Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 10:31 pm BST

PDB ID	:	1BE4
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 following versions of software and data (see references ⓘ) were used in the production of this report:

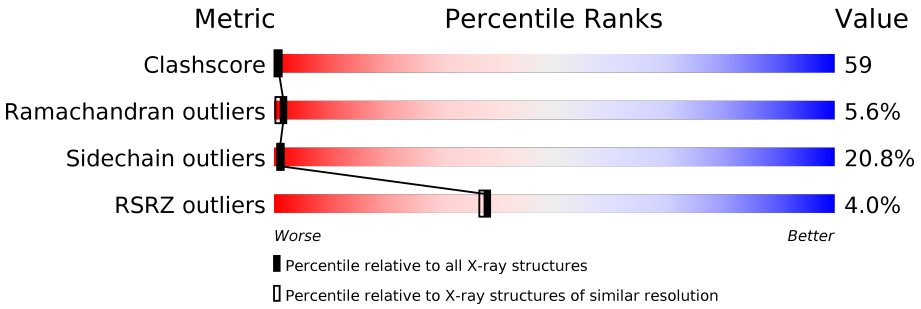
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 on 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 <=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	5% 5% 31% 52% 12%
1	B	151	6% 19% 30% 38% 13%
1	C	151	% 15% 37% 36% 12%

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

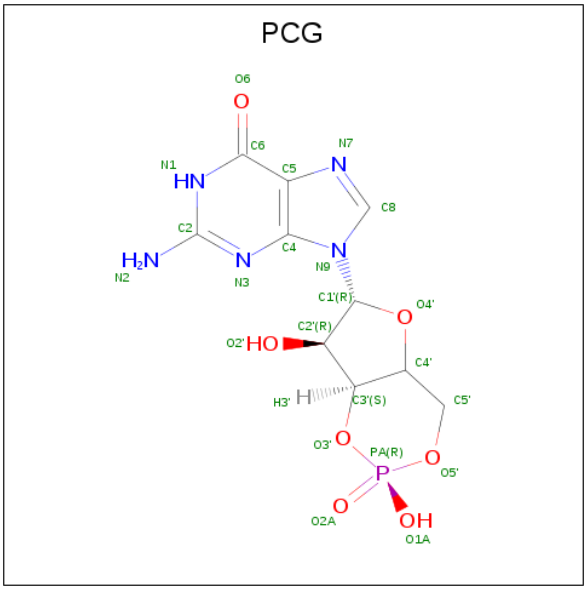
There are 3 unique types of molecules in this entry. The entry contains 3968 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: 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.

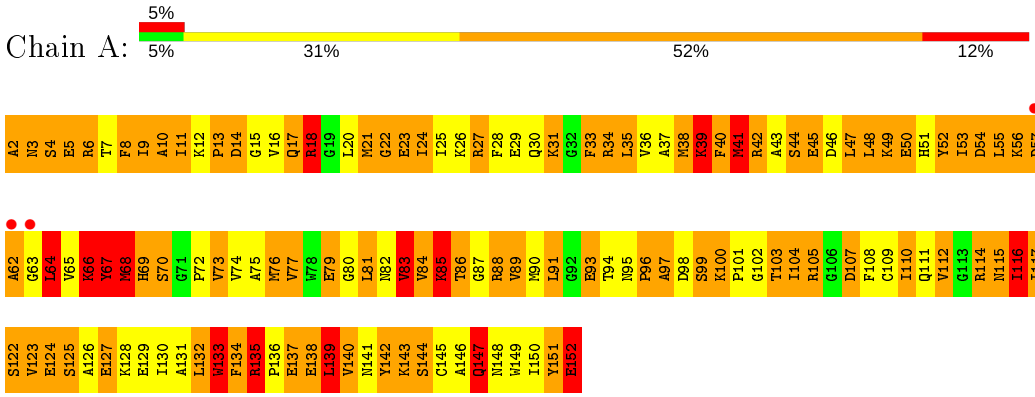
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	90	Total O 90 90	0	0
3	B	88	Total O 88 88	0	0
3	C	100	Total O 100 100	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

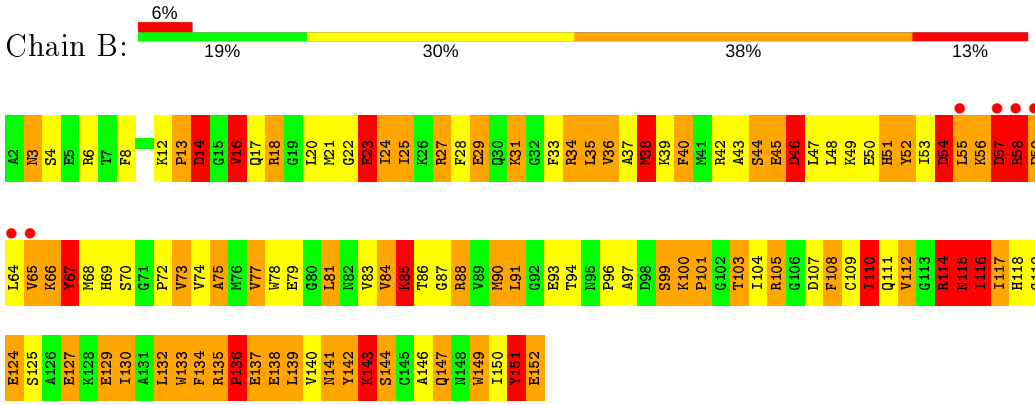
• Molecule 1: NUCLEOSIDE DIPHOSPHATE TRANSFERASE

Chain A:



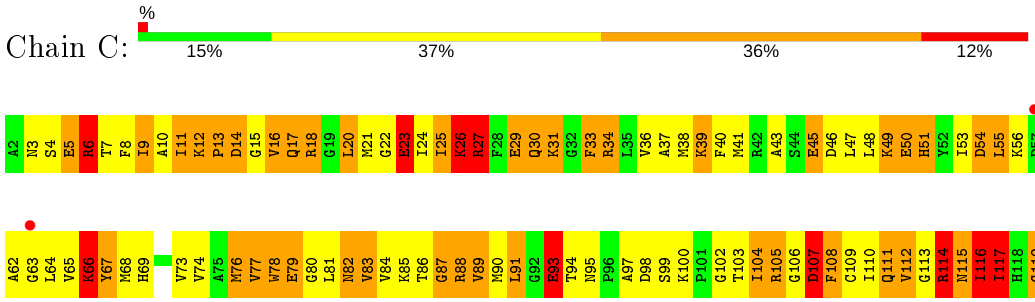
• Molecule 1: NUCLEOSIDE DIPHOSPHATE TRANSFERASE

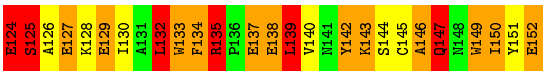
Chain B:



• Molecule 1: NUCLEOSIDE DIPHOSPHATE TRANSFERASE

Chain C:




E124
S125
A126
E127
K128
E129
I130
A131
L132
W133
F134
R135
P136
E137
E138
L139
V140
M141
Y142
K143
S144
C145
A146
Q147
N148
W149
I150
Y151
E152

4 Data and refinement statistics (i)

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 33.07 – 2.35	Depositor EDS
% Data completeness (in resolution range)	89.0 (20.00-2.40) 86.0 (33.07-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.34Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.198 , (Not available) 0.185 , (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)	0.35 , 166.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	1.54	15/1233 (1.2%)	3.47	177/1657 (10.7%)
1	B	1.42	8/1233 (0.6%)	2.94	130/1657 (7.8%)
1	C	1.58	17/1233 (1.4%)	3.09	156/1657 (9.4%)
All	All	1.51	40/3699 (1.1%)	3.18	463/4971 (9.3%)

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 (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23	GLU	CD-OE2	9.34	1.35	1.25
1	C	50	GLU	CD-OE2	9.34	1.35	1.25
1	B	137	GLU	CD-OE1	9.14	1.35	1.25
1	C	29	GLU	CD-OE2	9.13	1.35	1.25
1	C	79	GLU	CD-OE2	8.58	1.35	1.25
1	A	124	GLU	CD-OE2	8.44	1.34	1.25
1	C	137	GLU	CD-OE2	8.43	1.34	1.25
1	B	127	GLU	CD-OE2	8.42	1.34	1.25
1	B	23	GLU	CD-OE2	8.05	1.34	1.25
1	B	138	GLU	CD-OE2	8.04	1.34	1.25
1	C	124	GLU	CD-OE1	7.90	1.34	1.25
1	A	29	GLU	CD-OE2	7.85	1.34	1.25
1	C	5	GLU	CD-OE2	7.72	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	45	GLU	CD-OE2	7.70	1.34	1.25
1	C	127	GLU	CD-OE2	7.42	1.33	1.25
1	B	93	GLU	CD-OE2	7.20	1.33	1.25
1	C	93	GLU	CD-OE2	7.15	1.33	1.25
1	A	5	GLU	CD-OE2	7.03	1.33	1.25
1	A	147	GLN	C-N	7.00	1.50	1.34
1	A	79	GLU	CD-OE1	6.65	1.32	1.25
1	B	124	GLU	CD-OE2	6.44	1.32	1.25
1	C	23	GLU	CD-OE2	6.38	1.32	1.25
1	B	50	GLU	CD-OE1	6.00	1.32	1.25
1	C	45	GLU	CD-OE2	5.96	1.32	1.25
1	C	5	GLU	CD-OE1	-5.94	1.19	1.25
1	A	50	GLU	CD-OE1	5.83	1.32	1.25
1	A	6	ARG	CA-CB	-5.82	1.41	1.53
1	A	137	GLU	CD-OE2	5.72	1.31	1.25
1	C	133	TRP	CZ2-CH2	5.71	1.48	1.37
1	A	138	GLU	CD-OE2	-5.70	1.19	1.25
1	A	2	ALA	C-O	5.52	1.33	1.23
1	C	138	GLU	CD-OE1	5.43	1.31	1.25
1	A	93	GLU	CD-OE1	5.42	1.31	1.25
1	A	152	GLU	CD-OE2	5.38	1.31	1.25
1	A	14	ASP	CG-OD2	5.36	1.37	1.25
1	C	152	GLU	CD-OE1	5.25	1.31	1.25
1	C	115	ASN	C-O	5.24	1.33	1.23
1	C	25	ILE	C-O	5.18	1.33	1.23
1	C	129	GLU	CD-OE1	-5.14	1.20	1.25
1	A	127	GLU	CD-OE2	5.07	1.31	1.25

All (463) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	18	ARG	NE-CZ-NH1	27.10	133.85	120.30
1	A	98	ASP	CB-CG-OD2	-19.44	100.81	118.30
1	A	114	ARG	NE-CZ-NH1	18.61	129.60	120.30
1	C	67	TYR	CB-CG-CD2	-16.06	111.36	121.00
1	B	88	ARG	NE-CZ-NH1	-16.04	112.28	120.30
1	C	46	ASP	CB-CG-OD2	-15.63	104.23	118.30
1	B	18	ARG	NE-CZ-NH2	-15.35	112.63	120.30
1	A	67	TYR	CB-CG-CD2	-15.19	111.89	121.00
1	A	18	ARG	NH1-CZ-NH2	-15.14	102.75	119.40
1	A	6	ARG	NE-CZ-NH2	-14.82	112.89	120.30
1	A	61	PHE	CB-CG-CD2	13.87	130.51	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	34	ARG	NE-CZ-NH2	-13.80	113.40	120.30
1	A	103	THR	CA-CB-CG2	-13.73	93.17	112.40
1	A	6	ARG	NE-CZ-NH1	13.51	127.05	120.30
1	B	137	GLU	OE1-CD-OE2	13.26	139.22	123.30
1	B	27	ARG	NE-CZ-NH2	-13.14	113.73	120.30
1	C	107	ASP	CB-CG-OD1	13.04	130.04	118.30
1	C	98	ASP	CB-CG-OD2	-12.96	106.64	118.30
1	C	54	ASP	CB-CG-OD2	-12.81	106.77	118.30
1	A	52	TYR	CB-CG-CD2	12.36	128.41	121.00
1	A	67	TYR	CB-CG-CD1	12.32	128.39	121.00
1	B	6	ARG	NE-CZ-NH2	-12.31	114.15	120.30
1	C	127	GLU	N-CA-CB	-12.11	88.80	110.60
1	A	27	ARG	NE-CZ-NH2	11.99	126.29	120.30
1	C	121	ASP	CB-CG-OD2	-11.90	107.59	118.30
1	B	52	TYR	CB-CG-CD2	11.84	128.10	121.00
1	A	107	ASP	CB-CG-OD2	-11.83	107.65	118.30
1	C	88	ARG	NE-CZ-NH2	11.75	126.17	120.30
1	C	88	ARG	NE-CZ-NH1	-11.72	114.44	120.30
1	C	105	ARG	CD-NE-CZ	-11.64	107.31	123.60
1	A	34	ARG	NE-CZ-NH1	11.56	126.08	120.30
1	A	98	ASP	CB-CG-OD1	11.53	128.68	118.30
1	C	105	ARG	NE-CZ-NH1	-11.47	114.56	120.30
1	A	57	ASP	CB-CG-OD2	-11.39	108.05	118.30
1	C	34	ARG	NE-CZ-NH2	-11.38	114.61	120.30
1	B	103	THR	CA-CB-CG2	-11.28	96.61	112.40
1	C	123	VAL	CA-CB-CG1	-11.14	94.19	110.90
1	A	27	ARG	CD-NE-CZ	-11.10	108.06	123.60
1	A	145	CYS	CA-CB-SG	11.05	133.90	114.00
1	C	123	VAL	CA-CB-CG2	-10.97	94.44	110.90
1	A	145	CYS	N-CA-CB	10.96	130.33	110.60
1	A	70	SER	CB-CA-C	-10.91	89.37	110.10
1	A	45	GLU	OE1-CD-OE2	-10.76	110.39	123.30
1	B	137	GLU	CB-CA-C	-10.70	89.00	110.40
1	C	36	VAL	CA-CB-CG1	-10.62	94.97	110.90
1	A	121	ASP	CB-CG-OD1	10.59	127.83	118.30
1	A	114	ARG	NE-CZ-NH2	-10.39	115.11	120.30
1	A	83	VAL	CA-CB-CG1	-10.31	95.44	110.90
1	C	67	TYR	CB-CG-CD1	10.27	127.16	121.00
1	A	112	VAL	CA-CB-CG1	-10.21	95.58	110.90
1	A	21	MET	CG-SD-CE	10.17	116.47	100.20
1	C	26	LYS	CA-CB-CG	-10.15	91.07	113.40
1	A	41	MET	CG-SD-CE	-10.11	84.02	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	18	ARG	NE-CZ-NH1	10.07	125.33	120.30
1	A	134	PHE	CB-CG-CD1	-10.00	113.80	120.80
1	A	76	MET	CG-SD-CE	9.98	116.17	100.20
1	A	135	ARG	C-N-CD	-9.93	98.75	120.60
1	A	107	ASP	CB-CG-OD1	9.89	127.20	118.30
1	C	97	ALA	CB-CA-C	-9.82	95.37	110.10
1	B	14	ASP	CB-CG-OD2	-9.81	109.47	118.30
1	B	46	ASP	CB-CG-OD2	-9.79	109.49	118.30
1	A	135	ARG	NE-CZ-NH2	9.67	125.13	120.30
1	A	3	ASN	CA-CB-CG	-9.64	92.19	113.40
1	A	44	SER	N-CA-CB	9.59	124.88	110.50
1	A	31	LYS	O-C-N	-9.49	107.06	123.20
1	A	8	PHE	CD1-CE1-CZ	-9.46	108.75	120.10
1	B	38	MET	CG-SD-CE	9.44	115.31	100.20
1	C	31	LYS	C-N-CA	-9.38	102.60	122.30
1	B	100	LYS	CB-CA-C	-9.33	91.75	110.40
1	C	6	ARG	NE-CZ-NH2	-9.29	115.66	120.30
1	C	134	PHE	CB-CG-CD1	9.24	127.27	120.80
1	B	105	ARG	CD-NE-CZ	-9.20	110.72	123.60
1	C	27	ARG	NE-CZ-NH1	9.19	124.89	120.30
1	A	105	ARG	CD-NE-CZ	9.11	136.35	123.60
1	B	149	TRP	O-C-N	9.09	137.25	122.70
1	A	6	ARG	CA-CB-CG	-8.93	93.76	113.40
1	B	65	VAL	CB-CA-C	-8.90	94.49	111.40
1	A	52	TYR	CB-CG-CD1	-8.87	115.68	121.00
1	A	57	ASP	CB-CG-OD1	8.78	126.20	118.30
1	C	105	ARG	NE-CZ-NH2	8.67	124.63	120.30
1	A	151	TYR	CZ-CE2-CD2	8.66	127.59	119.80
1	C	23	GLU	CB-CG-CD	-8.63	90.90	114.20
1	C	62	ALA	CB-CA-C	-8.62	97.17	110.10
1	C	6	ARG	N-CA-CB	8.60	126.08	110.60
1	B	35	LEU	CB-CG-CD2	8.58	125.59	111.00
1	A	125	SER	N-CA-CB	-8.44	97.84	110.50
1	C	14	ASP	CB-CG-OD2	-8.44	110.71	118.30
1	B	24	ILE	CA-CB-CG1	-8.43	94.98	111.00
1	A	69	HIS	N-CA-CB	-8.40	95.47	110.60
1	A	91	LEU	CB-CG-CD2	-8.38	96.75	111.00
1	A	151	TYR	CG-CD2-CE2	-8.33	114.64	121.30
1	A	134	PHE	CB-CG-CD2	8.32	126.63	120.80
1	A	134	PHE	CZ-CE2-CD2	-8.25	110.20	120.10
1	A	31	LYS	CA-CB-CG	-8.21	95.34	113.40
1	C	133	TRP	CH2-CZ2-CE2	8.19	125.59	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	88	ARG	NE-CZ-NH2	8.15	124.38	120.30
1	B	140	VAL	CA-CB-CG1	8.13	123.10	110.90
1	A	137	GLU	OE1-CD-OE2	-8.04	113.65	123.30
1	A	136	PRO	O-C-N	8.04	135.56	122.70
1	B	52	TYR	CB-CG-CD1	-7.99	116.20	121.00
1	B	74	VAL	CA-CB-CG2	-7.99	98.91	110.90
1	C	36	VAL	O-C-N	-7.99	109.92	122.70
1	C	34	ARG	NE-CZ-NH1	7.97	124.28	120.30
1	C	125	SER	N-CA-CB	-7.96	98.55	110.50
1	B	29	GLU	OE1-CD-OE2	-7.94	113.77	123.30
1	A	38	MET	CG-SD-CE	7.90	112.84	100.20
1	A	133	TRP	CG-CD2-CE3	-7.87	126.82	133.90
1	B	149	TRP	N-CA-CB	7.85	124.73	110.60
1	B	60	PHE	N-CA-CB	7.84	124.70	110.60
1	A	54	ASP	CA-CB-CG	-7.81	96.22	113.40
1	C	67	TYR	CG-CD1-CE1	-7.79	115.07	121.30
1	A	42	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	B	140	VAL	CA-CB-CG2	7.77	122.55	110.90
1	A	29	GLU	N-CA-CB	-7.76	96.64	110.60
1	C	46	ASP	CB-CG-OD1	7.76	125.28	118.30
1	C	25	ILE	CG1-CB-CG2	-7.76	94.33	111.40
1	A	140	VAL	CG1-CB-CG2	-7.74	98.52	110.90
1	B	79	GLU	C-N-CA	-7.74	106.06	122.30
1	C	8	PHE	CZ-CE2-CD2	7.73	129.38	120.10
1	B	152	GLU	CG-CD-OE2	-7.70	102.91	118.30
1	C	88	ARG	CD-NE-CZ	-7.68	112.85	123.60
1	B	122	SER	CB-CA-C	-7.68	95.52	110.10
1	C	17	GLN	CA-CB-CG	-7.66	96.56	113.40
1	A	58	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	B	137	GLU	CG-CD-OE1	-7.63	103.04	118.30
1	B	14	ASP	CB-CG-OD1	7.59	125.13	118.30
1	B	78	TRP	CH2-CZ2-CE2	7.59	124.99	117.40
1	B	18	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	A	74	VAL	CA-C-N	-7.58	100.53	117.20
1	B	132	LEU	CB-CA-C	7.57	124.58	110.20
1	A	104	ILE	CA-CB-CG1	-7.53	96.70	111.00
1	A	10	ALA	CB-CA-C	-7.52	98.82	110.10
1	A	88	ARG	O-C-N	7.47	134.65	122.70
1	C	12	LYS	CB-CA-C	7.46	125.32	110.40
1	A	98	ASP	O-C-N	7.45	134.62	122.70
1	C	26	LYS	O-C-N	-7.42	110.82	122.70
1	A	112	VAL	CA-CB-CG2	-7.42	99.77	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	6	ARG	CD-NE-CZ	7.41	133.98	123.60
1	A	42	ARG	N-CA-CB	7.41	123.93	110.60
1	C	60	PHE	O-C-N	7.39	134.52	122.70
1	A	6	ARG	CB-CA-C	-7.37	95.66	110.40
1	A	65	VAL	CA-C-N	-7.34	101.04	117.20
1	C	121	ASP	N-CA-CB	7.32	123.78	110.60
1	B	130	ILE	CA-CB-CG2	-7.27	96.36	110.90
1	C	114	ARG	CD-NE-CZ	-7.25	113.45	123.60
1	B	109	CYS	CA-CB-SG	-7.22	100.99	114.00
1	B	109	CYS	CB-CA-C	7.20	124.79	110.40
1	A	28	PHE	O-C-N	7.16	134.15	122.70
1	C	119	GLY	N-CA-C	-7.10	95.35	113.10
1	A	133	TRP	C-N-CA	-7.08	104.00	121.70
1	A	89	VAL	CA-CB-CG2	-7.07	100.30	110.90
1	A	16	VAL	CA-CB-CG1	7.06	121.50	110.90
1	C	54	ASP	CB-CG-OD1	7.06	124.66	118.30
1	C	91	LEU	CA-C-N	-7.04	102.12	116.20
1	B	112	VAL	CB-CA-C	-7.03	98.04	111.40
1	B	108	PHE	CB-CA-C	-7.03	96.34	110.40
1	B	23	GLU	N-CA-CB	-7.01	97.99	110.60
1	C	98	ASP	CB-CG-OD1	6.99	124.59	118.30
1	C	16	VAL	CA-CB-CG2	6.97	121.36	110.90
1	C	66	LYS	N-CA-CB	-6.96	98.07	110.60
1	B	18	ARG	CB-CA-C	6.94	124.27	110.40
1	B	65	VAL	CA-CB-CG2	-6.91	100.53	110.90
1	B	79	GLU	CG-CD-OE2	-6.91	104.48	118.30
1	C	61	PHE	C-N-CA	-6.91	104.43	121.70
1	A	81	LEU	CB-CA-C	-6.87	97.15	110.20
1	C	108	PHE	N-CA-C	6.85	129.50	111.00
1	C	139	LEU	CB-CA-C	-6.84	97.20	110.20
1	C	29	GLU	OE1-CD-OE2	6.82	131.48	123.30
1	C	14	ASP	CB-CG-OD1	6.81	124.43	118.30
1	C	89	VAL	CA-CB-CG1	-6.81	100.69	110.90
1	A	108	PHE	N-CA-CB	-6.80	98.36	110.60
1	A	88	ARG	NE-CZ-NH2	6.79	123.69	120.30
1	A	99	SER	CA-CB-OG	-6.78	92.89	111.20
1	C	8	PHE	CG-CD1-CE1	6.75	128.23	120.80
1	C	149	TRP	CA-CB-CG	-6.75	100.87	113.70
1	B	14	ASP	CA-C-N	-6.74	102.72	116.20
1	B	129	GLU	C-N-CA	-6.74	104.85	121.70
1	A	108	PHE	CA-C-N	6.72	132.00	117.20
1	C	152	GLU	CB-CA-C	6.72	123.85	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	40	PHE	C-N-CA	-6.71	104.94	121.70
1	A	9	ILE	CA-CB-CG1	-6.70	98.27	111.00
1	C	107	ASP	OD1-CG-OD2	-6.70	110.57	123.30
1	A	147	GLN	N-CA-CB	-6.69	98.55	110.60
1	C	39	LYS	CA-C-N	-6.68	102.50	117.20
1	B	27	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	A	27	ARG	NH1-CZ-NH2	-6.67	112.07	119.40
1	A	61	PHE	CG-CD1-CE1	6.64	128.10	120.80
1	A	10	ALA	N-CA-CB	6.63	119.38	110.10
1	C	55	LEU	CB-CA-C	-6.63	97.61	110.20
1	A	22	GLY	O-C-N	-6.62	112.12	122.70
1	A	66	LYS	CA-C-N	-6.62	102.65	117.20
1	A	74	VAL	CA-CB-CG2	-6.60	101.00	110.90
1	A	22	GLY	CA-C-O	6.60	132.47	120.60
1	A	61	PHE	N-CA-CB	6.57	122.42	110.60
1	B	135	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	C	135	ARG	N-CA-CB	6.54	122.38	110.60
1	A	8	PHE	CA-C-N	-6.53	102.83	117.20
1	C	88	ARG	O-C-N	6.53	133.14	122.70
1	B	121	ASP	CB-CA-C	-6.53	97.35	110.40
1	C	142	TYR	CB-CG-CD2	-6.53	117.08	121.00
1	C	20	LEU	C-N-CA	-6.52	105.40	121.70
1	B	135	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	C	134	PHE	CG-CD1-CE1	6.51	127.96	120.80
1	C	121	ASP	C-N-CA	-6.50	105.45	121.70
1	C	142	TYR	CB-CG-CD1	6.50	124.90	121.00
1	C	21	MET	CA-C-N	-6.47	103.25	116.20
1	C	79	GLU	CA-C-N	-6.47	103.25	116.20
1	C	58	ARG	N-CA-C	-6.45	93.58	111.00
1	A	69	HIS	CA-CB-CG	-6.45	102.63	113.60
1	C	151	TYR	CB-CG-CD2	-6.45	117.13	121.00
1	B	99	SER	N-CA-CB	-6.44	100.84	110.50
1	A	64	LEU	CB-CG-CD2	-6.44	100.06	111.00
1	B	134	PHE	CB-CG-CD2	-6.43	116.30	120.80
1	B	88	ARG	N-CA-CB	6.43	122.17	110.60
1	C	133	TRP	CZ3-CH2-CZ2	-6.39	113.93	121.60
1	C	79	GLU	N-CA-CB	6.38	122.08	110.60
1	A	136	PRO	N-CA-CB	6.38	110.95	103.30
1	C	145	CYS	N-CA-CB	6.37	122.07	110.60
1	A	121	ASP	CB-CA-C	-6.37	97.67	110.40
1	A	105	ARG	C-N-CA	-6.36	108.94	122.30
1	A	139	LEU	CA-CB-CG	-6.36	100.67	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	89	VAL	N-CA-CB	-6.36	97.51	111.50
1	A	81	LEU	CB-CG-CD1	-6.34	100.23	111.00
1	A	133	TRP	CH2-CZ2-CE2	-6.34	111.06	117.40
1	B	129	GLU	CG-CD-OE2	-6.33	105.64	118.30
1	C	41	MET	N-CA-CB	-6.32	99.23	110.60
1	B	97	ALA	CB-CA-C	-6.32	100.62	110.10
1	A	54	ASP	CB-CG-OD2	-6.30	112.62	118.30
1	A	117	ILE	N-CA-CB	-6.30	96.30	110.80
1	A	35	LEU	N-CA-CB	6.28	122.96	110.40
1	C	137	GLU	O-C-N	6.28	132.75	122.70
1	B	6	ARG	NH1-CZ-NH2	6.27	126.29	119.40
1	C	100	LYS	CA-CB-CG	-6.26	99.62	113.40
1	B	39	LYS	CA-C-O	6.24	133.21	120.10
1	C	78	TRP	C-N-CA	-6.24	106.10	121.70
1	C	36	VAL	CG1-CB-CG2	6.24	120.88	110.90
1	A	52	TYR	N-CA-CB	-6.21	99.42	110.60
1	A	18	ARG	NE-CZ-NH2	6.21	123.40	120.30
1	A	147	GLN	C-N-CA	-6.20	106.20	121.70
1	B	79	GLU	CG-CD-OE1	6.20	130.69	118.30
1	C	114	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	123	VAL	CA-CB-CG1	6.18	120.17	110.90
1	A	66	LYS	CA-CB-CG	-6.17	99.83	113.40
1	B	129	GLU	CG-CD-OE1	6.17	130.63	118.30
1	B	40	PHE	CB-CG-CD1	-6.16	116.49	120.80
1	A	111	GLN	CA-C-N	-6.15	103.67	117.20
1	A	123	VAL	N-CA-CB	-6.15	97.97	111.50
1	A	79	GLU	CG-CD-OE1	-6.14	106.02	118.30
1	C	114	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	C	31	LYS	N-CA-CB	-6.13	99.57	110.60
1	C	11	ILE	O-C-N	6.11	132.48	122.70
1	A	68	MET	CB-CA-C	6.11	122.61	110.40
1	B	78	TRP	CA-C-N	-6.10	103.78	117.20
1	C	76	MET	CB-CA-C	-6.10	98.20	110.40
1	C	49	LYS	C-N-CA	-6.10	106.46	121.70
1	C	62	ALA	N-CA-CB	6.07	118.60	110.10
1	B	20	LEU	N-CA-CB	-6.06	98.28	110.40
1	C	60	PHE	N-CA-CB	6.06	121.51	110.60
1	C	82	ASN	N-CA-CB	6.05	121.50	110.60
1	A	94	THR	CB-CA-C	6.05	127.92	111.60
1	A	142	TYR	CG-CD1-CE1	6.04	126.14	121.30
1	A	136	PRO	CA-N-CD	-6.04	103.05	111.50
1	C	106	GLY	CA-C-O	-6.03	109.75	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	142	TYR	CZ-CE2-CD2	-6.03	114.38	119.80
1	B	105	ARG	N-CA-CB	-6.02	99.76	110.60
1	A	49	LYS	N-CA-CB	-6.02	99.77	110.60
1	B	84	VAL	CG1-CB-CG2	-6.01	101.29	110.90
1	C	33	PHE	CB-CA-C	-6.00	98.39	110.40
1	B	18	ARG	CD-NE-CZ	6.00	132.00	123.60
1	C	127	GLU	CA-C-O	6.00	132.70	120.10
1	C	12	LYS	CB-CG-CD	-5.99	96.02	111.60
1	C	137	GLU	OE1-CD-OE2	5.99	130.49	123.30
1	C	82	ASN	CA-CB-CG	-5.97	100.27	113.40
1	A	121	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	A	7	THR	N-CA-CB	5.94	121.58	110.30
1	A	39	LYS	CA-C-N	-5.91	104.21	117.20
1	B	58	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	11	ILE	CA-CB-CG2	-5.90	99.09	110.90
1	C	107	ASP	CA-C-N	-5.90	104.22	117.20
1	A	85	LYS	CG-CD-CE	5.90	129.60	111.90
1	B	141	ASN	N-CA-CB	5.89	121.21	110.60
1	C	9	ILE	CB-CG1-CD1	-5.89	97.41	113.90
1	C	34	ARG	N-CA-CB	-5.89	100.00	110.60
1	A	52	TYR	CZ-CE2-CD2	5.88	125.09	119.80
1	C	83	VAL	CA-CB-CG2	-5.86	102.11	110.90
1	B	51	HIS	CB-CA-C	-5.85	98.71	110.40
1	C	150	ILE	CA-CB-CG1	-5.85	99.89	111.00
1	A	33	PHE	CZ-CE2-CD2	-5.84	113.09	120.10
1	C	25	ILE	CA-C-N	-5.84	104.35	117.20
1	B	24	ILE	CA-CB-CG2	-5.84	99.23	110.90
1	B	150	ILE	CA-C-N	-5.83	104.37	117.20
1	C	66	LYS	CB-CA-C	-5.83	98.74	110.40
1	A	33	PHE	CG-CD2-CE2	5.83	127.21	120.80
1	C	105	ARG	CB-CA-C	5.80	122.01	110.40
1	A	146	ALA	CB-CA-C	-5.80	101.40	110.10
1	B	81	LEU	CA-C-O	5.80	132.28	120.10
1	B	31	LYS	CB-CA-C	-5.79	98.82	110.40
1	C	51	HIS	CA-CB-CG	-5.79	103.76	113.60
1	C	149	TRP	O-C-N	5.78	131.95	122.70
1	B	40	PHE	CG-CD1-CE1	-5.78	114.44	120.80
1	B	78	TRP	O-C-N	5.78	131.94	122.70
1	C	111	GLN	N-CA-CB	-5.78	100.20	110.60
1	A	5	GLU	N-CA-CB	-5.77	100.22	110.60
1	C	116	ILE	C-N-CA	-5.76	107.29	121.70
1	B	136	PRO	N-CA-CB	5.76	110.22	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	8	PHE	CG-CD1-CE1	5.75	127.13	120.80
1	A	108	PHE	CB-CA-C	-5.75	98.90	110.40
1	A	110	ILE	N-CA-C	5.75	126.52	111.00
1	B	31	LYS	CA-CB-CG	5.75	126.05	113.40
1	B	110	ILE	CA-C-N	-5.74	104.57	117.20
1	C	104	ILE	CG1-CB-CG2	-5.74	98.78	111.40
1	A	83	VAL	C-N-CA	-5.73	107.37	121.70
1	B	91	LEU	O-C-N	5.73	132.94	123.20
1	A	48	LEU	N-CA-CB	-5.72	98.96	110.40
1	C	127	GLU	CG-CD-OE1	5.72	129.75	118.30
1	A	140	VAL	CA-CB-CG1	-5.72	102.32	110.90
1	C	135	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	A	76	MET	CA-CB-CG	5.70	122.98	113.30
1	A	35	LEU	O-C-N	5.69	131.80	122.70
1	C	135	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	133	TRP	CH2-CZ2-CE2	-5.67	111.73	117.40
1	C	60	PHE	CA-C-N	-5.66	104.76	117.20
1	C	40	PHE	CB-CA-C	-5.65	99.11	110.40
1	A	13	PRO	N-CD-CG	-5.62	94.78	103.20
1	C	146	ALA	CB-CA-C	-5.61	101.68	110.10
1	B	93	GLU	OE1-CD-OE2	5.61	130.03	123.30
1	C	8	PHE	CE1-CZ-CE2	-5.60	109.92	120.00
1	B	115	ASN	N-CA-C	5.60	126.12	111.00
1	C	21	MET	O-C-N	5.60	132.72	123.20
1	C	93	GLU	N-CA-CB	-5.59	100.54	110.60
1	A	55	LEU	CB-CG-CD2	-5.58	101.51	111.00
1	A	127	GLU	O-C-N	5.57	131.61	122.70
1	C	133	TRP	C-N-CA	-5.56	107.79	121.70
1	A	142	TYR	CZ-CE2-CD2	5.56	124.80	119.80
1	B	78	TRP	NE1-CE2-CZ2	5.55	136.50	130.40
1	B	93	GLU	CG-CD-OE2	-5.54	107.22	118.30
1	C	77	VAL	CA-CB-CG2	-5.53	102.61	110.90
1	A	8	PHE	O-C-N	5.53	131.54	122.70
1	B	40	PHE	CZ-CE2-CD2	-5.52	113.47	120.10
1	C	23	GLU	CB-CA-C	-5.52	99.37	110.40
1	A	74	VAL	CA-C-O	5.51	131.68	120.10
1	B	18	ARG	O-C-N	-5.51	113.82	123.20
1	A	142	TYR	CA-CB-CG	-5.50	102.94	113.40
1	C	116	ILE	O-C-N	-5.50	113.89	122.70
1	A	10	ALA	CA-C-N	-5.50	105.10	117.20
1	A	73	VAL	CA-CB-CG1	-5.50	102.65	110.90
1	B	77	VAL	CA-CB-CG1	-5.50	102.65	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	34	ARG	O-C-N	5.50	131.50	122.70
1	A	85	LYS	CD-CE-NZ	5.50	124.34	111.70
1	B	116	ILE	CB-CG1-CD1	-5.49	98.52	113.90
1	A	103	THR	O-C-N	5.49	131.49	122.70
1	A	97	ALA	N-CA-CB	-5.49	102.41	110.10
1	B	13	PRO	CB-CA-C	5.49	125.72	112.00
1	A	41	MET	CA-CB-CG	5.47	122.61	113.30
1	A	60	PHE	CB-CA-C	5.47	121.35	110.40
1	C	27	ARG	CB-CA-C	-5.47	99.45	110.40
1	A	84	VAL	O-C-N	-5.47	113.95	122.70
1	B	105	ARG	O-C-N	-5.47	113.90	123.20
1	B	6	ARG	CB-CA-C	-5.47	99.47	110.40
1	B	35	LEU	CB-CG-CD1	-5.47	101.71	111.00
1	B	16	VAL	CG1-CB-CG2	-5.46	102.16	110.90
1	B	36	VAL	CA-CB-CG1	5.46	119.08	110.90
1	B	60	PHE	CB-CG-CD2	5.44	124.61	120.80
1	A	91	LEU	N-CA-CB	-5.44	99.52	110.40
1	B	107	ASP	CB-CA-C	-5.44	99.52	110.40
1	C	129	GLU	OE1-CD-OE2	-5.44	116.78	123.30
1	A	77	VAL	CA-C-N	-5.42	105.28	117.20
1	C	152	GLU	CA-CB-CG	5.42	125.31	113.40
1	A	96	PRO	O-C-N	-5.40	114.06	122.70
1	B	96	PRO	O-C-N	5.40	131.34	122.70
1	B	127	GLU	CB-CA-C	5.40	121.19	110.40
1	B	127	GLU	CA-CB-CG	-5.39	101.54	113.40
1	C	151	TYR	CB-CG-CD1	5.39	124.23	121.00
1	A	108	PHE	O-C-N	-5.38	114.09	122.70
1	C	147	GLN	CB-CG-CD	-5.38	97.62	111.60
1	A	35	LEU	CB-CG-CD1	5.37	120.14	111.00
1	B	105	ARG	NE-CZ-NH1	-5.37	117.61	120.30
1	C	18	ARG	CG-CD-NE	5.37	123.08	111.80
1	C	18	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	A	55	LEU	N-CA-CB	-5.37	99.67	110.40
1	A	140	VAL	CA-CB-CG2	5.37	118.95	110.90
1	A	8	PHE	CB-CG-CD1	-5.36	117.05	120.80
1	C	22	GLY	C-N-CA	-5.36	108.31	121.70
1	B	108	PHE	CB-CG-CD1	-5.35	117.06	120.80
1	A	33	PHE	N-CA-C	5.34	125.42	111.00
1	A	67	TYR	CG-CD1-CE1	-5.34	117.03	121.30
1	B	114	ARG	CB-CG-CD	5.34	125.48	111.60
1	B	141	ASN	CB-CA-C	5.33	121.06	110.40
1	A	58	ARG	CD-NE-CZ	5.33	131.06	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	85	LYS	CA-C-N	-5.32	105.50	117.20
1	A	49	LYS	CA-C-N	-5.31	105.52	117.20
1	C	49	LYS	N-CA-CB	5.31	120.15	110.60
1	C	116	ILE	CA-CB-CG2	5.31	121.51	110.90
1	C	20	LEU	N-CA-CB	-5.30	99.81	110.40
1	C	77	VAL	N-CA-C	-5.29	96.73	111.00
1	A	64	LEU	CB-CA-C	-5.28	100.18	110.20
1	C	13	PRO	CA-C-N	-5.27	105.60	117.20
1	B	54	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	B	73	VAL	O-C-N	5.27	131.13	122.70
1	B	34	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	A	18	ARG	CG-CD-NE	-5.26	100.75	111.80
1	A	133	TRP	CB-CG-CD1	5.26	133.84	127.00
1	A	135	ARG	CD-NE-CZ	5.26	130.96	123.60
1	C	78	TRP	CB-CA-C	-5.25	99.90	110.40
1	B	78	TRP	N-CA-CB	5.24	120.04	110.60
1	C	135	ARG	CD-NE-CZ	5.24	130.94	123.60
1	C	114	ARG	N-CA-CB	5.24	120.02	110.60
1	B	67	TYR	CA-CB-CG	5.23	123.34	113.40
1	A	47	LEU	CA-C-O	5.22	131.07	120.10
1	B	149	TRP	CE3-CZ3-CH2	5.22	126.94	121.20
1	B	24	ILE	O-C-N	-5.21	114.36	122.70
1	C	104	ILE	CA-C-N	-5.21	105.74	117.20
1	A	18	ARG	CB-CA-C	5.21	120.81	110.40
1	C	124	GLU	OE1-CD-OE2	5.19	129.53	123.30
1	A	133	TRP	CB-CG-CD2	-5.18	119.86	126.60
1	C	27	ARG	O-C-N	5.18	130.99	122.70
1	C	111	GLN	N-CA-C	5.17	124.96	111.00
1	C	112	VAL	CG1-CB-CG2	-5.17	102.63	110.90
1	A	3	ASN	O-C-N	5.17	130.97	122.70
1	C	132	LEU	N-CA-CB	-5.16	100.08	110.40
1	A	115	ASN	C-N-CA	5.16	134.59	121.70
1	C	67	TYR	CD1-CE1-CZ	5.16	124.44	119.80
1	B	152	GLU	OE1-CD-OE2	5.15	129.48	123.30
1	A	83	VAL	CB-CA-C	-5.15	101.61	111.40
1	B	133	TRP	CD1-CG-CD2	-5.15	102.18	106.30
1	C	8	PHE	CD1-CG-CD2	-5.15	111.61	118.30
1	B	6	ARG	CD-NE-CZ	5.14	130.80	123.60
1	C	17	GLN	CA-C-N	-5.14	105.89	117.20
1	A	61	PHE	CD1-CG-CD2	-5.14	111.62	118.30
1	C	91	LEU	CA-C-O	5.13	130.88	120.10
1	B	24	ILE	CB-CA-C	-5.13	101.34	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	39	LYS	CA-C-N	-5.13	105.92	117.20
1	B	78	TRP	CD2-CE2-CZ2	-5.13	116.14	122.30
1	B	116	ILE	CA-CB-CG2	5.13	121.15	110.90
1	C	33	PHE	CG-CD2-CE2	-5.13	115.16	120.80
1	B	101	PRO	C-N-CA	5.12	133.06	122.30
1	B	38	MET	CA-CB-CG	-5.12	104.60	113.30
1	A	38	MET	CB-CA-C	-5.12	100.17	110.40
1	B	134	PHE	N-CA-C	5.11	124.81	111.00
1	B	25	ILE	O-C-N	-5.11	114.53	122.70
1	C	147	GLN	CA-CB-CG	-5.10	102.17	113.40
1	B	151	TYR	CA-C-N	-5.10	105.98	117.20
1	B	58	ARG	C-N-CD	-5.10	109.39	120.60
1	C	140	VAL	CG1-CB-CG2	-5.09	102.75	110.90
1	C	87	GLY	C-N-CA	-5.09	108.98	121.70
1	A	145	CYS	O-C-N	-5.08	114.58	122.70
1	A	29	GLU	O-C-N	-5.07	114.58	122.70
1	B	78	TRP	CD1-CG-CD2	5.07	110.36	106.30
1	B	137	GLU	O-C-N	5.07	130.81	122.70
1	A	24	ILE	CA-CB-CG1	5.07	120.63	111.00
1	B	34	ARG	NE-CZ-NH2	5.06	122.83	120.30
1	A	122	SER	CA-C-N	-5.06	106.08	117.20
1	B	101	PRO	N-CA-CB	5.06	109.37	103.30
1	C	117	ILE	CA-C-O	-5.06	109.48	120.10
1	A	134	PHE	CE1-CZ-CE2	5.05	129.09	120.00
1	B	121	ASP	CB-CG-OD1	5.05	122.85	118.30
1	A	8	PHE	CE1-CZ-CE2	5.04	129.07	120.00
1	B	143	LYS	O-C-N	5.04	130.76	122.70
1	A	105	ARG	CB-CA-C	-5.03	100.34	110.40
1	B	18	ARG	C-N-CA	-5.03	111.74	122.30
1	B	75	ALA	N-CA-CB	5.03	117.14	110.10
1	C	9	ILE	CA-CB-CG2	5.01	120.92	110.90
1	C	6	ARG	NH1-CZ-NH2	5.01	124.91	119.40

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1207	0	1207	177	0
1	B	1207	0	1207	148	0
1	C	1207	0	1207	132	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	434	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 59.

All (434) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:VAL:HG11	1:B:122:SER:CA	2.07	0.84
1:B:139:LEU:H	1:B:139:LEU:HD22	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:HD23	1:A:139:LEU:N	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
1:A:42:ARG:HD3	1:A:69:HIS:O	1.84	0.78
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: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: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:B:16:VAL:HG21	1:B:72:PRO:O	1.89	0.73
1:B:61:PHE:O	1:B:62:ALA:C	2.24	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:5:GLU:HG2	1:A:83:VAL:HG23	1.72	0.71
1:B:60:PHE:O	1:B:61:PHE:C	2.28	0.71
1:A:93:GLU:O	1:A:105:ARG:HD2	1.91	0.71
1:C:26:LYS:O	1:C:26:LYS:HG2	1.80	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:LEU:HD21	1:A:38:MET:HB2	1.72	0.70
1:A:134:PHE:HD1	1:A:138:GLU:HG3	1.56	0.70
1:A:56:LYS:HA	1:A:61:PHE:CE1	2.26	0.70
1:B:27:ARG:HH11	1:B:104:ILE:HG13	1.56	0.70
1:A:56:LYS:NZ	1:A:56:LYS:O	2.22	0.70
1:A:96:PRO:HG3	1:A:109:CYS:SG	2.32	0.69
1:B:24:ILE:O	1:B:25:ILE:C	2.27	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:A:52:TYR:C	3:A:239:HOH:O	2.31	0.68
1:C:5:GLU:O	1:C:79:GLU:HB2	1.93	0.68
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:A:138:GLU:C	1:A:139:LEU:HD23	2.16	0.66
1:B:14:ASP:N	1:B:14:ASP:OD1	2.29	0.66
1:C:91:LEU:O	1:C:105:ARG:HB2	1.96	0.66
1:A:147:GLN:HA	1:A:147:GLN:HE21	1.60	0.65
1:C:10:ALA:O	1:C:117:ILE:HG12	1.95	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ASN:OD1	1:B:3:ASN:N	2.29	0.63
1:C:12:LYS:NZ	2:C:160:PCG:O1A	2.24	0.63
1:A:122:SER:HG	1:A:125:SER:H	1.47	0.63
1:B:136:PRO:HA	1:B:139:LEU:CD2	2.28	0.63
1:B:4:SER:HB3	3:B:306:HOH:O	1.98	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:105:ARG:HE	1:B:115:ASN:ND2	1.93	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:56:LYS:HA	1:B:61:PHE:CD1	2.34	0.62
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:B:101:PRO:HG2	1:C:103:THR:HG22	1.82	0.62
1:B:42:ARG:O	1:B:43:ALA:C	2.35	0.62
1:C:80:GLY:O	1:C:83:VAL:HB	2.00	0.61
1:A:66:LYS:C	1:A:66:LYS:HD2	2.19	0.61
1:C:4:SER:O	1:C:5:GLU:C	2.36	0.61
1:B:24:ILE:HG22	1:B:25:ILE:N	2.10	0.61
1:B:56:LYS:HG2	1:B:57:ASP:N	2.15	0.61
1:B:57:ASP:C	1:B:58:ARG:HG2	2.21	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:C:51:HIS:NE2	1:C:129:GLU:OE1	2.29	0.60
1:A:115:ASN:C	1:A:116:ILE:HG13	2.22	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: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:HD2	1:A:112:VAL:HA	1.83	0.59
1:A:96:PRO:O	1:A:99:SER:HB2	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:86:THR:O	1:B:90:MET:HG3	2.02	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:31:LYS:O	1:A:31:LYS:HG3	2.03	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
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: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:A:17:GLN:HG3	1:B:149:TRP:CE2	2.39	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: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: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:39:LYS:HE2	1:A:41:MET:HE2	1.87	0.56
1:A:86:THR:O	1:A:90:MET:HG3	2.05	0.56
1:A:2:ALA:C	1:A:4:SER:H	2.09	0.56
1:B:129:GLU:O	1:B:130:ILE:C	2.39	0.56
1:B:137:GLU:N	1:B:137:GLU:OE1	2.35	0.56
1:C:139:LEU:N	1:C:139:LEU:HD23	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:O	1:A:66:LYS:HD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:ARG:O	1:B:59:PRO:C	2.43	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: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: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: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:B:139:LEU:N	1:B:139:LEU:HD22	2.17	0.55
1:B:34:ARG:NH1	1:B:142:TYR:CE1	2.75	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: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:A:150:ILE:HG21	1:C:110:ILE:HD12	1.89	0.54
1:A:64:LEU:C	1:A:66:LYS:N	2.60	0.54
1:B:139:LEU:HD13	1:B:139:LEU:N	2.21	0.54
1:B:28:PHE:O	1:B:29:GLU:C	2.38	0.54
1:B:64:LEU:O	1:B:68:MET:N	2.30	0.54
1:C:43:ALA:O	1:C:69:HIS:ND1	2.40	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:113:GLY:N	3:C:445:HOH:O	2.27	0.54
1:C:66:LYS:HB3	1:C:66:LYS:NZ	2.23	0.54
1:C:13:PRO:O	1:C:17:GLN:HB2	2.08	0.54
1:C:115:ASN:O	1:C:117:ILE:N	2.41	0.53
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:PRO:O	1:B:60:PHE:C	2.47	0.52
1:A:3:ASN:HD21	1:A:81:LEU:CB	2.20	0.52
1:A:57:ASP:O	1:A:58:ARG:C	2.46	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:B:110:ILE:HG22	1:B:111:GLN:N	2.25	0.52
1:B:67:TYR:HA	1:B:70:SER:OG	2.10	0.52
1:A:33:PHE:CZ	1:A:86:THR:CG2	2.93	0.52
1:A:135:ARG:O	1:A:138:GLU:HG2	2.09	0.52
1:A:61:PHE:O	1:A:63:GLY:N	2.42	0.52
1:C:56:LYS:HB2	3:C:353:HOH:O	2.09	0.52
1:C:9:ILE:HD13	1:C:119:GLY:CA	2.40	0.52
1:B:143:LYS:HD3	1:B:147:GLN:HB2	1.93	0.51
1:B:44:SER:O	1:B:48:LEU:HG	2.10	0.51
1:B:65:VAL:O	1:B:69:HIS:N	2.36	0.51
1:C:15:GLY:O	1:C:16:VAL:C	2.46	0.51
1:B:34:ARG:NH1	1:B:36:VAL:HG22	2.26	0.51
1:A:147:GLN:NE2	1:A:147:GLN:HA	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:CB	1:B:58:ARG:HH11	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:C:123:VAL:HG22	1:C:124:GLU:N	2.18	0.50
1:C:146:ALA:O	1:C:147:GLN:C	2.48	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:C:139:LEU:N	1:C:139:LEU:CD2	2.72	0.50
1:C:85:LYS:O	1:C:88:ARG:HB2	2.12	0.50
1:C:115:ASN:C	1:C:116:ILE:HG12	2.32	0.50
1:C:66:LYS:NZ	3:C:435:HOH:O	2.43	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:B:47:LEU:HD12	1:B:47:LEU:C	2.31	0.49
1:C:45:GLU:O	1:C:49:LYS:HG3	2.12	0.49
1:C:7:THR:HB	1:C:84:VAL:CG2	2.40	0.49
1:B:67:TYR:O	1:B:70:SER:OG	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:43:ALA:O	1:A:69:HIS:ND1	2.46	0.49
1:C:86:THR:O	1:C:89:VAL:HB	2.13	0.49
1:A:80:GLY:O	1:A:81:LEU:C	2.49	0.49
1:A:53:ILE:CG2	1:A:54:ASP:N	2.76	0.49
1:B:53:ILE:O	1:B:54:ASP:O	2.30	0.49
1:A:149:TRP:O	1:C:114:ARG:HB3	2.12	0.49
1:C:146:ALA:O	1:C:149:TRP:N	2.45	0.49
1:C:23:GLU:OE1	3:C:299:HOH:O	2.20	0.49
1:B:135:ARG:O	1:B:138:GLU:N	2.41	0.48
1:B:67:TYR:HA	1:B:70:SER:CB	2.43	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: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:A:46:ASP:O	1:A:47:LEU:C	2.49	0.47
1:C:129:GLU:O	1:C:133:TRP:HD1	1.97	0.47
1:C:7:THR:CB	1:C:84:VAL:HG22	2.41	0.47
1:A:36:VAL:O	1:A:140:VAL:N	2.47	0.47
1:A:50:GLU:O	1:A:53:ILE:HB	2.14	0.47
1:A:6:ARG:HH21	1:A:127:GLU:CD	2.18	0.47
1:A:122:SER:HB2	1:A:124:GLU:HG3	1.96	0.47
1:A:84:VAL:O	1:A:88:ARG:HG2	2.14	0.47
1:B:100:LYS:O	1:B:101:PRO:C	2.52	0.47
1:B:83:VAL:O	1:B:84:VAL:C	2.52	0.47
1:B:37:ALA:HB1	1:B:134:PHE:CE2	2.49	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:B:123:VAL:O	1:B:124:GLU:C	2.53	0.47
1:B:33:PHE:CE1	1:B:83:VAL:HG12	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ASP:OD1	1:A:125:SER:OG	2.26	0.47
1:A:86:THR:O	1:A:87:GLY:C	2.50	0.47
1:A:45:GLU:O	1:A:49:LYS:HG3	2.15	0.46
1:C:48:LEU:CD2	1:C:68:MET:HB3	2.44	0.46
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:47:LEU:HD23	1:A:48:LEU:N	2.30	0.46
1:A:24:ILE:HG22	1:A:25:ILE:N	2.30	0.46
1:C:47:LEU:CD1	1:C:132:LEU:HD22	2.46	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:H	2.19	0.46
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:B:16:VAL:HG13	1:B:21:MET:SD	2.56	0.45
1:B:67:TYR:C	1:B:70:SER:H	2.20	0.45
1:A:100:LYS:HA	1:A:101:PRO:HD3	1.82	0.45
1:A:8:PHE:O	1:A:120:SER:N	2.48	0.45
1:A:101:PRO:HG2	1:B:103:THR:HG22	1.99	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:B:63:GLY:C	1:B:66:LYS:HG2	2.36	0.45
1:A:140:VAL:HG12	1:A:141:ASN:N	2.31	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:B:116:ILE:HG21	1:B:116:ILE:HD13	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:A:128:LYS:NZ	3:A:280:HOH:O	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:LEU:HD12	1:C:47:LEU:O	2.17	0.44
1:A:22:GLY:O	1:A:23:GLU:C	2.55	0.44
1:A:3:ASN:ND2	1:A:81:LEU:CD1	2.71	0.44
1:B:137:GLU:H	1:B:137:GLU:CD	2.20	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:C:37:ALA:HB2	1:C:139:LEU:HA	1.99	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:HA	1:A:66:LYS:HD2	1.53	0.44
1:A:143:LYS:HG3	1:A:144:SER:N	2.32	0.44
1:A:24:ILE:CG2	1:A:25:ILE:N	2.80	0.44
1:A:3:ASN:HD22	1:A:3:ASN:HA	1.34	0.44
1:B:94:THR:HG21	2:B:160:PCG:H3'	1.99	0.44
1:B:91:LEU:O	1:B:104:ILE:N	2.50	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:B:22:GLY:O	1:B:23:GLU:C	2.56	0.44
1:B:61:PHE:O	1:B:63:GLY:N	2.51	0.44
1:C:129:GLU:O	1:C:133:TRP:CD1	2.70	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:A:110:ILE:O	1:A:110:ILE:HG22	2.18	0.43
1:C:105:ARG:HH11	1:C:105:ARG:HD2	1.26	0.43
1:C:39:LYS:HE3	1:C:134:PHE:CE1	2.53	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: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: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:A:152:GLU:N	1:C:111:GLN:OE1	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:PHE:HB2	1:B:130:ILE:HG13	2.00	0.43
1:B:144:SER:C	1:B:146:ALA:H	2.22	0.43
1:A:124:GLU:HG3	1:A:124:GLU:H	1.46	0.42
1:A:64:LEU:C	1:A:66:LYS:H	2.20	0.42
1:B:118:HIS:CG	1:B:119:GLY:N	2.84	0.42
1:A:151:TYR:HE1	1:C:110:ILE:HG21	1.83	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: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:HE3	1:B:85:LYS:HB3	1.82	0.42
1:C:69:HIS:CD2	1:C:69:HIS:O	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:O	1:B:69:HIS:ND1	2.52	0.42
1:C:14:ASP:OD1	1:C:116:ILE:HA	2.19	0.42
1:A:114:ARG:HA	1:A:114:ARG:HD3	1.69	0.42
1:A:40:PHE:CE1	1:A:72:PRO:HB2	2.54	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:B:53:ILE:O	1:B:54:ASP:C	2.58	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:C:123:VAL:HG12	1:C:123:VAL:H	1.12	0.42
1:A:9:ILE:HB	1:A:76:MET:HE3	2.02	0.41
1:A:134:PHE:HD1	1:A:138:GLU:CG	2.30	0.41
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: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:HG13	1:A:104:ILE:H	1.51	0.41
1:B:59:PRO:N	3:B:356:HOH:O	2.53	0.41
1:C:47:LEU:HD12	1:C:47:LEU:C	2.40	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:40:PHE:O	1:A:41:MET:HB3	2.20	0.41
1:B:52:TYR:CE1	2:B:160:PCG:H5'2	2.56	0.41
1:B:53:ILE:HG13	1:B:53:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:TYR:HE1	1:C:110:ILE:CG2	2.33	0.41
1:A:61:PHE:C	1:A:63:GLY:N	2.74	0.41
1:B:56:LYS:CG	1:B:57:ASP:N	2.81	0.41
1:C:12:LYS:HE3	1:C:117:ILE:C	2.41	0.41
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

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	149/151 (99%)	128 (86%)	13 (9%)	8 (5%)	2	1
1	B	149/151 (99%)	120 (80%)	16 (11%)	13 (9%)	1	0
1	C	149/151 (99%)	131 (88%)	14 (9%)	4 (3%)	5	5
All	All	447/453 (99%)	379 (85%)	43 (10%)	25 (6%)	2	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

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Mol	Chain	Res	Type
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	128/128 (100%)	101 (79%)	27 (21%)	1 1
1	B	128/128 (100%)	100 (78%)	28 (22%)	1 1
1	C	128/128 (100%)	103 (80%)	25 (20%)	1 1
All	All	384/384 (100%)	304 (79%)	80 (21%)	1 1

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER

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Mol	Chain	Res	Type
1	A	17	GLN
1	A	18	ARG
1	A	39	LYS
1	A	41	MET
1	A	55	LEU
1	A	56	LYS
1	A	60	PHE
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	116	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	147	GLN
1	A	152	GLU
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	56	LYS
1	B	57	ASP
1	B	58	ARG
1	B	66	LYS
1	B	67	TYR
1	B	85	LYS
1	B	88	ARG
1	B	90	MET
1	B	110	ILE

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Mol	Chain	Res	Type
1	B	112	VAL
1	B	114	ARG
1	B	115	ASN
1	B	120	SER
1	B	121	ASP
1	B	127	GLU
1	B	132	LEU
1	B	139	LEU
1	B	141	ASN
1	B	143	LYS
1	B	144	SER
1	B	147	GLN
1	C	6	ARG
1	C	23	GLU
1	C	26	LYS
1	C	27	ARG
1	C	30	GLN
1	C	38	MET
1	C	53	ILE
1	C	54	ASP
1	C	66	LYS
1	C	67	TYR
1	C	93	GLU
1	C	107	ASP
1	C	114	ARG
1	C	117	ILE
1	C	122	SER
1	C	123	VAL
1	C	124	GLU
1	C	125	SER
1	C	132	LEU
1	C	135	ARG
1	C	137	GLU
1	C	139	LEU
1	C	142	TYR
1	C	143	LYS
1	C	144	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN

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Mol	Chain	Res	Type
1	A	51	HIS
1	B	51	HIS
1	C	82	ASN
1	C	147	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	-	22,26,26	2.48	5 (22%)	26,41,41	4.60	16 (61%)
2	PCG	A	160	-	22,26,26	2.67	7 (31%)	26,41,41	4.34	14 (53%)
2	PCG	B	160	-	22,26,26	2.55	8 (36%)	26,41,41	3.94	13 (50%)

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

All (20) 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	C6-N1	6.01	1.43	1.33
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	C6-N1	5.18	1.42	1.33
2	C	160	PCG	C6-N1	5.01	1.41	1.33
2	A	160	PCG	O3'-C3'	4.37	1.51	1.44
2	A	160	PCG	C4-N3	3.85	1.41	1.35
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	C	160	PCG	C2-N1	3.40	1.41	1.35
2	A	160	PCG	C2-N1	2.90	1.40	1.35
2	B	160	PCG	PA-O3'	-2.84	1.53	1.57
2	B	160	PCG	O6-C6	2.60	1.31	1.24
2	B	160	PCG	C2-N1	2.59	1.40	1.35
2	A	160	PCG	C6-C5	2.47	1.45	1.41
2	B	160	PCG	C6-C5	2.33	1.45	1.41
2	C	160	PCG	C8-N7	-2.14	1.30	1.34
2	B	160	PCG	C8-N7	-2.13	1.30	1.34

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	160	PCG	C5-C6-N1	-12.46	106.38	123.43
2	C	160	PCG	C5-C6-N1	-11.31	107.96	123.43
2	A	160	PCG	O5'-PA-O3'	-9.54	92.54	105.68
2	A	160	PCG	C5-C6-N1	-8.41	111.93	123.43
2	C	160	PCG	C2-N3-C4	-8.16	106.03	115.36
2	C	160	PCG	C1'-N9-C4	-8.05	112.49	126.64
2	A	160	PCG	C1'-N9-C4	-8.02	112.55	126.64
2	B	160	PCG	C6-N1-C2	7.76	128.26	115.93
2	C	160	PCG	C5'-C4'-C3'	7.66	128.01	112.49
2	A	160	PCG	O1A-PA-O3'	7.43	124.36	107.04
2	C	160	PCG	C6-N1-C2	7.00	127.05	115.93
2	A	160	PCG	C6-N1-C2	6.86	126.84	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	160	PCG	C2'-C3'-C4'	-6.67	91.40	103.22
2	B	160	PCG	C1'-N9-C4	6.66	138.34	126.64
2	B	160	PCG	C2-N3-C4	-6.44	108.01	115.36
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	C	160	PCG	O5'-PA-O3'	4.61	112.03	105.68
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'	-4.10	95.95	103.22
2	B	160	PCG	C2'-C3'-C4'	-3.56	96.91	103.22
2	B	160	PCG	O1A-PA-O3'	3.52	115.23	107.04
2	B	160	PCG	N2-C2-N1	-3.48	111.85	117.25
2	C	160	PCG	O3'-C3'-C2'	3.44	118.98	115.61
2	A	160	PCG	C6-C5-C4	-3.31	117.63	120.80
2	C	160	PCG	O4'-C4'-C3'	3.25	111.83	104.87
2	A	160	PCG	C2-N3-C4	-3.17	111.73	115.36
2	B	160	PCG	N2-C2-N3	3.03	122.73	117.79
2	A	160	PCG	N3-C2-N1	-2.91	123.34	127.22
2	C	160	PCG	N2-C2-N1	-2.84	112.83	117.25
2	A	160	PCG	O2'-C2'-C1'	-2.83	100.41	110.85
2	A	160	PCG	O3'-PA-O2A	2.78	116.35	110.39
2	A	160	PCG	C5'-C4'-C3'	-2.72	106.98	112.49
2	A	160	PCG	O2'-C2'-C3'	2.64	118.67	111.17
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	C	160	PCG	O4'-C4'-C5'	2.33	119.33	112.37
2	C	160	PCG	O4'-C1'-C2'	-2.26	103.62	106.93
2	B	160	PCG	O5'-PA-O3'	2.23	108.75	105.68
2	B	160	PCG	O2'-C2'-C3'	2.11	117.15	111.17
2	B	160	PCG	O2'-C2'-C1'	-2.08	103.17	110.85

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

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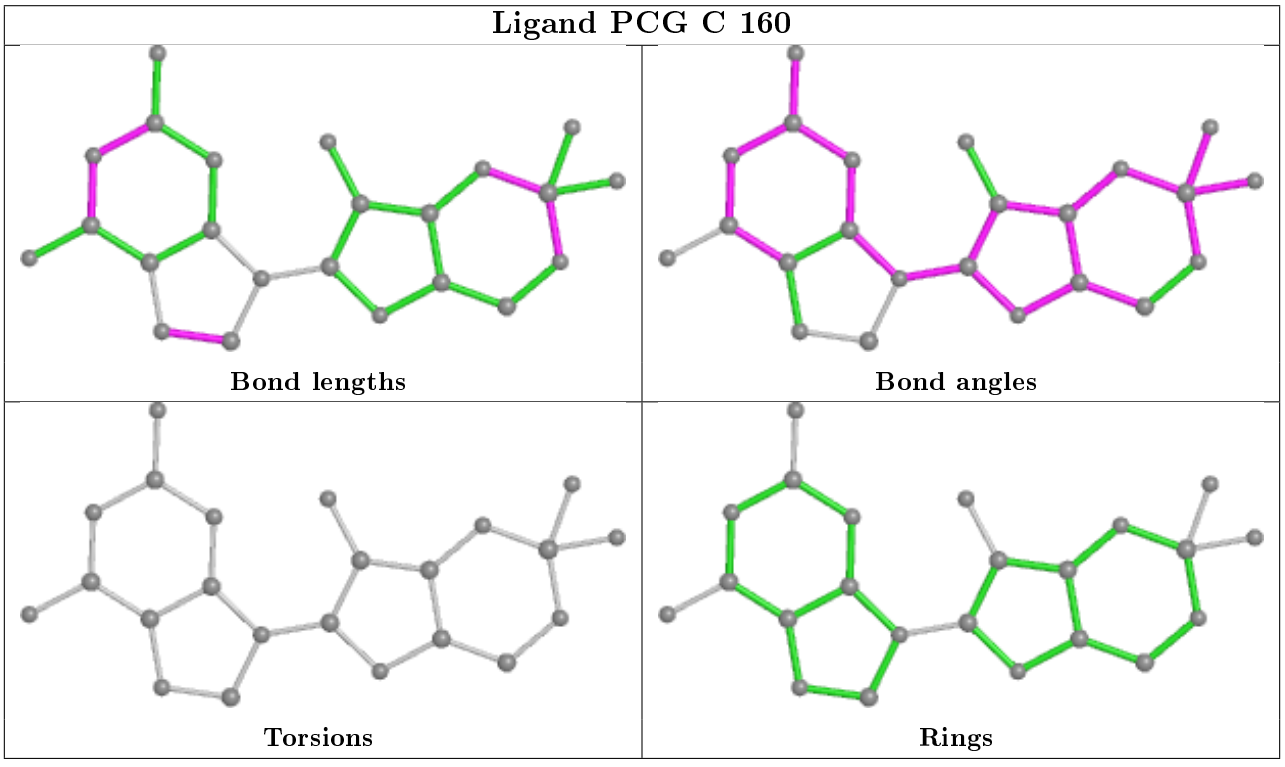
Mol	Chain	Res	Type	Atoms
2	A	160	PCG	C3'-C4'-C5'-O3'-O5'-PA

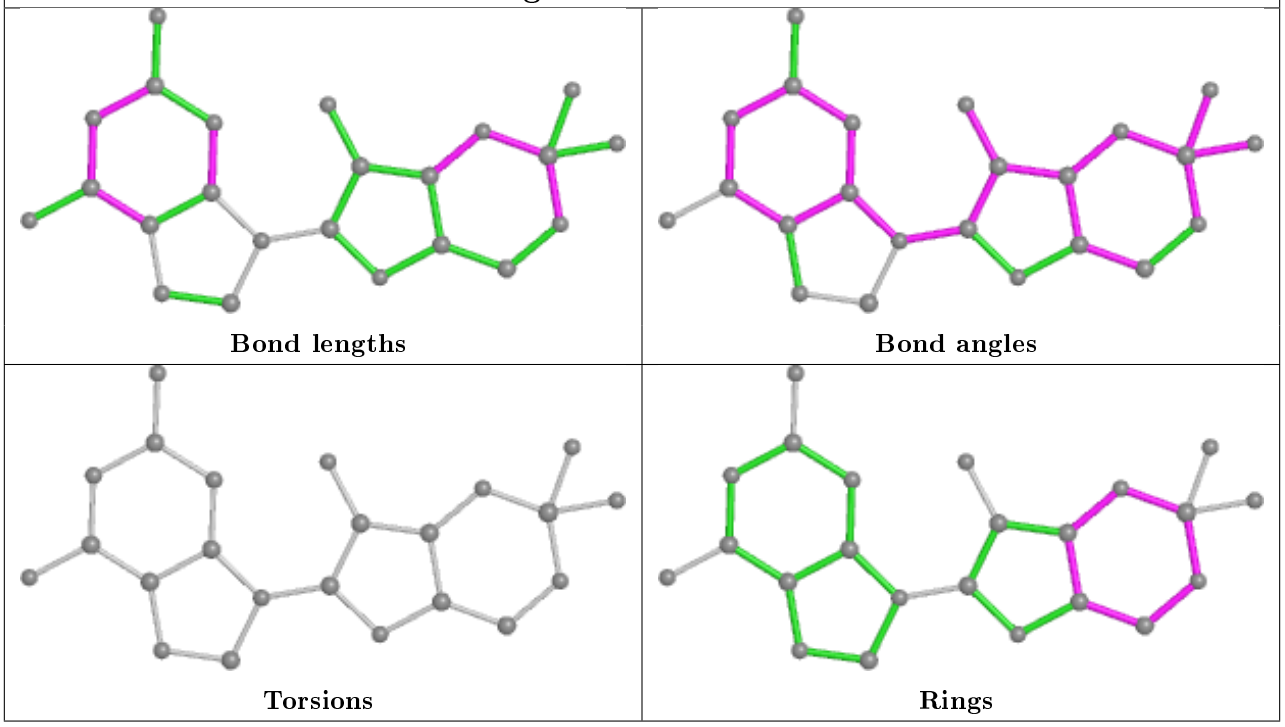
3 monomers are involved in 9 short contacts:

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

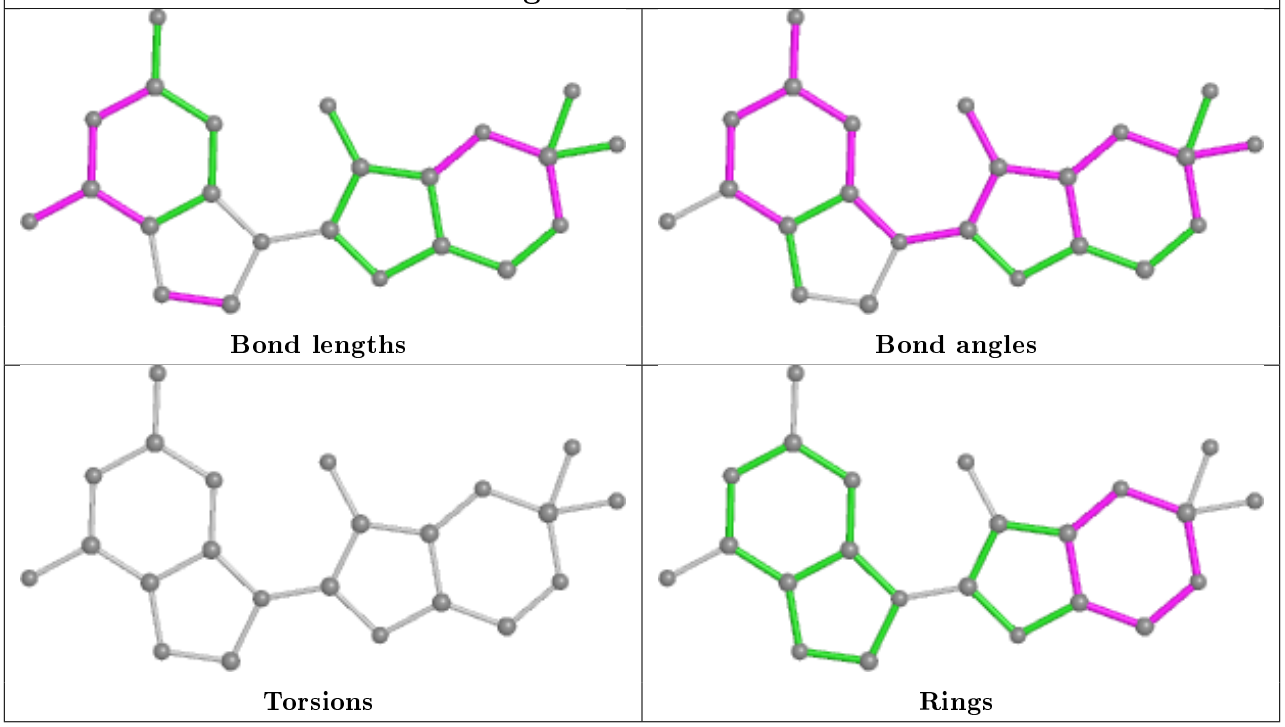
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.



Ligand PCG A 160



Ligand PCG B 160



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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%)	-0.31	7 (4%)	32	31	10, 28, 70, 92	0
1	B	151/151 (100%)	-0.14	9 (5%)	21	20	13, 34, 81, 100	0
1	C	151/151 (100%)	-0.37	2 (1%)	77	75	9, 26, 65, 81	0
All	All	453/453 (100%)	-0.27	18 (3%)	38	37	9, 30, 73, 100	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	60	PHE	4.6
1	B	59	PRO	4.3
1	B	61	PHE	4.1
1	B	63	GLY	3.8
1	B	60	PHE	3.2
1	A	61	PHE	3.2
1	B	55	LEU	3.0
1	B	65	VAL	3.0
1	A	59	PRO	2.9
1	B	58	ARG	2.8
1	A	63	GLY	2.3
1	B	57	ASP	2.3
1	B	64	LEU	2.2
1	A	57	ASP	2.2
1	A	62	ALA	2.1
1	C	57	ASP	2.1
1	A	58	ARG	2.1
1	C	63	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

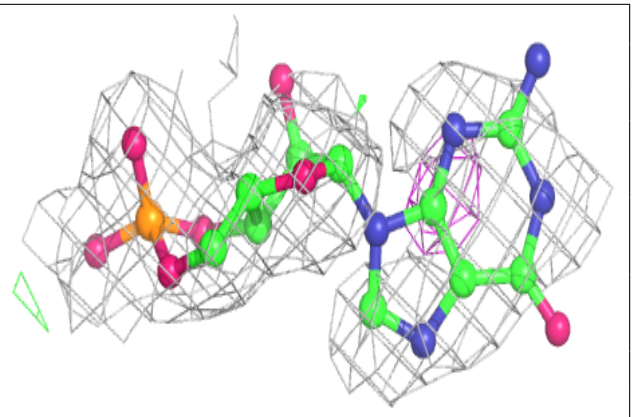
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

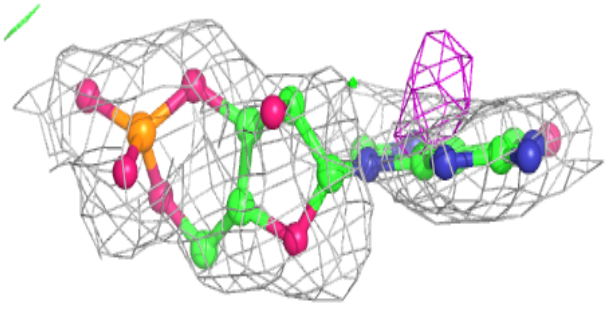
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PCG	A	160	23/23	0.89	0.21	19,74,99,99	0
2	PCG	B	160	23/23	0.90	0.20	28,78,99,99	0
2	PCG	C	160	23/23	0.95	0.18	15,41,86,99	0

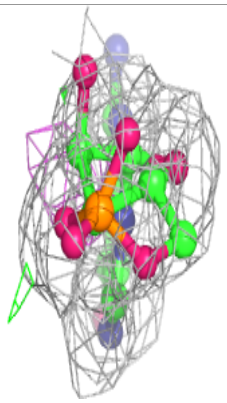
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

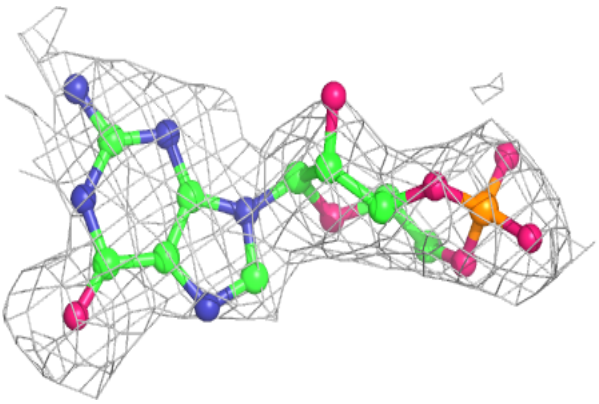


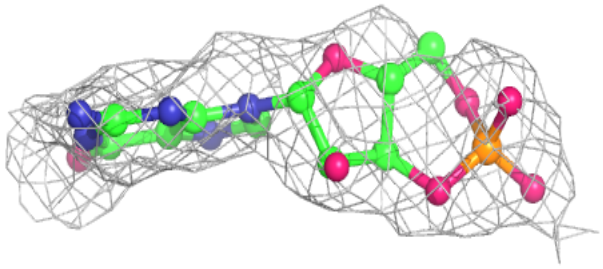


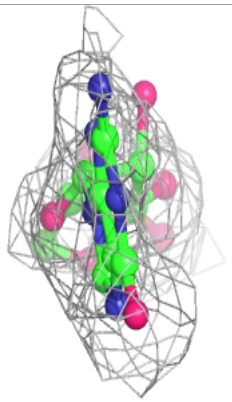


Electron density around PCG B 160:

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

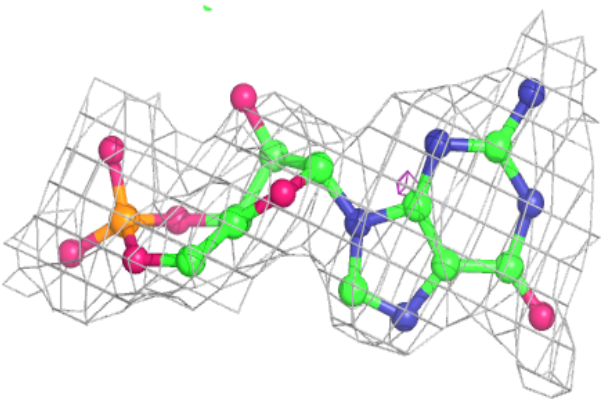


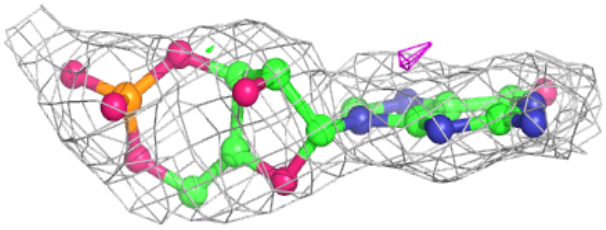


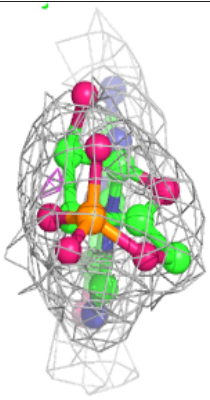


Electron density around PCG C 160:

$2mF_o$-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.