



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:33 AM GMT

PDB ID : 2HWC  
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 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/ValidationPDFNotes.html>

---

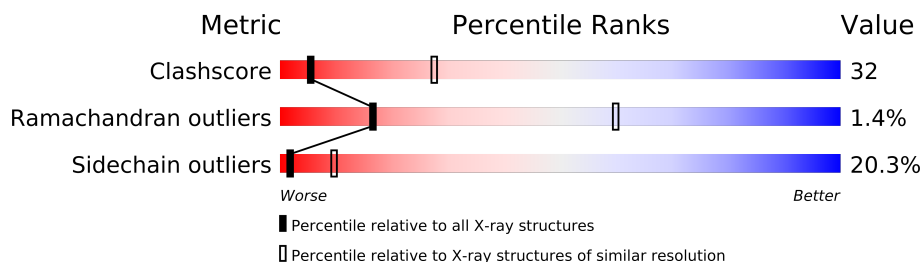
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 6292 atoms, of which 0 are hydrogen and 0 are deuterium.

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

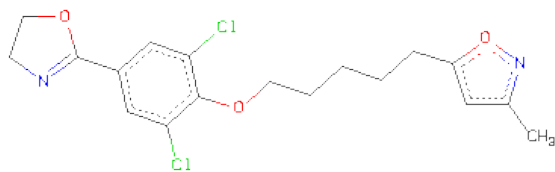
- Molecule 3 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP3).

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-(5-(2,6-DICHLORO-4-(4,5-DIHYDRO-2-OXAZOLY)PHENOXY)PENTYL)-3-METHYLISOXAZOLE (three-letter code: W54) (formula: C<sub>18</sub>H<sub>20</sub>Cl<sub>2</sub>N<sub>2</sub>O<sub>3</sub>).



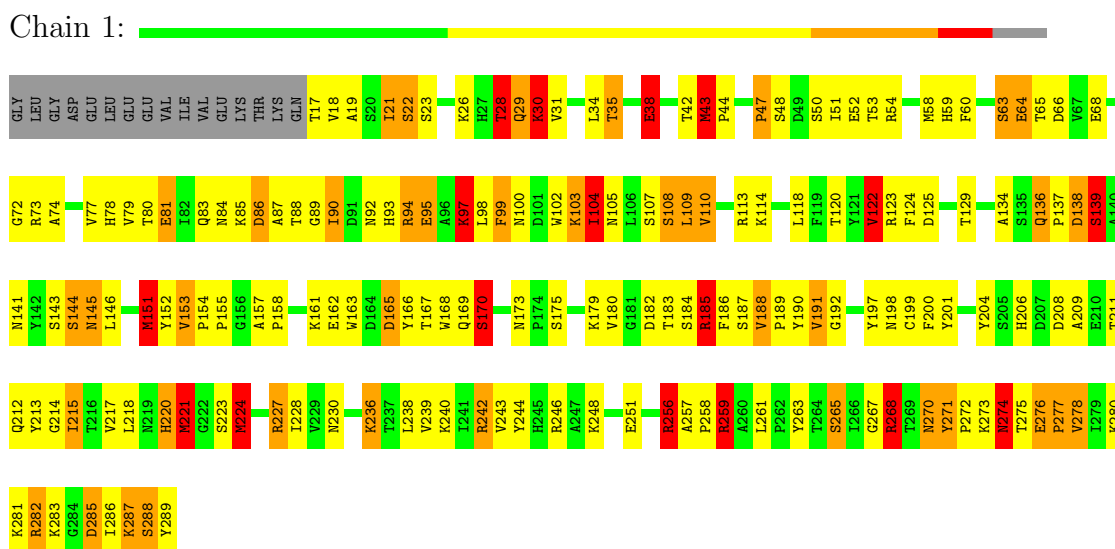
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
5	1	1	25	18	2	2	3	0	0

### 3 Residue-property plots

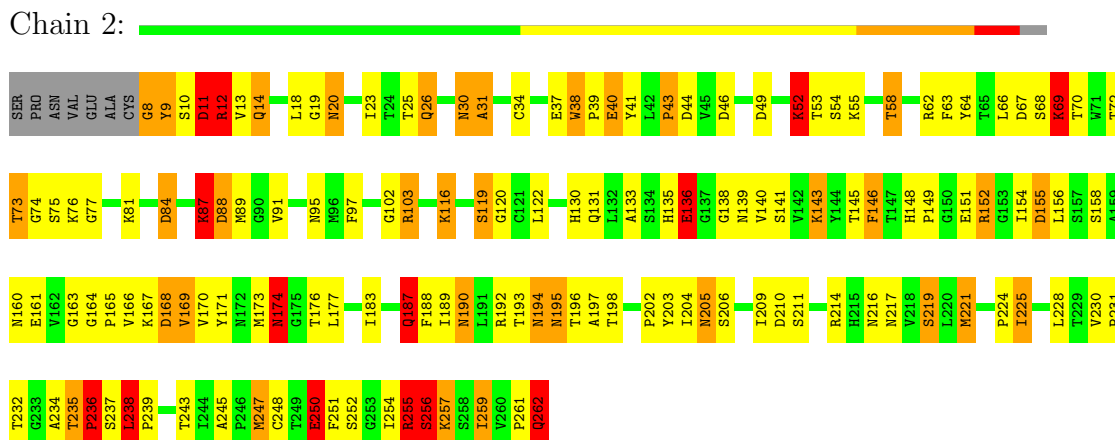
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

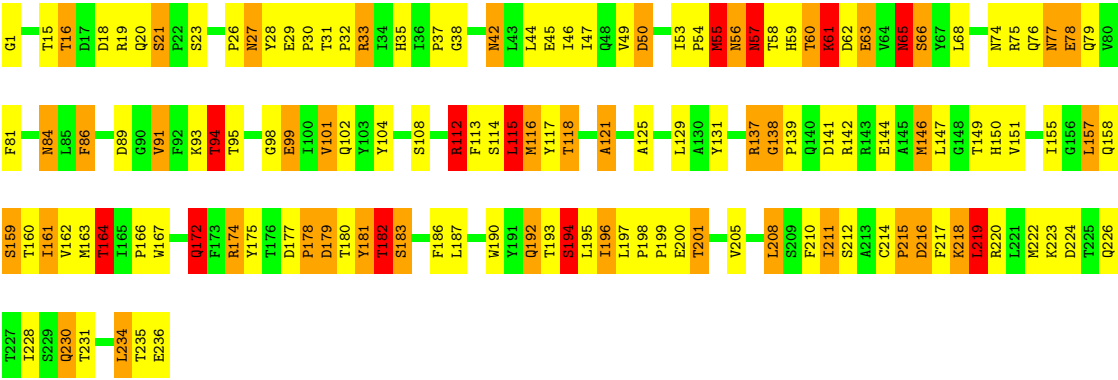


#### • Molecule 2: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP2)



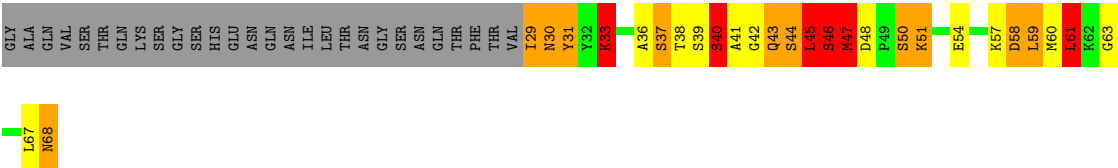
#### • Molecule 3: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP3)





● 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 will therefore be 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	6292	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	0.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: W54

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	1.66	31/2228 (1.4%)	2.12	90/3031 (3.0%)
2	2	1.86	33/2000 (1.6%)	2.16	76/2734 (2.8%)
3	3	1.83	22/1898 (1.2%)	2.17	74/2597 (2.8%)
4	4	2.30	13/302 (4.3%)	2.46	21/406 (5.2%)
All	All	1.81	99/6428 (1.5%)	2.16	261/8768 (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)
3	3	234	LEU	C-N	21.20	1.82	1.34
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	169	VAL	C-N	-10.24	1.10	1.34
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
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

*Continued on next page...*



*Continued from previous page...*

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	7.33	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	6.14	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

*Continued on next page...*

*Continued from previous page...*

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
2	2	219	SER	CB-OG	-5.49	1.35	1.42
2	2	236	PRO	C-O	5.43	1.34	1.23
4	4	50	SER	CB-OG	5.42	1.49	1.42
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	118	THR	CB-OG1	5.23	1.53	1.43
3	3	33	ARG	CZ-NH2	5.22	1.39	1.33
2	2	120	GLY	N-CA	5.21	1.53	1.46
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

*Continued on next page...*

*Continued from previous page...*

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 (261) 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	-18.66	110.97	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
1	1	282	ARG	NE-CZ-NH2	-14.11	113.25	120.30
2	2	255	ARG	NE-CZ-NH1	14.07	127.34	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	-10.01	109.59	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

*Continued on next page...*

*Continued from previous page...*

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
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
1	1	113	ARG	NE-CZ-NH2	7.29	123.94	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	282	ARG	NH1-CZ-NH2	7.27	127.39	119.40
3	3	234	LEU	O-C-N	7.23	134.26	122.70
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
3	3	234	LEU	CA-C-N	-6.93	101.95	117.20
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
3	3	45	GLU	CG-CD-OE2	6.59	131.49	118.30
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
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
3	3	74	ASN	CA-CB-CG	-6.48	99.14	113.40
1	1	288	SER	N-CA-CB	-6.48	100.78	110.50
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	168	ASP	OD1-CG-OD2	6.42	135.50	123.30
3	3	29	GLU	CB-CG-CD	6.42	131.52	114.20
1	1	274	ASN	O-C-N	6.40	132.94	122.70
2	2	97	PHE	CB-CG-CD1	-6.34	116.36	120.80
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	6.16	110.05	100.20
2	2	69	LYS	CA-CB-CG	6.14	126.92	113.40
1	1	221	MET	CG-SD-CE	6.14	110.03	100.20
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	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
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	169	VAL	CA-C-N	5.94	130.27	117.20
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	45	GLU	CG-CD-OE1	-5.88	106.55	118.30
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
1	1	185	ARG	NE-CZ-NH2	5.84	123.22	120.30
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
4	4	33	LYS	CD-CE-NZ	-5.83	98.30	111.70
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
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
3	3	234	LEU	C-N-CA	-5.53	107.87	121.70
1	1	122	VAL	CB-CA-C	5.53	121.91	111.40
1	1	244	TYR	CB-CG-CD2	-5.53	117.68	121.00
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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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	125.17	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
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
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
3	3	74	ASN	OD1-CG-ND2	5.22	133.91	121.90
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
1	1	275	THR	CA-C-O	-5.20	109.17	120.10
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
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
1	1	282	ARG	CG-CD-NE	-5.15	100.98	111.80
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
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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	141	ASN	CA-CB-CG	-5.11	102.16	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
1	1	274	ASN	CA-C-N	-5.05	106.09	117.20
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
3	3	178	PRO	O-C-N	5.02	130.73	122.70
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2170	0	2106	173	0
2	2	1951	0	1923	128	0
3	3	1849	0	1830	141	0
4	4	297	0	294	35	0
5	1	25	0	20	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6292	0	6173	403	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 32.

All (403) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:CE	2:2:52:LYS:NZ	1.68	1.53
3:3:234:LEU:C	3:3:235:THR:N	1.82	1.32
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:OD1	1:1:285:ASP:CA	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
2:2:12:ARG:HH11	2:2:12:ARG:HG3	1.27	0.93
1:1:285:ASP:CG	1:1:285:ASP:CA	2.37	0.93
1:1:152:TYR:O	1:1:154:PRO:HD3	1.69	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
1:1:103:LYS:HG3	1:1:103:LYS:O	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
1:1:102:TRP:CZ3	1:1:243:VAL:HG11	2.07	0.89
3:3:198:PRO:HD2	3:3:201:THR:HG21	1.55	0.89
1:1:47:PRO:HA	3:3:164:THR:CG2	2.03	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
1:1:191:VAL:O	1:1:191:VAL:HG23	1.75	0.86

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:CG	3:3:57:ASN:CA	2.45	0.84
2:2:195:ASN:ND2	2:2:196:THR:HG23	1.91	0.84
1:1:282:ARG:HD2	1:1:285:ASP:O	1.78	0.84
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:CD	2:2:52:LYS:NZ	2.43	0.82
4:4:68:ASN:OD1	4:4:68:ASN:N	2.11	0.82
1:1:103:LYS:O	1:1:103:LYS:CG	2.27	0.82
2:2:12:ARG:HH11	2:2:12:ARG:CG	1.89	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
1:1:47:PRO:CA	3:3:164:THR:HG21	2.15	0.77
2:2:12:ARG:CG	2:2:12:ARG:NH1	2.44	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
1:1:94:ARG:NH1	1:1:94:ARG:HG2	2.00	0.76
1:1:220:HIS:CG	1:1:220:HIS:O	2.39	0.75
2:2:262:GLN:C	2:2:262:GLN:HE21	1.91	0.74
1:1:92:ASN:OD1	1:1:95:GLU:HB2	1.87	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
1:1:258: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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
1:1:102:TRP:CZ3	1:1:224:MET:HE3	2.29	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
2:2:195:ASN:HD22	2:2:195:ASN:C	1.99	0.66
3:3:42:ASN:HD22	3:3:44:LEU:H	1.43	0.66
2:2:84:ASP:OD1	2:2:87:LYS:HE2	1.94	0.66
1:1:151:MET:SD	1:1:170:SER:HB2	2.35	0.66
1:1:285:ASP:CB	1:1:285:ASP:H	2.09	0.66
1:1:278:VAL:HG12	3:3:62:ASP:OD2	1.95	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
2:2:149:PRO:HG3	2:2:154:ILE:HG13	1.78	0.64
1:1:201:TYR:HD2	1:1:214:GLY:O	1.80	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
3:3:234:LEU:CA	3:3:235:THR:N	2.61	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
3:3:79:GLN:HB2	3:3:190:TRP:CE3	2.32	0.63
2:2:23:ILE:HD11	2:2:243:THR:HG21	1.79	0.63
2:2:13:VAL:O	2:2:14:GLN:HG2	1.99	0.63
1:1:83:GLN:CG	1:1:85:LYS:HE2	2.24	0.63
1:1:166:TYR:O	1:1:169:GLN:HB2	1.99	0.63
1:1:191:VAL:O	1:1:191:VAL:CG2	2.46	0.62
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:1:102:TRP:CE3	1:1:224:MET:HE3	2.34	0.62
2:2:205:ASN:HD22	2:2:206:SER:H	1.45	0.62
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	0.61
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
1:1:87:ALA:HA	1:1:90:ILE:HG12	1.80	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
3:3:131:TYR:HB3	3:3:149:THR:HB	1.82	0.60
1:1:265:SER:HB3	1:1:268:ARG:HG2	1.83	0.60
2:2:155:ASP:C	2:2:155:ASP:OD1	2.37	0.60
3:3:234:LEU:C	3:3:235:THR:CA	2.69	0.60
3:3:76:GLN:O	3:3:78:GLU:N	2.34	0.60
1:1:204:TYR:CE2	1:1:213:TYR:HB2	2.36	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
2:2:11:ASP:H	4:4:68:ASN:CG	2.06	0.59
1:1:259:ARG:HD2	1:1:263:TYR:CE1	2.38	0.59
2:2:30:ASN:HD21	4:4:58:ASP:H	1.51	0.58
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
3:3:180:THR:O	3:3:183:SER:HB3	2.02	0.58
1:1:58:MET:HE1	3:3:216:ASP:C	2.24	0.58
1:1:151:MET:HB2	1:1:175:SER:OG	2.04	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
1:1:78:HIS:NE2	1:1:102:TRP:HB2	2.19	0.58
1:1:104:ILE:HG12	1:1:223:SER:HA	1.86	0.57
1:1:93:HIS:CE1	1:1:163:TRP:HD1	2.22	0.57
1:1:209:ALA:HB2	2:2:261:PRO:HB3	1.85	0.57
2:2:52:LYS:HD3	2:2:52:LYS:NZ	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
2:2:10:SER:OG	2:2:12:ARG:CB	2.53	0.56
1:1:155:PRO:HB3	1:1:220:HIS:HE1	1.70	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
1:1:185:ARG:HG3	1:1:186:PHE:N	2.21	0.56
3:3:179:ASP:OD2	3:3:182:THR:CG2	2.52	0.56
4:4:43:GLN:O	4:4:45:LEU:HB3	2.05	0.56
2:2:204:ILE:HG12	3:3:37:PRO:HG2	1.87	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
3:3:197:LEU:HB3	3:3:201:THR:HG21	1.87	0.55
1:1:102:TRP:CH2	1:1:243:VAL:HG11	2.40	0.55
1:1:155:PRO:HB3	1:1:220:HIS:CE1	2.42	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
1:1:224:MET:HE2	5:1:500:W54:CL2	2.43	0.54
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
3:3:175:TYR:H	3:3:182:THR:CG2	2.21	0.54
1:1:102:TRP:HZ3	1:1:243:VAL:HG11	1.69	0.54
1:1:208:ASP:O	2:2:261:PRO:HG2	2.07	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
1:1:151:MET:HE1	1:1:168:TRP:HA	1.89	0.54
1:1:158:PRO:HB2	1:1:167:THR:HG22	1.90	0.54
1:1:104:ILE:HG21	5:1:500:W54:H3C1	1.90	0.53
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
3:3:55:MET:HA	3:3:91:VAL:HG11	1.90	0.53
3:3:57:ASN:C	3:3:57:ASN:HB3	2.27	0.53
3:3:117:TYR:CD1	3:3:155:ILE:HD13	2.44	0.53
3:3:86:PHE:CD1	3:3:178:PRO:HB3	2.44	0.53
1:1:35:THR:HG23	3:3:160:THR:HB	1.90	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:2:235:THR:CG2	2:2:236:PRO:CD	2.86	0.53
1:1:208:ASP:HB3	1:1:211:THR:HB	1.89	0.53
3:3:61:LYS:HG2	3:3:61:LYS:O	2.07	0.52
3:3:193:THR:O	3:3:194:SER:HB3	2.08	0.52
1:1:276:GLU:HB3	1:1:277:PRO:CD	2.39	0.52
3:3:210:PHE:N	3:3:210:PHE:CD1	2.77	0.52
1:1:190:TYR:HD1	1:1:197:TYR:CZ	2.28	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
1:1:151:MET:HE3	1:1:167:THR:O	2.09	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
1:1:273:LYS:O	1:1:274:ASN:O	2.28	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
3:3:84:ASN:HD22	3:3:86:PHE:N	2.08	0.51
3:3:214:CYS:HB3	3:3:215:PRO:HD2	1.92	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
1:1:129:THR:OG1	1:1:185:ARG:NH1	2.41	0.51
2:2:34:CYS:HB2	2:2:202:PRO:CD	2.41	0.51
1:1:153:VAL:HG12	1:1:157:ALA:HB3	1.91	0.51
2:2:205:ASN:HD22	2:2:206:SER:N	2.09	0.51
3:3:175:TYR:HB2	3:3:182:THR:HG21	1.92	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
1:1:265:SER:HB2	2:2:138:GLY:O	2.11	0.51
1:1:60:PHE:CD2	3:3:218:LYS:HB3	2.46	0.51
2:2:171:TYR:HA	2:2:176:THR:O	2.11	0.51
3:3:63:GLU:C	3:3:65:ASN:H	2.14	0.50
1:1:102:TRP:CZ3	1:1:224:MET:CE	2.94	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
2:2:8:GLY:C	2:2:9:TYR:HD1	2.14	0.49
3:3:54:PRO:O	3:3:91:VAL:HG12	2.12	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:1:179:LYS:O	1:1:182:ASP:HB2	2.12	0.49
4:4:59:LEU:HG	4:4:60:MET:N	2.27	0.49
1:1:208:ASP:C	2:2:261:PRO:HG2	2.32	0.49
2:2:19:GLY:HA2	2:2:58:THR:HG22	1.94	0.49
1:1:58:MET:CE	3:3:216:ASP:O	2.60	0.49
1:1:83:GLN:HG3	1:1:85:LYS:CE	2.31	0.49
1:1:280:LYS:HE3	3:3:89:ASP:OD1	2.13	0.49
3:3:112:ARG:HG2	3:3:112:ARG:NH1	2.27	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
3:3:125:ALA:HB3	3:3:155:ILE:HD12	1.95	0.48
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
3:3:112: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
1:1:58:MET:HE1	3:3:216:ASP:O	2.13	0.48
3:3:129:LEU:O	3:3:150:HIS:HA	2.13	0.48
2:2:10:SER:CB	4:4:68:ASN:OXT	2.61	0.48
1:1:103:LYS:HA	1:1:223:SER:CB	2.43	0.48
1:1:103:LYS:HD3	3:3:236:GLU:OE2	2.14	0.48
2:2:40:GLU:CG	2:2:40:GLU:O	2.61	0.48
1:1:215:ILE:O	1:1:218:LEU:N	2.43	0.48
3:3:95:THR:O	3:3:99:GLU:HB2	2.13	0.48
1:1:58:MET:O	1:1:59:HIS: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
1:1:92: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
3:3:190:TRP:CD1	3:3:190:TRP:N	2.81	0.47
1:1:198:ASN:ND2	2:2:206:SER:OG	2.40	0.47
3:3:115:LEU:HD22	3:3:129:LEU:HD21	1.96	0.47
1:1:74:ALA:HB3	3:3:15:THR:HB	1.97	0.47
1:1:83:GLN:OE1	1:1:236:LYS:HD2	2.15	0.47
1:1:228:ILE:HD11	1:1:239:VAL:HG21	1.97	0.47
2:2:135:HIS:CD2	2:2:160:ASN:HB3	2.49	0.46
3:3:101:VAL:HG22	3:3:219:LEU:HD11	1.98	0.46
1:1:200:PHE:CE2	1:1:256:ARG:HD2	2.50	0.46
1:1:43:MET:HE3	1:1:43:MET:HA	1.97	0.46
2:2:30:ASN:ND2	2:2:31:ALA:H	2.05	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:1:92:ASN:CG	1:1:95:GLU:HB2	2.36	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
1:1:188:VAL:HG23	1:1:189:PRO:O	2.16	0.46
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
2:2:187:GLN:NE2	2:2:198:THR:H	2.14	0.45
1:1:43:MET:CE	1:1:43:MET:HA	2.46	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
2:2:190:ASN:H	2:2:194:ASN:CB	2.30	0.45
2:2:156:LEU:HD11	2:2:173:MET:SD	2.56	0.45
2:2:13:VAL:C	2:2:14:GLN:CG	2.85	0.45
3:3:55:MET:HE2	3:3:91:VAL:HG21	1.99	0.45
3:3:197:LEU:HD21	3:3:205:VAL:HG11	1.99	0.45
3:3:174:ARG:HH11	3:3:174:ARG:HD3	1.64	0.45
2:2:91:VAL:HG12	2:2:95:ASN:HD22	1.82	0.45
2:2:195:ASN:ND2	2:2:195:ASN:C	2.66	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
3:3:50:ASP:HA	3:3:212:SER:HB3	1.98	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
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
1:1:285:ASP:HB3	1:1:288:SER:H	1.82	0.44
2:2:10:SER:OG	4:4:68:ASN:OXT	2.35	0.44
1:1:201:TYR:H	2:2:131:GLN:HE21	1.66	0.44
1:1:124:PHE:O	1:1:190:TYR:HB2	2.18	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
2:2:148:HIS:N	2:2:149:PRO:CD	2.79	0.44
1:1:146:LEU:HD13	1:1:228:ILE:HD13	1.99	0.44
3:3:61:LYS:O	3:3:63:GLU:HG3	2.16	0.44
1:1:289:TYR:CE2	3:3:138:GLY:HA3	2.53	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
1:1:190:TYR:CD1	1:1:197:TYR:CZ	3.05	0.44
2:2:37:GLU:CD	3:3:35:HIS:HE2	2.19	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:1:289:TYR:CD2	3:3:138:GLY:HA3	2.52	0.44
1:1:187:SER:O	3:3:23:SER:HA	2.17	0.44
3:3:57:ASN:H	3:3:57:ASN:CB	2.26	0.44
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	2.70	0.43
1:1:146:LEU:HA	1:1:230:ASN:OD1	2.18	0.43
1:1:103:LYS:HA	1:1:223:SER:HB3	2.00	0.43
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
1:1:104:ILE:HG12	1:1:104:ILE:H	1.62	0.43
2:2:13:VAL:C	2:2:14:GLN:HG2	2.39	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
2:2:143:LYS:HG2	2:2:143:LYS:H	1.56	0.43
1:1:221:MET:H	1:1:221:MET:HG2	1.66	0.43
1:1:214:GLY:O	1:1:217:VAL:CG1	2.67	0.43
2:2:91:VAL:HG12	2:2:95:ASN:ND2	2.34	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
1:1:286:ILE:HG21	1:1:286:ILE:HD13	1.77	0.43
3:3:47:ILE:HG21	3:3:47:ILE:HD13	1.51	0.43
3:3:151:VAL:HG11	3:3:161:ILE:HD11	2.01	0.43
2:2:70:THR:HG22	2:2:72:THR:HG22	2.01	0.43
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
1:1:190:TYR:CE1	1:1:192:GLY:HA3	2.54	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
2:2:228:LEU:HD11	2:2:238:LEU:HD22	2.02	0.42
1:1:136:GLN:HB2	1:1:136:GLN:HE21	1.13	0.42
2:2:225:ILE:O	3:3:68:LEU:HD21	2.20	0.42
1:1:110:VAL:HG13	3:3:230:GLN:CD	2.39	0.42
1:1:118:LEU:HA	1:1:118:LEU:HD12	1.91	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
1:1:146:LEU:HD13	1:1:228:ILE:CD1	2.50	0.42
4:4:30:ASN:HA	4:4:30:ASN:HD22	1.40	0.42
1:1:286:ILE:HG23	3:3:81:PHE:HA	2.00	0.42
1:1:285:ASP:HB3	1:1:288:SER:N	2.34	0.41
3:3:44:LEU:HD23	3:3:44:LEU:HA	1.79	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:3:18:ASP:CG	4:4:40:SER:HB2	2.41	0.41
2:2:235:THR:HG22	2:2:237:SER:N	2.35	0.41
1:1:86:ASP:OD1	1:1:88:THR:HB	2.20	0.41
1:1:97:LYS:C	1:1:99:PHE:N	2.71	0.41
3:3:112:ARG:HG2	3:3:112:ARG:HH11	1.83	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
1:1:103:LYS:O	1:1:104:ILE:C	2.58	0.41
1:1:87:ALA:HB2	1:1:98:LEU:HD11	2.02	0.41
1:1:38:GLU:CD	3:3:116:MET:CE	2.88	0.41
3:3:195:LEU:C	3:3:196:ILE:HG12	2.40	0.41
2:2:84:ASP:HB2	2:2:216:ASN:HD21	1.86	0.41
2:2:43:PRO:HG2	2:2:46:ASP:HB2	2.03	0.41
2:2:122:LEU:HD23	2:2:224:PRO:HA	2.02	0.41
2:2:255:ARG:CG	2:2:256:SER:H	1.99	0.41
1:1:289:TYR:CZ	3:3:139:PRO:HD2	2.55	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
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
3:3:20:GLN:NE2	4:4:30:ASN:HA	2.36	0.40
1:1:38:GLU:N	3:3:116:MET:HE3	2.37	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
3:3:57:ASN:HD21	3:3:91:VAL:HG13	1.84	0.40
4:4:43:GLN:O	4:4:44:SER:C	2.58	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
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

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%)	243 (90%)	22 (8%)	6 (2%)	10	45
2	2	253/262 (97%)	233 (92%)	18 (7%)	2 (1%)	27	76
3	3	234/236 (99%)	217 (93%)	15 (6%)	2 (1%)	25	73
4	4	38/68 (56%)	34 (90%)	3 (8%)	1 (3%)	8	39
All	All	796/855 (93%)	727 (91%)	58 (7%)	11 (1%)	16	60

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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%)	191 (80%)	48 (20%)	2	10
2	2	223/229 (97%)	180 (81%)	43 (19%)	2	12
3	3	209/209 (100%)	170 (81%)	39 (19%)	2	12
4	4	33/57 (58%)	20 (61%)	13 (39%)	0	0
All	All	704/748 (94%)	561 (80%)	143 (20%)	2	9

All (143) 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	103	LYS
1	1	104	ILE
1	1	105	ASN
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	188	VAL
1	1	191	VAL
1	1	215	ILE
1	1	220	HIS
1	1	221	MET
1	1	224	MET
1	1	240	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1	256	ARG
1	1	268	ARG
1	1	274	ASN
1	1	278	VAL
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	2	247	MET
2	2	250	GLU
2	2	254	ILE
2	2	255	ARG
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	3	226	GLN
3	3	228	ILE
3	3	230	GLN
4	4	29	ILE
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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
3	3	84	ASN
3	3	102	GLN
3	3	140	GLN
3	3	192	GLN
3	3	226	GLN
4	4	30	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	W54	1	500	-	27,27,27	2.80	4 (14%)	36,36,36	2.73	8 (22%)

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	W54	1	500	-	-	0/12/20/20	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	500	W54	C2A-N3A	11.61	1.43	1.27
5	1	500	W54	C4A-N3A	-6.45	1.36	1.47
5	1	500	W54	O1A-C2A	-4.09	1.29	1.36
5	1	500	W54	O1A-C5A	-2.81	1.38	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	500	W54	O1A-C2A-N3A	-8.72	110.09	118.38
5	1	500	W54	O1A-C2A-C4B	7.79	123.74	115.61
5	1	500	W54	C4A-N3A-C2A	6.07	112.70	106.68
5	1	500	W54	O1B-C1B-C6B	-5.83	115.00	121.08
5	1	500	W54	O1B-C1B-C2B	4.02	125.27	121.08
5	1	500	W54	C1C-C5-C4	2.97	134.97	128.51
5	1	500	W54	O1A-C5A-C4A	2.91	111.71	104.35
5	1	500	W54	C5C-O1B-C1B	2.17	120.53	114.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section 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.