Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:52 PM GMT

PDB ID	:	1MEC
Title	:	CONFORMATIONAL VARIABILITY OF A PICORNAVIRUS CAPSID: PH-DEPENDENT STRUCTURAL CHANGES OF MENGO VIRUS RELATED TO ITS HOST RECEPTOR ATTACHMENT SITE AND DISASSEMBLY
Authors	:	Rossmann, M.G.
Deposited on	:	1992-01-17
Resolution	:	3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

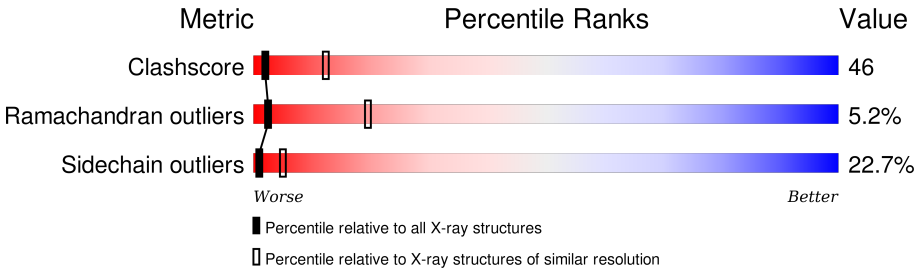
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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 >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	274	37% 40% 16% 7%
2	2	256	39% 39% 14% 8%
3	3	231	53% 31% 14% .
4	4	70	29% 17% 24% 19% 11%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	2	825	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6710 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 MENGO VIRUS COAT PROTEIN (SUBUNIT VP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	274	Total	C	N	O	S	0	0	0
			2139	1375	354	403	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	45	ARG	ALA	CONFLICT	UNP P12296

- Molecule 2 is a protein called MENGO VIRUS COAT PROTEIN (SUBUNIT VP2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	256	Total	C	N	O	S	0	0	0
			2031	1279	358	388	6			

- Molecule 3 is a protein called MENGO VIRUS COAT PROTEIN (SUBUNIT VP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	231	Total	C	N	O	S	0	0	0
			1773	1153	283	326	11			

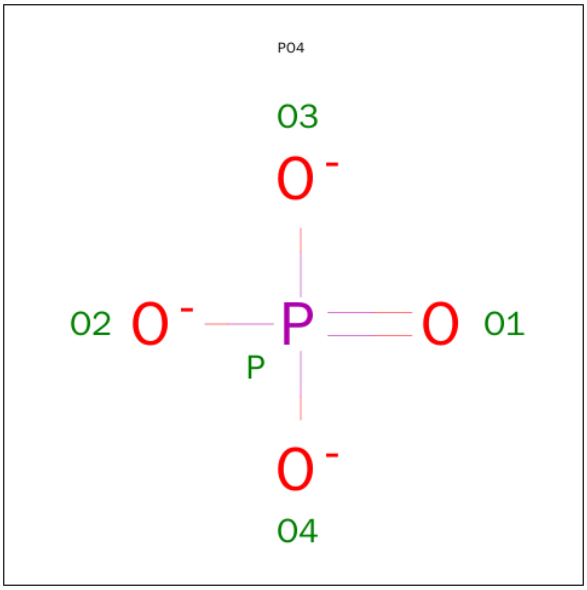
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	58	MET	VAL	CONFLICT	UNP P12296

- Molecule 4 is a protein called MENGO VIRUS COAT PROTEIN (SUBUNIT VP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	62	Total	C	N	O	S	0	0	0
			461	284	77	99	1			

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	2	1	Total O P 5 4 1	0	0
5	2	1	Total O P 5 4 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	1	114	Total O 114 114	0	0
6	2	122	Total O 122 122	0	0
6	3	50	Total O 50 50	0	0
6	4	10	Total O 10 10	0	0

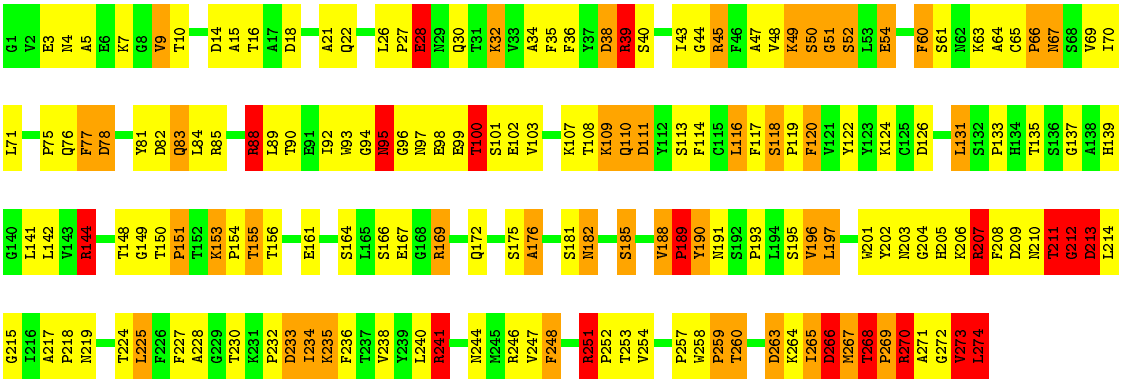
3 Residue-property plots (i)

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

Note EDS was not executed.

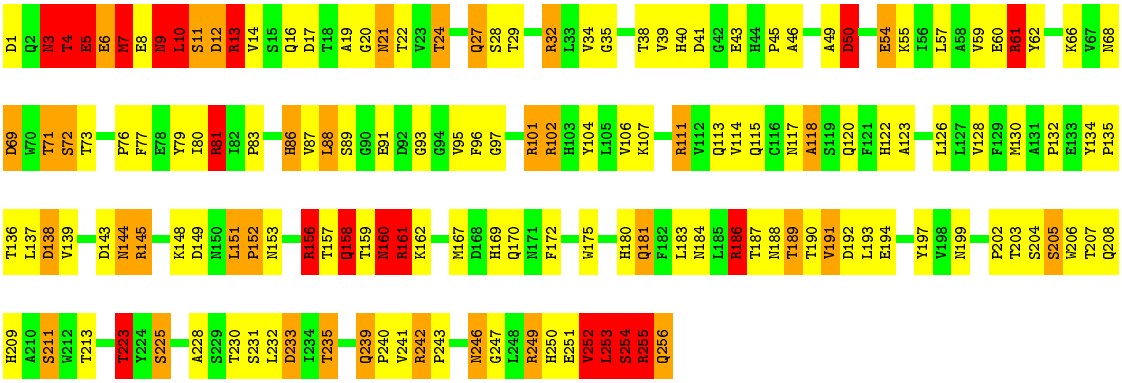
• Molecule 1: MENGO VIRUS COAT PROTEIN (SUBUNIT VP1)

Chain 1:



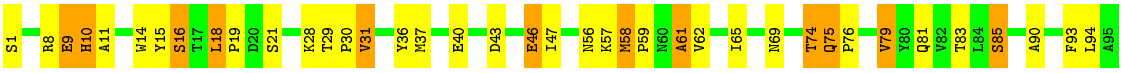
• Molecule 2: MENGO VIRUS COAT PROTEIN (SUBUNIT VP2)

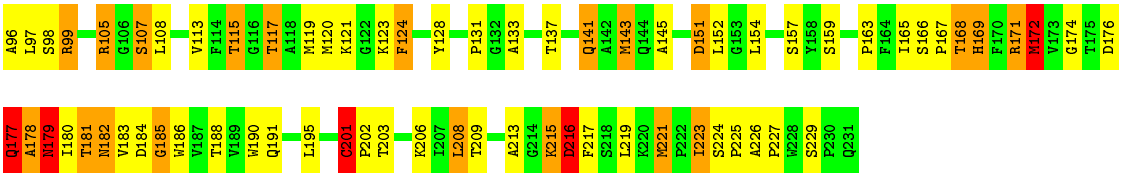
Chain 2:



• Molecule 3: MENGO VIRUS COAT PROTEIN (SUBUNIT VP1)

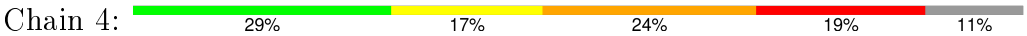
Chain 3:

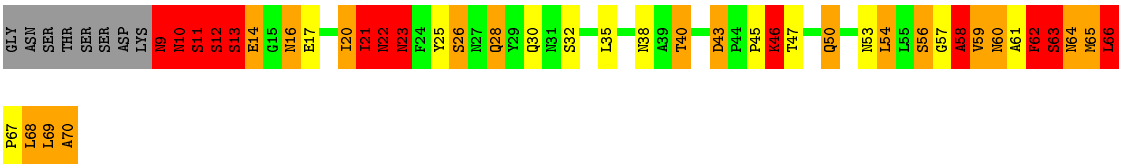




- Molecule 4: MENGO VIRUS COAT PROTEIN (SUBUNIT VP1)

Chain 4:





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	439.80Å 426.90Å 421.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.20)	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	6710	wwPDB-VP
Average B, all atoms (Å^2)	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: PO4

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	1.19	12/2208 (0.5%)	2.03	78/3018 (2.6%)
2	2	1.27	21/2086 (1.0%)	2.07	80/2854 (2.8%)
3	3	1.01	2/1830 (0.1%)	1.72	33/2512 (1.3%)
4	4	1.55	1/469 (0.2%)	3.92	27/638 (4.2%)
All	All	1.20	36/6593 (0.5%)	2.16	218/9022 (2.4%)

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	1
2	2	0	3
4	4	0	3
All	All	0	7

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	58	ALA	C-N	23.31	1.87	1.34
2	2	12	ASP	C-N	-16.79	0.95	1.34
1	1	274	LEU	N-CA	13.47	1.73	1.46
3	3	186	TRP	CA-CB	-12.89	1.25	1.53
2	2	6	GLU	CG-CD	12.03	1.70	1.51
1	1	268	THR	N-CA	9.64	1.65	1.46
1	1	273	VAL	CA-CB	9.56	1.74	1.54
1	1	270	ARG	CA-CB	-9.08	1.33	1.53
2	2	6	GLU	CB-CG	8.69	1.68	1.52
2	2	4	THR	C-N	8.28	1.53	1.34
1	1	273	VAL	N-CA	-7.85	1.30	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	255	ARG	C-N	-7.62	1.16	1.34
2	2	3	ASN	CA-C	7.62	1.72	1.52
1	1	274	LEU	CA-C	7.57	1.72	1.52
1	1	266	ASP	C-N	7.26	1.50	1.34
2	2	256	GLN	N-CA	-7.04	1.32	1.46
2	2	6	GLU	CA-CB	7.02	1.69	1.53
2	2	152	PRO	N-CD	6.94	1.57	1.47
2	2	5	GLU	N-CA	6.86	1.60	1.46
2	2	6	GLU	CD-OE1	6.31	1.32	1.25
2	2	6	GLU	CD-OE2	6.21	1.32	1.25
3	3	1	SER	CA-CB	-6.07	1.43	1.52
2	2	9	ASN	CA-CB	5.61	1.67	1.53
2	2	151	LEU	CA-C	-5.49	1.38	1.52
2	2	256	GLN	C-O	5.41	1.33	1.23
1	1	267	MET	CA-C	5.39	1.67	1.52
1	1	270	ARG	N-CA	5.36	1.57	1.46
2	2	255	ARG	NE-CZ	5.36	1.40	1.33
1	1	269	PRO	CA-C	5.24	1.63	1.52
2	2	160	ASN	N-CA	5.22	1.56	1.46
1	1	207	ARG	CG-CD	5.19	1.65	1.51
2	2	253	LEU	N-CA	-5.18	1.35	1.46
2	2	242	ARG	N-CA	5.11	1.56	1.46
2	2	252	VAL	C-N	-5.07	1.22	1.34
1	1	274	LEU	C-O	-5.06	1.13	1.23
2	2	5	GLU	C-O	-5.03	1.13	1.23

All (218) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	4	58	ALA	O-C-N	-56.32	32.59	122.70
4	4	9	ASN	O-C-N	-52.42	38.82	122.70
4	4	12	SER	O-C-N	24.06	161.20	122.70
1	1	241	ARG	NE-CZ-NH1	19.69	130.15	120.30
4	4	9	ASN	CA-C-N	18.36	157.58	117.20
2	2	152	PRO	CA-N-CD	-18.06	86.21	111.50
4	4	12	SER	CA-C-N	-16.76	80.33	117.20
2	2	12	ASP	C-N-CA	16.33	162.53	121.70
1	1	39	ARG	NE-CZ-NH2	16.26	128.43	120.30
3	3	178	ALA	CB-CA-C	15.68	133.61	110.10
1	1	265	ILE	O-C-N	15.10	146.87	122.70
2	2	12	ASP	O-C-N	-14.42	99.63	122.70
3	3	178	ALA	N-CA-CB	-13.60	91.06	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	5	GLU	CB-CA-C	-13.50	83.40	110.40
1	1	39	ARG	NE-CZ-NH1	-12.79	113.91	120.30
1	1	273	VAL	O-C-N	-12.74	102.31	122.70
1	1	45	ARG	NE-CZ-NH2	12.33	126.46	120.30
3	3	105	ARG	NE-CZ-NH2	12.07	126.33	120.30
2	2	255	ARG	NE-CZ-NH1	12.01	126.31	120.30
1	1	111	ASP	CB-CG-OD2	12.00	129.10	118.30
2	2	252	VAL	O-C-N	11.91	141.76	122.70
1	1	266	ASP	CB-CA-C	-11.56	87.28	110.40
2	2	6	GLU	N-CA-CB	11.52	131.33	110.60
1	1	273	VAL	CB-CA-C	11.21	132.70	111.40
1	1	273	VAL	CA-CB-CG2	11.16	127.64	110.90
2	2	17	ASP	CB-CG-OD2	11.14	128.32	118.30
1	1	265	ILE	CA-C-N	-10.96	93.08	117.20
1	1	270	ARG	NE-CZ-NH2	10.72	125.66	120.30
2	2	102	ARG	NE-CZ-NH2	-10.59	115.01	120.30
4	4	9	ASN	C-N-CA	-10.58	95.25	121.70
2	2	145	ARG	NE-CZ-NH1	10.22	125.41	120.30
2	2	152	PRO	N-CA-CB	10.11	115.43	103.30
2	2	4	THR	N-CA-CB	-10.08	91.14	110.30
2	2	156	ARG	NE-CZ-NH2	10.06	125.33	120.30
3	3	216	ASP	CB-CG-OD2	10.05	127.34	118.30
1	1	269	PRO	O-C-N	10.01	138.71	122.70
2	2	145	ARG	CD-NE-CZ	10.01	137.61	123.60
2	2	32	ARG	NE-CZ-NH2	9.97	125.28	120.30
2	2	101	ARG	NE-CZ-NH1	-9.77	115.41	120.30
1	1	241	ARG	NH1-CZ-NH2	-9.71	108.72	119.40
2	2	151	LEU	CB-CA-C	-9.70	91.77	110.20
2	2	6	GLU	C-N-CA	9.68	145.90	121.70
1	1	270	ARG	O-C-N	9.52	137.94	122.70
2	2	3	ASN	O-C-N	9.39	137.72	122.70
1	1	111	ASP	CB-CG-OD1	-9.37	109.87	118.30
3	3	179	ASN	CB-CA-C	9.37	129.14	110.40
1	1	66	PRO	C-N-CA	9.34	145.04	121.70
1	1	270	ARG	CA-CB-CG	-9.34	92.86	113.40
2	2	12	ASP	CA-C-N	9.20	137.43	117.20
1	1	269	PRO	C-N-CA	9.04	144.29	121.70
2	2	61	ARG	NE-CZ-NH1	8.99	124.79	120.30
2	2	252	VAL	CA-C-N	-8.97	97.47	117.20
4	4	43	ASP	CB-CG-OD1	-8.72	110.45	118.30
1	1	144	ARG	NE-CZ-NH2	8.69	124.65	120.30
1	1	265	ILE	C-N-CA	8.58	143.16	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	273	VAL	CA-C-N	8.49	135.87	117.20
2	2	8	GLU	C-N-CA	8.48	142.90	121.70
2	2	252	VAL	CB-CA-C	-8.45	95.34	111.40
4	4	12	SER	C-N-CA	8.42	142.75	121.70
3	3	186	TRP	CB-CA-C	-8.39	93.62	110.40
4	4	11	SER	C-N-CA	-8.36	100.81	121.70
1	1	38	ASP	CB-CG-OD1	-8.34	110.79	118.30
2	2	6	GLU	OE1-CD-OE2	-8.19	113.47	123.30
1	1	49	LYS	O-C-N	-8.00	109.89	122.70
2	2	4	THR	N-CA-C	7.94	132.43	111.00
2	2	50	ASP	N-CA-CB	-7.92	96.34	110.60
3	3	151	ASP	CB-CG-OD1	-7.92	111.17	118.30
1	1	273	VAL	C-N-CA	-7.87	102.02	121.70
1	1	28	GLU	CG-CD-OE2	7.81	133.93	118.30
2	2	9	ASN	N-CA-CB	-7.73	96.69	110.60
2	2	186	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	1	270	ARG	N-CA-C	7.69	131.75	111.00
1	1	169	ARG	NE-CZ-NH1	-7.59	116.51	120.30
2	2	10	LEU	O-C-N	7.53	134.74	122.70
3	3	215	LYS	C-N-CA	7.53	140.52	121.70
2	2	197	TYR	CB-CG-CD2	7.45	125.47	121.00
2	2	102	ARG	CD-NE-CZ	-7.41	113.23	123.60
4	4	12	SER	N-CA-CB	7.38	121.57	110.50
1	1	95	ASN	CA-CB-CG	-7.33	97.28	113.40
2	2	49	ALA	C-N-CA	7.30	139.94	121.70
1	1	266	ASP	N-CA-C	7.28	130.66	111.00
1	1	234	ILE	CB-CA-C	7.26	126.12	111.60
1	1	270	ARG	CA-C-N	-7.22	101.31	117.20
2	2	161	ARG	NE-CZ-NH2	7.17	123.89	120.30
2	2	81	ARG	NE-CZ-NH2	7.16	123.88	120.30
1	1	51	GLY	O-C-N	7.14	134.13	122.70
3	3	40	GLU	CA-CB-CG	7.11	129.03	113.40
4	4	12	SER	N-CA-C	7.07	130.09	111.00
2	2	246	ASN	CA-CB-CG	7.01	128.82	113.40
4	4	65	MET	O-C-N	7.00	133.89	122.70
3	3	105	ARG	CD-NE-CZ	6.90	133.26	123.60
4	4	58	ALA	CA-C-N	-6.88	102.07	117.20
1	1	266	ASP	O-C-N	6.84	133.65	122.70
2	2	152	PRO	N-CD-CG	6.78	113.37	103.20
3	3	59	PRO	CB-CA-C	-6.73	95.18	112.00
1	1	267	MET	CG-SD-CE	6.72	110.95	100.20
2	2	181	GLN	CA-CB-CG	6.72	128.18	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	8	GLU	CA-CB-CG	6.71	128.16	113.40
2	2	255	ARG	CD-NE-CZ	6.69	132.97	123.60
1	1	274	LEU	N-CA-C	6.67	129.01	111.00
3	3	105	ARG	NH1-CZ-NH2	-6.67	112.07	119.40
1	1	212	GLY	O-C-N	6.62	133.30	122.70
2	2	35	GLY	CA-C-N	6.58	131.67	117.20
1	1	211	THR	O-C-N	6.57	134.38	123.20
2	2	6	GLU	O-C-N	6.49	133.09	122.70
4	4	65	MET	CG-SD-CE	6.48	110.56	100.20
4	4	70	ALA	CB-CA-C	-6.45	100.43	110.10
3	3	171	ARG	NE-CZ-NH2	6.39	123.50	120.30
4	4	53	ASN	CB-CG-OD1	6.38	134.37	121.60
1	1	273	VAL	CG1-CB-CG2	-6.38	100.69	110.90
1	1	144	ARG	NH1-CZ-NH2	-6.36	112.40	119.40
2	2	255	ARG	O-C-N	6.35	132.86	122.70
1	1	260	THR	O-C-N	6.33	132.84	122.70
2	2	255	ARG	NH1-CZ-NH2	-6.32	112.45	119.40
2	2	111	ARG	NE-CZ-NH2	-6.32	117.14	120.30
2	2	35	GLY	N-CA-C	6.31	128.88	113.10
2	2	6	GLU	CB-CG-CD	6.29	131.19	114.20
2	2	54	GLU	OE1-CD-OE2	6.29	130.85	123.30
2	2	242	ARG	NE-CZ-NH2	6.29	123.44	120.30
1	1	116	LEU	CA-CB-CG	6.28	129.74	115.30
1	1	269	PRO	CA-C-N	-6.27	103.41	117.20
2	2	13	ARG	NE-CZ-NH1	6.22	123.41	120.30
2	2	233	ASP	CB-CG-OD1	-6.21	112.71	118.30
3	3	58	MET	CG-SD-CE	6.21	110.13	100.20
1	1	88	ARG	NE-CZ-NH2	6.16	123.38	120.30
3	3	168	THR	CA-CB-CG2	6.13	120.98	112.40
1	1	201	TRP	CA-CB-CG	6.12	125.33	113.70
2	2	21	ASN	C-N-CA	6.12	136.99	121.70
1	1	54	GLU	CG-CD-OE2	6.11	130.52	118.30
2	2	113	GLN	N-CA-CB	6.11	121.59	110.60
3	3	219	LEU	CA-CB-CG	6.08	129.29	115.30
3	3	177	GLN	N-CA-C	-6.06	94.63	111.00
2	2	5	GLU	N-CA-C	6.05	127.34	111.00
2	2	10	LEU	C-N-CA	6.02	136.76	121.70
1	1	190	TYR	N-CA-C	-6.00	94.81	111.00
3	3	172	MET	CG-SD-CE	6.00	109.79	100.20
2	2	3	ASN	C-N-CA	5.98	136.65	121.70
2	2	254	SER	O-C-N	-5.98	113.13	122.70
1	1	225	LEU	CA-CB-CG	5.97	129.03	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	60	PHE	N-CA-CB	-5.97	99.86	110.60
1	1	270	ARG	NH1-CZ-NH2	-5.95	112.85	119.40
2	2	10	LEU	CA-C-N	-5.93	104.15	117.20
3	3	179	ASN	CA-CB-CG	5.93	126.45	113.40
1	1	251	ARG	NE-CZ-NH2	5.93	123.26	120.30
3	3	190	TRP	CA-CB-CG	5.93	124.96	113.70
2	2	151	LEU	O-C-N	-5.91	109.87	121.10
1	1	85	ARG	N-CA-CB	-5.91	99.97	110.60
3	3	179	ASN	N-CA-CB	-5.87	100.03	110.60
2	2	151	LEU	C-N-CA	5.84	146.55	122.00
1	1	137	GLY	N-CA-C	-5.80	98.59	113.10
1	1	118	SER	N-CA-CB	5.79	119.19	110.50
1	1	45	ARG	NH1-CZ-NH2	-5.78	113.04	119.40
1	1	267	MET	CA-C-N	5.77	129.90	117.20
1	1	189	PRO	C-N-CA	5.77	136.13	121.70
2	2	156	ARG	CB-CA-C	5.75	121.90	110.40
2	2	61	ARG	CD-NE-CZ	5.67	131.54	123.60
4	4	12	SER	CB-CA-C	-5.67	99.33	110.10
3	3	177	GLN	CB-CA-C	5.63	121.67	110.40
2	2	117	ASN	CB-CA-C	-5.63	99.14	110.40
2	2	149	ASP	CB-CA-C	-5.63	99.14	110.40
1	1	109	LYS	CA-CB-CG	5.62	125.77	113.40
2	2	253	LEU	N-CA-C	-5.61	95.85	111.00
3	3	216	ASP	CB-CG-OD1	-5.60	113.26	118.30
1	1	18	ASP	CB-CG-OD2	-5.59	113.27	118.30
2	2	3	ASN	CA-C-N	-5.58	104.91	117.20
1	1	52	SER	N-CA-CB	-5.57	102.14	110.50
3	3	185	GLY	O-C-N	5.55	131.58	122.70
3	3	69	ASN	N-CA-CB	5.53	120.55	110.60
2	2	252	VAL	C-N-CA	5.52	135.49	121.70
3	3	74	THR	CA-CB-OG1	-5.51	97.44	109.00
1	1	28	GLU	CG-CD-OE1	-5.49	107.32	118.30
2	2	54	GLU	CG-CD-OE1	-5.47	107.35	118.30
3	3	182	ASN	CB-CA-C	-5.47	99.45	110.40
1	1	85	ARG	CA-CB-CG	5.46	125.42	113.40
4	4	21	ILE	CB-CA-C	-5.45	100.70	111.60
2	2	32	ARG	NE-CZ-NH1	-5.43	117.58	120.30
4	4	53	ASN	N-CA-C	-5.43	96.33	111.00
4	4	22	ASN	CB-CA-C	-5.43	99.54	110.40
1	1	155	THR	CA-CB-OG1	-5.42	97.61	109.00
2	2	3	ASN	N-CA-C	5.42	125.64	111.00
4	4	65	MET	CA-C-N	-5.42	105.27	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	212	GLY	CA-C-N	-5.41	105.29	117.20
3	3	15	TYR	CB-CG-CD2	5.41	124.25	121.00
1	1	211	THR	CA-C-N	-5.39	105.42	116.20
2	2	7	MET	CA-CB-CG	-5.39	104.14	113.30
1	1	155	THR	N-CA-CB	-5.37	100.09	110.30
2	2	6	GLU	CB-CA-C	-5.37	99.66	110.40
4	4	26	SER	N-CA-CB	-5.34	102.49	110.50
1	1	118	SER	CA-CB-OG	5.33	125.58	111.20
2	2	126	LEU	CA-CB-CG	5.30	127.50	115.30
1	1	188	VAL	CB-CA-C	5.30	121.46	111.40
1	1	241	ARG	CA-CB-CG	5.30	125.05	113.40
2	2	223	THR	CA-CB-OG1	-5.28	97.91	109.00
2	2	102	ARG	NH1-CZ-NH2	5.28	125.21	119.40
2	2	3	ASN	CB-CA-C	-5.28	99.84	110.40
2	2	10	LEU	CB-CA-C	-5.26	100.21	110.20
1	1	197	LEU	CA-CB-CG	5.24	127.36	115.30
2	2	181	GLN	CB-CA-C	5.22	120.85	110.40
1	1	44	GLY	C-N-CA	5.21	134.73	121.70
3	3	201	CYS	N-CA-CB	-5.21	101.21	110.60
1	1	189	PRO	O-C-N	-5.20	114.38	122.70
3	3	169	HIS	N-CA-CB	5.18	119.93	110.60
2	2	34	VAL	N-CA-C	-5.18	97.02	111.00
1	1	267	MET	N-CA-C	-5.16	97.08	111.00
1	1	207	ARG	CB-CG-CD	5.15	125.00	111.60
3	3	171	ARG	NH1-CZ-NH2	-5.15	113.74	119.40
4	4	11	SER	N-CA-CB	5.15	118.22	110.50
1	1	9	VAL	O-C-N	5.10	130.87	122.70
4	4	28	GLN	CB-CA-C	5.10	120.61	110.40
1	1	267	MET	O-C-N	-5.10	114.54	122.70
2	2	6	GLU	CG-CD-OE1	5.07	128.45	118.30
4	4	46	LYS	CB-CA-C	-5.07	100.26	110.40
3	3	1	SER	O-C-N	-5.07	111.47	121.10
4	4	70	ALA	N-CA-C	5.04	124.62	111.00
1	1	263	ASP	N-CA-CB	-5.04	101.54	110.60
4	4	54	LEU	CB-CG-CD2	-5.02	102.46	111.00
1	1	38	ASP	CB-CG-OD2	5.01	122.81	118.30
3	3	219	LEU	CB-CA-C	5.00	119.71	110.20

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	273	VAL	Peptide
2	2	12	ASP	Mainchain,Peptide
2	2	5	GLU	Peptide
4	4	11	SER	Peptide
4	4	9	ASN	Mainchain,Peptide

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	2139	0	2064	242	0
2	2	2031	0	1945	195	0
3	3	1773	0	1760	107	0
4	4	461	0	425	94	0
5	2	10	0	0	6	0
6	1	114	0	0	12	0
6	2	122	0	0	13	0
6	3	50	0	0	8	0
6	4	10	0	0	2	0
All	All	6710	0	6194	577	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 46.

All (577) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:273:VAL:CB	1:1:273:VAL:CA	1.74	1.62
1:1:268:THR:HG21	1:1:274:LEU:CD1	1.34	1.53
1:1:45:ARG:CZ	1:1:235:LYS:HG3	1.39	1.51
2:2:5:GLU:HG2	2:2:10:LEU:CB	1.45	1.47
1:1:274:LEU:CA	1:1:274:LEU:N	1.73	1.45
1:1:268:THR:CG2	1:1:274:LEU:HD12	1.43	1.44
1:1:45:ARG:NH1	1:1:235:LYS:HD2	1.33	1.39
1:1:45:ARG:CZ	1:1:235:LYS:CG	2.00	1.35
1:1:45:ARG:CZ	1:1:235:LYS:HD2	1.57	1.35
1:1:45:ARG:CZ	1:1:235:LYS:CD	2.07	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:7:MET:CE	2:2:120:GLN:HE22	1.47	1.27
1:1:45:ARG:NH2	1:1:235:LYS:HG3	1.51	1.26
1:1:246:ARG:HA	4:4:11:SER:OG	1.38	1.20
1:1:246:ARG:HG2	4:4:11:SER:CB	1.72	1.19
2:2:161:ARG:HG3	2:2:161:ARG:HH11	1.00	1.15
4:4:60:ASN:ND2	4:4:61:ALA:H	1.42	1.14
1:1:45:ARG:NE	1:1:235:LYS:HG3	1.62	1.14
1:1:45:ARG:NH1	1:1:235:LYS:CD	2.12	1.12
1:1:246:ARG:HG2	4:4:11:SER:HB2	1.29	1.12
1:1:268:THR:CG2	1:1:274:LEU:HA	1.70	1.11
2:2:7:MET:HA	2:2:7:MET:CE	1.81	1.11
4:4:9:ASN:HD22	4:4:10:ASN:HB2	0.95	1.08
2:2:5:GLU:CG	2:2:10:LEU:CB	2.31	1.08
1:1:99:GLU:O	1:1:100:THR:HB	1.46	1.08
2:2:158:GLN:HE21	2:2:158:GLN:HA	1.17	1.08
2:2:10:LEU:CG	2:2:11:SER:H	1.58	1.08
1:1:45:ARG:NE	1:1:235:LYS:CG	2.17	1.07
2:2:7:MET:HA	2:2:7:MET:HE2	1.13	1.07
1:1:34:ALA:HB2	4:4:11:SER:O	1.54	1.06
2:2:7:MET:HE1	2:2:120:GLN:HE22	1.20	1.06
2:2:5:GLU:HG2	2:2:10:LEU:HB3	1.37	1.06
4:4:12:SER:OG	4:4:13:SER:N	1.83	1.04
1:1:265:ILE:HG13	1:1:266:ASP:HB2	1.38	1.04
2:2:7:MET:SD	2:2:120:GLN:NE2	2.31	1.04
2:2:10:LEU:CD1	2:2:11:SER:H	1.70	1.03
1:1:268:THR:HG23	1:1:268:THR:O	1.59	1.03
1:1:268:THR:HG21	1:1:274:LEU:HD13	1.41	1.02
1:1:218:PRO:HB3	3:3:179:ASN:HD22	1.21	1.02
4:4:69:LEU:O	4:4:70:ALA:CB	2.07	1.01
4:4:9:ASN:ND2	4:4:10:ASN:HB2	1.74	1.01
1:1:246:ARG:CG	4:4:11:SER:HB2	1.90	1.01
2:2:251:GLU:O	2:2:252:VAL:HG23	1.59	1.01
2:2:5:GLU:CG	2:2:10:LEU:HB2	1.89	1.00
2:2:7:MET:CE	2:2:120:GLN:NE2	2.22	1.00
1:1:36:PHE:O	1:1:39:ARG:HD2	1.62	1.00
3:3:31:VAL:HG12	6:3:425:HOH:O	1.61	1.00
1:1:273:VAL:CB	1:1:273:VAL:HA	1.86	1.00
2:2:5:GLU:CG	2:2:10:LEU:HB3	1.91	1.00
2:2:5:GLU:HG2	2:2:10:LEU:HB2	1.03	0.99
4:4:10:ASN:ND2	4:4:13:SER:HA	1.75	0.99
1:1:270:ARG:NH2	1:1:271:ALA:O	1.96	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:10:LEU:HD12	2:2:11:SER:N	1.80	0.97
1:1:268:THR:CG2	1:1:274:LEU:CD1	2.19	0.96
1:1:218:PRO:CB	3:3:179:ASN:ND2	2.29	0.95
1:1:265:ILE:HG13	1:1:266:ASP:CB	1.96	0.95
2:2:10:LEU:O	2:2:13:ARG:HB2	1.65	0.95
2:2:158:GLN:NE2	2:2:158:GLN:HA	1.78	0.95
2:2:181:GLN:HG2	2:2:191:VAL:HG22	1.48	0.94
4:4:60:ASN:ND2	4:4:61:ALA:N	2.14	0.94
3:3:18:LEU:HD22	3:3:19:PRO:HD2	1.48	0.94
1:1:246:ARG:CA	4:4:11:SER:OG	2.15	0.93
1:1:218:PRO:HB3	3:3:179:ASN:ND2	1.84	0.93
2:2:22:THR:HG21	2:2:62:TYR:H	1.32	0.93
2:2:3:ASN:C	2:2:4:THR:OG1	2.06	0.93
2:2:24:THR:HG21	6:2:841:HOH:O	1.70	0.92
4:4:50:GLN:HA	6:4:78:HOH:O	1.68	0.92
1:1:268:THR:CG2	1:1:268:THR:O	2.18	0.92
1:1:265:ILE:CG1	1:1:266:ASP:N	2.29	0.92
2:2:5:GLU:O	2:2:6:GLU:HG2	1.70	0.91
3:3:79:VAL:HB	3:3:188:THR:HG22	1.53	0.91
2:2:10:LEU:HD12	2:2:11:SER:H	1.34	0.91
2:2:50:ASP:OD2	2:2:246:ASN:HB2	1.70	0.91
4:4:60:ASN:CG	4:4:61:ALA:H	1.70	0.90
2:2:71:THR:HG23	2:2:73:THR:H	1.33	0.90
1:1:45:ARG:NH2	1:1:235:LYS:CG	2.22	0.89
1:1:218:PRO:CB	3:3:179:ASN:HD22	1.87	0.88
1:1:45:ARG:HH11	1:1:235:LYS:HD2	1.35	0.88
2:2:161:ARG:NH1	2:2:161:ARG:HG3	1.80	0.88
1:1:273:VAL:HB	1:1:273:VAL:CA	2.01	0.88
3:3:180:ILE:HB	6:3:393:HOH:O	1.74	0.88
1:1:273:VAL:C	1:1:274:LEU:CA	2.43	0.87
2:2:71:THR:CG2	2:2:73:THR:H	1.86	0.87
1:1:14:ASP:OD1	1:1:16:THR:HB	1.74	0.87
1:1:45:ARG:HH12	1:1:235:LYS:HZ2	1.22	0.86
2:2:71:THR:CG2	2:2:73:THR:HB	2.06	0.86
1:1:99:GLU:O	1:1:100:THR:CB	2.23	0.85
4:4:69:LEU:O	4:4:70:ALA:HB3	1.75	0.85
4:4:10:ASN:HD21	4:4:13:SER:HA	1.35	0.85
4:4:16:ASN:O	4:4:17:GLU:HG2	1.75	0.85
1:1:61:SER:OG	1:1:82:ASP:HB2	1.75	0.85
4:4:62:PHE:HD1	4:4:63:SER:N	1.75	0.84
2:2:10:LEU:CG	2:2:11:SER:N	2.39	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:63:SER:OG	4:4:64:ASN:N	2.07	0.84
1:1:203:ASN:O	2:2:209:HIS:HD2	1.59	0.84
2:2:83:PRO:O	2:2:87:VAL:HG23	1.77	0.83
1:1:273:VAL:O	1:1:274:LEU:CA	2.26	0.83
1:1:169:ARG:HD2	3:3:223:ILE:O	1.79	0.83
1:1:246:ARG:HG2	4:4:11:SER:OG	1.79	0.83
2:2:10:LEU:HG	2:2:11:SER:H	1.44	0.82
1:1:273:VAL:O	1:1:274:LEU:HD13	1.79	0.82
1:1:45:ARG:NE	1:1:235:LYS:CD	2.41	0.82
3:3:81:GLN:NE2	3:3:183:VAL:HG11	1.94	0.82
3:3:56:ASN:O	3:3:61:ALA:HA	1.77	0.82
1:1:265:ILE:HG13	1:1:266:ASP:N	1.95	0.82
1:1:268:THR:HG21	1:1:274:LEU:CA	2.09	0.81
4:4:45:PRO:HA	4:4:46:LYS:HE3	1.61	0.81
1:1:268:THR:HG21	1:1:274:LEU:HD12	0.82	0.81
3:3:181:THR:HA	6:3:432:HOH:O	1.81	0.81
4:4:62:PHE:C	4:4:62:PHE:CD1	2.53	0.81
2:2:161:ARG:CG	2:2:161:ARG:HH11	1.87	0.81
3:3:143:MET:HG2	3:3:143:MET:O	1.82	0.79
1:1:135:THR:HB	1:1:234:ILE:HG21	1.63	0.79
1:1:63:LYS:HD3	1:1:235:LYS:NZ	1.97	0.79
2:2:254:SER:HB3	3:3:133:ALA:HB1	1.65	0.79
1:1:45:ARG:NE	1:1:235:LYS:HD2	1.97	0.78
1:1:218:PRO:HB2	3:3:179:ASN:ND2	1.98	0.78
1:1:95:ASN:OD1	1:1:107:LYS:HE3	1.83	0.78
1:1:63:LYS:HD3	1:1:235:LYS:HZ1	1.48	0.78
1:1:93:TRP:HA	2:2:160:ASN:HD21	1.47	0.78
4:4:12:SER:OG	4:4:13:SER:HB2	1.84	0.78
1:1:93:TRP:HB2	1:1:108:THR:HG23	1.65	0.78
1:1:270:ARG:HE	1:1:270:ARG:HA	1.49	0.77
2:2:40:HIS:O	2:2:242:ARG:NH1	2.17	0.77
1:1:268:THR:N	1:1:269:PRO:HD3	1.99	0.77
2:2:81:ARG:HD3	2:2:143:ASP:OD2	1.84	0.77
1:1:185:SER:HB2	3:3:10:HIS:HB3	1.66	0.77
1:1:45:ARG:NH1	1:1:235:LYS:NZ	2.34	0.76
1:1:208:PHE:CE2	3:3:131:PRO:CB	2.68	0.76
2:2:72:SER:HB2	6:2:942:HOH:O	1.85	0.76
2:2:69:ASP:HA	2:2:233:ASP:HA	1.68	0.76
2:2:162:LYS:HA	5:2:825:PO4:O4	1.86	0.75
1:1:208:PHE:CD2	3:3:131:PRO:HB2	2.20	0.75
1:1:3:GLU:HG2	1:1:10:THR:HG23	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:61:SER:H	1:1:83:GLN:NE2	1.84	0.75
1:1:7:LYS:HE3	1:1:9:VAL:O	1.86	0.75
2:2:13:ARG:O	2:2:29:THR:HG22	1.87	0.75
1:1:4:ASN:HB2	6:2:857:HOH:O	1.87	0.75
1:1:144:ARG:NH1	1:1:167:GLU:O	2.19	0.75
1:1:208:PHE:CE2	3:3:131:PRO:HB2	2.21	0.74
1:1:70:ILE:H	1:1:76:GLN:HE22	1.32	0.74
4:4:46:LYS:HG2	4:4:47:THR:HG22	1.69	0.74
1:1:274:LEU:CB	1:1:274:LEU:N	2.50	0.74
3:3:182:ASN:HB3	3:3:183:VAL:HG23	1.70	0.74
1:1:117:PHE:CD1	1:1:253:THR:HG21	2.22	0.73
1:1:268:THR:N	1:1:269:PRO:CD	2.51	0.73
4:4:13:SER:O	4:4:14:GLU:HB3	1.89	0.73
4:4:62:PHE:CD1	4:4:63:SER:N	2.56	0.73
2:2:188:ASN:ND2	2:2:190:THR:O	2.22	0.73
4:4:61:ALA:O	4:4:62:PHE:HB3	1.90	0.72
6:1:307:HOH:O	3:3:180:ILE:HG21	1.89	0.72
1:1:45:ARG:HH21	1:1:235:LYS:HG3	1.53	0.72
4:4:12:SER:OG	4:4:13:SER:CA	2.38	0.72
1:1:30:GLN:HG2	1:1:35:PHE:CE2	2.25	0.71
1:1:148:THR:H	1:1:191:ASN:ND2	1.88	0.71
2:2:71:THR:HG22	2:2:73:THR:HB	1.72	0.71
1:1:266:ASP:CG	1:1:267:MET:H	1.66	0.71
2:2:111:ARG:HD2	2:2:194:GLU:OE1	1.90	0.71
1:1:268:THR:HG22	1:1:274:LEU:HD12	1.66	0.70
4:4:59:VAL:HG13	4:4:60:ASN:N	2.05	0.70
4:4:69:LEU:O	4:4:70:ALA:HB2	1.89	0.70
1:1:122:TYR:HB3	1:1:196:VAL:HG13	1.71	0.70
1:1:172:GLN:HG3	6:1:362:HOH:O	1.92	0.70
1:1:273:VAL:HB	1:1:273:VAL:HA	1.64	0.70
4:4:9:ASN:HD22	4:4:10:ASN:CB	1.90	0.70
1:1:191:ASN:HA	3:3:221:MET:HE1	1.73	0.69
2:2:158:GLN:CA	2:2:158:GLN:HE21	1.95	0.69
2:2:60:GLU:HG2	6:2:906:HOH:O	1.92	0.69
4:4:59:VAL:HG13	4:4:60:ASN:H	1.58	0.69
2:2:202:PRO:HG3	3:3:169:HIS:CE1	2.28	0.69
1:1:209:ASP:HB3	1:1:211:THR:OG1	1.94	0.68
4:4:45:PRO:CA	4:4:46:LYS:HE3	2.23	0.68
4:4:13:SER:O	4:4:14:GLU:CB	2.42	0.68
3:3:113:VAL:HB	3:3:208:LEU:HB2	1.76	0.67
2:2:249:ARG:HG3	2:2:250:HIS:N	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:256:GLN:C	6:2:903:HOH:O	2.33	0.67
1:1:273:VAL:O	1:1:274:LEU:HA	1.93	0.67
1:1:63:LYS:O	1:1:64:ALA:HB3	1.95	0.67
2:2:80:ILE:HG23	2:2:143:ASP:HB2	1.76	0.67
3:3:123:LYS:NZ	3:3:151:ASP:OD1	2.27	0.67
2:2:254:SER:O	2:2:255:ARG:NE	2.28	0.66
1:1:28:GLU:HG2	1:1:30:GLN:H	1.60	0.66
1:1:273:VAL:CG1	1:1:273:VAL:CA	2.72	0.66
2:2:5:GLU:HG3	2:2:10:LEU:HB3	1.73	0.66
3:3:81:GLN:HE21	3:3:183:VAL:HG11	1.60	0.66
2:2:71:THR:CG2	2:2:73:THR:CB	2.73	0.66
1:1:45:ARG:NH1	1:1:235:LYS:HZ2	1.89	0.66
1:1:268:THR:CG2	1:1:274:LEU:CA	2.60	0.66
1:1:38:ASP:HB3	4:4:16:ASN:HB2	1.78	0.66
3:3:65:ILE:HG23	3:3:209:THR:HG21	1.78	0.66
2:2:122:HIS:CE1	2:2:228:ALA:HB1	2.31	0.65
1:1:268:THR:CB	1:1:274:LEU:HD12	2.25	0.65
1:1:34:ALA:CB	4:4:11:SER:O	2.39	0.65
4:4:12:SER:OG	4:4:13:SER:CB	2.43	0.65
2:2:254:SER:HB3	3:3:133:ALA:CB	2.25	0.65
1:1:82:ASP:OD1	1:1:82:ASP:N	2.27	0.65
2:2:123:ALA:HB3	2:2:223:THR:HG22	1.79	0.65
1:1:246:ARG:CG	4:4:11:SER:CB	2.57	0.65
2:2:162:LYS:HA	5:2:825:PO4:P	2.37	0.65
4:4:46:LYS:N	4:4:46:LYS:CE	2.60	0.65
3:3:124:PHE:HE1	3:3:152:LEU:HD13	1.62	0.64
1:1:218:PRO:HB2	3:3:179:ASN:HD21	1.62	0.64
2:2:79:TYR:C	2:2:79:TYR:CD1	2.72	0.64
1:1:45:ARG:NH1	1:1:235:LYS:CE	2.61	0.63
4:4:60:ASN:CG	4:4:61:ALA:N	2.45	0.63
2:2:22:THR:HG21	2:2:62:TYR:N	2.08	0.63
3:3:99:ARG:HG3	3:3:225:PRO:HB3	1.80	0.63
2:2:199:ASN:ND2	2:2:204:SER:HB2	2.12	0.63
1:1:265:ILE:HG12	1:1:266:ASP:N	2.13	0.63
4:4:60:ASN:HD22	4:4:61:ALA:N	1.93	0.63
6:1:307:HOH:O	3:3:180:ILE:HG12	1.97	0.63
2:2:252:VAL:HB	2:2:253:LEU:O	1.98	0.63
4:4:66:LEU:C	4:4:68:LEU:N	2.50	0.63
4:4:23:ASN:ND2	4:4:30:GLN:HE22	1.96	0.63
2:2:13:ARG:C	2:2:29:THR:HG22	2.19	0.63
3:3:137:THR:OG1	3:3:141:GLN:NE2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:171:ARG:NH1	6:3:432:HOH:O	2.33	0.62
1:1:139:HIS:HE1	1:1:141:LEU:HD22	1.64	0.62
2:2:240:PRO:HB2	2:2:243:PRO:HG3	1.81	0.62
4:4:66:LEU:C	4:4:68:LEU:H	2.01	0.61
1:1:49:LYS:HG2	1:1:50:SER:N	2.15	0.61
1:1:95:ASN:HB3	1:1:102:GLU:O	2.00	0.61
1:1:142:LEU:HD11	6:1:362:HOH:O	1.98	0.61
3:3:117:THR:CG2	3:3:119:MET:HB2	2.31	0.61
4:4:61:ALA:O	4:4:62:PHE:CB	2.48	0.61
1:1:214:LEU:HD11	2:2:138:ASP:HA	1.83	0.61
1:1:45:ARG:HE	1:1:235:LYS:HG3	1.59	0.61
2:2:104:TYR:CZ	3:3:131:PRO:HG2	2.36	0.61
2:2:21:ASN:OD1	2:2:61:ARG:NH1	2.32	0.61
3:3:94:LEU:HD13	3:3:213:ALA:HB2	1.82	0.61
2:2:5:GLU:HB2	2:2:6:GLU:HA	1.83	0.61
1:1:51:GLY:HA2	6:1:334:HOH:O	1.99	0.61
2:2:13:ARG:HA	2:2:29:THR:HG22	1.82	0.60
1:1:172:GLN:O	3:3:16:SER:HB3	2.01	0.60
4:4:23:ASN:HD21	4:4:30:GLN:HE22	1.48	0.60
1:1:71:LEU:HD11	1:1:225:LEU:HD13	1.82	0.60
2:2:50:ASP:OD2	2:2:246:ASN:CB	2.47	0.60
2:2:22:THR:CG2	2:2:62:TYR:HB2	2.32	0.60
3:3:62:VAL:CG2	6:3:399:HOH:O	2.50	0.60
2:2:19:ALA:HB1	2:2:61:ARG:HA	1.83	0.60
4:4:45:PRO:C	4:4:46:LYS:HD2	2.21	0.60
3:3:18:LEU:HD22	3:3:19:PRO:CD	2.29	0.59
2:2:250:HIS:HE1	3:3:133:ALA:O	1.84	0.59
2:2:252:VAL:HB	2:2:253:LEU:C	2.16	0.59
4:4:45:PRO:O	4:4:47:THR:N	2.35	0.59
1:1:77:PHE:O	1:1:78:ASP:HB3	2.02	0.59
2:2:1:ASP:OD1	2:2:1:ASP:O	2.20	0.59
3:3:177:GLN:O	3:3:182:ASN:ND2	2.36	0.59
2:2:66:LYS:HE3	2:2:233:ASP:HB2	1.84	0.59
1:1:77:PHE:O	1:1:78:ASP:CB	2.50	0.59
1:1:98:GLU:HA	2:2:161:ARG:HH11	1.68	0.59
1:1:268:THR:HG21	1:1:273:VAL:O	2.04	0.58
3:3:154:LEU:O	3:3:154:LEU:HG	2.03	0.58
2:2:186:ARG:NH1	2:2:187:THR:OG1	2.36	0.58
1:1:96:GLY:HA3	1:1:101:SER:HB3	1.85	0.58
2:2:7:MET:CA	2:2:7:MET:CE	2.65	0.58
1:1:268:THR:CG2	1:1:273:VAL:O	2.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:246:ARG:HG3	4:4:11:SER:HB2	1.80	0.58
3:3:117:THR:CG2	3:3:119:MET:H	2.17	0.57
3:3:131:PRO:HD3	3:3:185:GLY:N	2.19	0.57
3:3:137:THR:H	3:3:141:GLN:NE2	2.02	0.57
3:3:18:LEU:CD2	3:3:19:PRO:HD2	2.31	0.57
4:4:46:LYS:N	4:4:46:LYS:CD	2.67	0.57
1:1:270:ARG:HA	1:1:270:ARG:NE	2.11	0.57
1:1:61:SER:HB3	1:1:82:ASP:O	2.04	0.57
2:2:241:VAL:HG12	2:2:242:ARG:NH1	2.20	0.57
2:2:38:THR:HG22	2:2:39:VAL:N	2.18	0.57
2:2:241:VAL:CG1	2:2:242:ARG:NH1	2.68	0.57
1:1:148:THR:H	1:1:191:ASN:HD21	1.51	0.57
2:2:152:PRO:HD2	2:2:153:ASN:H	1.70	0.57
4:4:38:ASN:ND2	4:4:40:THR:HB	2.19	0.57
2:2:7:MET:HE2	2:2:120:GLN:HE22	1.61	0.56
2:2:162:LYS:CA	5:2:825:PO4:O4	2.52	0.56
2:2:162:LYS:HA	5:2:825:PO4:O3	2.05	0.56
3:3:107:SER:H	3:3:216:ASP:HB3	1.68	0.56
1:1:45:ARG:CD	1:1:235:LYS:HD2	2.36	0.56
1:1:98:GLU:HA	2:2:161:ARG:HG3	1.87	0.56
3:3:117:THR:HG23	3:3:119:MET:H	1.70	0.56
2:2:205:SER:OG	2:2:208:GLN:OE1	2.23	0.56
1:1:266:ASP:CG	1:1:267:MET:N	2.39	0.56
2:2:181:GLN:CG	2:2:191:VAL:HG22	2.28	0.56
1:1:122:TYR:HB3	1:1:196:VAL:CG1	2.35	0.56
2:2:186:ARG:HG3	2:2:186:ARG:NH1	2.19	0.56
3:3:28:LYS:O	3:3:30:PRO:HD3	2.04	0.56
2:2:251:GLU:O	2:2:252:VAL:CG2	2.46	0.56
3:3:117:THR:HG22	3:3:120:MET:H	1.71	0.56
4:4:10:ASN:HD22	4:4:13:SER:HA	1.70	0.55
1:1:49:LYS:HG2	1:1:50:SER:H	1.69	0.55
4:4:21:ILE:HG22	4:4:21:ILE:O	2.06	0.55
1:1:131:LEU:HD12	1:1:238:VAL:HG22	1.87	0.55
3:3:81:GLN:NE2	3:3:183:VAL:CG1	2.68	0.55
2:2:180:HIS:C	2:2:180:HIS:CD2	2.79	0.55
2:2:71:THR:HG21	2:2:73:THR:HB	1.84	0.55
1:1:230:THR:O	1:1:232:PRO:HD3	2.06	0.55
1:1:94:GLY:O	1:1:96:GLY:N	2.40	0.55
4:4:59:VAL:HG22	4:4:60:ASN:H	1.72	0.55
2:2:106:VAL:HG12	2:2:206:TRP:HB3	1.89	0.55
2:2:199:ASN:HD22	2:2:204:SER:HB2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:154:PRO:O	1:1:164:SER:OG	2.20	0.55
1:1:191:ASN:HA	3:3:221:MET:CE	2.35	0.55
2:2:118:ALA:HB2	2:2:232:LEU:HD13	1.88	0.55
1:1:244:ASN:ND2	4:4:9:ASN:O	2.40	0.54
4:4:46:LYS:HD2	4:4:47:THR:H	1.70	0.54
2:2:241:VAL:CG1	2:2:242:ARG:HH12	2.19	0.54
1:1:111:ASP:HB3	1:1:114:PHE:HB3	1.90	0.54
1:1:98:GLU:O	1:1:101:SER:N	2.31	0.54
2:2:161:ARG:CG	2:2:161:ARG:NH1	2.52	0.54
1:1:268:THR:HG21	1:1:274:LEU:HA	1.41	0.54
2:2:252:VAL:O	2:2:253:LEU:HD23	2.08	0.54
4:4:60:ASN:O	4:4:61:ALA:HB3	2.07	0.54
4:4:57:GLY:O	4:4:58:ALA:C	2.46	0.54
1:1:3:GLU:CG	1:1:10:THR:HG23	2.37	0.53
1:1:142:LEU:CD1	6:1:362:HOH:O	2.54	0.53
4:4:38:ASN:HD21	4:4:40:THR:HB	1.74	0.53
3:3:94:LEU:CD1	3:3:213:ALA:HB2	2.38	0.53
1:1:45:ARG:HH12	1:1:235:LYS:NZ	1.92	0.53
4:4:46:LYS:CG	4:4:47:THR:HG22	2.39	0.53
2:2:10:LEU:HG	2:2:11:SER:N	2.13	0.53
2:2:186:ARG:HG3	2:2:186:ARG:HH11	1.73	0.52
1:1:258:TRP:O	1:1:259:PRO:C	2.48	0.52
1:1:45:ARG:NE	1:1:235:LYS:CB	2.71	0.52
2:2:22:THR:HG21	2:2:62:TYR:HB2	1.92	0.52
1:1:175:SER:O	1:1:176:ALA:HB2	2.09	0.52
1:1:32:LYS:HB3	4:4:12:SER:O	2.09	0.52
1:1:267:MET:C	1:1:269:PRO:HD3	2.30	0.52
3:3:81:GLN:HE21	3:3:183:VAL:CG1	2.23	0.52
2:2:186:ARG:CG	2:2:186:ARG:HH11	2.22	0.52
2:2:156:ARG:HG3	2:2:160:ASN:HB3	1.92	0.52
2:2:41:ASP:OD1	2:2:41:ASP:N	2.42	0.52
2:2:7:MET:HE1	2:2:120:GLN:NE2	2.04	0.52
2:2:88:LEU:O	2:2:93:GLY:HA3	2.10	0.52
1:1:93:TRP:HA	2:2:160:ASN:ND2	2.22	0.51
4:4:57:GLY:O	4:4:59:VAL:N	2.43	0.51
1:1:76:GLN:O	1:1:77:PHE:CB	2.57	0.51
1:1:202:TYR:HB3	1:1:215:GLY:O	2.10	0.51
3:3:107:SER:OG	3:3:216:ASP:HB2	2.09	0.51
2:2:132:PRO:HA	2:2:211:SER:O	2.10	0.51
1:1:205:HIS:HD2	1:1:210:ASN:OD1	1.93	0.51
1:1:150:THR:HB	3:3:223:ILE:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:263:ASP:OD1	1:1:263:ASP:O	2.28	0.51
1:1:181:SER:HB2	3:3:9:GLU:O	2.10	0.51
1:1:265:ILE:CG1	1:1:266:ASP:CB	2.81	0.51
1:1:212:GLY:O	1:1:213:ASP:HB2	2.09	0.51
1:1:209:ASP:CB	1:1:211:THR:OG1	2.58	0.51
1:1:273:VAL:CB	1:1:273:VAL:N	2.57	0.51
1:1:218:PRO:HG2	3:3:180:ILE:CG1	2.41	0.51
3:3:83:THR:HG23	3:3:83:THR:O	2.09	0.51
2:2:7:MET:HE2	2:2:120:GLN:NE2	2.22	0.50
2:2:181:GLN:NE2	6:2:884:HOH:O	2.44	0.50
3:3:75:GLN:HG3	3:3:76:PRO:O	2.11	0.50
2:2:158:GLN:CA	2:2:158:GLN:NE2	2.56	0.50
2:2:206:TRP:CE3	2:2:207:THR:HA	2.47	0.50
1:1:98:GLU:HA	2:2:161:ARG:NH1	2.25	0.50
2:2:128:VAL:HB	2:2:191:VAL:HG11	1.94	0.50
2:2:114:VAL:HG11	2:2:128:VAL:HG11	1.93	0.50
2:2:181:GLN:HE21	2:2:191:VAL:HA	1.76	0.50
3:3:14:TRP:CH2	3:3:16:SER:HB2	2.47	0.50
3:3:94:LEU:HD21	3:3:108:LEU:HD22	1.92	0.50
2:2:14:VAL:HG22	2:2:27:GLN:HG3	1.93	0.50
1:1:265:ILE:HG13	1:1:266:ASP:CA	2.41	0.50
2:2:203:THR:HG23	3:3:167:PRO:HA	1.93	0.50
4:4:16:ASN:C	4:4:17:GLU:HG2	2.31	0.50
4:4:46:LYS:HE3	4:4:46:LYS:N	2.26	0.50
4:4:22:ASN:O	4:4:23:ASN:C	2.50	0.50
2:2:13:ARG:CA	2:2:29:THR:HG22	2.41	0.49
1:1:273:VAL:O	1:1:274:LEU:CD1	2.56	0.49
6:1:307:HOH:O	3:3:180:ILE:CG1	2.59	0.49
4:4:38:ASN:ND2	4:4:40:THR:H	2.11	0.49
1:1:208:PHE:CE1	3:3:180:ILE:HA	2.48	0.49
2:2:71:THR:HG22	2:2:73:THR:H	1.71	0.49
1:1:207:ARG:HH21	1:1:211:THR:HB	1.77	0.49
2:2:135:PRO:HB2	6:2:914:HOH:O	2.12	0.49
1:1:96:GLY:HA3	1:1:101:SER:CB	2.43	0.49
1:1:38:ASP:OD1	1:1:241:ARG:HD2	2.13	0.49
1:1:108:THR:OG1	1:1:110:GLN:NE2	2.45	0.49
1:1:135:THR:HB	1:1:234:ILE:HD13	1.95	0.49
1:1:205:HIS:CE1	1:1:214:LEU:CD2	2.96	0.49
1:1:126:ASP:HA	1:1:189:PRO:O	2.13	0.49
1:1:76:GLN:O	1:1:77:PHE:HB2	2.13	0.48
1:1:117:PHE:CE1	1:1:253:THR:HG21	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:43:ILE:HG21	1:1:240:LEU:HG	1.95	0.48
2:2:152:PRO:HD2	2:2:153:ASN:N	2.28	0.48
1:1:274:LEU:HB2	1:1:274:LEU:N	2.28	0.48
4:4:9:ASN:C	4:4:9:ASN:HD22	2.13	0.48
2:2:156:ARG:CG	2:2:160:ASN:HB3	2.43	0.48
4:4:50:GLN:NE2	6:4:76:HOH:O	2.46	0.48
1:1:182:ASN:HB3	6:1:282:HOH:O	2.13	0.48
1:1:63:LYS:HD3	1:1:235:LYS:HZ3	1.78	0.48
4:4:9:ASN:ND2	4:4:10:ASN:CB	2.63	0.48
2:2:249:ARG:HG3	2:2:250:HIS:H	1.79	0.48
1:1:47:ALA:HB3	1:1:65:CYS:O	2.13	0.48
2:2:59:VAL:HG22	2:2:96:PHE:HA	1.95	0.48
3:3:105:ARG:O	3:3:217:PHE:HA	2.13	0.48
1:1:97:ASN:O	2:2:161:ARG:NH1	2.46	0.48
2:2:86:HIS:H	2:2:86:HIS:CD2	2.31	0.48
1:1:218:PRO:HG2	3:3:180:ILE:HG13	1.96	0.48
1:1:246:ARG:CG	4:4:11:SER:OG	2.58	0.47
2:2:144:ASN:HD22	2:2:144:ASN:HA	1.36	0.47
4:4:46:LYS:HD2	4:4:46:LYS:N	2.30	0.47
3:3:36:TYR:CE2	3:3:37:MET:HE2	2.50	0.47
1:1:273:VAL:C	1:1:274:LEU:CB	2.82	0.47
6:1:307:HOH:O	3:3:180:ILE:CG2	2.56	0.47
1:1:101:SER:O	2:2:162:LYS:NZ	2.47	0.47
1:1:257:PRO:HG2	1:1:270:ARG:HD2	1.95	0.47
1:1:150:THR:HB	1:1:151:PRO:HD2	1.96	0.47
1:1:43:ILE:HD11	1:1:69:VAL:HG21	1.96	0.47
1:1:182:ASN:HD22	1:1:182:ASN:HA	1.44	0.47
1:1:90:THR:O	2:2:167:MET:HG2	2.14	0.47
2:2:5:GLU:CB	2:2:10:LEU:HB2	2.44	0.47
2:2:249:ARG:HH11	2:2:249:ARG:CG	2.27	0.47
2:2:59:VAL:HG23	2:2:95:VAL:HG12	1.97	0.47
4:4:23:ASN:CG	4:4:30:GLN:HE22	2.18	0.47
2:2:83:PRO:HB3	2:2:136:THR:HG21	1.98	0.46
3:3:117:THR:O	3:3:120:MET:HB2	2.15	0.46
2:2:61:ARG:O	2:2:239:GLN:HB2	2.15	0.46
1:1:45:ARG:CD	1:1:235:LYS:CD	2.91	0.46
4:4:20:ILE:HA	4:4:20:ILE:HD12	1.59	0.46
1:1:45:ARG:HD3	1:1:65:CYS:SG	2.56	0.46
2:2:115:GLN:HB2	2:2:235:THR:HG23	1.97	0.46
1:1:95:ASN:HA	1:1:107:LYS:HG2	1.98	0.46
2:2:28:SER:OG	2:2:189:THR:HB	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:6:GLU:HB3	2:2:7:MET:H	1.12	0.46
1:1:92:ILE:HG23	1:1:110:GLN:NE2	2.31	0.46
1:1:131:LEU:O	1:1:133:PRO:HD3	2.15	0.46
1:1:120:PHE:CG	1:1:247:VAL:HB	2.51	0.46
2:2:101:ARG:NH1	2:2:251:GLU:OE2	2.49	0.46
1:1:141:LEU:HD12	1:1:228:ALA:O	2.16	0.46
4:4:38:ASN:HD22	4:4:40:THR:H	1.63	0.46
2:2:114:VAL:C	2:2:115:GLN:HG3	2.34	0.46
2:2:71:THR:CG2	2:2:73:THR:N	2.67	0.46
3:3:8:ARG:NH1	3:3:9:GLU:OE2	2.49	0.46
3:3:9:GLU:C	3:3:11:ALA:H	2.18	0.46
3:3:178:ALA:O	3:3:179:ASN:HB3	2.14	0.45
3:3:178:ALA:O	3:3:179:ASN:CB	2.64	0.45
1:1:205:HIS:CD2	1:1:210:ASN:HA	2.52	0.45
1:1:48:VAL:HG23	1:1:236:PHE:HE1	1.81	0.45
2:2:86:HIS:NE2	2:2:206:TRP:O	2.49	0.45
1:1:233:ASP:N	1:1:233:ASP:OD1	2.48	0.45
1:1:32:LYS:CB	4:4:12:SER:O	2.64	0.45
4:4:59:VAL:CG1	4:4:60:ASN:N	2.75	0.45
1:1:270:ARG:HE	1:1:271:ALA:N	2.14	0.45
2:2:22:THR:HG23	2:2:62:TYR:HB2	1.98	0.45
3:3:128:TYR:O	3:3:145:ALA:HB1	2.16	0.45
2:2:32:ARG:HD2	6:2:845:HOH:O	2.14	0.45
2:2:101:ARG:HB2	2:2:251:GLU:HG3	1.98	0.45
2:2:4:THR:C	2:2:5:GLU:HG3	2.36	0.45
1:1:15:ALA:O	1:1:21:ALA:HB3	2.17	0.45
4:4:9:ASN:C	4:4:9:ASN:ND2	2.67	0.45
2:2:97:GLY:O	2:2:101:ARG:HG3	2.16	0.45
1:1:26:LEU:HA	1:1:27:PRO:HD2	1.74	0.45
1:1:45:ARG:HD3	1:1:235:LYS:CD	2.47	0.45
3:3:117:THR:HG21	3:3:201:CYS:SG	2.57	0.45
1:1:189:PRO:HB2	1:1:190:TYR:H	1.63	0.45
3:3:36:TYR:CE2	3:3:37:MET:CE	3.00	0.45
1:1:241:ARG:HH12	4:4:16:ASN:HB3	1.82	0.45
2:2:79:TYR:CE2	2:2:151:LEU:HD11	2.52	0.45
1:1:251:ARG:HB2	1:1:252:PRO:HD2	1.98	0.45
2:2:249:ARG:CG	2:2:250:HIS:N	2.78	0.45
1:1:81:TYR:HB3	1:1:84:LEU:HD12	1.98	0.45
1:1:203:ASN:O	2:2:209:HIS:CD2	2.51	0.45
3:3:62:VAL:HG21	6:3:399:HOH:O	2.15	0.45
2:2:54:GLU:OE2	2:2:55:LYS:HE3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:45:ARG:NE	1:1:235:LYS:HB2	2.32	0.45
2:2:111:ARG:NH1	2:2:194:GLU:OE1	2.49	0.44
3:3:201:CYS:HA	3:3:202:PRO:HD3	1.86	0.44
3:3:115:THR:HB	3:3:206:LYS:O	2.17	0.44
2:2:134:TYR:OH	2:2:175:TRP:CZ2	2.69	0.44
2:2:157:THR:O	2:2:160:ASN:N	2.49	0.44
4:4:56:SER:C	4:4:58:ALA:H	2.20	0.44
2:2:104:TYR:CE1	3:3:131:PRO:HG2	2.52	0.44
2:2:254:SER:CB	3:3:133:ALA:CB	2.94	0.44
3:3:9:GLU:H	3:3:9:GLU:HG3	1.29	0.44
2:2:156:ARG:NH2	5:2:825:PO4:O4	2.45	0.44
1:1:148:THR:N	1:1:191:ASN:ND2	2.61	0.44
4:4:11:SER:O	4:4:12:SER:C	2.51	0.44
2:2:81:ARG:HH11	2:2:143:ASP:CG	2.20	0.44
4:4:47:THR:HG23	4:4:47:THR:O	2.18	0.44
2:2:162:LYS:C	5:2:825:PO4:O4	2.56	0.44
2:2:183:LEU:HD23	2:2:183:LEU:C	2.38	0.44
1:1:96:GLY:C	1:1:97:ASN:HD22	2.22	0.43
3:3:163:PRO:HG2	3:3:165:ILE:CD1	2.48	0.43
2:2:169:HIS:O	2:2:170:GLN:HG2	2.17	0.43
2:2:104:TYR:HB3	2:2:247:GLY:HA3	2.00	0.43
1:1:208:PHE:CE2	3:3:131:PRO:HB3	2.51	0.43
4:4:23:ASN:OD1	4:4:30:GLN:NE2	2.50	0.43
2:2:7:MET:O	2:2:7:MET:HG3	2.17	0.43
4:4:66:LEU:O	4:4:67:PRO:C	2.52	0.43
1:1:95:ASN:CB	1:1:102:GLU:O	2.65	0.43
1:1:69:VAL:HG12	1:1:227:PHE:CZ	2.54	0.43
2:2:10:LEU:O	2:2:13:ARG:CB	2.53	0.43
4:4:66:LEU:HA	4:4:66:LEU:HD13	1.78	0.43
1:1:208:PHE:N	1:1:208:PHE:CD1	2.84	0.43
3:3:163:PRO:HG2	3:3:165:ILE:HD11	2.01	0.43
2:2:40:HIS:NE2	2:2:107:LYS:NZ	2.45	0.43
3:3:120:MET:CE	3:3:195:LEU:HD21	2.48	0.43
1:1:224:THR:HG22	1:1:225:LEU:N	2.34	0.43
1:1:133:PRO:HA	1:1:236:PHE:HB3	2.00	0.43
3:3:226:ALA:HA	3:3:227:PRO:HD3	1.86	0.43
2:2:223:THR:HG21	6:2:869:HOH:O	2.17	0.43
3:3:83:THR:C	3:3:85:SER:H	2.21	0.43
2:2:46:ALA:O	3:3:105:ARG:NH2	2.51	0.43
4:4:45:PRO:C	4:4:46:LYS:HE3	2.39	0.43
1:1:119:PRO:HB3	1:1:253:THR:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:208:PHE:HE1	6:3:393:HOH:O	2.02	0.42
1:1:254:VAL:HG23	2:2:169:HIS:CE1	2.54	0.42
2:2:122:HIS:HE1	2:2:228:ALA:HB1	1.78	0.42
2:2:9:ASN:HB3	2:2:27:GLN:O	2.19	0.42
1:1:270:ARG:CA	1:1:270:ARG:NE	2.78	0.42
1:1:60:PHE:O	1:1:66:PRO:HA	2.20	0.42
2:2:81:ARG:HB3	2:2:213:THR:CG2	2.48	0.42
1:1:167:GLU:HG2	6:1:298:HOH:O	2.19	0.42
2:2:71:THR:HG23	2:2:73:THR:N	2.16	0.42
2:2:19:ALA:CB	2:2:61:ARG:HA	2.48	0.42
1:1:43:ILE:CG2	1:1:240:LEU:HG	2.49	0.42
1:1:268:THR:HG23	1:1:274:LEU:HA	1.82	0.42
2:2:45:PRO:HB3	2:2:203:THR:HB	2.01	0.42
3:3:85:SER:OG	3:3:174:GLY:HA2	2.20	0.42
2:2:5:GLU:O	2:2:6:GLU:CG	2.55	0.42
1:1:75:PRO:HA	1:1:110:GLN:HB3	2.01	0.42
2:2:101:ARG:NH2	6:2:843:HOH:O	2.52	0.42
2:2:181:GLN:NE2	2:2:192:ASP:H	2.18	0.42
1:1:61:SER:HA	1:1:66:PRO:HA	2.01	0.42
1:1:191:ASN:HB3	3:3:221:MET:HE2	2.02	0.42
1:1:204:GLY:O	1:1:214:LEU:HA	2.20	0.42
1:1:202:TYR:CG	1:1:217:ALA:HB2	2.54	0.42
1:1:263:ASP:O	1:1:264:LYS:HB3	2.19	0.42
2:2:157:THR:HG22	2:2:159:THR:H	1.85	0.42
2:2:104:TYR:HA	2:2:249:ARG:HH21	1.84	0.42
1:1:70:ILE:HD13	1:1:88:ARG:HG2	2.00	0.42
3:3:83:THR:C	3:3:85:SER:N	2.74	0.42
4:4:57:GLY:C	4:4:59:VAL:N	2.73	0.42
3:3:43:ASP:O	3:3:46:GLU:HB2	2.20	0.42
4:4:23:ASN:HD22	4:4:25:TYR:H	1.68	0.41
1:1:268:THR:HG23	1:1:273:VAL:O	2.20	0.41
1:1:218:PRO:O	1:1:219:ASN:HB2	2.20	0.41
3:3:124:PHE:HE1	3:3:152:LEU:CD1	2.30	0.41
4:4:56:SER:C	4:4:58:ALA:N	2.73	0.41
4:4:66:LEU:O	4:4:68:LEU:N	2.52	0.41
2:2:136:THR:CG2	2:2:213:THR:OG1	2.68	0.41
3:3:81:GLN:HE22	3:3:183:VAL:HG11	1.81	0.41
1:1:265:ILE:CG1	1:1:266:ASP:CA	2.98	0.41
2:2:13:ARG:HA	2:2:29:THR:CG2	2.48	0.41
3:3:168:THR:CG2	6:3:432:HOH:O	2.69	0.41
1:1:67:ASN:O	1:1:227:PHE:CD2	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:93:PHE:HA	3:3:96:ALA:HB3	2.01	0.41
1:1:149:GLY:HA3	3:3:172:MET:HE2	2.02	0.41
2:2:54:GLU:HG2	6:2:936:HOH:O	2.20	0.41
3:3:47:ILE:HD11	3:3:93:PHE:CZ	2.56	0.41
2:2:253:LEU:HA	2:2:253:LEU:HD22	1.90	0.41
3:3:107:SER:OG	3:3:216:ASP:CB	2.69	0.41
4:4:64:ASN:O	4:4:67:PRO:HD2	2.20	0.41
4:4:46:LYS:HD2	4:4:47:THR:N	2.35	0.41
1:1:268:THR:HG22	1:1:274:LEU:CD1	2.36	0.41
2:2:6:GLU:OE2	2:2:13:ARG:NH1	2.54	0.41
1:1:61:SER:H	1:1:83:GLN:HE22	1.67	0.41
1:1:172:GLN:HB2	6:1:362:HOH:O	2.21	0.41
3:3:117:THR:HG22	3:3:119:MET:N	2.36	0.41
3:3:94:LEU:O	3:3:98:SER:HB2	2.20	0.41
1:1:202:TYR:N	1:1:215:GLY:O	2.54	0.41
1:1:15:ALA:HA	6:1:284:HOH:O	2.20	0.41
1:1:251:ARG:NH2	6:2:831:HOH:O	2.54	0.41
2:2:102:ARG:HH11	2:2:102:ARG:HD2	1.47	0.41
1:1:208:PHE:CD2	3:3:131:PRO:CB	2.94	0.41
4:4:46:LYS:HB3	4:4:46:LYS:HE2	1.84	0.41
1:1:248:PHE:N	1:1:248:PHE:CD1	2.88	0.41
2:2:76:PRO:O	2:2:77:PHE:HB2	2.21	0.41
1:1:45:ARG:HD3	1:1:235:LYS:HD2	2.03	0.40
1:1:98:GLU:O	1:1:99:GLU:C	2.59	0.40
2:2:114:VAL:CG1	2:2:128:VAL:HG11	2.50	0.40
1:1:153:LYS:HE3	1:1:153:LYS:HB2	1.58	0.40
2:2:225:SER:HB2	6:2:871:HOH:O	2.21	0.40
2:2:71:THR:HG22	2:2:73:THR:N	2.36	0.40
2:2:66:LYS:HE3	2:2:233:ASP:CB	2.51	0.40
4:4:59:VAL:HG22	4:4:60:ASN:N	2.35	0.40
2:2:239:GLN:CG	2:2:239:GLN:O	2.65	0.40
1:1:193:PRO:HG3	3:3:172:MET:SD	2.62	0.40
2:2:101:ARG:HD2	2:2:101:ARG:HH11	1.50	0.40
3:3:29:THR:HA	3:3:30:PRO:HD2	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	272/274 (99%)	222 (82%)	37 (14%)	13 (5%)	3 22
2	2	254/256 (99%)	214 (84%)	27 (11%)	13 (5%)	2 20
3	3	229/231 (99%)	205 (90%)	21 (9%)	3 (1%)	15 59
4	4	60/70 (86%)	39 (65%)	8 (13%)	13 (22%)	0 0
All	All	815/831 (98%)	680 (83%)	93 (11%)	42 (5%)	2 19

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	77	PHE
1	1	95	ASN
1	1	176	ALA
1	1	189	PRO
1	1	213	ASP
1	1	266	ASP
2	2	5	GLU
2	2	11	SER
2	2	13	ARG
2	2	252	VAL
4	4	10	ASN
4	4	46	LYS
4	4	58	ALA
4	4	62	PHE
4	4	66	LEU
4	4	69	LEU
1	1	100	THR
1	1	212	GLY
2	2	7	MET
2	2	86	HIS
3	3	90	ALA
4	4	63	SER

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Mol	Chain	Res	Type
2	2	9	ASN
2	2	118	ALA
3	3	61	ALA
4	4	23	ASN
4	4	68	LEU
1	1	78	ASP
2	2	4	THR
2	2	158	GLN
2	2	160	ASN
4	4	59	VAL
2	2	20	GLY
3	3	223	ILE
4	4	13	SER
4	4	14	GLU
4	4	32	SER
1	1	5	ALA
2	2	172	PHE
1	1	151	PRO
1	1	259	PRO
1	1	272	GLY

5.3.2 Protein sidechains (i)

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	238/238 (100%)	189 (79%)	49 (21%)	1 7
2	2	224/224 (100%)	176 (79%)	48 (21%)	1 6
3	3	195/195 (100%)	155 (80%)	40 (20%)	1 7
4	4	52/59 (88%)	28 (54%)	24 (46%)	0 0
All	All	709/716 (99%)	548 (77%)	161 (23%)	1 5

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	22	GLN

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Mol	Chain	Res	Type
1	1	28	GLU
1	1	32	LYS
1	1	39	ARG
1	1	40	SER
1	1	50	SER
1	1	52	SER
1	1	54	GLU
1	1	67	ASN
1	1	83	GLN
1	1	88	ARG
1	1	89	LEU
1	1	100	THR
1	1	103	VAL
1	1	109	LYS
1	1	110	GLN
1	1	113	SER
1	1	116	LEU
1	1	118	SER
1	1	120	PHE
1	1	124	LYS
1	1	131	LEU
1	1	144	ARG
1	1	153	LYS
1	1	155	THR
1	1	156	THR
1	1	161	GLU
1	1	166	SER
1	1	182	ASN
1	1	185	SER
1	1	188	VAL
1	1	195	SER
1	1	196	VAL
1	1	197	LEU
1	1	206	LYS
1	1	207	ARG
1	1	211	THR
1	1	213	ASP
1	1	233	ASP
1	1	235	LYS
1	1	241	ARG
1	1	248	PHE
1	1	251	ARG

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Mol	Chain	Res	Type
1	1	260	THR
1	1	266	ASP
1	1	268	THR
1	1	270	ARG
1	1	273	VAL
1	1	274	LEU
2	2	3	ASN
2	2	4	THR
2	2	5	GLU
2	2	7	MET
2	2	10	LEU
2	2	16	GLN
2	2	24	THR
2	2	27	GLN
2	2	43	GLU
2	2	50	ASP
2	2	57	LEU
2	2	61	ARG
2	2	68	ASN
2	2	69	ASP
2	2	71	THR
2	2	72	SER
2	2	81	ARG
2	2	88	LEU
2	2	89	SER
2	2	91	GLU
2	2	130	MET
2	2	137	LEU
2	2	138	ASP
2	2	139	VAL
2	2	144	ASN
2	2	145	ARG
2	2	148	LYS
2	2	156	ARG
2	2	158	GLN
2	2	160	ASN
2	2	161	ARG
2	2	184	ASN
2	2	186	ARG
2	2	189	THR
2	2	191	VAL
2	2	193	LEU

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Mol	Chain	Res	Type
2	2	205	SER
2	2	211	SER
2	2	223	THR
2	2	225	SER
2	2	230	THR
2	2	231	SER
2	2	235	THR
2	2	239	GLN
2	2	249	ARG
2	2	253	LEU
2	2	254	SER
2	2	255	ARG
3	3	9	GLU
3	3	10	HIS
3	3	16	SER
3	3	18	LEU
3	3	21	SER
3	3	31	VAL
3	3	46	GLU
3	3	57	LYS
3	3	58	MET
3	3	74	THR
3	3	75	GLN
3	3	79	VAL
3	3	85	SER
3	3	97	LEU
3	3	99	ARG
3	3	107	SER
3	3	115	THR
3	3	117	THR
3	3	121	LYS
3	3	124	PHE
3	3	141	GLN
3	3	143	MET
3	3	157	SER
3	3	159	SER
3	3	166	SER
3	3	172	MET
3	3	176	ASP
3	3	177	GLN
3	3	179	ASN
3	3	181	THR

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Mol	Chain	Res	Type
3	3	184	ASP
3	3	191	GLN
3	3	201	CYS
3	3	203	THR
3	3	208	LEU
3	3	215	LYS
3	3	216	ASP
3	3	221	MET
3	3	224	SER
3	3	229	SER
4	4	9	ASN
4	4	10	ASN
4	4	12	SER
4	4	13	SER
4	4	16	ASN
4	4	20	ILE
4	4	21	ILE
4	4	22	ASN
4	4	23	ASN
4	4	26	SER
4	4	28	GLN
4	4	35	LEU
4	4	40	THR
4	4	43	ASP
4	4	46	LYS
4	4	50	GLN
4	4	54	LEU
4	4	56	SER
4	4	60	ASN
4	4	62	PHE
4	4	63	SER
4	4	64	ASN
4	4	65	MET
4	4	66	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	4	ASN
1	1	76	GLN
1	1	97	ASN
1	1	110	GLN

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Mol	Chain	Res	Type
1	1	139	HIS
1	1	157	GLN
1	1	182	ASN
1	1	191	ASN
1	1	205	HIS
1	1	219	ASN
2	2	27	GLN
2	2	120	GLN
2	2	144	ASN
2	2	158	GLN
2	2	160	ASN
2	2	180	HIS
2	2	181	GLN
2	2	184	ASN
2	2	209	HIS
2	2	250	HIS
3	3	35	ASN
3	3	49	GLN
3	3	75	GLN
3	3	81	GLN
3	3	141	GLN
3	3	144	GLN
3	3	169	HIS
3	3	177	GLN
3	3	179	ASN
3	3	182	ASN
4	4	9	ASN
4	4	10	ASN
4	4	16	ASN
4	4	23	ASN
4	4	27	ASN
4	4	28	GLN
4	4	30	GLN
4	4	38	ASN
4	4	50	GLN
4	4	53	ASN
4	4	60	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	PO4	2	309	-	4,4,4	2.07	3 (75%)	6,6,6	0.26	0
5	PO4	2	825	-	4,4,4	2.06	3 (75%)	6,6,6	0.26	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PO4	2	309	-	-	0/0/0/0	0/0/0/0
5	PO4	2	825	-	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2	825	PO4	P-O3	-2.25	1.45	1.53
5	2	309	PO4	P-O4	-2.21	1.45	1.53
5	2	309	PO4	P-O3	-2.21	1.45	1.53
5	2	825	PO4	P-O2	-2.21	1.45	1.53
5	2	309	PO4	P-O2	-2.21	1.45	1.53
5	2	825	PO4	P-O4	-2.16	1.45	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	2	825	PO4	6	0

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.