



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:08 PM UTC

PDB ID : 1R09 / pdb_00001r09
Title : HUMAN RHINOVIRUS 14 COMPLEXED WITH ANTIVIRAL COM-
POUND R 61837
Authors : Chapman, M.S.; Minor, I.; Rossmann, M.G.; Diana, G.D.; Andries, K.
Deposited on : 1990-05-04
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

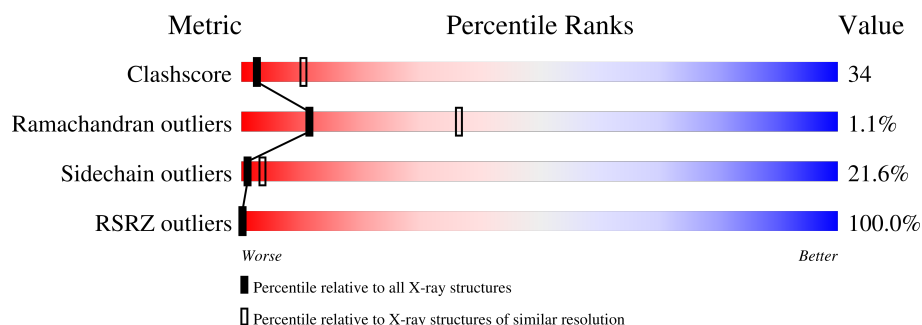
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	1	289	94% 22% 40% 26% 6% 6%
2	2	262	97% 24% 37% 27% 9% .
3	3	236	100% 24% 38% 29% 9%
4	4	68	59% 13% 21% 15% 10% 41%

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	JEN	1	1000	-	-	-	X
6	DMS	1	601	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6491 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP1).

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	255	Total	C	N	O	S	0	0	0
			1952	1238	330	372	12			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	170	LEU	ILE	conflict	UNP P03303

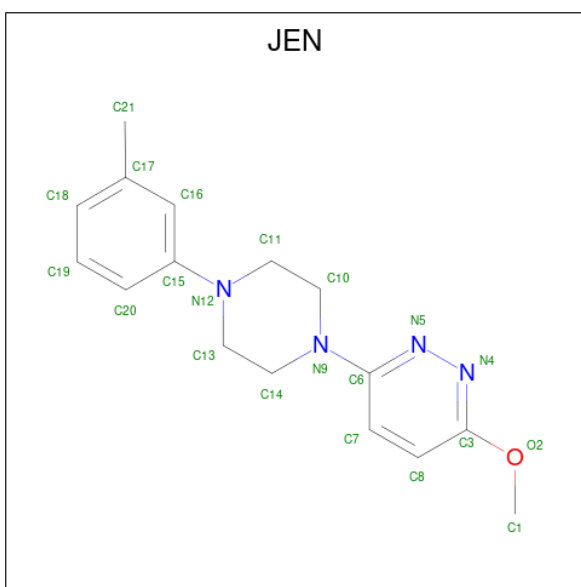
- Molecule 3 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP3).

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).

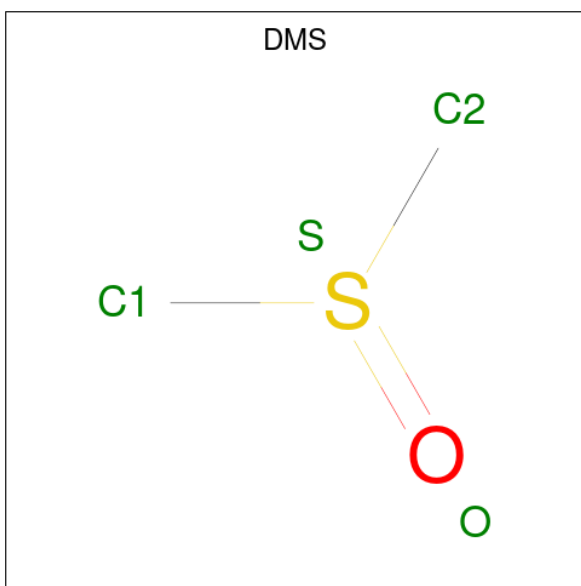
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	40	Total	C	N	O	S	0	0	0
			297	186	47	62	2			

- Molecule 5 is 3-METHOXY-6-[4-(3-METHYLPHENYL)-1-PIPERAZINYL]PYRIDAZINE (CCD ID: JEN) (formula: C₁₆H₂₀N₄O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	1	1	Total	C	N	O	0	0
			21	16	4	1		

- Molecule 6 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	1	1	Total	C	O	S	0	0
			4	2	1	1		

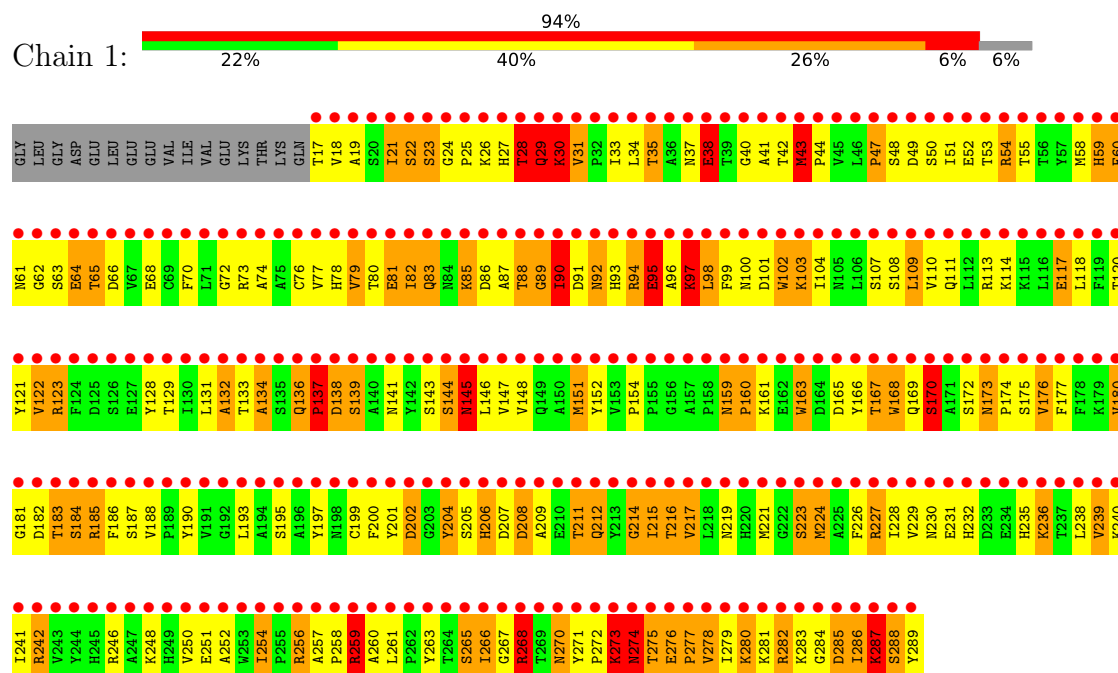
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	1	66	Total 66	O 66	0	0
7	2	66	Total 66	O 66	0	0
7	3	60	Total 60	O 60	0	0
7	4	6	Total 6	O 6	0	0

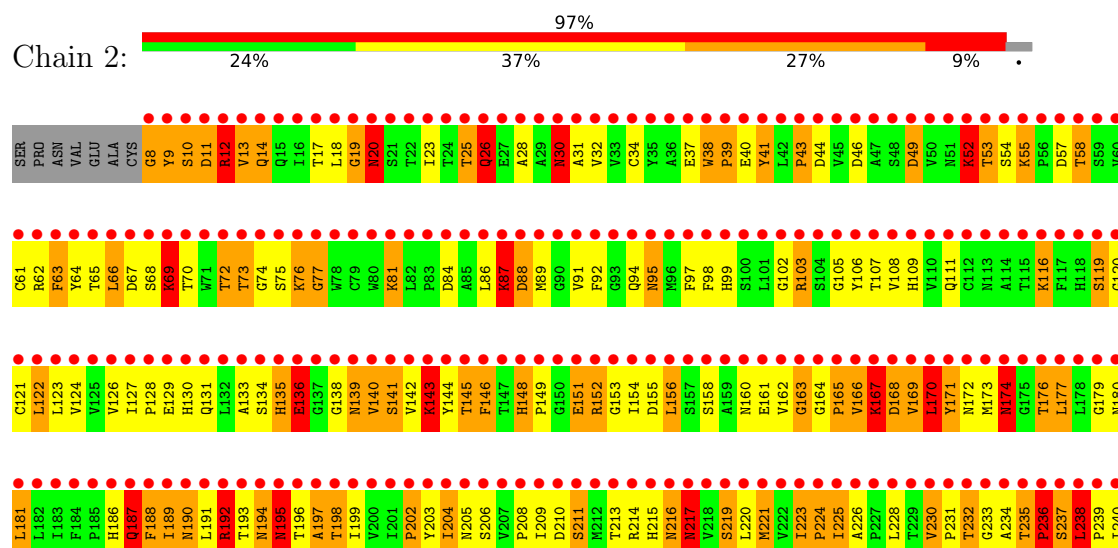
3 Residue-property plots

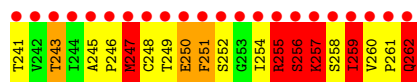
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

• Molecule 1: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP1)

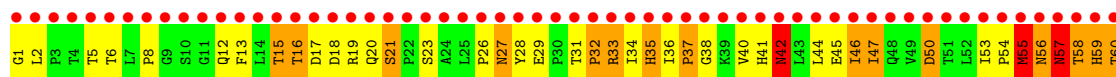
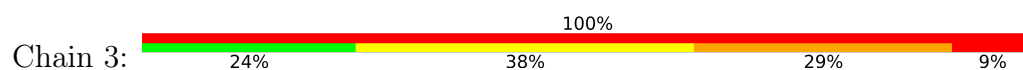


• Molecule 2: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP2)

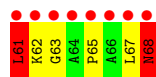
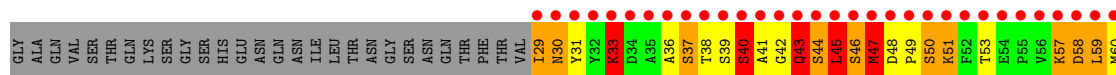
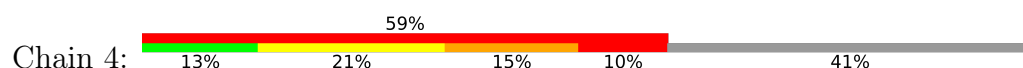




• Molecule 3: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP3)



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	445.10Å 445.10Å 445.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90 0.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90) 0.4 (0.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.54 (at 2.69Å)	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available) 0.210 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	15.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 25.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.126 for l,-k,h	Xtriage
F_o, F_c correlation	0.07	EDS
Total number of atoms	6491	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	2.21	82/2228 (3.7%)	2.56	191/3031 (6.3%)
2	2	2.40	96/2001 (4.8%)	2.77	193/2735 (7.1%)
3	3	2.31	81/1898 (4.3%)	2.80	192/2597 (7.4%)
4	4	2.62	14/302 (4.6%)	3.13	31/406 (7.6%)
All	All	2.32	273/6429 (4.2%)	2.73	607/8769 (6.9%)

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 (273) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	285	ASP	CA-CB	17.77	1.79	1.53
1	1	122	VAL	C-N	-14.79	1.14	1.33
4	4	41	ALA	C-O	13.33	1.41	1.24
3	3	57	ASN	CA-CB	12.78	1.75	1.53
4	4	42	GLY	N-CA	12.59	1.63	1.45
2	2	194	ASN	CA-CB	11.51	1.71	1.53
1	1	283	LYS	N-CA	10.88	1.61	1.46
1	1	144	SER	N-CA	10.33	1.58	1.45
3	3	164	THR	C-O	10.22	1.36	1.24
4	4	45	LEU	C-N	9.39	1.46	1.33
2	2	187	GLN	N-CA	9.31	1.57	1.45
2	2	256	SER	C-O	9.29	1.36	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	52	GLU	C-O	9.14	1.35	1.24
1	1	282	ARG	CD-NE	9.12	1.59	1.46
2	2	152	ARG	CD-NE	8.88	1.58	1.46
2	2	102	GLY	N-CA	8.88	1.54	1.45
2	2	168	ASP	C-O	8.82	1.34	1.24
1	1	175	SER	N-CA	8.68	1.56	1.45
3	3	21	SER	CA-CB	8.61	1.66	1.54
2	2	174	ASN	C-O	8.43	1.30	1.23
3	3	50	ASP	CA-CB	-8.28	1.40	1.53
3	3	232	VAL	N-CA	8.17	1.55	1.46
1	1	122	VAL	N-CA	8.04	1.55	1.46
1	1	73	ARG	C-O	8.02	1.33	1.23
2	2	77	GLY	N-CA	7.83	1.53	1.45
3	3	138	GLY	N-CA	7.83	1.55	1.44
2	2	236	PRO	C-O	7.80	1.34	1.24
2	2	161	GLU	CA-CB	-7.78	1.42	1.53
1	1	285	ASP	N-CA	-7.77	1.34	1.45
2	2	135	HIS	CE1-NE2	-7.66	1.24	1.32
3	3	1	GLY	N-CA	7.65	1.57	1.45
2	2	12	ARG	NE-CZ	7.59	1.41	1.33
1	1	72	GLY	C-O	7.53	1.34	1.23
2	2	52	LYS	N-CA	7.53	1.55	1.46
3	3	215	PRO	C-N	-7.47	1.23	1.33
1	1	143	SER	C-O	7.47	1.33	1.24
1	1	94	ARG	CD-NE	7.42	1.56	1.46
2	2	11	ASP	CA-CB	7.36	1.66	1.53
1	1	28	THR	CA-CB	7.34	1.64	1.53
1	1	288	SER	C-O	7.31	1.32	1.23
2	2	120	GLY	N-CA	7.22	1.53	1.45
1	1	132	ALA	C-O	7.20	1.32	1.24
3	3	77	ASN	C-O	7.17	1.33	1.24
3	3	60	THR	CA-CB	7.16	1.65	1.54
1	1	113	ARG	C-N	-7.16	1.24	1.33
2	2	260	VAL	N-CA	7.15	1.55	1.46
4	4	40	SER	CB-OG	7.05	1.56	1.42
2	2	108	VAL	C-O	7.01	1.32	1.24
2	2	219	SER	CA-CB	-7.01	1.41	1.53
1	1	30	LYS	C-O	7.00	1.32	1.23
2	2	9	TYR	C-O	6.99	1.32	1.23
1	1	276	GLU	C-O	6.97	1.30	1.24
2	2	58	THR	C-O	6.97	1.32	1.24
2	2	74	GLY	C-O	6.94	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	202	ASP	CA-CB	-6.86	1.42	1.53
4	4	49	PRO	C-N	-6.85	1.24	1.34
1	1	91	ASP	N-CA	6.84	1.55	1.46
1	1	133	THR	N-CA	6.84	1.54	1.45
1	1	288	SER	CA-CB	6.84	1.65	1.53
3	3	86	PHE	CA-CB	-6.84	1.42	1.52
1	1	23	SER	N-CA	6.81	1.54	1.45
2	2	223	ILE	CA-CB	6.80	1.59	1.54
3	3	6	THR	N-CA	6.76	1.54	1.45
1	1	170	SER	C-N	6.75	1.44	1.33
2	2	243	THR	C-O	6.74	1.32	1.24
2	2	193	THR	C-N	-6.73	1.23	1.33
2	2	152	ARG	CZ-NH2	6.73	1.42	1.33
2	2	194	ASN	N-CA	-6.72	1.37	1.45
3	3	216	ASP	CA-CB	6.72	1.64	1.53
2	2	197	ALA	C-O	6.71	1.31	1.23
1	1	73	ARG	N-CA	6.67	1.53	1.45
2	2	256	SER	CB-OG	6.67	1.55	1.42
2	2	10	SER	C-N	-6.66	1.25	1.33
1	1	251	GLU	CA-CB	-6.62	1.42	1.53
1	1	280	LYS	C-O	6.62	1.31	1.24
2	2	39	PRO	C-O	6.58	1.31	1.23
3	3	57	ASN	N-CA	-6.57	1.37	1.46
1	1	134	ALA	CA-CB	-6.56	1.42	1.53
2	2	109	HIS	CE1-NE2	-6.54	1.26	1.32
2	2	9	TYR	N-CA	6.54	1.53	1.46
3	3	15	THR	C-O	6.54	1.32	1.24
1	1	85	LYS	C-O	6.54	1.31	1.23
3	3	156	GLY	C-O	-6.51	1.18	1.24
2	2	190	ASN	CA-CB	-6.50	1.44	1.53
2	2	52	LYS	CE-NZ	6.50	1.68	1.49
4	4	62	LYS	C-O	6.50	1.31	1.24
4	4	44	SER	CB-OG	6.49	1.55	1.42
2	2	262	GLN	CD-OE1	6.46	1.35	1.23
1	1	79	VAL	C-N	-6.44	1.24	1.33
3	3	57	ASN	C-N	-6.43	1.25	1.33
2	2	30	ASN	N-CA	6.43	1.54	1.46
2	2	217	ASN	C-O	6.43	1.32	1.24
4	4	62	LYS	N-CA	6.42	1.54	1.46
1	1	231	GLU	CA-CB	-6.41	1.44	1.53
3	3	205	VAL	N-CA	6.35	1.53	1.46
1	1	22	SER	C-N	-6.33	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	95	GLU	CB-CG	6.33	1.71	1.52
2	2	8	GLY	N-CA	6.30	1.55	1.45
1	1	94	ARG	NE-CZ	6.29	1.40	1.33
4	4	63	GLY	N-CA	6.29	1.54	1.45
3	3	165	ILE	N-CA	6.28	1.54	1.46
3	3	5	THR	C-O	6.24	1.31	1.24
3	3	118	THR	CB-OG1	6.24	1.53	1.43
1	1	184	SER	N-CA	6.21	1.53	1.45
2	2	259	ILE	C-O	6.20	1.31	1.24
3	3	182	THR	CA-CB	6.20	1.62	1.53
3	3	75	ARG	C-N	-6.18	1.24	1.33
3	3	164	THR	N-CA	6.18	1.53	1.46
2	2	121	CYS	C-O	6.16	1.31	1.23
1	1	177	PHE	C-N	-6.16	1.25	1.33
3	3	16	THR	CA-CB	6.14	1.63	1.53
1	1	184	SER	C-O	6.14	1.31	1.23
4	4	45	LEU	N-CA	6.14	1.55	1.46
2	2	168	ASP	CA-CB	6.14	1.60	1.53
3	3	178	PRO	CA-CB	-6.13	1.45	1.53
1	1	251	GLU	N-CA	6.12	1.53	1.46
1	1	211	THR	N-CA	6.12	1.53	1.45
1	1	28	THR	N-CA	-6.10	1.37	1.45
2	2	162	VAL	N-CA	6.10	1.53	1.46
1	1	274	ASN	N-CA	6.10	1.54	1.46
3	3	215	PRO	CA-CB	-6.09	1.44	1.53
4	4	33	LYS	CE-NZ	6.08	1.67	1.49
1	1	24	GLY	N-CA	6.07	1.53	1.44
3	3	110	SER	N-CA	6.05	1.52	1.45
2	2	19	GLY	C-N	-6.05	1.25	1.33
2	2	190	ASN	N-CA	6.04	1.54	1.46
2	2	257	LYS	N-CA	6.04	1.53	1.46
3	3	57	ASN	C-O	6.03	1.31	1.24
1	1	131	LEU	C-O	6.02	1.31	1.23
3	3	155	ILE	N-CA	5.99	1.53	1.46
3	3	36	ILE	N-CA	5.99	1.53	1.46
3	3	135	GLY	C-O	5.99	1.31	1.24
2	2	208	PRO	C-N	-5.98	1.28	1.33
3	3	222	MET	CG-SD	5.96	1.95	1.80
1	1	88	THR	CB-OG1	5.93	1.53	1.43
2	2	180	ASN	C-N	-5.92	1.25	1.33
2	2	17	THR	C-N	-5.90	1.25	1.33
1	1	175	SER	CB-OG	-5.88	1.30	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	27	ASN	C-N	-5.87	1.25	1.33
1	1	38	GLU	CB-CG	-5.83	1.34	1.52
3	3	213	ALA	C-O	5.83	1.30	1.23
1	1	148	VAL	C-N	-5.82	1.25	1.33
3	3	219	LEU	C-N	-5.81	1.26	1.33
1	1	276	GLU	N-CA	5.80	1.54	1.45
2	2	55	LYS	N-CA	5.79	1.53	1.46
3	3	116	MET	N-CA	5.79	1.53	1.46
2	2	103	ARG	C-O	5.77	1.30	1.23
2	2	135	HIS	CG-CD2	-5.77	1.29	1.35
1	1	168	TRP	NE1-CE2	-5.76	1.31	1.37
1	1	287	LYS	C-O	5.75	1.31	1.24
2	2	88	ASP	C-O	5.74	1.32	1.24
3	3	33	ARG	NE-CZ	5.73	1.39	1.33
2	2	176	THR	N-CA	5.73	1.53	1.45
3	3	38	GLY	CA-C	-5.73	1.43	1.51
2	2	152	ARG	NE-CZ	5.72	1.39	1.33
1	1	274	ASN	CA-C	5.71	1.60	1.52
2	2	54	SER	CA-CB	-5.71	1.44	1.53
4	4	45	LEU	C-O	5.69	1.31	1.23
3	3	41	HIS	CE1-NE2	5.67	1.38	1.32
1	1	285	ASP	C-N	5.67	1.40	1.33
1	1	239	VAL	C-O	5.67	1.30	1.24
3	3	201	THR	C-O	5.66	1.30	1.23
2	2	103	ARG	N-CA	5.66	1.52	1.46
2	2	195	ASN	CA-CB	-5.66	1.44	1.54
3	3	35	HIS	C-N	-5.65	1.26	1.33
1	1	268	ARG	N-CA	5.65	1.52	1.45
3	3	158	GLN	C-O	5.65	1.30	1.24
1	1	25	PRO	CA-CB	-5.64	1.45	1.53
2	2	223	ILE	CA-C	-5.64	1.48	1.52
2	2	63	PHE	C-O	5.64	1.30	1.24
2	2	208	PRO	C-O	5.63	1.30	1.24
2	2	87	LYS	CB-CG	-5.63	1.35	1.52
1	1	63	SER	CB-OG	-5.62	1.30	1.42
1	1	267	GLY	C-O	5.62	1.32	1.24
3	3	82	GLY	N-CA	5.62	1.50	1.45
2	2	259	ILE	N-CA	5.62	1.53	1.46
1	1	180	VAL	C-O	5.62	1.29	1.24
2	2	75	SER	C-O	5.61	1.30	1.23
1	1	117	GLU	CD-OE2	5.59	1.35	1.25
3	3	172	GLN	CG-CD	-5.58	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	168	ASP	C-N	-5.58	1.26	1.33
1	1	137	PRO	C-O	5.58	1.31	1.24
2	2	194	ASN	C-O	5.58	1.30	1.23
1	1	254	ILE	CA-CB	5.57	1.61	1.54
3	3	82	GLY	C-N	-5.57	1.26	1.33
3	3	231	THR	CB-OG1	5.56	1.52	1.43
4	4	51	LYS	CE-NZ	5.55	1.66	1.49
3	3	75	ARG	N-CA	5.54	1.52	1.45
3	3	108	SER	CA-CB	-5.54	1.44	1.53
1	1	160	PRO	N-CA	-5.53	1.40	1.47
3	3	140	GLN	C-N	-5.52	1.26	1.33
2	2	109	HIS	C-O	5.51	1.30	1.24
3	3	66	SER	N-CA	5.51	1.53	1.46
3	3	61	LYS	CE-NZ	5.50	1.65	1.49
3	3	174	ARG	NE-CZ	5.50	1.39	1.33
2	2	153	GLY	C-N	-5.50	1.25	1.33
2	2	237	SER	C-O	5.49	1.30	1.23
2	2	237	SER	N-CA	5.49	1.52	1.46
2	2	151	GLU	CA-CB	-5.46	1.43	1.53
3	3	77	ASN	CG-OD1	5.45	1.33	1.23
1	1	25	PRO	C-N	-5.45	1.25	1.33
3	3	209	SER	N-CA	5.45	1.52	1.46
2	2	141	SER	N-CA	5.45	1.52	1.45
1	1	277	PRO	N-CA	5.44	1.53	1.47
3	3	40	VAL	C-O	5.44	1.30	1.24
3	3	37	PRO	CA-CB	-5.42	1.45	1.53
2	2	171	TYR	C-O	5.41	1.31	1.24
1	1	122	VAL	C-O	5.39	1.29	1.23
3	3	74	ASN	CA-CB	5.38	1.61	1.53
3	3	91	VAL	C-O	5.38	1.30	1.24
1	1	279	ILE	C-O	5.38	1.29	1.24
2	2	61	CYS	CA-C	-5.37	1.47	1.53
1	1	102	TRP	NE1-CE2	-5.36	1.31	1.37
1	1	163	TRP	NE1-CE2	-5.36	1.31	1.37
1	1	270	ASN	CA-C	5.36	1.59	1.52
2	2	103	ARG	CA-CB	-5.35	1.44	1.53
3	3	17	ASP	CG-OD2	5.35	1.35	1.25
2	2	72	THR	CB-OG1	5.34	1.52	1.43
3	3	209	SER	C-O	5.34	1.30	1.23
2	2	68	SER	CA-C	-5.34	1.45	1.52
2	2	211	SER	C-O	5.34	1.30	1.23
1	1	176	VAL	CA-C	5.33	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	148	HIS	ND1-CE1	5.32	1.37	1.32
2	2	256	SER	C-N	-5.32	1.26	1.33
4	4	61	LEU	C-O	5.32	1.30	1.24
2	2	219	SER	N-CA	5.30	1.52	1.46
1	1	30	LYS	CE-NZ	5.30	1.65	1.49
2	2	14	GLN	CD-NE2	5.29	1.44	1.33
2	2	123	LEU	C-N	-5.28	1.26	1.33
3	3	228	ILE	C-O	5.28	1.30	1.24
1	1	33	ILE	C-O	5.27	1.30	1.24
3	3	64	VAL	C-N	-5.26	1.25	1.33
3	3	2	LEU	CA-CB	5.25	1.63	1.53
1	1	89	GLY	C-O	5.25	1.31	1.23
2	2	246	PRO	C-O	5.23	1.29	1.23
2	2	99	HIS	C-N	-5.21	1.26	1.34
3	3	164	THR	CA-CB	5.21	1.61	1.53
1	1	283	LYS	CE-NZ	5.21	1.65	1.49
2	2	202	PRO	C-O	5.20	1.29	1.23
1	1	54	ARG	C-O	5.20	1.30	1.23
3	3	146	MET	C-O	5.19	1.30	1.24
3	3	77	ASN	C-N	-5.19	1.26	1.33
2	2	38	TRP	CA-C	-5.18	1.45	1.52
3	3	153	TRP	C-O	5.17	1.30	1.24
1	1	252	ALA	C-O	5.15	1.30	1.23
3	3	58	THR	CA-CB	5.15	1.62	1.53
3	3	133	PRO	CA-CB	-5.13	1.47	1.54
2	2	204	ILE	C-N	-5.13	1.26	1.33
3	3	112	ARG	CA-CB	-5.12	1.45	1.53
2	2	202	PRO	C-N	-5.10	1.26	1.33
3	3	136	ALA	C-O	5.10	1.30	1.23
3	3	205	VAL	C-O	5.10	1.29	1.23
1	1	85	LYS	N-CA	5.08	1.51	1.46
2	2	128	PRO	CA-CB	-5.08	1.46	1.53
1	1	209	ALA	C-N	-5.08	1.26	1.33
2	2	186	HIS	C-O	5.06	1.29	1.23
3	3	65	ASN	CA-CB	5.06	1.62	1.53
2	2	248	CYS	C-N	-5.06	1.26	1.33
3	3	232	VAL	C-O	5.05	1.29	1.23
2	2	233	GLY	C-O	5.05	1.30	1.24
1	1	42	THR	C-O	5.05	1.29	1.23
3	3	34	ILE	C-O	5.04	1.30	1.24
3	3	216	ASP	N-CA	-5.04	1.40	1.46
3	3	109	GLY	C-N	5.02	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	109	HIS	N-CA	5.02	1.53	1.46
2	2	12	ARG	N-CA	-5.01	1.40	1.46
3	3	164	THR	CA-C	-5.01	1.46	1.52
1	1	117	GLU	N-CA	5.01	1.52	1.46
2	2	220	LEU	C-N	-5.01	1.26	1.33
1	1	246	ARG	CD-NE	-5.00	1.39	1.46
2	2	223	ILE	N-CA	5.00	1.49	1.45
3	3	163	MET	C-N	-5.00	1.26	1.33
3	3	84	ASN	N-CA	5.00	1.51	1.45

All (607) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	50	ASP	CA-CB-CG	27.73	140.33	112.60
1	1	285	ASP	CA-CB-CG	-22.21	90.39	112.60
3	3	215	PRO	CA-C-N	20.36	149.20	120.29
3	3	215	PRO	C-N-CA	20.36	149.20	120.29
2	2	87	LYS	CA-CB-CG	19.05	152.21	114.10
2	2	11	ASP	CA-CB-CG	-18.96	93.64	112.60
1	1	145	ASN	OD1-CG-ND2	17.24	139.84	122.60
2	2	193	THR	CA-C-N	16.42	150.15	122.07
2	2	193	THR	C-N-CA	16.42	150.15	122.07
2	2	190	ASN	CA-CB-CG	16.38	128.98	112.60
2	2	194	ASN	CA-CB-CG	-14.89	97.71	112.60
2	2	11	ASP	CA-C-N	14.78	140.54	120.44
2	2	11	ASP	C-N-CA	14.78	140.54	120.44
3	3	57	ASN	CA-CB-CG	-13.74	98.86	112.60
1	1	38	GLU	CB-CG-CD	13.64	135.78	112.60
3	3	74	ASN	CA-CB-CG	-13.47	99.13	112.60
3	3	65	ASN	CA-CB-CG	-13.09	99.51	112.60
1	1	202	ASP	CA-CB-CG	12.96	125.56	112.60
3	3	27	ASN	CA-CB-CG	-12.94	99.66	112.60
1	1	145	ASN	CA-CB-CG	-12.89	99.71	112.60
2	2	194	ASN	N-CA-CB	-12.65	89.79	110.41
2	2	44	ASP	CA-CB-CG	12.64	125.24	112.60
1	1	94	ARG	CD-NE-CZ	-12.61	106.75	124.40
1	1	256	ARG	NE-CZ-NH2	12.57	130.51	119.20
2	2	67	ASP	CA-CB-CG	-12.45	100.15	112.60
2	2	256	SER	CA-C-O	-12.21	105.38	119.79
4	4	30	ASN	CA-CB-CG	-12.10	100.50	112.60
3	3	172	GLN	CB-CG-CD	12.03	133.05	112.60
4	4	45	LEU	N-CA-CB	-11.89	94.13	111.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	41	ALA	CA-C-O	-11.31	105.46	119.38
3	3	74	ASN	OD1-CG-ND2	11.30	133.90	122.60
2	2	14	GLN	OE1-CD-NE2	11.18	133.78	122.60
3	3	29	GLU	CB-CG-CD	11.13	131.52	112.60
1	1	285	ASP	N-CA-CB	-11.05	95.26	110.29
2	2	151	GLU	CA-CB-CG	11.04	136.19	114.10
1	1	173	ASN	CA-CB-CG	11.01	123.61	112.60
1	1	25	PRO	CA-C-O	-10.88	108.94	121.56
2	2	88	ASP	CA-CB-CG	-10.83	101.77	112.60
2	2	219	SER	CA-CB-OG	10.64	132.39	111.10
1	1	282	ARG	CD-NE-CZ	-10.62	109.53	124.40
2	2	97	PHE	CA-CB-CG	-10.60	103.20	113.80
4	4	48	ASP	CA-CB-CG	-10.60	102.00	112.60
1	1	141	ASN	CA-CB-CG	-10.45	102.15	112.60
3	3	57	ASN	N-CA-CB	-10.40	92.92	110.49
3	3	72	ASN	CA-CB-CG	-10.16	102.44	112.60
4	4	48	ASP	O-C-N	10.14	128.33	121.23
1	1	246	ARG	NE-CZ-NH1	10.01	131.51	121.50
1	1	63	SER	CB-CA-C	-10.00	94.20	110.79
1	1	54	ARG	CD-NE-CZ	-9.96	110.45	124.40
4	4	44	SER	CA-C-N	-9.87	107.96	122.07
4	4	44	SER	C-N-CA	-9.87	107.96	122.07
1	1	91	ASP	CA-CB-CG	-9.79	102.81	112.60
1	1	275	THR	CA-C-O	-9.78	109.17	121.88
1	1	285	ASP	N-CA-C	9.75	122.91	110.33
1	1	28	THR	CB-CA-C	-9.73	92.89	111.48
1	1	22	SER	CA-C-O	-9.71	109.62	120.69
1	1	208	ASP	CA-CB-CG	-9.69	102.92	112.60
1	1	256	ARG	NE-CZ-NH1	-9.66	111.83	121.50
3	3	33	ARG	CA-C-O	-9.66	110.04	121.05
3	3	137	ARG	NE-CZ-NH1	-9.63	111.87	121.50
1	1	53	THR	CA-CB-OG1	-9.54	95.30	109.60
1	1	246	ARG	CD-NE-CZ	9.44	137.62	124.40
1	1	79	VAL	CA-C-O	-9.42	110.59	120.39
1	1	38	GLU	CA-CB-CG	9.41	132.93	114.10
3	3	86	PHE	CA-CB-CG	9.40	123.20	113.80
3	3	89	ASP	CA-CB-CG	-9.37	103.23	112.60
3	3	57	ASN	CB-CA-C	-9.07	92.36	110.42
2	2	255	ARG	NE-CZ-NH2	-9.06	111.04	119.20
1	1	95	GLU	CB-CG-CD	-9.03	97.25	112.60
1	1	268	ARG	CD-NE-CZ	-9.03	111.76	124.40
4	4	50	SER	CA-C-O	-9.02	109.90	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	196	ILE	CA-C-O	-8.98	111.20	120.27
2	2	195	ASN	CA-CB-CG	8.94	121.54	112.60
2	2	136	GLU	CB-CG-CD	-8.84	97.57	112.60
2	2	250	GLU	CA-CB-CG	8.81	131.72	114.10
4	4	68	ASN	CA-CB-CG	-8.76	103.84	112.60
1	1	270	ASN	CA-CB-CG	8.67	121.27	112.60
1	1	251	GLU	CA-CB-CG	8.64	131.38	114.10
2	2	139	ASN	CA-CB-CG	-8.48	104.12	112.60
2	2	255	ARG	CA-CB-CG	8.48	131.07	114.10
2	2	73	THR	CA-CB-OG1	-8.47	96.89	109.60
1	1	259	ARG	CA-CB-CG	-8.44	97.22	114.10
4	4	58	ASP	O-C-N	8.43	132.83	123.22
3	3	174	ARG	CD-NE-CZ	-8.41	112.62	124.40
2	2	168	ASP	CA-C-O	-8.41	110.61	120.62
2	2	68	SER	N-CA-C	8.38	122.88	110.48
2	2	169	VAL	CA-C-O	-8.38	112.29	121.17
2	2	169	VAL	CB-CA-C	-8.37	101.25	111.97
4	4	41	ALA	N-CA-C	8.35	122.73	112.54
4	4	36	ALA	CA-C-N	-8.33	108.80	122.54
4	4	36	ALA	C-N-CA	-8.33	108.80	122.54
3	3	74	ASN	CA-C-O	-8.33	109.89	120.55
3	3	5	THR	CA-C-O	-8.29	111.11	120.32
3	3	172	GLN	CG-CD-NE2	8.25	128.77	116.40
3	3	219	LEU	CA-C-O	-8.22	111.21	120.66
1	1	82	ILE	CA-C-O	-8.20	113.06	121.67
3	3	182	THR	CA-CB-CG2	8.16	124.37	110.50
3	3	57	ASN	OD1-CG-ND2	8.15	130.75	122.60
3	3	16	THR	N-CA-CB	-8.15	98.30	110.61
3	3	21	SER	CB-CA-C	-8.13	95.50	108.91
4	4	57	LYS	CA-C-O	-8.12	112.33	120.70
1	1	29	GLN	N-CA-C	-8.11	102.43	113.30
2	2	49	ASP	CA-CB-CG	8.09	120.69	112.60
3	3	78	GLU	N-CA-C	8.00	120.85	110.53
3	3	233	ALA	CA-C-O	-8.00	112.39	121.19
3	3	60	THR	CA-CB-OG1	-8.00	97.61	109.60
2	2	187	GLN	CA-CB-CG	7.99	130.09	114.10
1	1	288	SER	CA-C-O	-7.98	113.09	121.55
2	2	248	CYS	CA-C-O	-7.97	112.29	121.54
3	3	27	ASN	O-C-N	7.96	131.95	122.00
1	1	94	ARG	NE-CZ-NH2	-7.95	112.05	119.20
3	3	111	LEU	CA-C-N	-7.94	111.80	123.00
3	3	111	LEU	C-N-CA	-7.94	111.80	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	231	THR	CA-CB-OG1	-7.91	97.74	109.60
2	2	223	ILE	N-CA-CB	-7.91	101.52	112.27
1	1	176	VAL	CA-C-O	-7.90	111.42	120.67
1	1	37	ASN	CB-CG-ND2	7.87	128.20	116.40
2	2	216	ASN	CA-C-O	-7.85	112.09	120.80
1	1	274	ASN	O-C-N	7.83	133.01	122.59
2	2	95	ASN	CA-CB-CG	-7.83	104.77	112.60
3	3	216	ASP	N-CA-CB	-7.79	98.63	110.16
4	4	45	LEU	CA-C-O	7.76	130.54	121.54
1	1	282	ARG	CA-C-N	-7.74	111.50	122.41
1	1	282	ARG	C-N-CA	-7.74	111.50	122.41
2	2	109	HIS	CA-C-O	-7.73	110.83	120.57
4	4	37	SER	CB-CA-C	7.71	122.96	110.09
1	1	176	VAL	CB-CA-C	-7.70	99.14	110.62
3	3	62	ASP	CA-CB-CG	7.68	120.28	112.60
1	1	64	GLU	CB-CG-CD	7.67	125.64	112.60
2	2	190	ASN	OD1-CG-ND2	-7.66	114.94	122.60
1	1	17	THR	CA-C-N	-7.65	110.26	122.50
1	1	17	THR	C-N-CA	-7.65	110.26	122.50
2	2	240	ILE	CA-C-O	-7.63	112.37	120.39
3	3	137	ARG	CD-NE-CZ	-7.62	113.74	124.40
1	1	61	ASN	CA-CB-CG	-7.61	104.99	112.60
3	3	59	HIS	CA-C-O	7.60	130.47	121.88
3	3	184	ALA	N-CA-C	7.58	122.72	113.17
3	3	142	ARG	CA-CB-CG	7.58	129.25	114.10
1	1	173	ASN	N-CA-CB	-7.57	97.08	109.94
2	2	87	LYS	CB-CG-CD	7.56	128.70	111.30
1	1	277	PRO	N-CD-CG	-7.54	91.88	103.20
3	3	27	ASN	N-CA-C	7.52	124.01	113.56
3	3	79	GLN	OE1-CD-NE2	-7.50	115.10	122.60
1	1	122	VAL	N-CA-CB	-7.50	97.90	111.92
1	1	175	SER	CB-CA-C	7.44	126.07	109.56
4	4	30	ASN	CA-C-O	-7.43	112.22	120.69
1	1	288	SER	N-CA-C	7.40	120.42	110.35
2	2	98	PHE	CA-C-O	-7.37	110.97	119.60
2	2	140	VAL	CA-C-O	-7.36	113.36	121.23
4	4	45	LEU	CB-CA-C	7.35	122.53	111.80
2	2	107	THR	CA-C-O	-7.34	112.24	120.32
3	3	129	LEU	CA-C-O	-7.34	112.93	120.71
2	2	39	PRO	CA-C-O	-7.31	113.01	121.34
3	3	27	ASN	CB-CA-C	-7.30	97.26	111.06
3	3	118	THR	CA-CB-OG1	-7.30	98.65	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	187	GLN	CB-CA-C	7.26	125.39	109.94
2	2	77	GLY	CA-C-O	-7.23	114.82	122.05
4	4	30	ASN	OD1-CG-ND2	7.23	129.83	122.60
3	3	46	ILE	CA-C-O	-7.23	112.45	120.25
3	3	61	LYS	CA-C-O	-7.23	112.68	121.06
2	2	169	VAL	N-CA-C	7.22	117.36	110.42
3	3	124	SER	CA-C-O	-7.22	113.53	121.33
1	1	26	LYS	CA-CB-CG	7.21	128.53	114.10
3	3	19	ARG	NE-CZ-NH2	7.21	125.69	119.20
2	2	180	ASN	CA-CB-CG	-7.21	105.39	112.60
2	2	103	ARG	CD-NE-CZ	-7.20	114.31	124.40
1	1	275	THR	CA-CB-OG1	-7.18	98.83	109.60
2	2	68	SER	O-C-N	-7.18	114.84	122.96
2	2	52	LYS	CA-C-O	-7.17	113.30	121.19
1	1	122	VAL	CA-C-N	7.16	133.17	121.86
1	1	122	VAL	C-N-CA	7.16	133.17	121.86
2	2	146	PHE	CA-CB-CG	-7.14	106.66	113.80
2	2	168	ASP	N-CA-CB	-7.14	97.90	109.60
1	1	59	HIS	CA-C-O	-7.12	111.98	120.81
1	1	284	GLY	CA-C-N	7.11	133.60	120.95
1	1	284	GLY	C-N-CA	7.11	133.60	120.95
4	4	47	MET	CA-CB-CG	-7.08	99.95	114.10
2	2	134	SER	CA-C-O	-7.06	113.01	121.05
1	1	285	ASP	CB-CA-C	-7.05	93.81	110.02
3	3	94	THR	O-C-N	7.04	131.65	122.42
2	2	259	ILE	CB-CG1-CD1	-7.04	99.03	113.80
3	3	13	PHE	CA-CB-CG	7.03	120.83	113.80
1	1	85	LYS	CA-C-O	-7.00	113.97	121.38
3	3	164	THR	N-CA-CB	-6.98	99.61	110.57
1	1	28	THR	OG1-CB-CG2	6.98	123.25	109.30
3	3	35	HIS	CA-C-O	-6.97	112.90	120.92
1	1	43	MET	CA-C-O	6.94	126.28	119.75
1	1	285	ASP	CB-CG-OD2	-6.93	102.46	118.40
3	3	109	GLY	CA-C-N	-6.93	110.86	122.64
3	3	109	GLY	C-N-CA	-6.93	110.86	122.64
3	3	121	ALA	CA-C-O	-6.93	112.27	120.10
3	3	66	SER	CB-CA-C	6.91	121.63	110.09
3	3	77	ASN	OD1-CG-ND2	-6.91	115.69	122.60
1	1	270	ASN	O-C-N	6.90	131.39	122.97
2	2	57	ASP	CB-CA-C	-6.88	108.65	116.63
1	1	138	ASP	CA-CB-CG	6.88	119.48	112.60
2	2	9	TYR	CB-CA-C	6.88	121.41	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	35	THR	CA-CB-OG1	-6.87	99.29	109.60
3	3	231	THR	CA-C-O	-6.85	110.49	119.06
4	4	44	SER	O-C-N	6.85	131.70	122.59
2	2	186	HIS	CA-CB-CG	-6.84	106.96	113.80
3	3	65	ASN	OD1-CG-ND2	6.84	129.44	122.60
2	2	219	SER	CB-CA-C	6.84	121.69	109.38
1	1	160	PRO	O-C-N	6.83	131.85	122.64
1	1	183	THR	CA-CB-OG1	-6.82	99.36	109.60
3	3	146	MET	CG-SD-CE	6.82	115.90	100.90
2	2	193	THR	O-C-N	-6.81	115.12	121.79
2	2	14	GLN	CB-CG-CD	-6.81	101.03	112.60
1	1	89	GLY	CA-C-N	-6.81	114.35	122.93
1	1	89	GLY	C-N-CA	-6.81	114.35	122.93
1	1	97	LYS	CB-CA-C	-6.80	100.77	111.51
1	1	42	THR	CA-CB-CG2	6.78	122.03	110.50
3	3	202	THR	CA-C-O	6.78	128.49	121.23
1	1	49	ASP	N-CA-C	-6.76	105.32	113.97
3	3	151	VAL	CA-C-O	-6.74	113.57	120.25
3	3	187	LEU	CA-C-O	-6.74	113.10	120.24
1	1	35	THR	N-CA-CB	-6.73	99.11	110.49
3	3	143	ARG	N-CA-C	-6.73	104.02	111.36
2	2	124	VAL	CA-C-O	-6.73	112.78	120.66
1	1	62	GLY	CA-C-N	6.73	129.29	120.28
1	1	62	GLY	C-N-CA	6.73	129.29	120.28
2	2	170	LEU	CD1-CG-CD2	-6.73	96.00	110.80
3	3	42	ASN	CA-C-O	-6.72	112.93	120.66
2	2	249	THR	CA-CB-OG1	-6.71	99.53	109.60
1	1	206	HIS	CA-C-O	-6.71	114.10	121.28
2	2	224	PRO	CA-C-O	-6.71	114.05	121.23
3	3	178	PRO	O-C-N	6.70	130.72	123.01
1	1	288	SER	CB-CA-C	-6.67	97.68	109.62
2	2	255	ARG	CB-CG-CD	6.66	126.61	111.30
1	1	282	ARG	NE-CZ-NH2	-6.65	113.22	119.20
3	3	227	THR	CA-CB-OG1	-6.65	99.63	109.60
1	1	95	GLU	CA-CB-CG	-6.64	100.82	114.10
1	1	90	ILE	CA-C-N	-6.62	109.74	122.06
1	1	90	ILE	C-N-CA	-6.62	109.74	122.06
1	1	259	ARG	CA-C-O	-6.62	113.20	120.81
2	2	198	THR	CA-C-O	-6.62	112.97	120.32
1	1	60	PHE	CA-C-O	-6.60	113.63	120.89
3	3	187	LEU	N-CA-CB	-6.59	100.42	110.77
1	1	147	VAL	CA-C-O	-6.59	113.48	120.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	134	PRO	CA-C-N	-6.59	116.32	123.30
3	3	134	PRO	C-N-CA	-6.59	116.32	123.30
1	1	25	PRO	CA-C-N	6.58	133.40	122.73
1	1	25	PRO	C-N-CA	6.58	133.40	122.73
3	3	202	THR	CA-CB-OG1	-6.58	99.73	109.60
2	2	145	THR	CA-CB-OG1	-6.57	99.75	109.60
1	1	118	LEU	CA-C-N	6.56	133.11	122.81
1	1	118	LEU	C-N-CA	6.56	133.11	122.81
2	2	161	GLU	CA-C-N	-6.54	114.52	122.90
2	2	161	GLU	C-N-CA	-6.54	114.52	122.90
2	2	38	TRP	N-CA-CB	-6.53	99.34	110.11
2	2	11	ASP	OD1-CG-OD2	6.52	138.55	122.90
2	2	226	ALA	N-CA-C	-6.52	99.14	109.04
4	4	48	ASP	OD1-CG-OD2	6.52	138.54	122.90
3	3	19	ARG	CA-CB-CG	6.51	127.13	114.10
2	2	18	LEU	CB-CA-C	6.51	119.84	110.79
2	2	12	ARG	N-CA-C	6.51	118.17	111.14
2	2	148	HIS	CA-CB-CG	6.50	120.30	113.80
2	2	163	GLY	O-C-N	6.50	130.17	122.50
1	1	277	PRO	CB-CA-C	6.48	119.87	111.64
3	3	74	ASN	N-CA-C	6.48	120.51	112.47
4	4	36	ALA	N-CA-C	-6.47	105.25	113.01
3	3	205	VAL	CB-CA-C	6.46	120.20	110.90
1	1	256	ARG	CD-NE-CZ	-6.45	115.37	124.40
4	4	39	SER	O-C-N	6.45	130.80	122.23
2	2	142	VAL	CA-C-O	-6.44	113.12	120.66
3	3	182	THR	CA-CB-OG1	-6.44	99.94	109.60
3	3	65	ASN	N-CA-CB	-6.44	100.94	110.53
3	3	57	ASN	N-CA-C	6.43	124.50	110.80
2	2	247	MET	CB-CA-C	6.43	122.41	109.68
2	2	193	THR	CA-C-O	6.43	126.47	119.40
2	2	194	ASN	N-CA-C	6.43	120.54	110.32
3	3	164	THR	CA-CB-OG1	-6.43	99.96	109.60
2	2	111	GLN	OE1-CD-NE2	-6.42	116.18	122.60
2	2	69	LYS	CA-CB-CG	6.41	126.91	114.10
3	3	216	ASP	CA-C-N	6.40	129.80	120.71
3	3	216	ASP	C-N-CA	6.40	129.80	120.71
1	1	205	SER	O-C-N	6.39	131.22	122.46
3	3	204	GLN	O-C-N	6.39	130.22	123.06
3	3	172	GLN	OE1-CD-NE2	-6.38	116.22	122.60
1	1	50	SER	CA-C-O	-6.38	110.45	118.43
2	2	203	TYR	CA-C-O	-6.38	113.18	120.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	99	GLU	CB-CG-CD	6.38	123.44	112.60
3	3	226	GLN	CB-CG-CD	-6.38	101.76	112.60
4	4	44	SER	CA-CB-OG	-6.37	98.36	111.10
1	1	239	VAL	CB-CA-C	6.36	120.04	110.63
2	2	223	ILE	CA-C-O	-6.35	116.64	119.94
3	3	41	HIS	CA-C-O	-6.34	112.38	119.67
1	1	144	SER	N-CA-CB	-6.33	100.79	110.42
1	1	166	TYR	N-CA-C	-6.33	104.81	112.54
2	2	235	THR	CB-CA-C	-6.33	99.52	109.52
1	1	250	VAL	N-CA-C	6.33	117.82	109.21
2	2	241	THR	CA-C-O	-6.32	114.01	120.71
3	3	181	TYR	O-C-N	6.32	128.82	122.12
1	1	137	PRO	CA-C-N	-6.31	113.05	122.39
1	1	137	PRO	C-N-CA	-6.31	113.05	122.39
3	3	80	VAL	CA-C-O	-6.31	113.96	120.71
1	1	265	SER	O-C-N	-6.31	115.95	123.27
3	3	202	THR	N-CA-C	6.29	118.42	108.79
2	2	145	THR	CA-C-O	-6.29	113.84	120.63
1	1	288	SER	N-CA-CB	-6.28	100.80	110.04
3	3	216	ASP	CB-CG-OD1	6.28	132.84	118.40
3	3	63	GLU	CB-CG-CD	-6.28	101.93	112.60
3	3	193	THR	CA-C-O	-6.27	111.54	120.51
3	3	83	THR	CA-CB-OG1	-6.27	100.19	109.60
1	1	117	GLU	CG-CD-OE1	6.26	132.81	118.40
2	2	103	ARG	CA-CB-CG	6.26	126.62	114.10
2	2	143	LYS	O-C-N	6.26	130.51	122.81
1	1	122	VAL	CB-CA-C	6.25	121.90	110.71
1	1	70	PHE	CA-CB-CG	6.23	120.03	113.80
3	3	183	SER	N-CA-CB	-6.23	100.82	110.29
4	4	65	PRO	CB-CA-C	-6.23	103.42	111.46
1	1	206	HIS	O-C-N	6.23	129.52	123.29
1	1	282	ARG	NH1-CZ-NH2	6.22	127.38	119.30
3	3	161	ILE	CA-C-O	-6.20	113.88	120.39
1	1	31	VAL	N-CA-CB	-6.20	102.53	111.21
3	3	196	ILE	N-CA-CB	-6.19	103.41	111.82
1	1	274	ASN	N-CA-CB	6.17	120.92	110.49
1	1	48	SER	CA-C-O	-6.17	108.19	119.36
2	2	28	ALA	CA-C-O	-6.17	114.85	121.94
3	3	27	ASN	N-CA-CB	-6.17	103.09	113.15
3	3	6	THR	CB-CA-C	6.17	120.05	109.51
3	3	132	THR	CA-C-O	-6.16	113.92	119.59
1	1	260	ALA	CA-C-O	-6.16	111.51	120.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	11	ASP	O-C-N	6.16	130.39	122.39
2	2	194	ASN	OD1-CG-ND2	6.15	128.75	122.60
2	2	111	GLN	CB-CG-CD	6.13	123.01	112.60
2	2	238	LEU	N-CA-CB	-6.13	98.78	110.42
1	1	236	LYS	CA-C-O	-6.12	114.25	121.16
2	2	179	GLY	CA-C-O	-6.12	114.21	120.45
3	3	163	MET	CA-CB-CG	-6.11	101.87	114.10
1	1	202	ASP	CB-CA-C	6.11	121.11	112.07
1	1	52	GLU	CA-C-O	-6.10	113.60	120.43
3	3	137	ARG	NE-CZ-NH2	6.09	124.68	119.20
3	3	170	GLY	CA-C-N	6.09	128.66	120.50
3	3	170	GLY	C-N-CA	6.09	128.66	120.50
1	1	252	ALA	CA-C-O	-6.08	113.67	120.66
3	3	193	THR	CA-CB-OG1	-6.08	100.48	109.60
2	2	12	ARG	CD-NE-CZ	-6.08	115.89	124.40
1	1	141	ASN	O-C-N	6.07	129.74	122.27
4	4	43	GLN	OE1-CD-NE2	-6.07	116.53	122.60
2	2	241	THR	CA-CB-OG1	-6.05	100.53	109.60
3	3	8	PRO	CA-C-O	-6.04	114.53	121.36
1	1	68	GLU	CG-CD-OE1	6.04	132.29	118.40
2	2	195	ASN	OD1-CG-ND2	-6.03	116.57	122.60
3	3	36	ILE	CA-C-O	-6.02	111.88	119.95
1	1	77	VAL	CA-C-O	-6.01	113.25	118.96
1	1	133	THR	CA-CB-OG1	-6.00	100.59	109.60
1	1	136	GLN	CG-CD-NE2	-6.00	107.39	116.40
2	2	86	LEU	CA-C-N	6.00	130.30	120.63
2	2	86	LEU	C-N-CA	6.00	130.30	120.63
3	3	47	ILE	CB-CG1-CD1	-6.00	101.19	113.80
1	1	41	ALA	CA-C-O	-6.00	114.64	121.72
2	2	169	VAL	N-CA-CB	5.99	117.56	110.55
3	3	121	ALA	CB-CA-C	-5.99	99.55	110.63
3	3	41	HIS	N-CA-CB	5.98	119.08	110.40
3	3	174	ARG	NH1-CZ-NH2	5.98	127.07	119.30
2	2	14	GLN	CA-CB-CG	-5.98	102.15	114.10
3	3	137	ARG	CA-C-O	-5.97	115.07	121.94
3	3	194	SER	N-CA-CB	-5.97	100.40	110.49
3	3	158	GLN	CA-C-O	5.95	127.70	120.62
2	2	105	GLY	N-CA-C	-5.94	102.31	112.64
2	2	136	GLU	CG-CD-OE2	-5.94	104.75	118.40
1	1	173	ASN	OD1-CG-ND2	-5.93	116.67	122.60
3	3	77	ASN	O-C-N	-5.93	114.71	122.59
3	3	207	LEU	CA-C-O	-5.91	114.23	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	160	THR	CA-CB-OG1	-5.91	100.74	109.60
1	1	22	SER	N-CA-CB	-5.90	100.80	109.95
1	1	265	SER	N-CA-CB	-5.90	100.55	111.53
1	1	55	THR	CA-CB-OG1	-5.90	100.75	109.60
2	2	161	GLU	CA-CB-CG	5.90	125.90	114.10
3	3	1	GLY	O-C-N	-5.90	113.57	123.00
3	3	57	ASN	O-C-N	-5.89	114.75	122.59
1	1	259	ARG	CB-CA-C	-5.89	100.47	109.89
2	2	41	TYR	N-CA-CB	5.89	118.45	110.38
3	3	55	MET	CA-CB-CG	-5.86	102.39	114.10
2	2	226	ALA	O-C-N	5.85	127.86	121.36
3	3	92	PHE	CA-CB-CG	-5.85	107.95	113.80
1	1	270	ASN	CB-CA-C	-5.84	100.29	109.70
1	1	280	LYS	CB-CA-C	-5.84	101.75	110.16
3	3	131	TYR	CA-C-O	-5.84	114.06	120.43
2	2	88	ASP	CA-C-O	-5.83	112.60	119.48
1	1	242	ARG	CD-NE-CZ	-5.82	116.25	124.40
1	1	267	GLY	CA-C-N	-5.82	113.04	122.81
1	1	267	GLY	C-N-CA	-5.82	113.04	122.81
2	2	198	THR	O-C-N	5.82	130.11	123.31
3	3	197	LEU	CB-CA-C	5.81	117.23	108.86
2	2	105	GLY	CA-C-O	-5.80	112.99	122.56
3	3	33	ARG	CB-CG-CD	-5.80	97.96	111.30
3	3	93	LYS	N-CA-C	5.80	118.38	111.71
2	2	54	SER	CA-C-N	-5.80	115.03	122.98
2	2	54	SER	C-N-CA	-5.80	115.03	122.98
3	3	59	HIS	CA-CB-CG	-5.80	108.00	113.80
2	2	255	ARG	NE-CZ-NH1	5.79	127.29	121.50
4	4	65	PRO	CA-C-O	-5.79	114.74	121.34
1	1	145	ASN	CB-CG-ND2	-5.78	107.73	116.40
1	1	175	SER	CA-CB-OG	5.77	122.63	111.10
2	2	235	THR	OG1-CB-CG2	5.76	120.83	109.30
1	1	68	GLU	CG-CD-OE2	-5.74	105.20	118.40
2	2	189	ILE	CA-C-O	-5.73	113.24	120.69
2	2	210	ASP	N-CA-CB	-5.73	100.56	110.87
1	1	182	ASP	CA-C-N	5.72	131.55	122.62
1	1	182	ASP	C-N-CA	5.72	131.55	122.62
1	1	94	ARG	CG-CD-NE	-5.71	99.43	112.00
2	2	86	LEU	CA-C-O	-5.71	112.88	119.56
3	3	38	GLY	N-CA-C	5.69	123.74	115.32
3	3	66	SER	N-CA-C	-5.69	106.00	113.17
1	1	83	GLN	CB-CG-CD	-5.68	102.94	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	45	GLU	CG-CD-OE1	5.68	131.47	118.40
3	3	137	ARG	O-C-N	5.68	129.64	122.65
3	3	112	ARG	CA-CB-CG	5.68	125.45	114.10
3	3	175	TYR	N-CA-CB	-5.68	101.49	110.06
1	1	139	SER	CA-CB-OG	-5.67	99.77	111.10
2	2	190	ASN	CB-CA-C	5.66	120.01	110.79
3	3	161	ILE	CA-CB-CG1	-5.66	100.79	110.40
2	2	199	ILE	CA-C-O	-5.65	114.37	120.36
1	1	28	THR	N-CA-C	5.64	118.08	109.95
1	1	232	HIS	CA-CB-CG	-5.64	108.16	113.80
1	1	94	ARG	NH1-CZ-NH2	5.63	126.62	119.30
3	3	235	THR	CA-CB-OG1	-5.61	101.18	109.60
1	1	208	ASP	CA-C-O	-5.61	114.66	121.28
3	3	180	THR	CA-CB-OG1	-5.61	101.18	109.60
3	3	42	ASN	CB-CG-ND2	5.60	124.80	116.40
2	2	99	HIS	CA-CB-CG	-5.58	108.22	113.80
1	1	241	ILE	N-CA-CB	-5.58	104.29	110.99
1	1	27	HIS	CA-CB-CG	5.58	119.38	113.80
2	2	217	ASN	CB-CA-C	5.58	118.92	109.55
2	2	251	PHE	CA-C-O	-5.58	114.81	121.11
2	2	262	GLN	OE1-CD-NE2	-5.57	117.03	122.60
2	2	106	TYR	CA-C-O	-5.56	115.33	121.33
2	2	215	HIS	CA-C-O	-5.55	112.50	120.11
1	1	273	LYS	CG-CD-CE	-5.55	98.54	111.30
3	3	166	PRO	CB-CA-C	5.55	118.62	111.46
2	2	9	TYR	CA-CB-CG	-5.54	103.93	113.90
3	3	190	TRP	CA-C-O	-5.54	115.14	121.40
2	2	94	GLN	CG-CD-NE2	-5.54	108.10	116.40
2	2	68	SER	N-CA-CB	-5.53	101.88	110.29
2	2	168	ASP	CA-C-N	5.53	127.52	120.56
2	2	168	ASP	C-N-CA	5.53	127.52	120.56
3	3	107	TRP	CA-C-O	-5.53	115.16	121.40
2	2	99	HIS	CA-C-N	5.51	128.22	120.28
2	2	99	HIS	C-N-CA	5.51	128.22	120.28
2	2	188	PHE	CA-C-O	-5.51	114.93	121.66
1	1	64	GLU	CA-CB-CG	5.51	125.12	114.10
1	1	235	HIS	CA-CB-CG	-5.51	108.29	113.80
3	3	57	ASN	CA-C-N	5.51	132.08	121.18
3	3	57	ASN	C-N-CA	5.51	132.08	121.18
3	3	76	GLN	CA-C-O	-5.50	115.18	121.68
1	1	122	VAL	O-C-N	-5.50	116.73	123.00
2	2	192	ARG	CA-C-O	-5.49	111.92	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	140	GLN	CA-CB-CG	-5.49	103.12	114.10
1	1	169	GLN	O-C-N	5.48	127.92	122.12
1	1	63	SER	O-C-N	5.48	127.92	122.12
3	3	63	GLU	CG-CD-OE2	-5.47	105.83	118.40
2	2	123	LEU	CA-C-O	-5.46	114.47	120.43
2	2	43	PRO	N-CD-CG	-5.46	95.01	103.20
2	2	167	LYS	CA-C-O	5.46	126.11	119.78
1	1	144	SER	CA-C-N	-5.45	115.37	123.11
1	1	144	SER	C-N-CA	-5.45	115.37	123.11
2	2	26	GLN	OE1-CD-NE2	-5.45	117.15	122.60
2	2	92	PHE	N-CA-C	-5.45	105.03	110.97
2	2	258	SER	O-C-N	5.45	129.51	122.81
2	2	38	TRP	CB-CA-C	5.45	116.25	108.68
3	3	164	THR	CB-CA-C	5.45	119.14	109.72
2	2	187	GLN	CA-C-O	-5.44	114.89	120.99
3	3	34	ILE	CA-C-O	-5.44	113.97	120.78
3	3	168	THR	CA-CB-OG1	-5.44	101.43	109.60
1	1	21	ILE	CA-CB-CG1	-5.44	101.15	110.40
3	3	84	ASN	OD1-CG-ND2	5.44	128.04	122.60
2	2	53	THR	CA-C-O	-5.43	115.54	121.89
1	1	50	SER	CB-CA-C	5.42	117.48	109.29
4	4	50	SER	CA-CB-OG	-5.42	100.26	111.10
2	2	13	VAL	CA-C-O	-5.42	114.56	120.84
2	2	232	THR	CA-CB-OG1	-5.42	101.48	109.60
2	2	63	PHE	CA-CB-CG	5.41	119.21	113.80
3	3	78	GLU	CA-CB-CG	5.40	124.91	114.10
2	2	219	SER	N-CA-C	-5.40	100.89	109.59
3	3	90	GLY	CA-C-O	-5.40	114.87	121.68
2	2	129	GLU	CB-CA-C	-5.40	104.22	111.89
2	2	221	MET	CA-C-O	-5.38	114.34	120.32
2	2	81	LYS	CB-CG-CD	5.37	123.66	111.30
3	3	112	ARG	CB-CA-C	5.37	119.08	110.16
1	1	231	GLU	N-CA-C	-5.37	102.94	110.35
3	3	38	GLY	O-C-N	-5.36	116.00	122.38
3	3	116	MET	CB-CG-SD	-5.36	96.63	112.70
1	1	92	ASN	O-C-N	5.36	129.49	123.28
1	1	117	GLU	CG-CD-OE2	-5.35	106.09	118.40
1	1	123	ARG	NE-CZ-NH2	5.35	124.01	119.20
1	1	288	SER	CA-CB-OG	-5.35	100.41	111.10
2	2	120	GLY	CA-C-O	-5.35	114.41	122.54
3	3	195	LEU	CA-C-O	-5.34	114.97	121.05
2	2	210	ASP	CA-CB-CG	-5.33	107.27	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	286	ILE	O-C-N	5.33	127.82	121.80
2	2	177	LEU	N-CA-CB	-5.33	101.60	110.23
1	1	174	PRO	CA-C-O	-5.33	115.53	121.23
1	1	282	ARG	O-C-N	5.32	129.35	122.81
3	3	226	GLN	N-CA-C	-5.32	106.74	113.18
2	2	102	GLY	CA-C-O	-5.31	115.46	121.68
3	3	221	LEU	O-C-N	5.31	129.66	122.59
4	4	58	ASP	N-CA-CB	5.31	119.08	110.42
1	1	26	LYS	CG-CD-CE	-5.30	99.10	111.30
2	2	12	ARG	CB-CG-CD	-5.30	99.11	111.30
3	3	161	ILE	N-CA-CB	5.30	118.72	111.41
3	3	222	MET	CB-CG-SD	-5.30	96.80	112.70
2	2	72	THR	CA-CB-OG1	-5.28	101.68	109.60
3	3	143	ARG	O-C-N	5.28	128.17	122.15
2	2	262	GLN	CG-CD-NE2	5.28	124.32	116.40
3	3	16	THR	OG1-CB-CG2	5.28	119.85	109.30
3	3	86	PHE	CB-CA-C	5.28	120.49	111.68
3	3	204	GLN	CA-C-O	-5.28	115.03	121.36
3	3	192	GLN	N-CA-C	-5.27	105.13	112.45
1	1	60	PHE	N-CA-CB	-5.27	102.17	111.39
3	3	56	ASN	CA-C-N	5.27	131.60	121.54
3	3	56	ASN	C-N-CA	5.27	131.60	121.54
2	2	76	LYS	CA-C-O	-5.27	113.46	119.41
2	2	195	ASN	N-CA-C	-5.26	106.64	114.64
1	1	229	VAL	N-CA-C	-5.26	104.94	112.35
2	2	122	LEU	CA-C-O	-5.26	115.08	121.28
2	2	257	LYS	N-CA-CB	5.25	119.36	110.49
4	4	53	THR	CA-CB-OG1	-5.25	101.73	109.60
3	3	77	ASN	CA-CB-CG	-5.25	107.35	112.60
1	1	227	ARG	NE-CZ-NH2	5.24	123.92	119.20
2	2	168	ASP	OD1-CG-OD2	5.24	135.49	122.90
3	3	94	THR	CA-C-O	-5.24	113.18	119.15
1	1	201	TYR	CA-C-N	-5.23	114.79	122.06
1	1	201	TYR	C-N-CA	-5.23	114.79	122.06
3	3	208	LEU	CA-C-O	-5.23	114.99	120.80
1	1	279	ILE	CA-C-N	5.23	128.76	121.02
1	1	279	ILE	C-N-CA	5.23	128.76	121.02
2	2	20	ASN	CA-CB-CG	5.23	117.83	112.60
3	3	28	TYR	N-CA-CB	-5.23	102.29	109.97
3	3	144	GLU	CA-CB-CG	5.22	124.54	114.10
1	1	136	GLN	OE1-CD-NE2	5.22	127.82	122.60
2	2	75	SER	N-CA-CB	-5.22	101.95	109.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	63	SER	N-CA-C	5.21	116.96	111.28
3	3	158	GLN	CG-CD-OE1	5.21	131.22	120.80
2	2	243	THR	CA-C-O	-5.21	114.70	120.38
2	2	127	ILE	CA-C-O	-5.21	114.21	119.89
2	2	214	ARG	CD-NE-CZ	-5.20	117.12	124.40
1	1	282	ARG	CB-CA-C	-5.20	100.31	109.62
3	3	67	TYR	N-CA-C	-5.20	106.78	113.23
1	1	259	ARG	N-CA-CB	5.20	117.59	109.85
1	1	268	ARG	CB-CA-C	5.20	119.74	109.66
2	2	8	GLY	CA-C-N	-5.19	113.50	120.87
2	2	8	GLY	C-N-CA	-5.19	113.50	120.87
3	3	138	GLY	N-CA-C	-5.19	101.75	112.34
2	2	18	LEU	N-CA-CB	-5.18	102.78	110.71
2	2	38	TRP	CA-CB-CG	-5.18	103.77	113.60
2	2	213	THR	CA-CB-OG1	-5.17	101.84	109.60
1	1	257	ALA	N-CA-CB	-5.17	101.86	109.98
2	2	259	ILE	CA-C-O	-5.17	115.01	120.39
3	3	233	ALA	O-C-N	5.17	129.23	122.87
3	3	215	PRO	CB-CA-C	5.17	119.24	111.44
2	2	127	ILE	O-C-N	5.16	125.67	120.92
3	3	186	PHE	O-C-N	5.16	129.85	123.15
3	3	45	GLU	CG-CD-OE2	-5.15	106.55	118.40
1	1	23	SER	CA-C-O	-5.15	115.09	121.06
1	1	145	ASN	O-C-N	5.14	129.61	123.13
2	2	181	LEU	N-CA-C	-5.14	106.27	112.54
2	2	165	PRO	CA-C-O	-5.14	115.37	122.15
3	3	186	PHE	CA-CB-CG	-5.14	108.66	113.80
3	3	231	THR	CA-C-N	-5.14	115.39	122.69
3	3	231	THR	C-N-CA	-5.14	115.39	122.69
2	2	152	ARG	CD-NE-CZ	-5.13	117.22	124.40
2	2	143	LYS	CA-C-N	5.12	131.32	121.54
2	2	143	LYS	C-N-CA	5.12	131.32	121.54
1	1	204	TYR	CA-C-O	-5.12	115.64	121.58
3	3	125	ALA	CA-C-O	-5.11	115.48	121.10
2	2	259	ILE	CA-C-N	-5.11	112.68	122.13
2	2	259	ILE	C-N-CA	-5.11	112.68	122.13
3	3	109	GLY	N-CA-C	5.11	117.50	111.63
2	2	119	SER	O-C-N	5.10	129.34	123.17
1	1	27	HIS	CA-C-O	-5.10	113.09	122.62
1	1	285	ASP	CA-C-N	-5.09	111.95	120.30
1	1	285	ASP	C-N-CA	-5.09	111.95	120.30
2	2	32	VAL	O-C-N	5.09	128.33	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	82	GLY	N-CA-C	-5.09	103.03	110.87
3	3	32	PRO	CA-C-O	-5.08	115.67	121.56
2	2	126	VAL	CA-C-O	-5.08	115.09	120.53
2	2	65	THR	CA-CB-OG1	-5.08	101.98	109.60
3	3	1	GLY	N-CA-C	5.07	128.01	113.30
3	3	174	ARG	NE-CZ-NH2	-5.07	114.64	119.20
1	1	40	GLY	N-CA-C	-5.07	108.12	115.27
2	2	119	SER	CA-C-O	-5.07	115.67	121.40
2	2	215	HIS	CA-CB-CG	5.07	118.87	113.80
2	2	235	THR	CA-C-O	5.07	125.44	120.17
2	2	25	THR	CA-C-O	5.07	126.49	120.66
3	3	75	ARG	CD-NE-CZ	-5.07	117.31	124.40
3	3	217	PHE	N-CA-C	5.06	117.57	110.23
2	2	168	ASP	CB-CG-OD2	-5.06	106.76	118.40
1	1	133	THR	CA-C-O	-5.06	115.39	121.11
1	1	83	GLN	OE1-CD-NE2	5.06	127.66	122.60
3	3	95	THR	CA-CB-OG1	-5.05	102.02	109.60
3	3	177	ASP	N-CA-CB	-5.05	103.02	110.14
2	2	170	LEU	N-CA-C	-5.05	106.81	112.87
3	3	158	GLN	CB-CA-C	5.05	118.34	110.67
1	1	270	ASN	N-CA-CB	5.04	117.71	109.69
1	1	66	ASP	CA-C-O	-5.04	115.64	121.19
3	3	146	MET	CB-CA-C	5.03	120.43	110.17
2	2	261	PRO	CA-C-N	5.03	130.75	121.70
2	2	261	PRO	C-N-CA	5.03	130.75	121.70
1	1	65	THR	N-CA-C	-5.03	106.07	113.61
1	1	76	CYS	CA-C-O	-5.03	115.03	120.81
1	1	282	ARG	CG-CD-NE	-5.02	100.95	112.00
2	2	121	CYS	N-CA-CB	-5.02	102.31	110.59
3	3	217	PHE	CA-C-O	-5.02	115.67	121.19
1	1	214	GLY	O-C-N	5.01	127.61	122.85
1	1	68	GLU	N-CA-C	-5.01	106.01	111.82

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	259	ARG	Sidechain
1	1	268	ARG	Sidechain
2	2	12	ARG	Sidechain
2	2	255	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2170	0	2106	174	0
2	2	1952	0	1926	137	0
3	3	1849	0	1832	152	0
4	4	297	0	294	39	0
5	1	21	0	20	3	0
6	1	4	0	6	0	0
7	1	66	0	0	11	0
7	2	66	0	0	5	0
7	3	60	0	0	2	0
7	4	6	0	0	1	0
All	All	6491	0	6184	427	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 34.

All (427) 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)
3:3:57:ASN:CB	3:3:57:ASN:CA	1.75	1.58
4:4:33:LYS:CE	4:4:33:LYS:NZ	1.67	1.55
2:2:52:LYS:NZ	2:2:52:LYS:CE	1.68	1.54
1:1:285:ASP:CB	1:1:285:ASP:CA	1.79	1.54
3:3:179:ASP:OD1	3:3:182:THR:HB	1.41	1.17
2:2:158:SER:OG	2:2:167:LYS:HE2	1.46	1.14
3:3:21:SER:O	4:4:37:SER:HB2	1.54	1.07
1:1:285:ASP:CA	1:1:285:ASP:OD2	2.00	1.07
1:1:258:PRO:HG2	3:3:99:GLU:HG2	1.36	1.06
1:1:47:PRO:HA	3:3:164:THR:HG21	1.34	1.05
2:2:12:ARG:NH1	2:2:12:ARG:HG3	1.69	1.05
2:2:255:ARG:HG2	2:2:256:SER:H	1.24	1.03
1:1:282:ARG:HG3	3:3:57:ASN:HB3	1.41	1.02
1:1:145:ASN:HB2	7:1:1020:HOH:O	1.62	0.98
1:1:248:LYS:HE3	4:4:38:THR:O	1.63	0.98
2:2:136:GLU:HB3	2:2:140:VAL:HG21	1.44	0.97
3:3:57:ASN:CB	3:3:57:ASN:N	2.28	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1:1025:HOH:O	3:3:58:THR:HA	1.63	0.97
3:3:57:ASN:CB	3:3:57:ASN:C	2.37	0.96
1:1:285:ASP:CA	1:1:285:ASP:CG	2.37	0.95
1:1:83:GLN:HG3	1:1:85:LYS:HE2	1.47	0.94
1:1:285:ASP:CB	1:1:285:ASP:C	2.40	0.93
2:2:41:TYR:CE2	2:2:55:LYS:HD3	2.05	0.92
1:1:285:ASP:CB	1:1:285:ASP:N	2.34	0.91
2:2:235:THR:HG23	2:2:236:PRO:HD2	1.53	0.91
2:2:12:ARG:HG3	2:2:12:ARG:HH11	1.27	0.91
1:1:152:TYR:O	1:1:154:PRO:HD3	1.69	0.91
1:1:28:THR:HB	1:1:30:LYS:H	1.35	0.90
1:1:58:MET:HE1	3:3:216:ASP:O	1.71	0.90
2:2:11:ASP:HB2	4:4:68:ASN:OD1	1.71	0.90
3:3:175:TYR:HB2	3:3:182:THR:HG21	1.53	0.90
3:3:57:ASN:CA	3:3:57:ASN:CG	2.45	0.89
1:1:285:ASP:OD2	1:1:285:ASP:HA	1.73	0.88
3:3:198:PRO:HD2	3:3:201:THR:HG21	1.55	0.88
2:2:20:ASN:ND2	2:2:62:ARG:HE	1.72	0.87
1:1:47:PRO:HA	3:3:164:THR:CG2	2.03	0.87
2:2:195:ASN:ND2	2:2:196:THR:HG23	1.91	0.86
2:2:12:ARG:HH11	2:2:12:ARG:CG	1.89	0.85
2:2:116:LYS:HB3	3:3:121:ALA:HB3	1.57	0.85
1:1:165:ASP:CB	1:1:167:THR:OG1	2.24	0.85
1:1:90:ILE:HD13	1:1:90:ILE:N	1.92	0.84
1:1:282:ARG:HD2	1:1:285:ASP:O	1.78	0.84
2:2:158:SER:OG	2:2:167:LYS:CE	2.27	0.82
1:1:165:ASP:HB3	1:1:167:THR:OG1	1.80	0.82
2:2:10:SER:OG	2:2:12:ARG:HB2	1.78	0.82
2:2:30:ASN:HD22	2:2:31:ALA:H	1.27	0.82
2:2:52:LYS:NZ	2:2:52:LYS:CD	2.43	0.82
2:2:136:GLU:CB	2:2:140:VAL:HG21	2.09	0.82
1:1:38:GLU:CD	3:3:116:MET:HE2	2.05	0.81
1:1:151:MET:SD	1:1:170:SER:HB2	2.20	0.80
1:1:58:MET:CE	3:3:216:ASP:HA	2.11	0.80
2:2:9:TYR:HD1	2:2:9:TYR:N	1.77	0.80
4:4:68:ASN:OD1	4:4:68:ASN:N	2.11	0.79
2:2:195:ASN:HD22	2:2:196:THR:HG23	1.48	0.79
2:2:9:TYR:N	2:2:9:TYR:CD1	2.43	0.79
1:1:58:MET:HE1	3:3:216:ASP:C	2.08	0.78
1:1:200:PHE:CA	1:1:215:ILE:HD11	2.14	0.78
2:2:262:GLN:HE21	2:2:262:GLN:C	1.91	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:282:ARG:HG3	3:3:57:ASN:CB	2.15	0.77
2:2:255:ARG:HG2	2:2:256:SER:N	2.00	0.77
1:1:151:MET:HE1	1:1:167:THR:O	1.84	0.76
4:4:59:LEU:HD21	4:4:61:LEU:HD13	1.66	0.76
3:3:79:GLN:HB2	3:3:190:TRP:CZ3	2.19	0.76
1:1:94:ARG:NH1	1:1:94:ARG:HG2	2.00	0.76
1:1:200:PHE:HA	1:1:215:ILE:CD1	2.15	0.75
1:1:270:ASN:HA	2:2:133:ALA:HB1	1.68	0.75
3:3:179:ASP:OD1	3:3:182:THR:CB	2.31	0.74
2:2:174:ASN:C	2:2:174:ASN:HD22	1.93	0.74
3:3:197:LEU:HB3	3:3:201:THR:CG2	2.18	0.74
1:1:89:GLY:C	1:1:90:ILE:HD13	2.13	0.74
4:4:43:GLN:HG2	4:4:45:LEU:HB2	1.70	0.73
3:3:26:PRO:O	3:3:27:ASN:HB2	1.89	0.73
2:2:9:TYR:HA	7:2:293:HOH:O	1.88	0.73
2:2:188:PHE:O	2:2:194:ASN:ND2	2.22	0.73
1:1:282:ARG:CG	3:3:57:ASN:HB3	2.18	0.73
1:1:92:ASN:OD1	1:1:95:GLU:HB2	1.87	0.73
1:1:109:LEU:N	1:1:109:LEU:HD23	2.05	0.72
1:1:208:ASP:HB3	1:1:211:THR:CG2	2.18	0.72
1:1:47:PRO:CA	3:3:164:THR:HG21	2.15	0.72
1:1:58:MET:HE1	3:3:216:ASP:HA	1.71	0.71
1:1:258:PRO:CG	3:3:99:GLU:HG2	2.16	0.71
2:2:53:THR:HG22	2:2:252:SER:HB2	1.71	0.71
2:2:20:ASN:HD21	2:2:62:ARG:HE	1.39	0.71
4:4:33:LYS:NZ	4:4:33:LYS:CD	2.52	0.71
2:2:195:ASN:HD22	2:2:195:ASN:C	1.99	0.71
1:1:19:ALA:HB2	1:1:58:MET:HG2	1.72	0.71
2:2:230:VAL:CG2	2:2:234:ALA:HB3	2.20	0.71
3:3:57:ASN:CA	3:3:57:ASN:OD1	2.38	0.70
2:2:39:PRO:HG2	2:2:247:MET:HE2	1.74	0.70
2:2:235:THR:CG2	2:2:236:PRO:HD2	2.21	0.70
3:3:98:GLY:O	3:3:102:GLN:HG3	1.92	0.69
2:2:136:GLU:HB3	2:2:140:VAL:CG2	2.21	0.69
2:2:230:VAL:HG23	2:2:234:ALA:HB3	1.74	0.69
1:1:103:LYS:HA	1:1:223:SER:HB3	1.75	0.68
1:1:208:ASP:HB3	1:1:211:THR:HG22	1.75	0.68
4:4:29:ILE:HG22	4:4:29:ILE:O	1.94	0.68
3:3:20:GLN:HE22	4:4:31:TYR:H	1.42	0.68
1:1:83:GLN:CG	1:1:85:LYS:HE2	2.24	0.67
1:1:278:VAL:HG12	3:3:62:ASP:OD1	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:84:ASP:OD1	2:2:87:LYS:HE2	1.94	0.67
3:3:61:LYS:HD3	3:3:63:GLU:OE1	1.95	0.67
1:1:159:ASN:ND2	7:1:1045:HOH:O	2.28	0.67
1:1:200:PHE:HA	1:1:215:ILE:HD11	1.73	0.67
1:1:146:LEU:HD13	1:1:228:ILE:HD13	1.77	0.66
2:2:155:ASP:OD2	2:2:155:ASP:C	2.37	0.66
3:3:89:ASP:HA	3:3:93:LYS:HD2	1.78	0.66
1:1:165:ASP:HB2	1:1:167:THR:OG1	1.94	0.66
3:3:42:ASN:HD22	3:3:44:LEU:H	1.43	0.66
3:3:197:LEU:HB3	3:3:201:THR:HG22	1.77	0.66
1:1:285:ASP:CB	1:1:285:ASP:H	2.09	0.65
2:2:190:ASN:HD21	3:3:118:THR:HA	1.62	0.65
2:2:256:SER:O	2:2:257:LYS:HB3	1.96	0.65
2:2:149:PRO:HG3	2:2:154:ILE:HG13	1.78	0.64
2:2:205:ASN:HD22	2:2:206:SER:H	1.45	0.64
1:1:58:MET:HE1	3:3:216:ASP:CA	2.27	0.64
1:1:102:TRP:O	1:1:104:ILE:N	2.30	0.64
1:1:107:SER:HB2	1:1:266:ILE:HG12	1.78	0.64
1:1:248:LYS:CE	4:4:38:THR:O	2.44	0.64
3:3:79:GLN:HB2	3:3:190:TRP:CE3	2.32	0.64
2:2:12:ARG:HH21	3:3:157:LEU:HD21	1.63	0.64
2:2:30:ASN:HD22	2:2:31:ALA:N	1.94	0.64
2:2:23:ILE:HD11	2:2:243:THR:HG21	1.79	0.64
2:2:12:ARG:NH1	4:4:68:ASN:O	2.31	0.64
1:1:60:PHE:CE2	3:3:218:LYS:HB3	2.33	0.64
2:2:11:ASP:H	4:4:68:ASN:CG	2.06	0.63
2:2:39:PRO:CG	2:2:247:MET:HE2	2.29	0.63
2:2:205:ASN:ND2	2:2:206:SER:H	1.96	0.63
2:2:187:GLN:HE21	2:2:197:ALA:HA	1.63	0.63
1:1:87:ALA:HA	1:1:90:ILE:HG12	1.80	0.63
3:3:75:ARG:O	3:3:194:SER:HB2	1.99	0.62
2:2:40:GLU:HG3	2:2:41:TYR:O	2.00	0.62
3:3:84:ASN:ND2	3:3:86:PHE:H	1.98	0.62
2:2:13:VAL:O	2:2:14:GLN:HG2	1.99	0.61
2:2:38:TRP:CZ3	4:4:57:LYS:HD2	2.36	0.61
2:2:133:ALA:O	2:2:166:VAL:HG12	2.01	0.61
3:3:57:ASN:ND2	3:3:91:VAL:HG13	2.15	0.61
1:1:281:LYS:HD2	3:3:59:HIS:O	2.01	0.61
3:3:55:MET:HG3	3:3:55:MET:O	1.99	0.61
1:1:90:ILE:N	1:1:90:ILE:CD1	2.62	0.61
1:1:151:MET:HE2	1:1:168:TRP:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:175:TYR:H	3:3:182:THR:HG21	1.66	0.60
3:3:56:ASN:HB3	3:3:66:SER:HA	1.83	0.60
3:3:76:GLN:O	3:3:78:GLU:N	2.34	0.60
1:1:265:SER:HB3	1:1:268:ARG:HG2	1.83	0.60
1:1:51:ILE:HD13	3:3:166:PRO:HG3	1.82	0.59
3:3:131:TYR:HB3	3:3:149:THR:HB	1.82	0.59
2:2:256:SER:O	2:2:257:LYS:CB	2.50	0.59
1:1:94:ARG:NH1	1:1:94:ARG:CG	2.60	0.59
1:1:259:ARG:HD2	1:1:263:TYR:CE2	2.38	0.59
3:3:84:ASN:HD22	3:3:86:PHE:H	1.49	0.59
2:2:30:ASN:HD21	4:4:58:ASP:H	1.51	0.59
1:1:281:LYS:HE3	7:1:1025:HOH:O	2.03	0.58
3:3:180:THR:O	3:3:183:SER:HB3	2.02	0.58
1:1:97:LYS:HE3	7:1:1036:HOH:O	2.02	0.58
1:1:43:MET:HE3	1:1:43:MET:HA	1.85	0.57
2:2:177:LEU:HD11	3:3:94:THR:HG21	1.86	0.57
2:2:204:ILE:HG12	3:3:37:PRO:HG2	1.87	0.57
2:2:64:TYR:CD2	2:2:89:MET:HB3	2.39	0.57
1:1:151:MET:CE	1:1:168:TRP:HA	2.34	0.57
1:1:285:ASP:HB3	1:1:287:LYS:N	2.18	0.57
2:2:221:MET:HE2	2:2:223:ILE:HD11	1.87	0.57
1:1:117:GLU:HB3	1:1:200:PHE:HZ	1.68	0.57
1:1:165:ASP:HB3	1:1:167:THR:H	1.69	0.57
3:3:179:ASP:OD1	3:3:182:THR:CG2	2.52	0.57
2:2:52:LYS:NZ	2:2:52:LYS:HD3	2.20	0.57
3:3:57:ASN:HB3	3:3:57:ASN:C	2.28	0.57
1:1:43:MET:HG3	1:1:44:PRO:HD2	1.87	0.56
1:1:58:MET:HE3	3:3:216:ASP:HA	1.85	0.56
3:3:175:TYR:H	3:3:182:THR:CG2	2.19	0.56
1:1:85:LYS:HB3	1:1:236:LYS:HG3	1.87	0.56
2:2:174:ASN:C	2:2:174:ASN:ND2	2.63	0.56
3:3:31:THR:CG2	3:3:32:PRO:HD2	2.34	0.56
1:1:186:PHE:CD2	1:1:186:PHE:O	2.59	0.56
2:2:10:SER:OG	2:2:12:ARG:CB	2.53	0.56
2:2:192:ARG:NH1	7:2:326:HOH:O	2.02	0.56
3:3:53:ILE:HD11	3:3:211:ILE:HB	1.87	0.56
4:4:44:SER:O	4:4:45:LEU:C	2.48	0.56
1:1:236:LYS:HE3	1:1:238:LEU:HD13	1.88	0.56
2:2:189:ILE:HA	2:2:194:ASN:ND2	2.21	0.55
4:4:59:LEU:HD21	4:4:61:LEU:CD1	2.37	0.55
4:4:43:GLN:O	4:4:45:LEU:HB3	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:77:GLY:O	2:2:156:LEU:HB2	2.07	0.55
1:1:117:GLU:HB3	1:1:200:PHE:CZ	2.42	0.55
2:2:230:VAL:HG23	2:2:231:PRO:O	2.05	0.55
1:1:228:ILE:HD11	1:1:239:VAL:HG21	1.88	0.55
3:3:199:PRO:O	3:3:200:GLU:HB2	2.05	0.55
2:2:38:TRP:CD1	2:2:39:PRO:HD2	2.42	0.55
1:1:87:ALA:HB2	1:1:98:LEU:HD11	1.89	0.55
1:1:79:VAL:HG22	1:1:242:ARG:HG2	1.89	0.54
1:1:266:ILE:HD12	3:3:235:THR:HA	1.88	0.54
1:1:204:TYR:HD2	1:1:212:GLN:O	1.91	0.54
2:2:8:GLY:C	2:2:9:TYR:HD1	2.14	0.54
3:3:31:THR:HG23	3:3:32:PRO:HD2	1.87	0.54
3:3:198:PRO:O	3:3:201:THR:HB	2.07	0.54
2:2:230:VAL:HB	2:2:231:PRO:HD2	1.89	0.54
3:3:20:GLN:HE22	4:4:31:TYR:N	2.04	0.54
3:3:63:GLU:C	3:3:65:ASN:H	2.14	0.54
2:2:38:TRP:HZ3	4:4:57:LYS:HD2	1.70	0.54
1:1:35:THR:HG23	3:3:160:THR:HB	1.90	0.54
2:2:170:LEU:CD2	3:3:64:VAL:HA	2.38	0.54
3:3:193:THR:O	3:3:194:SER:CB	2.55	0.54
3:3:197:LEU:HB3	3:3:201:THR:HG21	1.87	0.54
3:3:55:MET:HA	3:3:91:VAL:HG11	1.90	0.54
3:3:117:TYR:CD2	3:3:155:ILE:HD13	2.44	0.53
1:1:273:LYS:O	1:1:274:ASN:C	2.52	0.53
2:2:195:ASN:ND2	2:2:195:ASN:C	2.66	0.53
1:1:99:PHE:C	1:1:99:PHE:CD2	2.87	0.53
1:1:271:TYR:HB2	1:1:272:PRO:HD2	1.89	0.53
1:1:200:PHE:CA	1:1:215:ILE:CD1	2.82	0.53
1:1:214:GLY:O	1:1:217:VAL:HG13	2.09	0.53
2:2:158:SER:HG	2:2:167:LYS:HE2	1.69	0.53
2:2:192:ARG:HD3	7:2:326:HOH:O	2.08	0.53
2:2:235:THR:CG2	2:2:236:PRO:CD	2.86	0.53
1:1:120:THR:O	1:1:199:CYS:HB2	2.08	0.53
1:1:129:THR:OG1	1:1:185:ARG:NH1	2.41	0.53
3:3:18:ASP:OD1	4:4:40:SER:HB2	2.09	0.53
3:3:86:PHE:CD1	3:3:178:PRO:HB3	2.44	0.53
1:1:187:SER:O	3:3:23:SER:HA	2.09	0.53
4:4:59:LEU:HG	4:4:60:MET:N	2.23	0.53
2:2:12:ARG:NH2	3:3:157:LEU:HD21	2.24	0.52
1:1:88:THR:O	1:1:90:ILE:HD13	2.10	0.52
1:1:83:GLN:HG3	1:1:85:LYS:CE	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:88:THR:O	1:1:90:ILE:CD1	2.58	0.52
1:1:276:GLU:HB3	1:1:277:PRO:CD	2.39	0.52
1:1:200:PHE:N	1:1:215:ILE:HD11	2.25	0.52
1:1:92:ASN:C	1:1:92:ASN:ND2	2.67	0.52
1:1:236:LYS:NZ	1:1:238:LEU:HD11	2.25	0.52
3:3:216:ASP:O	3:3:218:LYS:HE3	2.09	0.52
2:2:66:LEU:HD12	2:2:89:MET:HE3	1.91	0.52
1:1:82:ILE:HG22	1:1:100:ASN:HB2	1.91	0.52
2:2:262:GLN:C	2:2:262:GLN:NE2	2.66	0.51
4:4:44:SER:C	4:4:46:SER:N	2.68	0.51
1:1:236:LYS:HE3	1:1:238:LEU:CD1	2.40	0.51
2:2:177:LEU:CD1	3:3:94:THR:HG21	2.40	0.51
3:3:20:GLN:NE2	7:3:261:HOH:O	2.44	0.51
3:3:75:ARG:NH1	3:3:78:GLU:OE1	2.41	0.51
1:1:273:LYS:O	1:1:274:ASN:O	2.28	0.51
3:3:193:THR:O	3:3:194:SER:HB3	2.08	0.51
3:3:214:CYS:HB3	3:3:215:PRO:HD2	1.92	0.51
1:1:152:TYR:C	1:1:154:PRO:HD3	2.35	0.51
2:2:34:CYS:HB2	2:2:202:PRO:CD	2.41	0.51
3:3:84:ASN:ND2	3:3:84:ASN:C	2.69	0.51
1:1:38:GLU:OE1	3:3:116:MET:HE2	2.10	0.51
1:1:265:SER:HB2	2:2:138:GLY:O	2.11	0.51
3:3:210:PHE:N	3:3:210:PHE:CD1	2.77	0.51
1:1:190:TYR:O	1:1:190:TYR:CD2	2.64	0.51
1:1:94:ARG:CG	1:1:94:ARG:HH11	2.24	0.51
1:1:187:SER:OG	3:3:21:SER:HB2	2.11	0.51
3:3:84:ASN:HD22	3:3:86:PHE:N	2.08	0.51
1:1:92:ASN:CG	1:1:95:GLU:HB2	2.36	0.50
1:1:114:LYS:NZ	3:3:99:GLU:OE1	2.44	0.50
1:1:168:TRP:CH2	1:1:227:ARG:HB3	2.45	0.50
3:3:174:ARG:NH2	7:3:290:HOH:O	2.43	0.50
2:2:171:TYR:HA	2:2:176:THR:O	2.11	0.50
1:1:65:THR:HG22	3:3:104:TYR:CZ	2.46	0.50
2:2:139:ASN:N	2:2:139:ASN:OD1	2.44	0.50
2:2:255:ARG:CG	2:2:256:SER:H	2.00	0.50
1:1:60:PHE:CD2	3:3:218:LYS:HB3	2.46	0.50
3:3:84:ASN:HD22	3:3:84:ASN:C	2.20	0.49
2:2:13:VAL:C	2:2:14:GLN:CG	2.85	0.49
2:2:143:LYS:HG2	2:2:163:GLY:O	2.12	0.49
2:2:37:GLU:CD	3:3:35:HIS:HE2	2.19	0.49
2:2:235:THR:HG22	2:2:236:PRO:N	2.22	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:58:MET:O	1:1:59:HIS:HB2	2.13	0.49
1:1:109:LEU:N	1:1:109:LEU:CD2	2.74	0.49
2:2:205:ASN:HD22	2:2:206:SER:N	2.09	0.49
2:2:19:GLY:HA2	2:2:58:THR:HG22	1.94	0.49
3:3:95:THR:O	3:3:99:GLU:HB2	2.13	0.49
2:2:34:CYS:HB2	2:2:202:PRO:HD2	1.94	0.49
3:3:20:GLN:NE2	4:4:31:TYR:H	2.11	0.49
3:3:181:TYR:CD1	3:3:181:TYR:C	2.91	0.49
2:2:30:ASN:ND2	2:2:31:ALA:H	2.05	0.48
2:2:158:SER:HG	2:2:167:LYS:CE	2.24	0.48
2:2:217:ASN:ND2	7:2:266:HOH:O	2.45	0.48
3:3:54:PRO:O	3:3:91:VAL:HG12	2.12	0.48
3:3:125:ALA:HB3	3:3:155:ILE:HD12	1.95	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
2:2:170:LEU:HD21	3:3:64:VAL:HA	1.94	0.48
1:1:280:LYS:HE3	3:3:89:ASP:OD2	2.13	0.48
2:2:135:HIS:CD2	2:2:160:ASN:HB3	2.49	0.48
3:3:115:LEU:HD22	3:3:129:LEU:HD21	1.96	0.48
3:3:61:LYS:O	3:3:61:LYS:HG2	2.07	0.48
3:3:190:TRP:CD1	3:3:190:TRP:N	2.81	0.48
3:3:112:ARG:NH1	3:3:112:ARG:HG2	2.28	0.48
1:1:134:ALA:HB2	1:1:180:VAL:HG11	1.96	0.48
1:1:186:PHE:O	1:1:186:PHE:CG	2.66	0.48
3:3:20:GLN:HE22	4:4:30:ASN:HA	1.79	0.48
1:1:87:ALA:CA	1:1:90:ILE:HG12	2.44	0.47
3:3:112:ARG:HD3	3:3:162:VAL:CG1	2.43	0.47
3:3:195:LEU:C	3:3:196:ILE:HG12	2.40	0.47
1:1:224:MET:HG2	1:1:226:PHE:CZ	2.50	0.47
2:2:13:VAL:C	2:2:14:GLN:HG2	2.39	0.47
4:4:45:LEU:N	7:4:106:HOH:O	2.40	0.47
1:1:83:GLN:OE1	1:1:236:LYS:HD2	2.15	0.47
1:1:123:ARG:HD2	1:1:195:SER:O	2.15	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	2.14	0.47
2:2:177:LEU:CD1	3:3:94:THR:CG2	2.93	0.47
1:1:206:HIS:ND1	1:1:206:HIS:N	2.62	0.47
2:2:63:PHE:CD2	2:2:245:ALA:HB2	2.50	0.47
4:4:43:GLN:O	4:4:44:SER:C	2.58	0.47
1:1:145:ASN:CB	7:1:1020:HOH:O	2.36	0.47
4:4:59:LEU:CD2	4:4:61:LEU:HD13	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:98:LEU:HD23	1:1:98:LEU:HA	1.78	0.47
1:1:268:ARG:HH11	1:1:268:ARG:HD3	1.50	0.47
2:2:130:HIS:ND1	2:2:219:SER:OG	2.47	0.46
1:1:74:ALA:HB3	3:3:15:THR:HB	1.97	0.46
2:2:170:LEU:HD23	3:3:64:VAL:CG2	2.45	0.46
4:4:61:LEU:HD12	4:4:61:LEU:HA	1.62	0.46
1:1:87:ALA:CB	1:1:98:LEU:HD11	2.45	0.46
1:1:199:CYS:C	1:1:200:PHE:CD1	2.94	0.46
2:2:156:LEU:HD11	2:2:173:MET:SD	2.56	0.46
3:3:18:ASP:CG	4:4:40:SER:HB2	2.41	0.46
1:1:236:LYS:HE2	1:1:236:LYS:HB3	1.83	0.46
3:3:101:VAL:HG22	3:3:219:LEU:HD11	1.98	0.46
3:3:55:MET:CE	3:3:91:VAL:HG21	2.46	0.46
1:1:101:ASP:HA	1:1:224:MET:O	2.15	0.45
2:2:148:HIS:N	2:2:149:PRO:CD	2.79	0.45
1:1:159:ASN:O	1:1:160:PRO:C	2.56	0.45
3:3:57:ASN:CB	3:3:57:ASN:H	2.26	0.45
2:2:190:ASN:H	2:2:194:ASN:CB	2.30	0.45
2:2:228:LEU:CD1	2:2:238:LEU:HD22	2.47	0.45
4:4:30:ASN:HA	4:4:30:ASN:HD22	1.40	0.45
1:1:31:VAL:HG11	1:1:34:LEU:HD12	1.98	0.45
2:2:187:GLN:NE2	2:2:198:THR:H	2.14	0.45
3:3:50:ASP:HA	3:3:212:SER:HB3	1.97	0.45
2:2:170:LEU:HD23	3:3:64:VAL:HG22	1.99	0.45
3:3:55:MET:HE2	3:3:91:VAL:HG21	1.98	0.45
1:1:64:GLU:O	1:1:64:GLU:HG2	2.17	0.45
2:2:91:VAL:HG12	2:2:95:ASN:HD22	1.82	0.45
1:1:28:THR:HG22	1:1:29:GLN:H	1.81	0.45
2:2:190:ASN:H	2:2:194:ASN:HB3	1.82	0.45
1:1:215:ILE:HG22	1:1:216:THR:N	2.31	0.45
3:3:192:GLN:HE21	3:3:192:GLN:HA	1.81	0.45
1:1:285:ASP:HB3	1:1:288:SER:H	1.82	0.44
2:2:259:ILE:HG21	2:2:259:ILE:HD13	1.74	0.44
1:1:43:MET:HA	1:1:43:MET:CE	2.46	0.44
1:1:92:ASN:C	1:1:92:ASN:HD22	2.26	0.44
1:1:207:ASP:HA	2:2:144:TYR:CE1	2.52	0.44
1:1:268:ARG:NH1	3:3:236:GLU:O	2.46	0.44
3:3:57:ASN:N	3:3:57:ASN:HB2	2.25	0.44
3:3:61:LYS:O	3:3:63:GLU:HG3	2.17	0.44
1:1:93:HIS:CE1	1:1:163:TRP:HD1	2.35	0.44
1:1:289:TYR:CE1	3:3:138:GLY:HA3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:116:MET:HG3	3:3:159:SER:OG	2.17	0.44
4:4:43:GLN:O	4:4:45:LEU:CB	2.65	0.44
1:1:186:PHE:CD2	1:1:186:PHE:C	2.95	0.44
3:3:197:LEU:HD21	3:3:205:VAL:HG11	1.99	0.44
2:2:10:SER:OG	4:4:68:ASN:OXT	2.35	0.44
3:3:221:LEU:C	3:3:221:LEU:HD23	2.43	0.44
1:1:282:ARG:CG	3:3:57:ASN:CB	2.89	0.44
2:2:146:PHE:CG	2:2:164:GLY:HA2	2.52	0.44
1:1:289:TYR:CD1	3:3:138:GLY:HA3	2.53	0.44
4:4:43:GLN:HG3	4:4:45:LEU:H	1.82	0.44
1:1:47:PRO:HB3	3:3:166:PRO:HB3	1.99	0.43
1:1:286:ILE:HG23	3:3:81:PHE:HA	2.00	0.43
3:3:208:LEU:HA	3:3:208:LEU:HD12	1.73	0.43
2:2:190:ASN:O	2:2:191:LEU:C	2.61	0.43
1:1:38:GLU:N	3:3:116:MET:HE1	2.34	0.43
1:1:132:ALA:O	1:1:181:GLY:N	2.41	0.43
3:3:57:ASN:HD21	3:3:91:VAL:HG13	1.84	0.43
1:1:110:VAL:O	1:1:111:GLN:C	2.59	0.43
2:2:91:VAL:HG12	2:2:95:ASN:ND2	2.34	0.43
3:3:61:LYS:HG2	3:3:63:GLU:HG3	2.00	0.43
1:1:170:SER:O	1:1:170:SER:OG	2.33	0.43
2:2:10:SER:CB	2:2:12:ARG:HB2	2.48	0.43
3:3:112:ARG:HG2	3:3:112:ARG:HH11	1.83	0.43
1:1:285:ASP:C	1:1:285:ASP:HB3	2.38	0.43
2:2:70:THR:HG22	2:2:72:THR:HG22	2.01	0.43
3:3:151:VAL:HG11	3:3:161:ILE:HD11	2.01	0.43
2:2:95:ASN:HB3	2:2:251:PHE:CE2	2.53	0.43
2:2:205:ASN:ND2	2:2:206:SER:N	2.66	0.43
1:1:128:TYR:OH	5:1:1000:JEN:N12	2.53	0.42
4:4:43:GLN:C	4:4:45:LEU:N	2.74	0.42
1:1:137:PRO:HD2	7:1:1032:HOH:O	2.19	0.42
1:1:206:HIS:HB2	7:1:1023:HOH:O	2.18	0.42
1:1:89:GLY:C	1:1:90:ILE:CD1	2.89	0.42
1:1:96:ALA:C	1:1:97:LYS:HG2	2.43	0.42
1:1:104:ILE:HG13	1:1:223:SER:HA	2.00	0.42
1:1:206:HIS:NE2	1:1:208:ASP:HB2	2.34	0.42
3:3:174:ARG:HD2	3:3:182:THR:O	2.19	0.42
1:1:87:ALA:HB2	1:1:98:LEU:CD1	2.49	0.42
3:3:153:TRP:CD1	3:3:153:TRP:C	2.97	0.42
1:1:217:VAL:HG11	7:1:1029:HOH:O	2.20	0.42
2:2:122:LEU:HD23	2:2:224:PRO:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:225:ILE:O	3:3:68:LEU:HD21	2.19	0.42
3:3:226:GLN:HE21	3:3:226:GLN:HB2	1.21	0.42
1:1:104:ILE:HG21	5:1:1000:JEN:H112	2.01	0.42
2:2:40:GLU:O	2:2:40:GLU:CG	2.61	0.42
2:2:228:LEU:HD11	2:2:238:LEU:HD22	2.02	0.42
2:2:235:THR:CG2	2:2:236:PRO:N	2.79	0.42
1:1:215:ILE:HD13	2:2:131:GLN:HE22	1.85	0.42
1:1:285:ASP:HB3	1:1:288:SER:N	2.34	0.42
3:3:44:LEU:HA	3:3:44:LEU:HD23	1.79	0.42
1:1:289:TYR:CZ	3:3:139:PRO:HD2	2.55	0.42
4:4:43:GLN:HG2	4:4:43:GLN:O	2.18	0.42
1:1:261:LEU:HD11	2:2:171:TYR:CD1	2.55	0.41
1:1:286:ILE:HD13	1:1:286:ILE:HG21	1.77	0.41
7:1:1040:HOH:O	4:4:44:SER:HB2	2.19	0.41
2:2:69:LYS:O	2:2:239:PRO:HA	2.20	0.41
3:3:47:ILE:HG21	3:3:47:ILE:HD13	1.51	0.41
3:3:113:PHE:CE1	3:3:115:LEU:HD13	2.55	0.41
1:1:86:ASP:OD2	1:1:88:THR:HB	2.21	0.41
1:1:87:ALA:C	1:1:90:ILE:HG12	2.45	0.41
2:2:235:THR:HG22	2:2:237:SER:N	2.35	0.41
3:3:167:TRP:HZ2	3:3:172:GLN:HA	1.86	0.41
2:2:43:PRO:HG2	2:2:46:ASP:HB2	2.02	0.41
1:1:121:TYR:HA	1:1:197:TYR:O	2.21	0.41
3:3:137:ARG:HH11	3:3:137:ARG:HD3	1.22	0.41
1:1:146:LEU:HA	1:1:230:ASN:OD1	2.20	0.41
5:1:1000:JEN:H142	5:1:1000:JEN:H7	1.85	0.41
1:1:54:ARG:HH11	1:1:54:ARG:HD2	1.55	0.41
2:2:84:ASP:HB2	2:2:216:ASN:HD21	1.86	0.41
3:3:64:VAL:O	3:3:64:VAL:HG12	2.21	0.41
1:1:78:HIS:NE2	1:1:80:THR:HB	2.36	0.41
3:3:157:LEU:HD23	3:3:157:LEU:O	2.21	0.41
1:1:165:ASP:HB2	1:1:167:THR:HG1	1.84	0.40
2:2:13:VAL:HG22	2:2:26:GLN:HA	2.03	0.40
3:3:214:CYS:HB3	3:3:215:PRO:CD	2.51	0.40
3:3:231:THR:C	3:3:232:VAL:HG13	2.45	0.40
3:3:20:GLN:NE2	4:4:30:ASN:HA	2.36	0.40
1:1:265:SER:OG	2:2:139:ASN:HB3	2.21	0.40
2:2:168:ASP:HB3	7:2:308:HOH:O	2.20	0.40
3:3:101:VAL:HG13	3:3:176:THR:HB	2.04	0.40
1:1:81:GLU:CD	7:1:1036:HOH:O	2.64	0.40
2:2:172:ASN:CG	2:2:181:LEU:HD13	2.47	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	271/289 (94%)	242 (89%)	25 (9%)	4 (2%)	8	28
2	2	253/262 (97%)	233 (92%)	18 (7%)	2 (1%)	16	44
3	3	234/236 (99%)	217 (93%)	15 (6%)	2 (1%)	14	41
4	4	38/68 (56%)	34 (90%)	3 (8%)	1 (3%)	4	17
All	All	796/855 (93%)	726 (91%)	61 (8%)	9 (1%)	11	36

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	103	LYS
1	1	139	SER
3	3	57	ASN
3	3	77	ASN
1	1	212	GLN
2	2	255	ARG
2	2	257	LYS
1	1	108	SER
4	4	47	MET

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	239/253 (94%)	186 (78%)	53 (22%)	1	3
2	2	223/229 (97%)	176 (79%)	47 (21%)	1	4
3	3	209/209 (100%)	170 (81%)	39 (19%)	1	5
4	4	33/57 (58%)	20 (61%)	13 (39%)	0	0
All	All	704/748 (94%)	552 (78%)	152 (22%)	1	3

All (152) 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	81	GLU
1	1	90	ILE
1	1	95	GLU
1	1	97	LYS
1	1	98	LEU
1	1	109	LEU
1	1	122	VAL
1	1	136	GLN
1	1	137	PRO
1	1	138	ASP
1	1	144	SER
1	1	145	ASN
1	1	151	MET
1	1	159	ASN
1	1	161	LYS
1	1	167	THR
1	1	170	SER
1	1	172	SER
1	1	173	ASN
1	1	176	VAL
1	1	183	THR
1	1	184	SER
1	1	185	ARG

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Mol	Chain	Res	Type
1	1	188	VAL
1	1	193	LEU
1	1	202	ASP
1	1	215	ILE
1	1	216	THR
1	1	217	VAL
1	1	219	ASN
1	1	221	MET
1	1	223	SER
1	1	224	MET
1	1	240	LYS
1	1	254	ILE
1	1	256	ARG
1	1	266	ILE
1	1	268	ARG
1	1	273	LYS
1	1	274	ASN
1	1	275	THR
1	1	278	VAL
1	1	287	LYS
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	143	LYS
2	2	145	THR
2	2	151	GLU
2	2	152	ARG

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Mol	Chain	Res	Type
2	2	156	LEU
2	2	165	PRO
2	2	166	VAL
2	2	167	LYS
2	2	169	VAL
2	2	170	LEU
2	2	174	ASN
2	2	187	GLN
2	2	192	ARG
2	2	195	ASN
2	2	209	ILE
2	2	211	SER
2	2	217	ASN
2	2	225	ILE
2	2	230	VAL
2	2	232	THR
2	2	236	PRO
2	2	238	LEU
2	2	247	MET
2	2	250	GLU
2	2	254	ILE
2	2	255	ARG
2	2	256	SER
2	2	259	ILE
2	2	262	GLN
3	3	12	GLN
3	3	16	THR
3	3	33	ARG
3	3	42	ASN
3	3	46	ILE
3	3	55	MET
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

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Mol	Chain	Res	Type
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	218	LYS
3	3	219	LEU
3	3	220	ARG
3	3	223	LYS
3	3	226	GLN
3	3	228	ILE
3	3	230	GLN
4	4	29	ILE
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	61	ASN
1	1	92	ASN
1	1	100	ASN

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Mol	Chain	Res	Type
1	1	136	GLN
1	1	198	ASN
1	1	219	ASN
2	2	15	GLN
2	2	20	ASN
2	2	30	ASN
2	2	94	GLN
2	2	111	GLN
2	2	131	GLN
2	2	135	HIS
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	27	ASN
3	3	42	ASN
3	3	56	ASN
3	3	65	ASN
3	3	84	ASN
3	3	140	GLN
3	3	192	GLN
3	3	226	GLN
4	4	30	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
6	DMS	1	601	-	3,3,3	0.44	0	3,3,3	0.13	0
5	JEN	1	1000	-	23,23,23	0.86	1 (4%)	30,31,31	0.90	1 (3%)

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	JEN	1	1000	-	-	2/10/20/20	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	1000	JEN	C8-C7	-2.72	1.34	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	1000	JEN	C7-C6-N5	-2.03	120.86	123.84

There are no chirality outliers.

All (2) torsion outliers are listed below:

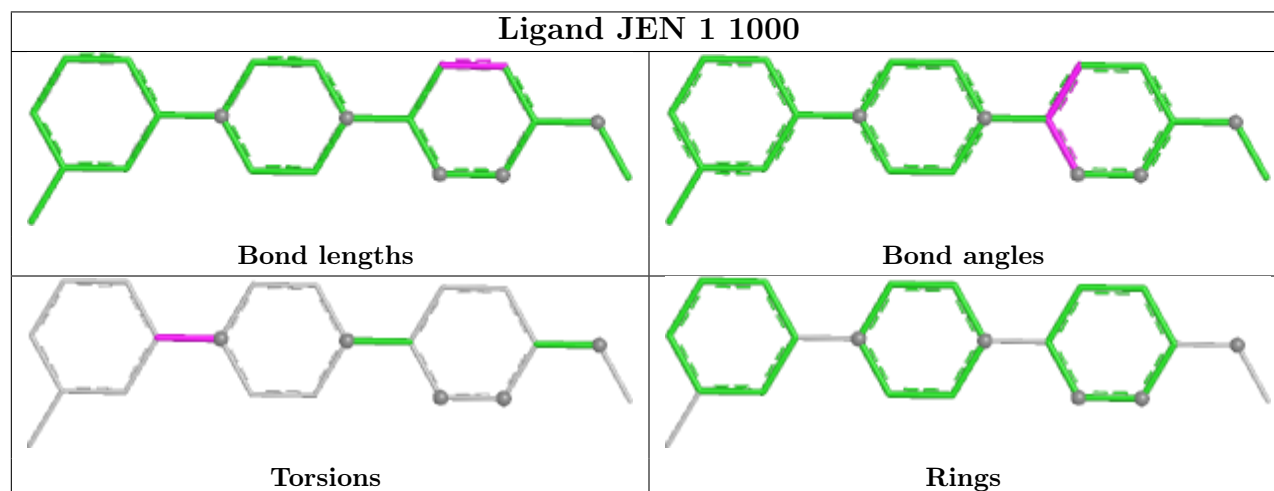
Mol	Chain	Res	Type	Atoms
5	1	1000	JEN	C16-C15-N12-C11
5	1	1000	JEN	C20-C15-N12-C11

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1	1000	JEN	3	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	122:VAL	C	123:ARG	N	1.14

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	273/289 (94%)	24.06	273 (100%) 0 0	4, 14, 30, 42	0
2	2	255/262 (97%)	25.54	255 (100%) 0 0	7, 12, 24, 42	0
3	3	236/236 (100%)	25.54	236 (100%) 0 0	8, 12, 23, 31	0
4	4	40/68 (58%)	22.34	40 (100%) 0 0	13, 24, 37, 38	0
All	All	804/855 (94%)	24.88	804 (100%) 0 0	4, 13, 28, 42	0

All (804) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	2	64	TYR	56.2
3	3	194	SER	55.6
2	2	248	CYS	55.3
2	2	137	GLY	53.9
1	1	48	SER	53.5
3	3	1	GLY	53.2
2	2	61	CYS	52.4
1	1	165	ASP	51.2
2	2	41	TYR	51.1
1	1	96	ALA	50.5
3	3	10	SER	50.4
2	2	252	SER	50.4
3	3	31	THR	49.6
2	2	21	SER	48.8
3	3	123	SER	48.7
3	3	29	GLU	48.0
2	2	15	GLN	48.0
1	1	157	ALA	47.8
3	3	181	TYR	47.8
3	3	138	GLY	47.7
3	3	21	SER	47.6

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Mol	Chain	Res	Type	RSRZ
1	1	23	SER	47.2
2	2	44	ASP	47.2
2	2	250	GLU	46.9
3	3	18	ASP	46.9
3	3	148	GLY	46.8
1	1	170	SER	46.4
3	3	179	ASP	46.3
2	2	118	HIS	46.2
2	2	20	ASN	46.2
4	4	37	SER	46.1
1	1	173	ASN	46.1
3	3	106	HIS	46.1
2	2	95	ASN	46.1
1	1	86	ASP	45.9
3	3	169	SER	45.8
2	2	47	ALA	45.8
3	3	12	GLN	45.7
1	1	158	PRO	45.1
3	3	5	THR	45.1
3	3	27	ASN	45.1
2	2	138	GLY	44.9
1	1	57	TYR	44.7
2	2	49	ASP	44.6
3	3	124	SER	44.5
2	2	117	PHE	44.4
1	1	27	HIS	44.4
2	2	51	ASN	44.4
1	1	93	HIS	44.4
1	1	166	TYR	44.3
2	2	54	SER	44.0
2	2	135	HIS	44.0
1	1	167	THR	43.9
2	2	53	THR	43.6
3	3	4	THR	43.6
1	1	139	SER	43.5
2	2	10	SER	43.4
3	3	175	TYR	43.4
3	3	143	ARG	43.3
3	3	182	THR	43.2
2	2	158	SER	43.0
3	3	200	GLU	42.8
2	2	59	SER	42.7

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Mol	Chain	Res	Type	RSRZ
1	1	206	HIS	42.6
1	1	24	GLY	42.6
1	1	22	SER	42.5
2	2	17	THR	42.4
2	2	22	THR	42.4
2	2	50	VAL	42.3
1	1	144	SER	42.2
2	2	253	GLY	42.2
2	2	48	SER	42.1
2	2	159	ALA	42.0
3	3	190	TRP	41.9
1	1	25	PRO	41.9
3	3	201	THR	41.9
3	3	171	VAL	41.7
1	1	132	ALA	41.6
2	2	43	PRO	41.6
3	3	3	PRO	41.6
2	2	261	PRO	41.6
2	2	93	GLY	41.4
1	1	55	THR	41.3
2	2	98	PHE	41.2
2	2	115	THR	41.2
2	2	89	MET	41.2
1	1	238	LEU	41.2
2	2	233	GLY	41.2
3	3	9	GLY	41.1
1	1	28	THR	41.0
2	2	94	GLN	41.0
3	3	141	ASP	41.0
2	2	237	SER	40.8
1	1	288	SER	40.7
3	3	8	PRO	40.5
4	4	31	TYR	40.3
3	3	144	GLU	40.3
1	1	53	THR	40.2
2	2	58	THR	40.2
2	2	25	THR	40.1
4	4	39	SER	40.0
1	1	233	ASP	40.0
1	1	59	HIS	40.0
2	2	230	VAL	40.0
3	3	199	PRO	39.9

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Mol	Chain	Res	Type	RSRZ
3	3	73	ALA	39.8
3	3	193	THR	39.8
3	3	170	GLY	39.8
2	2	235	THR	39.7
2	2	90	GLY	39.7
2	2	19	GLY	39.6
2	2	114	ALA	39.5
1	1	237	THR	39.4
1	1	141	ASN	39.4
1	1	58	MET	39.4
1	1	169	GLN	39.3
3	3	142	ARG	39.2
2	2	255	ARG	39.2
1	1	209	ALA	39.1
3	3	180	THR	39.0
1	1	156	GLY	39.0
1	1	171	ALA	38.9
4	4	38	THR	38.9
2	2	62	ARG	38.9
3	3	146	MET	38.8
2	2	232	THR	38.7
2	2	99	HIS	38.7
2	2	72	THR	38.6
2	2	256	SER	38.6
3	3	74	ASN	38.5
3	3	198	PRO	38.4
2	2	234	ALA	38.4
3	3	6	THR	38.4
3	3	17	ASP	38.3
2	2	45	VAL	38.3
4	4	30	ASN	38.2
1	1	284	GLY	38.2
1	1	137	PRO	38.1
3	3	30	PRO	38.1
1	1	20	SER	38.1
2	2	236	PRO	38.1
1	1	88	THR	38.0
3	3	14	LEU	38.0
3	3	72	ASN	37.9
2	2	56	PRO	37.9
1	1	89	GLY	37.8
3	3	76	GLN	37.8

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Mol	Chain	Res	Type	RSRZ
3	3	105	THR	37.8
1	1	182	ASP	37.7
2	2	155	ASP	37.6
1	1	52	GLU	37.6
1	1	142	TYR	37.5
2	2	13	VAL	37.5
1	1	235	HIS	37.3
2	2	52	LYS	37.3
4	4	34	ASP	37.2
3	3	172	GLN	37.1
1	1	19	ALA	37.1
1	1	92	ASN	37.0
2	2	229	THR	37.0
1	1	232	HIS	36.8
2	2	231	PRO	36.8
3	3	145	ALA	36.7
1	1	49	ASP	36.6
2	2	160	ASN	36.6
3	3	20	GLN	36.5
2	2	24	THR	36.5
1	1	56	THR	36.4
2	2	57	ASP	36.4
1	1	230	ASN	36.3
2	2	46	ASP	36.1
3	3	232	VAL	36.1
3	3	26	PRO	36.1
3	3	2	LEU	36.0
2	2	249	THR	36.0
1	1	18	VAL	35.9
2	2	91	VAL	35.8
2	2	140	VAL	35.8
3	3	137	ARG	35.7
3	3	231	THR	35.6
1	1	138	ASP	35.5
3	3	60	THR	35.4
1	1	140	ALA	35.3
3	3	183	SER	35.2
1	1	153	VAL	35.2
3	3	197	LEU	35.0
1	1	61	ASN	35.0
2	2	228	LEU	35.0
3	3	178	PRO	35.0

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Mol	Chain	Res	Type	RSRZ
1	1	168	TRP	34.7
3	3	23	SER	34.6
1	1	136	GLN	34.3
2	2	245	ALA	34.3
1	1	234	GLU	34.3
1	1	181	GLY	34.2
2	2	60	VAL	34.1
2	2	157	SER	34.0
1	1	172	SER	34.0
2	2	100	SER	33.9
3	3	77	ASN	33.8
1	1	277	PRO	33.6
3	3	7	LEU	33.6
3	3	32	PRO	33.5
1	1	187	SER	33.5
2	2	258	SER	33.5
2	2	112	CYS	33.5
1	1	54	ARG	33.4
2	2	55	LYS	33.3
3	3	11	GLY	33.3
3	3	28	TYR	33.1
1	1	274	ASN	33.1
2	2	139	ASN	33.0
4	4	32	TYR	33.0
2	2	163	GLY	32.9
1	1	17	THR	32.9
2	2	238	LEU	32.9
3	3	173	PHE	32.8
1	1	143	SER	32.4
1	1	135	SER	32.3
2	2	26	GLN	32.2
3	3	58	THR	32.1
1	1	154	PRO	31.9
1	1	285	ASP	31.8
2	2	251	PHE	31.8
1	1	155	PRO	31.6
3	3	13	PHE	31.5
3	3	177	ASP	31.5
3	3	221	LEU	31.4
2	2	134	SER	31.3
1	1	87	ALA	31.3
2	2	9	TYR	31.2

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Mol	Chain	Res	Type	RSRZ
1	1	29	GLN	31.2
3	3	136	ALA	31.2
3	3	108	SER	31.1
1	1	26	LYS	31.1
1	1	90	ILE	31.0
3	3	140	GLN	30.9
3	3	191	TYR	30.7
3	3	133	PRO	30.6
3	3	196	ILE	30.6
1	1	133	THR	30.6
2	2	71	TRP	30.6
3	3	125	ALA	30.5
1	1	272	PRO	30.5
3	3	139	PRO	30.4
1	1	180	VAL	30.2
1	1	21	ILE	30.2
4	4	29	ILE	30.0
3	3	16	THR	30.0
4	4	45	LEU	29.9
3	3	78	GLU	29.8
1	1	83	GLN	29.8
1	1	145	ASN	29.8
3	3	195	LEU	29.7
3	3	126	LYS	29.7
3	3	147	LEU	29.6
4	4	40	SER	29.5
2	2	145	THR	29.4
2	2	63	PHE	29.4
2	2	42	LEU	29.4
2	2	73	THR	29.2
3	3	192	GLN	29.2
1	1	159	ASN	29.2
1	1	164	ASP	29.2
2	2	161	GLU	28.9
1	1	134	ALA	28.9
2	2	162	VAL	28.7
1	1	281	LYS	28.6
1	1	162	GLU	28.6
2	2	23	ILE	28.6
3	3	56	ASN	28.6
3	3	79	GLN	28.5
2	2	119	SER	28.3

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Mol	Chain	Res	Type	RSRZ
1	1	60	PHE	28.3
2	2	113	ASN	28.2
2	2	136	GLU	28.2
1	1	239	VAL	28.2
2	2	70	THR	28.1
2	2	101	LEU	28.0
4	4	46	SER	28.0
1	1	192	GLY	28.0
1	1	273	LYS	28.0
1	1	146	LEU	27.9
1	1	283	LYS	27.8
3	3	135	GLY	27.7
2	2	16	ILE	27.7
2	2	65	THR	27.6
3	3	75	ARG	27.5
3	3	224	ASP	27.5
1	1	151	MET	27.5
2	2	262	GLN	27.4
2	2	259	ILE	27.3
1	1	91	ASP	27.2
2	2	75	SER	27.2
3	3	59	HIS	26.9
1	1	85	LYS	26.8
1	1	160	PRO	26.8
3	3	132	THR	26.6
3	3	167	TRP	26.6
3	3	122	LEU	26.6
1	1	282	ARG	26.5
2	2	254	ILE	26.5
3	3	134	PRO	26.4
1	1	208	ASP	26.3
3	3	15	THR	26.3
2	2	18	LEU	26.2
2	2	74	GLY	26.2
4	4	44	SER	26.0
2	2	246	PRO	25.9
1	1	98	LEU	25.9
2	2	239	PRO	25.8
1	1	231	GLU	25.8
3	3	82	GLY	25.6
3	3	24	ALA	25.5
1	1	161	LYS	25.5

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Mol	Chain	Res	Type	RSRZ
3	3	202	THR	25.5
2	2	27	GLU	25.4
2	2	14	GLN	25.4
2	2	164	GLY	25.4
3	3	216	ASP	25.3
2	2	88	ASP	25.2
1	1	176	VAL	25.2
2	2	260	VAL	25.1
2	2	257	LYS	25.1
4	4	36	ALA	25.1
3	3	121	ALA	25.0
1	1	84	ASN	24.9
3	3	19	ARG	24.8
1	1	178	PHE	24.6
2	2	243	THR	24.5
3	3	25	LEU	24.5
3	3	120	PRO	24.3
3	3	230	GLN	24.2
3	3	57	ASN	24.1
2	2	40	GLU	24.0
2	2	8	GLY	23.8
3	3	174	ARG	23.7
3	3	225	THR	23.7
1	1	175	SER	23.7
1	1	276	GLU	23.6
1	1	95	GLU	23.6
1	1	99	PHE	23.5
2	2	92	PHE	23.3
3	3	229	SER	23.3
4	4	43	GLN	23.2
3	3	71	LEU	23.1
2	2	102	GLY	23.0
3	3	203	GLY	22.9
1	1	205	SER	22.9
1	1	30	LYS	22.8
4	4	41	ALA	22.8
3	3	226	GLN	22.8
1	1	189	PRO	22.7
1	1	207	ASP	22.7
1	1	275	THR	22.6
1	1	129	THR	22.6
3	3	176	THR	22.6

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Mol	Chain	Res	Type	RSRZ
1	1	51	ILE	22.5
1	1	236	LYS	22.4
1	1	147	VAL	22.3
1	1	210	GLU	22.3
3	3	150	HIS	22.3
3	3	119	GLY	22.3
1	1	183	THR	22.2
3	3	168	THR	22.2
1	1	179	LYS	22.1
3	3	189	CYS	22.0
1	1	229	VAL	22.0
1	1	131	LEU	22.0
2	2	116	LYS	22.0
3	3	149	THR	22.0
3	3	204	GLN	21.8
1	1	50	SER	21.8
1	1	82	ILE	21.8
3	3	222	MET	21.8
1	1	265	SER	21.7
2	2	144	TYR	21.6
4	4	35	ALA	21.6
1	1	249	HIS	21.6
2	2	28	ALA	21.4
3	3	89	ASP	21.4
1	1	63	SER	21.3
1	1	188	VAL	21.3
1	1	163	TRP	21.3
1	1	211	THR	21.2
3	3	233	ALA	21.2
4	4	33	LYS	21.1
3	3	61	LYS	21.1
1	1	31	VAL	21.1
2	2	247	MET	20.9
1	1	130	ILE	20.8
1	1	149	GLN	20.6
3	3	154	ASP	20.6
2	2	97	PHE	20.5
1	1	62	GLY	20.4
3	3	227	THR	20.4
2	2	141	SER	20.3
1	1	148	VAL	20.2
3	3	51	THR	20.0

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Mol	Chain	Res	Type	RSRZ
3	3	235	THR	19.9
1	1	244	TYR	19.9
3	3	228	ILE	19.8
3	3	34	ILE	19.8
1	1	94	ARG	19.8
3	3	107	TRP	19.8
2	2	86	LEU	19.6
1	1	174	PRO	19.6
1	1	76	CYS	19.5
3	3	80	VAL	19.4
2	2	150	GLY	19.4
2	2	12	ARG	19.3
1	1	194	ALA	19.3
3	3	223	LYS	19.3
1	1	100	ASN	19.3
2	2	241	THR	19.2
1	1	125	ASP	19.2
1	1	271	TYR	19.2
1	1	177	PHE	19.2
1	1	286	ILE	19.2
3	3	220	ARG	19.2
1	1	127	GLU	19.2
2	2	37	GLU	19.1
1	1	77	VAL	19.1
2	2	66	LEU	19.1
2	2	244	ILE	19.1
1	1	270	ASN	19.0
4	4	48	ASP	19.0
3	3	22	PRO	19.0
1	1	262	PRO	18.9
3	3	234	LEU	18.9
2	2	36	ALA	18.9
3	3	50	ASP	18.8
2	2	143	LYS	18.8
2	2	191	LEU	18.8
1	1	287	LYS	18.8
1	1	47	PRO	18.8
3	3	127	LEU	18.7
2	2	193	THR	18.7
3	3	205	VAL	18.7
4	4	68	ASN	18.7
2	2	39	PRO	18.7

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Mol	Chain	Res	Type	RSRZ
3	3	155	ILE	18.6
2	2	195	ASN	18.6
1	1	121	TYR	18.5
2	2	194	ASN	18.5
1	1	243	VAL	18.5
1	1	105	ASN	18.5
1	1	80	THR	18.4
3	3	114	SER	18.4
1	1	190	TYR	18.3
2	2	165	PRO	18.3
3	3	49	VAL	18.3
4	4	58	ASP	18.3
1	1	248	LYS	18.3
3	3	81	PHE	18.3
3	3	164	THR	18.3
3	3	209	SER	18.2
1	1	106	LEU	18.2
1	1	195	SER	18.1
3	3	95	THR	18.1
2	2	207	VAL	18.1
3	3	33	ARG	18.0
1	1	81	GLU	18.0
2	2	171	TYR	18.0
3	3	41	HIS	18.0
4	4	63	GLY	17.9
2	2	240	ILE	17.9
2	2	216	ASN	17.9
2	2	156	LEU	17.9
3	3	152	VAL	17.9
3	3	96	LEU	17.8
1	1	258	PRO	17.8
1	1	101	ASP	17.8
3	3	67	TYR	17.8
2	2	126	VAL	17.8
1	1	37	ASN	17.8
2	2	166	VAL	17.7
2	2	218	VAL	17.7
1	1	107	SER	17.7
2	2	127	ILE	17.7
3	3	104	TYR	17.7
2	2	96	MET	17.6
1	1	184	SER	17.6

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Mol	Chain	Res	Type	RSRZ
4	4	52	PHE	17.6
1	1	215	ILE	17.5
3	3	236	GLU	17.5
3	3	212	SER	17.5
2	2	38	TRP	17.4
4	4	66	ALA	17.4
2	2	168	ASP	17.4
3	3	52	LEU	17.4
3	3	36	ILE	17.4
3	3	211	ILE	17.4
1	1	250	VAL	17.4
2	2	149	PRO	17.4
2	2	182	LEU	17.3
3	3	97	LEU	17.3
1	1	102	TRP	17.3
1	1	68	GLU	17.3
3	3	62	ASP	17.3
1	1	69	CYS	17.3
2	2	184	PHE	17.3
1	1	32	PRO	17.3
1	1	213	TYR	17.2
1	1	263	TYR	17.2
2	2	35	TYR	17.2
2	2	120	GLY	17.2
3	3	153	TRP	17.2
2	2	172	ASN	17.2
2	2	180	ASN	17.2
1	1	289	TYR	17.2
3	3	103	TYR	17.2
2	2	227	PRO	17.2
1	1	241	ILE	17.2
1	1	226	PHE	17.1
4	4	67	LEU	17.1
3	3	113	PHE	17.1
2	2	125	VAL	17.1
3	3	165	ILE	17.1
2	2	183	ILE	17.0
2	2	146	PHE	17.0
2	2	181	LEU	17.0
3	3	100	ILE	17.0
2	2	68	SER	17.0
3	3	65	ASN	17.0

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Mol	Chain	Res	Type	RSRZ
3	3	87	ILE	17.0
2	2	128	PRO	16.9
3	3	46	ILE	16.9
1	1	279	ILE	16.9
3	3	40	VAL	16.9
3	3	53	ILE	16.9
2	2	176	THR	16.9
2	2	201	ILE	16.8
1	1	67	VAL	16.8
2	2	106	TYR	16.8
1	1	124	PHE	16.8
2	2	67	ASP	16.8
3	3	219	LEU	16.8
3	3	47	ILE	16.7
2	2	186	HIS	16.7
3	3	160	THR	16.7
3	3	159	SER	16.7
1	1	97	LYS	16.7
1	1	257	ALA	16.7
3	3	217	PHE	16.7
3	3	128	ILE	16.7
1	1	219	ASN	16.7
1	1	35	THR	16.6
1	1	216	THR	16.6
1	1	119	PHE	16.6
1	1	278	VAL	16.6
1	1	228	ILE	16.5
3	3	83	THR	16.5
3	3	118	THR	16.5
1	1	191	VAL	16.5
2	2	217	ASN	16.5
1	1	201	TYR	16.5
3	3	54	PRO	16.5
1	1	65	THR	16.5
2	2	148	HIS	16.5
3	3	210	PHE	16.5
1	1	45	VAL	16.5
2	2	142	VAL	16.5
3	3	187	LEU	16.5
1	1	186	PHE	16.5
1	1	218	LEU	16.4
4	4	60	MET	16.4

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Mol	Chain	Res	Type	RSRZ
2	2	11	ASP	16.4
4	4	61	LEU	16.4
1	1	255	PRO	16.4
1	1	254	ILE	16.4
3	3	92	PHE	16.4
1	1	202	ASP	16.4
2	2	208	PRO	16.4
2	2	85	ALA	16.3
2	2	206	SER	16.3
2	2	185	PRO	16.3
2	2	110	VAL	16.3
4	4	53	THR	16.3
2	2	220	LEU	16.3
2	2	29	ALA	16.3
1	1	118	LEU	16.3
1	1	152	TYR	16.3
2	2	124	VAL	16.3
1	1	40	GLY	16.3
1	1	78	HIS	16.2
1	1	71	LEU	16.2
2	2	123	LEU	16.2
2	2	107	THR	16.2
3	3	156	GLY	16.2
2	2	188	PHE	16.2
1	1	74	ALA	16.2
2	2	190	ASN	16.2
3	3	184	ALA	16.2
1	1	66	ASP	16.2
2	2	222	VAL	16.2
3	3	161	ILE	16.2
3	3	70	PRO	16.1
2	2	154	ILE	16.1
2	2	130	HIS	16.1
2	2	174	ASN	16.1
2	2	213	THR	16.1
2	2	129	GLU	16.1
4	4	64	ALA	16.1
3	3	37	PRO	16.1
2	2	87	LYS	16.1
2	2	204	ILE	16.1
1	1	120	THR	16.1
4	4	56	VAL	16.0

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Mol	Chain	Res	Type	RSRZ
3	3	85	LEU	16.0
2	2	32	VAL	16.0
1	1	269	THR	16.0
2	2	147	THR	16.0
2	2	131	GLN	16.0
4	4	47	MET	16.0
1	1	247	ALA	16.0
2	2	242	VAL	16.0
2	2	225	ILE	16.0
3	3	208	LEU	16.0
1	1	42	THR	16.0
1	1	223	SER	16.0
2	2	223	ILE	15.9
3	3	185	GLY	15.9
3	3	162	VAL	15.9
1	1	46	LEU	15.9
2	2	179	GLY	15.9
3	3	111	LEU	15.9
3	3	115	LEU	15.9
1	1	39	THR	15.9
1	1	196	ALA	15.9
1	1	252	ALA	15.9
2	2	211	SER	15.9
1	1	112	LEU	15.9
2	2	122	LEU	15.9
2	2	178	LEU	15.9
2	2	198	THR	15.8
2	2	82	LEU	15.8
3	3	129	LEU	15.8
3	3	112	ARG	15.8
2	2	196	THR	15.8
1	1	104	ILE	15.8
2	2	219	SER	15.8
2	2	189	ILE	15.8
2	2	177	LEU	15.8
2	2	200	VAL	15.7
1	1	267	GLY	15.7
2	2	202	PRO	15.7
4	4	55	PRO	15.7
1	1	261	LEU	15.7
2	2	209	ILE	15.7
3	3	188	SER	15.7

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Mol	Chain	Res	Type	RSRZ
3	3	163	MET	15.6
2	2	83	PRO	15.6
1	1	266	ILE	15.6
1	1	150	ALA	15.6
3	3	69	ILE	15.6
2	2	108	VAL	15.6
3	3	64	VAL	15.5
3	3	43	LEU	15.5
2	2	33	VAL	15.5
3	3	130	ALA	15.5
3	3	48	GLN	15.5
2	2	203	TYR	15.5
1	1	108	SER	15.4
1	1	41	ALA	15.4
3	3	186	PHE	15.4
2	2	187	GLN	15.4
1	1	203	GLY	15.3
4	4	65	PRO	15.3
2	2	104	SER	15.3
2	2	69	LYS	15.3
1	1	122	VAL	15.3
1	1	70	PHE	15.3
2	2	192	ARG	15.3
2	2	132	LEU	15.3
1	1	200	PHE	15.3
1	1	116	LEU	15.3
3	3	166	PRO	15.3
3	3	131	TYR	15.3
1	1	193	LEU	15.2
2	2	199	ILE	15.2
3	3	158	GLN	15.2
3	3	94	THR	15.2
2	2	221	MET	15.2
1	1	256	ARG	15.2
3	3	66	SER	15.2
3	3	101	VAL	15.2
3	3	206	TYR	15.2
3	3	213	ALA	15.2
3	3	151	VAL	15.1
4	4	42	GLY	15.1
2	2	197	ALA	15.1
1	1	79	VAL	15.1

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Mol	Chain	Res	Type	RSRZ
3	3	207	LEU	15.1
1	1	128	TYR	15.1
2	2	133	ALA	15.0
3	3	44	LEU	15.0
1	1	75	ALA	15.0
3	3	42	ASN	15.0
1	1	240	LYS	14.9
1	1	214	GLY	14.9
1	1	227	ARG	14.9
1	1	126	SER	14.9
1	1	117	GLU	14.8
3	3	84	ASN	14.8
2	2	121	CYS	14.8
1	1	109	LEU	14.7
3	3	91	VAL	14.7
2	2	210	ASP	14.7
1	1	224	MET	14.7
4	4	59	LEU	14.7
2	2	105	GLY	14.7
2	2	81	LYS	14.6
1	1	264	THR	14.6
3	3	109	GLY	14.6
1	1	198	ASN	14.6
3	3	215	PRO	14.5
1	1	222	GLY	14.5
2	2	84	ASP	14.5
2	2	169	VAL	14.4
2	2	212	MET	14.3
4	4	49	PRO	14.3
3	3	110	SER	14.3
3	3	63	GLU	14.3
2	2	80	TRP	14.2
1	1	268	ARG	14.2
1	1	33	ILE	14.2
1	1	253	TRP	14.1
2	2	226	ALA	14.1
1	1	110	VAL	14.1
1	1	197	TYR	14.1
3	3	99	GLU	14.1
1	1	212	GLN	14.1
2	2	205	ASN	14.0
3	3	98	GLY	14.0

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Mol	Chain	Res	Type	RSRZ
3	3	90	GLY	14.0
1	1	225	ALA	13.9
2	2	153	GLY	13.9
1	1	217	VAL	13.9
3	3	35	HIS	13.9
2	2	78	TRP	13.9
1	1	103	LYS	13.9
2	2	76	LYS	13.8
3	3	68	LEU	13.8
1	1	38	GLU	13.6
2	2	170	LEU	13.6
3	3	157	LEU	13.6
2	2	31	ALA	13.6
1	1	123	ARG	13.5
3	3	117	TYR	13.5
2	2	215	HIS	13.5
1	1	260	ALA	13.4
1	1	246	ARG	13.3
3	3	214	CYS	13.3
4	4	51	LYS	13.3
1	1	115	LYS	13.2
3	3	88	GLY	13.2
2	2	175	GLY	13.2
4	4	62	LYS	13.2
2	2	152	ARG	13.1
2	2	34	CYS	13.1
4	4	54	GLU	13.1
1	1	204	TYR	13.0
1	1	43	MET	13.0
1	1	185	ARG	13.0
1	1	242	ARG	13.0
3	3	218	LYS	13.0
3	3	86	PHE	13.0
1	1	44	PRO	13.0
1	1	64	GLU	13.0
2	2	103	ARG	13.0
1	1	34	LEU	12.9
1	1	111	GLN	12.9
2	2	224	PRO	12.9
1	1	251	GLU	12.8
1	1	259	ARG	12.7
3	3	55	MET	12.6

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Mol	Chain	Res	Type	RSRZ
2	2	30	ASN	12.6
2	2	77	GLY	12.6
2	2	111	GLN	12.6
3	3	102	GLN	12.6
2	2	109	HIS	12.5
4	4	50	SER	12.5
2	2	79	CYS	12.5
2	2	173	MET	12.4
1	1	221	MET	12.4
1	1	72	GLY	12.4
3	3	38	GLY	12.4
2	2	167	LYS	12.4
3	3	116	MET	12.4
3	3	45	GLU	12.3
3	3	93	LYS	12.3
1	1	199	CYS	12.2
1	1	280	LYS	12.2
1	1	245	HIS	12.0
1	1	220	HIS	11.9
2	2	214	ARG	11.9
4	4	57	LYS	11.8
1	1	73	ARG	11.8
1	1	114	LYS	11.8
3	3	39	LYS	11.6
1	1	36	ALA	11.6
2	2	151	GLU	11.6
1	1	113	ARG	11.5

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

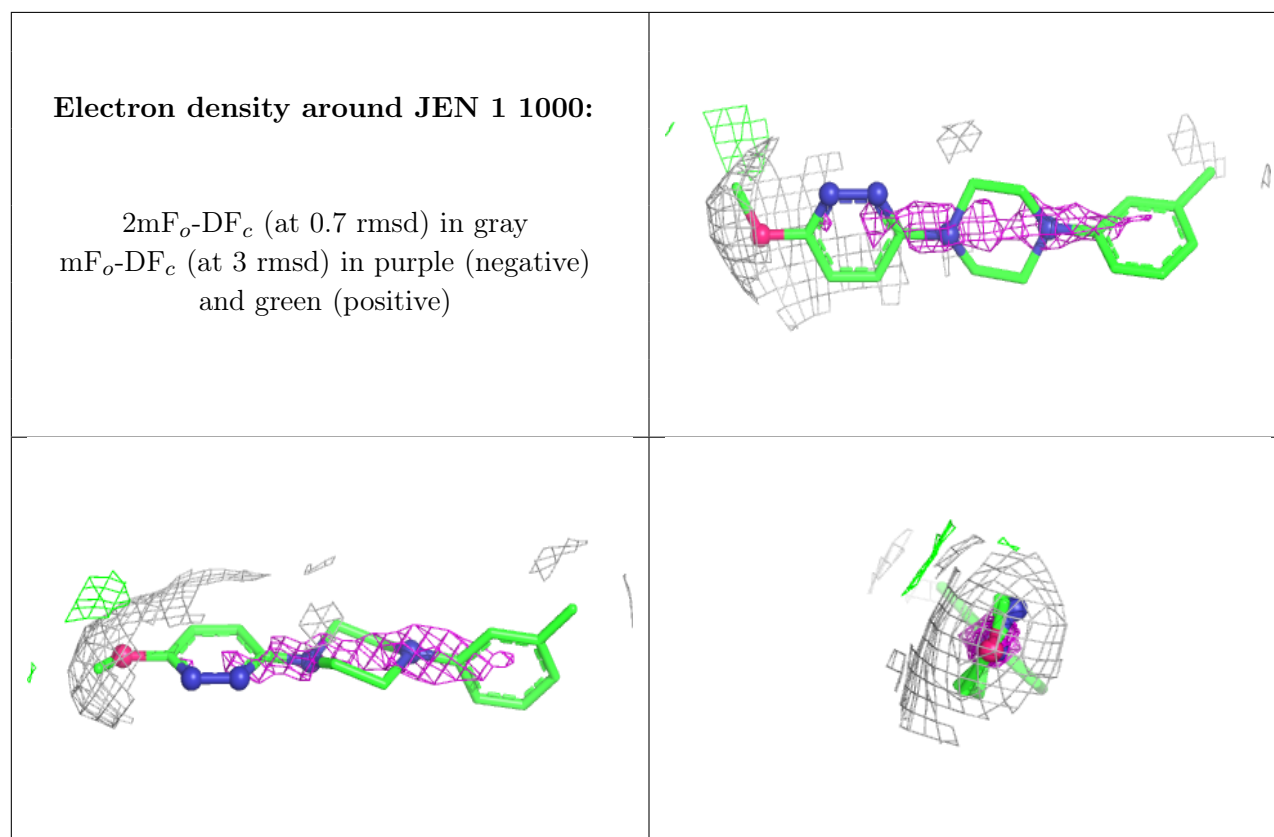
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	DMS	1	601	4/4	-0.96	2.19	1,1,1,1	0
5	JEN	1	1000	21/21	-0.67	1.66	1,1,1,1	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.