



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:55 PM UTC

PDB ID : 1BE4 / pdb_00001be4
Title : NUCLEOSIDE DIPHOSPHATE KINASE ISOFORM B FROM BOVINE RETINA
Authors : Ladner, J.E.; Abdulaev, N.G.; Kakuev, D.L.; Karaschuk, G.N.; Tordova, M.; Eisenstein, E.; Fujiwara, J.H.; Ridge, K.D.; Gilliland, G.L.
Deposited on : 1998-05-19
Resolution : 2.40 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

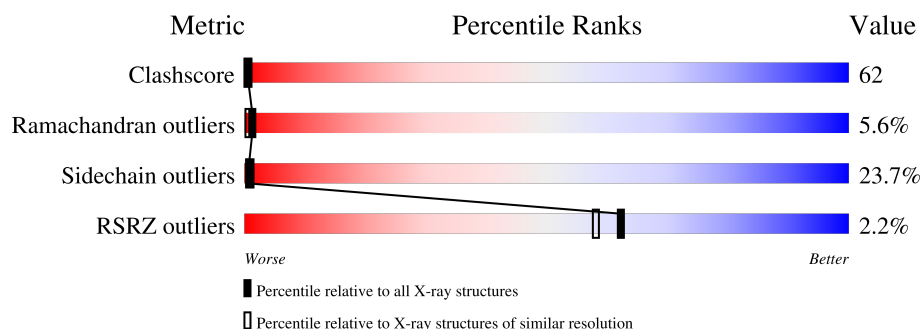
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	A	151	
1	B	151	
1	C	151	

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	PCG	C	160	X	-	-	-

2 Entry composition [i](#)

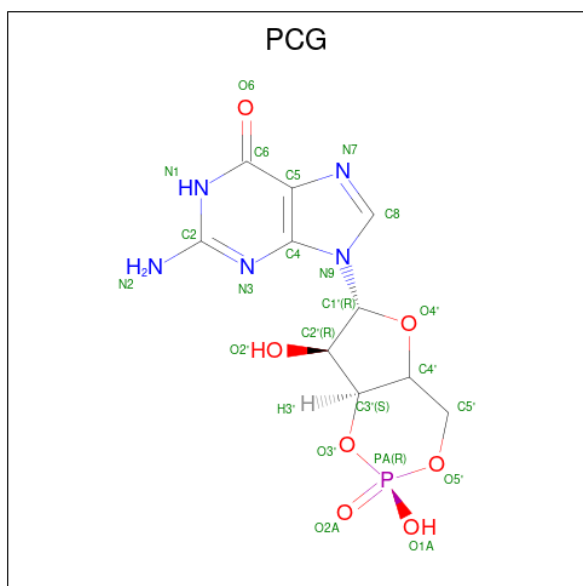
There are 3 unique types of molecules in this entry. The entry contains 3968 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NUCLEOSIDE DIPHOSPHATE TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	151	Total	C	N	O	S	0	0	0
			1207	770	211	218	8			
1	B	151	Total	C	N	O	S	0	0	0
			1207	770	211	218	8			
1	C	151	Total	C	N	O	S	0	0	0
			1207	770	211	218	8			

- Molecule 2 is CYCLIC GUANOSINE MONOPHOSPHATE (CCD ID: PCG) (formula: $C_{10}H_{12}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

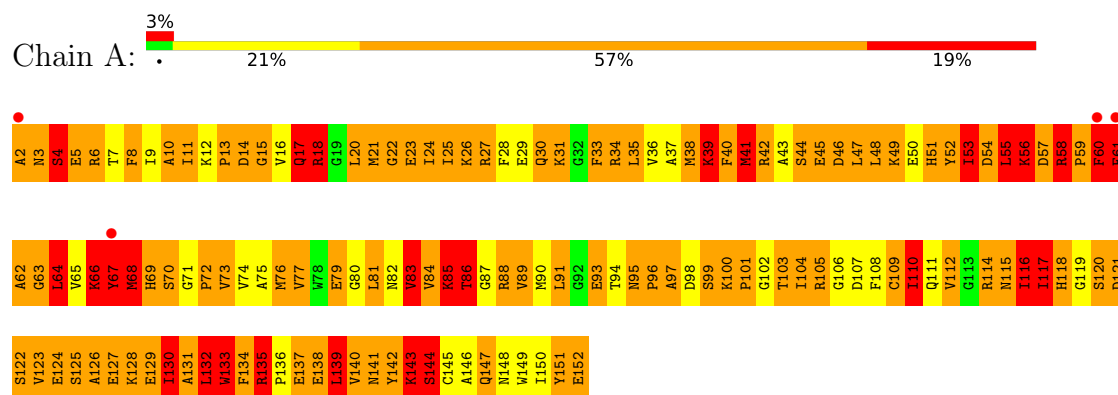
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	90	Total 90	O 90	0	0
3	B	88	Total 88	O 88	0	0
3	C	100	Total 100	O 100	0	0

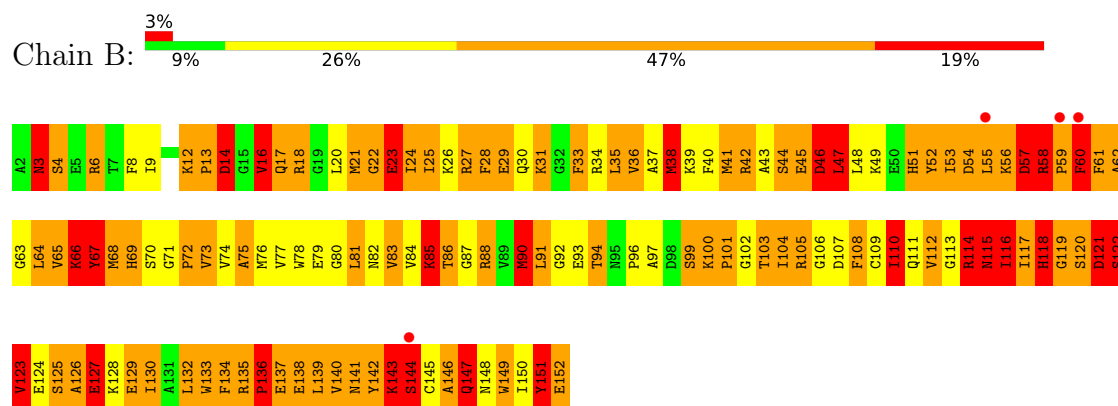
3 Residue-property plots

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.

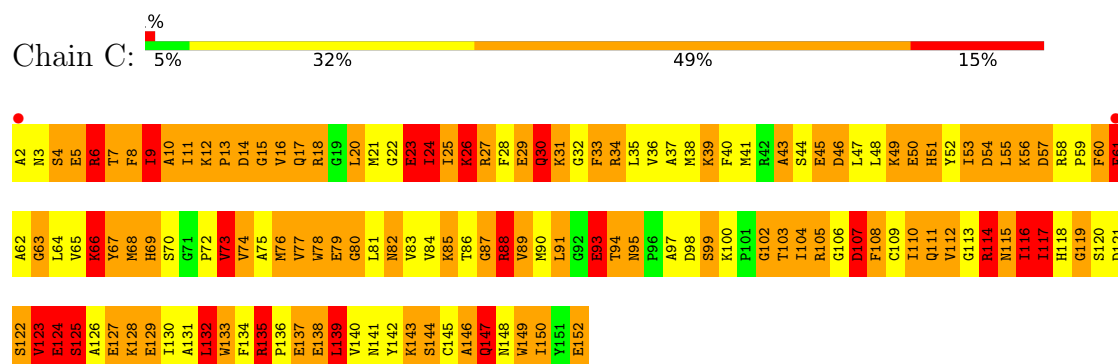
• Molecule 1: NUCLEOSIDE DIPHOSPHATE TRANSFERASE



• Molecule 1: NUCLEOSIDE DIPHOSPHATE TRANSFERASE



• Molecule 1: NUCLEOSIDE DIPHOSPHATE TRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	128.61Å 128.61Å 88.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	89.0 (20.00-2.40) 89.2 (20.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.34Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.198 , (Not available) 0.186 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.772	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 172.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3968	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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: PCG

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	1.93	26/1233 (2.1%)	3.88	315/1657 (19.0%)
1	B	1.76	21/1233 (1.7%)	3.47	232/1657 (14.0%)
1	C	1.89	30/1233 (2.4%)	3.73	283/1657 (17.1%)
All	All	1.86	77/3699 (2.1%)	3.70	830/4971 (16.7%)

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	2	1
1	B	0	3
All	All	2	4

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	GLN	C-N	11.59	1.50	1.33
1	C	25	ILE	C-O	8.03	1.33	1.24
1	B	150	ILE	N-CA	-7.07	1.40	1.46
1	C	104	ILE	C-O	6.97	1.32	1.24
1	B	149	TRP	CA-CB	-6.94	1.43	1.53
1	C	115	ASN	C-O	6.92	1.33	1.24
1	A	83	VAL	C-N	6.92	1.42	1.33
1	B	149	TRP	CA-C	-6.85	1.43	1.52
1	A	112	VAL	CA-C	-6.68	1.44	1.52
1	C	9	ILE	CA-C	-6.67	1.44	1.52
1	A	6	ARG	CA-CB	-6.62	1.41	1.53
1	A	118	HIS	CD2-NE2	6.62	1.45	1.37
1	B	29	GLU	N-CA	-6.60	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	21	MET	C-O	6.52	1.31	1.24
1	A	14	ASP	CG-OD2	6.49	1.37	1.25
1	A	128	LYS	C-N	6.37	1.41	1.33
1	C	107	ASP	CA-C	-6.24	1.44	1.52
1	A	145	CYS	CA-CB	6.16	1.63	1.53
1	A	8	PHE	C-O	6.14	1.31	1.24
1	B	14	ASP	N-CA	6.12	1.54	1.46
1	B	13	PRO	C-O	5.97	1.31	1.24
1	B	24	ILE	CA-CB	-5.97	1.47	1.54
1	C	89	VAL	CA-CB	-5.96	1.47	1.54
1	A	118	HIS	CG-ND1	5.94	1.44	1.38
1	C	119	GLY	N-CA	-5.93	1.39	1.45
1	A	88	ARG	CA-C	-5.92	1.45	1.52
1	C	76	MET	CA-C	-5.87	1.45	1.52
1	B	86	THR	N-CA	-5.86	1.39	1.46
1	C	121	ASP	CA-C	-5.85	1.44	1.52
1	B	29	GLU	C-O	-5.83	1.17	1.24
1	B	17	GLN	N-CA	5.83	1.53	1.46
1	C	133	TRP	CZ2-CH2	5.76	1.48	1.37
1	A	64	LEU	CA-C	-5.75	1.46	1.53
1	A	118	HIS	CE1-NE2	5.73	1.38	1.32
1	B	140	VAL	C-O	5.69	1.29	1.24
1	A	64	LEU	N-CA	-5.58	1.39	1.46
1	A	23	GLU	CD-OE2	5.57	1.35	1.25
1	C	50	GLU	CD-OE2	5.57	1.35	1.25
1	C	12	LYS	CA-C	-5.56	1.45	1.52
1	B	110	ILE	CA-C	-5.56	1.45	1.52
1	A	21	MET	N-CA	-5.53	1.39	1.46
1	C	32	GLY	N-CA	5.53	1.52	1.45
1	C	44	SER	C-O	5.51	1.31	1.23
1	C	115	ASN	CA-CB	5.51	1.60	1.53
1	B	133	TRP	CA-CB	5.50	1.62	1.53
1	C	28	PHE	C-N	5.49	1.40	1.33
1	B	104	ILE	CA-CB	-5.48	1.48	1.54
1	B	137	GLU	CD-OE1	5.45	1.35	1.25
1	C	85	LYS	CA-C	5.45	1.59	1.52
1	C	29	GLU	CD-OE2	5.44	1.35	1.25
1	A	116	ILE	CA-C	-5.40	1.45	1.52
1	B	100	LYS	CA-C	-5.38	1.46	1.52
1	C	57	ASP	CG-OD2	5.37	1.35	1.25
1	C	88	ARG	CA-C	-5.32	1.46	1.52
1	B	73	VAL	C-N	5.31	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	11	ILE	CA-C	-5.26	1.45	1.52
1	C	27	ARG	CA-C	-5.26	1.45	1.52
1	A	42	ARG	N-CA	5.25	1.52	1.46
1	B	21	MET	N-CA	-5.24	1.40	1.46
1	C	34	ARG	CA-C	-5.22	1.46	1.52
1	A	104	ILE	CA-CB	-5.22	1.47	1.54
1	B	105	ARG	CA-C	5.20	1.59	1.52
1	C	36	VAL	CA-CB	-5.16	1.47	1.54
1	A	18	ARG	NE-CZ	5.15	1.38	1.33
1	A	2	ALA	C-O	5.14	1.33	1.23
1	C	79	GLU	CD-OE2	5.12	1.35	1.25
1	C	106	GLY	C-N	5.09	1.41	1.33
1	C	40	PHE	N-CA	-5.09	1.39	1.46
1	A	66	LYS	N-CA	-5.08	1.39	1.46
1	A	103	THR	CA-C	-5.08	1.45	1.53
1	A	74	VAL	C-O	5.07	1.29	1.24
1	A	126	ALA	C-O	5.07	1.29	1.24
1	C	76	MET	CA-CB	5.07	1.62	1.53
1	B	96	PRO	N-CA	-5.07	1.40	1.47
1	A	124	GLU	CD-OE2	5.04	1.34	1.25
1	C	137	GLU	CD-OE2	5.04	1.34	1.25
1	B	127	GLU	CD-OE2	5.03	1.34	1.25

All (830) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	ASN	CA-CB-CG	-20.41	92.19	112.60
1	A	54	ASP	CA-CB-CG	-16.38	96.22	112.60
1	C	127	GLU	N-CA-CB	-14.17	88.80	110.06
1	A	145	CYS	N-CA-CB	13.97	130.33	110.07
1	C	31	LYS	CA-C-N	-13.87	102.60	122.29
1	C	31	LYS	C-N-CA	-13.87	102.60	122.29
1	B	65	VAL	CB-CA-C	-13.66	94.49	111.97
1	A	110	ILE	N-CA-C	13.26	126.52	113.53
1	C	23	GLU	CB-CG-CD	-12.76	90.90	112.60
1	A	18	ARG	NH1-CZ-NH2	-12.73	102.75	119.30
1	A	18	ARG	NE-CZ-NH1	12.35	133.85	121.50
1	C	82	ASN	CA-CB-CG	-12.33	100.27	112.60
1	A	88	ARG	O-C-N	12.21	134.65	122.07
1	C	105	ARG	CD-NE-CZ	-12.21	107.31	124.40
1	B	149	TRP	O-C-N	12.19	137.25	122.26
1	C	108	PHE	N-CA-C	12.14	129.50	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	TRP	CA-C-N	-11.94	104.00	122.62
1	A	133	TRP	C-N-CA	-11.94	104.00	122.62
1	C	117	ILE	CA-C-O	-11.89	109.48	121.49
1	A	70	SER	CB-CA-C	-11.80	89.37	110.37
1	C	89	VAL	N-CA-CB	-11.71	97.51	110.51
1	C	60	PHE	O-C-N	11.70	134.52	122.12
1	A	27	ARG	CD-NE-CZ	-11.67	108.06	124.40
1	C	116	ILE	CA-C-N	-11.59	107.29	123.17
1	C	116	ILE	C-N-CA	-11.59	107.29	123.17
1	C	26	LYS	CA-CB-CG	-11.52	91.07	114.10
1	A	31	LYS	O-C-N	-11.47	107.06	122.43
1	B	33	PHE	CA-CB-CG	-11.44	102.36	113.80
1	B	129	GLU	CA-C-N	-11.39	104.85	120.46
1	B	129	GLU	C-N-CA	-11.39	104.85	120.46
1	C	61	PHE	CA-C-N	-11.39	104.43	122.65
1	C	61	PHE	C-N-CA	-11.39	104.43	122.65
1	A	98	ASP	O-C-N	11.37	134.62	122.23
1	B	137	GLU	CB-CA-C	-11.29	89.00	110.67
1	A	22	GLY	CA-C-O	11.18	132.47	120.40
1	C	127	GLU	CA-C-O	11.17	132.70	120.63
1	A	69	HIS	CA-CB-CG	-11.17	102.63	113.80
1	C	20	LEU	CA-C-N	-11.06	105.40	120.44
1	C	20	LEU	C-N-CA	-11.06	105.40	120.44
1	C	30	GLN	N-CA-C	10.97	124.33	111.71
1	A	74	VAL	CA-C-O	10.86	131.68	120.39
1	A	21	MET	CA-C-O	-10.85	109.72	120.90
1	A	94	THR	CB-CA-C	10.78	127.92	110.90
1	B	115	ASN	N-CA-C	10.69	126.12	113.18
1	C	26	LYS	O-C-N	-10.66	110.82	122.12
1	C	53	ILE	N-CA-C	10.54	120.54	110.42
1	A	33	PHE	N-CA-C	10.47	125.42	110.23
1	A	28	PHE	O-C-N	10.38	134.15	122.11
1	A	83	VAL	CA-C-N	-10.30	107.37	120.56
1	A	83	VAL	C-N-CA	-10.30	107.37	120.56
1	B	39	LYS	CA-C-O	10.30	133.21	120.54
1	A	108	PHE	N-CA-C	10.29	124.45	112.72
1	C	88	ARG	O-C-N	10.23	133.14	122.09
1	A	103	THR	CA-CB-CG2	-10.19	93.17	110.50
1	A	6	ARG	CA-CB-CG	-10.17	93.76	114.10
1	A	44	SER	N-CA-CB	10.16	124.88	110.36
1	B	81	LEU	CA-C-O	10.09	132.28	120.58
1	C	51	HIS	CA-CB-CG	-10.04	103.76	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	137	GLU	O-C-N	10.02	132.75	122.12
1	C	141	ASN	CA-CB-CG	-9.96	102.64	112.60
1	C	78	TRP	CA-C-N	-9.95	106.10	122.21
1	C	78	TRP	C-N-CA	-9.95	106.10	122.21
1	A	147	GLN	CA-C-N	-9.90	106.20	122.54
1	A	147	GLN	C-N-CA	-9.90	106.20	122.54
1	B	100	LYS	CA-C-N	-9.89	109.59	119.78
1	B	100	LYS	C-N-CA	-9.89	109.59	119.78
1	B	79	GLU	CA-C-N	-9.88	106.06	120.97
1	B	79	GLU	C-N-CA	-9.88	106.06	120.97
1	C	21	MET	O-C-N	9.84	132.72	122.09
1	B	134	PHE	N-CA-C	9.80	124.81	109.81
1	B	105	ARG	CD-NE-CZ	-9.77	110.72	124.40
1	A	47	LEU	CA-C-O	9.76	131.07	120.82
1	C	91	LEU	CA-C-O	9.74	130.88	120.55
1	B	73	VAL	CA-C-N	9.71	133.38	122.22
1	B	73	VAL	C-N-CA	9.71	133.38	122.22
1	B	99	SER	CA-C-O	-9.70	110.62	121.87
1	A	136	PRO	O-C-N	9.57	135.56	122.64
1	A	33	PHE	CA-CB-CG	-9.56	104.24	113.80
1	A	22	GLY	O-C-N	-9.55	112.12	122.24
1	C	123	VAL	CA-CB-CG1	-9.54	94.19	110.40
1	C	111	GLN	N-CA-C	9.53	124.96	109.72
1	B	24	ILE	N-CA-CB	-9.51	99.42	110.55
1	C	133	TRP	CA-C-N	-9.51	107.79	122.62
1	C	133	TRP	C-N-CA	-9.51	107.79	122.62
1	C	140	VAL	N-CA-C	9.49	120.83	108.12
1	B	46	ASP	CA-CB-CG	-9.44	103.16	112.60
1	A	69	HIS	N-CA-CB	-9.40	95.47	110.98
1	C	123	VAL	CA-CB-CG2	-9.39	94.44	110.40
1	A	31	LYS	CA-CB-CG	-9.38	95.34	114.10
1	B	100	LYS	CB-CA-C	-9.35	91.75	110.17
1	C	98	ASP	CA-CB-CG	-9.35	103.25	112.60
1	A	14	ASP	CA-CB-CG	9.30	121.90	112.60
1	A	103	THR	CA-C-O	-9.26	110.79	121.72
1	B	88	ARG	NE-CZ-NH1	-9.22	112.28	121.50
1	A	67	TYR	N-CA-C	-9.22	100.92	110.97
1	C	6	ARG	N-CA-CB	9.21	126.08	111.43
1	A	99	SER	CA-CB-OG	-9.10	92.89	111.10
1	C	139	LEU	CA-C-O	-9.10	110.24	120.43
1	C	36	VAL	CA-CB-CG1	-9.07	94.97	110.40
1	B	24	ILE	CA-CB-CG1	-9.07	94.98	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	ILE	N-CA-CB	-9.05	96.30	111.23
1	C	119	GLY	N-CA-C	-9.03	95.35	110.80
1	C	138	GLU	CA-C-N	-9.02	110.12	122.30
1	C	138	GLU	C-N-CA	-9.02	110.12	122.30
1	C	97	ALA	CB-CA-C	-9.01	95.37	110.68
1	C	22	GLY	N-CA-C	-8.97	101.79	112.64
1	C	121	ASP	CA-C-N	-8.95	105.45	122.09
1	C	121	ASP	C-N-CA	-8.95	105.45	122.09
1	C	11	ILE	O-C-N	8.87	132.48	122.99
1	C	26	LYS	CA-C-O	8.85	130.19	120.63
1	B	85	LYS	CA-C-N	8.85	131.94	120.44
1	B	85	LYS	C-N-CA	8.85	131.94	120.44
1	B	53	ILE	N-CA-C	8.84	120.63	111.00
1	C	147	GLN	CB-CG-CD	-8.81	97.62	112.60
1	A	83	VAL	CA-CB-CG1	-8.80	95.44	110.40
1	C	17	GLN	CA-CB-CG	-8.77	96.56	114.10
1	A	112	VAL	CA-CB-CG1	-8.71	95.58	110.40
1	A	40	PHE	CA-C-N	-8.69	104.94	121.54
1	A	40	PHE	C-N-CA	-8.69	104.94	121.54
1	A	48	LEU	CA-C-O	8.69	129.91	120.10
1	B	135	ARG	O-C-N	8.68	129.11	121.39
1	C	49	LYS	CA-C-N	-8.64	106.46	121.66
1	C	49	LYS	C-N-CA	-8.64	106.46	121.66
1	A	42	ARG	N-CA-CB	8.63	123.93	110.21
1	B	149	TRP	N-CA-CB	8.63	124.73	110.92
1	B	144	SER	N-CA-C	8.60	121.70	110.43
1	B	74	VAL	CA-C-O	-8.59	112.59	121.70
1	B	13	PRO	CB-CA-C	8.59	125.72	111.56
1	B	14	ASP	CA-C-O	8.57	129.76	120.24
1	C	13	PRO	CA-C-O	8.57	131.94	119.34
1	C	46	ASP	CA-CB-CG	-8.57	104.03	112.60
1	A	130	ILE	N-CA-CB	-8.56	100.53	110.55
1	A	98	ASP	N-CA-C	-8.55	100.39	113.89
1	A	105	ARG	CD-NE-CZ	8.54	136.35	124.40
1	B	28	PHE	CA-C-N	-8.52	109.40	120.65
1	B	28	PHE	C-N-CA	-8.52	109.40	120.65
1	B	79	GLU	N-CA-C	8.52	122.78	108.90
1	A	29	GLU	CA-C-O	8.50	130.44	120.92
1	C	121	ASP	N-CA-CB	8.49	123.78	110.46
1	A	28	PHE	CA-C-O	-8.48	111.89	120.80
1	A	63	GLY	N-CA-C	-8.48	101.12	115.62
1	A	145	CYS	CA-CB-SG	8.48	133.90	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	TRP	N-CA-C	8.47	123.43	113.18
1	C	22	GLY	CA-C-N	-8.44	108.31	120.29
1	C	22	GLY	C-N-CA	-8.44	108.31	120.29
1	A	17	GLN	N-CA-C	-8.43	102.44	112.89
1	B	129	GLU	CA-C-O	8.43	129.35	120.42
1	C	87	GLY	CA-C-N	-8.42	108.98	120.44
1	C	87	GLY	C-N-CA	-8.42	108.98	120.44
1	B	60	PHE	N-CA-CB	8.41	124.70	110.49
1	A	15	GLY	N-CA-C	-8.39	102.12	113.37
1	B	108	PHE	CB-CA-C	-8.36	96.34	109.80
1	A	21	MET	N-CA-C	8.34	120.29	111.03
1	C	55	LEU	CB-CA-C	-8.33	97.61	111.02
1	B	130	ILE	CA-CB-CG2	-8.32	96.36	110.50
1	C	145	CYS	N-CA-CB	8.31	122.07	110.01
1	B	24	ILE	CB-CA-C	-8.31	101.34	111.97
1	C	21	MET	N-CA-C	8.29	120.09	111.14
1	A	144	SER	N-CA-C	8.29	120.60	110.41
1	A	108	PHE	N-CA-CB	-8.28	98.36	110.70
1	C	66	LYS	N-CA-CB	-8.28	98.07	110.07
1	A	79	GLU	N-CA-C	8.25	123.45	110.17
1	C	88	ARG	CD-NE-CZ	-8.25	112.85	124.40
1	B	150	ILE	CA-C-O	8.22	128.40	119.35
1	A	138	GLU	CA-C-O	8.22	128.88	119.18
1	B	45	GLU	CA-C-O	8.21	129.12	120.42
1	A	31	LYS	CA-C-O	8.20	129.47	119.38
1	B	107	ASP	N-CA-C	8.18	122.52	112.54
1	B	103	THR	CA-CB-CG2	-8.17	96.61	110.50
1	A	125	SER	N-CA-CB	-8.12	97.84	109.94
1	A	114	ARG	NE-CZ-NH1	8.11	129.60	121.50
1	B	112	VAL	CB-CA-C	-8.08	98.04	111.29
1	C	36	VAL	O-C-N	-8.08	109.92	122.04
1	A	29	GLU	N-CA-CB	-8.06	96.64	109.78
1	A	104	ILE	CA-CB-CG1	-8.06	96.70	110.40
1	C	95	ASN	CB-CA-C	8.06	119.35	110.08
1	C	27	ARG	N-CA-C	8.04	121.15	111.82
1	B	110	ILE	CA-C-N	-8.04	111.28	122.93
1	B	110	ILE	C-N-CA	-8.04	111.28	122.93
1	A	127	GLU	O-C-N	8.03	131.61	122.22
1	A	83	VAL	CB-CA-C	-8.02	101.61	111.88
1	B	23	GLU	N-CA-CB	-8.02	97.99	109.94
1	C	131	ALA	CA-C-O	8.00	129.27	120.63
1	B	20	LEU	N-CA-CB	-8.00	98.28	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	106	GLY	CA-C-O	7.98	129.12	120.66
1	A	85	LYS	CG-CD-CE	7.96	129.60	111.30
1	A	139	LEU	CA-C-N	-7.95	112.84	123.10
1	A	139	LEU	C-N-CA	-7.95	112.84	123.10
1	C	107	ASP	CA-C-N	-7.94	109.63	122.26
1	C	107	ASP	C-N-CA	-7.94	109.63	122.26
1	B	74	VAL	N-CA-CB	7.93	119.75	112.06
1	A	72	PRO	CB-CA-C	7.92	121.66	110.17
1	C	62	ALA	CB-CA-C	-7.92	97.17	110.56
1	A	127	GLU	CA-C-N	7.90	131.37	120.63
1	A	127	GLU	C-N-CA	7.90	131.37	120.63
1	A	74	VAL	N-CA-CB	7.89	121.90	111.64
1	C	25	ILE	O-C-N	7.88	129.64	121.91
1	A	27	ARG	NE-CZ-NH2	7.88	126.29	119.20
1	C	77	VAL	N-CA-C	-7.87	96.73	108.46
1	C	33	PHE	CA-CB-CG	-7.87	105.93	113.80
1	A	118	HIS	ND1-CG-CD2	7.87	113.97	106.10
1	B	65	VAL	O-C-N	7.83	129.58	121.91
1	C	114	ARG	CD-NE-CZ	-7.82	113.45	124.40
1	B	30	GLN	CA-C-O	-7.82	110.03	119.49
1	A	127	GLU	N-CA-C	7.82	120.70	111.71
1	C	31	LYS	N-CA-C	-7.81	103.73	113.18
1	C	9	ILE	CB-CG1-CD1	-7.80	97.41	113.80
1	C	50	GLU	CA-C-N	-7.80	110.30	120.44
1	C	50	GLU	C-N-CA	-7.80	110.30	120.44
1	A	65	VAL	O-C-N	7.80	129.78	121.90
1	A	110	ILE	N-CA-CB	-7.80	101.59	112.12
1	A	65	VAL	CA-C-O	7.80	129.14	120.64
1	C	139	LEU	CB-CA-C	-7.79	97.20	110.22
1	B	91	LEU	O-C-N	7.78	132.94	122.59
1	B	121	ASP	CB-CA-C	-7.78	97.35	110.81
1	C	75	ALA	CA-C-O	-7.78	112.10	121.28
1	B	58	ARG	O-C-N	7.76	128.38	121.32
1	C	60	PHE	N-CA-CB	7.75	121.51	110.12
1	C	88	ARG	NE-CZ-NH2	7.75	126.17	119.20
1	A	118	HIS	CA-C-N	-7.75	115.64	121.61
1	A	118	HIS	C-N-CA	-7.75	115.64	121.61
1	C	76	MET	CA-C-O	-7.75	112.94	121.23
1	C	122	SER	CA-C-N	-7.70	109.48	120.42
1	C	122	SER	C-N-CA	-7.70	109.48	120.42
1	B	24	ILE	O-C-N	-7.70	114.36	121.91
1	C	66	LYS	CB-CA-C	-7.69	98.74	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	LEU	N-CA-CB	7.69	122.96	110.42
1	C	12	LYS	CB-CA-C	7.69	125.32	110.17
1	A	41	MET	CG-SD-CE	-7.67	84.02	100.90
1	B	12	LYS	O-C-N	7.67	130.29	121.31
1	A	147	GLN	N-CA-CB	-7.67	98.55	110.06
1	A	98	ASP	CB-CG-OD2	-7.65	100.81	118.40
1	A	84	VAL	O-C-N	-7.65	113.95	121.90
1	A	103	THR	O-C-N	7.63	131.49	122.94
1	A	121	ASP	CB-CA-C	-7.63	97.67	110.56
1	B	73	VAL	O-C-N	7.63	131.13	122.97
1	A	52	TYR	N-CA-CB	-7.62	99.42	110.47
1	A	22	GLY	N-CA-C	-7.61	103.27	113.24
1	A	128	LYS	O-C-N	7.60	130.24	122.03
1	A	108	PHE	CA-CB-CG	-7.58	106.22	113.80
1	C	125	SER	N-CA-CB	-7.57	98.55	110.28
1	B	132	LEU	CB-CA-C	7.54	124.58	110.63
1	A	35	LEU	O-C-N	7.52	131.80	123.22
1	C	55	LEU	N-CA-C	-7.52	103.42	112.59
1	C	25	ILE	N-CA-CB	-7.51	101.76	110.55
1	C	51	HIS	CA-C-O	7.49	128.69	120.82
1	B	122	SER	CB-CA-C	-7.49	95.52	110.42
1	B	140	VAL	CA-CB-CG1	7.47	123.10	110.40
1	C	80	GLY	CA-C-O	-7.43	114.25	121.83
1	B	69	HIS	CA-CB-CG	-7.42	106.38	113.80
1	B	60	PHE	CA-CB-CG	7.42	121.22	113.80
1	B	25	ILE	O-C-N	-7.41	114.53	121.94
1	A	71	GLY	CA-C-N	-7.41	112.59	120.66
1	A	71	GLY	C-N-CA	-7.41	112.59	120.66
1	B	3	ASN	CA-CB-CG	-7.41	105.19	112.60
1	B	22	GLY	CA-C-O	7.40	128.50	120.66
1	A	46	ASP	CA-CB-CG	7.39	120.00	112.60
1	B	33	PHE	CA-C-O	-7.38	113.45	121.94
1	A	97	ALA	N-CA-C	7.38	121.97	113.19
1	B	147	GLN	CA-C-O	7.36	128.39	119.49
1	B	73	VAL	CA-C-O	-7.35	113.07	121.75
1	B	85	LYS	O-C-N	7.35	129.94	122.08
1	B	45	GLU	N-CA-C	-7.34	103.35	111.36
1	C	58	ARG	N-CA-C	-7.34	93.58	109.81
1	A	136	PRO	N-CA-CB	7.33	110.95	103.25
1	C	52	TYR	N-CA-C	7.33	120.74	112.97
1	A	48	LEU	N-CA-CB	-7.31	98.96	110.22
1	A	109	CYS	CA-C-O	-7.30	113.42	121.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	18	ARG	NE-CZ-NH2	-7.30	112.63	119.20
1	A	108	PHE	CB-CA-C	-7.30	98.90	110.94
1	C	98	ASP	CA-C-N	-7.28	112.95	123.00
1	C	98	ASP	C-N-CA	-7.28	112.95	123.00
1	B	116	ILE	CB-CG1-CD1	-7.28	98.52	113.80
1	C	34	ARG	O-C-N	7.26	131.50	123.22
1	C	23	GLU	CA-C-N	-7.26	111.42	120.56
1	C	23	GLU	C-N-CA	-7.26	111.42	120.56
1	B	115	ASN	CA-CB-CG	-7.25	105.34	112.60
1	B	21	MET	O-C-N	7.24	129.91	122.09
1	C	100	LYS	CA-CB-CG	-7.24	99.62	114.10
1	B	24	ILE	CA-C-O	7.24	128.84	121.17
1	C	41	MET	N-CA-CB	-7.24	99.23	111.31
1	C	152	GLU	CB-CA-C	7.24	123.85	110.10
1	B	142	TYR	CA-C-N	-7.22	111.35	122.62
1	B	142	TYR	C-N-CA	-7.22	111.35	122.62
1	B	109	CYS	CB-CA-C	7.22	124.79	110.42
1	A	6	ARG	CB-CA-C	-7.22	95.66	109.66
1	A	91	LEU	N-CA-CB	-7.21	99.52	110.12
1	C	95	ASN	OD1-CG-ND2	7.21	129.81	122.60
1	C	149	TRP	O-C-N	7.18	131.95	122.33
1	C	7	THR	CA-C-O	7.17	129.02	120.99
1	A	129	GLU	CA-C-O	7.16	128.56	120.90
1	B	140	VAL	CA-CB-CG2	7.15	122.55	110.40
1	B	51	HIS	CB-CA-C	-7.14	98.71	110.85
1	A	9	ILE	CA-CB-CG1	-7.14	98.27	110.40
1	A	66	LYS	CA-CB-CG	-7.13	99.83	114.10
1	A	8	PHE	O-C-N	7.13	131.54	123.27
1	C	98	ASP	N-CA-C	7.12	120.84	112.72
1	A	139	LEU	O-C-N	-7.11	115.11	123.22
1	A	97	ALA	CA-C-N	-7.10	110.91	121.99
1	A	97	ALA	C-N-CA	-7.10	110.91	121.99
1	B	88	ARG	N-CA-CB	7.10	122.17	110.39
1	C	118	HIS	CA-CB-CG	-7.10	106.70	113.80
1	C	27	ARG	O-C-N	7.09	130.99	122.27
1	C	105	ARG	CB-CA-C	7.09	122.01	110.88
1	A	133	TRP	CG-CD2-CE3	-7.08	126.82	133.90
1	A	20	LEU	CA-C-N	-7.08	111.00	120.63
1	A	20	LEU	C-N-CA	-7.08	111.00	120.63
1	A	115	ASN	CA-C-O	7.08	129.69	121.34
1	A	21	MET	CG-SD-CE	7.08	116.47	100.90
1	A	123	VAL	N-CA-CB	-7.07	97.97	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	88	ARG	NE-CZ-NH1	-7.06	114.44	121.50
1	A	61	PHE	N-CA-CB	7.06	122.42	110.49
1	C	40	PHE	CB-CA-C	-7.04	99.11	111.22
1	A	41	MET	CA-C-N	-7.02	113.08	122.42
1	A	41	MET	C-N-CA	-7.02	113.08	122.42
1	A	115	ASN	CA-C-N	7.01	134.59	121.97
1	A	115	ASN	C-N-CA	7.01	134.59	121.97
1	A	6	ARG	NE-CZ-NH2	-7.01	112.89	119.20
1	C	23	GLU	N-CA-C	7.01	119.00	111.36
1	A	49	LYS	N-CA-CB	-7.00	99.77	110.13
1	A	55	LEU	N-CA-CB	-6.99	99.67	111.20
1	B	51	HIS	CA-CB-CG	-6.98	106.82	113.80
1	B	101	PRO	CA-C-N	6.98	133.06	122.86
1	B	101	PRO	C-N-CA	6.98	133.06	122.86
1	A	145	CYS	O-C-N	-6.96	114.58	122.09
1	B	137	GLU	O-C-N	6.94	130.81	122.27
1	C	116	ILE	O-C-N	-6.94	113.89	122.57
1	A	76	MET	CA-C-N	6.94	132.69	123.11
1	A	76	MET	C-N-CA	6.94	132.69	123.11
1	A	76	MET	CG-SD-CE	6.94	116.17	100.90
1	C	135	ARG	N-CA-CB	6.94	122.38	109.68
1	C	105	ARG	NE-CZ-NH1	-6.94	114.56	121.50
1	B	93	GLU	CA-C-O	-6.93	114.00	121.56
1	B	101	PRO	N-CA-CB	6.92	109.37	103.35
1	C	20	LEU	N-CA-CB	-6.91	99.81	111.20
1	A	115	ASN	N-CA-C	6.90	121.17	111.30
1	A	151	TYR	N-CA-C	6.90	120.64	109.40
1	B	141	ASN	CB-CA-C	6.87	121.06	109.80
1	C	132	LEU	N-CA-CB	-6.85	100.08	110.01
1	A	110	ILE	CB-CA-C	-6.84	103.94	110.65
1	A	6	ARG	CD-NE-CZ	6.84	133.98	124.40
1	A	34	ARG	CA-C-O	6.84	128.85	121.05
1	C	93	GLU	CB-CG-CD	6.83	124.21	112.60
1	A	93	GLU	CA-C-N	6.81	129.70	120.44
1	A	93	GLU	C-N-CA	6.81	129.70	120.44
1	C	95	ASN	CA-C-O	6.81	123.71	119.29
1	B	149	TRP	CA-C-O	-6.81	111.92	119.95
1	B	137	GLU	OE1-CD-OE2	6.80	139.22	122.90
1	C	119	GLY	O-C-N	-6.80	117.72	123.23
1	B	96	PRO	O-C-N	6.79	131.34	122.24
1	C	146	ALA	CA-C-O	6.79	127.62	119.61
1	A	134	PHE	CA-C-O	-6.78	113.17	121.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	VAL	CA-CB-CG2	-6.76	98.91	110.40
1	C	23	GLU	CB-CA-C	-6.75	99.37	110.85
1	A	49	LYS	N-CA-C	-6.74	103.18	111.40
1	B	152	GLU	CG-CD-OE2	-6.74	102.91	118.40
1	B	78	TRP	O-C-N	6.73	131.94	123.19
1	C	68	MET	CA-C-O	6.73	127.58	119.10
1	A	108	PHE	O-C-N	-6.71	114.09	122.35
1	B	92	GLY	CA-C-O	-6.71	115.92	121.76
1	A	11	ILE	CA-CB-CG2	-6.71	99.09	110.50
1	C	104	ILE	CA-C-O	6.71	127.93	120.95
1	B	75	ALA	CA-C-O	6.71	128.36	120.58
1	C	107	ASP	CA-C-O	6.70	126.79	119.15
1	B	141	ASN	N-CA-CB	6.70	121.21	110.16
1	C	149	TRP	CA-CB-CG	-6.70	100.87	113.60
1	C	93	GLU	N-CA-CB	-6.70	100.54	110.85
1	A	129	GLU	CB-CG-CD	-6.68	101.24	112.60
1	C	76	MET	CB-CA-C	-6.68	98.20	110.62
1	B	137	GLU	CG-CD-OE1	-6.68	103.04	118.40
1	A	115	ASN	CA-CB-CG	-6.67	105.93	112.60
1	A	81	LEU	CB-CA-C	-6.67	97.15	110.42
1	A	64	LEU	N-CA-C	-6.67	101.36	111.56
1	A	122	SER	CA-C-O	6.67	128.43	121.10
1	A	105	ARG	CA-C-N	-6.66	108.94	120.79
1	A	105	ARG	C-N-CA	-6.66	108.94	120.79
1	B	99	SER	N-CA-CB	-6.66	100.84	110.36
1	A	4	SER	CA-CB-OG	-6.66	97.79	111.10
1	A	126	ALA	CA-C-O	6.65	128.37	120.92
1	A	24	ILE	CA-C-O	-6.65	113.08	120.46
1	C	12	LYS	CB-CG-CD	-6.65	96.02	111.30
1	A	46	ASP	CA-C-N	-6.64	111.81	120.44
1	A	46	ASP	C-N-CA	-6.64	111.81	120.44
1	B	136	PRO	N-CA-CB	6.63	110.22	103.25
1	B	24	ILE	CA-CB-CG2	-6.63	99.23	110.50
1	C	53	ILE	CB-CA-C	6.62	120.45	111.97
1	B	18	ARG	CB-CA-C	6.61	124.27	110.32
1	A	69	HIS	CA-C-O	6.61	127.28	119.48
1	A	9	ILE	O-C-N	6.61	130.12	123.18
1	A	135	ARG	NE-CZ-NH2	6.59	125.13	119.20
1	B	18	ARG	O-C-N	-6.59	113.82	122.39
1	A	147	GLN	N-CA-C	-6.58	103.37	111.33
1	B	64	LEU	N-CA-C	-6.57	104.05	111.14
1	A	114	ARG	N-CA-CB	-6.56	101.60	111.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	SER	N-CA-C	-6.55	105.03	113.16
1	B	38	MET	CG-SD-CE	6.55	115.31	100.90
1	A	69	HIS	ND1-CG-CD2	6.55	112.65	106.10
1	A	29	GLU	O-C-N	-6.54	114.58	122.11
1	B	26	LYS	CA-C-N	-6.53	110.38	120.31
1	B	26	LYS	C-N-CA	-6.53	110.38	120.31
1	B	105	ARG	O-C-N	-6.53	113.90	122.39
1	C	5	GLU	CB-CA-C	6.53	119.92	109.61
1	A	16	VAL	CA-CB-CG1	6.53	121.50	110.40
1	C	82	ASN	N-CA-CB	6.51	121.50	110.49
1	B	47	LEU	N-CA-CB	-6.50	100.55	109.98
1	C	8	PHE	CA-CB-CG	-6.50	107.30	113.80
1	C	15	GLY	CA-C-N	-6.50	111.55	120.46
1	C	15	GLY	C-N-CA	-6.50	111.55	120.46
1	B	113	GLY	N-CA-C	-6.50	107.52	114.67
1	B	127	GLU	CB-CA-C	6.49	121.19	110.81
1	A	120	SER	O-C-N	-6.48	114.89	122.87
1	C	116	ILE	CA-CB-CG2	6.48	121.51	110.50
1	C	43	ALA	O-C-N	-6.46	115.24	122.86
1	C	144	SER	CA-C-N	-6.46	112.04	120.44
1	C	144	SER	C-N-CA	-6.46	112.04	120.44
1	B	57	ASP	CA-CB-CG	6.45	119.05	112.60
1	C	31	LYS	N-CA-CB	-6.45	99.57	110.41
1	C	49	LYS	N-CA-CB	6.45	120.15	110.22
1	A	34	ARG	NE-CZ-NH2	-6.45	113.40	119.20
1	C	16	VAL	CA-CB-CG2	6.45	121.36	110.40
1	B	16	VAL	CA-C-N	-6.44	111.65	120.28
1	B	16	VAL	C-N-CA	-6.44	111.65	120.28
1	A	124	GLU	CB-CG-CD	6.43	123.53	112.60
1	B	18	ARG	CA-C-N	-6.43	111.74	121.51
1	B	18	ARG	C-N-CA	-6.43	111.74	121.51
1	A	135	ARG	C-N-CD	-6.40	98.75	125.00
1	C	150	ILE	CA-C-N	-6.40	113.34	122.94
1	C	150	ILE	C-N-CA	-6.40	113.34	122.94
1	A	136	PRO	CA-N-CD	-6.39	103.05	112.00
1	C	4	SER	CA-C-N	-6.39	111.78	121.31
1	C	4	SER	C-N-CA	-6.39	111.78	121.31
1	C	34	ARG	N-CA-CB	-6.39	100.00	110.42
1	B	94	THR	CA-C-O	6.39	127.53	120.63
1	C	20	LEU	CA-C-O	6.38	127.67	119.95
1	B	148	ASN	OD1-CG-ND2	6.37	128.97	122.60
1	C	111	GLN	N-CA-CB	-6.36	100.20	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	PRO	O-C-N	-6.36	114.06	122.64
1	B	118	HIS	N-CA-C	-6.35	99.02	108.99
1	C	39	LYS	O-C-N	6.34	130.58	123.48
1	A	135	ARG	N-CA-C	-6.33	99.61	109.87
1	A	49	LYS	O-C-N	6.33	129.83	122.17
1	A	49	LYS	CA-C-N	-6.33	112.22	120.44
1	A	49	LYS	C-N-CA	-6.33	112.22	120.44
1	C	108	PHE	O-C-N	6.33	130.13	122.35
1	C	137	GLU	CA-C-O	-6.32	113.86	120.55
1	B	85	LYS	N-CA-C	6.31	118.72	111.02
1	C	24	ILE	CB-CG1-CD1	6.29	127.01	113.80
1	C	67	TYR	CB-CG-CD2	-6.29	111.36	120.80
1	C	33	PHE	CB-CA-C	-6.29	98.39	109.71
1	C	94	THR	CB-CA-C	6.28	120.86	110.81
1	B	127	GLU	CA-CB-CG	-6.28	101.54	114.10
1	A	16	VAL	CB-CA-C	-6.28	102.09	112.26
1	C	128	LYS	N-CA-C	6.28	117.81	110.97
1	B	67	TYR	N-CA-C	-6.27	104.69	112.90
1	B	116	ILE	CA-CB-CG2	6.27	121.15	110.50
1	B	142	TYR	O-C-N	6.26	129.66	123.46
1	A	112	VAL	CA-CB-CG2	-6.25	99.77	110.40
1	B	78	TRP	CD2-CE2-CZ2	-6.25	116.14	122.40
1	A	123	VAL	CA-C-O	6.25	127.22	120.47
1	A	8	PHE	CD1-CE1-CZ	-6.25	108.75	120.00
1	B	93	GLU	CB-CG-CD	-6.24	101.99	112.60
1	C	45	GLU	CA-C-N	-6.24	112.33	120.44
1	C	45	GLU	C-N-CA	-6.24	112.33	120.44
1	C	140	VAL	CA-C-N	-6.24	113.88	122.30
1	C	140	VAL	C-N-CA	-6.24	113.88	122.30
1	B	68	MET	O-C-N	6.23	129.51	122.22
1	A	121	ASP	O-C-N	6.22	129.81	122.34
1	C	62	ALA	O-C-N	6.22	129.81	122.34
1	C	133	TRP	CH2-CZ2-CE2	6.22	125.59	117.50
1	C	106	GLY	CA-C-O	-6.22	109.75	120.57
1	C	139	LEU	CA-C-N	6.22	132.14	121.63
1	C	139	LEU	C-N-CA	6.22	132.14	121.63
1	B	105	ARG	N-CA-CB	-6.21	99.76	110.32
1	A	86	THR	N-CA-CB	-6.21	101.07	110.07
1	A	118	HIS	CG-CD2-NE2	-6.20	101.00	107.20
1	B	126	ALA	CA-C-N	6.20	128.90	120.54
1	B	126	ALA	C-N-CA	6.20	128.90	120.54
1	A	10	ALA	CB-CA-C	-6.19	98.82	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	80	GLY	CA-C-N	6.18	129.54	120.82
1	C	80	GLY	C-N-CA	6.18	129.54	120.82
1	C	150	ILE	CA-CB-CG1	-6.18	99.89	110.40
1	A	108	PHE	CA-C-N	-6.18	110.31	121.62
1	A	108	PHE	C-N-CA	-6.18	110.31	121.62
1	B	114	ARG	CA-C-N	6.18	133.63	121.58
1	B	114	ARG	C-N-CA	6.18	133.63	121.58
1	B	114	ARG	CB-CG-CD	6.17	125.48	111.30
1	A	122	SER	CA-CB-OG	-6.16	98.78	111.10
1	B	144	SER	CA-CB-OG	-6.16	98.78	111.10
1	C	46	ASP	CB-CG-OD2	-6.16	104.23	118.40
1	A	77	VAL	O-C-N	6.15	129.00	123.03
1	A	9	ILE	CA-C-N	-6.13	112.02	122.33
1	A	9	ILE	C-N-CA	-6.13	112.02	122.33
1	C	9	ILE	CA-CB-CG2	6.13	120.92	110.50
1	A	68	MET	CB-CA-C	6.13	122.61	110.42
1	C	18	ARG	CA-C-O	-6.13	111.89	119.18
1	B	127	GLU	CA-C-N	-6.12	112.48	120.44
1	B	127	GLU	C-N-CA	-6.12	112.48	120.44
1	C	87	GLY	CA-C-O	6.12	127.01	120.40
1	B	143	LYS	O-C-N	6.11	130.76	123.24
1	A	31	LYS	N-CA-C	-6.11	105.09	112.54
1	C	45	GLU	CA-C-O	6.11	127.00	120.10
1	A	142	TYR	CA-C-O	6.10	127.92	121.33
1	A	48	LEU	N-CA-C	6.10	118.72	111.71
1	C	17	GLN	CA-C-O	6.10	126.88	119.38
1	C	95	ASN	CB-CG-ND2	-6.09	107.26	116.40
1	A	137	GLU	N-CA-C	-6.09	104.97	113.37
1	A	142	TYR	CA-CB-CG	-6.09	102.94	113.90
1	C	51	HIS	N-CA-C	-6.08	104.57	111.07
1	B	27	ARG	NE-CZ-NH2	-6.08	113.73	119.20
1	A	5	GLU	N-CA-CB	-6.06	100.22	109.92
1	C	91	LEU	CA-C-N	-6.06	112.31	122.62
1	C	91	LEU	C-N-CA	-6.06	112.31	122.62
1	A	116	ILE	CB-CA-C	6.05	121.22	111.29
1	B	79	GLU	CG-CD-OE2	-6.05	104.48	118.40
1	C	122	SER	N-CA-C	-6.05	98.94	108.14
1	A	25	ILE	O-C-N	-6.04	115.77	121.87
1	B	150	ILE	CB-CA-C	-6.04	104.95	110.63
1	C	105	ARG	NE-CZ-NH2	6.04	124.63	119.20
1	C	132	LEU	CA-C-O	6.03	127.15	120.82
1	A	116	ILE	CA-C-N	-6.02	111.13	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	ILE	C-N-CA	-6.02	111.13	121.97
1	A	122	SER	CA-C-N	-6.02	110.42	120.30
1	A	122	SER	C-N-CA	-6.02	110.42	120.30
1	A	24	ILE	CA-CB-CG1	6.01	120.63	110.40
1	C	20	LEU	CD1-CG-CD2	-6.01	97.57	110.80
1	A	51	HIS	O-C-N	-6.01	115.88	122.07
1	A	25	ILE	CA-C-O	6.01	127.00	120.57
1	B	41	MET	N-CA-C	6.01	116.21	108.34
1	A	18	ARG	CB-CA-C	6.00	120.81	110.01
1	A	41	MET	O-C-N	5.99	130.56	122.59
1	B	74	VAL	CA-C-N	5.99	129.86	121.24
1	B	74	VAL	C-N-CA	5.99	129.86	121.24
1	B	127	GLU	CA-C-O	5.98	127.30	120.90
1	A	131	ALA	N-CA-C	-5.97	104.68	111.07
1	C	79	GLU	N-CA-CB	5.97	122.08	111.69
1	B	31	LYS	CA-CB-CG	5.97	126.05	114.10
1	B	150	ILE	CA-C-N	-5.97	112.44	122.29
1	B	150	ILE	C-N-CA	-5.97	112.44	122.29
1	C	147	GLN	CA-CB-CG	-5.96	102.17	114.10
1	C	53	ILE	O-C-N	-5.96	116.07	121.91
1	A	15	GLY	CA-C-N	-5.96	110.53	120.30
1	A	15	GLY	C-N-CA	-5.96	110.53	120.30
1	C	54	ASP	CA-CB-CG	-5.96	106.64	112.60
1	A	57	ASP	CA-CB-CG	-5.95	106.65	112.60
1	A	67	TYR	CB-CG-CD2	-5.94	111.89	120.80
1	A	7	THR	N-CA-CB	5.94	121.58	111.66
1	A	89	VAL	CA-CB-CG2	-5.94	100.30	110.40
1	B	146	ALA	CA-C-N	-5.94	111.10	120.60
1	B	146	ALA	C-N-CA	-5.94	111.10	120.60
1	A	117	ILE	CA-CB-CG2	5.94	120.59	110.50
1	B	23	GLU	CB-CA-C	-5.93	101.32	110.81
1	B	97	ALA	CB-CA-C	-5.92	100.62	110.68
1	C	23	GLU	N-CA-CB	5.91	118.91	110.16
1	B	99	SER	CA-CB-OG	-5.91	99.28	111.10
1	A	24	ILE	CB-CG1-CD1	-5.91	101.40	113.80
1	A	69	HIS	ND1-CE1-NE2	5.91	114.31	108.40
1	A	128	LYS	CA-C-O	-5.90	114.83	120.90
1	A	23	GLU	N-CA-C	5.89	117.70	111.28
1	A	89	VAL	O-C-N	-5.89	115.92	121.87
1	A	146	ALA	N-CA-C	5.89	120.88	111.81
1	A	89	VAL	CA-C-N	5.88	128.09	120.44
1	A	89	VAL	C-N-CA	5.88	128.09	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	79	GLU	O-C-N	5.88	130.28	123.17
1	C	56	LYS	CA-C-N	5.87	132.04	123.12
1	C	56	LYS	C-N-CA	5.87	132.04	123.12
1	A	130	ILE	N-CA-C	5.86	116.05	110.42
1	B	136	PRO	O-C-N	5.86	130.55	122.64
1	C	29	GLU	N-CA-C	-5.86	104.08	111.11
1	A	130	ILE	O-C-N	5.86	127.65	121.91
1	C	52	TYR	N-CA-CB	-5.85	102.34	110.65
1	A	93	GLU	CB-CG-CD	-5.84	102.67	112.60
1	C	27	ARG	CB-CA-C	-5.84	99.45	110.67
1	A	18	ARG	N-CA-CB	5.84	119.38	110.44
1	A	70	SER	N-CA-C	5.83	120.02	113.02
1	B	109	CYS	CA-CB-SG	-5.83	100.99	114.40
1	A	45	GLU	CA-CB-CG	-5.82	102.45	114.10
1	C	133	TRP	CZ3-CH2-CZ2	-5.82	113.93	121.50
1	C	117	ILE	CA-CB-CG2	5.82	120.39	110.50
1	C	129	GLU	O-C-N	5.81	128.78	122.15
1	A	64	LEU	CB-CA-C	-5.80	100.18	111.03
1	B	65	VAL	CA-CB-CG2	-5.80	100.53	110.40
1	C	35	LEU	CB-CA-C	-5.80	101.60	110.88
1	B	25	ILE	CA-CB-CG2	5.79	120.35	110.50
1	C	26	LYS	N-CA-C	5.79	118.34	111.33
1	A	146	ALA	CB-CA-C	-5.78	101.40	111.23
1	C	91	LEU	CD1-CG-CD2	-5.78	98.09	110.80
1	A	61	PHE	CB-CG-CD2	5.77	130.51	120.70
1	A	40	PHE	CB-CA-C	-5.76	100.74	110.19
1	B	78	TRP	CH2-CZ2-CE2	5.76	124.99	117.50
1	B	88	ARG	NE-CZ-NH2	5.75	124.38	119.20
1	A	123	VAL	CA-CB-CG1	5.75	120.17	110.40
1	A	22	GLY	CA-C-N	-5.74	112.58	120.28
1	A	22	GLY	C-N-CA	-5.74	112.58	120.28
1	A	17	GLN	CB-CG-CD	5.74	122.36	112.60
1	A	133	TRP	CE2-CD2-CE3	5.73	124.53	118.80
1	C	136	PRO	CA-C-N	5.73	127.96	120.28
1	C	136	PRO	C-N-CA	5.73	127.96	120.28
1	A	47	LEU	N-CA-CB	-5.72	101.72	110.01
1	A	111	GLN	CA-C-O	5.72	127.46	120.60
1	C	89	VAL	CA-CB-CG1	-5.71	100.69	110.40
1	C	35	LEU	O-C-N	-5.69	114.74	122.48
1	A	24	ILE	N-CA-C	-5.69	105.55	111.58
1	B	129	GLU	CB-CA-C	-5.69	101.18	110.85
1	A	132	LEU	CB-CA-C	-5.69	102.20	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	CYS	N-CA-CB	5.69	119.14	110.44
1	C	16	VAL	CA-C-O	5.69	126.86	120.95
1	C	53	ILE	CA-C-O	5.68	127.19	121.17
1	B	82	ASN	CB-CA-C	-5.67	103.67	111.73
1	A	73	VAL	N-CA-C	-5.67	100.52	108.80
1	A	38	MET	CB-CA-C	-5.67	100.17	109.80
1	C	110	ILE	CA-C-N	5.66	131.70	122.81
1	C	110	ILE	C-N-CA	5.66	131.70	122.81
1	C	148	ASN	CA-CB-CG	5.66	118.26	112.60
1	C	73	VAL	CB-CA-C	5.66	119.40	110.52
1	A	11	ILE	O-C-N	5.65	129.78	122.77
1	A	68	MET	CA-C-N	-5.64	113.68	122.37
1	A	68	MET	C-N-CA	-5.64	113.68	122.37
1	B	112	VAL	N-CA-C	5.64	121.07	109.34
1	C	72	PRO	O-C-N	5.64	130.00	123.01
1	C	16	VAL	O-C-N	-5.64	116.40	121.87
1	B	103	THR	N-CA-CB	5.64	118.50	110.44
1	A	139	LEU	N-CA-C	-5.63	100.11	109.46
1	A	105	ARG	O-C-N	5.63	129.88	122.33
1	B	42	ARG	CB-CA-C	5.63	120.03	111.76
1	A	58	ARG	CA-C-O	5.62	127.87	120.16
1	A	86	THR	CB-CA-C	5.62	119.79	110.90
1	A	13	PRO	N-CD-CG	-5.62	94.78	103.20
1	B	6	ARG	NE-CZ-NH2	-5.62	114.15	119.20
1	A	143	LYS	CA-CB-CG	-5.61	102.88	114.10
1	C	152	GLU	CA-CB-CG	5.61	125.31	114.10
1	C	14	ASP	CB-CA-C	5.60	119.75	110.90
1	A	105	ARG	CA-CB-CG	-5.60	102.90	114.10
1	C	8	PHE	CE1-CZ-CE2	-5.60	109.92	120.00
1	C	116	ILE	N-CA-C	5.60	120.99	109.34
1	A	131	ALA	CA-C-O	5.60	126.70	120.82
1	C	142	TYR	N-CA-C	5.60	116.78	108.60
1	C	11	ILE	CB-CG1-CD1	-5.60	102.04	113.80
1	A	145	CYS	CB-CA-C	5.60	119.75	110.90
1	A	56	LYS	CA-C-N	-5.59	113.28	122.79
1	A	56	LYS	C-N-CA	-5.59	113.28	122.79
1	A	138	GLU	CB-CA-C	5.59	119.72	109.99
1	A	6	ARG	N-CA-C	5.59	118.67	109.85
1	A	140	VAL	CG1-CB-CG2	-5.58	98.52	110.80
1	B	116	ILE	CA-C-N	-5.58	111.93	121.97
1	B	116	ILE	C-N-CA	-5.58	111.93	121.97
1	A	46	ASP	CA-C-O	5.58	126.68	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	50	GLU	CA-C-O	5.58	125.80	119.27
1	C	103	THR	N-CA-C	-5.57	101.20	110.17
1	A	27	ARG	NH1-CZ-NH2	-5.56	112.07	119.30
1	C	46	ASP	N-CA-CB	-5.56	101.95	110.01
1	A	6	ARG	NE-CZ-NH1	5.55	127.05	121.50
1	C	105	ARG	O-C-N	5.55	127.79	122.07
1	A	39	LYS	O-C-N	5.55	129.70	123.48
1	B	129	GLU	CG-CD-OE2	-5.55	105.64	118.40
1	C	35	LEU	CD1-CG-CD2	-5.55	98.60	110.80
1	A	116	ILE	O-C-N	5.54	129.49	122.57
1	A	74	VAL	CA-CB-CG2	-5.53	101.00	110.40
1	B	74	VAL	N-CA-C	5.53	114.56	106.55
1	B	42	ARG	O-C-N	-5.52	115.64	122.82
1	A	29	GLU	CB-CG-CD	-5.52	103.21	112.60
1	C	118	HIS	CA-C-N	-5.52	114.64	121.38
1	C	118	HIS	C-N-CA	-5.52	114.64	121.38
1	B	152	GLU	CA-CB-CG	-5.51	103.08	114.10
1	C	62	ALA	N-CA-CB	5.51	118.60	110.56
1	B	31	LYS	CB-CA-C	-5.50	98.82	110.31
1	B	116	ILE	CA-CB-CG1	5.49	119.74	110.40
1	A	60	PHE	CB-CA-C	5.49	121.35	110.42
1	C	27	ARG	CA-C-N	-5.49	111.20	120.58
1	C	27	ARG	C-N-CA	-5.49	111.20	120.58
1	B	94	THR	O-C-N	-5.48	116.31	122.12
1	C	23	GLU	CA-C-O	5.48	126.23	120.42
1	C	75	ALA	O-C-N	5.47	129.40	123.10
1	A	13	PRO	O-C-N	-5.47	115.16	122.22
1	B	3	ASN	O-C-N	5.47	130.42	122.43
1	A	126	ALA	CA-C-N	-5.46	112.42	120.28
1	A	126	ALA	C-N-CA	-5.46	112.42	120.28
1	C	39	LYS	CA-C-O	5.46	126.89	120.89
1	C	25	ILE	CG1-CB-CG2	-5.46	94.33	110.70
1	B	80	GLY	CA-C-N	-5.45	113.39	121.24
1	B	80	GLY	C-N-CA	-5.45	113.39	121.24
1	A	110	ILE	CA-C-O	5.44	124.59	118.98
1	A	134	PHE	CZ-CE2-CD2	-5.44	110.20	120.00
1	B	134	PHE	CA-CB-CG	5.44	119.24	113.80
1	A	77	VAL	CA-C-O	5.43	125.63	120.31
1	A	38	MET	CG-SD-CE	5.43	112.84	100.90
1	B	18	ARG	CD-NE-CZ	5.43	132.00	124.40
1	B	72	PRO	CB-CA-C	-5.42	102.88	110.63
1	B	103	THR	CA-C-N	-5.42	114.11	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	THR	C-N-CA	-5.42	114.11	120.72
1	C	58	ARG	CA-C-O	5.42	127.58	120.16
1	B	16	VAL	N-CA-CB	5.41	120.15	111.23
1	C	74	VAL	N-CA-CB	5.40	119.17	111.82
1	A	101	PRO	N-CA-C	-5.40	102.21	110.95
1	C	18	ARG	CB-CA-C	5.39	120.07	109.72
1	A	47	LEU	O-C-N	-5.39	116.52	122.07
1	A	79	GLU	CG-CD-OE1	-5.38	106.02	118.40
1	B	6	ARG	NH1-CZ-NH2	5.38	126.29	119.30
1	B	94	THR	CA-CB-OG1	5.38	117.66	109.60
1	B	52	TYR	CA-C-N	-5.37	111.95	120.55
1	B	52	TYR	C-N-CA	-5.37	111.95	120.55
1	A	117	ILE	CB-CA-C	-5.37	102.48	111.29
1	B	13	PRO	O-C-N	-5.37	115.39	122.64
1	B	108	PHE	CA-C-N	-5.37	111.29	121.54
1	B	108	PHE	C-N-CA	-5.37	111.29	121.54
1	A	74	VAL	N-CA-C	-5.36	99.92	107.75
1	C	94	THR	N-CA-CB	5.36	117.93	109.94
1	B	65	VAL	CA-C-N	-5.36	113.04	120.38
1	B	65	VAL	C-N-CA	-5.36	113.04	120.38
1	B	18	ARG	CA-C-O	5.35	125.97	119.49
1	C	33	PHE	CA-C-N	-5.35	115.66	122.77
1	C	33	PHE	C-N-CA	-5.35	115.66	122.77
1	B	79	GLU	CG-CD-OE1	5.35	130.69	118.40
1	C	59	PRO	O-C-N	5.33	129.84	122.64
1	C	124	GLU	CA-C-N	-5.33	112.21	120.31
1	C	124	GLU	C-N-CA	-5.33	112.21	120.31
1	C	44	SER	CA-C-N	-5.33	112.61	120.28
1	C	44	SER	C-N-CA	-5.33	112.61	120.28
1	B	110	ILE	CB-CA-C	-5.33	102.56	111.29
1	B	129	GLU	CG-CD-OE1	5.32	130.63	118.40
1	B	110	ILE	O-C-N	5.32	129.22	122.57
1	B	27	ARG	CA-CB-CG	-5.31	103.48	114.10
1	C	140	VAL	O-C-N	-5.31	116.69	122.64
1	A	14	ASP	CB-CA-C	-5.31	101.82	110.85
1	B	42	ARG	CA-C-N	-5.31	113.40	121.31
1	B	42	ARG	C-N-CA	-5.31	113.40	121.31
1	A	21	MET	CA-C-N	5.31	126.77	120.14
1	A	21	MET	C-N-CA	5.31	126.77	120.14
1	B	125	SER	O-C-N	5.30	127.54	122.03
1	C	120	SER	N-CA-C	5.30	117.92	110.23
1	B	83	VAL	N-CA-CB	5.30	117.75	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	63	GLY	O-C-N	5.30	129.59	122.70
1	A	66	LYS	O-C-N	5.29	129.63	122.59
1	B	66	LYS	CB-CA-C	5.29	119.68	110.68
1	A	104	ILE	N-CA-CB	-5.29	102.50	111.23
1	B	58	ARG	N-CA-CB	-5.29	103.75	111.20
1	C	102	GLY	O-C-N	-5.28	116.68	122.65
1	C	133	TRP	CA-C-O	5.28	125.78	119.60
1	A	67	TYR	N-CA-CB	-5.27	102.21	109.91
1	B	102	GLY	N-CA-C	-5.27	108.42	114.69
1	A	27	ARG	CA-CB-CG	-5.26	103.58	114.10
1	A	125	SER	CA-C-O	5.26	126.53	120.90
1	C	106	GLY	CA-C-N	-5.26	113.17	122.26
1	C	106	GLY	C-N-CA	-5.26	113.17	122.26
1	C	10	ALA	O-C-N	5.25	129.98	123.15
1	C	125	SER	CA-C-N	-5.25	112.83	120.29
1	C	125	SER	C-N-CA	-5.25	112.83	120.29
1	B	67	TYR	CA-CB-CG	5.25	123.34	113.90
1	B	73	VAL	CB-CA-C	-5.25	103.34	110.90
1	A	117	ILE	CB-CG1-CD1	-5.25	102.79	113.80
1	B	78	TRP	N-CA-CB	5.24	120.04	111.08
1	B	90	MET	N-CA-CB	-5.23	102.17	110.22
1	C	124	GLU	CA-C-O	5.22	126.00	120.10
1	B	83	VAL	CB-CA-C	-5.22	105.09	112.14
1	A	35	LEU	CA-C-O	-5.22	114.78	120.36
1	A	45	GLU	OE1-CD-OE2	-5.21	110.39	122.90
1	C	8	PHE	CZ-CE2-CD2	5.21	129.38	120.00
1	C	46	ASP	O-C-N	5.20	127.42	122.07
1	B	119	GLY	N-CA-C	-5.19	102.92	111.38
1	C	69	HIS	CA-C-O	5.19	125.30	119.18
1	A	115	ASN	N-CA-CB	-5.18	103.76	111.43
1	C	99	SER	CA-C-N	5.18	128.24	120.83
1	C	99	SER	C-N-CA	5.18	128.24	120.83
1	C	120	SER	N-CA-CB	5.18	117.65	109.83
1	C	150	ILE	CB-CA-C	-5.17	104.37	111.65
1	B	107	ASP	CB-CA-C	-5.16	99.52	110.31
1	C	100	LYS	N-CA-C	5.16	115.92	109.57
1	B	17	GLN	CA-CB-CG	-5.16	103.78	114.10
1	C	70	SER	CA-CB-OG	-5.15	100.79	111.10
1	B	71	GLY	CA-C-N	-5.15	114.68	120.14
1	B	71	GLY	C-N-CA	-5.15	114.68	120.14
1	B	123	VAL	CA-C-N	-5.15	113.09	120.82
1	B	123	VAL	C-N-CA	-5.15	113.09	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	136	PRO	CA-C-O	5.15	127.77	119.64
1	C	107	ASP	OD1-CG-OD2	-5.14	110.57	122.90
1	A	85	LYS	N-CA-CB	-5.12	102.59	110.12
1	A	52	TYR	CA-CB-CG	-5.12	104.68	113.90
1	B	88	ARG	N-CA-C	5.12	118.79	112.54
1	B	114	ARG	CA-CB-CG	-5.12	103.86	114.10
1	C	78	TRP	N-CA-C	-5.12	100.69	109.24
1	A	30	GLN	CG-CD-NE2	5.12	124.08	116.40
1	C	98	ASP	CB-CG-OD2	-5.12	106.64	118.40
1	A	18	ARG	CG-CD-NE	-5.11	100.75	112.00
1	C	26	LYS	CG-CD-CE	5.11	123.06	111.30
1	A	18	ARG	N-CA-C	5.11	119.50	113.16
1	B	36	VAL	CA-CB-CG1	5.11	119.08	110.40
1	B	148	ASN	CA-C-N	-5.11	114.55	122.67
1	B	148	ASN	C-N-CA	-5.11	114.55	122.67
1	A	10	ALA	N-CA-CB	5.10	119.38	110.81
1	C	34	ARG	NE-CZ-NH2	-5.10	114.61	119.20
1	C	73	VAL	CA-C-O	-5.09	116.65	121.64
1	A	79	GLU	CA-C-N	-5.09	113.11	122.27
1	A	79	GLU	C-N-CA	-5.09	113.11	122.27
1	C	97	ALA	CA-C-N	-5.09	114.53	122.73
1	C	97	ALA	C-N-CA	-5.09	114.53	122.73
1	C	144	SER	N-CA-C	5.09	118.24	110.20
1	C	45	GLU	N-CA-C	-5.09	105.86	111.71
1	B	23	GLU	CA-C-N	-5.09	114.15	120.56
1	B	23	GLU	C-N-CA	-5.09	114.15	120.56
1	A	95	ASN	CB-CA-C	-5.08	102.07	109.38
1	A	52	TYR	CB-CG-CD2	5.08	128.41	120.80
1	A	106	GLY	N-CA-C	-5.07	108.03	114.16
1	A	67	TYR	CB-CG-CD1	5.06	128.39	120.80
1	A	141	ASN	CA-C-N	-5.06	113.00	121.75
1	A	141	ASN	C-N-CA	-5.06	113.00	121.75
1	C	107	ASP	CB-CG-OD1	5.06	130.04	118.40
1	A	17	GLN	CA-CB-CG	5.06	124.22	114.10
1	A	85	LYS	N-CA-C	5.06	116.79	111.28
1	C	54	ASP	CB-CG-OD2	-5.06	106.77	118.40
1	A	53	ILE	CA-C-O	-5.05	114.47	120.78
1	A	134	PHE	CE1-CZ-CE2	5.05	129.09	120.00
1	C	36	VAL	CA-C-O	5.05	125.22	119.92
1	B	138	GLU	CA-C-O	5.04	125.80	120.10
1	A	8	PHE	CE1-CZ-CE2	5.04	129.07	120.00
1	B	26	LYS	O-C-N	-5.04	115.84	122.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	121	ASP	O-C-N	5.04	128.82	122.37
1	C	18	ARG	CG-CD-NE	5.04	123.08	112.00
1	B	64	LEU	CA-C-O	5.04	125.89	120.70
1	B	151	TYR	O-C-N	5.03	129.11	123.27
1	A	33	PHE	CA-C-O	-5.03	115.66	121.19
1	A	54	ASP	N-CA-C	5.03	121.52	110.80
1	A	140	VAL	CA-CB-CG2	5.03	118.95	110.40
1	A	20	LEU	N-CA-CB	5.02	119.48	111.20
1	C	6	ARG	CA-C-N	5.01	130.73	121.85
1	C	6	ARG	C-N-CA	5.01	130.73	121.85
1	C	103	THR	OG1-CB-CG2	5.01	119.33	109.30
1	A	2	ALA	CA-C-O	5.01	129.32	120.80
1	A	66	LYS	CA-C-O	5.01	127.67	120.51
1	A	72	PRO	N-CA-CB	5.01	108.51	102.85
1	C	36	VAL	N-CA-CB	-5.01	101.02	111.24
1	A	28	PHE	CA-CB-CG	-5.00	108.80	113.80

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	18	ARG	CA
1	A	24	ILE	CB

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	ASN	Mainchain
1	B	151	TYR	Sidechain
1	B	3	ASN	Sidechain
1	B	99	SER	Mainchain

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	1207	0	1207	184	0
1	B	1207	0	1207	158	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1207	0	1207	135	0
2	A	23	0	11	1	0
2	B	23	0	11	3	0
2	C	23	0	10	5	0
3	A	90	0	0	6	0
3	B	88	0	0	3	0
3	C	100	0	0	18	0
All	All	3968	0	3653	454	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 62.

All (454) 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:84:VAL:HG11	1:B:122:SER:HA	1.30	1.06
1:A:114:ARG:NH1	1:B:152:GLU:HB3	1.73	1.02
1:A:3:ASN:HD21	1:A:81:LEU:HD13	1.29	0.96
1:A:51:HIS:HD2	1:A:133:TRP:HE1	1.14	0.92
1:B:63:GLY:HA2	1:B:66:LYS:HG2	1.49	0.91
1:B:58:ARG:NH1	1:B:58:ARG:HB3	1.87	0.90
1:B:105:ARG:HE	1:B:115:ASN:HD22	1.17	0.89
1:A:126:ALA:O	1:A:130:ILE:HG13	1.73	0.88
1:A:3:ASN:ND2	1:A:81:LEU:HB2	1.88	0.88
1:A:38:MET:HG3	1:A:76:MET:CG	2.06	0.84
1:B:63:GLY:CA	1:B:66:LYS:HG2	2.06	0.84
1:B:84:VAL:HG11	1:B:122:SER:CA	2.07	0.84
1:B:139:LEU:HD22	1:B:139:LEU:H	1.42	0.83
1:A:110:ILE:HG23	3:A:232:HOH:O	1.78	0.83
1:C:55:LEU:HD13	1:C:60:PHE:HE1	1.43	0.83
1:A:51:HIS:CD2	1:A:133:TRP:HE1	1.96	0.83
1:C:55:LEU:HD13	1:C:60:PHE:CE1	2.14	0.82
1:A:79:GLU:HG2	1:A:80:GLY:N	1.95	0.82
1:A:15:GLY:CA	1:A:116:ILE:HG22	2.11	0.81
1:A:139:LEU:N	1:A:139:LEU:HD23	1.93	0.81
1:C:135:ARG:HG2	1:C:138:GLU:OE1	1.82	0.80
1:A:95:ASN:HA	1:A:112:VAL:HG22	1.64	0.80
1:C:125:SER:O	1:C:129:GLU:HG3	1.82	0.80
1:B:81:LEU:HB2	1:B:151:TYR:HE1	1.45	0.79
1:C:109:CYS:HA	3:C:457:HOH:O	1.82	0.78
1:A:27:ARG:NH2	1:A:107:ASP:OD2	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ARG:HD3	1:A:69:HIS:O	1.84	0.78
1:B:61:PHE:O	1:B:62:ALA:C	2.24	0.77
1:C:50:GLU:O	1:C:128:LYS:NZ	2.15	0.77
1:A:3:ASN:HD21	1:A:81:LEU:HB2	1.48	0.77
1:B:114:ARG:HG2	1:C:149:TRP:O	1.86	0.76
1:B:60:PHE:O	1:B:61:PHE:C	2.28	0.76
1:A:38:MET:HG3	1:A:76:MET:HG2	1.68	0.76
1:B:58:ARG:HB3	1:B:58:ARG:HH11	1.48	0.75
1:C:85:LYS:HG2	1:C:86:THR:N	2.00	0.75
1:A:88:ARG:NH1	1:A:119:GLY:O	2.19	0.75
1:C:7:THR:HB	1:C:84:VAL:HG22	1.67	0.75
1:B:105:ARG:NE	1:B:115:ASN:HD22	1.85	0.75
1:A:38:MET:HG3	1:A:76:MET:HG3	1.68	0.74
1:B:24:ILE:O	1:B:25:ILE:C	2.27	0.74
1:B:36:VAL:HB	1:B:77:VAL:HG12	1.69	0.73
1:A:62:ALA:O	1:A:66:LYS:HB2	1.89	0.73
1:A:3:ASN:ND2	1:A:81:LEU:HD13	2.02	0.73
1:A:52:TYR:C	3:A:239:HOH:O	2.31	0.73
1:B:16:VAL:HG21	1:B:72:PRO:O	1.89	0.73
1:A:3:ASN:HD21	1:A:81:LEU:CD1	2.02	0.72
1:C:23:GLU:HB3	3:C:299:HOH:O	1.89	0.72
1:B:136:PRO:HA	1:B:139:LEU:HD23	1.71	0.72
1:A:53:ILE:HG22	3:A:280:HOH:O	1.89	0.72
1:C:12:LYS:HE3	1:C:117:ILE:O	1.90	0.72
1:A:33:PHE:HZ	1:A:86:THR:HG21	1.55	0.72
1:A:39:LYS:HE2	1:A:41:MET:HE3	1.72	0.71
1:A:5:GLU:HG2	1:A:83:VAL:HG23	1.72	0.71
1:A:93:GLU:O	1:A:105:ARG:HD2	1.91	0.71
1:C:26:LYS:HG2	1:C:26:LYS:O	1.80	0.71
1:A:35:LEU:HD21	1:A:38:MET:HB2	1.72	0.70
1:A:56:LYS:HA	1:A:61:PHE:CE1	2.26	0.70
1:A:134:PHE:HD1	1:A:138:GLU:HG3	1.56	0.70
1:A:138:GLU:C	1:A:139:LEU:HD23	2.16	0.70
1:B:27:ARG:HH11	1:B:104:ILE:HG13	1.56	0.70
1:A:96:PRO:HG3	1:A:109:CYS:SG	2.32	0.69
1:A:105:ARG:NH2	1:A:117:ILE:O	2.25	0.69
1:C:93:GLU:H	1:C:99:SER:HB3	1.58	0.69
1:A:112:VAL:HG23	3:A:395:HOH:O	1.91	0.69
1:A:123:VAL:HA	1:A:126:ALA:HB3	1.73	0.69
1:B:125:SER:O	1:B:129:GLU:HG3	1.91	0.69
1:C:5:GLU:O	1:C:79:GLU:HB2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:GLY:O	1:C:91:LEU:HD13	1.94	0.68
1:A:61:PHE:O	1:A:64:LEU:N	2.24	0.67
1:A:61:PHE:O	1:A:64:LEU:HB2	1.95	0.67
1:B:81:LEU:CB	1:B:151:TYR:HE1	2.07	0.67
1:C:143:LYS:HG3	1:C:147:GLN:HE22	1.59	0.67
1:A:135:ARG:NH1	3:A:271:HOH:O	2.28	0.67
2:C:160:PCG:H8	3:C:443:HOH:O	1.95	0.67
1:B:147:GLN:OE1	1:B:147:GLN:HA	1.95	0.67
1:B:108:PHE:CD1	1:C:30:GLN:HG3	2.30	0.66
1:B:12:LYS:HG3	1:B:117:ILE:N	2.09	0.66
1:B:14:ASP:OD1	1:B:14:ASP:N	2.29	0.66
1:C:91:LEU:O	1:C:105:ARG:HB2	1.96	0.66
1:A:147:GLN:HE21	1:A:147:GLN:HA	1.60	0.65
1:C:10:ALA:O	1:C:117:ILE:HG12	1.95	0.65
1:A:56:LYS:O	1:A:56:LYS:NZ	2.22	0.65
1:B:122:SER:O	1:B:125:SER:HB2	1.96	0.65
1:B:56:LYS:O	1:B:58:ARG:N	2.28	0.65
1:C:3:ASN:OD1	1:C:81:LEU:HB2	1.96	0.65
1:A:88:ARG:HD3	1:A:120:SER:O	1.97	0.65
1:A:66:LYS:HD2	1:A:66:LYS:C	2.19	0.65
1:A:115:ASN:C	1:A:116:ILE:HG13	2.22	0.65
1:B:81:LEU:HB2	1:B:151:TYR:CE1	2.30	0.65
1:C:18:ARG:NH2	1:C:108:PHE:O	2.28	0.65
1:B:12:LYS:HB3	1:B:13:PRO:HD2	1.78	0.64
1:B:57:ASP:C	1:B:58:ARG:HG2	2.21	0.64
1:A:15:GLY:N	1:A:116:ILE:HG22	2.12	0.64
1:B:56:LYS:HA	1:B:61:PHE:CE1	2.32	0.64
1:B:42:ARG:O	1:B:43:ALA:C	2.35	0.64
1:A:122:SER:HG	1:A:125:SER:H	1.44	0.64
1:B:67:TYR:HD1	3:B:461:HOH:O	1.81	0.63
1:A:56:LYS:HA	1:A:61:PHE:CD1	2.33	0.63
1:B:111:GLN:NE2	1:C:152:GLU:OE1	2.30	0.63
1:B:3:ASN:OD1	1:B:3:ASN:N	2.29	0.63
1:B:4:SER:HB3	3:B:306:HOH:O	1.98	0.63
1:B:136:PRO:HA	1:B:139:LEU:CD2	2.28	0.63
1:A:31:LYS:HA	1:C:107:ASP:O	1.98	0.63
1:A:152:GLU:OE1	2:C:160:PCG:N2	2.32	0.63
1:B:53:ILE:HD11	1:B:56:LYS:HD3	1.80	0.63
1:B:53:ILE:HD11	1:B:56:LYS:NZ	2.14	0.63
1:B:105:ARG:HE	1:B:115:ASN:ND2	1.93	0.63
1:B:56:LYS:HA	1:B:61:PHE:CD1	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:VAL:HG12	3:C:227:HOH:O	1.98	0.62
1:C:12:LYS:HB3	1:C:13:PRO:HD2	1.80	0.62
1:C:63:GLY:O	1:C:66:LYS:HB2	2.00	0.62
1:C:83:VAL:HG22	1:C:83:VAL:O	1.99	0.62
1:C:4:SER:O	1:C:5:GLU:C	2.36	0.62
1:B:101:PRO:HG2	1:C:103:THR:HG22	1.82	0.62
1:C:80:GLY:O	1:C:83:VAL:HB	2.00	0.61
1:B:56:LYS:HG2	1:B:57:ASP:N	2.15	0.61
1:B:66:LYS:O	1:B:70:SER:HB3	2.00	0.61
1:A:8:PHE:O	1:A:119:GLY:HA2	2.01	0.61
1:A:2:ALA:C	1:A:4:SER:H	2.09	0.60
1:C:51:HIS:NE2	1:C:129:GLU:OE1	2.29	0.60
1:A:37:ALA:HB2	1:A:139:LEU:HD22	1.83	0.60
1:C:34:ARG:O	1:C:79:GLU:N	2.26	0.60
1:A:114:ARG:HH12	1:B:152:GLU:HB3	1.63	0.60
1:B:46:ASP:HA	1:B:49:LYS:HD2	1.82	0.60
1:C:104:ILE:O	1:C:108:PHE:HB2	2.00	0.60
1:C:128:LYS:O	1:C:132:LEU:HB2	2.02	0.60
1:B:58:ARG:O	1:B:59:PRO:C	2.43	0.60
1:B:108:PHE:CE1	1:C:30:GLN:HG3	2.36	0.60
1:B:27:ARG:NH1	1:B:104:ILE:HG13	2.17	0.60
1:C:10:ALA:HA	1:C:74:VAL:O	2.01	0.60
1:A:96:PRO:O	1:A:99:SER:HB2	2.02	0.59
1:A:96:PRO:HD2	1:A:112:VAL:HA	1.83	0.59
1:C:112:VAL:HG23	3:C:340:HOH:O	2.00	0.59
1:C:146:ALA:HB1	1:C:150:ILE:CD1	2.33	0.59
1:C:27:ARG:HD2	3:C:251:HOH:O	2.02	0.59
1:A:151:TYR:CE1	1:C:110:ILE:HG21	2.37	0.59
1:C:12:LYS:HB3	1:C:13:PRO:CD	2.33	0.59
1:C:86:THR:O	1:C:90:MET:HG3	2.02	0.59
1:A:110:ILE:HD13	1:B:33:PHE:CE1	2.37	0.59
1:B:28:PHE:O	1:B:29:GLU:C	2.38	0.59
1:B:86:THR:O	1:B:90:MET:HG3	2.02	0.59
1:B:129:GLU:O	1:B:130:ILE:C	2.39	0.59
1:A:114:ARG:CZ	1:B:152:GLU:HB3	2.32	0.58
1:C:55:LEU:CD1	1:C:60:PHE:HE1	2.13	0.58
1:B:110:ILE:HG22	1:B:111:GLN:HB2	1.84	0.58
1:A:50:GLU:OE2	1:A:53:ILE:HD12	2.03	0.58
1:B:63:GLY:HA2	1:B:66:LYS:CG	2.30	0.58
1:A:3:ASN:ND2	1:A:81:LEU:CB	2.66	0.58
1:C:48:LEU:HD22	1:C:68:MET:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ARG:NH1	1:A:142:TYR:H	2.02	0.58
1:C:135:ARG:N	1:C:138:GLU:OE1	2.32	0.58
1:A:134:PHE:CD1	1:A:138:GLU:HG3	2.38	0.57
1:C:7:THR:O	1:C:77:VAL:HA	2.03	0.57
1:A:17:GLN:HG3	1:B:149:TRP:CE2	2.39	0.57
1:A:44:SER:O	1:A:48:LEU:HB2	2.04	0.57
1:B:122:SER:O	1:B:125:SER:N	2.37	0.57
1:B:53:ILE:CD1	1:B:56:LYS:HD3	2.34	0.57
1:C:126:ALA:O	1:C:130:ILE:HG13	2.05	0.57
1:B:59:PRO:O	1:B:60:PHE:C	2.47	0.57
1:C:56:LYS:HA	1:C:61:PHE:CD2	2.40	0.57
1:A:8:PHE:HB3	1:A:120:SER:OG	2.04	0.57
1:A:57:ASP:O	1:A:58:ARG:C	2.46	0.57
1:A:130:ILE:O	1:A:134:PHE:N	2.36	0.57
1:C:6:ARG:NH1	1:C:79:GLU:OE1	2.37	0.56
1:A:80:GLY:O	1:A:83:VAL:HG22	2.04	0.56
1:A:86:THR:O	1:A:90:MET:HG3	2.05	0.56
1:B:137:GLU:OE1	1:B:137:GLU:N	2.35	0.56
1:C:139:LEU:HD23	1:C:139:LEU:N	2.21	0.56
1:C:20:LEU:O	1:C:24:ILE:HD12	2.05	0.56
1:A:60:PHE:HD1	1:A:64:LEU:CD2	2.19	0.56
1:A:33:PHE:HZ	1:A:86:THR:CG2	2.19	0.56
1:A:42:ARG:HD2	1:A:69:HIS:CE1	2.40	0.56
1:A:66:LYS:HD2	1:A:66:LYS:O	2.06	0.56
1:C:127:GLU:HA	3:C:286:HOH:O	2.05	0.56
1:A:39:LYS:HE2	1:A:41:MET:CE	2.36	0.56
1:B:108:PHE:HA	1:C:31:LYS:HA	1.87	0.55
2:C:160:PCG:H5'1	3:C:443:HOH:O	2.05	0.55
1:A:60:PHE:HD1	1:A:64:LEU:HD23	1.71	0.55
1:A:64:LEU:C	1:A:66:LYS:N	2.60	0.55
1:C:146:ALA:HB1	1:C:150:ILE:HD11	1.88	0.55
1:A:82:ASN:O	1:A:86:THR:HB	2.07	0.55
1:B:47:LEU:HD12	1:B:47:LEU:C	2.31	0.55
1:B:58:ARG:HB3	1:B:58:ARG:CZ	2.36	0.55
1:A:47:LEU:O	1:A:51:HIS:N	2.32	0.55
1:B:14:ASP:O	1:B:18:ARG:N	2.31	0.55
1:C:146:ALA:O	1:C:147:GLN:C	2.48	0.55
1:B:53:ILE:HD11	1:B:56:LYS:HZ2	1.71	0.55
1:B:33:PHE:CZ	1:B:83:VAL:HG12	2.42	0.55
1:C:115:ASN:C	1:C:116:ILE:HG12	2.32	0.55
1:B:34:ARG:NH1	1:B:142:TYR:CE1	2.75	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:LEU:HD22	1:B:139:LEU:N	2.17	0.55
1:A:128:LYS:O	1:A:131:ALA:HB3	2.07	0.54
1:B:53:ILE:HD12	1:B:56:LYS:HB2	1.88	0.54
1:A:123:VAL:O	1:A:127:GLU:N	2.39	0.54
1:A:150:ILE:HG21	1:C:110:ILE:HD12	1.89	0.54
1:B:40:PHE:CZ	1:B:72:PRO:HB2	2.42	0.54
1:B:51:HIS:CD2	1:B:133:TRP:HE1	2.25	0.54
1:B:64:LEU:O	1:B:68:MET:N	2.30	0.54
1:B:139:LEU:N	1:B:139:LEU:HD13	2.21	0.54
1:C:43:ALA:O	1:C:69:HIS:ND1	2.40	0.54
1:A:115:ASN:C	1:A:117:ILE:H	2.16	0.54
1:A:13:PRO:HA	1:A:72:PRO:O	2.07	0.54
1:A:100:LYS:O	1:A:103:THR:OG1	2.25	0.54
1:C:66:LYS:NZ	1:C:66:LYS:HB3	2.23	0.54
1:C:113:GLY:N	3:C:445:HOH:O	2.27	0.54
1:A:80:GLY:O	1:A:81:LEU:C	2.49	0.54
1:C:13:PRO:O	1:C:17:GLN:HB2	2.08	0.54
1:C:48:LEU:CD1	1:C:69:HIS:HB2	2.38	0.53
1:C:93:GLU:HB2	1:C:99:SER:HB3	1.89	0.53
1:C:115:ASN:O	1:C:117:ILE:N	2.41	0.53
1:C:15:GLY:O	1:C:16:VAL:C	2.46	0.53
1:A:95:ASN:CA	1:A:112:VAL:HG22	2.36	0.53
1:A:125:SER:O	1:A:129:GLU:HG3	2.07	0.53
1:A:57:ASP:O	1:A:58:ARG:O	2.27	0.53
1:A:112:VAL:O	1:A:112:VAL:HG12	2.06	0.53
1:A:14:ASP:O	1:A:18:ARG:HG3	2.09	0.53
1:B:110:ILE:HD12	1:C:31:LYS:O	2.07	0.53
1:C:128:LYS:HE2	1:C:132:LEU:HD12	1.91	0.53
1:C:30:GLN:NE2	3:C:203:HOH:O	2.40	0.53
1:A:6:ARG:NH2	1:A:127:GLU:OE1	2.42	0.53
1:B:13:PRO:HD3	1:B:73:VAL:HG12	1.91	0.53
1:A:3:ASN:HD21	1:A:81:LEU:CB	2.20	0.52
1:B:135:ARG:N	1:B:138:GLU:OE2	2.41	0.52
1:A:122:SER:O	1:A:125:SER:HB2	2.09	0.52
1:A:46:ASP:O	1:A:47:LEU:C	2.49	0.52
1:B:67:TYR:HA	1:B:70:SER:OG	2.10	0.52
1:B:110:ILE:HG22	1:B:111:GLN:N	2.25	0.52
1:C:12:LYS:NZ	2:C:160:PCG:O1A	2.24	0.52
1:A:6:ARG:HH21	1:A:127:GLU:CD	2.18	0.52
1:A:33:PHE:CZ	1:A:86:THR:CG2	2.93	0.52
1:B:83:VAL:O	1:B:84:VAL:C	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LYS:O	1:B:101:PRO:C	2.52	0.52
1:B:9:ILE:O	1:B:76:MET:HE3	2.09	0.52
1:A:61:PHE:O	1:A:63:GLY:N	2.42	0.52
1:A:135:ARG:O	1:A:138:GLU:HG2	2.09	0.52
1:C:9:ILE:HD13	1:C:119:GLY:CA	2.40	0.52
1:C:56:LYS:HB2	3:C:353:HOH:O	2.09	0.52
1:B:44:SER:O	1:B:48:LEU:HG	2.10	0.51
1:B:123:VAL:O	1:B:124:GLU:C	2.53	0.51
1:B:143:LYS:HD3	1:B:147:GLN:HB2	1.93	0.51
1:B:65:VAL:O	1:B:69:HIS:N	2.36	0.51
1:A:86:THR:O	1:A:87:GLY:C	2.50	0.51
1:B:34:ARG:NH1	1:B:36:VAL:HG22	2.26	0.51
1:A:147:GLN:HA	1:A:147:GLN:NE2	2.26	0.51
1:B:90:MET:O	1:B:104:ILE:N	2.44	0.51
1:B:56:LYS:HE2	1:B:57:ASP:OD1	2.11	0.51
1:B:58:ARG:HH11	1:B:58:ARG:CB	2.18	0.51
1:C:79:GLU:HG3	1:C:80:GLY:N	2.23	0.51
1:A:87:GLY:O	1:A:90:MET:HB2	2.10	0.51
1:B:81:LEU:N	1:B:151:TYR:OH	2.32	0.51
1:C:95:ASN:HA	1:C:112:VAL:HG22	1.91	0.51
1:A:85:LYS:O	1:A:89:VAL:HG23	2.11	0.50
1:A:61:PHE:C	1:A:63:GLY:H	2.19	0.50
1:B:143:LYS:HD2	1:B:144:SER:N	2.26	0.50
1:C:9:ILE:HD13	1:C:119:GLY:HA2	1.93	0.50
1:B:67:TYR:C	1:B:70:SER:H	2.20	0.50
1:C:85:LYS:O	1:C:88:ARG:HB2	2.12	0.50
1:C:139:LEU:N	1:C:139:LEU:CD2	2.72	0.50
1:C:66:LYS:NZ	3:C:435:HOH:O	2.43	0.50
1:B:63:GLY:C	1:B:66:LYS:HG2	2.36	0.50
1:B:66:LYS:HG3	1:B:67:TYR:N	2.26	0.50
1:A:67:TYR:O	1:A:69:HIS:N	2.44	0.49
1:B:116:ILE:O	1:B:117:ILE:HB	2.11	0.49
1:A:31:LYS:O	1:A:31:LYS:HG3	2.03	0.49
1:C:7:THR:HB	1:C:84:VAL:CG2	2.40	0.49
1:C:45:GLU:O	1:C:49:LYS:HG3	2.12	0.49
1:B:67:TYR:O	1:B:70:SER:OG	2.27	0.49
1:B:12:LYS:HG3	1:B:117:ILE:CA	2.41	0.49
1:B:135:ARG:O	1:B:138:GLU:HB2	2.11	0.49
1:B:137:GLU:H	1:B:137:GLU:CD	2.20	0.49
1:A:22:GLY:O	1:A:23:GLU:C	2.55	0.49
1:A:43:ALA:O	1:A:69:HIS:ND1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:THR:O	1:C:89:VAL:HB	2.13	0.49
1:A:53:ILE:CG2	1:A:54:ASP:N	2.76	0.49
1:A:149:TRP:O	1:C:114:ARG:HB3	2.12	0.49
1:B:53:ILE:O	1:B:54:ASP:O	2.30	0.49
1:C:23:GLU:OE1	3:C:299:HOH:O	2.20	0.49
1:C:146:ALA:O	1:C:149:TRP:N	2.45	0.49
1:B:67:TYR:HA	1:B:70:SER:CB	2.43	0.48
1:B:135:ARG:O	1:B:138:GLU:N	2.41	0.48
1:A:11:ILE:O	1:A:73:VAL:HA	2.13	0.48
1:A:51:HIS:CD2	1:A:133:TRP:NE1	2.74	0.48
1:B:22:GLY:O	1:B:23:GLU:C	2.56	0.48
1:B:24:ILE:HG22	1:B:25:ILE:N	2.10	0.48
1:B:52:TYR:HE1	2:B:160:PCG:H5'2	1.78	0.48
1:C:60:PHE:O	1:C:63:GLY:N	2.39	0.48
1:B:67:TYR:HA	1:B:70:SER:HB3	1.96	0.48
1:C:93:GLU:HA	1:C:93:GLU:OE1	2.14	0.48
1:A:122:SER:OG	1:A:125:SER:N	2.31	0.48
1:B:52:TYR:O	1:B:61:PHE:HE1	1.96	0.48
1:C:23:GLU:N	3:C:202:HOH:O	2.40	0.48
1:C:88:ARG:O	1:C:91:LEU:HB2	2.13	0.48
1:B:52:TYR:HE2	1:B:68:MET:HG3	1.79	0.48
1:A:39:LYS:O	1:A:75:ALA:N	2.37	0.47
1:C:48:LEU:HD12	1:C:69:HIS:HB2	1.95	0.47
1:C:7:THR:CB	1:C:84:VAL:HG22	2.41	0.47
1:C:129:GLU:O	1:C:133:TRP:HD1	1.97	0.47
1:A:36:VAL:O	1:A:140:VAL:N	2.47	0.47
1:A:121:ASP:OD1	1:A:125:SER:OG	2.26	0.47
1:A:50:GLU:O	1:A:53:ILE:HB	2.14	0.47
1:B:144:SER:C	1:B:146:ALA:H	2.22	0.47
1:A:84:VAL:O	1:A:88:ARG:HG2	2.14	0.47
1:A:122:SER:HB2	1:A:124:GLU:HG3	1.96	0.47
1:A:12:LYS:HE3	1:A:118:HIS:HB2	1.96	0.47
1:A:12:LYS:NZ	2:A:160:PCG:O2'	2.47	0.47
1:A:60:PHE:CD1	1:A:64:LEU:CD2	2.98	0.47
1:A:64:LEU:C	1:A:66:LYS:H	2.20	0.47
1:B:37:ALA:HB1	1:B:134:PHE:CE2	2.49	0.47
1:B:33:PHE:CE1	1:B:83:VAL:HG12	2.50	0.47
1:A:45:GLU:O	1:A:49:LYS:HG3	2.15	0.46
1:B:53:ILE:O	1:B:54:ASP:C	2.58	0.46
1:C:48:LEU:CD2	1:C:68:MET:HB3	2.44	0.46
1:A:47:LEU:HD23	1:A:48:LEU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ASN:O	1:A:117:ILE:N	2.32	0.46
1:A:129:GLU:O	1:A:133:TRP:HD1	1.99	0.46
1:A:11:ILE:HG13	1:A:76:MET:HE2	1.96	0.46
1:C:47:LEU:CD1	1:C:132:LEU:HD22	2.46	0.46
1:A:128:LYS:NZ	3:A:280:HOH:O	2.45	0.46
1:C:4:SER:HA	1:C:79:GLU:OE2	2.16	0.46
1:B:40:PHE:CZ	1:B:72:PRO:CB	2.99	0.46
1:B:87:GLY:HA2	1:B:90:MET:HG3	1.97	0.46
1:B:17:GLN:HG3	1:C:149:TRP:CZ2	2.51	0.46
1:A:60:PHE:CD1	1:A:64:LEU:HD21	2.51	0.46
1:B:12:LYS:HB3	1:B:13:PRO:CD	2.46	0.46
1:A:61:PHE:C	1:A:63:GLY:N	2.74	0.45
1:B:101:PRO:HB2	1:C:102:GLY:O	2.16	0.45
1:C:33:PHE:O	1:C:78:TRP:HZ3	1.99	0.45
1:C:55:LEU:O	1:C:61:PHE:HB2	2.16	0.45
1:A:15:GLY:HA2	1:A:116:ILE:HG22	1.94	0.45
1:A:24:ILE:HG22	1:A:25:ILE:N	2.30	0.45
1:B:16:VAL:HG13	1:B:21:MET:SD	2.56	0.45
1:C:12:LYS:HE3	1:C:117:ILE:C	2.41	0.45
1:C:123:VAL:HG22	1:C:124:GLU:N	2.18	0.45
1:A:8:PHE:O	1:A:120:SER:N	2.48	0.45
1:A:100:LYS:HA	1:A:101:PRO:HD3	1.82	0.45
1:A:101:PRO:HG2	1:B:103:THR:HG22	1.99	0.45
1:B:76:MET:HE3	1:B:76:MET:HB2	1.78	0.45
1:A:95:ASN:OD1	1:A:97:ALA:HB3	2.16	0.45
1:B:53:ILE:CD1	1:B:56:LYS:NZ	2.79	0.45
1:C:47:LEU:C	1:C:47:LEU:HD12	2.40	0.45
1:A:30:GLN:HG3	1:C:107:ASP:O	2.16	0.45
1:A:64:LEU:HA	1:A:64:LEU:HD22	1.73	0.45
1:A:140:VAL:HG12	1:A:141:ASN:N	2.31	0.45
1:B:116:ILE:HD13	1:B:116:ILE:HG21	1.41	0.45
1:B:121:ASP:O	1:B:122:SER:HB3	2.17	0.45
1:C:17:GLN:HG2	3:C:228:HOH:O	2.17	0.45
1:A:21:MET:O	1:A:25:ILE:HG13	2.17	0.45
1:B:63:GLY:O	1:B:66:LYS:HG2	2.17	0.45
1:C:112:VAL:HG12	1:C:112:VAL:O	2.16	0.45
1:B:27:ARG:HD2	1:B:104:ILE:HD11	1.99	0.45
1:B:45:GLU:O	1:B:49:LYS:HG3	2.17	0.45
1:A:151:TYR:CE1	1:C:110:ILE:CG2	3.00	0.44
1:C:47:LEU:HD12	1:C:47:LEU:O	2.17	0.44
1:A:3:ASN:ND2	1:A:81:LEU:CD1	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:ALA:HB2	1:C:139:LEU:HA	1.99	0.44
1:C:93:GLU:O	1:C:105:ARG:HD3	2.18	0.44
1:C:135:ARG:O	1:C:138:GLU:HB2	2.17	0.44
1:A:91:LEU:HG	1:A:117:ILE:HD13	2.00	0.44
1:B:3:ASN:ND2	1:B:151:TYR:CD1	2.85	0.44
1:C:11:ILE:O	1:C:73:VAL:HB	2.17	0.44
1:A:59:PRO:O	1:A:61:PHE:N	2.51	0.44
1:A:66:LYS:HD2	1:A:66:LYS:HA	1.53	0.44
1:A:24:ILE:CG2	1:A:25:ILE:N	2.80	0.44
1:A:143:LYS:HG3	1:A:144:SER:N	2.32	0.44
1:A:3:ASN:HD22	1:A:3:ASN:HA	1.34	0.44
1:B:91:LEU:O	1:B:104:ILE:N	2.50	0.44
1:B:94:THR:HG21	2:B:160:PCG:H3'	1.99	0.44
1:C:39:LYS:CE	1:C:134:PHE:CE1	3.01	0.44
1:C:51:HIS:CD2	1:C:133:TRP:HE1	2.35	0.44
1:A:12:LYS:HB3	1:A:13:PRO:HD3	2.00	0.44
1:A:95:ASN:OD1	1:A:97:ALA:N	2.41	0.44
1:C:23:GLU:HG2	3:C:202:HOH:O	2.16	0.44
1:C:37:ALA:HB1	3:C:247:HOH:O	2.17	0.44
1:C:129:GLU:O	1:C:133:TRP:CD1	2.70	0.44
1:A:54:ASP:C	1:A:55:LEU:HG	2.41	0.43
1:A:110:ILE:O	1:A:110:ILE:HG22	2.18	0.43
1:C:39:LYS:HE3	1:C:134:PHE:CE1	2.53	0.43
1:C:105:ARG:HH11	1:C:105:ARG:HD2	1.26	0.43
1:A:85:LYS:O	1:A:88:ARG:HB2	2.18	0.43
1:A:14:ASP:O	1:A:18:ARG:N	2.51	0.43
1:B:36:VAL:HB	1:B:77:VAL:CG1	2.45	0.43
1:A:20:LEU:O	1:A:24:ILE:HD12	2.19	0.43
1:A:59:PRO:C	1:A:61:PHE:H	2.27	0.43
1:C:11:ILE:HG13	1:C:76:MET:CE	2.49	0.43
1:C:94:THR:CG2	2:C:160:PCG:H3'	2.48	0.43
1:A:33:PHE:CZ	1:A:86:THR:HG21	2.44	0.43
1:A:152:GLU:N	1:C:111:GLN:OE1	2.34	0.43
1:B:8:PHE:HB3	1:B:120:SER:OG	2.19	0.43
1:B:33:PHE:CE1	1:B:83:VAL:CG1	3.02	0.43
1:B:125:SER:O	1:B:126:ALA:C	2.61	0.43
1:C:12:LYS:CB	1:C:13:PRO:CD	2.94	0.43
1:C:56:LYS:HA	1:C:61:PHE:CE2	2.54	0.43
1:B:8:PHE:HB2	1:B:130:ILE:HG13	2.00	0.43
1:B:118:HIS:CD2	1:B:118:HIS:C	2.94	0.43
1:B:41:MET:HE2	1:B:43:ALA:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:GLU:HG3	1:A:124:GLU:H	1.46	0.42
1:A:151:TYR:HE1	1:C:110:ILE:HG21	1.83	0.42
1:B:118:HIS:CG	1:B:119:GLY:N	2.84	0.42
1:A:10:ALA:O	1:A:117:ILE:HA	2.19	0.42
1:A:77:VAL:HG23	1:A:134:PHE:CE2	2.55	0.42
1:B:53:ILE:O	1:B:56:LYS:HB3	2.19	0.42
1:C:8:PHE:C	1:C:9:ILE:HG12	2.44	0.42
1:B:115:ASN:ND2	1:B:115:ASN:C	2.77	0.42
1:C:5:GLU:OE2	1:C:84:VAL:N	2.50	0.42
1:A:10:ALA:O	1:A:118:HIS:N	2.44	0.42
1:B:85:LYS:HB3	1:B:85:LYS:HE3	1.82	0.42
1:C:69:HIS:O	1:C:69:HIS:CD2	2.73	0.42
1:A:22:GLY:O	1:A:26:LYS:HB2	2.19	0.42
1:B:58:ARG:HA	1:B:59:PRO:HD2	1.53	0.42
1:B:69:HIS:ND1	1:B:69:HIS:O	2.52	0.42
1:C:14:ASP:OD1	1:C:116:ILE:HA	2.19	0.42
1:B:61:PHE:O	1:B:63:GLY:N	2.51	0.42
1:A:40:PHE:CE1	1:A:72:PRO:HB2	2.54	0.42
1:A:114:ARG:HA	1:A:114:ARG:HD3	1.69	0.42
1:C:116:ILE:O	1:C:117:ILE:HB	2.18	0.42
1:A:139:LEU:HD22	1:A:139:LEU:HA	1.28	0.42
1:B:14:ASP:OD1	1:B:67:TYR:CE1	2.72	0.42
1:C:25:ILE:O	1:C:29:GLU:HG3	2.19	0.42
1:C:64:LEU:HB3	1:C:65:VAL:H	1.46	0.42
1:B:12:LYS:O	1:B:16:VAL:HG23	2.19	0.42
1:B:127:GLU:O	1:B:128:LYS:C	2.59	0.42
1:C:123:VAL:HG12	1:C:123:VAL:H	1.12	0.42
1:A:5:GLU:O	1:A:83:VAL:CG2	2.68	0.41
1:A:48:LEU:CD1	1:A:69:HIS:HB2	2.51	0.41
1:A:134:PHE:HD1	1:A:138:GLU:CG	2.30	0.41
1:B:64:LEU:O	1:B:65:VAL:C	2.63	0.41
1:C:45:GLU:O	1:C:46:ASP:C	2.62	0.41
1:A:24:ILE:HD13	1:A:24:ILE:HG21	1.64	0.41
1:B:38:MET:HA	1:B:75:ALA:O	2.20	0.41
1:A:104:ILE:H	1:A:104:ILE:HG13	1.51	0.41
1:B:59:PRO:N	3:B:356:HOH:O	2.53	0.41
1:A:27:ARG:NH1	1:A:102:GLY:O	2.54	0.41
1:A:38:MET:CG	1:A:76:MET:HG2	2.45	0.41
1:A:59:PRO:C	1:A:61:PHE:N	2.78	0.41
1:A:40:PHE:O	1:A:41:MET:HB3	2.20	0.41
1:C:2:ALA:C	1:C:4:SER:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LEU:C	1:A:57:ASP:H	2.29	0.41
1:A:151:TYR:HE1	1:C:110:ILE:CG2	2.33	0.41
1:B:52:TYR:CE1	2:B:160:PCG:H5'2	2.56	0.41
1:B:53:ILE:O	1:B:53:ILE:HG13	2.20	0.41
1:B:56:LYS:C	1:B:58:ARG:N	2.79	0.41
1:B:35:LEU:O	1:B:142:TYR:OH	2.34	0.41
1:B:56:LYS:CG	1:B:57:ASP:N	2.81	0.41
1:A:12:LYS:HB2	1:A:116:ILE:C	2.45	0.40
1:A:17:GLN:HG3	1:B:149:TRP:CZ2	2.55	0.40
1:A:43:ALA:HB1	1:A:48:LEU:HG	2.02	0.40
1:B:48:LEU:HD22	1:B:68:MET:HB3	2.04	0.40
1:B:55:LEU:O	1:B:61:PHE:CD1	2.74	0.40
1:A:122:SER:OG	1:A:125:SER:HB2	2.21	0.40
1:C:18:ARG:NH1	3:C:457:HOH:O	2.55	0.40
1:A:96:PRO:CG	1:A:109:CYS:SG	3.06	0.40
1:C:12:LYS:HA	1:C:13:PRO:HD3	1.75	0.40
1:A:47:LEU:HG	1:A:132:LEU:HD22	2.04	0.40
1:A:125:SER:O	1:A:126:ALA:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	149/151 (99%)	128 (86%)	13 (9%)	8 (5%)	1	1
1	B	149/151 (99%)	120 (80%)	16 (11%)	13 (9%)	0	0
1	C	149/151 (99%)	131 (88%)	14 (9%)	4 (3%)	4	4
All	All	447/453 (99%)	379 (85%)	43 (10%)	25 (6%)	1	1

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	PHE
1	A	61	PHE
1	A	116	ILE
1	B	55	LEU
1	B	59	PRO
1	B	61	PHE
1	B	62	ALA
1	B	122	SER
1	C	116	ILE
1	A	68	MET
1	B	54	ASP
1	B	60	PHE
1	B	116	ILE
1	B	123	VAL
1	A	59	PRO
1	C	61	PHE
1	C	82	ASN
1	B	38	MET
1	A	58	ARG
1	B	57	ASP
1	C	147	GLN
1	A	62	ALA
1	B	117	ILE
1	B	136	PRO
1	A	53	ILE

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	128/128 (100%)	98 (77%)	30 (23%)	1	1
1	B	128/128 (100%)	96 (75%)	32 (25%)	0	1
1	C	128/128 (100%)	99 (77%)	29 (23%)	1	1
All	All	384/384 (100%)	293 (76%)	91 (24%)	1	1

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	17	GLN
1	A	18	ARG
1	A	26	LYS
1	A	39	LYS
1	A	41	MET
1	A	53	ILE
1	A	55	LEU
1	A	56	LYS
1	A	64	LEU
1	A	66	LYS
1	A	67	TYR
1	A	68	MET
1	A	70	SER
1	A	83	VAL
1	A	85	LYS
1	A	86	THR
1	A	100	LYS
1	A	110	ILE
1	A	116	ILE
1	A	117	ILE
1	A	130	ILE
1	A	132	LEU
1	A	133	TRP
1	A	135	ARG
1	A	137	GLU
1	A	139	LEU
1	A	143	LYS
1	A	144	SER
1	A	152	GLU
1	B	6	ARG
1	B	14	ASP
1	B	16	VAL
1	B	23	GLU
1	B	31	LYS
1	B	35	LEU
1	B	44	SER
1	B	46	ASP
1	B	47	LEU
1	B	56	LYS
1	B	57	ASP
1	B	58	ARG
1	B	66	LYS

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Mol	Chain	Res	Type
1	B	67	TYR
1	B	85	LYS
1	B	88	ARG
1	B	90	MET
1	B	110	ILE
1	B	112	VAL
1	B	114	ARG
1	B	115	ASN
1	B	118	HIS
1	B	120	SER
1	B	121	ASP
1	B	127	GLU
1	B	132	LEU
1	B	139	LEU
1	B	140	VAL
1	B	141	ASN
1	B	143	LYS
1	B	144	SER
1	B	147	GLN
1	C	6	ARG
1	C	9	ILE
1	C	23	GLU
1	C	24	ILE
1	C	26	LYS
1	C	30	GLN
1	C	38	MET
1	C	53	ILE
1	C	54	ASP
1	C	57	ASP
1	C	66	LYS
1	C	67	TYR
1	C	73	VAL
1	C	88	ARG
1	C	93	GLU
1	C	107	ASP
1	C	112	VAL
1	C	114	ARG
1	C	117	ILE
1	C	122	SER
1	C	123	VAL
1	C	124	GLU
1	C	125	SER

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Mol	Chain	Res	Type
1	C	132	LEU
1	C	135	ARG
1	C	137	GLU
1	C	139	LEU
1	C	143	LYS
1	C	144	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	51	HIS
1	B	17	GLN
1	B	51	HIS
1	C	82	ASN
1	C	147	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](#)

3 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	PCG	C	160	-	26,26,26	1.99	2 (7%)	39,41,41	2.92	16 (41%)
2	PCG	B	160	-	26,26,26	2.06	5 (19%)	39,41,41	2.13	13 (33%)
2	PCG	A	160	-	26,26,26	2.22	5 (19%)	39,41,41	2.97	11 (28%)

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	PCG	C	160	-	1/1/5/5	0/4/31/31	0/4/4/4
2	PCG	B	160	-	-	0/4/31/31	1/4/4/4
2	PCG	A	160	-	-	0/4/31/31	1/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	160	PCG	PA-O5'	-7.47	1.49	1.57
2	C	160	PCG	PA-O5'	-7.27	1.49	1.57
2	B	160	PCG	PA-O5'	-5.92	1.50	1.57
2	B	160	PCG	O3'-C3'	5.44	1.52	1.44
2	A	160	PCG	O3'-C3'	4.36	1.51	1.44
2	B	160	PCG	O6-C6	3.97	1.31	1.23
2	A	160	PCG	PA-O3'	-3.85	1.51	1.57
2	C	160	PCG	PA-O3'	-3.77	1.51	1.57
2	A	160	PCG	C4-N3	3.25	1.41	1.34
2	B	160	PCG	PA-O3'	-2.84	1.53	1.57
2	A	160	PCG	C5-N7	2.74	1.44	1.39
2	B	160	PCG	C6-N1	2.49	1.43	1.38

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	160	PCG	O5'-PA-O3'	-9.83	92.54	105.70
2	C	160	PCG	C5'-C4'-C3'	8.22	128.01	112.56
2	A	160	PCG	O1A-PA-O3'	7.43	124.36	107.04
2	A	160	PCG	C2'-C3'-C4'	-6.76	91.40	103.24
2	A	160	PCG	O3'-C3'-C2'	6.43	121.91	115.61
2	C	160	PCG	O3'-C3'-C4'	-6.16	106.06	110.71
2	B	160	PCG	C1'-N9-C8	-5.28	111.74	126.73
2	C	160	PCG	C1'-N9-C4	-4.74	112.49	126.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	160	PCG	O5'-PA-O3'	4.73	112.03	105.70
2	A	160	PCG	C1'-N9-C4	-4.72	112.55	126.49
2	C	160	PCG	O5'-PA-O2A	-4.57	99.91	110.44
2	C	160	PCG	O1A-PA-O5'	4.44	117.99	107.16
2	B	160	PCG	O3'-C3'-C2'	4.35	119.87	115.61
2	C	160	PCG	C2'-C3'-C4'	-4.16	95.95	103.24
2	B	160	PCG	C1'-N9-C4	4.01	138.34	126.49
2	A	160	PCG	C1'-N9-C8	4.00	138.08	126.73
2	C	160	PCG	C1'-N9-C8	3.97	138.00	126.73
2	C	160	PCG	O4'-C1'-N9	-3.87	99.58	108.36
2	C	160	PCG	C2-N3-C4	-3.63	106.03	112.30
2	B	160	PCG	C2'-C3'-C4'	-3.61	96.91	103.24
2	B	160	PCG	O1A-PA-O3'	3.52	115.23	107.04
2	C	160	PCG	O3'-C3'-C2'	3.44	118.98	115.61
2	C	160	PCG	O4'-C4'-C3'	3.28	111.83	104.92
2	A	160	PCG	C5'-C4'-C3'	-2.97	106.98	112.56
2	B	160	PCG	C4'-O4'-C1'	-2.94	102.98	109.47
2	A	160	PCG	O2'-C2'-C1'	-2.81	100.41	110.10
2	A	160	PCG	O3'-PA-O2A	2.78	116.35	110.39
2	B	160	PCG	C5-C6-N1	-2.70	106.38	113.25
2	A	160	PCG	O2'-C2'-C3'	2.68	118.67	111.19
2	C	160	PCG	O3'-PA-O2A	2.64	116.05	110.39
2	B	160	PCG	O3'-C3'-C4'	2.57	112.65	110.71
2	B	160	PCG	C2-N3-C4	-2.49	108.01	112.30
2	B	160	PCG	N2-C2-N1	-2.33	111.85	116.76
2	C	160	PCG	C5-C4-N3	2.32	132.09	128.39
2	C	160	PCG	O4'-C4'-C5'	2.30	119.33	112.38
2	B	160	PCG	O5'-PA-O3'	2.28	108.75	105.70
2	A	160	PCG	C4'-O4'-C1'	-2.17	104.67	109.47
2	B	160	PCG	O2'-C2'-C3'	2.13	117.15	111.19
2	C	160	PCG	C5-C6-N1	-2.08	107.96	113.25
2	B	160	PCG	O2'-C2'-C1'	-2.01	103.17	110.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	160	PCG	C4'

There are no torsion outliers.

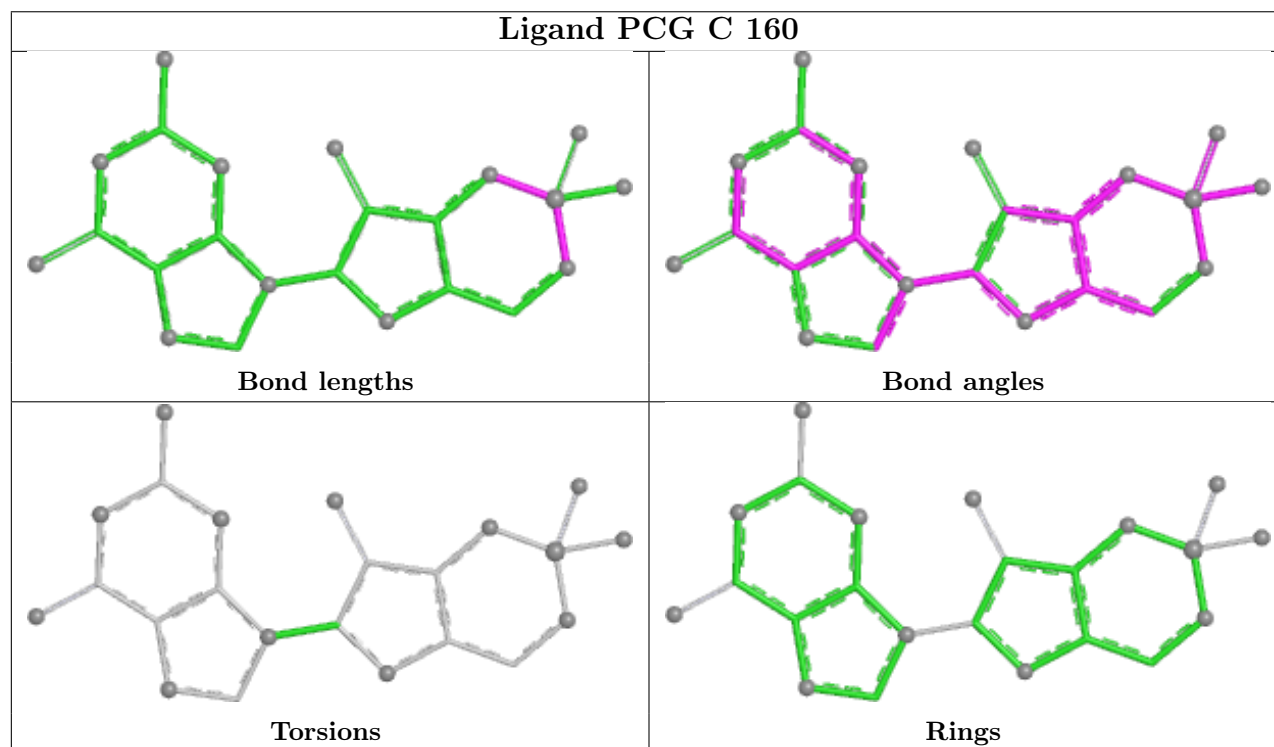
All (2) ring outliers are listed below:

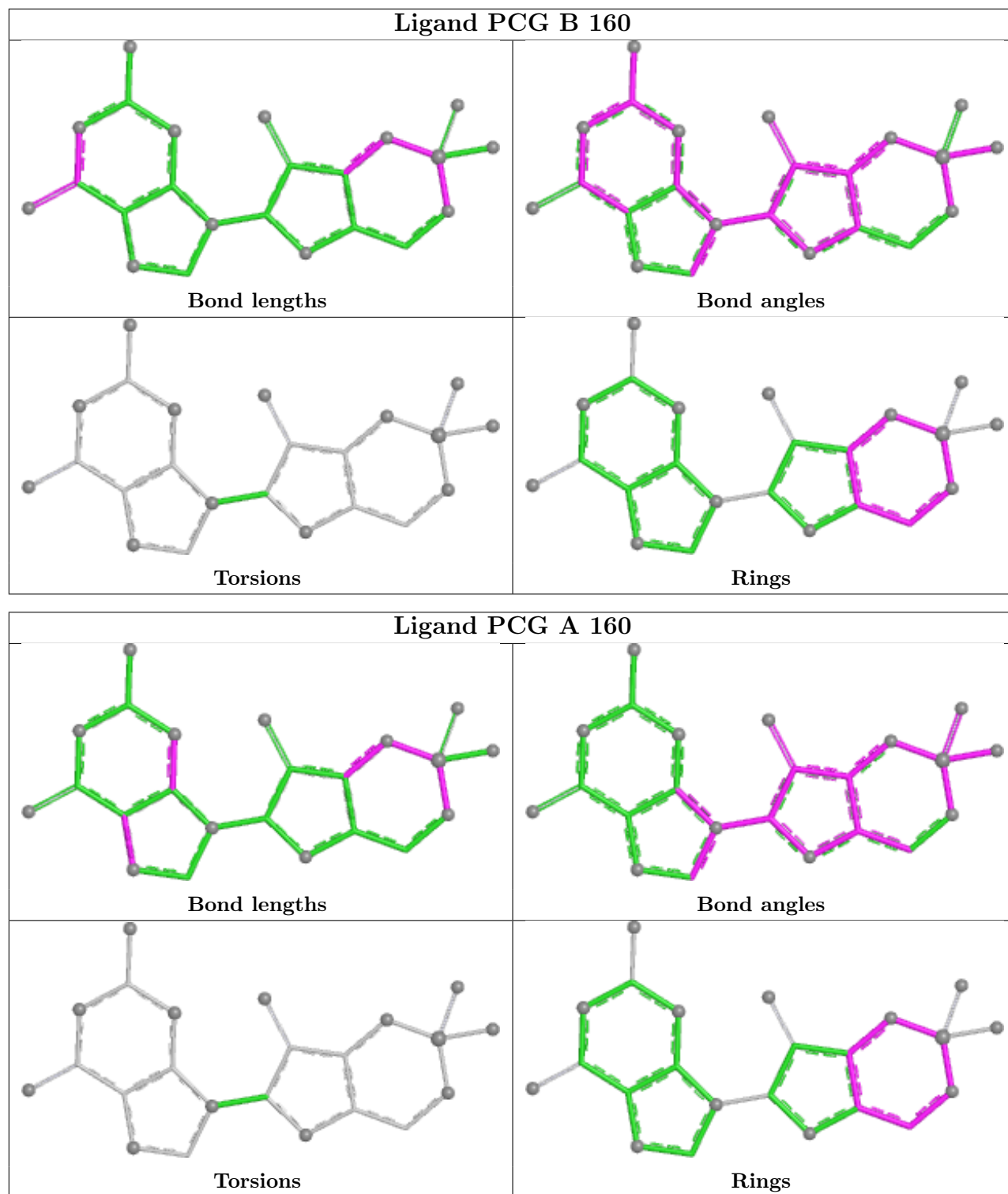
Mol	Chain	Res	Type	Atoms
2	B	160	PCG	C3'-C4'-C5'-O3'-O5'-PA
2	A	160	PCG	C3'-C4'-C5'-O3'-O5'-PA

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	160	PCG	5	0
2	B	160	PCG	3	0
2	A	160	PCG	1	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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	A	151/151 (100%)	-0.28	4 (2%) 57 53	10, 28, 70, 92	0
1	B	151/151 (100%)	-0.15	4 (2%) 57 53	13, 34, 81, 100	0
1	C	151/151 (100%)	-0.41	2 (1%) 75 71	9, 26, 65, 81	0
All	All	453/453 (100%)	-0.28	10 (2%) 62 58	9, 30, 73, 100	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	55	LEU	3.5
1	A	2	ALA	3.0
1	C	2	ALA	2.7
1	B	60	PHE	2.5
1	A	67	TYR	2.3
1	A	60	PHE	2.2
1	C	61	PHE	2.2
1	A	61	PHE	2.1
1	B	59	PRO	2.1
1	B	144	SER	2.0

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](#)

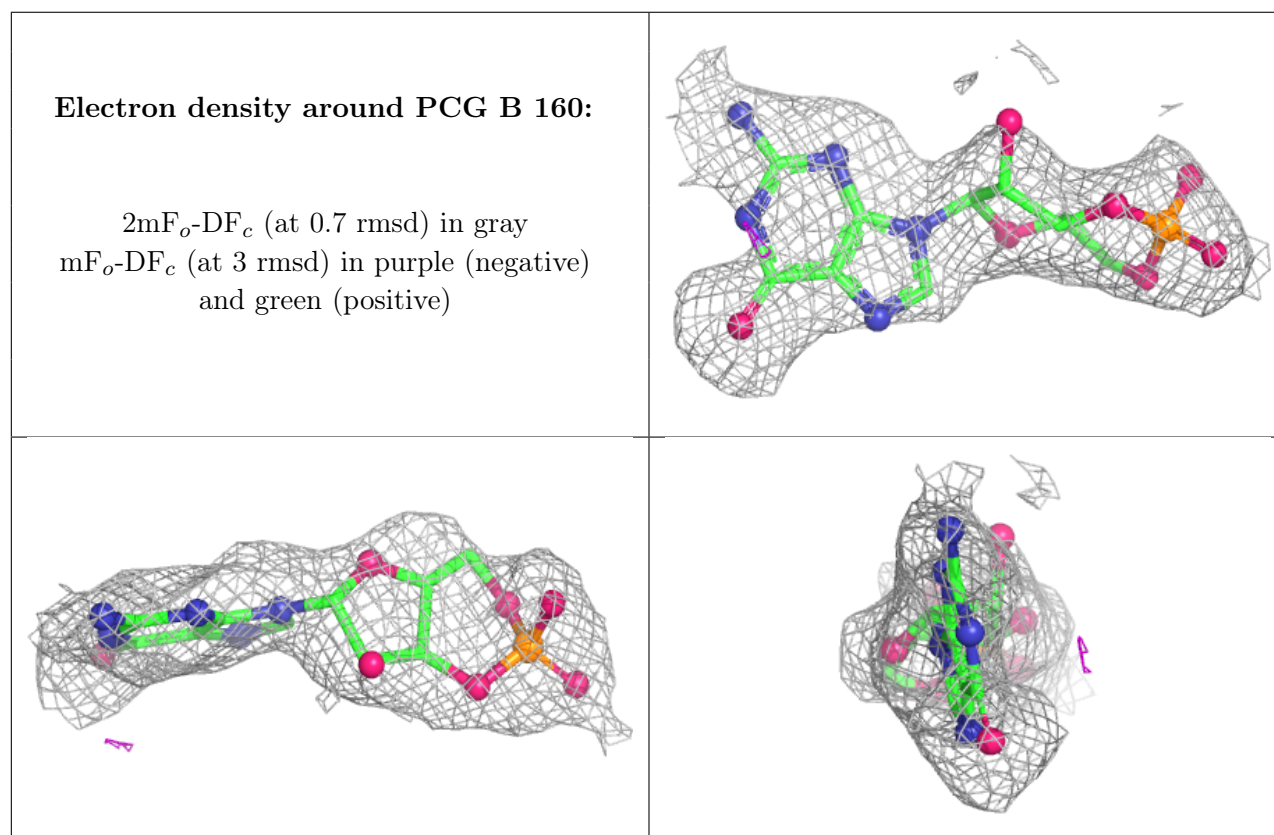
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

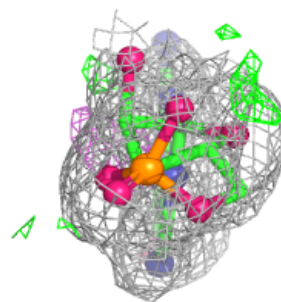
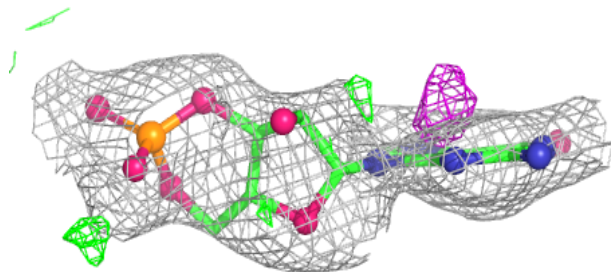
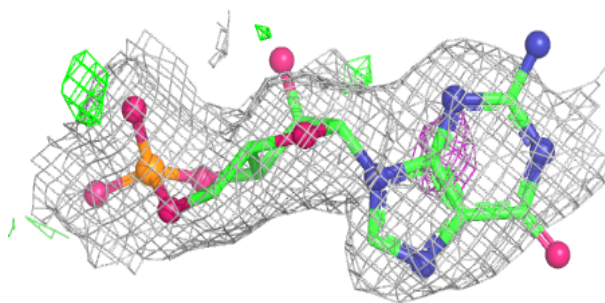
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PCG	B	160	23/23	0.90	0.12	28,78,99,99	0
2	PCG	A	160	23/23	0.91	0.13	19,74,99,99	0
2	PCG	C	160	23/23	0.95	0.09	15,41,86,99	0

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.

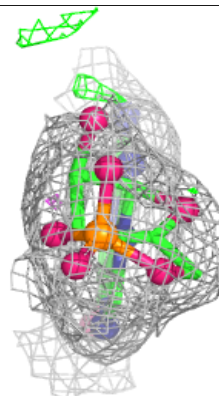
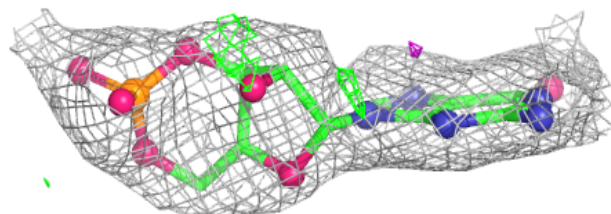
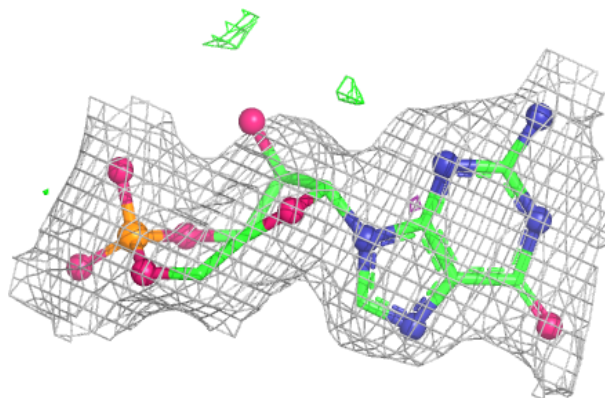


Electron density around PCG A 160:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around PCG C 160:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.