



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:44 PM UTC

PDB ID : 3PMG / pdb_00003pmg
Title : STRUCTURE OF RABBIT MUSCLE PHOSPHOGLUCOMUTASE AT 2.4
ANGSTROMS RESOLUTION. USE OF FREEZING POINT DEPRESSANT
AND REDUCED TEMPERATURE TO ENHANCE DIFFRACTIVITY
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Deposited on : 1995-03-02
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

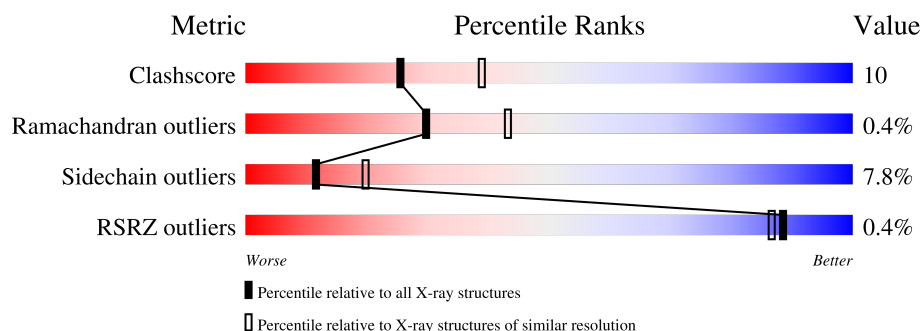
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	561	52% 35% 11% .
1	B	561	% 57% 35% 7% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12092 atoms, of which 2930 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 Phosphoglucomutase-1.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
1	A	561	Total	C	H	N	O	P	S		0	0	0
			5304	2753	971	743	820	1	16				
1	B	561	Total	C	H	N	O	P	S		0	0	0
			5304	2753	971	743	820	1	16				

- 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 water.

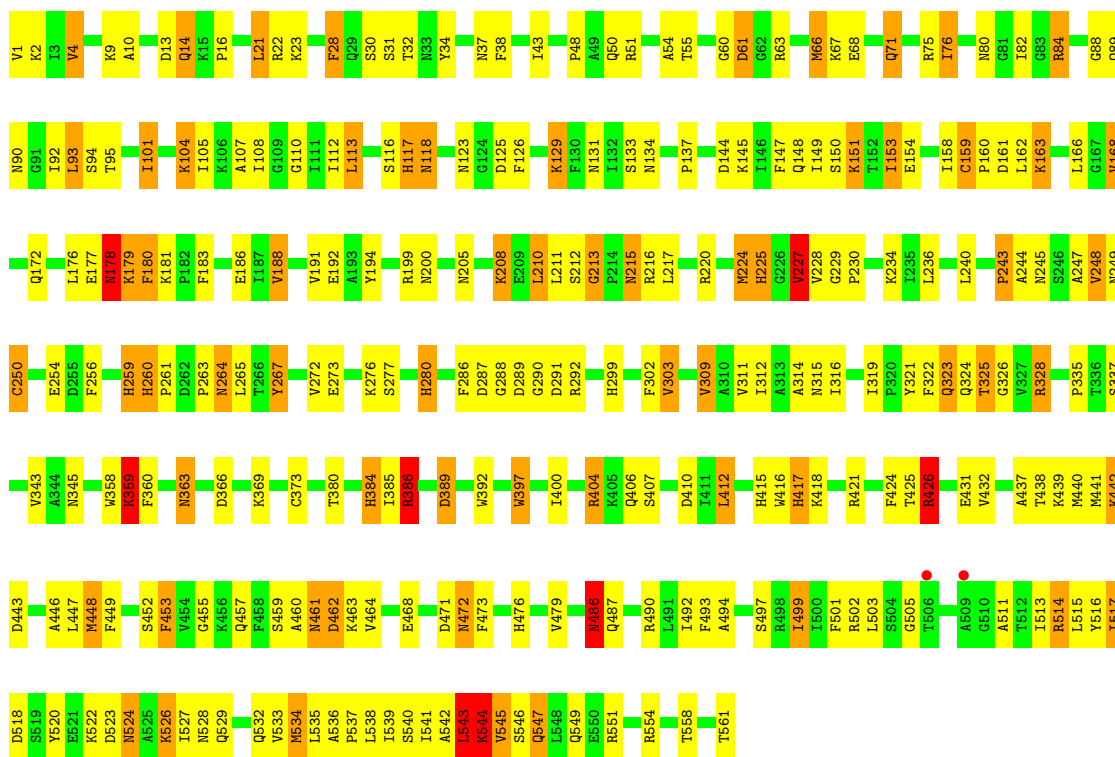
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	201	Total	H	O	0	0
			603	402	201		
3	B	293	Total	H	O	0	0
			879	586	293		

3 Residue-property plots

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

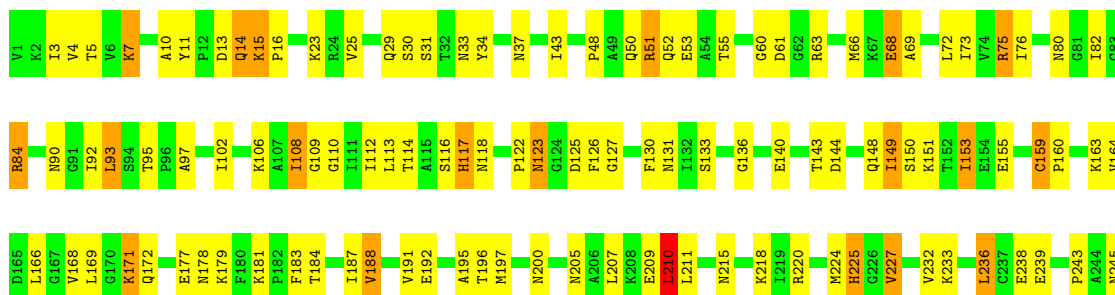
• Molecule 1: Phosphoglucumutase-1

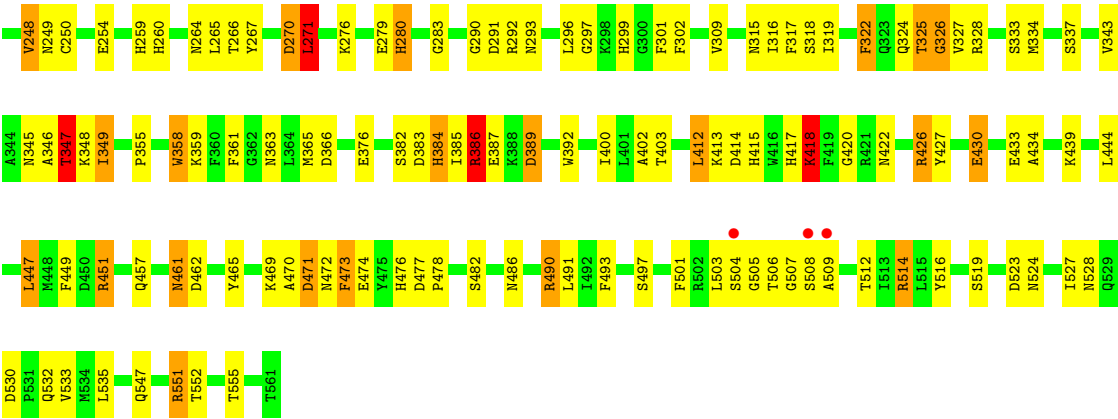
Chain A: 



• Molecule 1: Phosphoglucumutase-1

Chain B: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	174.42Å 174.42Å 101.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.40 6.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	87.0 (6.00-2.40) 81.0 (6.00-2.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.40 (at 2.28Å)	Xtriage
Refinement program	X-PLOR 3.1, HOMOLOGY, MAPMAN	Depositor
R, R_{free}	0.163 , 0.191 0.156 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 67.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12092	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.24	17/4409 (0.4%)	2.22	216/5958 (3.6%)
1	B	1.31	28/4409 (0.6%)	2.21	210/5958 (3.5%)
All	All	1.28	45/8818 (0.5%)	2.21	426/11916 (3.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	ILE	CA-CB	7.70	1.63	1.53
1	B	225	HIS	CD2-NE2	-7.03	1.30	1.37
1	B	327	VAL	CA-CB	-6.84	1.46	1.54
1	A	384	HIS	CD2-NE2	-6.71	1.30	1.37
1	B	280	HIS	CD2-NE2	-6.56	1.30	1.37
1	B	319	ILE	CA-C	6.53	1.58	1.53
1	B	243	PRO	CA-CB	-6.52	1.45	1.53
1	B	117	HIS	CD2-NE2	-6.48	1.30	1.37
1	A	260	HIS	CD2-NE2	-6.47	1.30	1.37
1	B	349	ILE	CA-CB	6.43	1.63	1.54
1	A	117	HIS	CD2-NE2	-6.25	1.30	1.37
1	B	384	HIS	CD2-NE2	-6.16	1.31	1.37
1	B	476	HIS	CD2-NE2	-6.12	1.31	1.37
1	B	417	HIS	CD2-NE2	-6.10	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	GLU	CA-CB	-6.06	1.44	1.53
1	A	280	HIS	CD2-NE2	-6.05	1.31	1.37
1	B	260	HIS	CD2-NE2	-6.03	1.31	1.37
1	A	225	HIS	CD2-NE2	-5.89	1.31	1.37
1	B	478	PRO	CA-CB	-5.88	1.45	1.53
1	A	243	PRO	CA-CB	-5.83	1.45	1.53
1	B	348	LYS	CA-CB	-5.82	1.44	1.53
1	A	415	HIS	CD2-NE2	-5.80	1.31	1.37
1	A	319	ILE	CA-C	5.80	1.57	1.53
1	A	384	HIS	CG-ND1	-5.76	1.31	1.38
1	B	299	HIS	CD2-NE2	-5.72	1.31	1.37
1	A	476	HIS	CD2-NE2	-5.64	1.31	1.37
1	A	259	HIS	CD2-NE2	-5.53	1.31	1.37
1	B	37	ASN	CG-ND2	-5.53	1.21	1.33
1	B	427	TYR	CA-CB	-5.50	1.46	1.53
1	B	102	ILE	CA-CB	5.47	1.60	1.54
1	B	358	TRP	CG-CD2	-5.46	1.33	1.43
1	B	168	VAL	CA-CB	5.45	1.60	1.53
1	A	299	HIS	CG-ND1	-5.43	1.32	1.38
1	B	420	GLY	CA-C	5.34	1.57	1.52
1	A	37	ASN	CG-ND2	-5.33	1.22	1.33
1	B	415	HIS	CD2-NE2	-5.32	1.32	1.37
1	B	417	HIS	CG-ND1	-5.30	1.32	1.38
1	B	76	ILE	CA-CB	5.29	1.61	1.54
1	B	14	GLN	CA-C	-5.25	1.47	1.53
1	A	76	ILE	CA-CB	5.20	1.61	1.54
1	B	225	HIS	CG-ND1	-5.15	1.32	1.38
1	B	319	ILE	CA-CB	5.13	1.60	1.54
1	B	266	THR	CA-CB	5.08	1.61	1.53
1	A	280	HIS	CG-ND1	-5.03	1.32	1.38
1	B	259	HIS	CD2-NE2	-5.01	1.32	1.37

All (426) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	GLN	OE1-CD-NE2	-13.76	108.84	122.60
1	B	461	ASN	OD1-CG-ND2	-13.26	109.34	122.60
1	B	345	ASN	OD1-CG-ND2	-12.54	110.06	122.60
1	A	345	ASN	OD1-CG-ND2	-12.35	110.25	122.60
1	A	309	VAL	CB-CA-C	-11.96	96.00	112.14
1	B	528	ASN	CA-CB-CG	-11.71	100.89	112.60
1	B	430	GLU	N-CA-C	11.71	128.72	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	ARG	N-CA-C	10.65	122.97	111.36
1	A	30	SER	N-CA-C	10.60	127.50	113.72
1	A	463	LYS	N-CA-C	10.36	125.88	109.50
1	B	13	ASP	N-CA-C	10.28	125.56	112.92
1	A	199	ARG	NE-CZ-NH2	-10.14	110.07	119.20
1	B	524	ASN	OD1-CG-ND2	-10.08	112.52	122.60
1	A	524	ASN	OD1-CG-ND2	-10.04	112.56	122.60
1	A	529	GLN	OE1-CD-NE2	-10.01	112.59	122.60
1	B	363	ASN	OD1-CG-ND2	-9.99	112.61	122.60
1	A	178	ASN	OD1-CG-ND2	-9.95	112.65	122.60
1	B	547	GLN	OE1-CD-NE2	-9.88	112.72	122.60
1	A	192	GLU	N-CA-C	9.87	123.06	111.02
1	B	200	ASN	OD1-CG-ND2	-9.70	112.90	122.60
1	B	51	ARG	N-CA-C	9.54	121.76	111.36
1	A	487	GLN	OE1-CD-NE2	-9.51	113.09	122.60
1	A	172	GLN	OE1-CD-NE2	-9.45	113.15	122.60
1	B	490	ARG	NE-CZ-NH1	9.37	130.87	121.50
1	A	324	GLN	OE1-CD-NE2	-9.34	113.26	122.60
1	B	490	ARG	NE-CZ-NH2	-9.12	110.99	119.20
1	B	33	ASN	OD1-CG-ND2	-9.12	113.48	122.60
1	A	13	ASP	N-CA-C	9.11	124.64	112.88
1	B	418	LYS	CA-CB-CG	9.07	132.23	114.10
1	A	249	ASN	OD1-CG-ND2	-9.04	113.56	122.60
1	A	37	ASN	OD1-CG-ND2	-8.95	113.65	122.60
1	A	457	GLN	OE1-CD-NE2	-8.91	113.69	122.60
1	B	259	HIS	CA-CB-CG	-8.86	104.94	113.80
1	B	205	ASN	OD1-CG-ND2	-8.79	113.81	122.60
1	B	293	ASN	OD1-CG-ND2	-8.78	113.82	122.60
1	A	462	ASP	CA-CB-CG	8.75	121.35	112.60
1	A	549	GLN	OE1-CD-NE2	-8.75	113.85	122.60
1	B	279	GLU	N-CA-C	8.73	120.57	111.14
1	A	486	ASN	CA-CB-CG	8.72	121.32	112.60
1	A	205	ASN	OD1-CG-ND2	-8.67	113.93	122.60
1	B	345	ASN	CB-CG-ND2	8.61	129.31	116.40
1	B	10	ALA	N-CA-C	8.60	121.69	110.43
1	A	322	PHE	CA-CB-CG	-8.58	105.22	113.80
1	A	299	HIS	CA-CB-CG	-8.54	105.26	113.80
1	A	309	VAL	N-CA-CB	8.53	122.14	110.54
1	A	178	ASN	CB-CG-ND2	8.51	129.16	116.40
1	B	462	ASP	N-CA-C	8.50	121.77	111.40
1	B	509	ALA	CA-C-N	8.47	129.79	121.57
1	B	509	ALA	C-N-CA	8.47	129.79	121.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	GLN	OE1-CD-NE2	-8.45	114.15	122.60
1	B	168	VAL	N-CA-C	8.42	120.06	107.51
1	B	254	GLU	N-CA-C	8.39	122.94	112.87
1	A	288	GLY	N-CA-C	8.38	122.78	112.64
1	A	71	GLN	OE1-CD-NE2	-8.37	114.23	122.60
1	B	434	ALA	N-CA-C	8.36	121.32	111.71
1	A	260	HIS	CA-CB-CG	8.34	122.14	113.80
1	A	345	ASN	CB-CG-ND2	8.34	128.90	116.40
1	A	118	ASN	OD1-CG-ND2	-8.31	114.29	122.60
1	A	363	ASN	OD1-CG-ND2	-8.23	114.37	122.60
1	A	248	VAL	O-C-N	-8.13	114.52	122.98
1	A	250	CYS	N-CA-C	8.13	121.99	112.72
1	B	192	GLU	N-CA-C	8.09	119.72	111.07
1	A	267	TYR	N-CA-C	8.04	120.96	111.71
1	B	50	GLN	OE1-CD-NE2	-8.02	114.58	122.60
1	B	462	ASP	N-CA-CB	-7.96	98.34	110.13
1	B	524	ASN	CB-CG-ND2	7.95	128.33	116.40
1	A	264	ASN	OD1-CG-ND2	-7.93	114.67	122.60
1	A	249	ASN	CB-CG-ND2	7.88	128.22	116.40
1	B	61	ASP	N-CA-C	7.88	122.47	113.02
1	A	386	ARG	NE-CZ-NH1	7.86	129.36	121.50
1	B	547	GLN	CG-CD-NE2	7.83	128.14	116.40
1	A	168	VAL	N-CA-CB	-7.82	101.64	111.41
1	A	532	GLN	OE1-CD-NE2	-7.79	114.81	122.60
1	B	430	GLU	O-C-N	-7.78	110.84	122.28
1	A	80	ASN	OD1-CG-ND2	-7.77	114.83	122.60
1	A	472	ASN	OD1-CG-ND2	-7.68	114.92	122.60
1	B	291	ASP	CA-CB-CG	7.60	120.20	112.60
1	A	518	ASP	CA-CB-CG	7.60	120.20	112.60
1	B	317	PHE	CA-CB-CG	-7.58	106.22	113.80
1	A	92	ILE	N-CA-C	7.57	118.84	108.84
1	A	490	ARG	N-CA-C	7.56	121.24	109.07
1	B	509	ALA	O-C-N	7.56	130.13	122.12
1	A	471	ASP	CA-CB-CG	7.55	120.15	112.60
1	A	325	THR	CA-CB-OG1	-7.53	98.30	109.60
1	A	547	GLN	OE1-CD-NE2	-7.53	115.07	122.60
1	B	172	GLN	OE1-CD-NE2	-7.52	115.08	122.60
1	A	200	ASN	CA-CB-CG	-7.52	105.08	112.60
1	A	123	ASN	OD1-CG-ND2	-7.51	115.09	122.60
1	A	90	ASN	CA-CB-CG	-7.50	105.10	112.60
1	A	461	ASN	OD1-CG-ND2	-7.48	115.12	122.60
1	B	144	ASP	CA-CB-CG	-7.47	105.13	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	473	PHE	N-CA-C	7.47	121.22	110.24
1	A	80	ASN	CA-CB-CG	-7.44	105.16	112.60
1	B	160	PRO	N-CA-C	7.43	123.51	113.84
1	A	227	VAL	N-CA-C	7.38	122.51	111.89
1	A	328	ARG	NE-CZ-NH2	-7.33	112.61	119.20
1	B	430	GLU	CA-C-N	-7.29	113.14	123.20
1	B	430	GLU	C-N-CA	-7.29	113.14	123.20
1	A	316	ILE	N-CA-C	7.28	122.37	111.89
1	B	358	TRP	CE2-CD2-CE3	7.27	126.07	118.80
1	B	178	ASN	OD1-CG-ND2	-7.24	115.36	122.60
1	B	472	ASN	OD1-CG-ND2	-7.21	115.39	122.60
1	A	148	GLN	CG-CD-NE2	7.20	127.19	116.40
1	B	530	ASP	CA-CB-CG	7.15	119.75	112.60
1	B	80	ASN	OD1-CG-ND2	-7.13	115.47	122.60
1	B	68	GLU	CB-CG-CD	7.10	124.67	112.60
1	A	358	TRP	CE2-CD2-CE3	7.07	125.87	118.80
1	A	417	HIS	CB-CG-CD2	-7.07	122.01	131.20
1	A	10	ALA	N-CA-C	7.06	120.46	110.23
1	B	29	GLN	OE1-CD-NE2	-7.04	115.56	122.60
1	B	224	MET	CG-SD-CE	-7.02	85.45	100.90
1	A	287	ASP	CA-CB-CG	7.02	119.62	112.60
1	B	514	ARG	CG-CD-NE	-7.01	96.59	112.00
1	B	37	ASN	OD1-CG-ND2	-7.00	115.61	122.60
1	B	123	ASN	CA-CB-CG	-6.99	105.61	112.60
1	B	265	LEU	N-CA-C	6.98	120.68	111.75
1	A	22	ARG	O-C-N	-6.98	115.27	123.22
1	A	133	SER	N-CA-C	6.96	121.39	112.34
1	A	43	ILE	CB-CG1-CD1	-6.96	99.19	113.80
1	A	533	VAL	N-CA-C	-6.90	103.94	110.42
1	A	208	LYS	N-CA-C	-6.88	103.84	111.82
1	B	211	LEU	N-CA-C	6.87	121.95	113.50
1	B	471	ASP	CA-CB-CG	6.86	119.46	112.60
1	B	293	ASN	N-CA-C	6.83	119.71	108.99
1	B	476	HIS	CB-CG-CD2	-6.82	122.34	131.20
1	A	315	ASN	OD1-CG-ND2	-6.79	115.81	122.60
1	B	551	ARG	CG-CD-NE	-6.74	97.17	112.00
1	A	199	ARG	NE-CZ-NH1	6.72	128.22	121.50
1	B	195	ALA	O-C-N	-6.69	114.52	122.15
1	B	473	PHE	N-CA-C	6.69	120.08	110.24
1	B	188	VAL	N-CA-CB	-6.69	99.56	111.93
1	B	271	LEU	N-CA-C	-6.68	104.08	111.36
1	B	389	ASP	CA-CB-CG	6.67	119.27	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	514	ARG	NE-CZ-NH2	-6.67	113.20	119.20
1	B	84	ARG	N-CA-C	6.65	119.54	109.23
1	A	492	ILE	N-CA-CB	-6.64	103.44	111.21
1	B	322	PHE	CA-CB-CG	-6.64	107.16	113.80
1	A	50	GLN	OE1-CD-NE2	-6.64	115.96	122.60
1	A	494	ALA	N-CA-C	6.63	120.63	112.54
1	B	13	ASP	N-CA-CB	-6.60	100.92	110.56
1	A	453	PHE	CA-CB-CG	-6.59	107.21	113.80
1	B	461	ASN	CB-CG-ND2	6.53	126.20	116.40
1	A	534	MET	N-CA-C	6.51	119.20	111.71
1	A	416	TRP	O-C-N	-6.50	115.23	122.12
1	A	154	GLU	CB-CG-CD	6.49	123.63	112.60
1	A	461	ASN	CB-CG-ND2	6.49	126.13	116.40
1	B	290	GLY	N-CA-C	6.48	123.96	115.47
1	A	452	SER	N-CA-C	6.48	121.33	113.17
1	B	361	PHE	CA-C-N	6.45	127.28	119.99
1	B	361	PHE	C-N-CA	6.45	127.28	119.99
1	B	523	ASP	CA-C-O	6.45	128.12	120.70
1	B	236	LEU	N-CA-C	6.45	118.39	111.36
1	A	314	ALA	O-C-N	-6.44	113.81	122.43
1	B	552	THR	N-CA-C	6.42	122.59	114.31
1	A	527	ILE	N-CA-C	6.42	117.93	110.62
1	B	245	ASN	OD1-CG-ND2	-6.41	116.19	122.60
1	B	501	PHE	CA-CB-CG	6.40	120.20	113.80
1	B	507	GLY	O-C-N	6.39	131.01	122.70
1	B	358	TRP	N-CA-C	6.39	118.32	111.36
1	A	28	PHE	N-CA-C	6.38	117.92	110.97
1	A	67	LYS	N-CA-C	6.38	117.90	111.07
1	B	462	ASP	CA-C-O	6.36	127.36	120.55
1	A	215	ASN	CA-CB-CG	6.36	118.95	112.60
1	A	260	HIS	CB-CA-C	-6.35	99.19	109.67
1	A	499	ILE	N-CA-C	-6.35	98.90	108.17
1	B	309	VAL	CA-CB-CG2	-6.34	99.63	110.40
1	B	472	ASN	N-CA-C	-6.33	94.97	107.69
1	B	97	ALA	N-CA-C	-6.33	104.46	111.36
1	B	215	ASN	OD1-CG-ND2	-6.32	116.28	122.60
1	A	487	GLN	CG-CD-NE2	6.32	125.87	116.40
1	A	188	VAL	N-CA-CB	-6.30	96.95	111.81
1	A	302	PHE	CA-CB-CG	6.29	120.09	113.80
1	A	544	LYS	CA-CB-CG	6.29	126.67	114.10
1	A	162	LEU	N-CA-C	6.29	119.47	110.10
1	B	75	ARG	CA-CB-CG	-6.27	101.55	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	528	ASN	OD1-CG-ND2	-6.27	116.33	122.60
1	B	95	THR	O-C-N	-6.26	114.91	120.48
1	A	386	ARG	NH1-CZ-NH2	-6.25	111.17	119.30
1	B	333	SER	O-C-N	-6.25	115.67	122.79
1	B	151	LYS	CA-CB-CG	6.24	126.58	114.10
1	B	227	VAL	N-CA-C	6.24	118.85	111.05
1	A	459	SER	N-CA-C	6.23	118.61	108.76
1	B	118	ASN	OD1-CG-ND2	-6.22	116.38	122.60
1	B	270	ASP	CA-CB-CG	-6.22	106.38	112.60
1	A	486	ASN	OD1-CG-ND2	-6.21	116.39	122.60
1	B	131	ASN	OD1-CG-ND2	-6.19	116.41	122.60
1	B	324	GLN	CA-CB-CG	-6.18	101.74	114.10
1	A	514	ARG	CG-CD-NE	-6.17	98.42	112.00
1	A	104	LYS	O-C-N	-6.17	115.72	122.07
1	B	92	ILE	N-CA-C	6.17	117.67	108.54
1	B	280	HIS	CA-CB-CG	-6.16	107.64	113.80
1	B	427	TYR	CA-C-O	-6.16	113.77	120.36
1	A	137	PRO	N-CA-CB	6.15	108.79	103.31
1	A	473	PHE	CA-C-O	6.14	127.66	120.96
1	B	326	GLY	O-C-N	-6.14	115.53	122.78
1	A	549	GLN	CG-CD-NE2	6.13	125.60	116.40
1	B	55	THR	OG1-CB-CG2	-6.12	97.05	109.30
1	A	229	GLY	CA-C-N	6.12	125.61	119.24
1	A	229	GLY	C-N-CA	6.12	125.61	119.24
1	B	260	HIS	CB-CG-CD2	-6.12	123.24	131.20
1	A	493	PHE	O-C-N	-6.12	116.09	122.94
1	B	347	THR	CA-CB-OG1	-6.09	100.47	109.60
1	B	355	PRO	N-CA-C	-6.08	102.70	111.22
1	A	343	VAL	N-CA-C	-6.07	105.21	110.74
1	A	406	GLN	OE1-CD-NE2	-6.07	116.53	122.60
1	B	239	GLU	N-CA-C	6.06	119.15	111.69
1	A	254	GLU	N-CA-C	6.06	119.50	111.75
1	B	299	HIS	CB-CG-CD2	-6.05	123.33	131.20
1	B	127	GLY	O-C-N	-6.04	118.66	123.49
1	B	187	ILE	O-C-N	-6.04	115.59	122.72
1	A	524	ASN	CB-CG-ND2	6.04	125.46	116.40
1	A	160	PRO	CA-C-N	6.04	130.94	120.68
1	A	160	PRO	C-N-CA	6.04	130.94	120.68
1	A	359	LYS	CB-CA-C	-6.04	99.47	110.63
1	B	140	GLU	CB-CG-CD	6.03	122.86	112.60
1	B	415	HIS	CA-C-N	6.03	128.36	120.28
1	B	415	HIS	C-N-CA	6.03	128.36	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	527	ILE	N-CA-C	6.02	121.86	109.34
1	B	80	ASN	CB-CG-ND2	6.01	125.42	116.40
1	A	131	ASN	OD1-CG-ND2	-5.99	116.61	122.60
1	B	400	ILE	N-CA-C	-5.99	104.67	110.72
1	A	191	VAL	N-CA-C	5.97	121.77	109.34
1	A	415	HIS	CA-C-N	5.97	128.28	120.28
1	A	415	HIS	C-N-CA	5.97	128.28	120.28
1	B	283	GLY	O-C-N	-5.96	118.05	123.36
1	A	527	ILE	N-CA-CB	-5.96	103.02	110.47
1	A	32	THR	CA-CB-OG1	-5.95	100.68	109.60
1	B	413	LYS	CG-CD-CE	-5.94	97.63	111.30
1	A	61	ASP	CA-CB-CG	5.92	118.52	112.60
1	B	497	SER	O-C-N	-5.92	116.11	122.85
1	A	161	ASP	CA-CB-CG	5.91	118.51	112.60
1	A	324	GLN	CG-CD-NE2	5.90	125.25	116.40
1	A	84	ARG	CB-CG-CD	-5.89	97.75	111.30
1	A	277	SER	N-CA-C	5.88	119.93	112.87
1	B	347	THR	N-CA-CB	-5.88	100.81	110.40
1	A	211	LEU	N-CA-C	5.88	120.45	113.28
1	B	200	ASN	CA-CB-CG	-5.87	106.73	112.60
1	A	517	ILE	N-CA-C	5.87	116.30	107.80
1	B	108	ILE	CA-CB-CG1	-5.87	100.43	110.40
1	B	249	ASN	CB-CG-ND2	5.86	125.19	116.40
1	B	250	CYS	N-CA-C	5.86	119.50	112.93
1	B	473	PHE	CA-C-O	5.86	127.35	120.96
1	B	334	MET	N-CA-C	5.85	120.86	113.25
1	B	191	VAL	N-CA-C	5.82	121.84	113.16
1	A	71	GLN	CG-CD-NE2	5.82	125.13	116.40
1	B	30	SER	CA-CB-OG	5.82	122.73	111.10
1	B	4	VAL	N-CA-CB	-5.81	103.35	111.25
1	A	113	LEU	CA-C-O	5.79	127.30	120.70
1	B	276	LYS	N-CA-C	5.79	118.37	111.71
1	B	328	ARG	CA-CB-CG	-5.78	102.53	114.10
1	A	244	ALA	N-CA-C	5.78	118.36	111.71
1	A	325	THR	O-C-N	-5.78	114.15	122.36
1	B	249	ASN	OD1-CG-ND2	-5.78	116.82	122.60
1	A	471	ASP	N-CA-C	5.76	116.16	108.38
1	B	260	HIS	O-C-N	-5.76	116.05	121.35
1	A	325	THR	OG1-CB-CG2	5.75	120.80	109.30
1	B	93	LEU	O-C-N	-5.73	116.48	123.36
1	B	30	SER	O-C-N	-5.72	115.56	122.48
1	A	22	ARG	N-CA-C	5.70	118.02	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	HIS	CB-CG-CD2	-5.69	123.80	131.20
1	B	238	GLU	CA-C-O	-5.66	115.05	121.00
1	B	347	THR	CA-CB-CG2	5.66	120.13	110.50
1	B	415	HIS	CB-CG-CD2	-5.66	123.84	131.20
1	B	260	HIS	CB-CG-ND1	5.66	131.19	122.70
1	A	463	LYS	CA-C-O	5.66	127.73	121.11
1	A	245	ASN	N-CA-C	5.66	118.21	111.71
1	A	455	GLY	N-CA-C	-5.66	106.90	114.25
1	B	508	SER	N-CA-C	-5.63	99.94	107.88
1	B	507	GLY	CA-C-N	5.62	132.46	122.45
1	B	507	GLY	C-N-CA	5.62	132.46	122.45
1	A	373	CYS	N-CA-C	5.62	117.81	108.99
1	A	303	VAL	CA-C-O	5.61	126.53	120.53
1	B	417	HIS	CA-CB-CG	-5.61	108.19	113.80
1	A	224	MET	N-CA-C	5.61	119.17	111.54
1	A	101	ILE	CA-C-O	-5.60	114.91	120.85
1	B	477	ASP	CA-C-O	5.60	125.00	119.51
1	B	7	LYS	CA-C-O	5.59	127.43	121.05
1	A	407	SER	O-C-N	-5.59	115.77	122.65
1	A	457	GLN	CG-CD-NE2	5.59	124.79	116.40
1	A	108	ILE	CA-CB-CG1	-5.59	100.90	110.40
1	B	92	ILE	CB-CA-C	-5.58	104.55	111.08
1	B	207	LEU	CD1-CG-CD2	-5.58	98.52	110.80
1	A	290	GLY	N-CA-C	5.57	122.94	115.59
1	B	7	LYS	CB-CG-CD	5.54	124.05	111.30
1	A	412	LEU	CA-C-O	-5.53	115.00	120.70
1	B	153	ILE	N-CA-C	5.52	116.19	109.30
1	A	392	TRP	CE2-CD2-CG	-5.51	100.58	107.20
1	B	376	GLU	CA-C-O	5.50	126.15	119.49
1	A	532	GLN	CA-C-N	5.50	127.43	120.72
1	A	532	GLN	C-N-CA	5.50	127.43	120.72
1	A	54	ALA	N-CA-C	5.50	118.25	110.50
1	A	95	THR	CA-C-N	5.49	124.84	118.85
1	A	95	THR	C-N-CA	5.49	124.84	118.85
1	A	421	ARG	N-CA-C	5.49	118.43	109.59
1	B	200	ASN	CB-CG-ND2	5.49	124.64	116.40
1	A	448	MET	N-CA-C	5.48	117.33	111.36
1	A	21	LEU	N-CA-C	5.48	117.16	108.67
1	A	360	PHE	CA-C-N	5.47	127.56	120.44
1	A	360	PHE	C-N-CA	5.47	127.56	120.44
1	B	491	LEU	N-CA-C	-5.47	98.30	107.99
1	B	270	ASP	N-CA-C	5.46	116.91	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	ASP	N-CA-C	5.45	119.64	113.15
1	B	205	ASN	N-CA-C	-5.45	104.98	111.69
1	B	109	GLY	O-C-N	-5.44	118.70	123.92
1	B	386	ARG	CA-C-N	5.42	131.54	121.62
1	B	386	ARG	C-N-CA	5.42	131.54	121.62
1	A	323	GLN	OE1-CD-NE2	-5.42	117.18	122.60
1	A	213	GLY	CA-C-N	5.41	126.60	119.84
1	A	213	GLY	C-N-CA	5.41	126.60	119.84
1	A	172	GLN	CG-CD-NE2	5.41	124.51	116.40
1	B	392	TRP	CE2-CD2-CG	-5.40	100.72	107.20
1	B	552	THR	O-C-N	5.40	128.28	122.34
1	B	196	THR	N-CA-C	-5.40	105.40	111.28
1	A	464	VAL	CA-C-O	5.39	126.00	120.39
1	B	346	ALA	N-CA-C	5.39	117.15	111.28
1	A	95	THR	CA-CB-CG2	5.38	119.65	110.50
1	B	486	ASN	N-CA-C	5.38	119.00	111.74
1	B	420	GLY	N-CA-C	-5.37	105.91	112.68
1	A	526	LYS	CA-C-O	5.37	125.04	119.14
1	B	118	ASN	CA-CB-CG	-5.37	107.23	112.60
1	A	337	SER	N-CA-C	5.36	117.45	110.43
1	B	4	VAL	N-CA-C	5.35	115.67	108.17
1	B	474	GLU	N-CA-CB	-5.35	101.31	111.00
1	A	32	THR	CA-CB-CG2	5.35	119.59	110.50
1	B	5	THR	CA-CB-OG1	-5.35	101.58	109.60
1	A	180	PHE	N-CA-C	5.34	117.18	111.36
1	A	359	LYS	N-CA-C	5.34	117.85	111.71
1	A	468	GLU	CA-C-O	5.33	125.44	119.41
1	B	171	LYS	N-CA-C	5.33	118.31	109.46
1	A	397	TRP	CG-CD2-CE3	5.32	139.22	133.90
1	B	183	PHE	O-C-N	-5.32	116.99	123.16
1	A	417	HIS	CA-CB-CG	-5.31	108.49	113.80
1	A	129	LYS	O-C-N	-5.31	117.27	123.27
1	B	476	HIS	CB-CG-ND1	5.31	130.66	122.70
1	A	148	GLN	CB-CG-CD	5.30	121.61	112.60
1	A	328	ARG	CB-CA-C	-5.29	99.25	110.31
1	A	134	ASN	N-CA-C	-5.27	106.62	113.16
1	B	328	ARG	N-CA-C	5.27	119.56	113.18
1	B	533	VAL	O-C-N	-5.26	116.75	121.91
1	A	286	PHE	N-CA-C	5.26	117.68	109.52
1	B	457	GLN	CA-CB-CG	-5.26	103.58	114.10
1	B	130	PHE	CA-CB-CG	5.26	119.06	113.80
1	B	387	GLU	O-C-N	-5.25	117.80	123.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	303	VAL	N-CA-C	-5.25	100.19	107.80
1	B	75	ARG	CD-NE-CZ	-5.25	117.05	124.40
1	B	97	ALA	O-C-N	-5.25	116.17	122.15
1	A	84	ARG	N-CA-C	5.24	117.22	108.99
1	B	315	ASN	OD1-CG-ND2	-5.24	117.36	122.60
1	B	149	ILE	CB-CG1-CD1	-5.24	102.79	113.80
1	A	319	ILE	CA-C-O	5.24	123.03	119.20
1	B	133	SER	N-CA-C	5.24	118.77	112.38
1	B	297	GLY	N-CA-C	-5.24	105.39	112.57
1	B	136	GLY	CA-C-N	5.23	125.15	119.76
1	B	136	GLY	C-N-CA	5.23	125.15	119.76
1	B	359	LYS	CB-CG-CD	5.23	123.33	111.30
1	A	410	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	254	GLU	CA-C-O	5.22	125.67	119.10
1	B	110	GLY	O-C-N	-5.21	119.01	123.23
1	A	543	LEU	CA-C-N	5.20	127.51	120.44
1	A	543	LEU	C-N-CA	5.20	127.51	120.44
1	A	359	LYS	N-CA-CB	5.19	118.22	110.22
1	B	400	ILE	O-C-N	-5.19	116.49	121.83
1	B	528	ASN	N-CA-C	5.19	119.30	112.92
1	A	244	ALA	CA-C-N	5.18	127.75	120.28
1	A	244	ALA	C-N-CA	5.18	127.75	120.28
1	A	404	ARG	N-CA-C	5.18	118.76	112.23
1	A	316	ILE	N-CA-CB	-5.18	100.52	110.78
1	B	555	THR	OG1-CB-CG2	5.18	119.66	109.30
1	B	293	ASN	CB-CG-ND2	5.17	124.16	116.40
1	A	107	ALA	O-C-N	-5.17	116.90	122.79
1	B	29	GLN	N-CA-C	5.17	119.43	113.18
1	A	558	THR	CB-CA-C	-5.16	102.77	110.88
1	B	505	GLY	N-CA-C	-5.15	100.98	113.18
1	B	482	SER	N-CA-C	5.14	121.76	110.80
1	A	178	ASN	CB-CA-C	-5.14	104.24	111.95
1	B	113	LEU	CA-C-O	5.14	127.14	121.39
1	B	346	ALA	CA-C-N	5.14	130.13	121.14
1	B	346	ALA	C-N-CA	5.14	130.13	121.14
1	A	186	GLU	O-C-N	-5.13	116.66	123.13
1	B	97	ALA	CA-C-O	-5.13	114.98	120.42
1	B	309	VAL	CA-CB-CG1	5.13	119.12	110.40
1	A	66	MET	O-C-N	-5.12	116.69	122.12
1	A	325	THR	CA-CB-CG2	5.12	119.21	110.50
1	A	426	ARG	CB-CG-CD	-5.12	99.52	111.30
1	A	9	LYS	CB-CG-CD	-5.11	99.55	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	ASN	CA-CB-CG	5.11	117.71	112.60
1	A	494	ALA	CA-C-O	5.11	125.66	119.38
1	A	212	SER	CA-CB-OG	5.11	121.32	111.10
1	B	164	VAL	O-C-N	-5.10	117.67	123.18
1	B	358	TRP	CD2-CE3-CZ3	-5.10	111.97	118.60
1	A	153	ILE	N-CA-C	5.10	116.25	109.37
1	B	159	CYS	O-C-N	-5.10	115.46	121.32
1	A	4	VAL	N-CA-CB	-5.09	101.36	111.91
1	B	532	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	B	33	ASN	CB-CG-ND2	5.09	124.03	116.40
1	A	514	ARG	CA-C-O	5.08	125.90	120.46
1	B	503	LEU	CA-C-O	5.08	127.36	121.11
1	B	422	ASN	CA-CB-CG	-5.07	107.53	112.60
1	B	532	GLN	CB-CG-CD	5.07	121.23	112.60
1	A	134	ASN	O-C-N	-5.07	115.38	122.37
1	A	389	ASP	CA-CB-CG	5.07	117.67	112.60
1	B	426	ARG	CA-CB-CG	-5.07	103.97	114.10
1	A	245	ASN	CA-CB-CG	-5.06	107.54	112.60
1	A	513	ILE	CA-C-O	5.06	126.11	120.59
1	B	155	GLU	N-CA-C	5.06	116.94	108.99
1	B	418	LYS	CB-CA-C	-5.06	101.44	110.70
1	A	37	ASN	CA-CB-CG	5.06	117.66	112.60
1	B	461	ASN	O-C-N	-5.05	115.87	122.59
1	B	302	PHE	CA-CB-CG	5.05	118.85	113.80
1	A	463	LYS	CA-CB-CG	5.05	124.20	114.10
1	A	289	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	492	ILE	O-C-N	-5.04	116.31	122.97
1	B	210	LEU	O-C-N	-5.04	116.78	122.12
1	A	110	GLY	O-C-N	-5.03	119.15	123.23
1	A	476	HIS	CB-CG-CD2	-5.03	124.66	131.20
1	A	319	ILE	O-C-N	-5.03	117.53	121.46
1	A	224	MET	CG-SD-CE	-5.03	89.83	100.90
1	B	125	ASP	CA-CB-CG	-5.03	107.57	112.60
1	A	131	ASN	CB-CG-ND2	5.03	123.94	116.40
1	A	267	TYR	CA-CB-CG	-5.03	104.85	113.90
1	A	14	GLN	OE1-CD-NE2	-5.02	117.58	122.60
1	B	131	ASN	CB-CG-ND2	5.02	123.94	116.40
1	A	159	CYS	N-CA-C	-5.02	98.72	109.81
1	B	90	ASN	OD1-CG-ND2	-5.02	117.58	122.60
1	B	148	GLN	OE1-CD-NE2	-5.00	117.59	122.60
1	A	476	HIS	CB-CG-ND1	5.00	130.21	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	194	TYR	Sidechain
1	A	386	ARG	Sidechain
1	B	514	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4333	971	4331	94	0
1	B	4333	971	4331	73	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	201	402	0	17	0
3	B	293	586	0	15	0
All	All	9162	2930	8662	167	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 10.

All (167) 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:63:ARG:HD2	3:A:758:HOH:O	1.77	0.84
1:B:383:ASP:HB2	1:B:386:ARG:NH2	1.94	0.83
1:A:280:HIS:HD2	3:A:753:HOH:O	1.65	0.78
1:A:112:ILE:HD12	1:A:129:LYS:HD3	1.68	0.74
1:B:365:MET:HB3	1:B:386:ARG:NH2	2.03	0.73
1:B:383:ASP:HB2	1:B:386:ARG:HH21	1.56	0.70
1:B:471:ASP:OD1	1:B:490:ARG:HD3	1.91	0.69
1:B:325:THR:HG22	1:B:326:GLY:O	1.92	0.69
1:A:178:ASN:HB2	3:A:714:HOH:O	1.93	0.69
1:A:359:LYS:HE2	3:A:644:HOH:O	1.92	0.69
1:A:547:GLN:HB2	1:A:551:ARG:NH1	2.10	0.67
1:B:444:LEU:HD12	1:B:447:LEU:HD22	1.80	0.64
1:B:68:GLU:HB2	3:B:773:HOH:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:PHE:HB2	1:B:490:ARG:HD2	1.81	0.63
1:B:280:HIS:HD2	3:B:643:HOH:O	1.81	0.63
1:B:382:SER:OG	1:B:384:HIS:HD2	1.81	0.63
1:A:437:ALA:HB1	1:A:503:LEU:HD11	1.82	0.62
1:A:259:HIS:NE2	1:A:267:TYR:HD1	1.98	0.61
1:A:272:VAL:O	1:A:276:LYS:HG2	2.01	0.60
1:A:321:TYR:O	1:A:325:THR:HB	2.01	0.60
1:A:384:HIS:HE1	1:A:389:ASP:OD2	1.86	0.59
1:A:384:HIS:CE1	1:A:385:ILE:HG12	2.38	0.58
1:A:440:MET:HG3	1:A:546:SER:O	2.01	0.58
1:A:505:GLY:HA2	1:A:511:ALA:HA	1.86	0.58
1:A:247:ALA:HB1	1:A:250:CYS:SG	2.44	0.58
1:B:220:ARG:NH1	1:B:248:VAL:HG21	2.19	0.58
1:B:75:ARG:HD2	1:B:159:CYS:O	2.04	0.58
1:B:11:TYR:OH	1:B:31:SER:HB3	2.04	0.57
1:A:499:ILE:HD13	1:A:542:ALA:HB2	1.87	0.57
1:B:197:MET:HA	3:B:576:HOH:O	2.03	0.57
1:B:426:ARG:HG3	1:B:516:TYR:CD2	2.40	0.57
1:B:451:ARG:HD3	1:B:451:ARG:H	1.71	0.56
1:B:384:HIS:HE1	1:B:389:ASP:OD2	1.88	0.55
1:A:499:ILE:HD11	1:A:538:LEU:HD22	1.88	0.55
1:B:318:SER:HB2	1:B:403:THR:HG21	1.89	0.55
1:A:426:ARG:HG3	1:A:516:TYR:CE2	2.41	0.54
1:B:15:LYS:NZ	1:B:15:LYS:HB3	2.22	0.54
1:A:536:ALA:HB3	1:A:537:PRO:HD3	1.90	0.54
1:A:147:PHE:CZ	1:A:151:LYS:HD2	2.43	0.54
1:A:554:ARG:NH1	3:A:763:HOH:O	2.34	0.54
1:A:448:MET:HA	1:A:453:PHE:CD2	2.44	0.53
1:B:16:PRO:HG2	1:B:143:THR:HB	1.91	0.53
1:A:228:VAL:HG12	3:A:627:HOH:O	2.08	0.53
1:A:55:THR:OG1	1:A:84:ARG:HD3	2.09	0.53
1:B:14:GLN:HE21	1:B:150:SER:HB2	1.73	0.52
1:B:69:ALA:O	1:B:73:ILE:HG13	2.09	0.52
1:B:106:LYS:HD3	3:B:787:HOH:O	2.10	0.52
1:B:53:GLU:HG2	3:B:805:HOH:O	2.08	0.52
1:A:31:SER:HB2	1:A:34:TYR:HB2	1.92	0.51
1:B:117:HIS:HB3	1:B:292:ARG:HH21	1.75	0.51
1:B:280:HIS:CD2	3:B:643:HOH:O	2.60	0.51
1:B:504:SER:OG	1:B:512:THR:HB	2.10	0.51
1:B:210:LEU:HG	1:B:402:ALA:HB2	1.93	0.51
1:B:271:LEU:HD13	1:B:296:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:PHE:CD1	1:A:261:PRO:HG3	2.47	0.50
1:B:60:GLY:HA3	1:B:66:MET:SD	2.52	0.50
1:A:449:PHE:CD1	1:A:449:PHE:N	2.78	0.50
1:A:145:LYS:O	1:A:149:ILE:HG13	2.11	0.50
1:A:425:THR:CG2	1:A:535:LEU:HD13	2.41	0.50
1:A:220:ARG:CZ	1:A:248:VAL:HG21	2.42	0.50
1:B:63:ARG:HD2	3:B:793:HOH:O	2.11	0.50
1:B:264:ASN:HD21	1:B:267:TYR:HD2	1.59	0.49
1:B:384:HIS:CE1	1:B:385:ILE:HG12	2.47	0.49
1:A:76:ILE:HG13	1:A:158:ILE:HD12	1.94	0.49
1:B:301:PHE:HE2	1:B:412:LEU:HD13	1.78	0.49
1:B:177:GLU:HB3	3:B:779:HOH:O	2.12	0.49
1:A:404:ARG:NH2	3:A:694:HOH:O	2.45	0.49
1:B:316:ILE:HG12	1:B:322:PHE:CD2	2.47	0.49
1:A:71:GLN:HB3	1:A:75:ARG:HH12	1.77	0.49
1:A:180:PHE:HB3	1:A:181:LYS:HD2	1.95	0.49
1:B:347:THR:HG22	1:B:349:ILE:HG12	1.95	0.48
1:A:425:THR:HG22	1:A:535:LEU:HD13	1.94	0.48
1:A:369:LYS:HE2	3:A:737:HOH:O	2.13	0.48
1:B:383:ASP:CB	1:B:386:ARG:HH21	2.25	0.48
1:A:259:HIS:CE1	1:A:260:HIS:O	2.65	0.48
1:A:539:ILE:HG22	1:A:543:LEU:HD22	1.94	0.48
1:A:71:GLN:HB3	1:A:75:ARG:NH1	2.28	0.48
1:B:280:HIS:CD2	1:B:280:HIS:N	2.82	0.48
1:B:225:HIS:HD2	3:B:767:HOH:O	1.96	0.48
1:A:460:ALA:HB3	1:A:537:PRO:HB3	1.96	0.47
1:B:470:ALA:HA	1:B:490:ARG:O	2.14	0.47
1:A:432:VAL:HG22	1:A:511:ALA:O	2.14	0.47
1:A:264:ASN:HB2	3:A:622:HOH:O	2.14	0.47
1:B:343:VAL:O	1:B:347:THR:HB	2.15	0.47
1:A:117:HIS:HB3	1:A:292:ARG:NH2	2.29	0.47
1:A:234:LYS:NZ	3:A:749:HOH:O	2.47	0.47
1:A:335:PRO:HG3	1:A:502:ARG:HD2	1.97	0.47
1:B:451:ARG:HD3	1:B:451:ARG:N	2.30	0.47
1:A:230:PRO:O	1:A:234:LYS:HB2	2.14	0.47
1:B:52:GLN:HG2	3:B:594:HOH:O	2.14	0.47
1:A:443:ASP:O	1:A:446:ALA:HB3	2.15	0.46
1:A:505:GLY:CA	1:A:511:ALA:HA	2.45	0.46
1:B:439:LYS:HE3	1:B:551:ARG:NE	2.30	0.46
1:B:181:LYS:HD3	3:B:592:HOH:O	2.14	0.46
1:B:414:ASP:O	1:B:418:LYS:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:LYS:HE3	1:A:418:LYS:HB2	1.69	0.46
1:B:365:MET:HB3	1:B:386:ARG:CZ	2.45	0.46
1:A:438:THR:O	1:A:442:LYS:HB2	2.16	0.46
1:B:117:HIS:HB3	1:B:292:ARG:NH2	2.31	0.46
1:B:366:ASP:OD1	1:B:386:ARG:NH1	2.45	0.46
1:B:68:GLU:CB	3:B:773:HOH:O	2.57	0.46
1:B:280:HIS:CD2	1:B:280:HIS:H	2.33	0.46
1:A:236:LEU:HD23	1:A:240:LEU:HD12	1.96	0.45
1:B:149:ILE:O	1:B:153:ILE:HB	2.16	0.45
1:A:61:ASP:HA	1:A:227:VAL:CG2	2.46	0.45
1:A:163:LYS:NZ	3:A:592:HOH:O	2.47	0.45
1:A:265:LEU:HD12	3:A:622:HOH:O	2.17	0.45
1:A:551:ARG:NH1	3:A:674:HOH:O	2.48	0.45
1:B:123:ASN:HB2	3:B:776:HOH:O	2.15	0.45
1:A:210:LEU:HD22	1:A:217:LEU:HB2	1.99	0.45
1:B:519:SER:HB3	1:B:535:LEU:HD23	1.97	0.45
1:A:273:GLU:CD	1:A:276:LYS:HZ2	2.25	0.45
1:B:23:LYS:HE3	1:B:34:TYR:OH	2.16	0.45
1:B:218:LYS:HE2	1:B:218:LYS:HB3	1.85	0.45
1:A:88:GLY:HA3	1:A:93:LEU:HD13	1.98	0.45
1:A:441:MET:HG3	1:A:503:LEU:HD22	1.99	0.45
1:A:366:ASP:OD1	1:A:386:ARG:HD2	2.16	0.44
1:A:176:LEU:HD11	1:A:183:PHE:HB2	1.98	0.44
1:A:178:ASN:O	1:A:179:LYS:HG2	2.17	0.44
1:A:312:ILE:HA	1:A:400:ILE:HD11	1.99	0.44
1:B:465:TYR:HB3	1:B:493:PHE:CD1	2.53	0.44
1:A:426:ARG:HG3	1:A:516:TYR:CD2	2.53	0.44
1:B:84:ARG:HA	1:B:184:THR:O	2.18	0.44
1:B:232:VAL:O	1:B:236:LEU:HB2	2.18	0.44
1:A:101:ILE:O	1:A:105:ILE:HG12	2.18	0.44
1:A:520:TYR:CE2	1:A:522:LYS:HB2	2.53	0.44
1:B:112:ILE:HG22	1:B:114:THR:HG22	2.00	0.44
1:B:469:LYS:NZ	3:B:717:HOH:O	2.50	0.44
1:A:28:PHE:CD2	1:A:126:PHE:HB3	2.53	0.43
1:A:224:MET:HG2	3:A:612:HOH:O	2.18	0.43
1:B:426:ARG:HG3	1:B:516:TYR:CE2	2.52	0.43
1:B:551:ARG:HA	1:B:551:ARG:HD3	1.90	0.43
1:A:280:HIS:CD2	3:A:753:HOH:O	2.51	0.43
1:A:273:GLU:O	1:A:276:LYS:HB2	2.18	0.43
1:A:2:LYS:O	1:A:159:CYS:HA	2.19	0.43
1:A:60:GLY:HA3	1:A:66:MET:SD	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:ASP:OD2	1:A:526:LYS:HG3	2.17	0.43
1:B:382:SER:OG	1:B:384:HIS:CD2	2.66	0.43
1:A:225:HIS:HD2	3:A:713:HOH:O	2.00	0.43
1:A:363:ASN:HB3	1:A:479:VAL:HB	2.00	0.43
1:A:501:PHE:CE2	1:A:515:LEU:HD13	2.54	0.42
1:A:540:SER:O	1:A:544:LYS:HB2	2.19	0.42
1:A:537:PRO:O	1:A:541:ILE:HG13	2.20	0.42
1:A:14:GLN:HE21	1:A:150:SER:HB2	1.83	0.42
1:B:3:ILE:HD12	1:B:179:LYS:HE3	2.01	0.42
1:B:449:PHE:HE1	1:B:471:ASP:HA	1.85	0.42
1:B:325:THR:HG21	3:B:785:HOH:O	2.19	0.42
1:A:325:THR:O	1:A:328:ARG:NH2	2.53	0.41
1:A:526:LYS:HB3	1:A:534:MET:HE1	2.02	0.41
1:A:497:SER:HB3	1:A:538:LEU:HD11	2.02	0.41
1:A:14:GLN:O	1:A:16:PRO:HD3	2.21	0.41
1:B:383:ASP:CB	1:B:386:ARG:NH2	2.77	0.41
1:A:94:SER:HA	1:A:227:VAL:HG11	2.03	0.41
1:A:311:VAL:HG11	1:A:397:TRP:CH2	2.56	0.41
1:B:31:SER:HB2	1:B:34:TYR:HB2	2.03	0.41
1:B:48:PRO:HA	1:B:51:ARG:CD	2.51	0.41
1:A:447:LEU:HD21	1:A:545:VAL:HG22	2.03	0.41
1:A:177:GLU:O	1:A:177:GLU:HG3	2.20	0.40
1:A:325:THR:HG22	1:A:326:GLY:O	2.21	0.40
1:A:303:VAL:HG22	1:A:412:LEU:CD1	2.52	0.40
1:A:424:PHE:HA	1:A:517:ILE:O	2.22	0.40
1:B:25:VAL:HG22	1:B:126:PHE:HB2	2.02	0.40
1:A:21:LEU:HD11	1:A:23:LYS:HE3	2.02	0.40
1:B:220:ARG:HH11	1:B:248:VAL:HG21	1.84	0.40
1:A:16:PRO:HG3	1:A:38:PHE:CZ	2.56	0.40
1:A:104:LYS:NZ	3:A:605:HOH:O	2.52	0.40
1:A:472:ASN:OD1	1:A:486:ASN:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	558/561 (100%)	533 (96%)	22 (4%)	3 (0%)	24	37
1	B	558/561 (100%)	533 (96%)	24 (4%)	1 (0%)	43	58
All	All	1116/1122 (100%)	1066 (96%)	46 (4%)	4 (0%)	30	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	ARG
1	B	461	ASN
1	A	213	GLY
1	A	263	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	461/461 (100%)	421 (91%)	40 (9%)	9	16
1	B	461/461 (100%)	429 (93%)	32 (7%)	14	24
All	All	922/922 (100%)	850 (92%)	72 (8%)	11	20

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL
1	A	4	VAL
1	A	48	PRO
1	A	68	GLU
1	A	93	LEU
1	A	113	LEU
1	A	118	ASN
1	A	125	ASP
1	A	144	ASP

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Mol	Chain	Res	Type
1	A	151	LYS
1	A	153	ILE
1	A	163	LYS
1	A	166	LEU
1	A	168	VAL
1	A	178	ASN
1	A	179	LYS
1	A	188	VAL
1	A	208	LYS
1	A	210	LEU
1	A	215	ASN
1	A	227	VAL
1	A	243	PRO
1	A	309	VAL
1	A	323	GLN
1	A	359	LYS
1	A	380	THR
1	A	417	HIS
1	A	426	ARG
1	A	431	GLU
1	A	439	LYS
1	A	442	LYS
1	A	461	ASN
1	A	462	ASP
1	A	486	ASN
1	A	514	ARG
1	A	524	ASN
1	A	543	LEU
1	A	544	LYS
1	A	545	VAL
1	A	561	THR
1	B	7	LYS
1	B	15	LYS
1	B	43	ILE
1	B	72	LEU
1	B	82	ILE
1	B	93	LEU
1	B	108	ILE
1	B	122	PRO
1	B	163	LYS
1	B	166	LEU
1	B	169	LEU

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Mol	Chain	Res	Type
1	B	171	LYS
1	B	188	VAL
1	B	209	GLU
1	B	210	LEU
1	B	227	VAL
1	B	233	LYS
1	B	248	VAL
1	B	270	ASP
1	B	271	LEU
1	B	325	THR
1	B	337	SER
1	B	347	THR
1	B	358	TRP
1	B	386	ARG
1	B	412	LEU
1	B	418	LYS
1	B	430	GLU
1	B	433	GLU
1	B	447	LEU
1	B	451	ARG
1	B	506	THR

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	14	GLN
1	A	40	GLN
1	A	80	ASN
1	A	172	GLN
1	A	205	ASN
1	A	280	HIS
1	A	293	ASN
1	A	345	ASN
1	A	384	HIS
1	A	486	ASN
1	A	547	GLN
1	B	14	GLN
1	B	29	GLN
1	B	173	GLN
1	B	280	HIS
1	B	384	HIS
1	B	422	ASN

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Mol	Chain	Res	Type
1	B	547	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	SEP	A	116	1,2	8,9,10	1.33	1 (12%)	7,12,14	1.06	0
1	SEP	B	116	1,2	8,9,10	1.23	1 (12%)	7,12,14	2.99	1 (14%)

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
1	SEP	A	116	1,2	-	2/6/8/10	-
1	SEP	B	116	1,2	-	4/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	116	SEP	P-OG	-3.07	1.50	1.60
1	A	116	SEP	P-OG	-2.70	1.51	1.60

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	SEP	OG-CB-CA	-7.59	100.76	108.14

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	116	SEP	N-CA-CB-OG
1	A	116	SEP	CB-OG-P-O2P
1	B	116	SEP	CB-OG-P-O1P
1	B	116	SEP	CB-OG-P-O2P
1	B	116	SEP	CB-OG-P-O3P
1	B	116	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	560/561 (99%)	-0.68	2 (0%) 88 86	7, 24, 57, 74	0
1	B	560/561 (99%)	-0.93	3 (0%) 87 85	4, 17, 40, 64	0
All	All	1120/1122 (99%)	-0.80	5 (0%) 88 86	4, 21, 52, 74	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	508	SER	3.2
1	A	506	THR	2.7
1	B	509	ALA	2.7
1	A	509	ALA	2.2
1	B	504	SER	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SEP	A	116	10/11	0.89	0.11	0,45,60,61	0
1	SEP	B	116	10/11	0.91	0.10	0,40,53,54	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	B	562	1/1	0.70	0.11	28,28,28,28	0
2	MG	A	562	1/1	0.83	0.09	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.