



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:55 PM UTC

PDB ID : 2YPI / pdb_00002ypi
Title : CRYSTALLOGRAPHIC ANALYSIS OF THE COMPLEX BETWEEN
TRIOSEPHOSPHATE ISOMERASE AND 2-PHOSPHOGLYCOLATE AT
2.5-ANGSTROMS RESOLUTION. IMPLICATIONS FOR CATALYSIS
Authors : Lolis, E.; Petsko, G.A.
Deposited on : 1990-01-12
Resolution : 2.50 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

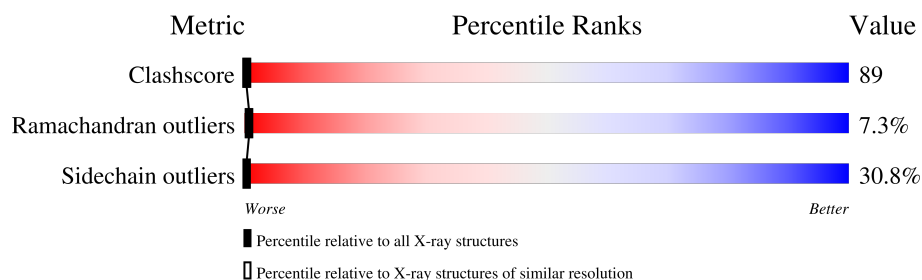
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	247	
1	B	247	

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
2	PGA	B	249	-	X	-	-

2 Entry composition [i](#)

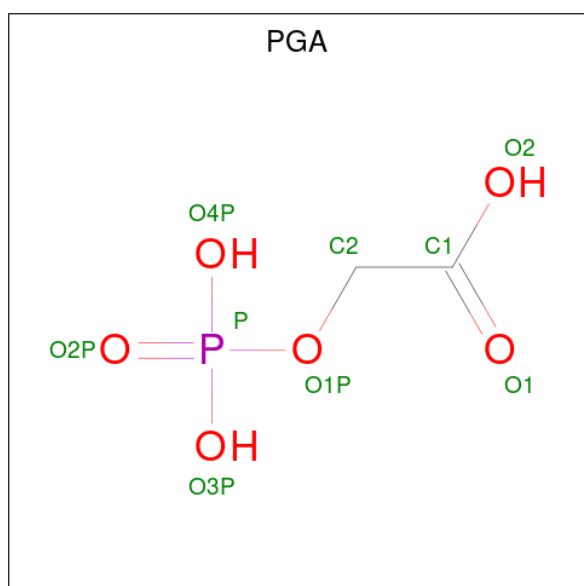
There are 3 unique types of molecules in this entry. The entry contains 3809 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRIOSEPHOSPHATE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			1883	1196	320	365	2			
1	B	247	Total	C	N	O	S	0	0	0
			1883	1196	320	365	2			

- Molecule 2 is 2-PHOSPHOGLYCOLIC ACID (CCD ID: PGA) (formula: $C_2H_5O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			9	2	6	1		
2	B	1	Total	C	O	P	0	0
			9	2	6	1		

- Molecule 3 is water.

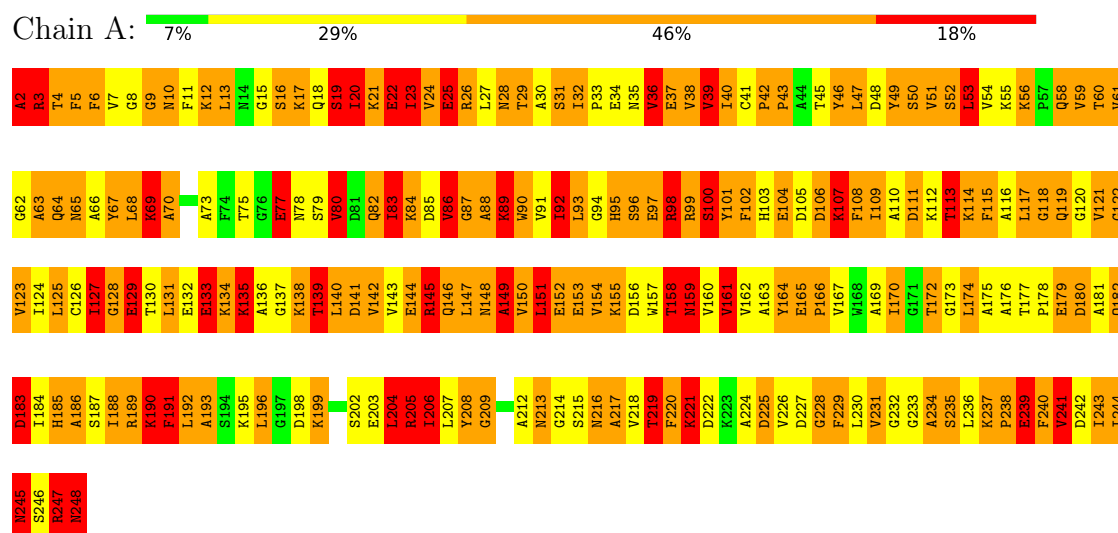
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total 12	O 12	0	0
3	B	13	Total 13	O 13	0	0

3 Residue-property plots

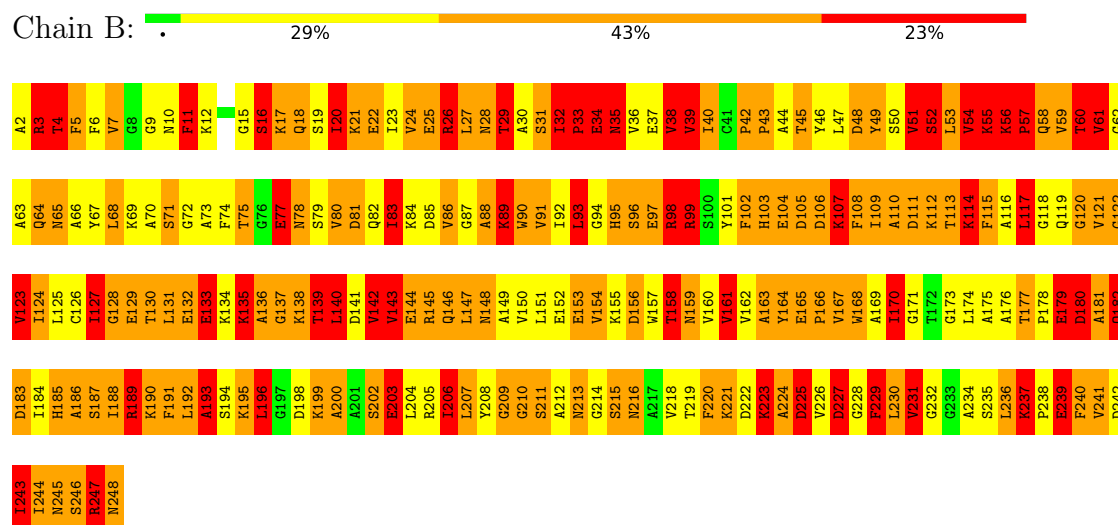
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: TRIOSEPHOSPHATE ISOMERASE



• Molecule 1: TRIOSEPHOSPHATE ISOMERASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.35Å 83.97Å 38.67Å 90.00° 99.70° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.177 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3809	wwPDB-VP
Average B, all atoms (Å ²)	6.0	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: PGA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.62	121/1915 (6.3%)	3.47	336/2590 (13.0%)
1	B	2.59	119/1915 (6.2%)	3.32	314/2590 (12.1%)
All	All	2.61	240/3830 (6.3%)	3.40	650/5180 (12.5%)

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

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

All (240) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	SER	CA-C	11.83	1.67	1.52
1	A	108	PHE	N-CA	11.53	1.59	1.46
1	A	162	VAL	CA-CB	-10.69	1.40	1.54
1	A	48	ASP	N-CA	10.41	1.59	1.45
1	A	100	SER	N-CA	10.18	1.58	1.46
1	A	155	LYS	C-O	10.15	1.32	1.23
1	B	7	VAL	CA-C	9.95	1.64	1.52
1	B	139	THR	C-O	9.90	1.36	1.24
1	A	3	ARG	N-CA	-9.89	1.33	1.46
1	B	74	PHE	N-CA	9.07	1.58	1.46
1	A	185	HIS	C-N	-8.78	1.23	1.33
1	A	170	ILE	CA-CB	-8.76	1.42	1.54
1	A	113	THR	C-N	-8.70	1.22	1.33
1	B	209	GLY	C-O	8.64	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	5	PHE	C-N	-8.32	1.22	1.33
1	B	33	PRO	CA-CB	8.30	1.65	1.53
1	B	247	ARG	NE-CZ	8.22	1.42	1.33
1	A	130	THR	CA-C	8.20	1.63	1.52
1	A	95	HIS	CE1-NE2	8.18	1.40	1.32
1	B	98	ARG	NE-CZ	8.09	1.42	1.33
1	A	121	VAL	N-CA	7.98	1.55	1.46
1	B	170	ILE	N-CA	7.97	1.55	1.46
1	A	247	ARG	C-N	-7.96	1.22	1.33
1	A	87	GLY	N-CA	7.91	1.56	1.45
1	A	245	ASN	C-O	7.90	1.34	1.24
1	A	28	ASN	CA-C	7.87	1.62	1.52
1	A	50	SER	N-CA	7.76	1.55	1.46
1	A	19	SER	C-N	-7.75	1.25	1.34
1	A	219	THR	CB-OG1	-7.71	1.31	1.43
1	B	194	SER	N-CA	7.60	1.54	1.46
1	A	39	VAL	N-CA	7.50	1.54	1.46
1	B	170	ILE	C-O	7.47	1.31	1.24
1	B	205	ARG	CD-NE	-7.47	1.35	1.46
1	A	141	ASP	CA-CB	-7.46	1.40	1.53
1	A	28	ASN	C-N	-7.41	1.24	1.34
1	A	208	TYR	C-N	-7.34	1.24	1.33
1	B	38	VAL	C-O	7.33	1.32	1.24
1	A	133	GLU	CA-CB	-7.26	1.41	1.53
1	B	186	ALA	C-O	7.24	1.32	1.24
1	A	23	ILE	CA-CB	-7.24	1.44	1.54
1	A	120	GLY	N-CA	7.23	1.55	1.45
1	B	22	GLU	CD-OE2	7.22	1.39	1.25
1	A	58	GLN	CA-CB	7.20	1.64	1.53
1	B	224	ALA	C-O	7.20	1.32	1.24
1	A	228	GLY	N-CA	7.18	1.52	1.45
1	A	89	LYS	C-N	-7.18	1.22	1.33
1	B	7	VAL	C-N	7.15	1.39	1.33
1	A	126	CYS	CA-C	7.13	1.61	1.52
1	A	3	ARG	C-O	7.12	1.32	1.24
1	B	31	SER	N-CA	7.11	1.55	1.46
1	B	245	ASN	CA-C	7.11	1.61	1.52
1	A	86	VAL	CA-C	7.10	1.60	1.52
1	B	74	PHE	CA-CB	-7.09	1.42	1.52
1	B	33	PRO	N-CA	-7.08	1.38	1.47
1	B	31	SER	C-N	7.08	1.41	1.33
1	A	109	ILE	N-CA	7.06	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	97	GLU	N-CA	7.06	1.54	1.46
1	A	132	GLU	CD-OE2	7.05	1.38	1.25
1	B	142	VAL	C-N	-7.05	1.24	1.33
1	B	99	ARG	CD-NE	-7.01	1.36	1.46
1	B	75	THR	N-CA	6.97	1.55	1.46
1	B	131	LEU	C-N	-6.92	1.25	1.33
1	B	227	ASP	N-CA	6.81	1.55	1.46
1	A	113	THR	N-CA	-6.80	1.37	1.46
1	A	198	ASP	CA-C	-6.76	1.43	1.52
1	A	70	ALA	C-N	-6.75	1.25	1.33
1	B	28	ASN	CA-CB	6.74	1.66	1.53
1	A	26	ARG	CD-NE	-6.73	1.36	1.46
1	A	242	ASP	C-O	-6.73	1.16	1.24
1	B	132	GLU	C-O	-6.73	1.16	1.24
1	A	90	TRP	CA-CB	6.72	1.63	1.53
1	A	25	GLU	CD-OE2	6.72	1.38	1.25
1	A	86	VAL	C-O	6.71	1.32	1.24
1	A	111	ASP	N-CA	6.70	1.54	1.46
1	A	84	LYS	CA-C	6.70	1.61	1.52
1	A	145	ARG	NE-CZ	6.68	1.40	1.33
1	A	62	GLY	N-CA	6.67	1.55	1.45
1	B	61	VAL	C-N	-6.67	1.24	1.33
1	A	154	VAL	N-CA	6.64	1.54	1.46
1	B	95	HIS	CG-ND1	6.64	1.45	1.38
1	A	190	LYS	CA-C	6.62	1.61	1.52
1	B	58	GLN	N-CA	6.60	1.54	1.46
1	B	21	LYS	C-O	6.58	1.31	1.24
1	A	37	GLU	N-CA	6.55	1.54	1.46
1	A	150	VAL	C-O	6.55	1.31	1.23
1	B	73	ALA	CA-CB	6.54	1.61	1.52
1	B	25	GLU	CD-OE2	6.54	1.37	1.25
1	A	141	ASP	N-CA	6.53	1.54	1.46
1	B	87	GLY	C-O	6.53	1.32	1.23
1	B	155	LYS	CA-CB	6.51	1.63	1.53
1	B	214	GLY	C-O	6.46	1.32	1.23
1	B	64	GLN	C-O	6.45	1.32	1.24
1	B	153	GLU	C-O	6.45	1.32	1.24
1	A	13	LEU	C-O	6.42	1.32	1.23
1	A	133	GLU	CD-OE2	6.37	1.37	1.25
1	B	47	LEU	C-O	6.37	1.31	1.24
1	A	96	SER	C-N	-6.32	1.25	1.33
1	B	135	LYS	C-O	6.32	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	85	ASP	N-CA	6.30	1.54	1.46
1	B	195	LYS	CA-C	6.30	1.60	1.52
1	B	101	TYR	CA-C	6.29	1.60	1.52
1	A	86	VAL	C-N	-6.28	1.24	1.33
1	B	157	TRP	CA-CB	-6.27	1.44	1.53
1	B	140	LEU	N-CA	6.19	1.54	1.46
1	B	223	LYS	N-CA	6.19	1.54	1.46
1	B	146	GLN	C-O	6.17	1.31	1.24
1	B	148	ASN	CA-C	-6.15	1.45	1.52
1	A	102	PHE	C-N	-6.10	1.25	1.33
1	B	160	VAL	C-O	6.07	1.30	1.24
1	B	179	GLU	CD-OE2	6.07	1.36	1.25
1	A	155	LYS	C-N	-6.06	1.25	1.33
1	B	39	VAL	CA-C	6.05	1.59	1.52
1	B	92	ILE	N-CA	6.05	1.53	1.46
1	A	166	PRO	N-CD	6.04	1.56	1.47
1	B	148	ASN	C-O	6.04	1.31	1.24
1	A	43	PRO	C-O	6.03	1.31	1.23
1	A	188	ILE	CA-C	6.03	1.60	1.52
1	A	203	GLU	CD-OE2	6.02	1.36	1.25
1	B	132	GLU	C-N	6.01	1.42	1.33
1	B	133	GLU	N-CA	6.00	1.53	1.46
1	A	226	VAL	CA-C	-5.98	1.47	1.53
1	B	117	LEU	C-O	5.96	1.31	1.24
1	B	25	GLU	N-CA	5.94	1.53	1.46
1	A	139	THR	N-CA	-5.94	1.38	1.45
1	A	100	SER	CA-C	-5.94	1.46	1.52
1	A	247	ARG	CA-CB	5.93	1.62	1.53
1	A	15	GLY	CA-C	-5.92	1.44	1.51
1	A	209	GLY	CA-C	5.92	1.57	1.51
1	B	229	PHE	C-N	5.91	1.43	1.33
1	B	226	VAL	CA-CB	-5.87	1.46	1.54
1	B	48	ASP	CG-OD1	5.86	1.36	1.25
1	A	107	LYS	N-CA	-5.85	1.39	1.46
1	A	216	ASN	C-N	-5.82	1.26	1.33
1	B	101	TYR	C-N	-5.82	1.25	1.33
1	B	187	SER	N-CA	-5.82	1.39	1.46
1	A	99	ARG	C-O	5.82	1.31	1.24
1	A	198	ASP	C-O	5.78	1.31	1.24
1	B	209	GLY	C-N	-5.77	1.25	1.33
1	B	220	PHE	N-CA	5.77	1.53	1.46
1	A	226	VAL	N-CA	5.76	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	56	LYS	C-O	5.76	1.31	1.24
1	B	192	LEU	N-CA	5.74	1.53	1.46
1	A	128	GLY	N-CA	5.74	1.50	1.45
1	A	159	ASN	CA-CB	5.73	1.62	1.53
1	B	230	LEU	C-N	-5.71	1.26	1.33
1	B	171	GLY	C-O	5.69	1.31	1.23
1	B	198	ASP	CA-CB	5.68	1.62	1.53
1	B	183	ASP	N-CA	5.68	1.53	1.46
1	A	213	ASN	N-CA	5.67	1.53	1.45
1	B	106	ASP	C-O	5.67	1.30	1.24
1	A	189	ARG	C-O	5.65	1.30	1.24
1	B	81	ASP	C-N	-5.64	1.25	1.33
1	B	98	ARG	CA-C	-5.63	1.45	1.52
1	B	232	GLY	N-CA	5.63	1.53	1.45
1	A	45	THR	CB-OG1	-5.62	1.34	1.43
1	B	176	ALA	N-CA	5.61	1.53	1.45
1	B	156	ASP	CG-OD1	5.61	1.36	1.25
1	B	39	VAL	N-CA	-5.60	1.38	1.46
1	A	173	GLY	N-CA	5.58	1.53	1.45
1	B	73	ALA	C-O	5.58	1.29	1.23
1	A	63	ALA	N-CA	5.57	1.53	1.45
1	A	178	PRO	CA-CB	5.56	1.61	1.53
1	A	208	TYR	C-O	5.56	1.30	1.24
1	A	118	GLY	CA-C	5.54	1.58	1.52
1	A	30	ALA	N-CA	-5.54	1.39	1.46
1	B	173	GLY	N-CA	5.54	1.52	1.45
1	B	187	SER	C-O	5.53	1.30	1.24
1	A	8	GLY	CA-C	5.52	1.57	1.52
1	A	247	ARG	NE-CZ	5.52	1.39	1.33
1	A	148	ASN	CA-CB	-5.50	1.45	1.53
1	A	13	LEU	N-CA	5.49	1.53	1.46
1	B	204	LEU	C-O	5.48	1.30	1.23
1	A	185	HIS	C-O	5.48	1.30	1.24
1	B	72	GLY	C-N	-5.48	1.27	1.33
1	B	123	VAL	C-O	5.47	1.29	1.24
1	A	185	HIS	CD2-NE2	-5.46	1.31	1.37
1	A	10	ASN	CA-CB	5.44	1.60	1.52
1	B	34	GLU	CD-OE2	5.43	1.35	1.25
1	A	175	ALA	C-O	5.43	1.31	1.23
1	A	239	GLU	CD-OE2	5.40	1.35	1.25
1	B	195	LYS	CA-CB	-5.39	1.44	1.53
1	B	85	ASP	C-N	-5.38	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	158	THR	CB-OG1	-5.38	1.35	1.43
1	B	241	VAL	CA-C	-5.37	1.45	1.52
1	A	237	LYS	C-N	-5.35	1.27	1.33
1	A	24	VAL	C-O	5.34	1.30	1.24
1	B	11	PHE	C-O	5.34	1.30	1.24
1	A	161	VAL	CA-CB	-5.32	1.47	1.53
1	B	27	LEU	CA-C	5.32	1.59	1.52
1	B	121	VAL	CA-CB	-5.31	1.47	1.54
1	B	71	SER	N-CA	5.30	1.52	1.46
1	B	52	SER	N-CA	5.29	1.53	1.46
1	A	95	HIS	CA-CB	-5.29	1.44	1.53
1	B	166	PRO	N-CA	5.28	1.53	1.47
1	B	105	ASP	CG-OD1	5.28	1.35	1.25
1	B	15	GLY	CA-C	5.27	1.59	1.51
1	A	149	ALA	N-CA	5.25	1.52	1.46
1	A	7	VAL	C-O	-5.24	1.18	1.24
1	A	60	THR	C-O	5.24	1.30	1.23
1	A	131	LEU	C-N	-5.23	1.26	1.33
1	B	214	GLY	CA-C	-5.21	1.44	1.51
1	A	16	SER	C-N	-5.21	1.26	1.33
1	A	212	ALA	C-N	-5.20	1.26	1.33
1	A	234	ALA	C-O	5.20	1.31	1.24
1	B	162	VAL	N-CA	-5.20	1.40	1.46
1	B	31	SER	C-O	5.19	1.30	1.24
1	B	187	SER	C-N	5.19	1.40	1.33
1	A	34	GLU	C-N	5.18	1.39	1.33
1	B	142	VAL	C-O	5.18	1.30	1.24
1	B	153	GLU	CD-OE2	5.17	1.35	1.25
1	B	152	GLU	CD-OE1	-5.16	1.15	1.25
1	A	158	THR	C-O	-5.16	1.17	1.24
1	A	69	LYS	CA-C	5.15	1.58	1.52
1	A	132	GLU	CG-CD	-5.14	1.39	1.52
1	B	224	ALA	C-N	-5.14	1.26	1.33
1	A	222	ASP	N-CA	5.13	1.50	1.46
1	A	26	ARG	C-O	5.12	1.30	1.24
1	A	133	GLU	C-O	-5.11	1.18	1.24
1	B	240	PHE	N-CA	5.11	1.52	1.46
1	B	133	GLU	CD-OE2	5.10	1.35	1.25
1	A	206	ILE	CA-CB	-5.10	1.47	1.54
1	B	26	ARG	CD-NE	-5.10	1.39	1.46
1	B	39	VAL	C-O	5.09	1.30	1.24
1	A	82	GLN	C-O	5.09	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	206	ILE	N-CA	-5.09	1.39	1.46
1	B	34	GLU	CA-CB	5.08	1.62	1.53
1	A	205	ARG	CA-CB	5.08	1.60	1.53
1	B	235	SER	N-CA	5.07	1.52	1.46
1	A	247	ARG	CA-C	-5.07	1.46	1.53
1	B	75	THR	CA-C	-5.07	1.46	1.52
1	B	175	ALA	CA-C	-5.02	1.46	1.53
1	A	123	VAL	C-N	-5.02	1.27	1.33
1	A	179	GLU	N-CA	-5.02	1.40	1.46
1	B	77	GLU	CB-CG	5.02	1.67	1.52
1	B	240	PHE	CA-CB	-5.01	1.45	1.53
1	A	165	GLU	CA-CB	-5.01	1.47	1.53
1	B	185	HIS	CE1-NE2	5.01	1.37	1.32
1	A	179	GLU	C-O	5.01	1.30	1.24
1	A	67	TYR	N-CA	-5.01	1.39	1.45
1	A	166	PRO	C-O	5.00	1.29	1.23

All (650) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	ALA	CA-C-N	28.02	175.06	121.54
1	A	2	ALA	C-N-CA	28.02	175.06	121.54
1	B	26	ARG	CD-NE-CZ	26.33	161.27	124.40
1	B	111	ASP	CA-CB-CG	20.20	132.80	112.60
1	A	17	LYS	CA-CB-CG	16.58	147.25	114.10
1	A	132	GLU	CB-CG-CD	16.33	140.36	112.60
1	A	108	PHE	CA-CB-CG	16.04	129.84	113.80
1	A	141	ASP	CA-CB-CG	15.89	128.49	112.60
1	B	195	LYS	N-CA-C	-14.40	93.83	111.40
1	B	5	PHE	CA-CB-CG	13.39	127.19	113.80
1	B	33	PRO	N-CA-C	13.32	139.91	112.47
1	A	138	LYS	CA-C-N	12.97	143.38	122.11
1	A	138	LYS	C-N-CA	12.97	143.38	122.11
1	B	198	ASP	CA-C-O	-12.97	107.34	120.70
1	A	32	ILE	CB-CA-C	12.71	121.79	109.33
1	B	33	PRO	CA-C-O	12.60	143.53	120.60
1	B	54	VAL	CA-C-N	12.57	145.56	121.54
1	B	54	VAL	C-N-CA	12.57	145.56	121.54
1	A	36	VAL	CA-C-O	12.39	133.90	121.63
1	B	101	TYR	CA-CB-CG	12.35	136.12	113.90
1	A	17	LYS	N-CA-C	-11.98	98.30	111.36
1	B	128	GLY	CA-C-O	-11.87	109.06	121.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	156	ASP	CA-CB-CG	11.85	124.44	112.60
1	A	152	GLU	CA-CB-CG	11.77	137.63	114.10
1	B	39	VAL	N-CA-CB	11.47	126.03	112.15
1	A	29	THR	CA-C-N	11.39	137.04	120.87
1	A	29	THR	C-N-CA	11.39	137.04	120.87
1	A	191	PHE	CA-CB-CG	-11.28	102.52	113.80
1	A	32	ILE	N-CA-C	-11.24	99.97	109.19
1	B	3	ARG	CA-C-N	11.24	143.01	121.54
1	B	3	ARG	C-N-CA	11.24	143.01	121.54
1	B	148	ASN	CA-CB-CG	-11.11	101.49	112.60
1	A	87	GLY	CA-C-N	11.11	137.14	120.82
1	A	87	GLY	C-N-CA	11.11	137.14	120.82
1	A	132	GLU	CA-CB-CG	10.86	135.83	114.10
1	A	247	ARG	N-CA-C	10.81	126.30	111.39
1	B	223	LYS	CB-CG-CD	10.67	135.85	111.30
1	A	117	LEU	N-CA-C	-10.66	99.67	112.89
1	A	121	VAL	CB-CA-C	10.65	126.24	110.90
1	B	146	GLN	CA-C-N	10.58	135.52	120.28
1	B	146	GLN	C-N-CA	10.58	135.52	120.28
1	B	99	ARG	CG-CD-NE	10.55	135.22	112.00
1	A	111	ASP	CA-CB-CG	10.52	123.12	112.60
1	A	24	VAL	CA-C-O	-10.50	110.35	121.27
1	B	166	PRO	CB-CA-C	10.40	124.77	111.56
1	A	151	LEU	O-C-N	10.38	133.12	122.12
1	A	21	LYS	N-CA-C	-10.37	98.94	111.69
1	A	48	ASP	CB-CA-C	10.32	126.40	109.07
1	A	103	HIS	CA-CB-CG	-10.29	103.51	113.80
1	A	245	ASN	OD1-CG-ND2	-10.15	112.45	122.60
1	B	189	ARG	N-CA-C	-10.15	99.44	112.23
1	B	92	ILE	N-CA-C	-10.06	96.72	109.30
1	A	124	ILE	CA-C-N	9.89	135.48	121.24
1	A	124	ILE	C-N-CA	9.89	135.48	121.24
1	B	15	GLY	CA-C-N	9.88	138.85	121.75
1	B	15	GLY	C-N-CA	9.88	138.85	121.75
1	A	159	ASN	CA-CB-CG	-9.86	102.74	112.60
1	A	31	SER	N-CA-CB	9.82	125.83	110.21
1	A	5	PHE	CA-CB-CG	9.75	123.55	113.80
1	B	200	ALA	O-C-N	9.69	132.50	122.03
1	B	212	ALA	CA-C-O	-9.69	109.88	120.92
1	B	226	VAL	O-C-N	9.68	134.67	122.57
1	B	207	LEU	O-C-N	9.65	133.87	123.06
1	A	126	CYS	CA-C-O	9.62	130.87	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	PHE	CA-C-N	9.61	139.89	121.54
1	B	102	PHE	C-N-CA	9.61	139.89	121.54
1	A	31	SER	O-C-N	9.59	134.44	122.93
1	A	225	ASP	CA-CB-CG	-9.56	103.04	112.60
1	B	148	ASN	CB-CA-C	9.47	125.87	110.90
1	B	224	ALA	CA-C-O	-9.34	109.51	120.62
1	A	133	GLU	CA-CB-CG	9.26	132.62	114.10
1	A	153	GLU	CB-CG-CD	9.23	128.29	112.60
1	B	88	ALA	CA-C-O	-9.22	110.39	121.28
1	A	181	ALA	O-C-N	9.21	131.55	122.07
1	A	113	THR	CA-C-N	9.19	132.98	120.38
1	A	113	THR	C-N-CA	9.19	132.98	120.38
1	A	15	GLY	N-CA-C	9.19	124.60	111.00
1	A	116	ALA	O-C-N	9.18	132.97	122.22
1	A	30	ALA	N-CA-C	9.09	123.73	110.28
1	B	176	ALA	N-CA-C	-9.03	97.12	110.48
1	B	227	ASP	CA-CB-CG	9.00	121.60	112.60
1	B	213	ASN	CA-CB-CG	-8.98	103.62	112.60
1	A	68	LEU	CA-C-N	8.96	136.87	122.81
1	A	68	LEU	C-N-CA	8.96	136.87	122.81
1	B	214	GLY	CA-C-N	8.92	138.58	121.54
1	B	214	GLY	C-N-CA	8.92	138.58	121.54
1	A	164	TYR	CA-C-O	-8.82	110.55	120.43
1	A	28	ASN	CA-C-N	8.80	132.96	120.28
1	A	28	ASN	C-N-CA	8.80	132.96	120.28
1	A	46	TYR	CA-CB-CG	8.77	129.69	113.90
1	A	235	SER	N-CA-C	-8.76	102.49	113.01
1	A	28	ASN	O-C-N	8.76	132.14	122.15
1	A	102	PHE	N-CA-C	8.75	123.68	112.92
1	A	183	ASP	O-C-N	8.74	131.53	122.09
1	B	248	ASN	CA-CB-CG	-8.73	103.87	112.60
1	B	193	ALA	CA-C-N	-8.66	109.49	122.83
1	B	193	ALA	C-N-CA	-8.66	109.49	122.83
1	A	146	GLN	OE1-CD-NE2	-8.66	113.94	122.60
1	A	69	LYS	CB-CG-CD	8.65	131.19	111.30
1	A	108	PHE	N-CA-C	-8.65	100.47	111.02
1	B	113	THR	N-CA-C	-8.65	101.82	111.07
1	B	230	LEU	N-CA-CB	8.64	125.06	110.46
1	B	145	ARG	NE-CZ-NH2	8.60	126.94	119.20
1	B	47	LEU	O-C-N	-8.58	112.77	122.03
1	B	166	PRO	N-CA-C	-8.56	97.62	111.15
1	A	92	ILE	CA-C-O	-8.54	110.95	121.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	TRP	CA-C-O	-8.52	111.29	121.60
1	B	161	VAL	CB-CA-C	8.51	120.11	110.41
1	B	26	ARG	CG-CD-NE	8.51	130.71	112.00
1	B	60	THR	CA-CB-CG2	8.50	124.95	110.50
1	B	205	ARG	CA-C-O	8.50	131.31	121.28
1	B	59	VAL	N-CA-CB	-8.50	101.27	111.21
1	A	91	VAL	CA-C-O	-8.46	110.21	120.78
1	A	60	THR	CA-C-O	-8.44	111.54	120.99
1	A	205	ARG	NE-CZ-NH2	8.41	126.77	119.20
1	B	58	GLN	N-CA-C	-8.41	103.03	113.28
1	A	146	GLN	CA-CB-CG	8.39	130.89	114.10
1	A	131	LEU	CA-C-N	8.36	132.17	120.29
1	A	131	LEU	C-N-CA	8.36	132.17	120.29
1	A	161	VAL	CA-C-O	-8.29	111.36	120.48
1	A	164	TYR	O-C-N	8.28	132.65	123.13
1	B	64	GLN	OE1-CD-NE2	8.26	130.86	122.60
1	B	4	THR	CA-CB-OG1	-8.24	97.24	109.60
1	A	220	PHE	CA-C-N	8.23	137.25	121.54
1	A	220	PHE	C-N-CA	8.23	137.25	121.54
1	A	102	PHE	CA-CB-CG	-8.21	105.59	113.80
1	A	247	ARG	N-CA-CB	-8.21	99.55	111.70
1	A	189	ARG	NE-CZ-NH2	8.15	126.54	119.20
1	B	247	ARG	O-C-N	-8.10	111.82	122.59
1	A	56	LYS	CA-C-N	8.06	128.50	119.32
1	A	56	LYS	C-N-CA	8.06	128.50	119.32
1	B	216	ASN	CA-CB-CG	8.05	120.65	112.60
1	A	248	ASN	OD1-CG-ND2	-8.02	114.58	122.60
1	A	106	ASP	CA-C-N	7.97	131.87	120.79
1	A	106	ASP	C-N-CA	7.97	131.87	120.79
1	A	190	LYS	CA-C-O	7.96	129.36	121.00
1	B	55	LYS	N-CA-CB	7.96	123.94	110.49
1	A	136	ALA	CA-C-O	7.96	128.91	119.28
1	A	132	GLU	CG-CD-OE1	7.93	136.65	118.40
1	A	32	ILE	O-C-N	7.93	126.69	121.69
1	A	121	VAL	N-CA-CB	-7.91	99.19	112.47
1	A	193	ALA	O-C-N	7.89	130.20	122.07
1	B	73	ALA	CA-C-O	-7.89	112.78	122.64
1	A	22	GLU	CA-CB-CG	7.84	129.77	114.10
1	B	53	LEU	CA-C-O	-7.83	111.55	120.24
1	B	27	LEU	N-CA-C	-7.81	102.70	111.14
1	A	26	ARG	CD-NE-CZ	7.81	135.33	124.40
1	B	59	VAL	CB-CA-C	7.80	121.67	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	VAL	CB-CA-C	7.78	122.38	111.34
1	B	128	GLY	O-C-N	7.78	130.99	123.76
1	B	22	GLU	CA-CB-CG	7.77	129.65	114.10
1	A	28	ASN	CA-C-O	-7.76	112.20	120.42
1	A	96	SER	N-CA-C	-7.75	103.28	112.89
1	B	73	ALA	O-C-N	7.75	132.71	122.56
1	A	181	ALA	CA-C-O	-7.75	112.69	120.82
1	B	18	GLN	CB-CG-CD	-7.74	99.44	112.60
1	A	96	SER	N-CA-CB	7.73	122.99	110.40
1	A	107	LYS	CA-CB-CG	7.70	129.50	114.10
1	A	2	ALA	O-C-N	-7.68	110.71	123.00
1	B	225	ASP	O-C-N	7.67	132.80	122.59
1	B	101	TYR	N-CA-CB	7.67	121.19	110.07
1	B	163	ALA	CA-C-O	7.67	128.51	120.54
1	A	181	ALA	N-CA-CB	7.66	121.12	110.01
1	B	32	ILE	CA-C-N	7.66	129.42	119.84
1	B	32	ILE	C-N-CA	7.66	129.42	119.84
1	B	133	GLU	CB-CG-CD	7.64	125.59	112.60
1	B	161	VAL	CA-C-O	-7.63	113.43	120.22
1	A	139	THR	CA-CB-OG1	-7.61	98.19	109.60
1	A	86	VAL	CA-C-O	-7.61	109.73	119.39
1	B	93	LEU	CA-C-O	-7.59	111.90	120.32
1	A	84	LYS	CA-CB-CG	7.56	129.22	114.10
1	B	241	VAL	CB-CA-C	7.54	122.62	112.22
1	B	47	LEU	CA-C-N	7.53	130.37	120.28
1	B	47	LEU	C-N-CA	7.53	130.37	120.28
1	A	69	LYS	CA-CB-CG	7.52	129.13	114.10
1	B	154	VAL	CA-C-O	7.51	128.28	120.39
1	B	57	PRO	N-CA-C	-7.50	97.01	112.47
1	A	26	ARG	NE-CZ-NH2	7.49	125.94	119.20
1	A	177	THR	O-C-N	7.49	129.82	121.43
1	A	49	TYR	N-CA-C	-7.49	103.05	111.14
1	B	127	ILE	CA-C-O	-7.45	112.64	121.28
1	A	148	ASN	CA-CB-CG	7.44	120.04	112.60
1	A	175	ALA	CA-C-O	-7.43	113.52	121.99
1	B	63	ALA	CA-C-O	-7.42	112.72	121.11
1	A	50	SER	N-CA-C	-7.40	102.90	110.97
1	A	24	VAL	N-CA-CB	7.40	118.72	110.51
1	A	106	ASP	CA-C-O	7.39	128.58	120.82
1	B	99	ARG	CD-NE-CZ	7.38	134.74	124.40
1	A	41	CYS	CA-C-N	7.37	127.97	120.38
1	A	41	CYS	C-N-CA	7.37	127.97	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	ASN	CA-CB-CG	7.37	119.97	112.60
1	B	245	ASN	N-CA-C	-7.34	102.61	113.61
1	A	101	TYR	CA-CB-CG	7.32	127.07	113.90
1	B	115	PHE	CA-C-O	7.31	128.52	120.63
1	B	203	GLU	CA-CB-CG	7.31	128.71	114.10
1	A	224	ALA	N-CA-C	7.30	120.29	111.82
1	A	10	ASN	CA-C-O	-7.30	113.98	122.37
1	B	44	ALA	CA-C-O	7.29	128.50	120.63
1	A	117	LEU	CA-CB-CG	7.28	141.76	116.30
1	A	161	VAL	N-CA-CB	7.27	121.06	111.90
1	B	198	ASP	O-C-N	7.26	129.93	122.09
1	A	22	GLU	CA-C-O	7.24	130.87	120.51
1	B	51	VAL	CB-CA-C	7.24	123.16	111.29
1	B	133	GLU	CB-CA-C	7.21	124.77	110.42
1	B	170	ILE	N-CA-CB	-7.21	102.88	110.95
1	A	153	GLU	CA-CB-CG	7.19	128.48	114.10
1	A	129	GLU	CA-C-N	7.18	133.31	121.39
1	A	129	GLU	C-N-CA	7.18	133.31	121.39
1	B	199	LYS	CA-C-O	7.18	128.97	120.92
1	A	165	GLU	O-C-N	7.18	127.40	121.44
1	A	212	ALA	CA-C-O	-7.18	112.43	120.54
1	A	224	ALA	O-C-N	-7.18	113.44	122.27
1	A	247	ARG	CA-C-O	-7.16	113.53	121.84
1	A	98	ARG	CA-C-N	7.16	131.19	120.31
1	A	98	ARG	C-N-CA	7.16	131.19	120.31
1	A	3	ARG	N-CA-C	7.16	126.05	110.80
1	A	83	ILE	CA-CB-CG2	7.15	122.65	110.50
1	B	164	TYR	N-CA-CB	7.14	122.16	110.37
1	A	26	ARG	NH1-CZ-NH2	-7.14	110.02	119.30
1	B	109	ILE	O-C-N	7.08	128.74	121.87
1	B	107	LYS	O-C-N	7.08	130.97	122.27
1	B	7	VAL	N-CA-CB	7.07	120.71	112.15
1	B	75	THR	CB-CA-C	7.07	120.92	109.90
1	B	167	VAL	CA-C-O	-7.04	111.11	119.85
1	B	92	ILE	N-CA-CB	7.03	118.96	110.31
1	B	159	ASN	O-C-N	7.03	130.71	121.99
1	A	111	ASP	N-CA-C	-7.03	102.68	112.45
1	B	247	ARG	NE-CZ-NH2	-7.03	112.88	119.20
1	A	153	GLU	N-CA-C	7.02	121.89	113.12
1	A	50	SER	O-C-N	7.01	129.33	122.03
1	A	238	PRO	CA-C-O	7.01	129.21	119.18
1	B	91	VAL	O-C-N	7.01	131.33	122.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	HIS	CA-CB-CG	7.00	120.80	113.80
1	B	123	VAL	CB-CA-C	7.00	121.90	110.69
1	B	182	GLN	CB-CA-C	-6.98	99.20	110.79
1	A	182	GLN	CA-C-N	6.98	129.93	120.44
1	A	182	GLN	C-N-CA	6.98	129.93	120.44
1	B	144	GLU	CA-CB-CG	6.98	128.05	114.10
1	B	89	LYS	O-C-N	6.97	130.00	122.34
1	A	29	THR	CA-CB-CG2	6.95	122.32	110.50
1	A	89	LYS	CA-C-N	6.95	136.38	123.32
1	A	89	LYS	C-N-CA	6.95	136.38	123.32
1	B	16	SER	CA-C-O	-6.94	113.83	121.33
1	B	162	VAL	CB-CA-C	-6.93	102.97	111.08
1	B	23	ILE	CB-CA-C	6.93	120.57	111.70
1	A	242	ASP	O-C-N	6.91	129.45	122.12
1	A	133	GLU	N-CA-CB	6.90	120.37	110.16
1	A	170	ILE	CA-C-N	6.90	134.93	121.41
1	A	170	ILE	C-N-CA	6.90	134.93	121.41
1	A	25	GLU	CG-CD-OE1	6.88	134.22	118.40
1	B	43	PRO	CA-C-N	6.86	129.78	120.38
1	B	43	PRO	C-N-CA	6.86	129.78	120.38
1	A	224	ALA	CA-C-O	6.86	127.86	119.97
1	A	104	GLU	CB-CG-CD	6.84	124.24	112.60
1	A	77	GLU	N-CA-C	6.83	120.50	110.59
1	B	99	ARG	NH1-CZ-NH2	-6.83	110.42	119.30
1	A	113	THR	CA-CB-OG1	-6.80	99.39	109.60
1	A	204	LEU	O-C-N	6.80	131.19	122.89
1	B	74	PHE	CB-CA-C	6.77	120.84	111.23
1	B	205	ARG	CD-NE-CZ	6.77	133.88	124.40
1	B	180	ASP	CB-CA-C	6.76	123.88	110.42
1	A	129	GLU	CA-CB-CG	6.76	127.62	114.10
1	B	153	GLU	CA-C-O	6.75	126.25	118.55
1	A	198	ASP	CA-C-O	-6.75	112.21	119.97
1	A	8	GLY	CA-C-O	6.74	127.55	120.94
1	B	220	PHE	N-CA-C	-6.74	104.18	112.88
1	A	238	PRO	CA-C-N	6.73	137.27	121.52
1	A	238	PRO	C-N-CA	6.73	137.27	121.52
1	B	24	VAL	O-C-N	6.73	128.40	121.87
1	A	99	ARG	CD-NE-CZ	-6.73	114.98	124.40
1	A	9	GLY	CA-C-N	6.72	132.24	122.16
1	A	9	GLY	C-N-CA	6.72	132.24	122.16
1	A	88	ALA	O-C-N	6.72	131.42	122.82
1	B	75	THR	N-CA-CB	-6.71	99.42	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	ARG	CB-CA-C	-6.71	102.37	111.89
1	B	56	LYS	N-CA-C	6.69	124.60	109.81
1	A	202	SER	O-C-N	6.68	131.29	122.33
1	B	3	ARG	CB-CA-C	6.68	123.02	111.86
1	A	205	ARG	CA-C-N	-6.68	114.21	123.10
1	A	205	ARG	C-N-CA	-6.68	114.21	123.10
1	B	110	ALA	N-CA-CB	-6.66	100.18	109.91
1	A	147	LEU	CA-C-O	6.65	127.05	119.27
1	A	232	GLY	CA-C-N	6.63	134.41	121.41
1	A	232	GLY	C-N-CA	6.63	134.41	121.41
1	A	213	ASN	CA-CB-CG	6.62	119.22	112.60
1	A	199	LYS	N-CA-CB	6.62	120.41	110.22
1	B	56	LYS	O-C-N	6.61	128.92	121.32
1	B	177	THR	N-CA-C	-6.60	100.61	110.24
1	B	241	VAL	CA-C-O	-6.58	113.88	120.85
1	B	9	GLY	CA-C-N	6.56	131.36	122.84
1	B	9	GLY	C-N-CA	6.56	131.36	122.84
1	A	5	PHE	CB-CA-C	6.55	123.46	110.42
1	A	101	TYR	CA-C-O	-6.55	113.61	120.55
1	B	29	THR	CA-CB-OG1	-6.55	99.78	109.60
1	A	111	ASP	CB-CA-C	6.54	122.46	110.11
1	B	133	GLU	CA-C-N	6.53	134.01	121.54
1	B	133	GLU	C-N-CA	6.53	134.01	121.54
1	A	193	ALA	CA-C-O	-6.52	113.97	120.82
1	B	22	GLU	N-CA-C	-6.52	104.09	111.07
1	B	140	LEU	CA-C-N	6.51	129.29	120.44
1	B	140	LEU	C-N-CA	6.51	129.29	120.44
1	A	28	ASN	N-CA-CB	6.50	119.78	110.16
1	B	95	HIS	CA-C-N	6.50	131.01	120.60
1	B	95	HIS	C-N-CA	6.50	131.01	120.60
1	A	141	ASP	N-CA-C	-6.49	96.97	110.80
1	A	208	TYR	CA-C-N	6.49	127.62	121.46
1	A	208	TYR	C-N-CA	6.49	127.62	121.46
1	A	99	ARG	CA-C-N	-6.48	111.77	122.79
1	A	99	ARG	C-N-CA	-6.48	111.77	122.79
1	A	17	LYS	O-C-N	6.46	129.51	122.15
1	B	173	GLY	N-CA-C	-6.46	106.23	114.37
1	A	212	ALA	N-CA-C	-6.45	98.75	109.46
1	B	108	PHE	CA-C-N	6.44	129.28	120.46
1	B	108	PHE	C-N-CA	6.44	129.28	120.46
1	B	132	GLU	O-C-N	6.44	129.72	122.32
1	A	124	ILE	CA-C-O	-6.43	113.86	121.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	GLN	CB-CG-CD	6.42	123.52	112.60
1	B	61	VAL	O-C-N	6.42	129.44	122.76
1	A	185	HIS	CA-C-N	6.41	129.70	120.79
1	A	185	HIS	C-N-CA	6.41	129.70	120.79
1	B	74	PHE	CA-CB-CG	6.39	120.19	113.80
1	B	63	ALA	N-CA-CB	-6.37	100.18	111.08
1	B	85	ASP	CA-CB-CG	6.37	118.97	112.60
1	A	34	GLU	N-CA-CB	6.36	119.89	110.53
1	B	117	LEU	CB-CA-C	6.36	122.89	110.67
1	B	4	THR	N-CA-C	6.35	124.32	110.80
1	A	48	ASP	CA-C-N	6.33	129.05	120.44
1	A	48	ASP	C-N-CA	6.33	129.05	120.44
1	A	61	VAL	CB-CA-C	6.32	121.10	111.68
1	B	71	SER	CB-CA-C	6.32	121.05	110.43
1	B	28	ASN	CA-CB-CG	-6.32	106.28	112.60
1	A	189	ARG	NH1-CZ-NH2	-6.32	111.09	119.30
1	A	53	LEU	CB-CA-C	6.31	120.29	109.24
1	A	215	SER	CA-C-O	-6.31	113.85	120.92
1	B	229	PHE	N-CA-C	6.31	118.76	109.24
1	B	247	ARG	N-CA-C	6.30	124.23	110.80
1	B	52	SER	N-CA-CB	-6.30	99.84	110.49
1	B	99	ARG	CA-CB-CG	6.30	126.70	114.10
1	A	209	GLY	CA-C-O	-6.30	115.80	121.47
1	B	68	LEU	N-CA-C	6.30	120.82	113.20
1	B	205	ARG	CA-C-N	6.29	131.56	123.13
1	B	205	ARG	C-N-CA	6.29	131.56	123.13
1	B	45	THR	O-C-N	-6.28	115.50	122.03
1	B	83	ILE	N-CA-C	-6.28	103.77	112.50
1	A	238	PRO	O-C-N	-6.27	113.83	122.24
1	A	186	ALA	N-CA-C	-6.27	103.37	111.02
1	A	177	THR	CA-CB-OG1	-6.27	100.20	109.60
1	A	138	LYS	CA-C-O	6.27	127.57	120.80
1	A	129	GLU	CB-CG-CD	6.26	123.25	112.60
1	A	146	GLN	O-C-N	6.26	130.72	122.33
1	A	103	HIS	ND1-CE1-NE2	6.26	114.66	108.40
1	A	139	THR	N-CA-CB	-6.25	101.98	110.67
1	A	115	PHE	CA-CB-CG	-6.25	107.55	113.80
1	B	77	GLU	O-C-N	6.23	130.88	122.59
1	A	206	ILE	CB-CA-C	6.23	119.61	110.77
1	A	32	ILE	CA-C-O	-6.22	114.38	121.59
1	B	18	GLN	CG-CD-NE2	-6.22	107.07	116.40
1	A	190	LYS	N-CA-C	-6.21	104.20	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	23	ILE	CA-C-N	6.21	128.96	120.46
1	B	23	ILE	C-N-CA	6.21	128.96	120.46
1	B	145	ARG	NE-CZ-NH1	-6.20	115.30	121.50
1	B	232	GLY	N-CA-C	-6.20	98.48	113.18
1	A	225	ASP	CB-CA-C	6.20	120.44	110.09
1	B	49	TYR	N-CA-C	-6.20	104.44	111.07
1	B	75	THR	CA-CB-OG1	-6.20	100.30	109.60
1	B	200	ALA	CA-C-O	-6.20	114.52	120.90
1	B	95	HIS	ND1-CE1-NE2	6.19	114.59	108.40
1	B	196	LEU	N-CA-C	6.18	118.79	110.88
1	B	133	GLU	CA-C-O	6.18	129.34	120.51
1	A	6	PHE	N-CA-C	6.17	118.57	108.52
1	A	133	GLU	CG-CD-OE2	-6.16	104.22	118.40
1	B	22	GLU	CG-CD-OE2	-6.16	104.23	118.40
1	B	223	LYS	CG-CD-CE	6.16	125.47	111.30
1	A	241	VAL	O-C-N	6.15	130.24	121.82
1	B	246	SER	CA-C-N	6.14	133.28	121.54
1	B	246	SER	C-N-CA	6.14	133.28	121.54
1	B	246	SER	O-C-N	-6.13	114.67	122.34
1	B	103	HIS	ND1-CG-CD2	6.13	112.23	106.10
1	B	4	THR	CA-C-N	6.13	130.09	121.02
1	B	4	THR	C-N-CA	6.13	130.09	121.02
1	B	157	TRP	O-C-N	6.12	130.39	122.19
1	B	226	VAL	CB-CA-C	6.12	121.32	111.29
1	B	243	ILE	CA-C-O	-6.12	113.14	120.78
1	A	225	ASP	CA-C-N	-6.11	115.87	122.59
1	A	225	ASP	C-N-CA	-6.11	115.87	122.59
1	A	69	LYS	N-CA-CB	6.11	121.52	111.08
1	A	29	THR	O-C-N	-6.10	115.09	122.22
1	B	35	ASN	CA-CB-CG	-6.09	106.51	112.60
1	A	42	PRO	N-CA-CB	6.08	108.98	103.08
1	A	35	ASN	O-C-N	6.07	130.94	122.08
1	A	133	GLU	O-C-N	6.07	129.07	122.15
1	B	29	THR	N-CA-CB	-6.07	101.76	110.80
1	B	127	ILE	CA-CB-CG2	6.05	120.79	110.50
1	B	72	GLY	CA-C-N	6.04	131.54	122.23
1	B	72	GLY	C-N-CA	6.04	131.54	122.23
1	A	7	VAL	CA-C-O	-6.04	114.11	120.39
1	B	37	GLU	CG-CD-OE2	-6.04	104.51	118.40
1	A	65	ASN	CB-CA-C	6.04	120.57	110.43
1	A	98	ARG	CD-NE-CZ	6.03	132.85	124.40
1	A	148	ASN	O-C-N	6.03	129.10	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	136	ALA	N-CA-C	-6.02	105.99	113.15
1	B	182	GLN	OE1-CD-NE2	6.02	128.62	122.60
1	A	135	LYS	CA-C-N	6.02	133.27	122.38
1	A	135	LYS	C-N-CA	6.02	133.27	122.38
1	B	228	GLY	N-CA-C	6.01	119.05	110.46
1	B	189	ARG	CA-C-O	6.00	126.87	119.79
1	A	189	ARG	CB-CG-CD	6.00	125.09	111.30
1	A	60	THR	O-C-N	5.99	130.10	123.33
1	A	247	ARG	CA-CB-CG	-5.99	102.13	114.10
1	B	182	GLN	O-C-N	5.99	128.47	122.12
1	B	7	VAL	O-C-N	5.97	129.95	122.66
1	A	228	GLY	CA-C-O	5.97	127.62	121.35
1	B	229	PHE	CA-C-O	5.97	128.15	121.40
1	B	122	GLY	N-CA-C	-5.97	102.99	112.66
1	B	81	ASP	CA-C-O	-5.96	112.58	119.61
1	B	204	LEU	N-CA-C	5.94	119.59	110.20
1	B	26	ARG	NE-CZ-NH2	5.94	124.55	119.20
1	B	130	THR	CB-CA-C	5.93	121.57	109.76
1	B	33	PRO	CB-CA-C	-5.92	101.79	111.56
1	B	28	ASN	CB-CG-ND2	5.92	125.27	116.40
1	B	105	ASP	N-CA-C	5.92	118.40	109.41
1	A	148	ASN	N-CA-C	-5.91	103.62	111.24
1	A	166	PRO	CB-CA-C	5.91	118.00	111.56
1	A	42	PRO	O-C-N	5.90	128.42	121.46
1	B	34	GLU	N-CA-C	5.90	123.37	110.80
1	A	185	HIS	CA-C-O	-5.89	114.64	120.70
1	B	129	GLU	CG-CD-OE1	5.88	131.92	118.40
1	A	102	PHE	CA-C-N	5.88	130.47	122.07
1	A	102	PHE	C-N-CA	5.88	130.47	122.07
1	B	226	VAL	CA-C-O	-5.87	113.44	120.78
1	A	91	VAL	O-C-N	5.87	129.91	122.57
1	A	99	ARG	NE-CZ-NH2	-5.87	113.92	119.20
1	B	59	VAL	CA-C-O	5.86	126.98	120.59
1	B	211	SER	CB-CA-C	5.86	119.60	111.63
1	A	20	ILE	CB-CG1-CD1	-5.86	101.50	113.80
1	A	237	LYS	CA-C-N	5.85	125.53	119.56
1	A	237	LYS	C-N-CA	5.85	125.53	119.56
1	A	49	TYR	CA-CB-CG	5.83	124.40	113.90
1	A	139	THR	O-C-N	5.83	129.54	122.48
1	A	245	ASN	CB-CG-ND2	5.83	125.14	116.40
1	B	38	VAL	CA-C-O	5.83	126.66	120.48
1	B	140	LEU	CB-CA-C	5.83	121.36	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	ARG	NH1-CZ-NH2	-5.80	111.77	119.30
1	B	244	ILE	CA-C-O	5.79	127.03	120.42
1	B	145	ARG	N-CA-C	-5.78	104.35	111.40
1	B	220	PHE	CA-CB-CG	5.77	119.57	113.80
1	B	110	ALA	O-C-N	5.77	128.03	122.03
1	B	90	TRP	N-CA-C	5.76	118.63	109.81
1	A	159	ASN	CB-CG-ND2	-5.76	107.76	116.40
1	A	59	VAL	N-CA-CB	-5.76	102.37	110.26
1	A	180	ASP	CB-CA-C	5.76	121.72	110.67
1	B	247	ARG	CD-NE-CZ	-5.75	116.35	124.40
1	B	168	TRP	CB-CG-CD1	5.75	135.52	126.90
1	A	163	ALA	CB-CA-C	5.74	119.69	110.16
1	B	142	VAL	N-CA-CB	-5.74	101.76	111.23
1	A	93	LEU	O-C-N	-5.74	116.19	123.24
1	A	24	VAL	O-C-N	5.73	127.67	121.94
1	B	121	VAL	CB-CA-C	5.72	119.32	110.50
1	A	235	SER	CA-C-O	5.71	126.48	119.05
1	B	146	GLN	OE1-CD-NE2	5.71	128.31	122.60
1	B	121	VAL	CA-C-O	-5.71	114.27	120.67
1	B	200	ALA	N-CA-C	-5.71	104.69	111.03
1	B	54	VAL	CA-CB-CG2	5.71	120.11	110.40
1	B	69	LYS	CA-C-O	-5.70	114.10	120.66
1	B	226	VAL	N-CA-C	-5.70	97.49	109.34
1	B	23	ILE	CA-C-O	5.69	127.33	121.41
1	A	84	LYS	CB-CA-C	-5.69	102.20	110.96
1	A	221	LYS	N-CA-C	5.68	122.91	110.80
1	A	205	ARG	O-C-N	5.68	129.70	123.22
1	B	17	LYS	CA-C-N	5.68	133.75	121.64
1	B	17	LYS	C-N-CA	5.68	133.75	121.64
1	A	243	ILE	O-C-N	5.67	127.37	121.87
1	B	147	LEU	CA-CB-CG	5.67	136.15	116.30
1	A	100	SER	N-CA-C	-5.67	105.39	112.93
1	A	229	PHE	N-CA-CB	-5.66	101.00	111.53
1	A	69	LYS	N-CA-C	-5.66	100.66	109.72
1	B	144	GLU	CA-C-O	-5.66	113.47	119.97
1	A	28	ASN	CB-CA-C	-5.65	101.24	110.85
1	B	182	GLN	N-CA-C	5.65	117.44	111.28
1	A	127	ILE	O-C-N	-5.65	116.77	123.04
1	B	121	VAL	N-CA-C	-5.65	100.05	108.46
1	A	229	PHE	N-CA-C	5.64	117.98	109.23
1	A	119	GLN	CA-C-O	5.64	126.38	119.05
1	A	26	ARG	CA-CB-CG	5.63	125.37	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	58	GLN	CA-C-O	5.62	125.87	119.18
1	A	62	GLY	N-CA-C	-5.62	99.86	113.18
1	B	183	ASP	CB-CA-C	5.62	121.60	110.42
1	B	104	GLU	CB-CG-CD	-5.61	103.06	112.60
1	B	78	ASN	CB-CG-ND2	-5.60	108.00	116.40
1	B	177	THR	CA-CB-OG1	-5.60	101.21	109.60
1	A	139	THR	OG1-CB-CG2	5.59	120.49	109.30
1	A	129	GLU	CG-CD-OE1	5.59	131.26	118.40
1	B	34	GLU	CG-CD-OE2	-5.59	105.54	118.40
1	A	122	GLY	N-CA-C	-5.59	102.54	112.54
1	A	217	ALA	CB-CA-C	5.58	120.06	110.79
1	A	152	GLU	CB-CG-CD	5.57	122.06	112.60
1	B	176	ALA	O-C-N	5.57	129.25	122.96
1	B	94	GLY	N-CA-C	5.56	122.76	115.36
1	B	37	GLU	OE1-CD-OE2	5.56	136.25	122.90
1	B	42	PRO	O-C-N	5.56	128.02	121.46
1	B	137	GLY	O-C-N	5.56	129.93	122.70
1	A	212	ALA	O-C-N	5.55	129.55	123.22
1	B	65	ASN	CA-CB-CG	5.55	118.15	112.60
1	A	51	VAL	N-CA-CB	-5.55	102.08	111.23
1	A	4	THR	OG1-CB-CG2	5.54	120.39	109.30
1	A	184	ILE	CB-CA-C	5.54	119.62	112.14
1	B	38	VAL	CB-CA-C	5.54	119.08	110.83
1	B	152	GLU	CA-C-N	5.53	130.55	122.08
1	B	152	GLU	C-N-CA	5.53	130.55	122.08
1	A	155	LYS	CA-C-N	5.53	129.74	121.72
1	A	155	LYS	C-N-CA	5.53	129.74	121.72
1	B	3	ARG	N-CA-C	-5.53	97.06	108.18
1	A	132	GLU	OE1-CD-OE2	-5.52	109.64	122.90
1	A	177	THR	N-CA-CB	5.52	118.74	110.02
1	A	25	GLU	CG-CD-OE2	-5.52	105.71	118.40
1	A	231	VAL	N-CA-CB	-5.51	104.77	111.21
1	A	77	GLU	N-CA-CB	5.50	118.79	110.42
1	A	58	GLN	CA-CB-CG	-5.49	103.11	114.10
1	A	61	VAL	CG1-CB-CG2	-5.49	98.72	110.80
1	A	147	LEU	CA-C-N	5.49	129.77	120.88
1	A	147	LEU	C-N-CA	5.49	129.77	120.88
1	B	112	LYS	O-C-N	5.49	130.16	122.36
1	A	26	ARG	CB-CG-CD	5.49	123.92	111.30
1	A	130	THR	CA-CB-OG1	-5.48	101.38	109.60
1	B	102	PHE	N-CA-CB	-5.48	102.52	110.47
1	A	10	ASN	O-C-N	5.47	128.97	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	VAL	O-C-N	5.47	127.43	121.90
1	B	223	LYS	CB-CA-C	5.47	120.42	111.23
1	A	103	HIS	ND1-CG-CD2	5.47	111.57	106.10
1	B	185	HIS	CA-CB-CG	-5.47	108.33	113.80
1	A	119	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	B	11	PHE	CA-CB-CG	5.46	119.26	113.80
1	B	17	LYS	CB-CG-CD	5.45	123.84	111.30
1	A	203	GLU	CB-CA-C	5.45	119.21	109.29
1	A	188	ILE	CB-CA-C	-5.44	104.92	111.88
1	B	215	SER	CA-CB-OG	-5.42	100.26	111.10
1	B	246	SER	N-CA-CB	-5.41	102.48	110.49
1	A	230	LEU	CA-C-N	5.41	129.83	122.90
1	A	230	LEU	C-N-CA	5.41	129.83	122.90
1	A	188	ILE	N-CA-CB	5.40	116.51	110.51
1	B	154	VAL	CB-CA-C	5.40	118.62	110.63
1	A	122	GLY	CA-C-N	5.40	130.28	123.10
1	A	122	GLY	C-N-CA	5.40	130.28	123.10
1	B	59	VAL	CA-CB-CG2	-5.39	101.24	110.40
1	B	193	ALA	CB-CA-C	-5.39	99.70	110.42
1	A	159	ASN	N-CA-C	5.38	120.12	113.50
1	B	245	ASN	CB-CA-C	5.38	119.35	109.99
1	B	57	PRO	CB-CA-C	5.37	120.42	111.56
1	A	48	ASP	CA-CB-CG	5.35	117.95	112.60
1	B	207	LEU	CA-C-O	-5.35	114.94	121.36
1	B	33	PRO	CA-C-N	5.35	131.76	121.54
1	B	33	PRO	C-N-CA	5.35	131.76	121.54
1	A	109	ILE	CA-C-O	-5.35	114.10	120.78
1	B	181	ALA	N-CA-CB	5.35	119.53	110.49
1	A	172	THR	CA-CB-OG1	-5.34	101.59	109.60
1	B	216	ASN	CB-CG-ND2	5.33	124.40	116.40
1	B	42	PRO	CB-CA-C	-5.33	104.42	110.92
1	A	86	VAL	O-C-N	5.32	128.71	122.17
1	A	216	ASN	CA-C-N	5.31	127.39	120.28
1	A	216	ASN	C-N-CA	5.31	127.39	120.28
1	B	56	LYS	CA-C-O	-5.31	112.89	120.16
1	A	240	PHE	CA-C-O	5.30	126.06	119.97
1	A	176	ALA	O-C-N	5.29	129.19	123.10
1	B	86	VAL	CA-C-N	5.29	131.78	121.41
1	B	86	VAL	C-N-CA	5.29	131.78	121.41
1	B	158	THR	CA-CB-OG1	-5.28	101.68	109.60
1	B	222	ASP	CA-C-N	-5.28	115.16	123.13
1	B	222	ASP	C-N-CA	-5.28	115.16	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	GLU	CG-CD-OE2	-5.27	106.29	118.40
1	B	131	LEU	O-C-N	-5.26	115.43	122.43
1	A	20	ILE	N-CA-C	-5.26	106.16	113.00
1	A	113	THR	CA-C-O	-5.26	112.98	120.51
1	B	35	ASN	CB-CA-C	5.26	120.09	110.36
1	B	43	PRO	CB-CA-C	5.26	120.24	111.56
1	B	155	LYS	N-CA-C	5.26	119.69	113.12
1	A	158	THR	CA-CB-OG1	-5.25	101.73	109.60
1	A	226	VAL	CB-CA-C	5.24	118.95	112.45
1	B	124	ILE	CB-CA-C	5.22	117.65	111.59
1	A	247	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	A	144	GLU	N-CA-C	-5.21	107.05	113.41
1	B	94	GLY	CA-C-N	5.21	128.48	120.82
1	B	94	GLY	C-N-CA	5.21	128.48	120.82
1	A	32	ILE	CA-C-N	5.21	125.94	120.11
1	A	32	ILE	C-N-CA	5.21	125.94	120.11
1	B	213	ASN	CA-C-O	-5.21	115.88	121.45
1	A	142	VAL	CA-C-O	-5.20	114.28	120.78
1	B	10	ASN	CB-CA-C	-5.20	102.45	110.78
1	B	124	ILE	CA-C-N	5.20	130.60	122.17
1	B	124	ILE	C-N-CA	5.20	130.60	122.17
1	B	202	SER	CA-C-O	-5.20	113.81	120.31
1	B	112	LYS	N-CA-CB	5.20	118.12	110.33
1	B	237	LYS	CA-C-O	5.18	127.26	120.16
1	B	195	LYS	O-C-N	5.18	128.44	122.17
1	A	179	GLU	CA-CB-CG	5.18	124.46	114.10
1	B	154	VAL	CA-C-N	5.17	132.46	122.53
1	B	154	VAL	C-N-CA	5.17	132.46	122.53
1	B	78	ASN	O-C-N	5.17	129.91	123.19
1	B	179	GLU	CG-CD-OE1	5.17	130.29	118.40
1	A	3	ARG	CA-C-O	-5.17	113.12	120.51
1	A	80	VAL	N-CA-CB	-5.16	102.43	110.54
1	A	103	HIS	N-CA-CB	-5.16	104.15	111.84
1	B	155	LYS	N-CA-CB	-5.13	102.57	110.42
1	B	240	PHE	N-CA-C	-5.13	105.13	111.33
1	A	192	LEU	N-CA-CB	-5.12	102.04	110.14
1	B	35	ASN	N-CA-C	-5.12	107.05	113.15
1	A	10	ASN	CB-CA-C	-5.12	104.04	112.03
1	A	164	TYR	CA-CB-CG	-5.12	104.69	113.90
1	A	222	ASP	CB-CA-C	5.12	121.20	110.45
1	A	69	LYS	CA-C-O	-5.12	115.33	121.11
1	A	242	ASP	CA-CB-CG	-5.12	107.48	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	THR	N-CA-CB	-5.11	102.34	110.22
1	A	91	VAL	N-CA-CB	5.11	119.67	111.23
1	A	115	PHE	CA-C-O	5.11	126.19	120.82
1	A	12	LYS	CA-C-O	-5.11	113.53	120.83
1	A	77	GLU	CA-C-N	5.11	130.19	122.99
1	A	77	GLU	C-N-CA	5.11	130.19	122.99
1	B	165	GLU	CA-C-O	5.11	125.90	120.08
1	B	211	SER	CA-C-N	5.10	128.01	120.82
1	B	211	SER	C-N-CA	5.10	128.01	120.82
1	A	130	THR	O-C-N	5.10	128.72	122.96
1	B	189	ARG	CB-CA-C	5.09	120.77	110.38
1	A	19	SER	CB-CA-C	-5.09	100.50	110.11
1	B	22	GLU	CG-CD-OE1	5.08	130.09	118.40
1	A	11	PHE	CA-C-O	-5.08	112.70	119.10
1	A	124	ILE	CB-CA-C	-5.07	106.17	112.45
1	A	195	LYS	CG-CD-CE	5.07	122.95	111.30
1	A	176	ALA	N-CA-C	-5.06	102.02	110.17
1	B	247	ARG	N-CA-CB	-5.06	101.94	110.49
1	B	60	THR	CA-C-N	5.06	129.73	122.45
1	B	60	THR	C-N-CA	5.06	129.73	122.45
1	A	203	GLU	O-C-N	-5.05	115.72	122.49
1	B	99	ARG	NE-CZ-NH2	5.05	123.75	119.20
1	A	26	ARG	N-CA-CB	5.05	118.01	109.78
1	B	245	ASN	CA-CB-CG	5.04	117.64	112.60
1	A	222	ASP	CA-C-O	5.04	124.04	118.65
1	B	132	GLU	N-CA-C	-5.03	103.86	111.56
1	B	120	GLY	CA-C-N	5.03	129.93	122.94
1	B	120	GLY	C-N-CA	5.03	129.93	122.94
1	B	226	VAL	CA-C-N	-5.03	113.92	122.56
1	B	226	VAL	C-N-CA	-5.03	113.92	122.56
1	B	242	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	64	GLN	CA-C-O	-5.01	114.67	120.24
1	B	222	ASP	O-C-N	5.01	129.26	122.59
1	A	34	GLU	CB-CG-CD	-5.01	104.08	112.60
1	B	180	ASP	O-C-N	-5.01	115.93	122.59
1	B	231	VAL	CA-CB-CG2	5.01	118.91	110.40
1	A	167	VAL	CA-CB-CG1	5.00	118.91	110.40
1	B	21	LYS	CA-C-N	5.00	126.94	120.44
1	B	21	LYS	C-N-CA	5.00	126.94	120.44
1	A	96	SER	O-C-N	5.00	129.36	122.46

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	ALA	Peptide
1	A	205	ARG	Sidechain
1	B	189	ARG	Sidechain
1	B	247	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	A	1883	0	1891	286	0
1	B	1883	0	1892	411	0
2	A	9	0	2	0	0
2	B	9	0	3	2	0
3	A	12	0	0	5	0
3	B	13	0	0	6	0
All	All	3809	0	3788	671	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 89.

All (671) 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:B:186:ALA:HA	1:B:225:ASP:OD1	1.28	1.27
1:A:111:ASP:HA	1:A:114:LYS:CE	1.65	1.25
1:A:28:ASN:ND2	1:A:55:LYS:H	1.35	1.23
1:B:3:ARG:NH2	1:B:203:GLU:HA	1.51	1.21
1:A:28:ASN:HD21	1:A:55:LYS:N	1.38	1.21
1:B:224:ALA:O	1:B:225:ASP:HB2	1.37	1.18
1:B:178:PRO:O	1:B:181:ALA:HB3	1.46	1.14
1:B:32:ILE:N	1:B:33:PRO:HD3	1.65	1.12
1:B:3:ARG:HH22	1:B:203:GLU:CA	1.62	1.11
1:A:2:ALA:N	3:A:612:HOH:O	1.83	1.11
1:A:192:LEU:HD22	1:A:196:LEU:HD21	1.31	1.10
1:B:54:VAL:CG2	1:B:55:LYS:H	1.66	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:VAL:HG12	1:B:143:VAL:H	1.16	1.06
1:B:56:LYS:NZ	1:B:56:LYS:HB3	1.70	1.04
1:B:91:VAL:CG1	1:B:93:LEU:HD22	1.88	1.04
1:B:91:VAL:HG13	1:B:93:LEU:HD22	1.35	1.03
1:B:186:ALA:CA	1:B:225:ASP:OD1	2.07	1.02
1:A:111:ASP:HA	1:A:114:LYS:HE2	1.06	1.02
1:B:246:SER:C	1:B:247:ARG:HG3	1.85	1.02
1:B:179:GLU:HG3	1:B:180:ASP:H	1.25	1.01
1:A:111:ASP:CA	1:A:114:LYS:HE2	1.90	1.01
1:B:127:ILE:HG13	1:B:143:VAL:HG22	1.38	1.01
1:A:105:ASP:O	1:A:109:ILE:HD12	1.61	1.01
1:B:24:VAL:HG11	1:B:53:LEU:HB3	1.41	1.01
1:B:32:ILE:HG22	1:B:245:ASN:ND2	1.76	1.01
1:B:56:LYS:HA	1:B:59:VAL:O	1.61	1.01
1:B:70:ALA:HB2	1:B:115:PHE:HZ	1.25	0.99
1:B:32:ILE:HG21	1:B:241:VAL:CG1	1.92	0.99
1:A:2:ALA:CA	3:A:612:HOH:O	2.10	0.98
1:A:17:LYS:HB3	1:A:49:TYR:CE1	1.99	0.98
1:B:127:ILE:CG1	1:B:143:VAL:HG22	1.95	0.96
1:B:142:VAL:O	1:B:145:ARG:HG2	1.66	0.96
1:B:190:LYS:O	1:B:193:ALA:N	1.98	0.95
1:B:56:LYS:HB3	1:B:56:LYS:HZ3	1.25	0.95
1:B:32:ILE:HG12	1:B:244:ILE:HD11	1.49	0.95
1:B:104:GLU:HB3	1:B:108:PHE:HD2	1.31	0.95
1:B:16:SER:OG	1:B:18:GLN:HG2	1.66	0.93
1:A:221:LYS:O	1:A:221:LYS:HG2	1.66	0.93
1:B:54:VAL:HB	1:B:59:VAL:HG12	1.50	0.93
1:B:51:VAL:HG12	1:B:61:VAL:HG11	1.51	0.92
1:B:231:VAL:CG1	1:B:234:ALA:HB3	2.00	0.92
1:B:32:ILE:HG22	1:B:245:ASN:HD21	1.35	0.92
1:B:218:VAL:O	1:B:221:LYS:HB2	1.69	0.92
1:A:70:ALA:HB2	1:A:115:PHE:HZ	1.34	0.92
1:B:148:ASN:HD21	1:B:191:PHE:HE1	1.03	0.92
1:A:56:LYS:O	1:A:59:VAL:HG12	1.70	0.91
1:B:51:VAL:O	1:B:53:LEU:N	2.04	0.91
1:B:224:ALA:O	1:B:225:ASP:CB	2.20	0.90
1:B:182:GLN:HG2	1:B:223:LYS:HG2	1.55	0.89
1:B:32:ILE:H	1:B:33:PRO:HD3	1.37	0.89
1:B:164:TYR:CZ	1:B:166:PRO:HG3	2.08	0.89
1:B:213:ASN:C	1:B:213:ASN:OD1	2.13	0.89
1:A:142:VAL:O	1:A:146:GLN:HG3	1.71	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:GLN:CG	1:B:223:LYS:HG2	2.02	0.88
1:B:189:ARG:NH1	1:B:227:ASP:OD2	2.07	0.87
1:B:247:ARG:HH11	1:B:247:ARG:HG2	1.34	0.87
1:B:56:LYS:NZ	1:B:56:LYS:CB	2.32	0.86
1:A:86:VAL:HG23	1:A:86:VAL:O	1.75	0.86
1:A:110:ALA:O	1:A:114:LYS:HG2	1.75	0.86
1:A:131:LEU:O	1:A:135:LYS:HG2	1.77	0.85
1:B:114:LYS:HG3	1:B:153:GLU:OE2	1.76	0.85
1:B:24:VAL:HG11	1:B:53:LEU:CB	2.06	0.85
1:B:60:THR:HG21	1:B:89:LYS:NZ	1.92	0.85
1:A:85:ASP:OD1	1:B:46:TYR:OH	1.94	0.84
1:A:87:GLY:O	1:A:89:LYS:NZ	2.10	0.84
1:A:28:ASN:ND2	1:A:55:LYS:N	2.08	0.84
1:B:32:ILE:N	1:B:33:PRO:CD	2.40	0.84
1:B:79:SER:O	1:B:80:VAL:C	2.20	0.84
1:A:88:ALA:O	1:A:89:LYS:NZ	2.08	0.84
1:B:148:ASN:ND2	1:B:191:PHE:CE1	2.46	0.84
1:B:32:ILE:HG21	1:B:241:VAL:HG12	1.59	0.83
1:B:244:ILE:HG21	3:B:620:HOH:O	1.76	0.83
1:A:188:ILE:O	1:A:191:PHE:HB3	1.78	0.83
1:B:136:ALA:HB3	1:B:138:LYS:NZ	1.94	0.83
1:B:142:VAL:HG12	1:B:143:VAL:N	1.87	0.83
1:B:56:LYS:HE2	1:B:89:LYS:HD2	1.61	0.83
1:A:47:LEU:HD23	1:A:61:VAL:HG12	1.61	0.83
1:A:73:ALA:HA	1:B:12:LYS:HD3	1.59	0.82
1:B:20:ILE:O	1:B:24:VAL:HG23	1.77	0.82
1:B:231:VAL:HG11	1:B:234:ALA:HB3	1.61	0.82
1:B:40:ILE:HD11	1:B:54:VAL:HG11	1.60	0.82
1:A:52:SER:C	1:A:53:LEU:HD23	2.04	0.82
1:B:142:VAL:CG1	1:B:143:VAL:H	1.92	0.82
1:B:177:THR:OG1	1:B:179:GLU:HG2	1.80	0.82
1:A:127:ILE:HG13	1:A:146:GLN:OE1	1.78	0.81
1:B:6:PHE:CZ	1:B:39:VAL:HG13	2.16	0.81
1:B:104:GLU:HB3	1:B:108:PHE:CD2	2.16	0.81
1:B:244:ILE:HD13	3:B:620:HOH:O	1.80	0.81
1:A:111:ASP:HA	1:A:114:LYS:NZ	1.95	0.81
1:A:67:TYR:HB2	1:A:77:GLU:HG2	1.61	0.81
1:B:196:LEU:N	1:B:196:LEU:HD13	1.95	0.81
1:A:143:VAL:O	1:A:147:LEU:HB2	1.80	0.81
1:B:54:VAL:CG2	1:B:55:LYS:N	2.41	0.80
1:B:216:ASN:O	1:B:219:THR:OG1	1.99	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:VAL:HG11	1:B:45:THR:CG2	2.11	0.80
1:B:145:ARG:HG3	1:B:146:GLN:N	1.94	0.80
1:B:185:HIS:ND1	1:B:206:ILE:HG22	1.96	0.80
1:A:66:ALA:O	1:A:112:LYS:HE2	1.81	0.80
1:B:51:VAL:O	1:B:54:VAL:N	2.15	0.80
1:A:238:PRO:O	1:A:241:VAL:HG12	1.82	0.80
1:B:129:GLU:HB3	1:B:139:THR:HG23	1.63	0.79
1:B:136:ALA:CB	1:B:138:LYS:HZ2	1.95	0.79
1:B:32:ILE:CG1	1:B:244:ILE:HD11	2.12	0.79
1:B:56:LYS:CB	1:B:56:LYS:HZ2	1.93	0.78
1:A:127:ILE:HG23	1:A:143:VAL:HG22	1.64	0.78
1:B:54:VAL:HG23	1:B:55:LYS:H	1.48	0.78
1:B:83:ILE:O	1:B:88:ALA:HB3	1.83	0.78
1:B:55:LYS:O	1:B:56:LYS:HG2	1.82	0.78
1:A:186:ALA:O	1:A:190:LYS:N	2.15	0.78
1:B:54:VAL:HG23	1:B:55:LYS:N	2.00	0.77
1:A:138:LYS:HD3	1:A:141:ASP:OD1	1.85	0.77
1:A:188:ILE:HD13	1:A:206:ILE:HD13	1.65	0.76
1:A:78:ASN:ND2	3:A:632:HOH:O	2.07	0.76
1:B:17:LYS:O	1:B:49:TYR:HE1	1.68	0.76
1:B:56:LYS:HD2	1:B:89:LYS:HD3	1.68	0.76
1:A:92:ILE:O	1:A:93:LEU:HD23	1.86	0.75
1:A:40:ILE:O	1:A:42:PRO:HD3	1.86	0.75
1:A:47:LEU:O	1:A:51:VAL:HG23	1.86	0.75
1:B:165:GLU:HG2	1:B:209:GLY:C	2.12	0.75
1:B:190:LYS:O	1:B:191:PHE:C	2.29	0.75
1:A:65:ASN:HD21	1:A:112:LYS:NZ	1.85	0.75
1:B:33:PRO:HB3	1:B:34:GLU:OE1	1.86	0.75
1:B:188:ILE:HD12	1:B:192:LEU:CD1	2.17	0.75
1:A:3:ARG:HB3	1:A:3:ARG:CZ	2.16	0.74
1:A:115:PHE:HZ	1:A:119:GLN:HE21	1.32	0.74
1:B:5:PHE:CE1	1:B:248:ASN:HA	2.23	0.74
1:B:129:GLU:CG	1:B:139:THR:HG23	2.18	0.74
1:B:33:PRO:O	1:B:36:VAL:HG12	1.86	0.74
1:B:54:VAL:HG22	1:B:55:LYS:H	1.49	0.74
1:B:32:ILE:HG21	1:B:241:VAL:HG13	1.69	0.73
1:B:136:ALA:HB3	1:B:138:LYS:HZ2	1.50	0.73
1:A:28:ASN:HD22	1:A:55:LYS:C	1.96	0.73
1:B:142:VAL:CG1	1:B:143:VAL:N	2.49	0.73
1:A:42:PRO:C	1:A:64:GLN:NE2	2.46	0.73
1:B:70:ALA:HB2	1:B:115:PHE:CZ	2.16	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:VAL:CG1	1:B:45:THR:CG2	2.66	0.73
1:A:238:PRO:O	1:A:241:VAL:CG1	2.37	0.73
1:B:31:SER:C	1:B:32:ILE:HG23	2.14	0.73
1:A:6:PHE:CD2	1:A:207:LEU:HD11	2.24	0.73
1:A:32:ILE:HA	1:A:245:ASN:HD21	1.53	0.73
1:A:151:LEU:HD13	1:A:157:TRP:HZ2	1.54	0.72
1:A:216:ASN:O	1:A:219:THR:HG22	1.90	0.72
1:B:136:ALA:CB	1:B:138:LYS:NZ	2.51	0.72
1:B:17:LYS:O	1:B:49:TYR:CE1	2.43	0.71
1:B:170:ILE:HA	2:B:249:PGA:O3P	1.90	0.71
1:B:247:ARG:O	1:B:248:ASN:HB2	1.90	0.71
1:B:2:ALA:C	1:B:3:ARG:HG2	2.14	0.71
1:B:96:SER:HA	1:B:99:ARG:HG3	1.71	0.71
1:A:190:LYS:O	1:A:193:ALA:HB3	1.90	0.71
1:B:106:ASP:O	1:B:110:ALA:HB2	1.90	0.71
1:A:32:ILE:HG21	1:A:244:ILE:HD11	1.71	0.71
1:A:22:GLU:O	1:A:23:ILE:C	2.33	0.71
1:A:70:ALA:HB2	1:A:115:PHE:CZ	2.22	0.71
1:B:21:LYS:HG3	1:B:53:LEU:CD1	2.21	0.71
1:B:24:VAL:CG1	1:B:53:LEU:HB3	2.19	0.70
1:A:128:GLY:HA3	1:A:165:GLU:O	1.91	0.70
1:B:60:THR:HG21	1:B:89:LYS:HZ3	1.56	0.70
1:A:47:LEU:HD23	1:A:61:VAL:CG1	2.21	0.70
1:B:51:VAL:HG22	1:B:52:SER:H	1.55	0.70
1:B:113:THR:O	1:B:117:LEU:HG	1.91	0.70
1:A:82:GLN:HB3	1:B:46:TYR:CE1	2.26	0.70
1:A:21:LYS:O	1:A:25:GLU:HB2	1.91	0.70
1:A:28:ASN:O	1:A:56:LYS:HE3	1.91	0.70
1:A:39:VAL:HA	1:A:60:THR:O	1.91	0.70
1:B:5:PHE:CD1	1:B:248:ASN:HA	2.27	0.70
1:B:148:ASN:ND2	1:B:191:PHE:HE1	1.83	0.70
1:A:105:ASP:OD2	1:A:107:LYS:HB3	1.92	0.70
1:A:111:ASP:CB	1:A:114:LYS:HE2	2.22	0.70
1:B:21:LYS:HG3	1:B:53:LEU:HD13	1.72	0.70
1:A:217:ALA:O	1:A:248:ASN:ND2	2.24	0.69
1:B:131:LEU:O	1:B:135:LYS:HD3	1.92	0.69
1:B:117:LEU:O	1:B:120:GLY:N	2.22	0.69
1:B:213:ASN:OD1	1:B:213:ASN:O	2.10	0.69
1:A:188:ILE:HD13	1:A:206:ILE:CD1	2.23	0.69
1:B:20:ILE:O	1:B:24:VAL:CG2	2.40	0.69
1:B:51:VAL:O	1:B:52:SER:C	2.34	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:LEU:HD13	1:B:191:PHE:CE2	2.28	0.69
1:B:3:ARG:NH2	1:B:3:ARG:HB3	2.08	0.68
1:B:129:GLU:CB	1:B:139:THR:HG23	2.24	0.68
1:B:182:GLN:HG3	1:B:223:LYS:HG2	1.74	0.68
1:A:38:VAL:O	1:A:59:VAL:HA	1.92	0.68
1:A:2:ALA:CB	3:A:612:HOH:O	2.40	0.68
1:A:66:ALA:O	1:A:112:LYS:CE	2.41	0.68
1:A:96:SER:O	1:A:100:SER:OG	2.10	0.68
1:A:134:LYS:O	1:A:137:GLY:N	2.26	0.68
1:A:2:ALA:HB2	3:A:612:HOH:O	1.93	0.68
1:A:28:ASN:HA	1:A:56:LYS:HG3	1.75	0.68
1:B:49:TYR:O	1:B:52:SER:HB3	1.94	0.68
1:B:238:PRO:O	1:B:240:PHE:N	2.27	0.68
1:A:65:ASN:HD21	1:A:112:LYS:HZ3	1.41	0.68
1:B:164:TYR:CE2	1:B:166:PRO:HG3	2.28	0.68
1:A:157:TRP:O	1:A:159:ASN:N	2.28	0.67
1:A:52:SER:O	1:A:53:LEU:HD23	1.94	0.67
1:B:48:ASP:HB2	1:B:86:VAL:CG1	2.24	0.67
1:B:67:TYR:O	3:B:622:HOH:O	2.12	0.67
1:B:179:GLU:HG3	1:B:180:ASP:CG	2.19	0.67
1:A:28:ASN:ND2	1:A:55:LYS:CA	2.57	0.67
1:B:188:ILE:HD11	1:B:206:ILE:HD11	1.77	0.67
1:B:7:VAL:HG21	1:B:244:ILE:HG22	1.76	0.67
1:B:33:PRO:HB2	1:B:34:GLU:HG2	1.77	0.67
1:B:60:THR:HG21	1:B:89:LYS:HZ2	1.60	0.66
1:B:179:GLU:CG	1:B:180:ASP:H	1.99	0.66
1:A:129:GLU:HB2	1:A:133:GLU:HG3	1.76	0.66
1:B:129:GLU:HG3	1:B:139:THR:HG23	1.75	0.66
1:B:56:LYS:HZ2	1:B:56:LYS:HB2	1.59	0.66
1:B:132:GLU:O	1:B:133:GLU:C	2.39	0.66
1:A:90:TRP:CZ3	1:A:161:VAL:HG13	2.29	0.66
1:A:42:PRO:C	1:A:64:GLN:HE21	2.03	0.66
1:A:2:ALA:N	1:A:227:ASP:OD1	2.29	0.66
1:A:36:VAL:HG12	1:A:58:GLN:HG2	1.77	0.66
1:A:207:LEU:HD22	1:A:228:GLY:HA3	1.78	0.65
1:B:56:LYS:HE2	1:B:89:LYS:CD	2.25	0.65
1:B:113:THR:HG23	1:B:123:VAL:HG11	1.78	0.65
1:A:83:ILE:HG23	1:A:88:ALA:HB3	1.76	0.65
1:A:129:GLU:HB2	1:A:133:GLU:CG	2.26	0.65
1:B:140:LEU:O	1:B:144:GLU:HB3	1.96	0.65
1:B:179:GLU:C	1:B:181:ALA:N	2.54	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LYS:O	1:A:59:VAL:CG1	2.44	0.65
1:A:151:LEU:HD13	1:A:157:TRP:CZ2	2.32	0.65
1:B:147:LEU:HD13	1:B:191:PHE:HE2	1.59	0.65
1:A:182:GLN:O	1:A:182:GLN:HG3	1.94	0.65
1:B:108:PHE:CZ	1:B:112:LYS:HE2	2.32	0.65
1:B:188:ILE:HD12	1:B:192:LEU:HD11	1.77	0.65
1:B:142:VAL:O	1:B:145:ARG:CG	2.45	0.64
1:A:16:SER:O	1:A:20:ILE:HG23	1.96	0.64
1:A:113:THR:HG23	1:A:123:VAL:HG11	1.79	0.64
1:B:61:VAL:CG2	1:B:62:GLY:N	2.61	0.64
1:A:28:ASN:ND2	1:A:55:LYS:C	2.55	0.64
1:A:79:SER:O	1:A:83:ILE:HD12	1.98	0.64
1:B:98:ARG:HA	1:B:102:PHE:HB2	1.80	0.64
1:B:142:VAL:O	1:B:145:ARG:N	2.31	0.64
1:A:5:PHE:CD1	1:A:248:ASN:O	2.51	0.64
1:B:178:PRO:O	1:B:181:ALA:CB	2.35	0.64
1:A:147:LEU:O	1:A:151:LEU:HD22	1.98	0.64
1:A:156:ASP:CG	1:A:158:THR:HG22	2.22	0.64
1:B:48:ASP:HB2	1:B:86:VAL:HG11	1.79	0.63
1:A:75:THR:HG23	1:B:64:GLN:HB3	1.79	0.63
1:A:141:ASP:HB3	1:A:145:ARG:CZ	2.28	0.63
1:A:75:THR:OG1	1:B:97:GLU:OE1	2.16	0.63
1:B:177:THR:OG1	1:B:179:GLU:CG	2.46	0.63
1:A:156:ASP:OD1	1:A:158:THR:HG22	1.98	0.63
1:B:90:TRP:CZ3	1:B:122:GLY:HA3	2.33	0.63
1:B:190:LYS:O	1:B:193:ALA:CB	2.46	0.63
1:B:148:ASN:OD1	1:B:151:LEU:HD12	1.98	0.63
1:B:185:HIS:ND1	1:B:206:ILE:CG2	2.62	0.63
1:A:32:ILE:CG2	1:A:244:ILE:HD11	2.29	0.62
1:B:129:GLU:HG3	1:B:139:THR:CG2	2.28	0.62
1:B:133:GLU:HG2	1:B:142:VAL:HG21	1.81	0.62
1:A:47:LEU:CD2	1:A:61:VAL:HG12	2.27	0.62
1:B:107:LYS:O	1:B:110:ALA:HB3	1.98	0.62
1:B:5:PHE:CE1	1:B:248:ASN:CA	2.81	0.62
1:A:185:HIS:HB3	1:A:225:ASP:HB3	1.80	0.62
1:A:32:ILE:HA	1:A:245:ASN:ND2	2.14	0.62
1:B:18:GLN:CG	1:B:19:SER:N	2.62	0.62
1:B:165:GLU:HG2	1:B:209:GLY:O	1.99	0.62
1:B:184:ILE:O	1:B:185:HIS:C	2.40	0.62
1:A:47:LEU:HD11	1:A:63:ALA:HB2	1.81	0.62
1:B:32:ILE:HA	1:B:245:ASN:OD1	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:PRO:C	1:B:36:VAL:HG12	2.24	0.61
1:B:80:VAL:HG23	1:B:81:ASP:N	2.14	0.61
1:A:47:LEU:O	1:A:51:VAL:CG2	2.49	0.61
1:A:129:GLU:OE1	1:A:164:TYR:OH	2.17	0.61
1:B:114:LYS:HZ2	1:B:153:GLU:HB3	1.64	0.61
1:B:127:ILE:CD1	1:B:143:VAL:HG22	2.29	0.61
1:A:127:ILE:HG21	1:A:143:VAL:HG13	1.82	0.61
1:B:140:LEU:HD22	1:B:141:ASP:N	2.15	0.61
1:B:80:VAL:HG21	1:B:119:GLN:HG3	1.81	0.61
1:B:178:PRO:C	1:B:181:ALA:HB3	2.26	0.61
1:B:179:GLU:HG3	1:B:180:ASP:OD1	2.00	0.61
1:A:148:ASN:C	1:A:150:VAL:N	2.59	0.60
1:B:244:ILE:CG2	3:B:620:HOH:O	2.43	0.60
1:B:18:GLN:HG3	1:B:19:SER:N	2.15	0.60
1:A:148:ASN:O	1:A:150:VAL:N	2.34	0.60
1:B:56:LYS:CD	1:B:89:LYS:HD3	2.31	0.60
1:B:112:LYS:O	1:B:116:ALA:HB2	2.01	0.60
1:B:188:ILE:O	1:B:192:LEU:HB2	2.02	0.60
1:B:31:SER:O	1:B:32:ILE:CG2	2.49	0.60
1:B:179:GLU:O	1:B:180:ASP:C	2.45	0.60
1:B:140:LEU:O	1:B:144:GLU:CB	2.50	0.60
1:A:127:ILE:CG1	1:A:146:GLN:OE1	2.48	0.60
1:B:91:VAL:HG11	1:B:93:LEU:HD22	1.78	0.60
1:B:99:ARG:NH1	1:B:109:ILE:HD12	2.16	0.60
1:A:221:LYS:O	1:A:221:LYS:CG	2.47	0.60
1:B:91:VAL:HG13	1:B:91:VAL:O	2.01	0.59
1:B:239:GLU:O	1:B:243:ILE:HG13	2.02	0.59
1:A:95:HIS:CG	1:B:75:THR:HG21	2.37	0.59
1:A:139:THR:HG22	1:A:140:LEU:HD23	1.85	0.59
1:A:247:ARG:HH21	1:A:247:ARG:HG3	1.66	0.59
1:A:31:SER:C	1:A:32:ILE:HG23	2.27	0.59
1:B:56:LYS:HD2	1:B:60:THR:OG1	2.03	0.59
1:B:31:SER:C	1:B:32:ILE:CG2	2.75	0.59
1:B:185:HIS:CE1	1:B:206:ILE:HG22	2.38	0.58
1:A:10:ASN:ND2	1:A:12:LYS:HE2	2.18	0.58
1:A:190:LYS:O	1:A:191:PHE:C	2.46	0.58
1:B:107:LYS:HZ2	1:B:110:ALA:HB3	1.67	0.58
1:B:117:LEU:O	1:B:118:GLY:C	2.45	0.58
1:B:48:ASP:CG	1:B:86:VAL:HG13	2.28	0.58
1:B:247:ARG:HG2	1:B:247:ARG:NH1	2.13	0.58
1:A:77:GLU:HG3	1:A:78:ASN:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:TRP:O	1:A:158:THR:C	2.46	0.58
1:A:220:PHE:HB3	1:A:248:ASN:HD22	1.68	0.58
1:B:99:ARG:NH1	1:B:109:ILE:CD1	2.67	0.58
1:A:2:ALA:HB2	1:A:189:ARG:CZ	2.34	0.58
1:A:86:VAL:HG11	1:B:45:THR:HG23	1.84	0.58
1:B:78:ASN:ND2	3:B:630:HOH:O	2.31	0.58
1:B:117:LEU:HD23	1:B:123:VAL:CG1	2.34	0.58
1:A:40:ILE:HG13	1:A:61:VAL:HG22	1.85	0.57
1:A:115:PHE:CZ	1:A:119:GLN:NE2	2.66	0.57
1:A:115:PHE:O	1:A:118:GLY:N	2.37	0.57
1:B:126:CYS:HA	1:B:163:ALA:O	2.04	0.57
1:B:134:LYS:HE2	1:B:168:TRP:CZ2	2.39	0.57
1:A:105:ASP:OD2	1:A:107:LYS:CB	2.52	0.57
1:B:25:GLU:HA	1:B:28:ASN:HB2	1.86	0.57
1:B:138:LYS:O	1:B:141:ASP:HB2	2.04	0.57
1:A:83:ILE:HG23	1:A:88:ALA:CB	2.34	0.57
1:B:99:ARG:CZ	1:B:109:ILE:CD1	2.83	0.57
1:A:53:LEU:O	1:A:55:LYS:HG3	2.04	0.57
1:B:179:GLU:O	1:B:181:ALA:N	2.38	0.56
1:B:247:ARG:HH11	1:B:247:ARG:CG	2.09	0.56
1:A:95:HIS:CB	1:B:75:THR:HG21	2.35	0.56
1:B:48:ASP:CB	1:B:86:VAL:HG13	2.35	0.56
1:B:164:TYR:OH	1:B:166:PRO:HG3	2.04	0.56
1:A:234:ALA:C	1:A:236:LEU:N	2.63	0.56
1:B:77:GLU:OE2	1:B:77:GLU:HA	2.01	0.56
1:B:169:ALA:HB1	1:B:210:GLY:O	2.05	0.56
1:B:48:ASP:CB	1:B:86:VAL:CG1	2.84	0.56
1:B:182:GLN:HG2	1:B:223:LYS:CG	2.32	0.56
1:A:9:GLY:HA2	1:A:231:VAL:O	2.06	0.56
1:B:165:GLU:OE2	1:B:209:GLY:HA3	2.05	0.56
1:A:40:ILE:C	1:A:42:PRO:HD3	2.31	0.56
1:B:135:LYS:C	1:B:137:GLY:H	2.14	0.56
1:B:64:GLN:O	1:B:65:ASN:HB2	2.05	0.56
1:A:6:PHE:HD2	1:A:207:LEU:HD11	1.68	0.55
1:A:90:TRP:HZ3	1:A:161:VAL:HG13	1.72	0.55
1:A:140:LEU:HD11	1:A:187:SER:HB3	1.87	0.55
1:A:180:ASP:O	1:A:183:ASP:HB2	2.06	0.55
1:B:50:SER:O	1:B:51:VAL:O	2.24	0.55
1:A:114:LYS:HB3	1:A:154:VAL:HG22	1.89	0.55
1:B:114:LYS:HG3	1:B:153:GLU:HB3	1.87	0.55
1:A:105:ASP:C	1:A:109:ILE:HD12	2.28	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ARG:HH22	1:B:203:GLU:HA	0.66	0.55
1:B:195:LYS:C	1:B:196:LEU:HD13	2.31	0.55
1:A:46:TYR:CE1	1:B:82:GLN:HG2	2.41	0.55
1:B:112:LYS:O	1:B:116:ALA:CB	2.55	0.55
1:A:111:ASP:HB3	1:A:114:LYS:HE2	1.88	0.55
1:B:105:ASP:O	1:B:106:ASP:C	2.50	0.55
1:B:188:ILE:O	1:B:192:LEU:HD12	2.06	0.55
1:A:141:ASP:OD2	1:A:145:ARG:NH2	2.40	0.55
1:A:82:GLN:HA	1:B:46:TYR:OH	2.07	0.55
1:A:83:ILE:CG2	1:A:88:ALA:HB3	2.37	0.55
1:A:199:LYS:O	1:A:199:LYS:HG2	2.06	0.55
1:A:247:ARG:HG3	1:A:247:ARG:NH2	2.22	0.55
1:A:31:SER:O	1:A:245:ASN:OD1	2.25	0.55
1:A:53:LEU:HD23	1:A:53:LEU:N	2.14	0.55
1:B:107:LYS:NZ	1:B:111:ASP:OD2	2.40	0.55
1:B:142:VAL:C	1:B:145:ARG:HG2	2.32	0.55
1:A:148:ASN:O	1:A:149:ALA:C	2.50	0.54
1:A:169:ALA:HB2	1:A:174:LEU:O	2.07	0.54
1:B:169:ALA:O	1:B:211:SER:OG	2.20	0.54
1:A:86:VAL:HG11	1:B:45:THR:HG22	1.88	0.54
1:A:46:TYR:OH	1:B:82:GLN:HG2	2.08	0.54
1:B:190:LYS:C	1:B:193:ALA:H	2.12	0.54
1:A:31:SER:O	1:A:32:ILE:HG23	2.08	0.54
1:B:11:PHE:N	1:B:11:PHE:CD2	2.74	0.54
1:B:179:GLU:HG3	1:B:180:ASP:N	2.09	0.54
1:A:79:SER:HB3	1:A:82:GLN:HG3	1.90	0.54
1:B:104:GLU:CB	1:B:108:PHE:HD2	2.12	0.54
1:A:111:ASP:CA	1:A:114:LYS:NZ	2.69	0.54
1:B:20:ILE:HD13	1:B:42:PRO:HB3	1.90	0.54
1:B:199:LYS:HG2	1:B:203:GLU:OE1	2.07	0.54
1:A:40:ILE:O	1:A:42:PRO:CD	2.54	0.54
1:A:75:THR:CG2	1:B:64:GLN:HB3	2.37	0.54
1:B:34:GLU:C	1:B:36:VAL:H	2.16	0.54
1:B:138:LYS:C	1:B:140:LEU:N	2.64	0.54
1:B:148:ASN:ND2	1:B:191:PHE:CZ	2.76	0.54
1:A:80:VAL:HG22	1:A:121:VAL:HG11	1.89	0.54
1:A:151:LEU:CD1	1:A:157:TRP:CZ2	2.91	0.54
1:B:31:SER:O	1:B:32:ILE:HG22	2.08	0.53
1:A:5:PHE:HE2	1:A:244:ILE:O	1.91	0.53
1:A:86:VAL:CG1	1:B:45:THR:HG22	2.38	0.53
1:A:104:GLU:OE1	1:A:112:LYS:NZ	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:SER:OG	1:A:19:SER:HB3	2.08	0.53
1:A:114:LYS:HZ3	1:A:153:GLU:HG3	1.73	0.53
1:A:186:ALA:O	1:A:187:SER:C	2.49	0.53
1:B:143:VAL:HG11	1:B:188:ILE:HG21	1.90	0.53
1:A:73:ALA:HA	1:B:12:LYS:CD	2.36	0.53
1:B:114:LYS:NZ	1:B:153:GLU:HB3	2.23	0.53
1:B:19:SER:O	1:B:20:ILE:C	2.46	0.53
1:B:188:ILE:CD1	1:B:206:ILE:HD11	2.38	0.53
1:A:98:ARG:HA	1:A:102:PHE:HD1	1.74	0.53
1:B:169:ALA:HB3	1:B:210:GLY:HA3	1.90	0.53
1:B:50:SER:O	1:B:51:VAL:C	2.52	0.53
1:B:138:LYS:O	1:B:140:LEU:N	2.42	0.53
1:B:185:HIS:HB3	1:B:225:ASP:O	2.09	0.53
1:B:188:ILE:CG1	1:B:206:ILE:HD11	2.40	0.52
1:B:54:VAL:HG23	1:B:55:LYS:C	2.34	0.52
1:A:84:LYS:HG3	1:A:121:VAL:CG2	2.40	0.52
1:B:191:PHE:CD2	1:B:192:LEU:N	2.77	0.52
1:A:125:LEU:HD11	1:A:150:VAL:HG21	1.92	0.52
1:A:17:LYS:CB	1:A:49:TYR:CE1	2.84	0.52
1:B:134:LYS:HE2	1:B:168:TRP:CE2	2.44	0.52
1:A:111:ASP:CA	1:A:114:LYS:CE	2.61	0.52
1:B:3:ARG:HB3	1:B:3:ARG:CZ	2.40	0.52
1:B:11:PHE:N	1:B:11:PHE:HD2	2.07	0.52
1:B:178:PRO:HB3	1:B:223:LYS:HE2	1.92	0.52
1:B:138:LYS:O	1:B:141:ASP:N	2.43	0.52
1:A:86:VAL:O	1:A:86:VAL:CG2	2.45	0.52
1:A:117:LEU:HD21	1:A:160:VAL:HG23	1.92	0.52
1:A:155:LYS:O	1:A:157:TRP:HD1	1.93	0.52
1:A:246:SER:O	1:A:247:ARG:HB2	2.10	0.52
1:B:114:LYS:NZ	1:B:153:GLU:O	2.40	0.52
1:A:95:HIS:O	1:A:99:ARG:HG3	2.10	0.52
1:B:91:VAL:CG1	1:B:91:VAL:O	2.56	0.52
1:A:17:LYS:HD3	1:A:49:TYR:CZ	2.45	0.51
1:A:84:LYS:O	1:A:85:ASP:C	2.53	0.51
1:A:141:ASP:O	1:A:144:GLU:N	2.35	0.51
1:A:33:PRO:HD3	1:A:245:ASN:ND2	2.25	0.51
1:A:220:PHE:CB	1:A:248:ASN:HD22	2.23	0.51
1:B:140:LEU:HD22	1:B:140:LEU:C	2.35	0.51
1:A:114:LYS:NZ	1:A:153:GLU:HG3	2.26	0.51
1:B:91:VAL:CG1	1:B:93:LEU:CD2	2.76	0.51
1:A:147:LEU:HD23	1:A:191:PHE:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:LEU:HD11	1:A:196:LEU:CD2	2.40	0.51
1:B:83:ILE:O	1:B:88:ALA:CB	2.57	0.51
1:B:95:HIS:O	1:B:99:ARG:HG2	2.11	0.51
1:B:133:GLU:HG2	1:B:142:VAL:CG2	2.40	0.51
1:B:42:PRO:C	1:B:64:GLN:NE2	2.68	0.51
1:B:190:LYS:HA	1:B:193:ALA:HB2	1.92	0.51
1:B:56:LYS:O	1:B:57:PRO:O	2.28	0.51
1:A:95:HIS:HB3	1:B:75:THR:HG21	1.93	0.51
1:B:16:SER:OG	1:B:18:GLN:CG	2.51	0.51
1:B:238:PRO:C	1:B:240:PHE:N	2.69	0.51
1:A:26:ARG:NE	1:A:238:PRO:HA	2.26	0.50
1:B:30:ALA:CB	1:B:241:VAL:HG11	2.42	0.50
1:B:5:PHE:CE1	1:B:248:ASN:N	2.79	0.50
1:A:18:GLN:O	1:A:18:GLN:HG3	2.10	0.50
1:A:214:GLY:HA2	1:A:243:ILE:HG13	1.94	0.50
1:B:95:HIS:O	1:B:99:ARG:CG	2.59	0.50
1:B:145:ARG:CG	1:B:146:GLN:N	2.69	0.50
1:B:247:ARG:O	1:B:248:ASN:CB	2.60	0.50
1:B:6:PHE:CD1	1:B:6:PHE:C	2.90	0.50
1:B:30:ALA:O	1:B:32:ILE:HG13	2.11	0.50
1:B:51:VAL:C	1:B:53:LEU:N	2.68	0.50
1:A:47:LEU:CD2	1:A:88:ALA:HB2	2.42	0.50
1:A:50:SER:O	1:A:53:LEU:N	2.31	0.50
1:B:150:VAL:O	1:B:154:VAL:N	2.45	0.50
1:A:32:ILE:HD13	1:A:244:ILE:HD11	1.92	0.50
1:B:32:ILE:HD13	1:B:244:ILE:HD12	1.93	0.50
1:B:196:LEU:N	1:B:196:LEU:CD1	2.73	0.50
1:A:94:GLY:O	1:A:99:ARG:NE	2.45	0.49
1:A:2:ALA:CB	1:A:189:ARG:NH2	2.75	0.49
1:A:234:ALA:C	1:A:236:LEU:H	2.17	0.49
1:B:48:ASP:HB2	1:B:86:VAL:HG13	1.95	0.49
1:B:237:LYS:HB3	1:B:238:PRO:HD2	1.93	0.49
1:A:2:ALA:CB	1:A:204:LEU:O	2.60	0.49
1:A:85:ASP:OD1	1:B:46:TYR:CZ	2.66	0.49
1:A:90:TRP:HA	1:A:122:GLY:O	2.12	0.49
1:A:157:TRP:C	1:A:159:ASN:N	2.68	0.49
1:B:61:VAL:HG23	1:B:62:GLY:N	2.27	0.49
1:B:130:THR:HA	1:B:167:VAL:HB	1.94	0.49
1:B:158:THR:HB	1:B:159:ASN:OD1	2.13	0.49
1:B:238:PRO:O	1:B:241:VAL:N	2.35	0.49
1:A:191:PHE:CD2	1:A:192:LEU:HG	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:PHE:O	1:A:109:ILE:C	2.54	0.49
1:B:51:VAL:CG2	1:B:52:SER:N	2.75	0.49
1:B:186:ALA:CB	1:B:225:ASP:OD1	2.60	0.49
1:B:238:PRO:O	1:B:239:GLU:C	2.54	0.49
1:A:33:PRO:HD3	1:A:245:ASN:HD22	1.77	0.49
1:B:20:ILE:HD12	1:B:46:TYR:HB2	1.94	0.49
1:B:4:THR:HG23	1:B:35:ASN:O	2.13	0.49
1:B:89:LYS:NZ	1:B:90:TRP:HE1	2.11	0.49
1:B:143:VAL:O	1:B:147:LEU:HB2	2.12	0.49
1:A:192:LEU:O	1:A:196:LEU:N	2.41	0.48
1:B:39:VAL:HG11	1:B:90:TRP:CD1	2.48	0.48
1:A:213:ASN:O	1:A:214:GLY:C	2.57	0.48
1:B:138:LYS:C	1:B:140:LEU:H	2.20	0.48
1:B:98:ARG:NH2	1:B:104:GLU:OE1	2.47	0.48
1:B:136:ALA:HB1	1:B:138:LYS:HZ2	1.75	0.48
1:A:109:ILE:O	1:A:109:ILE:HG22	2.13	0.48
1:A:235:SER:HA	1:A:240:PHE:CD1	2.49	0.48
1:B:148:ASN:O	1:B:151:LEU:HB2	2.12	0.48
1:A:73:ALA:CA	1:B:12:LYS:HD3	2.40	0.48
1:B:243:ILE:HG22	1:B:243:ILE:O	2.12	0.48
1:A:111:ASP:O	1:A:114:LYS:HG3	2.14	0.48
1:B:61:VAL:HG23	1:B:62:GLY:H	1.78	0.48
1:B:208:TYR:O	1:B:229:PHE:HA	2.14	0.48
1:A:117:LEU:HD11	1:A:154:VAL:HG11	1.95	0.48
1:B:68:LEU:HB3	1:B:112:LYS:HG2	1.95	0.47
1:B:145:ARG:HG3	1:B:146:GLN:H	1.73	0.47
1:A:235:SER:HA	1:A:240:PHE:CG	2.50	0.47
1:A:69:LYS:HE2	1:A:69:LYS:HA	1.96	0.47
1:B:179:GLU:CG	1:B:180:ASP:N	2.72	0.47
1:A:42:PRO:CB	1:A:43:PRO:HD2	2.45	0.47
1:B:6:PHE:C	1:B:6:PHE:HD1	2.22	0.47
1:B:32:ILE:CG2	1:B:241:VAL:HG12	2.38	0.47
1:B:117:LEU:HG	1:B:117:LEU:H	1.46	0.47
1:A:25:GLU:O	1:A:26:ARG:C	2.57	0.47
1:B:51:VAL:HG22	1:B:52:SER:N	2.27	0.47
1:B:51:VAL:CG2	1:B:52:SER:H	2.24	0.47
1:B:95:HIS:HA	1:B:126:CYS:HB2	1.97	0.47
1:A:169:ALA:CB	1:A:174:LEU:O	2.62	0.47
1:A:189:ARG:O	1:A:193:ALA:HB2	2.14	0.47
1:B:190:LYS:O	1:B:193:ALA:CA	2.62	0.47
1:B:96:SER:CA	1:B:99:ARG:HG3	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ILE:HD11	1:B:206:ILE:CD1	2.44	0.47
1:A:188:ILE:CD1	1:A:206:ILE:CD1	2.92	0.47
1:B:129:GLU:OE2	1:B:164:TYR:OH	2.26	0.46
1:A:164:TYR:HB2	1:A:206:ILE:HD11	1.95	0.46
1:B:129:GLU:CG	1:B:139:THR:CG2	2.89	0.46
1:A:75:THR:O	1:B:98:ARG:NE	2.42	0.46
1:A:106:ASP:O	1:A:110:ALA:N	2.49	0.46
1:A:247:ARG:NH2	1:A:247:ARG:CG	2.78	0.46
1:B:21:LYS:O	1:B:25:GLU:N	2.39	0.46
1:B:114:LYS:HZ2	1:B:153:GLU:C	2.24	0.46
1:B:124:ILE:HG13	1:B:161:VAL:HG23	1.98	0.46
1:A:85:ASP:OD1	1:B:46:TYR:CE2	2.68	0.46
1:B:80:VAL:HG23	1:B:81:ASP:H	1.80	0.46
1:A:129:GLU:HB2	1:A:133:GLU:HG2	1.96	0.46
1:A:170:ILE:O	1:A:172:THR:HG23	2.15	0.46
1:B:80:VAL:CG2	1:B:119:GLN:HG3	2.46	0.46
1:B:107:LYS:HD2	1:B:107:LYS:HA	1.55	0.46
1:B:178:PRO:HA	1:B:181:ALA:CB	2.46	0.46
1:A:140:LEU:HA	1:A:140:LEU:HD22	1.61	0.46
1:B:32:ILE:CD1	1:B:32:ILE:C	2.88	0.46
1:B:67:TYR:CG	1:B:77:GLU:HG3	2.51	0.46
1:B:113:THR:O	1:B:116:ALA:HB3	2.16	0.46
1:B:165:GLU:HG2	1:B:209:GLY:CA	2.45	0.46
1:B:191:PHE:O	1:B:195:LYS:HG2	2.16	0.46
1:A:17:LYS:O	1:A:49:TYR:HE1	1.99	0.46
1:A:75:THR:CB	1:B:97:GLU:OE1	2.64	0.46
1:B:32:ILE:O	1:B:36:VAL:HG11	2.15	0.46
1:B:66:ALA:HA	1:B:78:ASN:HB2	1.97	0.46
1:B:127:ILE:HD12	1:B:127:ILE:HG21	1.79	0.46
1:A:114:LYS:HA	1:A:117:LEU:HD12	1.98	0.46
1:B:38:VAL:HG13	1:B:59:VAL:HG22	1.98	0.46
1:B:132:GLU:CD	1:B:132:GLU:N	2.74	0.45
1:B:165:GLU:O	1:B:166:PRO:C	2.59	0.45
1:A:157:TRP:CG	1:A:196:LEU:HD13	2.51	0.45
1:B:42:PRO:HG3	1:B:50:SER:OG	2.16	0.45
1:B:127:ILE:HD11	1:B:143:VAL:HG22	1.97	0.45
1:A:13:LEU:HG	1:B:79:SER:HB2	1.98	0.45
1:A:127:ILE:CG2	1:A:143:VAL:HG13	2.46	0.45
1:A:205:ARG:HE	1:A:205:ARG:HB2	1.60	0.45
1:A:82:GLN:O	1:A:86:VAL:N	2.41	0.45
1:A:240:PHE:HA	1:A:243:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:ARG:H	1:B:98:ARG:HG2	1.50	0.45
1:A:165:GLU:OE2	1:A:209:GLY:HA3	2.17	0.45
1:B:136:ALA:HB1	1:B:138:LYS:NZ	2.29	0.45
1:B:230:LEU:HD12	1:B:230:LEU:HA	1.71	0.45
1:A:17:LYS:HD3	1:A:49:TYR:CE2	2.52	0.45
1:B:39:VAL:O	1:B:39:VAL:CG2	2.65	0.45
1:B:98:ARG:NH1	1:B:102:PHE:CD2	2.85	0.45
1:A:141:ASP:O	1:A:142:VAL:C	2.60	0.45
1:B:93:LEU:HB2	1:B:123:VAL:HG23	1.98	0.45
2:B:249:PGA:H21	3:B:643:HOH:O	2.16	0.45
1:B:122:GLY:HA2	1:B:159:ASN:O	2.17	0.44
1:A:190:LYS:O	1:A:193:ALA:CB	2.63	0.44
1:B:247:ARG:NH1	1:B:247:ARG:CG	2.76	0.44
1:A:17:LYS:HB3	1:A:49:TYR:CZ	2.49	0.44
1:B:7:VAL:CG2	1:B:244:ILE:HG22	2.44	0.44
1:B:142:VAL:O	1:B:143:VAL:C	2.60	0.44
1:A:97:GLU:HG2	1:A:101:TYR:HE2	1.82	0.44
1:B:32:ILE:C	1:B:32:ILE:HD12	2.42	0.44
1:B:54:VAL:HG23	1:B:55:LYS:O	2.16	0.44
1:B:25:GLU:O	1:B:28:ASN:N	2.50	0.44
1:B:80:VAL:CG2	1:B:81:ASP:N	2.78	0.44
1:B:188:ILE:HG13	1:B:206:ILE:HD11	1.98	0.44
1:A:32:ILE:CB	1:A:244:ILE:HD11	2.47	0.44
1:A:108:PHE:O	1:A:110:ALA:N	2.50	0.44
1:A:2:ALA:HB2	1:A:189:ARG:NH2	2.33	0.44
1:A:97:GLU:HB2	1:B:75:THR:HB	1.98	0.44
1:A:111:ASP:CG	1:A:114:LYS:HZ1	2.17	0.44
1:A:127:ILE:HG22	1:A:164:TYR:HD1	1.83	0.44
1:B:3:ARG:HH12	1:B:203:GLU:HB3	1.82	0.44
1:B:89:LYS:HZ1	1:B:90:TRP:HE1	1.66	0.44
1:A:36:VAL:HG13	1:A:58:GLN:HB3	1.99	0.44
1:A:6:PHE:HA	1:A:37:GLU:O	2.18	0.43
1:B:188:ILE:HD12	1:B:192:LEU:HD12	1.97	0.43
1:A:115:PHE:CZ	1:A:119:GLN:HG3	2.53	0.43
1:B:56:LYS:CD	1:B:89:LYS:CD	2.96	0.43
1:B:127:ILE:HG13	1:B:143:VAL:CG2	2.28	0.43
1:A:84:LYS:HG3	1:A:121:VAL:HG22	2.00	0.43
1:B:215:SER:O	1:B:218:VAL:HG12	2.18	0.43
1:B:90:TRP:CZ3	1:B:161:VAL:HG22	2.54	0.43
1:B:91:VAL:HG11	1:B:93:LEU:CD2	2.46	0.43
1:B:93:LEU:HD13	1:B:93:LEU:HA	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ASN:CG	1:B:151:LEU:HD12	2.44	0.43
1:A:247:ARG:HA	1:A:247:ARG:HD3	1.18	0.43
1:B:34:GLU:OE1	1:B:34:GLU:CA	2.65	0.43
1:B:143:VAL:HG12	1:B:144:GLU:N	2.33	0.43
1:A:18:GLN:O	1:A:21:LYS:HG2	2.18	0.43
1:A:82:GLN:O	1:A:86:VAL:HG13	2.18	0.43
1:A:185:HIS:HB3	1:A:225:ASP:CB	2.48	0.43
1:A:239:GLU:O	1:A:239:GLU:CG	2.64	0.43
1:B:20:ILE:HD12	1:B:46:TYR:CB	2.49	0.43
1:B:181:ALA:CB	1:B:220:PHE:CE2	3.01	0.43
1:B:25:GLU:O	1:B:26:ARG:C	2.60	0.43
1:B:32:ILE:HD13	1:B:244:ILE:CD1	2.48	0.43
1:A:135:LYS:HG2	1:A:135:LYS:H	1.66	0.42
1:B:51:VAL:HA	1:B:54:VAL:HG22	2.01	0.42
1:B:185:HIS:N	1:B:185:HIS:CD2	2.87	0.42
1:A:6:PHE:CD2	1:A:6:PHE:C	2.97	0.42
1:A:64:GLN:O	1:A:65:ASN:HB2	2.19	0.42
1:A:53:LEU:HD22	1:A:53:LEU:HA	1.51	0.42
1:A:89:LYS:O	1:A:122:GLY:N	2.45	0.42
1:A:208:TYR:O	1:A:229:PHE:HD2	2.02	0.42
1:B:238:PRO:C	1:B:240:PHE:H	2.27	0.42
1:A:3:ARG:HB3	1:A:3:ARG:NH1	2.35	0.42
1:B:180:ASP:O	1:B:181:ALA:C	2.62	0.42
1:A:2:ALA:N	1:A:227:ASP:CG	2.77	0.42
1:A:47:LEU:HD22	1:A:88:ALA:HB2	2.01	0.42
1:A:115:PHE:C	1:A:118:GLY:H	2.28	0.42
1:B:20:ILE:CD1	1:B:42:PRO:HB3	2.48	0.42
1:B:131:LEU:O	1:B:135:LYS:CD	2.65	0.42
1:B:179:GLU:O	1:B:182:GLN:N	2.52	0.42
1:B:208:TYR:CD2	1:B:208:TYR:C	2.98	0.42
1:A:133:GLU:CD	1:A:142:VAL:HG21	2.45	0.42
1:A:159:ASN:HD22	1:A:159:ASN:HA	1.25	0.42
1:A:22:GLU:O	1:A:23:ILE:O	2.36	0.42
1:A:148:ASN:C	1:A:150:VAL:H	2.25	0.42
1:A:221:LYS:HA	1:A:248:ASN:CG	2.45	0.42
1:B:26:ARG:HA	1:B:29:THR:HG22	2.02	0.42
1:B:236:LEU:HA	1:B:236:LEU:HD12	1.75	0.42
1:A:4:THR:HB	1:A:205:ARG:HH21	1.85	0.42
1:B:56:LYS:CE	1:B:89:LYS:CD	2.97	0.42
1:B:114:LYS:HZ3	1:B:153:GLU:CD	2.27	0.42
1:B:183:ASP:O	1:B:186:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:PRO:HB2	1:B:43:PRO:CD	2.50	0.41
1:B:134:LYS:CE	1:B:168:TRP:CE2	3.03	0.41
1:B:199:LYS:HD3	1:B:203:GLU:OE1	2.20	0.41
1:A:108:PHE:C	1:A:110:ALA:N	2.76	0.41
1:A:157:TRP:C	1:A:159:ASN:H	2.28	0.41
1:A:165:GLU:HA	1:A:166:PRO:HD3	1.75	0.41
1:B:19:SER:O	1:B:21:LYS:N	2.53	0.41
1:A:6:PHE:CD1	1:A:37:GLU:HG2	2.55	0.41
1:B:29:THR:O	1:B:29:THR:HG23	2.20	0.41
1:B:138:LYS:O	1:B:139:THR:C	2.60	0.41
1:B:32:ILE:CD1	1:B:32:ILE:O	2.69	0.41
1:B:145:ARG:O	1:B:146:GLN:C	2.63	0.41
1:B:179:GLU:C	1:B:181:ALA:H	2.26	0.41
1:A:31:SER:C	1:A:32:ILE:CG2	2.94	0.41
1:A:156:ASP:OD1	1:A:158:THR:CG2	2.67	0.41
1:A:2:ALA:CB	1:A:189:ARG:NH1	2.84	0.41
1:A:2:ALA:HB1	1:A:204:LEU:O	2.20	0.41
1:A:187:SER:O	1:A:190:LYS:HB3	2.20	0.41
1:A:88:ALA:C	1:A:89:LYS:HZ2	2.12	0.41
1:A:188:ILE:CD1	1:A:206:ILE:HD11	2.50	0.41
1:B:185:HIS:HD1	1:B:206:ILE:HG22	1.81	0.41
1:A:190:LYS:O	1:A:193:ALA:N	2.54	0.41
1:A:107:LYS:O	1:A:108:PHE:C	2.64	0.41
1:A:213:ASN:HB2	1:A:239:GLU:OE2	2.21	0.41
1:A:229:PHE:HB3	1:A:231:VAL:CG2	2.51	0.41
1:B:128:GLY:HA3	1:B:165:GLU:O	2.21	0.41
1:B:140:LEU:C	1:B:140:LEU:CD2	2.93	0.41
1:B:190:LYS:C	1:B:192:LEU:N	2.76	0.41
1:A:115:PHE:O	1:A:118:GLY:CA	2.69	0.41
1:B:142:VAL:HA	1:B:145:ARG:HG2	2.03	0.41
1:B:24:VAL:HG11	1:B:53:LEU:HB2	1.98	0.40
1:B:51:VAL:CG1	1:B:61:VAL:HG11	2.35	0.40
1:B:80:VAL:CG2	1:B:81:ASP:H	2.34	0.40
1:B:185:HIS:CD2	1:B:185:HIS:H	2.39	0.40
1:A:46:TYR:HE1	1:B:82:GLN:HG2	1.84	0.40
1:A:187:SER:HA	1:A:190:LYS:HD3	2.02	0.40
1:B:237:LYS:CB	1:B:238:PRO:CD	2.99	0.40
1:A:82:GLN:HB3	1:B:46:TYR:HE1	1.85	0.40
1:B:5:PHE:CZ	1:B:248:ASN:N	2.89	0.40
1:B:200:ALA:C	1:B:202:SER:N	2.75	0.40
1:B:220:PHE:HA	1:B:223:LYS:HE2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:SER:O	1:B:32:ILE:HG23	2.19	0.40
1:B:48:ASP:OD2	1:B:86:VAL:HG13	2.21	0.40
1:B:80:VAL:HG22	1:B:115:PHE:CE2	2.56	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	A	245/247 (99%)	191 (78%)	43 (18%)	11 (4%)	2	2
1	B	245/247 (99%)	181 (74%)	39 (16%)	25 (10%)	0	0
All	All	490/494 (99%)	372 (76%)	82 (17%)	36 (7%)	1	1

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	23	ILE
1	A	149	ALA
1	B	33	PRO
1	B	51	VAL
1	B	52	SER
1	B	55	LYS
1	B	57	PRO
1	B	77	GLU
1	B	103	HIS
1	B	142	VAL
1	B	179	GLU
1	B	239	GLU
1	A	158	THR
1	A	191	PHE

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Mol	Chain	Res	Type
1	B	4	THR
1	B	54	VAL
1	B	80	VAL
1	B	143	VAL
1	B	225	ASP
1	B	247	ARG
1	A	113	THR
1	A	134	LYS
1	B	34	GLU
1	B	149	ALA
1	B	193	ALA
1	A	135	LYS
1	A	221	LYS
1	B	20	ILE
1	B	139	THR
1	A	22	GLU
1	B	32	ILE
1	B	114	LYS
1	B	133	GLU
1	B	210	GLY
1	A	233	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	200/200 (100%)	145 (72%)	55 (28%)	0	1
1	B	200/200 (100%)	132 (66%)	68 (34%)	0	0
All	All	400/400 (100%)	277 (69%)	123 (31%)	0	0

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	SER
1	A	20	ILE

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Mol	Chain	Res	Type
1	A	24	VAL
1	A	25	GLU
1	A	27	LEU
1	A	29	THR
1	A	36	VAL
1	A	38	VAL
1	A	39	VAL
1	A	40	ILE
1	A	47	LEU
1	A	52	SER
1	A	53	LEU
1	A	54	VAL
1	A	68	LEU
1	A	69	LYS
1	A	77	GLU
1	A	80	VAL
1	A	83	ILE
1	A	86	VAL
1	A	89	LYS
1	A	92	ILE
1	A	97	GLU
1	A	98	ARG
1	A	100	SER
1	A	107	LYS
1	A	114	LYS
1	A	125	LEU
1	A	127	ILE
1	A	129	GLU
1	A	133	GLU
1	A	139	THR
1	A	140	LEU
1	A	145	ARG
1	A	151	LEU
1	A	152	GLU
1	A	159	ASN
1	A	161	VAL
1	A	174	LEU
1	A	179	GLU
1	A	183	ASP
1	A	190	LYS
1	A	196	LEU
1	A	204	LEU

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Mol	Chain	Res	Type
1	A	205	ARG
1	A	206	ILE
1	A	218	VAL
1	A	219	THR
1	A	237	LYS
1	A	239	GLU
1	A	241	VAL
1	A	244	ILE
1	A	245	ASN
1	A	247	ARG
1	A	248	ASN
1	B	3	ARG
1	B	11	PHE
1	B	16	SER
1	B	20	ILE
1	B	22	GLU
1	B	26	ARG
1	B	27	LEU
1	B	29	THR
1	B	32	ILE
1	B	34	GLU
1	B	35	ASN
1	B	38	VAL
1	B	39	VAL
1	B	40	ILE
1	B	51	VAL
1	B	54	VAL
1	B	56	LYS
1	B	58	GLN
1	B	60	THR
1	B	61	VAL
1	B	71	SER
1	B	83	ILE
1	B	84	LYS
1	B	89	LYS
1	B	93	LEU
1	B	96	SER
1	B	98	ARG
1	B	99	ARG
1	B	107	LYS
1	B	114	LYS
1	B	117	LEU

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Mol	Chain	Res	Type
1	B	121	VAL
1	B	123	VAL
1	B	125	LEU
1	B	127	ILE
1	B	133	GLU
1	B	135	LYS
1	B	138	LYS
1	B	139	THR
1	B	140	LEU
1	B	142	VAL
1	B	143	VAL
1	B	156	ASP
1	B	158	THR
1	B	161	VAL
1	B	170	ILE
1	B	174	LEU
1	B	180	ASP
1	B	182	GLN
1	B	187	SER
1	B	188	ILE
1	B	190	LYS
1	B	191	PHE
1	B	196	LEU
1	B	203	GLU
1	B	206	ILE
1	B	207	LEU
1	B	221	LYS
1	B	223	LYS
1	B	225	ASP
1	B	227	ASP
1	B	229	PHE
1	B	231	VAL
1	B	236	LEU
1	B	237	LYS
1	B	239	GLU
1	B	243	ILE
1	B	247	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN

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Mol	Chain	Res	Type
1	A	65	ASN
1	A	82	GLN
1	A	159	ASN
1	A	245	ASN
1	B	18	GLN
1	B	58	GLN
1	B	64	GLN
1	B	82	GLN

5.3.3 RNA [i](#)

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 oligosaccharides 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	$\# Z > 2$
2	PGA	A	249	-	8,8,8	2.38	1 (12%)	10,11,11	2.15	3 (30%)
2	PGA	B	249	-	8,8,8	1.89	4 (50%)	10,11,11	4.69	7 (70%)

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
2	PGA	A	249	-	-	2/6/6/6	-
2	PGA	B	249	-	-	3/6/6/6	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	249	PGA	O1P-C2	-5.75	1.37	1.43
2	B	249	PGA	P-O1P	2.76	1.69	1.60
2	B	249	PGA	P-O2P	-2.15	1.43	1.50
2	B	249	PGA	P-O3P	2.14	1.62	1.54
2	B	249	PGA	C2-C1	-2.05	1.44	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	249	PGA	O1P-C2-C1	11.11	127.28	110.54
2	B	249	PGA	O3P-P-O1P	-5.84	91.44	106.67
2	B	249	PGA	O2-C1-O1	-5.25	109.83	123.33
2	A	249	PGA	O4P-P-O1P	-4.13	95.91	106.67
2	A	249	PGA	O1P-P-O2P	3.92	117.02	106.44
2	B	249	PGA	O3P-P-O2P	3.03	122.63	110.83
2	B	249	PGA	O1P-P-O2P	2.88	114.23	106.44
2	B	249	PGA	O4P-P-O1P	-2.37	100.49	106.67
2	B	249	PGA	O4P-P-O2P	2.25	119.60	110.83
2	A	249	PGA	O3P-P-O1P	-2.21	100.92	106.67

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	249	PGA	C2-O1P-P-O3P
2	B	249	PGA	C2-O1P-P-O3P
2	B	249	PGA	C2-O1P-P-O4P
2	A	249	PGA	C2-O1P-P-O4P
2	B	249	PGA	C2-O1P-P-O2P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	249	PGA	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.