



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2017 – 07:32 PM EDT

PDB ID : 1K0G
Title : THE CRYSTAL STRUCTURE OF AMINODEOXYCHORISMATE SYNTHASE FROM PHOSPHATE GROWN CRYSTALS
Authors : Parsons, J.F.; Jensen, P.Y.; Pachikara, A.S.; Howard, A.J.; Eisenstein, E.; Ladner, J.E.
Deposited on : unknown
Resolution : 2.05 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

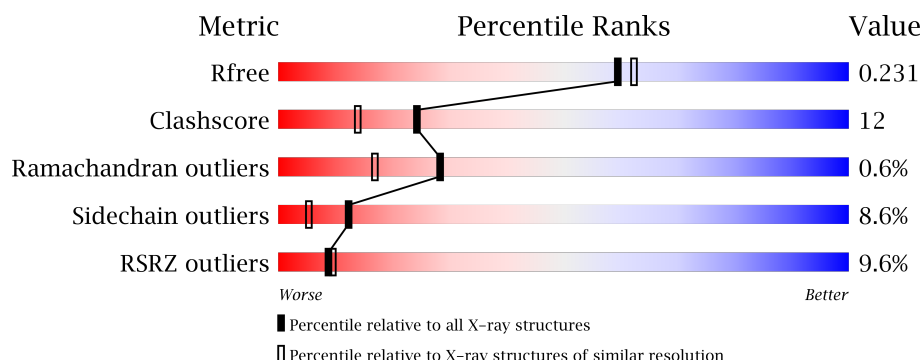
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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))
R_{free}	100719	1316 (2.04-2.04)
Clashscore	112137	1394 (2.04-2.04)
Ramachandran outliers	110173	1383 (2.04-2.04)
Sidechain outliers	110143	1383 (2.04-2.04)
RSRZ outliers	101464	1319 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	453	<div> <div>8%</div> <div> <div></div> <div>53%</div> <div>30%</div> <div>9%</div> <div>•</div> <div>7%</div> </div> </div>
1	B	453	<div> <div>10%</div> <div> <div></div> <div>48%</div> <div>32%</div> <div>9%</div> <div>•</div> <div>8%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	701	-	X	-	-
2	PO4	B	702	-	-	X	-

2 Entry composition [i](#)

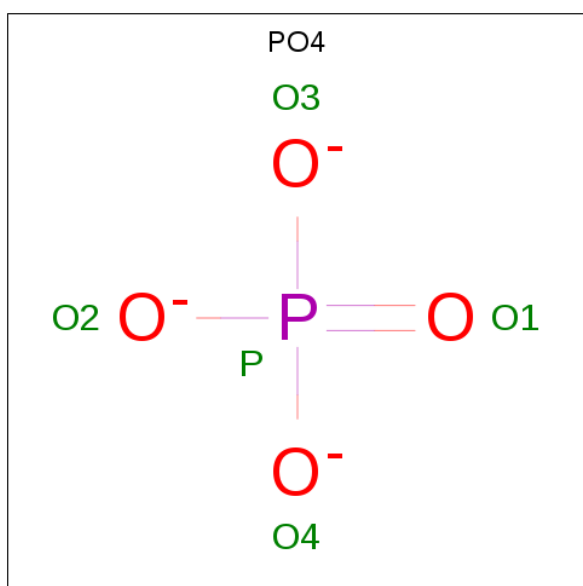
There are 4 unique types of molecules in this entry. The entry contains 7228 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 p-aminobenzoate synthase component I.

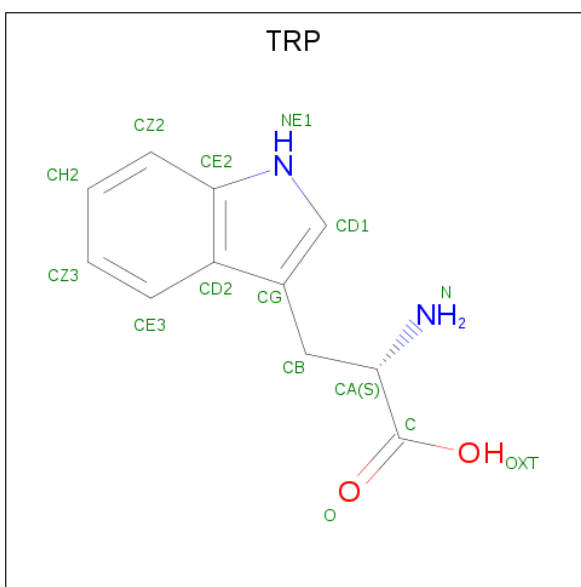
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3340	2106	580	640	14			
1	B	415	Total	C	N	O	S	0	0	0
			3288	2073	571	630	14			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is TRYPTOPHAN (three-letter code: TRP) (formula: C₁₁H₁₂N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	11	2	2		
3	B	1	Total	C	N	O	0	0
			15	11	2	2		

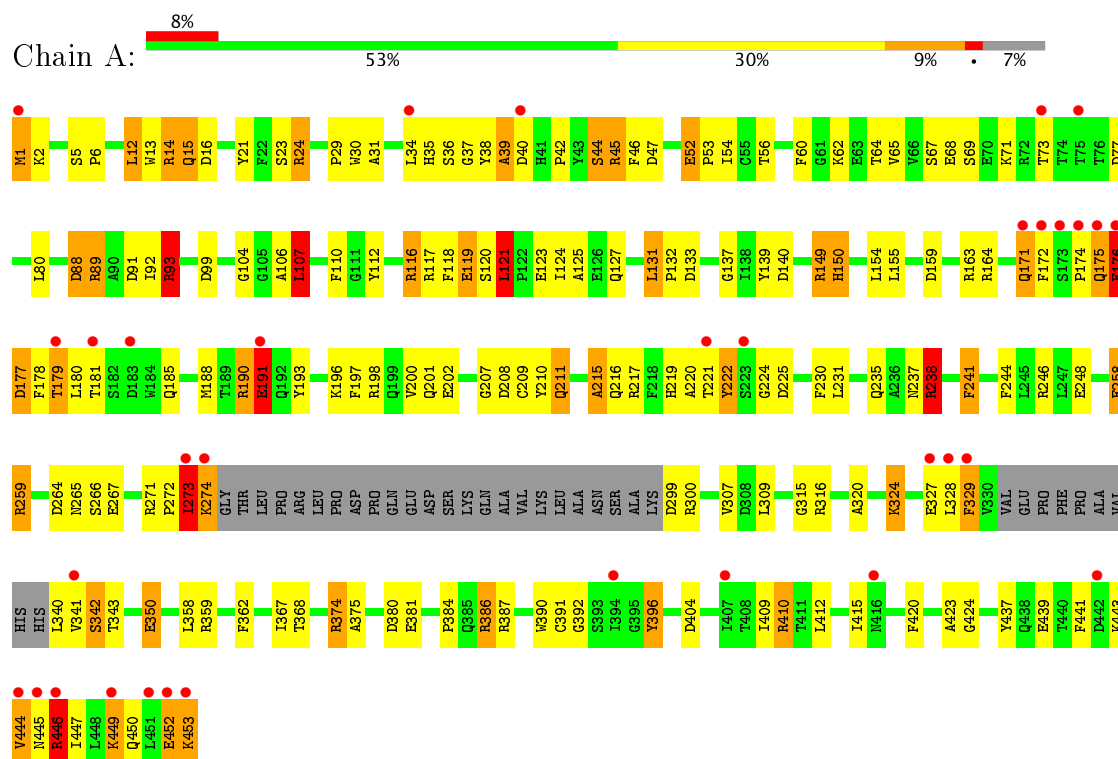
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	286	Total	O	0	0
			286	286		
4	B	274	Total	O	0	0
			274	274		

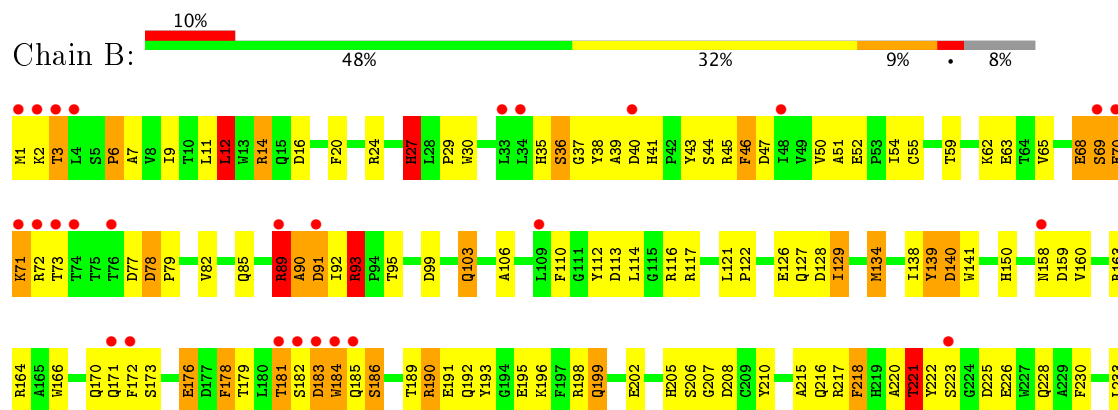
3 Residue-property plots

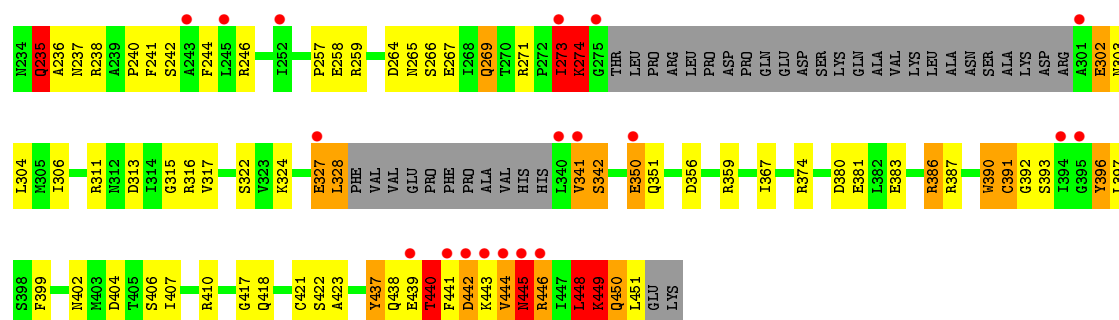
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: p-aminobenzoate synthase component I



• Molecule 1: p-aminobenzoate synthase component I





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.01Å 109.71Å 134.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.05 35.29 – 2.05	Depositor EDS
% Data completeness (in resolution range)	86.2 (10.00-2.05) 90.8 (35.29-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.05Å)	Xtriage
Refinement program	CNS, SHELXL-97	Depositor
R, R_{free}	0.172 , 0.238 0.177 , 0.231	Depositor DCC
R_{free} test set	4290 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 96.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7228	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	1.18	5/3410 (0.1%)	2.55	202/4626 (4.4%)
1	B	1.09	4/3357 (0.1%)	2.46	207/4557 (4.5%)
All	All	1.14	9/6767 (0.1%)	2.51	409/9183 (4.5%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	452	GLU	CD-OE1	22.80	1.50	1.25
1	A	452	GLU	CD-OE2	16.85	1.44	1.25
1	A	452	GLU	CG-CD	-9.04	1.38	1.51
1	B	383	GLU	CD-OE1	7.86	1.34	1.25
1	A	374	ARG	CZ-NH1	7.02	1.42	1.33
1	A	119	GLU	CB-CG	-5.95	1.40	1.52
1	B	406	SER	CB-OG	5.81	1.49	1.42
1	B	36	SER	CB-OG	5.17	1.49	1.42
1	B	393	SER	CA-CB	5.06	1.60	1.52

All (409) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	ARG	NE-CZ-NH1	25.30	132.95	120.30
1	A	45	ARG	NE-CZ-NH2	25.25	132.93	120.30
1	B	140	ASP	CB-CG-OD2	19.98	136.28	118.30
1	A	222	TYR	CB-CG-CD2	19.82	132.89	121.00
1	A	217	ARG	NE-CZ-NH1	18.14	129.37	120.30
1	B	316	ARG	NE-CZ-NH2	-17.36	111.62	120.30
1	A	238	ARG	NE-CZ-NH2	-16.80	111.90	120.30
1	B	246	ARG	NE-CZ-NH1	-16.73	111.94	120.30
1	B	410	ARG	NE-CZ-NH2	-16.57	112.02	120.30
1	A	45	ARG	NE-CZ-NH1	-16.46	112.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	ARG	NE-CZ-NH1	15.97	128.28	120.30
1	B	164	ARG	NE-CZ-NH1	-15.88	112.36	120.30
1	B	89	ARG	NE-CZ-NH2	-15.87	112.36	120.30
1	A	77	ASP	CB-CG-OD2	15.08	131.87	118.30
1	A	14	ARG	NE-CZ-NH2	-14.62	112.99	120.30
1	A	410	ARG	CA-CB-CG	14.62	145.56	113.40
1	B	246	ARG	NE-CZ-NH2	14.52	127.56	120.30
1	B	163	ARG	NE-CZ-NH1	14.37	127.48	120.30
1	A	446	ARG	NE-CZ-NH1	13.67	127.13	120.30
1	B	164	ARG	NE-CZ-NH2	13.29	126.94	120.30
1	A	387	ARG	NE-CZ-NH1	-12.96	113.82	120.30
1	A	185	GLN	CA-CB-CG	12.94	141.86	113.40
1	A	446	ARG	CD-NE-CZ	12.88	141.63	123.60
1	B	140	ASP	OD1-CG-OD2	-12.88	98.84	123.30
1	A	116	ARG	NE-CZ-NH2	12.49	126.55	120.30
1	A	386	ARG	NE-CZ-NH1	-12.42	114.09	120.30
1	A	374	ARG	NE-CZ-NH1	12.35	126.48	120.30
1	A	198	ARG	NE-CZ-NH1	12.24	126.42	120.30
1	B	271	ARG	NE-CZ-NH2	-12.23	114.18	120.30
1	B	159	ASP	CB-CG-OD2	-12.18	107.34	118.30
1	B	183	ASP	CB-CG-OD1	11.53	128.68	118.30
1	A	133	ASP	CB-CG-OD2	-11.51	107.94	118.30
1	A	410	ARG	NE-CZ-NH2	11.40	126.00	120.30
1	A	238	ARG	CA-CB-CG	11.22	138.08	113.40
1	A	52	GLU	OE1-CD-OE2	11.21	136.75	123.30
1	A	112	TYR	CD1-CE1-CZ	-11.15	109.77	119.80
1	B	78	ASP	CB-CG-OD1	10.79	128.01	118.30
1	A	24	ARG	NE-CZ-NH2	-10.73	114.94	120.30
1	B	222	TYR	CB-CG-CD1	-10.72	114.56	121.00
1	B	93	ARG	NE-CZ-NH2	-10.53	115.03	120.30
1	B	328	LEU	CA-C-O	-10.37	98.32	120.10
1	B	68	GLU	OE1-CD-OE2	10.36	135.73	123.30
1	B	78	ASP	CB-CG-OD2	-10.34	109.00	118.30
1	A	107	LEU	CA-CB-CG	10.31	139.02	115.30
1	A	198	ARG	NE-CZ-NH2	-10.25	115.18	120.30
1	B	259	ARG	NE-CZ-NH1	-10.08	115.26	120.30
1	B	89	ARG	NH1-CZ-NH2	10.04	130.44	119.40
1	A	149	ARG	NE-CZ-NH2	-10.00	115.30	120.30
1	A	273	ILE	C-N-CA	9.90	146.45	121.70
1	B	163	ARG	NE-CZ-NH2	-9.87	115.36	120.30
1	B	24	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	B	230	PHE	CB-CG-CD2	9.79	127.65	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	14	ARG	NE-CZ-NH1	9.78	125.19	120.30
1	A	210	TYR	CB-CG-CD2	-9.77	115.14	121.00
1	A	452	GLU	C-N-CA	9.63	145.77	121.70
1	A	178	PHE	CB-CG-CD2	9.54	127.48	120.80
1	B	91	ASP	CB-CG-OD2	-9.35	109.89	118.30
1	A	178	PHE	CG-CD2-CE2	9.28	131.01	120.80
1	B	311	ARG	NE-CZ-NH2	-9.16	115.72	120.30
1	B	182	SER	N-CA-CB	9.09	124.13	110.50
1	A	164	ARG	NE-CZ-NH2	9.07	124.84	120.30
1	A	210	TYR	CZ-CE2-CD2	-9.04	111.66	119.80
1	A	359	ARG	NE-CZ-NH2	9.03	124.82	120.30
1	B	190	ARG	NE-CZ-NH1	9.03	124.81	120.30
1	B	198	ARG	NE-CZ-NH1	8.99	124.80	120.30
1	B	43	TYR	CB-CG-CD1	8.98	126.39	121.00
1	A	222	TYR	CB-CG-CD1	-8.91	115.66	121.00
1	B	12	LEU	CA-CB-CG	-8.90	94.83	115.30
1	A	386	ARG	CD-NE-CZ	-8.88	111.17	123.60
1	B	316	ARG	CD-NE-CZ	8.81	135.93	123.60
1	B	176	GLU	OE1-CD-OE2	8.73	133.77	123.30
1	B	112	TYR	CB-CG-CD1	-8.71	115.77	121.00
1	A	271	ARG	CD-NE-CZ	-8.69	111.43	123.60
1	A	452	GLU	OE1-CD-OE2	-8.59	112.99	123.30
1	A	176	GLU	OE1-CD-OE2	-8.53	113.06	123.30
1	A	210	TYR	CG-CD1-CE1	-8.50	114.50	121.30
1	A	446	ARG	NE-CZ-NH2	-8.49	116.06	120.30
1	A	193	TYR	CB-CG-CD1	-8.46	115.93	121.00
1	A	244	PHE	CB-CG-CD1	8.44	126.71	120.80
1	A	40	ASP	CA-CB-CG	8.44	131.96	113.40
1	B	116	ARG	NE-CZ-NH2	-8.43	116.09	120.30
1	B	445	ASN	CA-CB-CG	8.41	131.90	113.40
1	B	235	GLN	O-C-N	8.36	136.08	122.70
1	A	415	ILE	CA-CB-CG1	8.32	126.81	111.00
1	A	178	PHE	CZ-CE2-CD2	-8.31	110.12	120.10
1	A	149	ARG	CD-NE-CZ	-8.29	112.00	123.60
1	A	193	TYR	CB-CG-CD2	8.24	125.95	121.00
1	A	230	PHE	CB-CG-CD1	-8.19	115.07	120.80
1	A	359	ARG	NE-CZ-NH1	-8.17	116.22	120.30
1	B	91	ASP	CB-CG-OD1	8.16	125.65	118.30
1	A	316	ARG	NE-CZ-NH1	8.11	124.35	120.30
1	A	178	PHE	CB-CG-CD1	-8.04	115.17	120.80
1	B	410	ARG	NE-CZ-NH1	7.99	124.29	120.30
1	B	440	THR	O-C-N	-7.98	109.94	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	ARG	CD-NE-CZ	-7.97	112.44	123.60
1	B	450	GLN	O-C-N	-7.92	110.03	122.70
1	A	89	ARG	NE-CZ-NH2	7.91	124.25	120.30
1	B	116	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	B	258	GLU	OE1-CD-OE2	-7.88	113.84	123.30
1	A	258	GLU	CB-CA-C	-7.87	94.67	110.40
1	A	40	ASP	CB-CG-OD2	7.77	125.29	118.30
1	B	450	GLN	CA-C-N	7.74	134.24	117.20
1	A	342	SER	N-CA-CB	-7.72	98.93	110.50
1	A	116	ARG	NE-CZ-NH1	-7.69	116.45	120.30
1	B	45	ARG	NE-CZ-NH2	7.69	124.14	120.30
1	B	225	ASP	CB-CG-OD1	7.66	125.19	118.30
1	A	119	GLU	CB-CG-CD	7.66	134.87	114.20
1	A	222	TYR	CG-CD1-CE1	7.61	127.39	121.30
1	A	93	ARG	CA-C-O	7.61	136.09	120.10
1	B	205	HIS	CA-CB-CG	-7.61	100.66	113.60
1	A	225	ASP	O-C-N	7.60	134.86	122.70
1	A	15	GLN	CA-CB-CG	7.59	130.09	113.40
1	B	421	CYS	CA-C-N	7.53	133.77	117.20
1	B	139	TYR	CD1-CE1-CZ	-7.49	113.06	119.80
1	A	404	ASP	CB-CG-OD1	7.49	125.04	118.30
1	A	42	PRO	O-C-N	7.47	134.66	122.70
1	B	316	ARG	NH1-CZ-NH2	7.43	127.58	119.40
1	B	181	THR	CA-CB-CG2	7.43	122.80	112.40
1	A	60	PHE	CZ-CE2-CD2	7.41	128.99	120.10
1	A	163	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	B	43	TYR	CB-CG-CD2	-7.38	116.57	121.00
1	B	393	SER	N-CA-CB	7.38	121.57	110.50
1	B	210	TYR	CG-CD2-CE2	7.37	127.19	121.30
1	B	198	ARG	NE-CZ-NH2	-7.37	116.62	120.30
1	A	40	ASP	O-C-N	-7.36	110.92	122.70
1	A	112	TYR	CB-CG-CD1	-7.36	116.59	121.00
1	B	238	ARG	CD-NE-CZ	7.35	133.90	123.60
1	B	448	LEU	CA-CB-CG	7.34	132.18	115.30
1	A	244	PHE	CB-CG-CD2	-7.33	115.67	120.80
1	B	140	ASP	CB-CG-OD1	7.31	124.88	118.30
1	B	51	ALA	N-CA-CB	7.27	120.28	110.10
1	B	16	ASP	CB-CG-OD1	7.24	124.82	118.30
1	B	393	SER	CB-CA-C	-7.22	96.39	110.10
1	B	236	ALA	CB-CA-C	-7.20	99.30	110.10
1	A	139	TYR	CB-CG-CD2	-7.19	116.69	121.00
1	A	381	GLU	CG-CD-OE2	-7.19	103.93	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	417	GLY	O-C-N	7.14	134.12	122.70
1	B	112	TYR	CG-CD1-CE1	-7.12	115.60	121.30
1	B	396	TYR	CZ-CE2-CD2	-7.12	113.39	119.80
1	B	202	GLU	OE1-CD-OE2	7.07	131.79	123.30
1	A	36	SER	C-N-CA	7.07	137.15	122.30
1	B	163	ARG	CD-NE-CZ	-7.07	113.71	123.60
1	B	184	TRP	O-C-N	-7.06	111.41	122.70
1	A	159	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	B	52	GLU	OE1-CD-OE2	-7.00	114.89	123.30
1	A	88	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	A	222	TYR	CZ-CE2-CD2	6.98	126.08	119.80
1	B	24	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	B	6	PRO	O-C-N	-6.93	111.60	122.70
1	B	40	ASP	O-C-N	-6.91	111.65	122.70
1	B	391	CYS	CA-CB-SG	-6.90	101.57	114.00
1	B	45	ARG	NE-CZ-NH1	-6.87	116.86	120.30
1	A	13	TRP	CE3-CZ3-CH2	6.86	128.75	121.20
1	A	40	ASP	CA-C-N	6.84	132.24	117.20
1	A	341	VAL	CA-CB-CG1	-6.83	100.66	110.90
1	B	183	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	A	241	PHE	CB-CG-CD2	-6.79	116.05	120.80
1	B	386	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	B	230	PHE	CB-CG-CD1	-6.77	116.06	120.80
1	A	39	ALA	O-C-N	-6.74	111.92	122.70
1	B	443	LYS	N-CA-CB	6.73	122.72	110.60
1	B	47	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	A	36	SER	O-C-N	-6.67	111.85	123.20
1	B	184	TRP	CG-CD2-CE3	-6.67	127.89	133.90
1	A	178	PHE	CG-CD1-CE1	-6.67	113.46	120.80
1	B	117	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	B	259	ARG	NH1-CZ-NH2	6.66	126.72	119.40
1	B	150	HIS	CA-CB-CG	-6.64	102.31	113.60
1	A	110	PHE	CZ-CE2-CD2	-6.64	112.13	120.10
1	A	52	GLU	CB-CG-CD	-6.63	96.29	114.20
1	A	209	CYS	CA-CB-SG	-6.63	102.06	114.00
1	B	217	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	24	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	176	GLU	CA-CB-CG	6.60	127.92	113.40
1	A	374	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	A	241	PHE	CG-CD2-CE2	-6.59	113.56	120.80
1	B	442	ASP	CA-CB-CG	6.58	127.87	113.40
1	A	230	PHE	CB-CG-CD2	6.57	125.40	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	PHE	CB-CG-CD1	6.57	125.40	120.80
1	B	244	PHE	CB-CG-CD1	-6.50	116.25	120.80
1	B	139	TYR	CG-CD2-CE2	-6.49	116.11	121.30
1	B	374	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	A	16	ASP	CB-CG-OD1	6.48	124.13	118.30
1	A	248	GLU	OE1-CD-OE2	-6.46	115.55	123.30
1	A	415	ILE	CB-CA-C	-6.44	98.72	111.60
1	B	110	PHE	CD1-CE1-CZ	-6.42	112.39	120.10
1	B	274	LYS	C-N-CA	6.42	135.79	122.30
1	B	315	GLY	CA-C-O	6.42	132.16	120.60
1	A	197	PHE	CB-CG-CD1	6.41	125.28	120.80
1	A	119	GLU	CB-CA-C	-6.39	97.62	110.40
1	A	110	PHE	CB-CG-CD1	-6.39	116.33	120.80
1	B	122	PRO	O-C-N	-6.37	112.51	122.70
1	A	197	PHE	CB-CG-CD2	-6.36	116.35	120.80
1	B	304	LEU	O-C-N	-6.36	112.53	122.70
1	B	139	TYR	CG-CD1-CE1	6.34	126.37	121.30
1	B	110	PHE	CB-CG-CD2	-6.33	116.37	120.80
1	B	178	PHE	O-C-N	6.32	132.82	122.70
1	A	208	ASP	CB-CG-OD1	6.32	123.99	118.30
1	A	272	PRO	O-C-N	-6.31	112.60	122.70
1	B	327	GLU	OE1-CD-OE2	-6.29	115.75	123.30
1	B	241	PHE	CA-CB-CG	-6.28	98.83	113.90
1	B	264	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	A	174	PRO	O-C-N	6.26	132.72	122.70
1	A	273	ILE	O-C-N	6.26	132.72	122.70
1	A	64	THR	O-C-N	6.25	132.71	122.70
1	B	441	PHE	CB-CG-CD2	6.25	125.17	120.80
1	A	380	ASP	CB-CG-OD2	6.23	123.91	118.30
1	A	40	ASP	OD1-CG-OD2	-6.22	111.48	123.30
1	B	89	ARG	NE-CZ-NH1	-6.22	117.19	120.30
1	A	238	ARG	CD-NE-CZ	6.21	132.30	123.60
1	A	176	GLU	CB-CG-CD	6.20	130.93	114.20
1	A	211	GLN	O-C-N	6.20	132.61	122.70
1	A	121	LEU	CA-CB-CG	6.18	129.52	115.30
1	B	417	GLY	CA-C-O	-6.18	109.47	120.60
1	A	99	ASP	CB-CG-OD1	6.17	123.85	118.30
1	A	220	ALA	N-CA-CB	6.16	118.73	110.10
1	A	380	ASP	CB-CG-OD1	6.14	123.82	118.30
1	A	264	ASP	CB-CG-OD1	6.13	123.82	118.30
1	B	172	PHE	CZ-CE2-CD2	-6.12	112.76	120.10
1	B	302	GLU	CA-CB-CG	-6.11	99.95	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	327	GLU	CA-C-N	6.11	130.65	117.20
1	B	221	THR	CA-CB-OG1	-6.08	96.24	109.00
1	B	242	SER	O-C-N	-6.07	112.98	122.70
1	A	200	VAL	O-C-N	-6.07	112.99	122.70
1	B	442	ASP	CB-CG-OD1	6.06	123.76	118.30
1	B	181	THR	N-CA-CB	-6.03	98.84	110.30
1	B	437	TYR	CB-CG-CD2	6.03	124.62	121.00
1	A	343	THR	CA-CB-CG2	-6.01	103.99	112.40
1	A	93	ARG	O-C-N	-6.00	109.70	121.10
1	A	38	TYR	CG-CD1-CE1	-6.00	116.50	121.30
1	B	402	ASN	CB-CG-ND2	-5.99	102.34	116.70
1	A	21	TYR	O-C-N	-5.98	113.14	122.70
1	A	215	ALA	CB-CA-C	-5.97	101.14	110.10
1	A	381	GLU	CB-CA-C	-5.97	98.45	110.40
1	A	210	TYR	CD1-CG-CD2	5.97	124.46	117.90
1	B	210	TYR	CZ-CE2-CD2	-5.95	114.44	119.80
1	A	77	ASP	CB-CG-OD1	-5.95	112.95	118.30
1	B	342	SER	N-CA-CB	-5.94	101.59	110.50
1	B	11	LEU	C-N-CA	-5.92	106.89	121.70
1	A	201	GLN	CA-CB-CG	-5.89	100.43	113.40
1	B	222	TYR	CB-CG-CD2	5.89	124.54	121.00
1	B	186	SER	O-C-N	-5.89	113.28	122.70
1	B	438	GLN	CB-CG-CD	5.89	126.91	111.60
1	A	93	ARG	CD-NE-CZ	-5.87	115.38	123.60
1	A	452	GLU	CB-CG-CD	-5.87	98.36	114.20
1	A	222	TYR	CD1-CG-CD2	-5.86	111.45	117.90
1	A	21	TYR	CA-C-N	5.86	130.09	117.20
1	B	89	ARG	CD-NE-CZ	-5.86	115.40	123.60
1	B	207	GLY	O-C-N	-5.85	113.34	122.70
1	A	150	HIS	CA-CB-CG	-5.84	103.67	113.60
1	B	359	ARG	CD-NE-CZ	-5.84	115.42	123.60
1	A	217	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	B	380	ASP	CB-CG-OD1	5.83	123.54	118.30
1	B	443	LYS	CA-C-N	-5.82	104.39	117.20
1	A	380	ASP	OD1-CG-OD2	-5.81	112.27	123.30
1	A	300	ARG	NE-CZ-NH1	-5.81	117.40	120.30
1	A	117	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	38	TYR	CD1-CE1-CZ	5.79	125.02	119.80
1	A	180	LEU	O-C-N	-5.77	113.46	122.70
1	A	46	PHE	CG-CD1-CE1	5.75	127.12	120.80
1	B	410	ARG	CD-NE-CZ	5.75	131.65	123.60
1	A	410	ARG	NE-CZ-NH1	-5.74	117.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	VAL	CG1-CB-CG2	5.74	120.08	110.90
1	B	226	GLU	OE1-CD-OE2	-5.73	116.42	123.30
1	A	374	ARG	CA-C-O	5.73	132.13	120.10
1	B	218	PHE	CB-CG-CD1	-5.72	116.80	120.80
1	B	63	GLU	CB-CG-CD	5.72	129.63	114.20
1	B	46	PHE	CB-CG-CD1	-5.71	116.80	120.80
1	B	184	TRP	CZ3-CH2-CZ2	5.70	128.44	121.60
1	A	231	LEU	CA-C-O	5.69	132.04	120.10
1	A	80	LEU	CA-C-O	5.67	132.02	120.10
1	A	191	GLU	N-CA-CB	-5.67	100.39	110.60
1	A	386	ARG	NH1-CZ-NH2	5.67	125.64	119.40
1	B	208	ASP	CA-CB-CG	-5.67	100.93	113.40
1	A	47	ASP	N-CA-CB	5.66	120.79	110.60
1	A	177	ASP	C-N-CA	-5.66	107.55	121.70
1	A	131	LEU	CB-CA-C	5.66	120.95	110.20
1	A	207	GLY	CA-C-O	-5.65	110.42	120.60
1	A	53	PRO	O-C-N	-5.64	113.67	122.70
1	B	106	ALA	O-C-N	5.64	131.73	122.70
1	A	180	LEU	C-N-CA	-5.64	107.60	121.70
1	A	309	LEU	N-CA-CB	-5.63	99.15	110.40
1	B	78	ASP	O-C-N	5.62	131.78	121.10
1	A	117	ARG	CD-NE-CZ	5.62	131.47	123.60
1	B	199	GLN	CA-CB-CG	5.62	125.76	113.40
1	A	202	GLU	OE1-CD-OE2	-5.61	116.56	123.30
1	B	271	ARG	CD-NE-CZ	-5.61	115.74	123.60
1	B	404	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	A	217	ARG	NH1-CZ-NH2	-5.60	113.24	119.40
1	B	444	VAL	O-C-N	5.59	131.65	122.70
1	B	99	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	B	178	PHE	CD1-CE1-CZ	-5.59	113.39	120.10
1	A	176	GLU	CG-CD-OE1	5.59	129.47	118.30
1	A	259	ARG	CG-CD-NE	-5.58	100.09	111.80
1	A	112	TYR	CG-CD1-CE1	5.58	125.76	121.30
1	B	273	ILE	CA-C-O	-5.57	108.40	120.10
1	B	350	GLU	O-C-N	-5.57	113.79	122.70
1	B	172	PHE	CG-CD2-CE2	5.56	126.92	120.80
1	A	65	VAL	O-C-N	-5.56	113.81	122.70
1	B	390	TRP	CG-CD1-NE1	-5.54	104.56	110.10
1	A	384	PRO	C-N-CA	-5.53	107.89	121.70
1	B	68	GLU	C-N-CA	5.52	135.51	121.70
1	B	38	TYR	CG-CD1-CE1	-5.52	116.89	121.30
1	A	267	GLU	OE1-CD-OE2	5.49	129.89	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	184	TRP	CH2-CZ2-CE2	-5.49	111.92	117.40
1	A	89	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	A	40	ASP	CB-CG-OD1	5.47	123.23	118.30
1	B	313	ASP	CB-CG-OD2	5.47	123.22	118.30
1	B	210	TYR	CA-CB-CG	-5.47	103.01	113.40
1	A	246	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	316	ARG	O-C-N	-5.46	113.96	122.70
1	B	241	PHE	CZ-CE2-CD2	-5.46	113.55	120.10
1	A	171	GLN	N-CA-CB	-5.46	100.78	110.60
1	A	452	GLU	CG-CD-OE2	5.45	129.19	118.30
1	A	31	ALA	O-C-N	-5.44	113.99	122.70
1	B	444	VAL	CA-C-O	-5.43	108.69	120.10
1	B	215	ALA	CB-CA-C	-5.43	101.96	110.10
1	B	215	ALA	O-C-N	5.43	131.38	122.70
1	B	178	PHE	CB-CG-CD2	-5.43	117.00	120.80
1	B	399	PHE	CB-CG-CD1	-5.42	117.00	120.80
1	A	125	ALA	O-C-N	-5.42	114.03	122.70
1	A	149	ARG	NH1-CZ-NH2	5.41	125.35	119.40
1	B	160	VAL	CA-CB-CG1	5.40	119.00	110.90
1	A	320	ALA	N-CA-CB	-5.40	102.55	110.10
1	B	241	PHE	CE1-CZ-CE2	5.39	129.71	120.00
1	B	380	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	B	210	TYR	CG-CD1-CE1	-5.37	117.01	121.30
1	B	7	ALA	CA-C-O	-5.36	108.84	120.10
1	B	421	CYS	CA-C-O	-5.36	108.85	120.10
1	B	182	SER	O-C-N	5.35	131.27	122.70
1	B	193	TYR	CB-CG-CD2	5.35	124.21	121.00
1	A	392	GLY	N-CA-C	-5.35	99.73	113.10
1	A	191	GLU	CB-CG-CD	-5.34	99.78	114.20
1	B	121	LEU	CA-C-O	-5.34	108.89	120.10
1	B	217	ARG	CG-CD-NE	-5.33	100.61	111.80
1	B	404	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	65	VAL	CA-CB-CG2	-5.32	102.92	110.90
1	B	173	SER	N-CA-CB	5.32	118.47	110.50
1	A	396	TYR	CB-CG-CD1	5.31	124.19	121.00
1	B	387	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	B	134	MET	CG-SD-CE	5.30	108.68	100.20
1	A	386	ARG	O-C-N	5.29	131.16	122.70
1	B	39	ALA	N-CA-CB	5.29	117.51	110.10
1	B	90	ALA	O-C-N	5.28	131.15	122.70
1	B	304	LEU	CA-C-O	5.28	131.19	120.10
1	B	274	LYS	CA-CB-CG	5.27	125.00	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	LYS	CB-CA-C	5.27	120.93	110.40
1	A	208	ASP	CA-C-O	-5.25	109.08	120.10
1	A	118	PHE	C-N-CA	5.25	134.81	121.70
1	A	375	ALA	O-C-N	-5.25	114.31	122.70
1	A	178	PHE	CD1-CE1-CZ	5.24	126.39	120.10
1	B	103	GLN	O-C-N	5.24	132.11	123.20
1	A	62	LYS	C-N-CA	-5.24	108.61	121.70
1	B	11	LEU	O-C-N	5.24	131.08	122.70
1	A	190	ARG	CA-C-O	5.24	131.09	120.10
1	B	16	ASP	C-N-CA	-5.24	108.61	121.70
1	B	404	ASP	CA-CB-CG	-5.23	101.89	113.40
1	B	269	GLN	N-CA-CB	5.23	120.01	110.60
1	A	374	ARG	CG-CD-NE	5.22	122.77	111.80
1	A	104	GLY	N-CA-C	-5.22	100.05	113.10
1	B	158	ASN	C-N-CA	-5.21	108.67	121.70
1	B	193	TYR	CB-CG-CD1	-5.21	117.88	121.00
1	A	164	ARG	NH1-CZ-NH2	-5.20	113.68	119.40
1	B	443	LYS	N-CA-C	-5.19	96.99	111.00
1	A	246	ARG	CD-NE-CZ	-5.19	116.33	123.60
1	B	128	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	B	267	GLU	OE1-CD-OE2	-5.19	117.08	123.30
1	A	452	GLU	CA-CB-CG	-5.19	101.99	113.40
1	A	31	ALA	N-CA-CB	5.18	117.36	110.10
1	A	217	ARG	O-C-N	-5.18	114.41	122.70
1	B	241	PHE	CB-CG-CD1	-5.18	117.17	120.80
1	B	392	GLY	O-C-N	-5.18	114.42	122.70
1	B	356	ASP	CB-CG-OD2	5.17	122.96	118.30
1	B	27	HIS	O-C-N	-5.17	114.43	122.70
1	B	443	LYS	CA-CB-CG	5.16	124.76	113.40
1	B	206	SER	C-N-CA	-5.16	111.47	122.30
1	A	179	THR	C-N-CA	-5.15	108.83	121.70
1	B	59	THR	O-C-N	-5.14	114.47	122.70
1	B	237	ASN	OD1-CG-ND2	5.14	133.72	121.90
1	B	341	VAL	CA-CB-CG2	-5.14	103.19	110.90
1	B	359	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	A	307	VAL	O-C-N	5.13	130.90	122.70
1	A	329	PHE	C-N-CA	5.13	134.52	121.70
1	A	444	VAL	CA-CB-CG2	-5.13	103.21	110.90
1	A	193	TYR	CZ-CE2-CD2	-5.12	115.19	119.80
1	A	174	PRO	C-N-CA	5.11	134.47	121.70
1	A	117	ARG	O-C-N	-5.10	114.53	122.70
1	B	418	GLN	CG-CD-OE1	-5.09	111.42	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	421	CYS	CA-CB-SG	-5.09	104.84	114.00
1	B	196	LYS	CB-CG-CD	-5.08	98.38	111.60
1	B	117	ARG	CG-CD-NE	-5.07	101.16	111.80
1	B	6	PRO	CA-C-N	5.07	128.35	117.20
1	A	299	ASP	CA-C-O	-5.07	109.46	120.10
1	B	222	TYR	CG-CD1-CE1	-5.06	117.25	121.30
1	B	407	ILE	C-N-CA	-5.06	109.05	121.70
1	A	315	GLY	O-C-N	-5.05	114.62	122.70
1	B	381	GLU	O-C-N	-5.04	114.63	122.70
1	A	219	HIS	CA-CB-CG	5.04	122.17	113.60
1	A	225	ASP	C-N-CA	-5.04	109.11	121.70
1	B	237	ASN	CA-CB-CG	-5.04	102.32	113.40
1	A	23	SER	CA-C-O	5.03	130.67	120.10
1	A	139	TYR	CG-CD1-CE1	-5.03	117.27	121.30
1	A	154	LEU	CA-C-O	5.03	130.66	120.10
1	A	155	LEU	CB-CG-CD1	5.02	119.53	111.00
1	B	311	ARG	CD-NE-CZ	-5.02	116.58	123.60
1	B	129	ILE	CB-CG1-CD1	-5.02	99.86	113.90
1	A	387	ARG	NH1-CZ-NH2	5.01	124.91	119.40
1	B	450	GLN	CA-CB-CG	-5.01	102.38	113.40
1	B	186	SER	CA-C-O	5.01	130.62	120.10

There are no chirality outliers.

There are no planarity outliers.

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	3340	0	3253	83	0
1	B	3288	0	3204	90	0
2	A	5	0	0	0	0
2	B	5	0	0	2	0
3	A	15	0	9	1	0
3	B	15	0	9	0	0
4	A	286	0	0	9	0
4	B	274	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7228	0	6475	163	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 12.

All (163) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:THR:HB	1:B:221:THR:HG22	1.54	0.90
1:B:444:VAL:HG23	1:B:448:LEU:HD11	1.65	0.78
1:A:15:GLN:HE22	1:B:178:PHE:H	1.32	0.77
1:B:216:GLN:HE21	1:B:440:THR:HG21	1.47	0.77
1:B:85:GLN:O	1:B:89:ARG:HG3	1.85	0.77
1:B:235:GLN:HA	1:B:235:GLN:OE1	1.85	0.76
1:B:35:HIS:HD2	1:B:37:GLY:H	1.32	0.74
1:A:328:LEU:HD21	4:A:1268:HOH:O	1.87	0.73
1:A:444:VAL:HA	1:A:446:ARG:NH2	2.03	0.73
1:A:35:HIS:HD2	1:A:37:GLY:H	1.38	0.70
1:A:191:GLU:HB2	4:A:1238:HOH:O	1.92	0.69
1:A:14:ARG:HA	1:B:228:GLN:HE22	1.57	0.68
1:A:235:GLN:HE22	1:B:449:LYS:HG2	1.57	0.67
1:A:12:LEU:HD22	1:A:12:LEU:H	1.60	0.64
1:A:116:ARG:NH1	1:A:121:LEU:HD13	2.12	0.64
1:B:322:SER:O	1:B:324:LYS:HE2	1.98	0.63
1:B:303:ASN:H	1:B:303:ASN:HD22	1.45	0.62
1:B:190:ARG:HD3	1:B:437:TYR:CE2	2.35	0.61
1:B:1:MET:O	1:B:2:LYS:HB3	1.99	0.61
1:B:442:ASP:HA	1:B:445:ASN:HB2	1.82	0.60
1:B:41:HIS:HB2	1:B:44:SER:OG	2.02	0.59
1:B:303:ASN:H	1:B:303:ASN:ND2	2.00	0.59
1:A:273:ILE:O	1:A:274:LYS:NZ	2.29	0.59
1:B:35:HIS:CD2	1:B:37:GLY:H	2.17	0.59
1:A:446:ARG:NH2	1:A:447:ILE:HD12	2.18	0.58
1:B:269:GLN:HE21	1:B:342:SER:CB	2.15	0.58
1:A:1:MET:CG	1:A:93:ARG:HD2	2.33	0.58
1:A:15:GLN:HE22	1:B:178:PHE:N	2.00	0.58
1:B:68:GLU:HB3	1:B:71:LYS:HZ3	1.67	0.58
1:B:216:GLN:HE21	1:B:440:THR:CG2	2.14	0.58
1:A:412:LEU:HA	1:A:420:PHE:O	2.04	0.58
1:B:2:LYS:HD3	1:B:95:THR:CG2	2.33	0.57
1:A:273:ILE:HD12	1:A:342:SER:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:HIS:CD2	1:A:37:GLY:H	2.22	0.56
1:B:35:HIS:HD2	1:B:37:GLY:N	2.01	0.55
1:B:442:ASP:HA	1:B:445:ASN:H	1.71	0.55
1:B:269:GLN:HE21	1:B:342:SER:HB3	1.70	0.55
1:B:442:ASP:CA	1:B:445:ASN:HB2	2.37	0.55
1:B:273:ILE:HG22	1:B:341:VAL:O	2.07	0.54
1:B:233:LEU:HD11	1:B:451:LEU:HD11	1.89	0.54
1:A:237:ASN:ND2	1:A:446:ARG:HD2	2.22	0.54
1:B:367:ILE:HD13	1:B:391:CYS:HB3	1.88	0.54
1:B:79:PRO:HB2	1:B:134:MET:HE3	1.91	0.53
1:A:449:LYS:O	1:A:453:LYS:O	2.27	0.53
1:B:126:GLU:HG3	1:B:127:GLN:N	2.22	0.53
1:A:446:ARG:HG2	4:A:1215:HOH:O	2.08	0.53
1:B:2:LYS:HG3	1:B:3:THR:H	1.74	0.52
1:B:79:PRO:HB2	1:B:134:MET:CE	2.38	0.52
1:A:116:ARG:HG2	1:A:121:LEU:CD1	2.40	0.52
4:A:1528:HOH:O	1:B:12:LEU:HD22	2.09	0.52
1:A:15:GLN:H	1:B:228:GLN:NE2	2.08	0.52
1:B:240:PRO:HD2	1:B:257:PRO:HA	1.92	0.52
1:A:177:ASP:O	1:A:224:GLY:HA3	2.08	0.51
1:A:15:GLN:NE2	1:B:178:PHE:H	2.02	0.51
1:A:215:ALA:HA	1:A:424:GLY:HA2	1.91	0.51
1:A:37:GLY:O	1:A:238:ARG:HA	2.09	0.51
1:A:265:ASN:O	1:A:266:SER:HB2	2.11	0.50
1:A:176:GLU:OE1	1:A:177:ASP:O	2.29	0.50
1:A:238:ARG:CB	1:A:238:ARG:HH11	2.24	0.50
1:B:2:LYS:HD3	1:B:95:THR:HG23	1.93	0.50
1:A:175:GLN:O	1:A:175:GLN:OE1	2.30	0.50
1:A:54:ILE:HD13	1:A:140:ASP:OD2	2.12	0.50
1:A:30:TRP:CE2	1:A:56:THR:HG21	2.47	0.50
1:A:1:MET:SD	1:A:93:ARG:HD2	2.52	0.50
1:B:444:VAL:O	1:B:448:LEU:HG	2.12	0.50
1:A:450:GLN:OE1	1:A:450:GLN:O	2.31	0.49
1:B:68:GLU:HB3	1:B:71:LYS:NZ	2.27	0.49
1:A:92:ILE:O	1:A:93:ARG:HG3	2.12	0.49
1:A:39:ALA:O	1:A:44:SER:OG	2.31	0.48
1:B:50:VAL:HB	1:B:139:TYR:CD2	2.47	0.48
1:A:444:VAL:HA	1:A:446:ARG:HH21	1.78	0.48
1:A:12:LEU:HD11	1:B:20:PHE:CD1	2.48	0.48
1:B:444:VAL:CG2	1:B:448:LEU:HD21	2.42	0.48
1:A:390:TRP:O	1:A:391:CYS:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ASP:HB2	1:B:82:VAL:CG2	2.43	0.47
1:B:195:GLU:HG3	4:B:1537:HOH:O	2.14	0.47
1:A:12:LEU:HD21	1:B:20:PHE:HD1	1.79	0.47
1:A:12:LEU:HD21	1:B:20:PHE:CD1	2.49	0.47
1:A:12:LEU:HD13	1:A:12:LEU:N	2.30	0.47
1:B:2:LYS:HD3	1:B:95:THR:HG22	1.96	0.47
1:A:54:ILE:O	1:A:68:GLU:HG3	2.15	0.47
1:B:113:ASP:OD1	2:B:702:PO4:O2	2.33	0.47
1:B:71:LYS:HZ3	1:B:71:LYS:HG2	1.57	0.46
1:A:211:GLN:NE2	4:A:1260:HOH:O	2.48	0.46
1:A:190:ARG:HD3	1:A:437:TYR:CD2	2.50	0.46
1:A:238:ARG:HH11	1:A:238:ARG:CA	2.29	0.46
1:B:190:ARG:HD3	1:B:437:TYR:CD2	2.50	0.46
1:A:235:GLN:NE2	1:B:449:LYS:HG2	2.27	0.46
1:B:72:ARG:O	1:B:72:ARG:HG2	2.15	0.46
1:B:129:ILE:HD13	1:B:129:ILE:HG21	1.40	0.46
1:B:265:ASN:O	1:B:266:SER:HB2	2.15	0.46
1:A:350:GLU:O	1:A:350:GLU:HG3	2.05	0.46
1:B:386:ARG:HG2	2:B:702:PO4:O3	2.16	0.46
1:A:340:LEU:HA	1:A:340:LEU:HD23	1.76	0.46
1:A:188:MET:HE2	1:A:196:LYS:HE3	1.98	0.46
1:A:89:ARG:NH1	4:A:1290:HOH:O	2.48	0.46
1:B:68:GLU:O	1:B:70:GLU:N	2.49	0.45
1:A:107:LEU:HD22	1:A:396:TYR:HB3	1.97	0.45
1:B:269:GLN:HE21	1:B:342:SER:HB2	1.81	0.45
1:B:2:LYS:HB2	1:B:2:LYS:HE3	1.33	0.45
1:B:3:THR:CG2	1:B:93:ARG:H	2.29	0.45
1:B:444:VAL:HB	1:B:448:LEU:HD21	1.97	0.45
1:A:441:PHE:O	1:A:445:ASN:N	2.49	0.45
1:B:55:CYS:HB3	1:B:138:ILE:HB	1.99	0.45
1:B:186:SER:HB2	1:B:218:PHE:CE1	2.52	0.45
1:A:106:ALA:HA	1:A:137:GLY:O	2.16	0.45
1:B:2:LYS:HG3	1:B:3:THR:N	2.31	0.45
1:A:88:ASP:O	1:A:93:ARG:NH2	2.48	0.45
1:A:116:ARG:HG2	1:A:121:LEU:HD11	1.98	0.45
1:A:324:LYS:NZ	4:A:1508:HOH:O	2.50	0.45
1:A:258:GLU:HG2	1:A:409:ILE:HD11	1.99	0.45
1:A:181:THR:N	1:A:221:THR:O	2.45	0.45
1:B:27:HIS:H	1:B:27:HIS:CD2	2.35	0.45
1:B:396:TYR:C	1:B:397:LEU:HD12	2.37	0.44
1:A:5:SER:HB2	1:A:6:PRO:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:PHE:CZ	1:A:259:ARG:HB2	2.53	0.43
1:A:443:LYS:O	1:A:446:ARG:NH2	2.50	0.43
1:B:166:TRP:O	1:B:170:GLN:HG2	2.18	0.43
1:B:90:ALA:O	1:B:92:ILE:HG13	2.18	0.43
1:A:367:ILE:HD12	1:A:368:THR:HG23	2.00	0.43
1:A:131:LEU:HA	1:A:132:PRO:HD3	1.90	0.43
1:B:71:LYS:HB3	1:B:71:LYS:HZ2	1.84	0.43
1:A:449:LYS:HG3	1:A:452:GLU:OE2	2.19	0.43
1:A:149:ARG:O	1:A:150:HIS:HB2	2.18	0.43
1:A:386:ARG:HH11	1:A:386:ARG:HD2	1.21	0.42
1:B:114:LEU:HD21	1:B:134:MET:CE	2.49	0.42
1:A:258:GLU:HB3	4:A:1515:HOH:O	2.19	0.42
1:A:29:PRO:O	1:A:30:TRP:HB2	2.20	0.42
1:A:35:HIS:HD2	1:A:37:GLY:N	2.13	0.42
1:B:9:ILE:HD13	1:B:9:ILE:HG21	1.88	0.42
1:B:41:HIS:CD2	1:B:274:LYS:HD2	2.54	0.42
1:B:29:PRO:O	1:B:30:TRP:HB2	2.20	0.42
1:A:123:GLU:HG2	1:A:123:GLU:H	1.57	0.42
1:A:123:GLU:HG2	4:A:1549:HOH:O	2.19	0.42
1:A:1:MET:SD	1:A:91:ASP:HA	2.60	0.42
1:B:444:VAL:HB	1:B:448:LEU:CD2	2.49	0.42
1:A:45:ARG:HH21	1:A:149:ARG:HD3	1.86	0.41
1:B:390:TRP:CE2	1:B:422:SER:HB2	2.55	0.41
1:B:6:PRO:CD	1:B:103:GLN:HE21	2.32	0.41
1:B:79:PRO:CG	1:B:114:LEU:HD11	2.49	0.41
1:A:127:GLN:O	1:A:127:GLN:HG2	2.20	0.41
1:A:358:LEU:O	1:A:362:PHE:HB2	2.20	0.41
1:B:184:TRP:HA	1:B:220:ALA:HB2	2.02	0.41
1:B:140:ASP:OD1	1:B:141:TRP:HD1	2.04	0.41
1:B:189:THR:OG1	1:B:192:GLN:HG3	2.21	0.41
1:B:303:ASN:N	1:B:303:ASN:ND2	2.68	0.41
1:B:390:TRP:CD2	1:B:422:SER:HB2	2.55	0.41
1:A:54:ILE:HD13	1:A:140:ASP:CG	2.41	0.41
1:A:181:THR:H	1:A:222:TYR:HA	1.85	0.41
1:B:179:THR:N	1:B:223:SER:O	2.48	0.41
1:B:176:GLU:O	1:B:228:GLN:HG3	2.21	0.41
1:A:124:ILE:HG21	1:A:124:ILE:HD13	1.81	0.41
1:A:237:ASN:HD21	1:A:446:ARG:HD2	1.85	0.40
1:B:450:GLN:HE21	1:B:450:GLN:HB2	1.54	0.40
1:A:34:LEU:HB3	3:A:601:TRP:CE2	2.56	0.40
1:B:306:ILE:HD13	1:B:306:ILE:HG21	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:ALA:HB2	1:B:444:VAL:CG1	2.52	0.40
1:B:41:HIS:HD2	1:B:274:LYS:NZ	2.20	0.40
1:B:306:ILE:HD13	1:B:328:LEU:HD12	2.03	0.40
1:B:36:SER:OG	1:B:46:PHE:O	2.37	0.40
1:A:120:SER:O	1:A:121:LEU:HB3	2.21	0.40
1:A:24:ARG:HD3	1:A:172:PHE:CZ	2.57	0.40
1:A:216:GLN:N	1:A:423:ALA:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	414/453 (91%)	399 (96%)	15 (4%)	0	100	100
1	B	409/453 (90%)	382 (93%)	22 (5%)	5 (1%)	15	6
All	All	823/906 (91%)	781 (95%)	37 (4%)	5 (1%)	28	17

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	69	SER
1	B	274	LYS
1	B	445	ASN
1	B	446	ARG
1	B	449	LYS

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	362/390 (93%)	332 (92%)	30 (8%)	13	6
1	B	356/390 (91%)	324 (91%)	32 (9%)	11	5
All	All	718/780 (92%)	656 (91%)	62 (9%)	12	5

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

Mol	Chain	Res	Type
1	A	1	MET
1	A	12	LEU
1	A	44	SER
1	A	52	GLU
1	A	67	SER
1	A	69	SER
1	A	71	LYS
1	A	73	THR
1	A	93	ARG
1	A	107	LEU
1	A	119	GLU
1	A	121	LEU
1	A	171	GLN
1	A	175	GLN
1	A	176	GLU
1	A	179	THR
1	A	191	GLU
1	A	238	ARG
1	A	273	ILE
1	A	274	LYS
1	A	324	LYS
1	A	327	GLU
1	A	329	PHE
1	A	350	GLU
1	A	374	ARG
1	A	410	ARG
1	A	439	GLU
1	A	446	ARG
1	A	449	LYS
1	A	453	LYS
1	B	3	THR
1	B	12	LEU
1	B	14	ARG

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Mol	Chain	Res	Type
1	B	27	HIS
1	B	54	ILE
1	B	62	LYS
1	B	69	SER
1	B	70	GLU
1	B	71	LYS
1	B	73	THR
1	B	78	ASP
1	B	89	ARG
1	B	91	ASP
1	B	93	ARG
1	B	171	GLN
1	B	183	ASP
1	B	185	GLN
1	B	191	GLU
1	B	199	GLN
1	B	221	THR
1	B	235	GLN
1	B	273	ILE
1	B	302	GLU
1	B	317	VAL
1	B	327	GLU
1	B	350	GLU
1	B	351	GLN
1	B	439	GLU
1	B	440	THR
1	B	446	ARG
1	B	448	LEU
1	B	449	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	35	HIS
1	A	171	GLN
1	A	199	GLN
1	A	211	GLN
1	A	235	GLN
1	A	237	ASN
1	B	27	HIS
1	B	35	HIS

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Mol	Chain	Res	Type
1	B	41	HIS
1	B	103	GLN
1	B	170	GLN
1	B	211	GLN
1	B	216	GLN
1	B	228	GLN
1	B	237	ASN
1	B	269	GLN
1	B	303	ASN
1	B	450	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TRP	A	601	-	11,16,16	0.93	0	11,22,22	1.92	4 (36%)
2	PO4	A	701	-	4,4,4	2.20	2 (50%)	6,6,6	2.33	3 (50%)
3	TRP	B	602	-	11,16,16	1.36	2 (18%)	11,22,22	1.66	3 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	B	702	-	4,4,4	0.78	0	6,6,6	0.73	0

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
3	TRP	A	601	-	-	0/3/8/8	0/2/2/2
2	PO4	A	701	-	-	0/0/0/0	0/0/0/0
3	TRP	B	602	-	-	0/3/8/8	0/2/2/2
2	PO4	B	702	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	PO4	P-O3	-2.09	1.47	1.54
3	B	602	TRP	CH2-CZ2	2.11	1.41	1.36
3	B	602	TRP	CH2-CZ3	2.86	1.45	1.38
2	A	701	PO4	P-O1	3.50	1.58	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	TRP	CH2-CZ2-CE2	-3.71	114.48	120.07
2	A	701	PO4	O4-P-O2	-3.24	96.00	107.90
3	B	602	TRP	CB-CG-CD1	-2.81	124.50	127.97
3	A	601	TRP	CB-CG-CD1	-2.41	124.99	127.97
3	A	601	TRP	CZ3-CE3-CD2	-2.40	117.45	120.88
3	B	602	TRP	CZ3-CH2-CZ2	-2.29	117.19	120.45
2	A	701	PO4	O3-P-O2	2.43	116.82	107.90
3	A	601	TRP	CZ3-CH2-CZ2	2.50	124.02	120.45
3	B	602	TRP	CB-CG-CD2	2.62	130.33	126.25
2	A	701	PO4	O4-P-O3	3.46	120.63	107.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	TRP	1	0
2	B	702	PO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	420/453 (92%)	0.51	34 (8%) 13 13	13, 23, 58, 102	0
1	B	415/453 (91%)	0.64	46 (11%) 6 6	11, 23, 60, 106	0
All	All	835/906 (92%)	0.58	80 (9%) 9 9	11, 23, 59, 106	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	8.9
1	B	301	ALA	8.7
1	B	70	GLU	7.4
1	B	442	ASP	6.0
1	B	69	SER	5.9
1	A	1	MET	5.6
1	B	273	ILE	5.5
1	B	71	LYS	5.4
1	B	72	ARG	5.3
1	A	416	ASN	5.2
1	A	453	LYS	5.2
1	A	273	ILE	5.1
1	A	274	LYS	4.9
1	B	441	PHE	4.9
1	B	340	LEU	4.7
1	A	329	PHE	4.6
1	A	176	GLU	4.6
1	B	181	THR	4.4
1	A	173	SER	4.2
1	A	175	GLN	4.0
1	B	444	VAL	3.7
1	A	327	GLU	3.7
1	B	445	ASN	3.7
1	A	445	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	171	GLN	3.6
1	A	174	PRO	3.6
1	A	179	THR	3.5
1	B	446	ARG	3.5
1	A	40	ASP	3.5
1	B	33	LEU	3.5
1	B	73	THR	3.3
1	A	172	PHE	3.3
1	B	183	ASP	3.2
1	B	34	LEU	3.1
1	A	444	VAL	3.1
1	B	394	ILE	3.0
1	B	2	LYS	3.0
1	B	443	LYS	3.0
1	B	252	ILE	2.9
1	B	275	GLY	2.9
1	B	158	ASN	2.9
1	B	341	VAL	2.9
1	A	171	GLN	2.9
1	B	74	THR	2.9
1	B	243	ALA	2.9
1	A	452	GLU	2.9
1	B	327	GLU	2.9
1	A	183	ASP	2.8
1	B	172	PHE	2.8
1	B	89	ARG	2.8
1	B	48	ILE	2.7
1	B	350	GLU	2.6
1	B	40	ASP	2.6
1	A	191	GLU	2.5
1	A	73	THR	2.5
1	B	439	GLU	2.5
1	A	223	SER	2.5
1	B	182	SER	2.5
1	A	181	THR	2.4
1	A	394	ILE	2.4
1	B	185	GLN	2.4
1	B	109	LEU	2.4
1	A	221	THR	2.4
1	A	341	VAL	2.4
1	B	4	LEU	2.3
1	B	245	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	449	LYS	2.3
1	A	328	LEU	2.3
1	A	446	ARG	2.3
1	B	76	THR	2.3
1	B	223	SER	2.2
1	A	34	LEU	2.2
1	A	75	THR	2.1
1	A	407	ILE	2.1
1	A	451	LEU	2.1
1	B	184	TRP	2.1
1	B	395	GLY	2.0
1	B	3	THR	2.0
1	A	442	ASP	2.0
1	B	91	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	TRP	A	601	15/15	0.96	0.16	0.33	12,16,18,22	0
3	TRP	B	602	15/15	0.95	0.19	0.19	11,16,21,22	0
2	PO4	A	701	5/5	0.98	0.12	-0.84	19,24,26,32	0
2	PO4	B	702	5/5	0.98	0.11	-0.87	15,16,19,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.