.15	0.77
1:1:282:ARG:HG3	3:3:57:ASN:CB	2.15	0.77
3:3:79:GLN:HB2	3:3:190:TRP:CZ3	2.19	0.77
2:2:255:ARG:HG2	2:2:256:SER:N	2.00	0.76
1:1:220:HIS:CG	1:1:220:HIS:O	2.39	0.76
1:1:94:ARG:NH1	1:1:94:ARG:HG2	2.00	0.76
1:1:92:ASN:OD1	1:1:95:GLU:HB2	1.87	0.74
2:2:262:GLN:C	2:2:262:GLN:HE21	1.91	0.74
1:1:270:ASN:HA	2:2:133:ALA:HB1	1.68	0.74
3:3:197:LEU:HB3	3:3:201:THR:CG2	2.18	0.74
4:4:43:GLN:HG2	4:4:45:LEU:HB2	1.70	0.74
1:1:103:LYS:HA	1:1:223:SER:HB3	1.68	0.74
1:1:258:PRO:CG	3:3:99:GLU:HG2	2.16	0.73
2:2:188:PHE:O	2:2:194:ASN:ND2	2.22	0.73
3:3:26:PRO:O	3:3:27:ASN:HB2	1.89	0.73
4:4:33:LYS:NZ	4:4:33:LYS:CD	2.52	0.72
2:2:230:VAL:CG2	2:2:234:ALA:HB3	2.20	0.72
1:1:19:ALA:HB2	1:1:58:MET:HG2	1.72	0.71
2:2:53:THR:HG22	2:2:252:SER:HB2	1.71	0.71
2:2:136:GLU:HB3	2:2:140:VAL:CG2	2.21	0.71
3:3:57:ASN:CA	3:3:57:ASN:OD1	2.38	0.71
2:2:174:ASN:C	2:2:174:ASN:HD22	1.93	0.70
1:1:282:ARG:CG	3:3:57:ASN:HB3	2.18	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:20:ASN:HD21	2:2:62:ARG:HE	1.39	0.70
2:2:235:THR:CG2	2:2:236:PRO:HD2	2.21	0.70
1:1:89:GLY:C	1:1:90:ILE:HD13	2.13	0.69
3:3:98:GLY:O	3:3:102:GLN:HG3	1.92	0.69
1:1:170:SER:OG	1:1:170:SER:O	2.09	0.68
4:4:29:ILE:O	4:4:29:ILE:HG22	1.94	0.68
2:2:230:VAL:HG23	2:2:234:ALA:HB3	1.74	0.68
3:3:20:GLN:HE22	4:4:31:TYR:H	1.42	0.67
3:3:42:ASN:HD22	3:3:44:LEU:H	1.43	0.67
2:2:195:ASN:HD22	2:2:195:ASN:C	1.99	0.66
2:2:84:ASP:OD1	2:2:87:LYS:HE2	1.94	0.66
1:1:185:ARG:HG3	1:1:186:PHE:N	2.10	0.66
1:1:151:MET:SD	1:1:170:SER:HB2	2.35	0.66
1:1:278:VAL:HG12	3:3:62:ASP:OD2	1.95	0.66
1:1:285:ASP:CB	1:1:285:ASP:H	2.09	0.66
3:3:197:LEU:HB3	3:3:201:THR:HG22	1.77	0.66
2:2:256:SER:O	2:2:257:LYS:HB3	1.96	0.65
3:3:179:ASP:OD2	3:3:182:THR:CB	2.31	0.65
3:3:89:ASP:HA	3:3:93:LYS:HD2	1.78	0.65
3:3:61:LYS:HD3	3:3:63:GLU:OE2	1.95	0.65
2:2:30:ASN:HD22	2:2:31:ALA:N	1.94	0.65
1:1:201:TYR:HD2	1:1:214:GLY:O	1.80	0.64
2:2:149:PRO:HG3	2:2:154:ILE:HG13	1.78	0.64
1:1:163:TRP:O	1:1:227:ARG:NH1	2.30	0.64
2:2:190:ASN:HD21	3:3:118:THR:HA	1.62	0.64
2:2:12:ARG:HH21	3:3:157:LEU:HD21	1.63	0.64
2:2:12:ARG:NH1	4:4:68:ASN:O	2.31	0.64
1:1:78:HIS:NE2	1:1:102:TRP:HB2	2.13	0.64
1:1:94:ARG:CG	1:1:94:ARG:NH1	2.60	0.63
2:2:187:GLN:HE21	2:2:197:ALA:HA	1.63	0.63
2:2:205:ASN:ND2	2:2:206:SER:H	1.97	0.63
2:2:23:ILE:HD11	2:2:243:THR:HG21	1.79	0.63
3:3:79:GLN:HB2	3:3:190:TRP:CE3	2.32	0.63
2:2:13:VAL:O	2:2:14:GLN:HG2	1.99	0.63
1:1:166:TYR:O	1:1:169:GLN:HB2	1.99	0.63
1:1:83:GLN:CG	1:1:85:LYS:HE2	2.24	0.63
1:1:103:LYS:O	1:1:104:ILE:O	2.17	0.63
2:2:170:VAL:CG1	2:2:170:VAL:O	2.48	0.62
1:1:60:PHE:CE2	3:3:218:LYS:HB3	2.33	0.62
2:2:40:GLU:HG3	2:2:41:TYR:O	2.00	0.62
2:2:205:ASN:HD22	2:2:206:SER:H	1.45	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:90:ILE:N	1:1:90:ILE:CD1	2.62	0.62
3:3:55:MET:O	3:3:55:MET:HG3	1.99	0.62
1:1:38:GLU:CD	3:3:116:MET:HE1	2.20	0.61
3:3:75:ARG:O	3:3:194:SER:HB2	1.99	0.61
3:3:57:ASN:ND2	3:3:91:VAL:HG13	2.15	0.61
3:3:84:ASN:ND2	3:3:86:PHE:H	1.98	0.61
1:1:120:THR:O	1:1:199:CYS:HB2	1.99	0.61
1:1:103:LYS:HA	1:1:223:SER:CB	2.30	0.61
1:1:87:ALA:HA	1:1:90:ILE:HG12	1.81	0.61
2:2:133:ALA:O	2:2:166:VAL:HG12	2.01	0.61
1:1:51:ILE:HD13	3:3:166:PRO:HG3	1.82	0.61
3:3:56:ASN:HB3	3:3:66:SER:HA	1.83	0.61
1:1:281:LYS:HD2	3:3:59:HIS:O	2.01	0.61
1:1:265:SER:HB3	1:1:268:ARG:HG2	1.83	0.60
3:3:131:TYR:HB3	3:3:149:THR:HB	1.82	0.60
2:2:155:ASP:OD1	2:2:155:ASP:C	2.37	0.60
1:1:204:TYR:CE2	1:1:213:TYR:HB2	2.36	0.60
3:3:76:GLN:O	3:3:78:GLU:N	2.34	0.60
2:2:38:TRP:CZ3	4:4:57:LYS:HD2	2.36	0.60
3:3:84:ASN:HD22	3:3:86:PHE:H	1.49	0.59
1:1:204:TYR:HD2	1:1:212:GLN:O	1.85	0.59
3:3:175:TYR:H	3:3:182:THR:HG21	1.68	0.59
1:1:259:ARG:HD2	1:1:263:TYR:CE1	2.38	0.59
2:2:11:ASP:H	4:4:68:ASN:CG	2.06	0.59
1:1:206:HIS:CE1	1:1:208:ASP:HB2	2.38	0.58
1:1:285:ASP:HB3	1:1:287:LYS:N	2.18	0.58
2:2:30:ASN:HD21	4:4:58:ASP:H	1.51	0.58
3:3:180:THR:O	3:3:183:SER:HB3	2.02	0.58
1:1:151:MET:HB2	1:1:175:SER:OG	2.04	0.58
1:1:58:MET:HE1	3:3:216:ASP:C	2.24	0.58
2:2:256:SER:O	2:2:257:LYS:CB	2.50	0.58
2:2:177:LEU:HD11	3:3:94:THR:HG21	1.86	0.58
1:1:209:ALA:HB2	2:2:261:PRO:HB3	1.85	0.57
1:1:93:HIS:CE1	1:1:163:TRP:HD1	2.22	0.57
1:1:155:PRO:HB3	1:1:220:HIS:HE1	1.69	0.57
2:2:52:LYS:NZ	2:2:52:LYS:HD3	2.20	0.57
3:3:199:PRO:O	3:3:200:GLU:HB2	2.05	0.57
3:3:53:ILE:HD11	3:3:211:ILE:HB	1.87	0.57
1:1:85:LYS:HB3	1:1:236:LYS:HG3	1.87	0.56
2:2:230:VAL:HG23	2:2:231:PRO:O	2.05	0.56
3:3:31:THR:CG2	3:3:32:PRO:HD2	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:10:SER:OG	2:2:12:ARG:CB	2.53	0.56
2:2:64:TYR:CD1	2:2:89:MET:HB3	2.39	0.56
2:2:38:TRP:HZ3	4:4:57:LYS:HD2	1.70	0.56
3:3:179:ASP:OD2	3:3:182:THR:CG2	2.52	0.56
1:1:155:PRO:HB3	1:1:220:HIS:CE1	2.41	0.56
2:2:204:ILE:HG12	3:3:37:PRO:HG2	1.87	0.56
4:4:43:GLN:O	4:4:45:LEU:HB3	2.05	0.56
1:1:93:HIS:CE1	1:1:162:GLU:HG2	2.41	0.55
2:2:170:VAL:HG12	2:2:170:VAL:O	2.05	0.55
1:1:266:ILE:HD12	3:3:235:THR:HA	1.88	0.55
3:3:197:LEU:HB3	3:3:201:THR:HG21	1.87	0.55
1:1:43:MET:HG3	1:1:44:PRO:HD2	1.87	0.55
2:2:230:VAL:HB	2:2:231:PRO:HD2	1.89	0.55
1:1:271:TYR:HB2	1:1:272:PRO:HD2	1.89	0.55
2:2:189:ILE:HA	2:2:194:ASN:ND2	2.21	0.55
3:3:198:PRO:O	3:3:201:THR:HB	2.07	0.55
3:3:31:THR:HG23	3:3:32:PRO:HD2	1.88	0.55
3:3:193:THR:O	3:3:194:SER:CB	2.55	0.54
3:3:20:GLN:HE22	4:4:31:TYR:N	2.04	0.54
1:1:208:ASP:O	2:2:261:PRO:HG2	2.07	0.54
3:3:175:TYR:H	3:3:182:THR:CG2	2.21	0.54
1:1:79:VAL:HG22	1:1:242:ARG:HG2	1.89	0.54
1:1:236:LYS:HE3	1:1:238:LEU:HD13	1.88	0.54
2:2:77:GLY:O	2:2:156:LEU:HB2	2.07	0.54
1:1:158:PRO:HB2	1:1:167:THR:HG22	1.90	0.54
1:1:151:MET:HE1	1:1:168:TRP:HA	1.89	0.54
1:1:104:ILE:HD12	5:1:700:W91:H3C2	1.90	0.54
1:1:204:TYR:HE2	1:1:213:TYR:HB2	1.72	0.53
2:2:38:TRP:CD1	2:2:39:PRO:HD2	2.42	0.53
3:3:117:TYR:CD1	3:3:155:ILE:HD13	2.44	0.53
3:3:57:ASN:C	3:3:57:ASN:HB3	2.27	0.53
1:1:35:THR:HG23	3:3:160:THR:HB	1.90	0.53
3:3:86:PHE:CD1	3:3:178:PRO:HB3	2.44	0.53
3:3:55:MET:HA	3:3:91:VAL:HG11	1.91	0.53
2:2:12:ARG:NH2	3:3:157:LEU:HD21	2.24	0.53
3:3:216:ASP:O	3:3:218:LYS:HE3	2.09	0.53
1:1:208:ASP:HB3	1:1:211:THR:HB	1.89	0.53
2:2:235:THR:CG2	2:2:236:PRO:CD	2.86	0.53
3:3:193:THR:O	3:3:194:SER:HB3	2.08	0.52
3:3:61:LYS:HG2	3:3:61:LYS:O	2.07	0.52
1:1:276:GLU:HB3	1:1:277:PRO:CD	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:210:PHE:N	3:3:210:PHE:CD1	2.77	0.52
3:3:18:ASP:OD2	4:4:40:SER:HB2	2.09	0.52
1:1:88:THR:O	1:1:90:ILE:CD1	2.58	0.52
2:2:174:ASN:C	2:2:174:ASN:ND2	2.63	0.52
3:3:75:ARG:NH1	3:3:78:GLU:OE2	2.41	0.52
1:1:88:THR:O	1:1:90:ILE:HD13	2.10	0.52
1:1:129:THR:OG1	1:1:185:ARG:NH1	2.41	0.52
1:1:151:MET:HE3	1:1:167:THR:O	2.09	0.52
1:1:273:LYS:O	1:1:274:ASN:O	2.27	0.52
2:2:235:THR:HG22	2:2:236:PRO:N	2.22	0.52
4:4:59:LEU:HD21	4:4:61:LEU:CD1	2.34	0.52
1:1:236:LYS:HE3	1:1:238:LEU:CD1	2.40	0.52
4:4:44:SER:O	4:4:45:LEU:C	2.48	0.52
1:1:114:LYS:NZ	3:3:99:GLU:OE2	2.43	0.52
2:2:177:LEU:CD1	3:3:94:THR:HG21	2.40	0.52
3:3:214:CYS:HB3	3:3:215:PRO:HD2	1.92	0.51
3:3:84:ASN:HD22	3:3:86:PHE:N	2.08	0.51
1:1:236:LYS:NZ	1:1:238:LEU:HD11	2.25	0.51
1:1:84:ASN:HB2	1:1:228:ILE:HD12	1.91	0.51
1:1:153:VAL:HG12	1:1:157:ALA:HB3	1.91	0.51
2:2:34:CYS:HB2	2:2:202:PRO:CD	2.41	0.51
2:2:205:ASN:HD22	2:2:206:SER:N	2.09	0.51
1:1:122:VAL:HG13	1:1:124:PHE:CE2	2.45	0.51
1:1:65:THR:HG22	3:3:104:TYR:CZ	2.46	0.51
3:3:175:TYR:HB2	3:3:182:THR:HG21	1.92	0.51
1:1:265:SER:HB2	2:2:138:GLY:O	2.11	0.51
2:2:171:TYR:HA	2:2:176:THR:O	2.11	0.51
1:1:60:PHE:CD2	3:3:218:LYS:HB3	2.46	0.51
3:3:63:GLU:C	3:3:65:ASN:H	2.14	0.50
1:1:151:MET:CE	1:1:167:THR:O	2.60	0.50
3:3:57:ASN:N	3:3:57:ASN:HB2	2.25	0.50
1:1:94:ARG:CG	1:1:94:ARG:HH11	2.24	0.50
2:2:139:ASN:N	2:2:139:ASN:OD1	2.44	0.50
1:1:190:TYR:HD1	1:1:197:TYR:CZ	2.30	0.50
2:2:8:GLY:C	2:2:9:TYR:HD1	2.14	0.49
1:1:179:LYS:O	1:1:182:ASP:HB2	2.12	0.49
3:3:54:PRO:O	3:3:91:VAL:HG12	2.12	0.49
4:4:59:LEU:HG	4:4:60:MET:N	2.27	0.49
2:2:19:GLY:HA2	2:2:58:THR:HG22	1.94	0.49
1:1:208:ASP:C	2:2:261:PRO:HG2	2.32	0.49
1:1:58:MET:CE	3:3:216:ASP:O	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:83:GLN:HG3	1:1:85:LYS:CE	2.31	0.49
3:3:112:ARG:HG2	3:3:112:ARG:NH1	2.27	0.49
1:1:280:LYS:HE3	3:3:89:ASP:OD1	2.13	0.49
2:2:143:LYS:HG2	2:2:163:GLY:O	2.12	0.49
3:3:20:GLN:NE2	4:4:31:TYR:H	2.11	0.49
1:1:134:ALA:HB2	1:1:180:VAL:HG11	1.95	0.48
2:2:34:CYS:HB2	2:2:202:PRO:HD2	1.95	0.48
3:3:125:ALA:HB3	3:3:155:ILE:HD12	1.95	0.48
3:3:112:ARG:HD3	3:3:162:VAL:CG1	2.43	0.48
3:3:20:GLN:HE22	4:4:30:ASN:HA	1.78	0.48
3:3:129:LEU:O	3:3:150:HIS:HA	2.13	0.48
1:1:58:MET:HE1	3:3:216:ASP:O	2.13	0.48
2:2:10:SER:CB	4:4:68:ASN:OXT	2.61	0.48
1:1:215:ILE:O	1:1:218:LEU:N	2.43	0.48
1:1:58:MET:O	1:1:59:HIS:HB2	2.12	0.48
2:2:40:GLU:CG	2:2:40:GLU:O	2.61	0.48
3:3:95:THR:O	3:3:99:GLU:HB2	2.13	0.48
1:1:268:ARG:HH11	1:1:268:ARG:HD3	1.50	0.48
2:2:130:HIS:ND1	2:2:219:SER:OG	2.47	0.48
1:1:268:ARG:NH1	3:3:236:GLU:O	2.46	0.48
1:1:92:ASN:C	1:1:92:ASN:ND2	2.67	0.47
1:1:273:LYS:O	1:1:274:ASN:C	2.52	0.47
1:1:268:ARG:CZ	2:2:139:ASN:HB2	2.44	0.47
2:2:13:VAL:HA	2:2:25:THR:O	2.15	0.47
2:2:177:LEU:CD1	3:3:94:THR:CG2	2.93	0.47
3:3:115:LEU:HD22	3:3:129:LEU:HD21	1.96	0.47
3:3:190:TRP:CD1	3:3:190:TRP:N	2.81	0.47
1:1:74:ALA:HB3	3:3:15:THR:HB	1.97	0.47
1:1:198:ASN:ND2	2:2:206:SER:OG	2.40	0.47
1:1:228:ILE:HD11	1:1:239:VAL:HG21	1.97	0.47
1:1:83:GLN:OE1	1:1:236:LYS:HD2	2.15	0.47
2:2:135:HIS:CD2	2:2:160:ASN:HB3	2.49	0.46
1:1:200:PHE:CE2	1:1:256:ARG:HD2	2.50	0.46
3:3:101:VAL:HG22	3:3:219:LEU:HD11	1.98	0.46
1:1:43:MET:HE3	1:1:43:MET:HA	1.97	0.46
1:1:174:PRO:O	5:1:700:W91:H4A2	2.14	0.46
1:1:92:ASN:CG	1:1:95:GLU:HB2	2.36	0.46
2:2:30:ASN:ND2	2:2:31:ALA:H	2.05	0.46
3:3:84:ASN:ND2	3:3:84:ASN:C	2.69	0.46
4:4:61:LEU:HD12	4:4:61:LEU:HA	1.62	0.46
2:2:63:PHE:CD1	2:2:245:ALA:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:87:ALA:CA	1:1:90:ILE:HG12	2.44	0.45
3:3:192:GLN:HA	3:3:192:GLN:HE21	1.81	0.45
1:1:43:MET:CE	1:1:43:MET:HA	2.46	0.45
2:2:187:GLN:NE2	2:2:198:THR:H	2.14	0.45
2:2:156:LEU:HD11	2:2:173:MET:SD	2.56	0.45
2:2:190:ASN:H	2:2:194:ASN:CB	2.30	0.45
3:3:55:MET:CE	3:3:91:VAL:HG21	2.46	0.45
4:4:44:SER:C	4:4:46:SER:N	2.68	0.45
2:2:13:VAL:C	2:2:14:GLN:CG	2.85	0.45
2:2:91:VAL:HG12	2:2:95:ASN:HD22	1.82	0.45
3:3:174:ARG:HH11	3:3:174:ARG:HD3	1.64	0.45
3:3:55:MET:HE2	3:3:91:VAL:HG21	1.99	0.45
2:2:195:ASN:ND2	2:2:195:ASN:C	2.66	0.45
3:3:197:LEU:HD21	3:3:205:VAL:HG11	1.99	0.45
3:3:50:ASP:HA	3:3:212:SER:HB3	1.98	0.45
4:4:43:GLN:HG3	4:4:45:LEU:H	1.82	0.45
1:1:215:ILE:C	1:1:217:VAL:H	2.20	0.45
1:1:28:THR:HG22	1:1:29:GLN:H	1.82	0.45
1:1:64:GLU:O	1:1:64:GLU:HG2	2.17	0.45
2:2:146:PHE:CG	2:2:164:GLY:HA2	2.52	0.45
1:1:285:ASP:HB3	1:1:288:SER:H	1.82	0.44
3:3:116:MET:HG3	3:3:159:SER:OG	2.17	0.44
3:3:181:TYR:CD1	3:3:181:TYR:C	2.91	0.44
1:1:201:TYR:H	2:2:131:GLN:HE21	1.66	0.44
2:2:10:SER:OG	4:4:68:ASN:OXT	2.35	0.44
1:1:31:VAL:HG11	1:1:34:LEU:HD12	1.98	0.44
1:1:77:VAL:C	1:1:109:LEU:CD2	2.86	0.44
2:2:228:LEU:CD1	2:2:238:LEU:HD22	2.47	0.44
1:1:146:LEU:HD13	1:1:228:ILE:HD13	1.99	0.44
2:2:148:HIS:N	2:2:149:PRO:CD	2.79	0.44
1:1:289:TYR:CE2	3:3:138:GLY:HA3	2.53	0.44
3:3:61:LYS:O	3:3:63:GLU:HG3	2.16	0.44
1:1:47:PRO:HB3	3:3:166:PRO:HB3	1.99	0.44
1:1:98:LEU:O	1:1:99:PHE:HB3	2.18	0.44
2:2:37:GLU:CD	3:3:35:HIS:HE2	2.19	0.44
1:1:289:TYR:CD2	3:3:138:GLY:HA3	2.52	0.44
3:3:57:ASN:H	3:3:57:ASN:CB	2.26	0.44
1:1:146:LEU:HA	1:1:230:ASN:OD1	2.18	0.43
1:1:282:ARG:CG	3:3:57:ASN:CB	2.89	0.43
4:4:59:LEU:CD2	4:4:61:LEU:HD13	2.41	0.43
1:1:215:ILE:C	1:1:217:VAL:N	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:190:ASN:H	2:2:194:ASN:HB3	1.82	0.43
2:2:95:ASN:HB3	2:2:251:PHE:CE2	2.53	0.43
2:2:13:VAL:C	2:2:14:GLN:HG2	2.39	0.43
2:2:143:LYS:HG2	2:2:143:LYS:H	1.56	0.43
3:3:61:LYS:HG2	3:3:63:GLU:HG3	2.00	0.43
3:3:84:ASN:HD22	3:3:84:ASN:C	2.20	0.43
1:1:128:TYR:HB2	1:1:186:PHE:CZ	2.54	0.43
1:1:214:GLY:O	1:1:217:VAL:CG1	2.67	0.43
1:1:286:ILE:HG21	1:1:286:ILE:HD13	1.77	0.43
1:1:87:ALA:HB2	1:1:98:LEU:CD1	2.48	0.43
2:2:262:GLN:C	2:2:262:GLN:NE2	2.66	0.43
2:2:91:VAL:HG12	2:2:95:ASN:ND2	2.34	0.43
3:3:47:ILE:HG21	3:3:47:ILE:HD13	1.51	0.43
1:1:104:ILE:HG12	1:1:223:SER:HA	2.00	0.43
2:2:70:THR:HG22	2:2:72:THR:HG22	2.01	0.43
3:3:151:VAL:HG11	3:3:161:ILE:HD11	2.01	0.43
1:1:103:LYS:O	1:1:104:ILE:C	2.57	0.42
4:4:43:GLN:O	4:4:45:LEU:CB	2.65	0.42
1:1:154:PRO:HD2	1:1:173:ASN:HD21	1.83	0.42
2:2:235:THR:CG2	2:2:236:PRO:N	2.79	0.42
2:2:259:ILE:HG21	2:2:259:ILE:HD13	1.74	0.42
1:1:261:LEU:HD11	2:2:171:TYR:CD2	2.55	0.42
1:1:190:TYR:CD1	1:1:197:TYR:CZ	3.07	0.42
1:1:103:LYS:O	1:1:103:LYS:CG	2.67	0.42
1:1:136:GLN:HB2	1:1:136:GLN:HE21	1.13	0.42
2:2:228:LEU:HD11	2:2:238:LEU:HD22	2.02	0.42
2:2:225:ILE:O	3:3:68:LEU:HD21	2.20	0.42
1:1:118:LEU:HA	1:1:118:LEU:HD12	1.91	0.42
1:1:110:VAL:HG13	3:3:230:GLN:CD	2.39	0.42
1:1:146:LEU:HD13	1:1:228:ILE:CD1	2.50	0.42
2:2:10:SER:CB	2:2:12:ARG:HB2	2.49	0.42
1:1:165:ASP:N	1:1:168:TRP:HD1	2.18	0.42
1:1:285:ASP:HB3	1:1:288:SER:N	2.34	0.42
1:1:286:ILE:HG23	3:3:81:PHE:HA	2.00	0.42
4:4:30:ASN:HA	4:4:30:ASN:HD22	1.40	0.42
1:1:104:ILE:CG1	1:1:223:SER:HA	2.50	0.41
3:3:18:ASP:CG	4:4:40:SER:HB2	2.41	0.41
3:3:44:LEU:HD23	3:3:44:LEU:HA	1.79	0.41
1:1:97:LYS:C	1:1:99:PHE:N	2.71	0.41
1:1:86:ASP:OD1	1:1:88:THR:HB	2.20	0.41
2:2:235:THR:HG22	2:2:237:SER:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:112:ARG:HG2	3:3:112:ARG:HH11	1.83	0.41
1:1:102:TRP:O	1:1:102:TRP:CG	2.73	0.41
3:3:113:PHE:CE2	3:3:115:LEU:HD13	2.55	0.41
3:3:208:LEU:HA	3:3:208:LEU:HD12	1.73	0.41
1:1:38:GLU:CD	3:3:116:MET:CE	2.88	0.41
1:1:87:ALA:HB2	1:1:98:LEU:HD11	2.02	0.41
3:3:195:LEU:C	3:3:196:ILE:HG12	2.40	0.41
2:2:43:PRO:HG2	2:2:46:ASP:HB2	2.03	0.41
2:2:84:ASP:HB2	2:2:216:ASN:HD21	1.86	0.41
1:1:289:TYR:CZ	3:3:139:PRO:HD2	2.55	0.41
2:2:122:LEU:HD23	2:2:224:PRO:HA	2.02	0.41
2:2:69:LYS:O	2:2:239:PRO:HA	2.20	0.41
1:1:78:HIS:NE2	1:1:80:THR:HB	2.36	0.41
2:2:255:ARG:CG	2:2:256:SER:H	2.00	0.41
3:3:214:CYS:HB3	3:3:215:PRO:CD	2.51	0.40
1:1:285:ASP:H	1:1:285:ASP:HB2	1.85	0.40
1:1:38:GLU:N	3:3:116:MET:HE3	2.37	0.40
3:3:20:GLN:NE2	4:4:30:ASN:HA	2.36	0.40
1:1:169:GLN:O	1:1:170:SER:C	2.59	0.40
4:4:43:GLN:HG2	4:4:43:GLN:O	2.18	0.40
2:2:13:VAL:HG22	2:2:26:GLN:HA	2.03	0.40
3:3:167:TRP:HZ2	3:3:172:GLN:HA	1.86	0.40
1:1:261:LEU:HD11	2:2:171:TYR:CE2	2.57	0.40
2:2:183:ILE:HD12	3:3:49:VAL:HG11	2.03	0.40
2:2:53:THR:OG1	2:2:250:GLU:HG2	2.22	0.40
3:3:86:PHE:CG	3:3:178:PRO:HB3	2.57	0.40
3:3:57:ASN:HD21	3:3:91:VAL:HG13	1.83	0.40
4:4:43:GLN:O	4:4:44:SER:C	2.58	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	1	271/289 (94%)	239 (88%)	25 (9%)	7 (3%)	5	27
2	2	253/262 (97%)	234 (92%)	17 (7%)	2 (1%)	19	57
3	3	234/236 (99%)	217 (93%)	15 (6%)	2 (1%)	17	55
4	4	38/68 (56%)	34 (90%)	3 (8%)	1 (3%)	5	27
All	All	796/855 (93%)	724 (91%)	60 (8%)	12 (2%)	10	42

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	103	LYS
1	1	104	ILE
1	1	139	SER
3	3	57	ASN
3	3	77	ASN
2	2	255	ARG
2	2	257	LYS
1	1	165	ASP
1	1	108	SER
1	1	170	SER
4	4	47	MET
1	1	99	PHE

### 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	1	239/253 (94%)	195 (82%)	44 (18%)	1	9
2	2	223/229 (97%)	180 (81%)	43 (19%)	1	8
3	3	209/209 (100%)	170 (81%)	39 (19%)	1	8
4	4	33/57 (58%)	20 (61%)	13 (39%)	0	0
All	All	704/748 (94%)	565 (80%)	139 (20%)	1	7

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	18	VAL
1	1	21	ILE
1	1	22	SER
1	1	23	SER
1	1	28	THR
1	1	29	GLN
1	1	30	LYS
1	1	38	GLU
1	1	43	MET
1	1	47	PRO
1	1	63	SER
1	1	81	GLU
1	1	90	ILE
1	1	97	LYS
1	1	100	ASN
1	1	104	ILE
1	1	107	SER
1	1	108	SER
1	1	109	LEU
1	1	110	VAL
1	1	122	VAL
1	1	136	GLN
1	1	137	PRO
1	1	138	ASP
1	1	139	SER
1	1	144	SER
1	1	145	ASN
1	1	151	MET
1	1	153	VAL
1	1	161	LYS
1	1	170	SER
1	1	183	THR
1	1	184	SER
1	1	185	ARG
1	1	215	ILE
1	1	216	THR
1	1	220	HIS
1	1	221	MET
1	1	240	LYS
1	1	256	ARG
1	1	268	ARG
1	1	274	ASN
1	1	278	VAL

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Mol	Chain	Res	Type
1	1	287	LYS
2	2	11	ASP
2	2	12	ARG
2	2	20	ASN
2	2	26	GLN
2	2	30	ASN
2	2	49	ASP
2	2	52	LYS
2	2	66	LEU
2	2	69	LYS
2	2	73	THR
2	2	76	LYS
2	2	81	LYS
2	2	87	LYS
2	2	88	ASP
2	2	103	ARG
2	2	116	LYS
2	2	119	SER
2	2	136	GLU
2	2	141	SER
2	2	145	THR
2	2	152	ARG
2	2	165	PRO
2	2	168	ASP
2	2	169	VAL
2	2	174	ASN
2	2	187	GLN
2	2	192	ARG
2	2	195	ASN
2	2	205	ASN
2	2	209	ILE
2	2	211	SER
2	2	217	ASN
2	2	221	MET
2	2	225	ILE
2	2	232	THR
2	2	236	PRO
2	2	238	LEU
2	2	247	MET
2	2	250	GLU
2	2	254	ILE
2	2	255	ARG

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Mol	Chain	Res	Type
2	2	256	SER
2	2	262	GLN
3	3	16	THR
3	3	33	ARG
3	3	46	ILE
3	3	55	MET
3	3	56	ASN
3	3	60	THR
3	3	61	LYS
3	3	65	ASN
3	3	84	ASN
3	3	91	VAL
3	3	94	THR
3	3	101	VAL
3	3	112	ARG
3	3	114	SER
3	3	115	LEU
3	3	137	ARG
3	3	146	MET
3	3	157	LEU
3	3	158	GLN
3	3	159	SER
3	3	164	THR
3	3	172	GLN
3	3	174	ARG
3	3	179	ASP
3	3	182	THR
3	3	192	GLN
3	3	194	SER
3	3	196	ILE
3	3	201	THR
3	3	208	LEU
3	3	211	ILE
3	3	217	PHE
3	3	218	LYS
3	3	219	LEU
3	3	220	ARG
3	3	223	LYS
3	3	226	GLN
3	3	228	ILE
3	3	230	GLN
4	4	29	ILE

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Mol	Chain	Res	Type
4	4	33	LYS
4	4	40	SER
4	4	43	GLN
4	4	45	LEU
4	4	46	SER
4	4	47	MET
4	4	50	SER
4	4	51	LYS
4	4	59	LEU
4	4	61	LEU
4	4	67	LEU
4	4	68	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	61	ASN
1	1	92	ASN
1	1	100	ASN
1	1	136	GLN
1	1	173	ASN
1	1	198	ASN
1	1	220	HIS
2	2	15	GLN
2	2	20	ASN
2	2	30	ASN
2	2	131	GLN
2	2	174	ASN
2	2	187	GLN
2	2	190	ASN
2	2	195	ASN
2	2	205	ASN
2	2	216	ASN
2	2	217	ASN
2	2	262	GLN
3	3	20	GLN
3	3	42	ASN
3	3	56	ASN
3	3	84	ASN
3	3	102	GLN
3	3	140	GLN
3	3	192	GLN

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Mol	Chain	Res	Type
3	3	226	GLN
4	4	30	ASN

### 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 ⓘ

1 ligand is 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$
5	W91	1	700	-	22,25,25	3.18	5 (22%)	29,34,34	2.69	7 (24%)

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
5	W91	1	700	-	-	1/10/18/18	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	700	W91	C2A-N3A	12.01	1.43	1.27
5	1	700	W91	C4A-N3A	-6.40	1.36	1.47
5	1	700	W91	C4-C5	-3.17	1.35	1.39
5	1	700	W91	O1A-C5A	-3.03	1.38	1.46
5	1	700	W91	O1A-C2A	-2.78	1.31	1.36

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	700	W91	O1A-C2A-N3A	-9.54	110.03	118.23
5	1	700	W91	C4A-N3A-C2A	6.30	112.40	106.77
5	1	700	W91	O1A-C2A-C4B	5.83	123.57	115.85
5	1	700	W91	O1A-C5A-C4A	3.74	111.91	104.28
5	1	700	W91	C3C-O1B-C1B	2.57	121.99	114.23
5	1	700	W91	C1C-C5-C4	2.56	135.25	128.60
5	1	700	W91	C5A-C4A-N3A	-2.07	99.42	104.35

There are no chirality outliers.

All (1) torsion outliers are listed below:

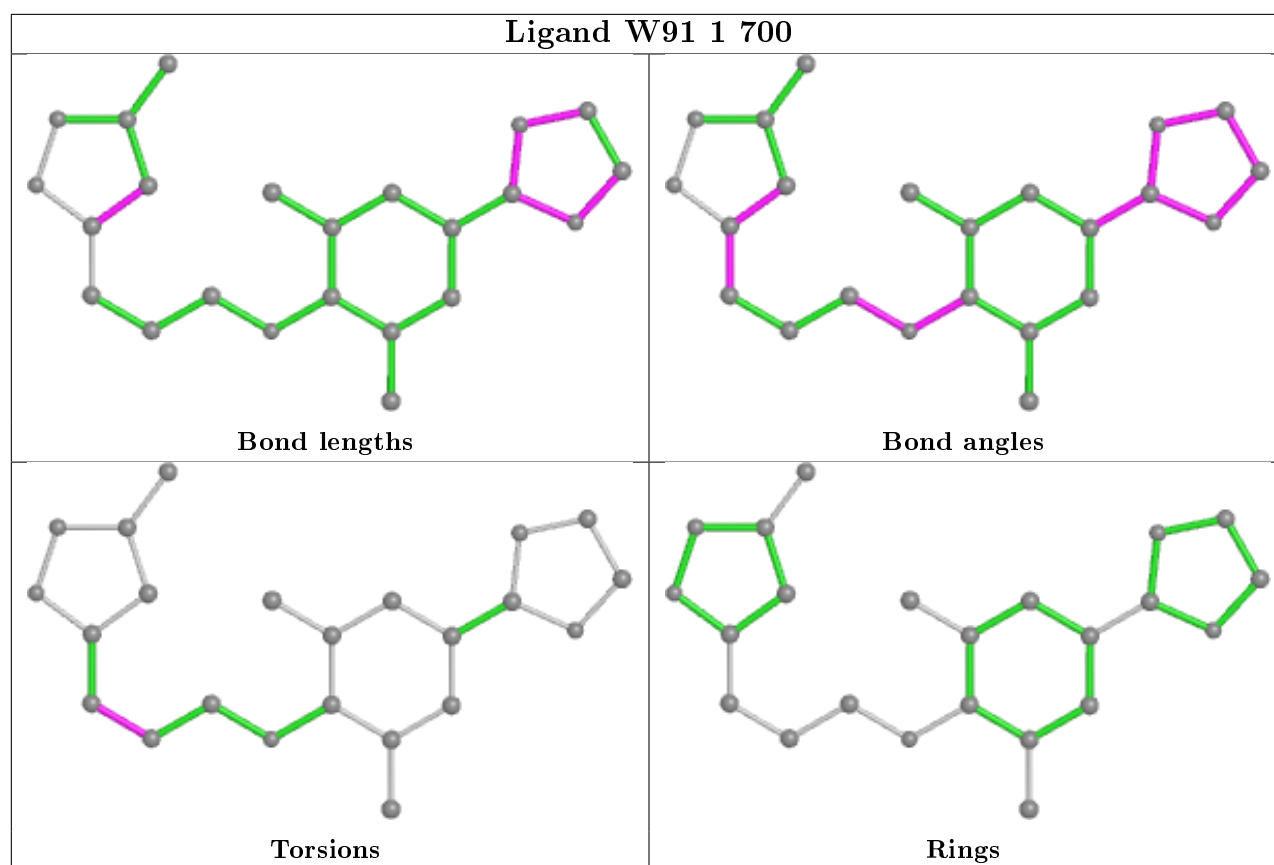
Mol	Chain	Res	Type	Atoms
5	1	700	W91	C5-C1C-C2C-C3C

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1	700	W91	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	169:VAL	C	170:VAL	N	1.11

## 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.