



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 08:05 AM UTC

PDB ID : 2ONE / pdb\_00002one  
Title : ASYMMETRIC YEAST ENOLASE DIMER COMPLEXED WITH RESOLVED 2'-PHOSPHOGLYCERATE AND PHOSPHOENOLPYRUVATE  
Authors : Lebioda, L.  
Deposited on : 1997-09-08  
Resolution : 2.00 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](mailto: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>.

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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)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

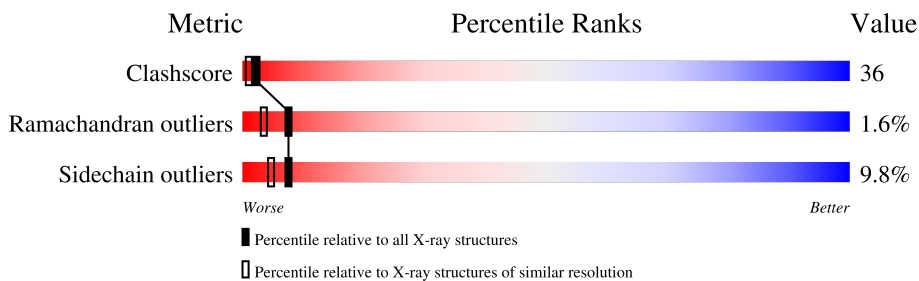
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	436	 42% 38% 14% 5%
1	B	436	 39% 41% 17% 1%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6964 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 ENOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	436	3292	2079	570	637	6	0	0	0
1	B	436	3292	2079	570	637	6	0	0	0

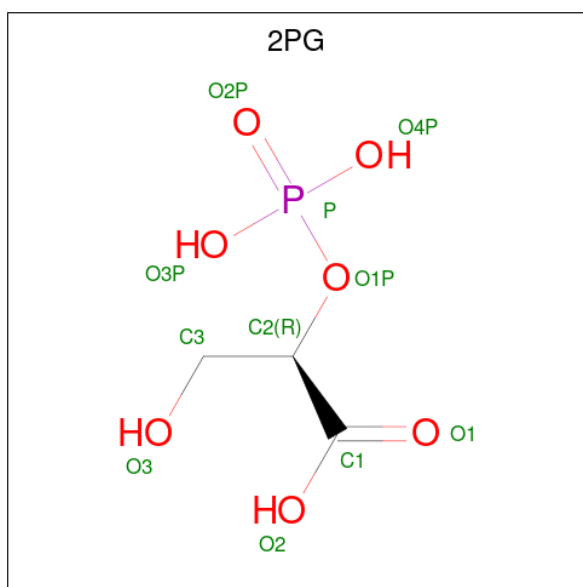
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is LITHIUM ION (CCD ID: LI) (formula: Li).

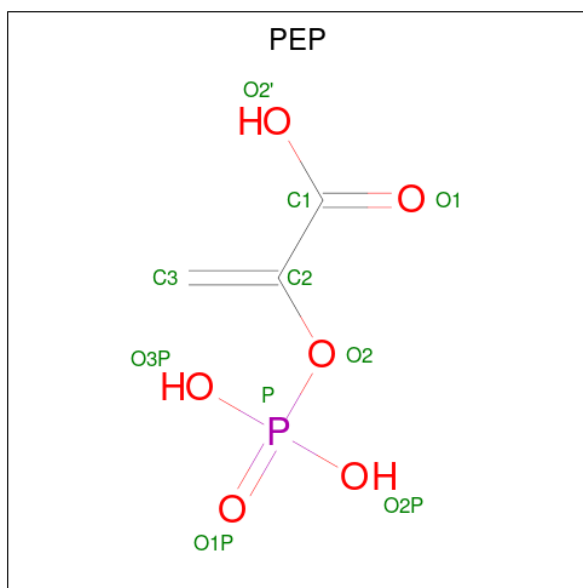
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Li	0	0
			1	1		

- Molecule 4 is 2-PHOSPHOGLYCERIC ACID (CCD ID: 2PG) (formula: C<sub>3</sub>H<sub>7</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			11	3	7	1		

- Molecule 5 is PHOSPHOENOLPYRUVATE (CCD ID: PEP) (formula:  $C_3H_5O_6P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 6 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	A	197	Total 197	O 197	0	0
6	B	159	Total 159	O 159	0	0

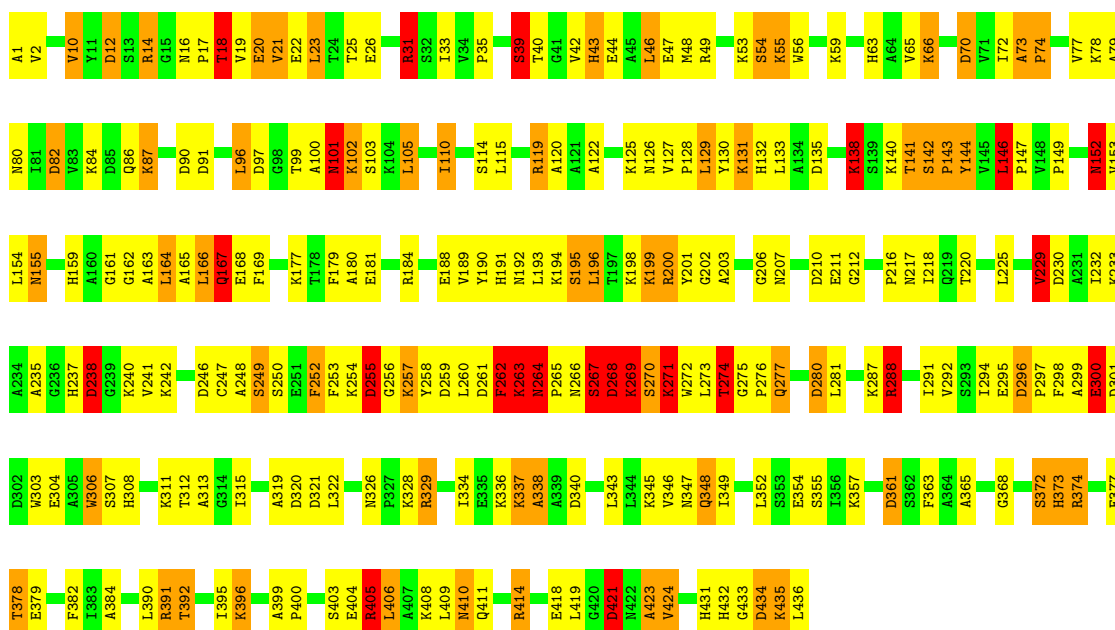
### 3 Residue-property plots

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

Note EDS was not executed.

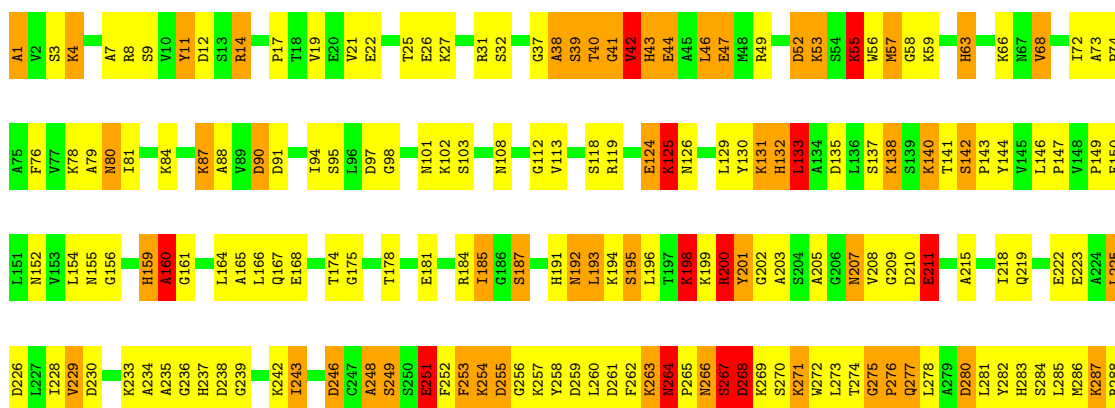
- Molecule 1: ENOLASE

Chain A: 



- Molecule 1: ENOLASE

Chain B: 





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.10Å 110.00Å 66.20Å 90.00° 113.00° 90.00°	Depositor
Resolution (Å)	9.00 – 2.00	Depositor
% Data completeness (in resolution range)	83.3 (9.00-2.00)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, $R_{free}$	0.137 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6964	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, LI, PEP, 2PG

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	1.20	4/3352 (0.1%)	2.68	235/4534 (5.2%)
1	B	1.13	1/3352 (0.0%)	2.47	217/4534 (4.8%)
All	All	1.16	5/6704 (0.1%)	2.58	452/9068 (5.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	17
1	B	0	7
All	All	0	24

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	264	ASN	C-O	15.25	1.41	1.24
1	A	264	ASN	C-N	13.67	1.47	1.34
1	A	268	ASP	N-CA	-5.52	1.39	1.46
1	A	312	THR	CA-CB	5.51	1.61	1.54
1	B	381	THR	CA-CB	5.16	1.60	1.53

All (452) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	ASN	O-C-N	-33.54	94.06	121.23
1	A	264	ASN	CA-C-O	-28.34	90.11	121.28
1	A	267	SER	CA-C-N	28.11	175.22	121.54
1	A	267	SER	C-N-CA	28.11	175.22	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	ASN	CA-C-N	20.52	142.89	120.12
1	A	264	ASN	C-N-CA	20.52	142.89	120.12
1	A	264	ASN	N-CA-C	17.03	137.70	108.75
1	B	391	ARG	CD-NE-CZ	16.99	148.19	124.40
1	A	262	PHE	CA-C-O	14.60	137.09	120.89
1	B	264	ASN	CA-CB-CG	-14.56	98.04	112.60
1	B	271	LYS	CA-C-N	13.29	141.34	123.00
1	B	271	LYS	C-N-CA	13.29	141.34	123.00
1	A	265	PRO	N-CA-C	-12.62	99.06	114.20
1	A	142	SER	O-C-N	11.64	128.25	121.27
1	B	238	ASP	CA-CB-CG	-10.32	102.28	112.60
1	A	165	ALA	CA-C-O	-10.28	110.31	120.90
1	B	58	GLY	CA-C-O	10.23	130.82	119.06
1	A	409	LEU	CA-C-O	-10.15	109.66	120.42
1	B	8	ARG	NE-CZ-NH1	10.12	131.62	121.50
1	A	265	PRO	N-CA-CB	9.89	113.08	103.19
1	B	81	ILE	CA-C-O	-9.79	109.05	121.48
1	B	91	ASP	CA-C-O	9.68	131.09	120.63
1	A	101	ASN	OD1-CG-ND2	-9.67	112.93	122.60
1	A	119	ARG	CA-C-N	9.61	133.16	120.28
1	A	119	ARG	C-N-CA	9.61	133.16	120.28
1	A	165	ALA	O-C-N	9.54	132.33	122.03
1	B	159	HIS	CA-C-O	-9.53	111.41	122.37
1	A	241	VAL	CA-C-O	9.39	130.32	120.36
1	A	155	ASN	CA-C-O	9.19	130.45	120.43
1	A	264	ASN	CB-CA-C	-9.19	97.76	111.27
1	B	192	ASN	CA-CB-CG	-9.11	103.49	112.60
1	A	101	ASN	CA-CB-CG	-9.01	103.59	112.60
1	A	54	SER	CA-C-N	8.97	134.16	121.24
1	A	54	SER	C-N-CA	8.97	134.16	121.24
1	A	404	GLU	N-CA-C	-8.89	102.42	113.18
1	A	126	ASN	OD1-CG-ND2	-8.86	113.74	122.60
1	B	167	GLN	OE1-CD-NE2	8.84	131.44	122.60
1	A	202	GLY	CA-C-O	-8.63	115.30	122.29
1	B	280	ASP	CA-CB-CG	-8.62	103.98	112.60
1	A	269	LYS	N-CA-CB	8.60	125.02	110.49
1	B	72	ILE	O-C-N	8.46	130.99	121.94
1	B	91	ASP	CA-CB-CG	8.45	121.05	112.60
1	B	246	ASP	N-CA-CB	8.44	123.99	110.65
1	B	52	ASP	CA-CB-CG	-8.43	104.17	112.60
1	A	12	ASP	O-C-N	8.38	132.55	121.83
1	A	152	ASN	CA-C-O	-8.36	111.95	120.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	248	ALA	CA-C-N	8.36	131.83	120.38
1	B	248	ALA	C-N-CA	8.36	131.83	120.38
1	A	217	ASN	OD1-CG-ND2	-8.32	114.28	122.60
1	B	187	SER	CA-C-O	-8.28	110.03	119.79
1	A	129	LEU	CA-C-O	-8.10	112.23	120.90
1	B	14	ARG	CD-NE-CZ	-8.00	113.20	124.40
1	B	187	SER	N-CA-CB	7.99	122.61	110.30
1	A	141	THR	CA-CB-OG1	-7.98	97.62	109.60
1	B	308	HIS	CA-CB-CG	-7.98	105.82	113.80
1	B	392	THR	CA-CB-OG1	-7.91	97.73	109.60
1	A	379	GLU	CA-CB-CG	7.91	129.92	114.10
1	A	361	ASP	CA-CB-CG	7.88	120.48	112.60
1	B	32	SER	CA-C-O	-7.86	111.62	120.66
1	A	31	ARG	NE-CZ-NH1	7.85	129.35	121.50
1	B	46	LEU	CA-C-O	7.82	129.18	120.43
1	B	291	ILE	CA-C-O	-7.81	111.82	121.11
1	A	143	PRO	CA-C-N	7.79	132.56	121.42
1	A	143	PRO	C-N-CA	7.79	132.56	121.42
1	B	4	LYS	CA-CB-CG	7.78	129.67	114.10
1	B	391	ARG	NE-CZ-NH2	-7.75	112.23	119.20
1	B	207	ASN	OD1-CG-ND2	-7.74	114.86	122.60
1	B	63	HIS	CA-CB-CG	-7.72	106.08	113.80
1	A	162	GLY	CA-C-O	-7.68	115.08	121.76
1	A	166	LEU	CB-CA-C	7.65	121.83	109.90
1	A	269	LYS	CA-C-N	-7.63	110.09	121.99
1	A	269	LYS	C-N-CA	-7.63	110.09	121.99
1	B	254	LYS	CA-C-N	7.62	136.10	121.54
1	B	254	LYS	C-N-CA	7.62	136.10	121.54
1	A	149	PRO	CA-C-N	7.62	134.04	122.77
1	A	149	PRO	C-N-CA	7.62	134.04	122.77
1	B	349	ILE	CB-CA-C	7.59	120.28	111.55
1	B	408	LYS	O-C-N	-7.58	114.27	122.07
1	A	146	LEU	CB-CA-C	7.55	121.64	109.41
1	A	384	ALA	N-CA-C	-7.53	102.67	111.03
1	B	266	ASN	CA-C-N	7.52	135.90	121.54
1	B	266	ASN	C-N-CA	7.52	135.90	121.54
1	B	192	ASN	O-C-N	7.48	130.08	122.08
1	B	118	SER	N-CA-CB	7.46	121.20	110.16
1	A	411	GLN	CA-C-N	7.45	130.26	120.28
1	A	411	GLN	C-N-CA	7.45	130.26	120.28
1	A	191	HIS	CA-CB-CG	-7.44	106.36	113.80
1	B	32	SER	O-C-N	7.44	132.35	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	ALA	CA-C-O	-7.43	112.60	120.63
1	A	319	ALA	CA-C-O	7.42	128.47	120.38
1	A	270	SER	CA-CB-OG	-7.42	96.25	111.10
1	A	200	ARG	CD-NE-CZ	-7.39	114.05	124.40
1	B	405	ARG	NE-CZ-NH2	-7.39	112.55	119.20
1	A	46	LEU	N-CA-C	7.37	120.43	109.59
1	B	277	GLN	CA-C-N	7.36	130.01	120.44
1	B	277	GLN	C-N-CA	7.36	130.01	120.44
1	B	339	ALA	CA-C-O	-7.36	113.56	121.36
1	B	384	ALA	CA-C-O	7.33	128.69	121.00
1	B	57	MET	CA-C-O	-7.31	111.75	120.81
1	A	409	LEU	CA-C-N	7.29	130.65	120.29
1	A	409	LEU	C-N-CA	7.29	130.65	120.29
1	B	430	PHE	CA-C-O	-7.26	111.89	120.10
1	B	113	VAL	CA-C-O	7.26	128.50	120.95
1	B	427	GLY	CA-C-N	7.26	131.34	120.31
1	B	427	GLY	C-N-CA	7.26	131.34	120.31
1	B	382	PHE	CA-C-O	-7.24	112.81	120.92
1	B	236	GLY	CA-C-O	7.24	126.78	118.96
1	A	280	ASP	CA-CB-CG	-7.21	105.39	112.60
1	B	307	SER	CA-C-O	7.20	128.38	120.82
1	A	300	GLU	CB-CG-CD	-7.16	100.44	112.60
1	B	195	SER	CA-C-N	7.15	130.19	120.54
1	B	195	SER	C-N-CA	7.15	130.19	120.54
1	B	422	ASN	OD1-CG-ND2	-7.14	115.46	122.60
1	A	192	ASN	CA-C-O	-7.12	113.36	120.70
1	A	163	ALA	N-CA-C	7.11	120.43	111.69
1	B	14	ARG	NE-CZ-NH1	-7.11	114.39	121.50
1	A	33	ILE	CA-C-O	-7.10	112.93	120.39
1	A	348	GLN	CA-C-N	7.08	131.06	122.63
1	A	348	GLN	C-N-CA	7.08	131.06	122.63
1	B	81	ILE	O-C-N	7.05	130.73	122.69
1	A	19	VAL	O-C-N	7.01	130.95	122.95
1	B	334	ILE	N-CA-C	-7.00	103.95	110.53
1	B	432	HIS	CA-CB-CG	-6.99	106.81	113.80
1	A	378	THR	O-C-N	6.98	132.06	122.78
1	A	101	ASN	N-CA-CB	-6.93	100.14	110.61
1	A	192	ASN	O-C-N	6.93	129.58	122.09
1	B	118	SER	CA-C-O	-6.93	113.08	120.42
1	B	156	GLY	CA-C-N	6.91	131.27	120.00
1	B	156	GLY	C-N-CA	6.91	131.27	120.00
1	B	4	LYS	N-CA-CB	6.91	124.37	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	330	ILE	CB-CG1-CD1	6.90	128.29	113.80
1	B	150	PHE	CA-CB-CG	-6.90	106.90	113.80
1	A	141	THR	CA-CB-CG2	6.89	122.22	110.50
1	B	167	GLN	N-CA-C	6.89	122.10	111.56
1	A	308	HIS	CA-CB-CG	-6.88	106.92	113.80
1	B	185	ILE	CA-C-N	6.85	127.70	120.03
1	B	185	ILE	C-N-CA	6.85	127.70	120.03
1	A	33	ILE	N-CA-CB	6.83	120.84	111.41
1	B	367	TRP	CA-CB-CG	6.82	126.56	113.60
1	B	175	GLY	CA-C-N	6.81	134.55	121.54
1	B	175	GLY	C-N-CA	6.81	134.55	121.54
1	B	161	GLY	N-CA-C	6.81	127.65	115.80
1	A	262	PHE	CA-C-N	6.78	134.50	121.54
1	A	262	PHE	C-N-CA	6.78	134.50	121.54
1	B	87	LYS	CB-CG-CD	6.74	126.81	111.30
1	B	193	LEU	CB-CA-C	6.74	121.59	110.81
1	B	80	ASN	OD1-CG-ND2	6.74	129.34	122.60
1	A	414	ARG	NE-CZ-NH2	6.71	125.24	119.20
1	B	326	ASN	CA-CB-CG	-6.71	105.89	112.60
1	A	263	LYS	N-CA-C	-6.69	96.55	110.80
1	B	351	THR	CA-C-N	6.68	129.12	120.44
1	B	351	THR	C-N-CA	6.68	129.12	120.44
1	A	202	GLY	O-C-N	6.67	130.65	122.78
1	A	202	GLY	N-CA-C	-6.66	104.30	112.68
1	A	268	ASP	N-CA-C	6.64	124.95	110.80
1	A	411	GLN	CA-C-O	-6.63	113.52	120.55
1	B	80	ASN	CA-C-O	6.62	131.05	122.45
1	A	138	LYS	CB-CA-C	-6.61	103.01	111.86
1	A	82	ASP	O-C-N	6.61	131.41	122.82
1	A	46	LEU	CA-C-O	-6.60	112.92	120.58
1	A	271	LYS	O-C-N	6.58	129.92	122.22
1	A	405	ARG	NE-CZ-NH2	-6.58	113.28	119.20
1	B	181	GLU	CB-CG-CD	6.57	123.77	112.60
1	A	155	ASN	CA-CB-CG	6.57	119.17	112.60
1	B	317	ILE	CB-CA-C	6.57	119.29	110.42
1	A	154	LEU	CB-CA-C	6.56	121.30	110.74
1	B	225	LEU	CA-C-O	-6.55	113.94	120.82
1	A	246	ASP	CA-C-O	-6.54	111.43	120.52
1	A	409	LEU	O-C-N	6.54	129.60	122.15
1	B	399	ALA	CA-C-O	-6.54	113.29	121.01
1	B	149	PRO	CA-C-O	-6.54	113.27	120.92
1	A	406	LEU	CD1-CG-CD2	6.53	125.16	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	ARG	O-C-N	-6.52	113.88	122.42
1	B	174	THR	CA-C-O	6.51	127.45	119.97
1	B	159	HIS	CB-CA-C	-6.51	101.88	112.03
1	B	25	THR	CA-CB-OG1	-6.50	99.85	109.60
1	A	220	THR	CA-C-N	6.50	128.88	120.44
1	A	220	THR	C-N-CA	6.50	128.88	120.44
1	B	68	VAL	O-C-N	6.47	128.86	121.94
1	B	400	PRO	N-CA-CB	6.46	107.14	102.81
1	A	307	SER	O-C-N	6.46	128.80	122.09
1	A	406	LEU	CA-C-O	-6.45	112.81	120.10
1	A	125	LYS	CA-C-O	-6.43	111.49	119.28
1	A	396	LYS	CA-C-O	6.43	127.15	120.40
1	A	101	ASN	CB-CG-OD1	6.38	133.56	120.80
1	A	189	VAL	O-C-N	6.37	128.15	121.91
1	B	207	ASN	CB-CA-C	6.36	122.71	109.68
1	A	271	LYS	CB-CA-C	-6.35	98.88	110.63
1	B	126	ASN	CA-CB-CG	-6.35	106.25	112.60
1	A	164	LEU	CA-C-O	6.35	127.66	120.80
1	A	423	ALA	O-C-N	6.34	130.84	123.17
1	B	184	ARG	NH1-CZ-NH2	-6.33	111.07	119.30
1	A	33	ILE	O-C-N	6.33	130.09	123.26
1	B	187	SER	O-C-N	6.32	130.79	122.33
1	A	10	VAL	O-C-N	6.30	129.54	122.92
1	A	313	ALA	N-CA-C	6.29	118.66	111.11
1	B	66	LYS	O-C-N	-6.29	114.53	122.27
1	B	211	GLU	CA-C-O	-6.29	112.04	120.15
1	B	200	ARG	CD-NE-CZ	-6.29	115.60	124.40
1	A	164	LEU	CB-CA-C	6.28	118.78	110.06
1	B	203	ALA	O-C-N	6.26	128.76	122.12
1	B	55	LYS	O-C-N	6.25	130.58	123.27
1	B	98	GLY	N-CA-C	6.25	123.67	115.36
1	B	94	ILE	N-CA-CB	-6.25	102.05	110.54
1	A	100	ALA	CA-C-O	6.24	127.15	119.97
1	B	284	SER	CA-C-O	-6.23	114.28	120.82
1	A	400	PRO	N-CA-C	-6.21	104.10	112.48
1	A	210	ASP	CA-C-O	-6.21	113.09	120.10
1	B	38	ALA	CA-C-N	6.21	133.39	121.54
1	B	38	ALA	C-N-CA	6.21	133.39	121.54
1	B	326	ASN	OD1-CG-ND2	6.21	128.81	122.60
1	B	320	ASP	CA-CB-CG	6.20	118.80	112.60
1	B	374	ARG	O-C-N	-6.20	114.08	122.94
1	B	209	GLY	N-CA-C	-6.19	104.09	112.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	335	GLU	CA-CB-CG	6.18	126.47	114.10
1	A	271	LYS	N-CA-C	-6.17	104.61	111.71
1	A	210	ASP	O-C-N	6.16	129.43	122.22
1	A	40	THR	CA-C-N	6.16	125.83	119.92
1	A	40	THR	C-N-CA	6.16	125.83	119.92
1	A	252	PHE	CA-CB-CG	6.14	119.94	113.80
1	A	254	LYS	CA-CB-CG	6.14	126.39	114.10
1	A	19	VAL	CA-C-N	-6.13	113.74	122.94
1	A	19	VAL	C-N-CA	-6.13	113.74	122.94
1	A	140	LYS	N-CA-CB	6.12	118.97	109.97
1	A	65	VAL	N-CA-C	-6.12	104.78	110.53
1	B	185	ILE	CA-CB-CG2	6.09	120.85	110.50
1	B	47	GLU	CA-C-O	-6.08	113.76	120.69
1	B	112	GLY	CA-C-O	-6.07	114.80	121.05
1	B	218	ILE	CB-CA-C	6.07	120.47	111.31
1	B	222	GLU	CB-CG-CD	6.06	122.91	112.60
1	B	317	ILE	CB-CG1-CD1	6.04	126.47	113.80
1	B	118	SER	N-CA-C	-6.03	104.79	111.36
1	A	434	ASP	CA-CB-CG	-6.02	106.58	112.60
1	A	320	ASP	O-C-N	6.02	127.69	121.79
1	A	82	ASP	CA-CB-CG	6.02	118.62	112.60
1	A	207	ASN	OD1-CG-ND2	6.01	128.62	122.60
1	B	124	GLU	CG-CD-OE1	-6.01	104.57	118.40
1	B	138	LYS	CB-CG-CD	6.00	125.11	111.30
1	B	300	GLU	N-CA-C	5.99	121.64	113.37
1	B	243	ILE	O-C-N	5.99	129.51	123.10
1	A	115	LEU	CA-C-O	-5.97	114.23	120.55
1	A	262	PHE	N-CA-C	5.96	118.51	109.63
1	A	87	LYS	CA-CB-CG	5.96	126.01	114.10
1	B	335	GLU	N-CA-CB	-5.96	101.36	110.12
1	B	349	ILE	CA-CB-CG2	5.95	120.62	110.50
1	B	1	ALA	N-CA-CB	5.94	119.31	110.40
1	A	167	GLN	OE1-CD-NE2	-5.93	116.67	122.60
1	B	264	ASN	N-CA-C	5.93	122.91	109.81
1	B	253	PHE	O-C-N	5.92	130.13	122.43
1	A	86	GLN	O-C-N	5.91	128.38	122.12
1	B	125	LYS	CG-CD-CE	5.90	124.87	111.30
1	B	8	ARG	NH1-CZ-NH2	-5.90	111.63	119.30
1	B	3	SER	CA-C-O	-5.90	112.75	119.41
1	B	14	ARG	NH1-CZ-NH2	5.89	126.95	119.30
1	A	164	LEU	CA-C-N	5.88	128.63	120.63
1	A	164	LEU	C-N-CA	5.88	128.63	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	SER	O-C-N	5.88	125.35	121.23
1	A	102	LYS	CA-C-O	5.88	128.10	120.81
1	A	82	ASP	CB-CG-OD1	5.88	131.91	118.40
1	A	274	THR	CA-C-O	-5.88	115.18	121.94
1	B	391	ARG	NE-CZ-NH1	5.88	127.38	121.50
1	A	368	GLY	N-CA-C	-5.87	103.62	112.89
1	B	263	LYS	CA-C-N	5.86	136.10	121.80
1	B	263	LYS	C-N-CA	5.86	136.10	121.80
1	B	357	LYS	CA-C-N	5.86	128.05	120.44
1	B	357	LYS	C-N-CA	5.86	128.05	120.44
1	A	217	ASN	CA-C-N	5.85	133.02	122.43
1	A	217	ASN	C-N-CA	5.85	133.02	122.43
1	A	288	ARG	N-CA-C	5.84	118.88	111.69
1	B	310	PHE	CA-CB-CG	-5.84	107.96	113.80
1	A	39	SER	CB-CA-C	-5.83	103.04	111.91
1	B	124	GLU	CA-C-O	5.83	126.68	120.10
1	A	31	ARG	CB-CG-CD	5.82	124.69	111.30
1	A	288	ARG	NE-CZ-NH1	-5.82	115.68	121.50
1	A	296	ASP	O-C-N	5.80	127.99	121.32
1	A	263	LYS	CA-C-O	5.80	128.80	120.51
1	A	212	GLY	CA-C-N	-5.79	115.31	121.45
1	A	212	GLY	C-N-CA	-5.79	115.31	121.45
1	A	298	PHE	CA-CB-CG	-5.79	108.00	113.80
1	B	164	LEU	CB-CA-C	5.79	118.93	109.90
1	B	55	LYS	CB-CA-C	-5.77	100.91	110.14
1	B	167	GLN	CA-CB-CG	-5.77	102.56	114.10
1	B	284	SER	N-CA-CB	5.77	118.37	110.01
1	B	201	TYR	CA-C-O	-5.75	112.53	119.03
1	A	232	ILE	O-C-N	5.75	127.55	121.91
1	A	410	ASN	CA-CB-CG	5.74	118.34	112.60
1	B	154	LEU	N-CA-CB	-5.74	100.74	111.13
1	B	184	ARG	NE-CZ-NH2	5.73	124.36	119.20
1	B	215	ALA	N-CA-CB	-5.73	103.95	111.23
1	B	42	VAL	O-C-N	5.72	127.64	121.87
1	B	9	SER	CB-CA-C	5.71	119.44	110.19
1	A	22	GLU	CB-CG-CD	5.70	122.29	112.60
1	A	63	HIS	N-CA-CB	5.69	118.56	110.13
1	A	146	LEU	N-CA-C	-5.69	102.48	109.65
1	A	190	TYR	CB-CG-CD2	5.69	129.33	120.80
1	B	381	THR	CA-C-O	5.68	126.65	119.95
1	B	222	GLU	CG-CD-OE1	5.68	131.46	118.40
1	A	313	ALA	CA-C-N	5.68	130.65	120.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	ALA	C-N-CA	5.68	130.65	120.77
1	A	90	ASP	CA-CB-CG	5.67	118.27	112.60
1	B	200	ARG	NE-CZ-NH1	-5.67	115.83	121.50
1	B	166	LEU	CB-CA-C	5.66	119.10	109.53
1	B	32	SER	CB-CA-C	-5.66	98.14	109.35
1	B	72	ILE	CA-C-O	-5.66	114.61	121.18
1	B	425	PHE	CA-CB-CG	-5.66	108.14	113.80
1	B	19	VAL	CA-C-O	5.63	127.07	120.71
1	B	198	LYS	N-CA-CB	5.63	118.49	110.16
1	A	300	GLU	CB-CA-C	-5.61	99.25	110.42
1	A	250	SER	O-C-N	5.60	128.05	122.12
1	A	424	VAL	N-CA-CB	-5.60	102.27	111.45
1	B	160	ALA	O-C-N	5.60	130.04	122.59
1	B	43	HIS	CA-CB-CG	-5.59	108.21	113.80
1	B	404	GLU	N-CA-C	-5.59	106.41	113.18
1	A	338	ALA	N-CA-C	5.59	120.23	112.90
1	A	31	ARG	CB-CA-C	5.58	120.03	109.37
1	B	382	PHE	O-C-N	5.58	128.52	122.11
1	A	53	LYS	CA-C-O	-5.57	114.64	120.55
1	A	363	PHE	CA-CB-CG	5.57	119.37	113.80
1	B	228	ILE	O-C-N	5.55	127.67	121.90
1	A	77	VAL	CA-C-O	-5.55	114.47	120.47
1	B	295	GLU	O-C-N	-5.55	116.72	123.10
1	A	287	LYS	CA-C-N	5.54	130.05	120.58
1	A	287	LYS	C-N-CA	5.54	130.05	120.58
1	A	181	GLU	CG-CD-OE1	5.53	131.12	118.40
1	B	159	HIS	N-CA-CB	5.53	118.04	110.57
1	B	208	VAL	CA-C-O	-5.52	115.46	121.92
1	A	241	VAL	N-CA-C	5.52	116.07	108.12
1	B	430	PHE	O-C-N	5.52	128.67	122.22
1	A	91	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	329	ARG	NE-CZ-NH2	5.51	124.16	119.20
1	A	20	GLU	CA-CB-CG	5.50	125.09	114.10
1	A	115	LEU	O-C-N	5.49	127.94	122.12
1	A	390	LEU	CA-C-N	5.48	129.91	122.07
1	A	390	LEU	C-N-CA	5.48	129.91	122.07
1	B	66	LYS	CA-C-O	5.48	126.28	119.97
1	A	264	ASN	CA-CB-CG	-5.48	107.12	112.60
1	B	185	ILE	CB-CG1-CD1	-5.47	102.31	113.80
1	A	18	THR	CA-CB-CG2	5.47	119.80	110.50
1	B	49	ARG	NH1-CZ-NH2	5.47	126.41	119.30
1	A	54	SER	CB-CA-C	5.46	121.29	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	GLY	O-C-N	5.46	129.79	122.70
1	B	138	LYS	CB-CA-C	5.44	119.03	111.63
1	B	316	GLN	CA-C-N	-5.43	115.26	122.98
1	B	316	GLN	C-N-CA	-5.43	115.26	122.98
1	B	40	THR	CA-C-O	5.43	128.27	120.51
1	B	80	ASN	CB-CA-C	5.43	122.29	112.30
1	B	311	LYS	N-CA-CB	5.43	118.63	109.78
1	B	408	LYS	CA-C-N	5.43	128.00	120.29
1	B	408	LYS	C-N-CA	5.43	128.00	120.29
1	B	84	LYS	N-CA-C	-5.42	105.93	112.54
1	B	380	ASP	CA-C-O	-5.41	115.24	121.19
1	A	16	ASN	CA-C-O	-5.39	115.08	120.96
1	A	82	ASP	CA-C-O	-5.39	114.50	120.60
1	B	230	ASP	CA-C-O	5.39	126.17	119.97
1	A	421	ASP	CA-C-O	-5.39	112.21	119.11
1	B	108	ASN	N-CA-CB	5.38	118.62	110.28
1	B	132	HIS	CA-C-O	5.38	126.12	120.42
1	B	90	ASP	CA-C-O	-5.38	114.72	120.42
1	A	255	ASP	CA-CB-CG	-5.36	107.24	112.60
1	A	404	GLU	N-CA-CB	5.35	119.40	110.41
1	A	270	SER	N-CA-CB	5.34	118.64	110.95
1	A	12	ASP	N-CA-C	-5.34	101.59	109.86
1	A	164	LEU	N-CA-C	5.33	118.30	110.30
1	A	340	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	200	ARG	N-CA-C	5.33	118.94	112.23
1	A	392	THR	CA-CB-CG2	5.32	119.55	110.50
1	B	255	ASP	CA-CB-CG	-5.32	107.28	112.60
1	B	80	ASN	N-CA-CB	-5.31	102.10	111.40
1	A	120	ALA	CA-C-N	5.31	127.83	120.29
1	A	120	ALA	C-N-CA	5.31	127.83	120.29
1	B	68	VAL	CA-C-N	5.31	127.34	120.44
1	B	68	VAL	C-N-CA	5.31	127.34	120.44
1	B	40	THR	OG1-CB-CG2	5.30	119.89	109.30
1	A	195	SER	CB-CA-C	5.29	119.19	110.88
1	B	42	VAL	CB-CA-C	-5.29	103.95	112.16
1	A	291	ILE	CA-C-O	-5.29	114.73	120.71
1	A	311	LYS	N-CA-CB	5.29	118.36	110.22
1	A	147	PRO	CB-CA-C	-5.27	101.94	110.21
1	A	235	ALA	O-C-N	5.26	130.12	122.43
1	A	110	ILE	CA-C-O	-5.26	115.08	121.18
1	A	202	GLY	CA-C-N	5.26	127.58	120.38
1	A	202	GLY	C-N-CA	5.26	127.58	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	GLU	CG-CD-OE1	5.25	130.48	118.40
1	A	49	ARG	CA-C-N	5.24	127.30	120.28
1	A	49	ARG	C-N-CA	5.24	127.30	120.28
1	A	96	LEU	CA-CB-CG	5.24	134.63	116.30
1	A	43	HIS	CA-CB-CG	-5.23	108.57	113.80
1	A	348	GLN	OE1-CD-NE2	-5.23	117.37	122.60
1	A	181	GLU	CA-CB-CG	5.23	124.56	114.10
1	B	40	THR	N-CA-C	5.23	121.94	110.80
1	A	277	GLN	O-C-N	5.23	127.45	122.07
1	B	76	PHE	CB-CA-C	5.22	119.08	110.88
1	B	239	GLY	CA-C-O	-5.22	113.21	119.06
1	B	364	ALA	CA-C-N	5.22	131.52	121.18
1	B	364	ALA	C-N-CA	5.22	131.52	121.18
1	B	408	LYS	CA-C-O	5.21	126.29	120.82
1	A	12	ASP	CA-C-N	-5.21	111.53	121.94
1	A	12	ASP	C-N-CA	-5.21	111.53	121.94
1	A	63	HIS	CA-C-O	-5.20	114.99	120.55
1	A	410	ASN	N-CA-C	-5.19	105.70	111.36
1	A	300	GLU	OE1-CD-OE2	5.19	135.36	122.90
1	B	318	VAL	N-CA-C	5.19	115.78	108.36
1	A	192	ASN	N-CA-C	-5.18	105.54	111.14
1	A	306	TRP	CA-CB-CG	5.18	123.44	113.60
1	B	405	ARG	NH1-CZ-NH2	5.18	126.03	119.30
1	B	95	SER	N-CA-CB	5.18	117.82	110.16
1	A	265	PRO	CA-N-CD	-5.17	104.76	112.00
1	B	358	ALA	O-C-N	5.17	127.40	122.07
1	A	238	ASP	CB-CA-C	5.17	117.96	109.90
1	A	70	ASP	CA-CB-CG	-5.17	107.44	112.60
1	A	216	PRO	CA-C-O	-5.17	115.57	121.56
1	B	356	ILE	CA-C-O	-5.17	115.32	121.05
1	A	229	VAL	CA-C-O	-5.16	115.05	120.57
1	A	294	ILE	CA-C-O	-5.16	114.89	120.36
1	B	343	LEU	N-CA-C	-5.13	100.94	109.46
1	A	21	VAL	CA-CB-CG2	5.13	119.12	110.40
1	A	374	ARG	N-CA-CB	5.12	118.73	110.85
1	A	23	LEU	CB-CA-C	5.12	119.07	109.71
1	B	303	TRP	CA-CB-CG	5.12	123.32	113.60
1	A	347	ASN	N-CA-C	-5.11	107.10	113.38
1	B	133	LEU	CB-CA-C	5.10	120.07	110.63
1	A	299	ALA	CA-C-N	5.09	131.26	121.54
1	A	299	ALA	C-N-CA	5.09	131.26	121.54
1	A	40	THR	CA-C-O	5.09	126.29	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	210	ASP	CA-C-N	-5.08	115.00	122.83
1	B	210	ASP	C-N-CA	-5.08	115.00	122.83
1	A	159	HIS	CB-CG-CD2	-5.07	124.61	131.20
1	B	94	ILE	CA-C-N	5.06	127.48	120.29
1	B	94	ILE	C-N-CA	5.06	127.48	120.29
1	B	55	LYS	CA-CB-CG	-5.06	103.98	114.10
1	B	44	GLU	CG-CD-OE2	-5.05	106.78	118.40
1	A	110	ILE	CA-CB-CG1	5.05	118.99	110.40
1	A	294	ILE	O-C-N	5.05	128.66	123.20
1	B	237	HIS	CA-CB-CG	-5.05	108.75	113.80
1	A	105	LEU	CB-CA-C	5.05	118.08	109.24
1	A	235	ALA	CA-C-O	-5.04	112.65	119.11
1	B	49	ARG	NE-CZ-NH2	-5.04	114.66	119.20
1	B	76	PHE	N-CA-C	-5.03	105.69	111.07
1	A	410	ASN	O-C-N	5.03	127.88	122.15
1	A	184	ARG	N-CA-CB	5.02	117.29	110.01
1	A	73	ALA	O-C-N	5.02	127.09	121.32
1	A	90	ASP	O-C-N	5.01	128.74	122.23
1	B	192	ASN	CA-C-O	-5.01	115.56	121.07
1	A	10	VAL	N-CA-C	-5.01	102.71	108.82
1	A	14	ARG	CA-CB-CG	-5.01	104.08	114.10
1	A	74	PRO	CA-C-N	5.01	126.99	120.28
1	A	74	PRO	C-N-CA	5.01	126.99	120.28
1	A	395	ILE	CA-C-O	5.00	126.58	121.28
1	A	254	LYS	CB-CA-C	-5.00	104.13	111.23
1	B	223	GLU	CA-C-N	5.00	126.94	120.44
1	B	223	GLU	C-N-CA	5.00	126.94	120.44
1	B	391	ARG	N-CA-CB	-5.00	104.31	111.91

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	LEU	Mainchain
1	A	119	ARG	Sidechain
1	A	14	ARG	Mainchain
1	A	144	TYR	Mainchain
1	A	152	ASN	Mainchain
1	A	167	GLN	Sidechain
1	A	201	TYR	Mainchain
1	A	23	LEU	Mainchain
1	A	249	SER	Mainchain

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Mol	Chain	Res	Type	Group
1	A	264	ASN	Peptide,Mainchain
1	A	267	SER	Peptide
1	A	268	ASP	Mainchain
1	A	338	ALA	Mainchain
1	A	346	VAL	Mainchain
1	A	35	PRO	Mainchain
1	A	405	ARG	Sidechain
1	B	11	TYR	Sidechain
1	B	119	ARG	Sidechain
1	B	178	THR	Mainchain
1	B	200	ARG	Mainchain
1	B	39	SER	Mainchain
1	B	395	ILE	Mainchain
1	B	399	ALA	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	3292	0	3300	227	0
1	B	3292	0	3301	255	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
4	A	11	0	4	2	0
5	B	10	0	2	3	0
6	A	197	0	0	42	1
6	B	159	0	0	36	0
All	All	6964	0	6607	476	1

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 36.

All (476) 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:A:274:THR:H	1:A:277:GLN:NE2	1.28	1.32
1:B:257:LYS:HB3	1:B:273:LEU:O	1.26	1.28
1:A:261:ASP:OD2	1:A:271:LYS:HB3	1.38	1.21
1:A:54:SER:C	6:A:621:HOH:O	1.80	1.20
1:A:122:ALA:HB2	6:A:811:HOH:O	1.37	1.18
1:B:415:ILE:HG22	6:B:881:HOH:O	1.43	1.15
1:A:48:MET:HE2	6:A:798:HOH:O	1.48	1.13
1:B:74:PRO:O	1:B:78:LYS:HD3	1.48	1.12
1:A:432:HIS:HD2	6:A:726:HOH:O	1.33	1.08
1:A:238:ASP:HB2	6:A:614:HOH:O	1.53	1.08
1:A:114:SER:HB2	6:A:865:HOH:O	1.54	1.07
1:A:432:HIS:CD2	6:A:726:HOH:O	2.07	1.06
1:A:252:PHE:CE2	6:A:866:HOH:O	2.08	1.05
1:B:257:LYS:HD2	1:B:272:TRP:O	1.55	1.05
1:B:235:ALA:HB2	6:B:777:HOH:O	1.57	1.04
1:A:274:THR:N	1:A:277:GLN:HE21	1.54	1.04
1:B:406:LEU:HD23	6:B:793:HOH:O	0.86	1.02
1:A:122:ALA:CB	6:A:811:HOH:O	1.96	1.02
1:A:255:ASP:HB3	1:A:257:LYS:NZ	1.76	1.01
1:B:415:ILE:CG2	6:B:881:HOH:O	1.99	1.00
1:A:274:THR:N	1:A:277:GLN:NE2	2.10	0.99
1:A:274:THR:HG23	1:A:277:GLN:NE2	1.76	0.99
1:A:268:ASP:O	1:A:270:SER:N	1.97	0.98
1:A:261:ASP:OD2	1:A:271:LYS:CB	2.10	0.97
1:A:264:ASN:C	1:A:264:ASN:OD1	2.07	0.97
1:A:110:ILE:O	6:A:865:HOH:O	1.82	0.95
1:B:219:GLN:HG2	6:B:870:HOH:O	1.66	0.95
1:B:14:ARG:HH22	1:B:38:ALA:HB2	1.32	0.95
1:A:132:HIS:CB	6:A:811:HOH:O	2.15	0.94
1:A:337:LYS:HA	1:A:337:LYS:HE3	1.47	0.93
1:A:39:SER:HB3	6:A:604:HOH:O	1.69	0.92
1:A:195:SER:O	1:A:199:LYS:HE2	1.69	0.92
1:A:255:ASP:HB3	1:A:257:LYS:HZ2	1.32	0.91
1:B:192:ASN:ND2	6:B:777:HOH:O	2.03	0.91
1:B:419:LEU:HD11	6:B:881:HOH:O	1.72	0.90
1:A:132:HIS:HB3	6:A:811:HOH:O	1.71	0.88
1:B:87:LYS:HG2	1:B:88:ALA:N	1.87	0.87
1:B:252:PHE:HB2	1:B:259:ASP:O	1.73	0.87
1:B:192:ASN:CG	6:B:777:HOH:O	2.15	0.87
1:A:198:LYS:HG2	1:A:203:ALA:HA	1.53	0.87
1:A:257:LYS:N	1:A:257:LYS:HD2	1.91	0.85
1:B:251:GLU:HG2	6:B:597:HOH:O	1.74	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ASN:OD1	1:B:264:ASN:C	2.14	0.85
1:A:252:PHE:CD2	6:A:866:HOH:O	2.26	0.85
1:B:254:LYS:HE2	1:B:272:TRP:CH2	2.12	0.85
1:B:288:ARG:NH2	6:B:673:HOH:O	2.09	0.84
1:A:233:LYS:HG3	1:A:238:ASP:OD1	1.77	0.84
1:B:14:ARG:NH2	1:B:38:ALA:HB2	1.92	0.84
1:A:46:LEU:HD22	1:A:103:SER:HA	1.60	0.84
1:B:101:ASN:H	1:B:101:ASN:HD22	1.26	0.83
1:B:419:LEU:CD1	6:B:881:HOH:O	2.23	0.83
1:A:261:ASP:HB3	1:A:271:LYS:HB2	1.61	0.83
1:B:274:THR:N	1:B:277:GLN:OE1	2.13	0.82
1:A:131:LYS:NZ	1:A:141:THR:HG21	1.94	0.82
1:A:432:HIS:HA	6:A:701:HOH:O	1.77	0.82
1:A:20:GLU:CD	1:A:31:ARG:HD3	2.05	0.81
1:A:55:LYS:N	6:A:621:HOH:O	2.02	0.81
1:A:196:LEU:O	1:A:200:ARG:HG3	1.80	0.81
1:B:168:GLU:HG2	6:B:644:HOH:O	1.79	0.81
1:A:432:HIS:HB3	1:A:435:LYS:HG3	1.62	0.80
1:B:254:LYS:HD3	1:B:259:ASP:OD2	1.80	0.80
1:B:40:THR:CG2	6:B:792:HOH:O	2.31	0.79
1:B:286:MET:CE	1:B:309:PHE:HZ	1.95	0.79
1:B:235:ALA:CB	6:B:777:HOH:O	2.22	0.79
1:B:42:VAL:HA	6:B:823:HOH:O	1.81	0.79
1:B:254:LYS:HB3	1:B:272:TRP:CZ3	2.18	0.79
1:B:101:ASN:HD22	1:B:101:ASN:N	1.79	0.78
1:A:262:PHE:CD2	6:A:648:HOH:O	2.38	0.77
1:B:261:ASP:OD1	1:B:264:ASN:HA	1.85	0.77
1:B:274:THR:O	1:B:277:GLN:HG3	1.85	0.76
1:A:373:HIS:HD2	1:A:405:ARG:HH11	1.33	0.76
1:A:262:PHE:HD2	6:A:648:HOH:O	1.67	0.76
1:A:101:ASN:C	1:A:101:ASN:HD22	1.94	0.75
1:B:391:ARG:NH2	1:B:436:LEU:O	2.17	0.75
1:A:255:ASP:C	1:A:257:LYS:H	1.93	0.75
1:A:188:GLU:OE1	1:A:237:HIS:NE2	2.14	0.75
1:A:274:THR:HG23	1:A:277:GLN:CD	2.10	0.75
1:B:254:LYS:N	1:B:257:LYS:O	2.20	0.75
1:B:273:LEU:HA	1:B:277:GLN:OE1	1.88	0.74
1:A:131:LYS:HZ2	1:A:141:THR:HG21	1.52	0.74
1:A:274:THR:H	1:A:277:GLN:HE21	0.74	0.74
1:A:198:LYS:HD2	1:A:206:GLY:HA3	1.70	0.74
1:B:40:THR:HG23	6:B:792:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:GLU:OE2	1:B:31:ARG:NH2	2.19	0.74
1:B:257:LYS:HB3	1:B:273:LEU:C	2.11	0.74
1:A:131:LYS:HG2	1:A:144:TYR:OH	1.88	0.73
1:B:257:LYS:CD	1:B:272:TRP:O	2.36	0.73
1:A:391:ARG:HH22	1:A:436:LEU:C	1.95	0.73
1:B:252:PHE:O	1:B:259:ASP:N	2.22	0.73
1:A:256:GLY:N	1:A:257:LYS:HD2	2.04	0.72
1:B:219:GLN:HG2	6:B:734:HOH:O	1.88	0.72
1:B:257:LYS:HD2	1:B:272:TRP:C	2.13	0.72
1:B:159:HIS:O	1:B:160:ALA:HB2	1.89	0.72
1:B:159:HIS:O	1:B:160:ALA:CB	2.38	0.72
1:A:101:ASN:H	1:A:101:ASN:ND2	1.86	0.72
1:B:315:ILE:O	1:B:317:ILE:HD12	1.91	0.71
1:A:130:TYR:OH	1:A:418:GLU:OE1	2.05	0.71
1:A:268:ASP:C	1:A:270:SER:H	1.98	0.70
1:A:271:LYS:HG3	1:A:271:LYS:O	1.91	0.70
1:B:235:ALA:CA	6:B:777:HOH:O	2.38	0.70
1:A:132:HIS:HB2	6:A:811:HOH:O	1.87	0.70
1:B:313:ALA:HB1	1:B:317:ILE:HD11	1.73	0.70
1:B:152:ASN:HD21	1:B:155:ASN:HD21	1.39	0.70
1:A:372:SER:HB2	1:A:396:LYS:HG2	1.74	0.70
1:B:264:ASN:ND2	1:B:267:SER:HA	2.07	0.69
1:A:43:HIS:ND1	1:A:329:ARG:NH1	2.41	0.69
1:A:233:LYS:CG	1:A:238:ASP:OD1	2.40	0.69
1:A:131:LYS:O	1:A:131:LYS:HD3	1.93	0.69
1:B:269:LYS:NZ	1:B:270:SER:OG	2.25	0.69
1:A:264:ASN:HD21	1:A:267:SER:HB2	1.58	0.69
1:B:42:VAL:O	6:B:823:HOH:O	2.09	0.69
1:A:403:SER:HB2	1:B:404:GLU:HB3	1.74	0.69
1:B:434:ASP:OD2	1:B:435:LYS:HD2	1.94	0.68
1:A:43:HIS:CE1	1:A:329:ARG:NH1	2.62	0.67
1:B:286:MET:HE1	1:B:309:PHE:CZ	2.28	0.67
1:A:194:LYS:HE3	6:A:859:HOH:O	1.95	0.67
1:B:40:THR:CG2	1:B:41:GLY:N	2.58	0.67
1:B:286:MET:CE	1:B:309:PHE:CZ	2.77	0.67
1:A:264:ASN:HD21	1:A:267:SER:CB	2.07	0.67
1:B:316:GLN:OE1	1:B:431:HIS:HD2	1.78	0.66
1:B:42:VAL:CA	6:B:823:HOH:O	2.41	0.66
1:B:264:ASN:HD22	1:B:267:SER:HA	1.61	0.66
1:A:357:LYS:HE2	1:A:361:ASP:OD1	1.95	0.66
1:B:41:GLY:O	6:B:792:HOH:O	2.12	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ASP:OD2	1:A:262:PHE:HB3	1.96	0.66
1:A:146:LEU:HD23	1:A:423:ALA:HB1	1.76	0.66
1:B:265:PRO:HD2	1:B:266:ASN:H	1.61	0.66
1:B:265:PRO:CD	1:B:266:ASN:H	2.06	0.66
1:B:74:PRO:HA	1:B:78:LYS:HZ3	1.61	0.65
1:A:59:LYS:HG2	6:A:575:HOH:O	1.97	0.65
1:A:264:ASN:C	1:A:266:ASN:H	2.03	0.65
1:B:257:LYS:HD3	1:B:274:THR:HG23	1.77	0.65
1:A:296:ASP:HA	1:A:306:TRP:CH2	2.32	0.65
1:B:264:ASN:HB3	1:B:265:PRO:CA	2.28	0.64
1:B:248:ALA:O	1:B:251:GLU:HB2	1.98	0.64
1:A:74:PRO:O	1:A:78:LYS:HG3	1.98	0.64
1:A:1:ALA:HB1	1:A:26:GLU:OE1	1.97	0.64
1:B:165:ALA:HB2	1:B:260:LEU:O	1.97	0.64
1:B:39:SER:O	1:B:40:THR:HB	1.98	0.64
1:B:37:GLY:HA3	1:B:374:ARG:NH2	2.13	0.64
1:B:194:LYS:O	1:B:198:LYS:HG2	1.97	0.64
1:B:274:THR:O	1:B:277:GLN:N	2.27	0.64
1:A:114:SER:CB	6:A:865:HOH:O	2.24	0.63
1:B:187:SER:O	1:B:191:HIS:ND1	2.31	0.63
1:A:66:LYS:HD2	1:A:70:ASP:OD2	1.98	0.63
1:B:275:GLY:O	1:B:277:GLN:N	2.32	0.63
1:B:264:ASN:OD1	1:B:264:ASN:O	2.16	0.63
1:B:269:LYS:C	1:B:271:LYS:H	2.07	0.63
1:B:251:GLU:OE1	1:B:251:GLU:CA	2.44	0.62
1:A:264:ASN:ND2	1:A:267:SER:CB	2.62	0.62
1:A:114:SER:N	6:A:865:HOH:O	2.20	0.62
1:A:260:LEU:HB2	1:A:271:LYS:HD3	1.82	0.62
1:B:39:SER:HB2	5:B:440:PEP:O3P	1.99	0.62
1:B:301:ASP:OD1	1:B:329:ARG:NH2	2.32	0.61
1:A:72:ILE:HA	1:A:96:LEU:HD21	1.81	0.61
1:B:74:PRO:HA	1:B:78:LYS:NZ	2.15	0.61
1:B:274:THR:OG1	1:B:277:GLN:HG3	2.00	0.61
1:B:257:LYS:CB	1:B:273:LEU:O	2.23	0.61
1:A:248:ALA:HB1	6:A:668:HOH:O	2.01	0.61
1:A:242:LYS:HD3	1:A:292:VAL:HG11	1.82	0.61
1:A:274:THR:O	1:A:277:GLN:HB2	2.01	0.61
1:B:411:GLN:O	1:B:415:ILE:HG13	2.01	0.61
1:A:225:LEU:O	1:A:229:VAL:HG13	2.00	0.60
1:A:255:ASP:C	1:A:257:LYS:N	2.60	0.60
1:A:274:THR:HG23	1:A:277:GLN:HE22	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:GLY:H	1:B:207:ASN:HD21	1.50	0.60
1:A:406:LEU:HD13	1:B:12:ASP:O	2.02	0.60
1:B:261:ASP:HA	6:B:627:HOH:O	2.01	0.60
1:A:261:ASP:H	1:A:271:LYS:HG2	1.66	0.59
1:A:373:HIS:HD2	1:A:405:ARG:NH1	2.00	0.59
1:B:373:HIS:ND1	1:B:405:ARG:NH1	2.50	0.59
1:B:53:LYS:N	1:B:53:LYS:HD2	2.17	0.59
1:A:349:ILE:HG12	1:A:354:GLU:HB3	1.83	0.59
1:A:101:ASN:ND2	1:A:103:SER:OG	2.36	0.59
1:B:226:ASP:OD1	1:B:289:TYR:OH	2.11	0.59
1:A:403:SER:CB	1:B:404:GLU:HB3	2.33	0.59
1:B:140:LYS:HE3	1:B:434:ASP:O	2.03	0.59
1:B:202:GLY:O	1:B:205:ALA:HB3	2.02	0.59
1:A:42:VAL:HG22	1:A:300:GLU:OE2	2.03	0.59
1:B:313:ALA:CB	1:B:317:ILE:HD11	2.31	0.59
1:B:235:ALA:HA	6:B:777:HOH:O	2.03	0.59
1:B:274:THR:O	1:B:275:GLY:C	2.46	0.58
1:A:73:ALA:N	1:A:74:PRO:HD2	2.18	0.58
1:A:433:GLY:HA2	1:A:436:LEU:HD13	1.85	0.58
1:A:372:SER:HB2	1:A:396:LYS:CG	2.33	0.58
1:B:313:ALA:HB3	1:B:317:ILE:HD13	1.85	0.58
1:A:260:LEU:CD1	1:A:273:LEU:HD12	2.34	0.58
1:A:281:LEU:O	1:A:281:LEU:HD12	2.03	0.58
1:B:42:VAL:C	6:B:823:HOH:O	2.46	0.58
1:B:46:LEU:HD23	1:B:103:SER:HB3	1.86	0.58
1:B:102:LYS:HE2	1:B:351:THR:HG23	1.85	0.57
1:B:334:ILE:HD13	1:B:365:ALA:HB2	1.86	0.57
1:B:39:SER:HB2	5:B:440:PEP:P	2.44	0.57
1:B:40:THR:HG22	1:B:41:GLY:N	2.20	0.57
1:A:240:LYS:NZ	6:A:833:HOH:O	2.25	0.57
1:A:255:ASP:CB	1:A:257:LYS:NZ	2.62	0.57
1:A:101:ASN:HD22	1:A:102:LYS:N	2.01	0.57
1:B:53:LYS:N	1:B:53:LYS:CD	2.66	0.57
1:A:66:LYS:O	1:A:66:LYS:HG3	2.04	0.57
1:A:255:ASP:HB3	1:A:257:LYS:HZ3	1.68	0.57
1:A:378:THR:O	1:A:408:LYS:NZ	2.38	0.56
1:B:275:GLY:C	1:B:277:GLN:N	2.62	0.56
1:B:152:ASN:HD21	1:B:155:ASN:ND2	2.02	0.56
1:A:300:GLU:O	1:A:322:LEU:HD12	2.06	0.56
1:B:264:ASN:HD21	1:B:268:ASP:CG	2.12	0.56
1:B:313:ALA:CB	1:B:317:ILE:CD1	2.83	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LEU:CD2	1:A:103:SER:HA	2.33	0.56
1:A:432:HIS:HB3	1:A:435:LYS:CG	2.35	0.56
1:B:276:PRO:O	1:B:280:ASP:OD2	2.23	0.56
1:B:55:LYS:HB3	1:B:56:TRP:CE3	2.40	0.56
1:A:274:THR:OG1	1:A:276:PRO:HD2	2.06	0.56
1:B:53:LYS:CD	1:B:53:LYS:H	2.16	0.56
1:B:53:LYS:HE2	6:B:848:HOH:O	2.05	0.56
1:A:391:ARG:NH2	1:A:436:LEU:OXT	2.39	0.56
1:A:264:ASN:ND2	1:A:267:SER:HB3	2.21	0.56
1:A:349:ILE:HG12	1:A:354:GLU:CB	2.35	0.56
1:B:261:ASP:O	1:B:262:PHE:C	2.46	0.56
1:B:229:VAL:O	1:B:233:LYS:HG3	2.06	0.56
1:A:260:LEU:HD11	1:A:273:LEU:HD12	1.88	0.55
1:B:14:ARG:HH22	1:B:38:ALA:CB	2.11	0.55
1:B:275:GLY:C	1:B:277:GLN:H	2.13	0.55
1:B:274:THR:H	1:B:277:GLN:CD	2.11	0.55
1:B:269:LYS:HG2	1:B:270:SER:N	2.22	0.55
1:B:271:LYS:HG2	1:B:271:LYS:O	2.07	0.55
1:A:101:ASN:HD22	1:A:103:SER:H	1.54	0.55
1:A:144:TYR:CD2	1:A:419:LEU:HD22	2.41	0.55
1:A:253:PHE:CE1	1:A:255:ASP:O	2.60	0.55
1:A:1:ALA:HB3	6:A:679:HOH:O	2.07	0.55
1:A:102:LYS:NZ	1:A:354:GLU:OE1	2.29	0.55
1:B:269:LYS:HG2	1:B:270:SER:H	1.71	0.55
1:A:373:HIS:CD2	1:A:405:ARG:HH11	2.20	0.54
1:A:43:HIS:HE1	1:A:301:ASP:OD2	1.91	0.54
1:B:46:LEU:HD23	1:B:103:SER:CB	2.36	0.54
1:B:152:ASN:HB2	6:B:893:HOH:O	2.07	0.54
1:A:101:ASN:C	1:A:101:ASN:ND2	2.65	0.54
1:A:272:TRP:N	1:A:272:TRP:CD1	2.74	0.54
1:B:74:PRO:CA	1:B:78:LYS:HZ3	2.20	0.54
1:A:273:LEU:HA	1:A:277:GLN:NE2	2.23	0.54
1:B:40:THR:HA	1:B:44:GLU:OE2	2.08	0.54
1:B:273:LEU:HB3	1:B:277:GLN:HB2	1.89	0.54
1:B:286:MET:HE3	1:B:309:PHE:HZ	1.72	0.54
1:B:349:ILE:HG12	1:B:354:GLU:HB3	1.90	0.54
1:A:261:ASP:N	1:A:271:LYS:HG2	2.23	0.53
1:A:166:LEU:HD22	1:A:247:CYS:HB3	1.89	0.53
1:A:261:ASP:OD1	1:A:267:SER:O	2.27	0.53
1:B:401:ALA:O	1:B:402:ARG:HB2	2.06	0.53
1:A:249:SER:HA	1:A:252:PHE:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ASN:HB3	1:B:265:PRO:C	2.33	0.53
1:B:283:HIS:O	1:B:287:LYS:HG3	2.09	0.53
1:A:373:HIS:CD2	1:A:405:ARG:NH1	2.76	0.53
1:A:59:LYS:CD	6:A:750:HOH:O	2.55	0.53
1:A:168:GLU:OE2	4:A:441:2PG:O3	2.26	0.53
1:B:27:LYS:HD3	1:B:124:GLU:HA	1.90	0.52
1:B:269:LYS:O	1:B:271:LYS:N	2.37	0.52
1:B:304:GLU:HG3	6:B:741:HOH:O	2.10	0.52
1:B:243:ILE:HD12	1:B:290:PRO:HD2	1.91	0.52
1:A:295:GLU:OE2	1:A:343:LEU:HD22	2.10	0.52
1:A:131:LYS:HD3	1:A:131:LYS:C	2.35	0.52
1:A:131:LYS:HZ3	1:A:141:THR:HG21	1.73	0.52
1:B:219:GLN:CG	6:B:734:HOH:O	2.51	0.52
1:B:43:HIS:ND1	1:B:329:ARG:NH1	2.58	0.52
1:A:73:ALA:HB3	1:A:74:PRO:HD3	1.92	0.52
1:A:79:ALA:O	1:A:80:ASN:C	2.53	0.52
1:A:261:ASP:HB3	1:A:271:LYS:CB	2.37	0.52
1:B:267:SER:O	1:B:269:LYS:N	2.43	0.52
1:B:38:ALA:N	5:B:440:PEP:O1P	2.36	0.51
1:B:301:ASP:O	1:B:303:TRP:N	2.35	0.51
1:B:137:SER:O	1:B:138:LYS:HB2	2.09	0.51
1:B:273:LEU:CA	1:B:277:GLN:OE1	2.56	0.51
1:A:10:VAL:C	6:A:695:HOH:O	2.53	0.51
1:B:90:ASP:OD2	1:B:353:SER:OG	2.22	0.51
1:B:265:PRO:CD	1:B:266:ASN:N	2.70	0.51
1:A:391:ARG:NH2	1:A:436:LEU:C	2.65	0.51
1:A:127:VAL:HB	1:A:128:PRO:HD2	1.91	0.51
1:B:253:PHE:CD1	1:B:258:TYR:CE1	2.99	0.51
1:B:254:LYS:HE2	1:B:272:TRP:HH2	1.67	0.51
1:A:268:ASP:C	1:A:268:ASP:OD1	2.54	0.51
1:A:42:VAL:HG23	1:A:43:HIS:CE1	2.46	0.50
1:B:43:HIS:CE1	1:B:329:ARG:NH1	2.80	0.50
1:B:147:PRO:HG3	1:B:387:VAL:CG1	2.41	0.50
1:A:262:PHE:HA	1:A:264:ASN:HB3	1.92	0.50
1:B:301:ASP:C	1:B:303:TRP:H	2.20	0.50
1:A:143:PRO:O	1:A:391:ARG:NH1	2.42	0.50
1:B:251:GLU:OE1	1:B:251:GLU:N	2.44	0.50
1:B:269:LYS:CE	1:B:270:SER:OG	2.60	0.50
1:A:262:PHE:CG	1:A:263:LYS:N	2.79	0.49
1:A:337:LYS:HA	1:A:337:LYS:CE	2.21	0.49
1:B:249:SER:HB2	1:B:296:ASP:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ASP:O	1:B:406:LEU:HD13	2.11	0.49
1:B:252:PHE:O	1:B:258:TYR:HA	2.12	0.49
1:A:127:VAL:O	6:A:699:HOH:O	2.19	0.49
1:A:233:LYS:HA	6:A:614:HOH:O	2.12	0.49
1:A:277:GLN:O	1:A:280:ASP:HB3	2.12	0.49
1:A:259:ASP:CG	1:A:262:PHE:HB3	2.37	0.49
1:B:53:LYS:H	1:B:53:LYS:HZ3	1.61	0.49
1:B:131:LYS:HD2	1:B:131:LYS:C	2.38	0.49
1:B:194:LYS:NZ	1:B:194:LYS:HB3	2.28	0.49
1:A:132:HIS:O	1:A:135:ASP:HB2	2.12	0.49
1:B:152:ASN:ND2	1:B:155:ASN:HD21	2.08	0.48
1:B:406:LEU:CD2	6:B:793:HOH:O	1.75	0.48
1:A:272:TRP:CD1	1:A:272:TRP:H	2.31	0.48
1:B:253:PHE:HA	1:B:257:LYS:O	2.13	0.48
1:A:17:PRO:HG3	1:A:56:TRP:CD1	2.49	0.48
1:A:253:PHE:CZ	1:A:255:ASP:O	2.66	0.48
1:A:300:GLU:HG3	1:A:321:ASP:HB3	1.95	0.48
1:B:323:THR:HB	1:B:330:ILE:CD1	2.43	0.48
1:B:39:SER:O	1:B:40:THR:CB	2.62	0.48
1:B:97:ASP:OD2	1:B:102:LYS:HA	2.13	0.48
1:B:130:TYR:CE1	1:B:419:LEU:HD21	2.49	0.48
1:B:147:PRO:HG3	1:B:387:VAL:HG11	1.95	0.48
1:B:192:ASN:O	1:B:195:SER:HB2	2.14	0.48
1:B:274:THR:O	1:B:277:GLN:CG	2.58	0.48
1:B:261:ASP:C	1:B:263:LYS:N	2.70	0.47
1:A:256:GLY:C	1:A:257:LYS:HD2	2.39	0.47
1:B:101:ASN:ND2	1:B:103:SER:OG	2.46	0.47
1:A:374:ARG:O	1:A:377:GLU:HG2	2.13	0.47
1:B:282:TYR:O	1:B:286:MET:HG3	2.14	0.47
1:A:99:THR:CB	1:A:101:ASN:HD21	2.27	0.47
1:A:257:LYS:N	1:A:257:LYS:CD	2.68	0.47
1:B:132:HIS:O	1:B:135:ASP:HB2	2.13	0.47
1:A:43:HIS:CE1	1:A:329:ARG:HH12	2.32	0.47
1:A:261:ASP:OD2	1:A:271:LYS:HB2	2.08	0.47
1:A:268:ASP:C	1:A:270:SER:N	2.54	0.47
1:A:421:ASP:OD1	1:A:421:ASP:N	2.46	0.47
1:B:52:ASP:OD1	1:B:52:ASP:C	2.54	0.47
1:B:257:LYS:HD3	1:B:274:THR:CG2	2.44	0.47
1:B:264:ASN:HB3	1:B:265:PRO:HA	1.97	0.47
1:A:258:TYR:HB2	1:A:273:LEU:O	2.15	0.47
1:A:82:ASP:OD1	1:A:84:LYS:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:LEU:HD12	1:B:47:GLU:O	2.14	0.47
1:B:74:PRO:CA	1:B:78:LYS:NZ	2.78	0.46
1:B:196:LEU:O	1:B:200:ARG:HG3	2.15	0.46
1:A:101:ASN:ND2	1:A:103:SER:H	2.12	0.46
1:B:330:ILE:HD12	1:B:342:LEU:HD13	1.97	0.46
1:B:296:ASP:N	1:B:297:PRO:CD	2.78	0.46
1:A:42:VAL:N	1:A:300:GLU:OE2	2.44	0.46
1:A:99:THR:HB	1:A:101:ASN:HD21	1.81	0.46
1:A:261:ASP:CB	1:A:271:LYS:HB2	2.37	0.46
1:A:274:THR:CG2	1:A:277:GLN:NE2	2.65	0.46
1:B:7:ALA:HB2	1:B:68:VAL:HG11	1.97	0.46
1:B:269:LYS:CG	1:B:270:SER:N	2.78	0.46
1:B:269:LYS:HZ3	1:B:270:SER:HG	1.55	0.46
1:B:304:GLU:HB2	6:B:741:HOH:O	2.16	0.46
1:B:283:HIS:CE1	1:B:309:PHE:CE1	3.04	0.46
1:B:303:TRP:CH2	1:B:332:THR:HB	2.50	0.46
1:A:271:LYS:O	1:A:271:LYS:CG	2.61	0.46
1:A:10:VAL:O	1:A:18:THR:N	2.39	0.46
1:A:42:VAL:CG2	1:A:43:HIS:CE1	2.99	0.46
1:B:185:ILE:HD13	1:B:185:ILE:HG21	1.56	0.46
1:A:138:LYS:HB2	1:A:138:LYS:HE3	1.26	0.45
1:A:2:VAL:HA	1:A:25:THR:HG22	1.99	0.45
1:A:44:GLU:HG2	1:A:348:GLN:HG2	1.98	0.45
1:A:406:LEU:HD22	1:B:11:TYR:HB2	1.98	0.45
1:B:326:ASN:C	1:B:328:LYS:H	2.23	0.45
1:B:57:MET:CE	1:B:59:LYS:NZ	2.80	0.45
1:B:252:PHE:CB	1:B:259:ASP:O	2.54	0.45
1:B:316:GLN:OE1	1:B:431:HIS:CD2	2.63	0.45
1:A:252:PHE:HE2	6:A:866:HOH:O	1.73	0.45
1:B:21:VAL:O	1:B:31:ARG:HA	2.17	0.45
1:A:177:LYS:HG2	6:A:833:HOH:O	2.16	0.45
1:A:55:LYS:HE2	6:A:787:HOH:O	2.16	0.45
1:B:264:ASN:CG	1:B:266:ASN:C	2.84	0.45
1:B:233:LYS:O	1:B:234:ALA:C	2.60	0.45
1:A:262:PHE:CE2	6:A:616:HOH:O	2.67	0.45
1:A:297:PRO:HD2	1:A:306:TRP:CH2	2.51	0.45
1:B:73:ALA:HB3	1:B:74:PRO:HD3	1.97	0.45
1:B:44:GLU:OE1	6:B:577:HOH:O	2.21	0.44
1:B:323:THR:HA	1:B:329:ARG:HB2	1.99	0.44
1:A:296:ASP:HA	1:A:306:TRP:HH2	1.81	0.44
1:B:361:ASP:O	1:B:364:ALA:HB3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:ALA:N	1:B:26:GLU:OE1	2.47	0.44
1:B:44:GLU:CD	1:B:348:GLN:HG2	2.42	0.44
1:B:281:LEU:O	1:B:282:TYR:C	2.59	0.44
1:A:303:TRP:CE3	1:A:336:LYS:HD2	2.52	0.44
1:A:326:ASN:OD1	1:A:326:ASN:C	2.60	0.44
1:A:431:HIS:CD2	1:A:432:HIS:CE1	3.06	0.44
1:A:55:LYS:CE	6:A:787:HOH:O	2.65	0.44
1:B:101:ASN:N	1:B:101:ASN:ND2	2.52	0.44
1:B:419:LEU:HD12	6:B:881:HOH:O	2.06	0.44
1:A:59:LYS:HD3	6:A:858:HOH:O	2.17	0.44
1:B:246:ASP:HA	1:B:295:GLU:HB3	1.99	0.44
1:B:248:ALA:HA	6:B:615:HOH:O	2.17	0.44
1:B:254:LYS:O	1:B:256:GLY:N	2.50	0.44
1:B:261:ASP:OD1	1:B:264:ASN:N	2.51	0.44
1:B:269:LYS:C	1:B:271:LYS:N	2.74	0.44
1:B:125:LYS:NZ	1:B:125:LYS:HB3	2.32	0.44
1:B:296:ASP:OD2	1:B:320:ASP:HB3	2.17	0.44
1:A:349:ILE:CG2	1:A:355:SER:OG	2.66	0.43
1:B:211:GLU:HG2	6:B:772:HOH:O	2.17	0.43
1:B:274:THR:OG1	1:B:277:GLN:CG	2.65	0.43
1:A:262:PHE:C	6:A:803:HOH:O	2.61	0.43
1:A:152:ASN:CG	1:A:155:ASN:ND2	2.76	0.43
1:A:262:PHE:O	1:A:263:LYS:HB2	2.18	0.43
1:B:264:ASN:CB	1:B:265:PRO:CA	2.97	0.43
1:A:275:GLY:N	1:A:276:PRO:HD2	2.34	0.43
1:A:179:PHE:O	1:A:180:ALA:C	2.60	0.43
1:A:334:ILE:HG12	1:A:365:ALA:HB1	2.00	0.43
1:B:131:LYS:HD2	1:B:131:LYS:O	2.19	0.43
1:B:269:LYS:HD3	1:B:270:SER:HB2	2.00	0.43
1:B:326:ASN:C	1:B:326:ASN:OD1	2.61	0.43
1:B:287:LYS:HB3	1:B:287:LYS:HE3	1.83	0.43
1:B:313:ALA:HB1	1:B:317:ILE:CD1	2.46	0.43
1:A:152:ASN:ND2	1:A:155:ASN:ND2	2.67	0.42
1:A:255:ASP:O	1:A:257:LYS:N	2.52	0.42
1:B:345:LYS:O	1:B:348:GLN:HB2	2.18	0.42
1:A:372:SER:OG	1:A:373:HIS:O	2.35	0.42
1:B:17:PRO:HG3	1:B:56:TRP:CD1	2.55	0.42
1:B:43:HIS:HB2	1:B:324:VAL:HG21	2.01	0.42
1:B:74:PRO:O	1:B:78:LYS:CD	2.41	0.42
1:A:153:VAL:HB	1:A:193:LEU:CD2	2.50	0.42
1:B:74:PRO:C	1:B:78:LYS:HZ3	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:LEU:HG	1:B:133:LEU:HD22	2.00	0.42
1:B:261:ASP:O	1:B:264:ASN:N	2.49	0.42
1:B:318:VAL:HG22	1:B:341:ALA:HB3	2.00	0.42
1:A:218:ILE:HD13	1:A:218:ILE:HG21	1.74	0.42
1:A:229:VAL:O	1:A:230:ASP:C	2.62	0.42
1:B:301:ASP:C	1:B:303:TRP:N	2.77	0.42
1:A:43:HIS:CE1	1:A:301:ASP:OD2	2.71	0.42
1:A:129:LEU:HD21	1:A:382:PHE:CE1	2.54	0.42
1:B:251:GLU:OE1	1:B:251:GLU:HA	2.18	0.42
1:B:401:ALA:O	1:B:402:ARG:CB	2.66	0.42
1:A:272:TRP:N	1:A:272:TRP:HD1	2.17	0.42
1:B:310:PHE:CD2	1:B:337:LYS:O	2.73	0.42
1:B:343:LEU:HD11	1:B:372:SER:HB2	2.01	0.42
1:A:48:MET:HE3	1:A:48:MET:HB2	1.72	0.42
1:A:84:LYS:HB2	1:A:84:LYS:HE2	1.88	0.42
1:A:211:GLU:OE2	4:A:441:2PG:O3	2.37	0.42
1:A:261:ASP:CG	1:A:271:LYS:CB	2.90	0.42
1:B:141:THR:HG22	1:B:144:TYR:CZ	2.55	0.42
1:B:261:ASP:O	1:B:263:LYS:N	2.52	0.42
1:A:21:VAL:O	1:A:31:ARG:HA	2.20	0.41
1:A:271:LYS:O	1:A:271:LYS:HE2	2.20	0.41
1:B:168:GLU:CG	6:B:644:HOH:O	2.52	0.41
1:B:326:ASN:OD1	1:B:327:PRO:N	2.53	0.41
1:A:142:SER:HA	1:A:143:PRO:HA	1.78	0.41
1:A:146:LEU:HD13	1:A:146:LEU:HA	1.84	0.41
1:A:343:LEU:CD2	1:A:345:LYS:HE3	2.50	0.41
1:B:63:HIS:CE1	6:B:856:HOH:O	2.74	0.41
1:B:79:ALA:O	1:B:80:ASN:C	2.62	0.41
1:B:261:ASP:OD1	1:B:261:ASP:O	2.37	0.41
1:B:140:LYS:HD3	1:B:391:ARG:NH2	2.34	0.41
1:B:320:ASP:CG	1:B:343:LEU:HD23	2.44	0.41
1:B:130:TYR:CE2	1:B:418:GLU:OE2	2.74	0.41
1:B:201:TYR:CD1	1:B:201:TYR:N	2.88	0.41
1:B:225:LEU:HD12	1:B:285:LEU:HD22	2.03	0.41
1:A:59:LYS:HD3	6:A:750:HOH:O	2.19	0.41
1:A:262:PHE:HB2	6:A:648:HOH:O	2.20	0.41
1:B:275:GLY:O	1:B:276:PRO:C	2.63	0.41
1:A:54:SER:HB2	6:A:621:HOH:O	2.20	0.41
1:A:288:ARG:HA	1:A:288:ARG:HD2	1.47	0.41
1:A:258:TYR:O	1:A:272:TRP:HA	2.21	0.41
1:B:27:LYS:HE2	1:B:27:LYS:HB3	1.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ASN:ND2	1:B:268:ASP:CG	2.77	0.41
1:A:42:VAL:HG23	1:A:43:HIS:CD2	2.56	0.41
1:A:97:ASP:CG	1:A:102:LYS:HA	2.46	0.41
1:A:259:ASP:OD1	1:A:259:ASP:C	2.64	0.41
1:A:352:LEU:HD12	1:A:352:LEU:HA	1.95	0.41
1:B:130:TYR:HE2	1:B:418:GLU:OE2	2.03	0.41
1:B:146:LEU:HA	1:B:147:PRO:HD3	1.96	0.41
1:B:269:LYS:HD3	1:B:270:SER:CB	2.50	0.41
1:B:274:THR:O	1:B:277:GLN:CB	2.69	0.41
1:A:164:LEU:HD21	1:A:169:PHE:CE1	2.56	0.40
1:A:255:ASP:CB	1:A:257:LYS:HZ3	2.31	0.40
1:B:142:SER:HA	1:B:143:PRO:HA	1.86	0.40
1:A:152:ASN:O	1:A:399:ALA:HB2	2.21	0.40
1:A:410:ASN:O	1:A:414:ARG:HG3	2.21	0.40
1:B:40:THR:HG23	1:B:41:GLY:N	2.36	0.40
1:B:381:THR:O	1:B:382:PHE:C	2.62	0.40
1:A:54:SER:CB	6:A:621:HOH:O	2.68	0.40
1:A:167:GLN:HB2	6:A:529:HOH:O	2.20	0.40
1:B:56:TRP:O	1:B:59:LYS:HB2	2.21	0.40
1:A:273:LEU:HD22	1:A:277:GLN:HB3	2.04	0.40
1:B:211:GLU:HG2	1:B:211:GLU:H	1.67	0.40
1:B:373:HIS:CG	1:B:397:THR:HA	2.57	0.40
1:B:225:LEU:HD23	1:B:225:LEU:HA	1.93	0.40
1:B:242:LYS:HD2	1:B:292:VAL:CG1	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ASN:ND2	6:A:520:HOH:O[1_556]	1.99	0.21

## 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	434/436 (100%)	407 (94%)	23 (5%)	4 (1%)	14	9
1	B	434/436 (100%)	394 (91%)	30 (7%)	10 (2%)	5	2
All	All	868/872 (100%)	801 (92%)	53 (6%)	14 (2%)	7	3

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	269	LYS
1	B	160	ALA
1	B	255	ASP
1	B	264	ASN
1	B	267	SER
1	B	268	ASP
1	A	268	ASP
1	B	251	GLU
1	B	275	GLY
1	A	263	LYS
1	B	276	PRO
1	A	300	GLU
1	B	302	ASP
1	B	402	ARG

### 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	344/344 (100%)	310 (90%)	34 (10%)	7	4
1	B	286/344 (83%)	258 (90%)	28 (10%)	7	5
All	All	630/688 (92%)	568 (90%)	62 (10%)	7	5

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	THR
1	A	31	ARG
1	A	39	SER
1	A	55	LYS
1	A	66	LYS
1	A	87	LYS
1	A	101	ASN
1	A	131	LYS
1	A	133	LEU
1	A	138	LYS
1	A	146	LEU
1	A	196	LEU
1	A	199	LYS
1	A	229	VAL
1	A	238	ASP
1	A	255	ASP
1	A	257	LYS
1	A	262	PHE
1	A	269	LYS
1	A	271	LYS
1	A	274	THR
1	A	288	ARG
1	A	304	GLU
1	A	315	ILE
1	A	328	LYS
1	A	337	LYS
1	A	372	SER
1	A	373	HIS
1	A	391	ARG
1	A	392	THR
1	A	421	ASP
1	A	424	VAL
1	A	434	ASP
1	A	435	LYS
1	B	4	LYS
1	B	42	VAL
1	B	53	LYS
1	B	55	LYS
1	B	125	LYS
1	B	131	LYS
1	B	133	LEU
1	B	140	LYS
1	B	193	LEU

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Mol	Chain	Res	Type
1	B	198	LYS
1	B	199	LYS
1	B	211	GLU
1	B	229	VAL
1	B	249	SER
1	B	251	GLU
1	B	267	SER
1	B	268	ASP
1	B	278	LEU
1	B	287	LYS
1	B	317	ILE
1	B	328	LYS
1	B	330	ILE
1	B	344	LEU
1	B	353	SER
1	B	375	SER
1	B	391	ARG
1	B	392	THR
1	B	403	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	101	ASN
1	A	152	ASN
1	A	155	ASN
1	A	159	HIS
1	A	207	ASN
1	A	219	GLN
1	A	264	ASN
1	A	277	GLN
1	A	373	HIS
1	A	432	HIS
1	B	155	ASN
1	B	167	GLN
1	B	207	ASN
1	B	266	ASN
1	B	283	HIS
1	B	348	GLN
1	B	431	HIS

### 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](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

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
4	2PG	A	441	2,3	9,10,10	2.47	3 (33%)	12,14,14	2.33	6 (50%)
5	PEP	B	440	2	9,9,9	2.23	3 (33%)	11,13,13	2.63	5 (45%)

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
4	2PG	A	441	2,3	-	0/11/11/11	-
5	PEP	B	440	2	-	1/9/9/9	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	441	2PG	P-O1P	5.11	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	440	PEP	O2'-C1	-4.26	1.19	1.30
5	B	440	PEP	C2-C1	4.11	1.53	1.49
4	A	441	2PG	C3-C2	3.60	1.60	1.52
4	A	441	2PG	C2-C1	-2.96	1.48	1.52
5	B	440	PEP	O1-C1	2.07	1.27	1.22

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	440	PEP	O1-C1-C2	-6.50	111.98	121.79
4	A	441	2PG	O3-C3-C2	4.81	123.96	111.73
5	B	440	PEP	O2'-C1-C2	3.51	119.89	113.91
4	A	441	2PG	O4P-P-O3P	3.12	119.50	107.80
4	A	441	2PG	P-O1P-C2	-2.98	116.21	123.04
4	A	441	2PG	O1-C1-C2	2.97	129.27	122.85
5	B	440	PEP	O3P-P-O2	-2.75	97.31	105.32
5	B	440	PEP	O3P-P-O1P	2.44	120.35	110.83
4	A	441	2PG	O3P-P-O2P	-2.44	101.32	110.83
5	B	440	PEP	O2P-P-O2	2.06	111.31	105.32
4	A	441	2PG	O2-C1-O1	-2.04	119.44	124.08

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	440	PEP	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	441	2PG	2	0
5	B	440	PEP	3	0

## 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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.