WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2023 – 04:58 AM EDT

PDB ID	:	1K7X
Title	:	CRYSTAL STRUCTURE OF THE BETA-SER178PRO MUTANT OF TRYPTOPHAN SYNTHASE
Authors	:	Weyand, M.; Schlichting, I.; Marabotti, A.; Mozzarelli, A.
Deposited on	:	2001-10-22
Resolution	:	1.70 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:

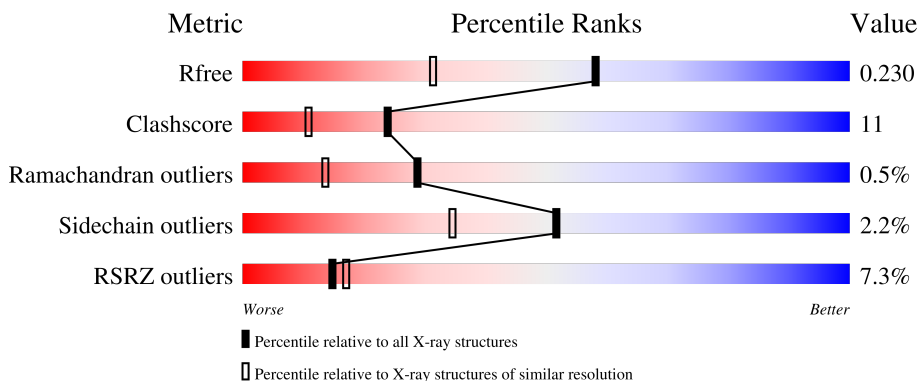|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.70 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	Percentile Ranks	Value
Rfree		0.230
Clashscore		11
Ramachandran outliers		0.5%
Sidechain outliers		2.2%
RSRZ outliers		7.3%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 <=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	268	12% / 37% 48% 9% · 5%
2	B	396	4% / 44% 46% 7% ··

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5326 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 TRYPTOPHAN SYNTHASE ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total 1917	C 1221	N 331	O 357	S 8	0	0	0

- Molecule 2 is a protein called TRYPTOPHAN SYNTHASE BETA CHAIN.

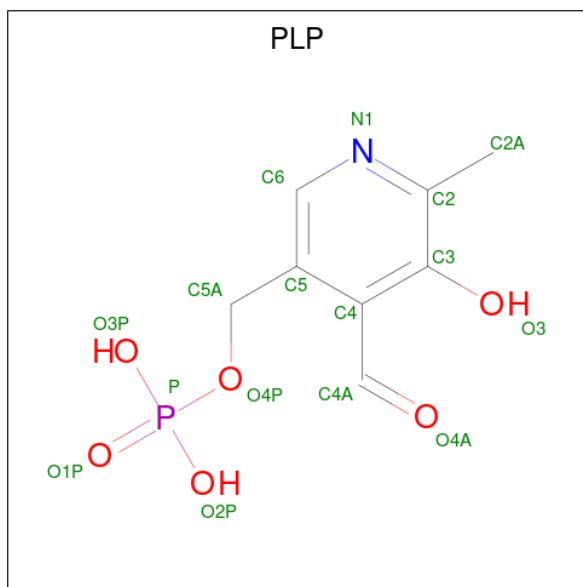| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	390	Total 2959	C 1861	N 517	O 561	S 20	0	3	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	34	SER	ARG	cloning artifact	UNP P0A2K1
B	178	PRO	SER	engineered mutation	UNP P0A2K1

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Na 1	0	0

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).

PLP

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

• Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	139	Total	O	0	0
			139	139		
5	B	295	Total	O	0	0
			295	295		

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: TRYPTOPHAN SYNTHASE ALPHA CHAIN
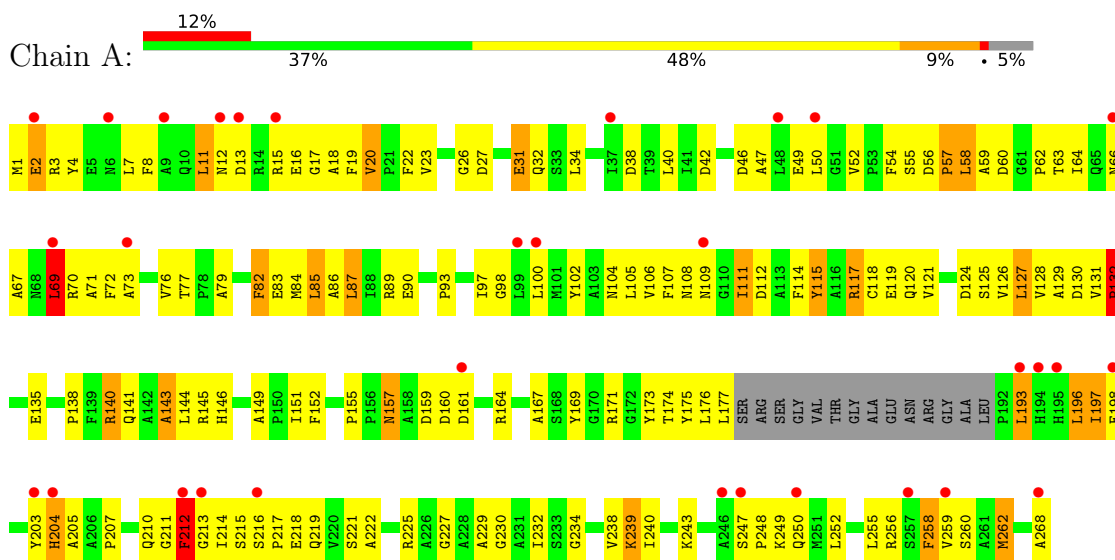
• Molecule 2: TRYPTOPHAN SYNTHASE BETA CHAIN
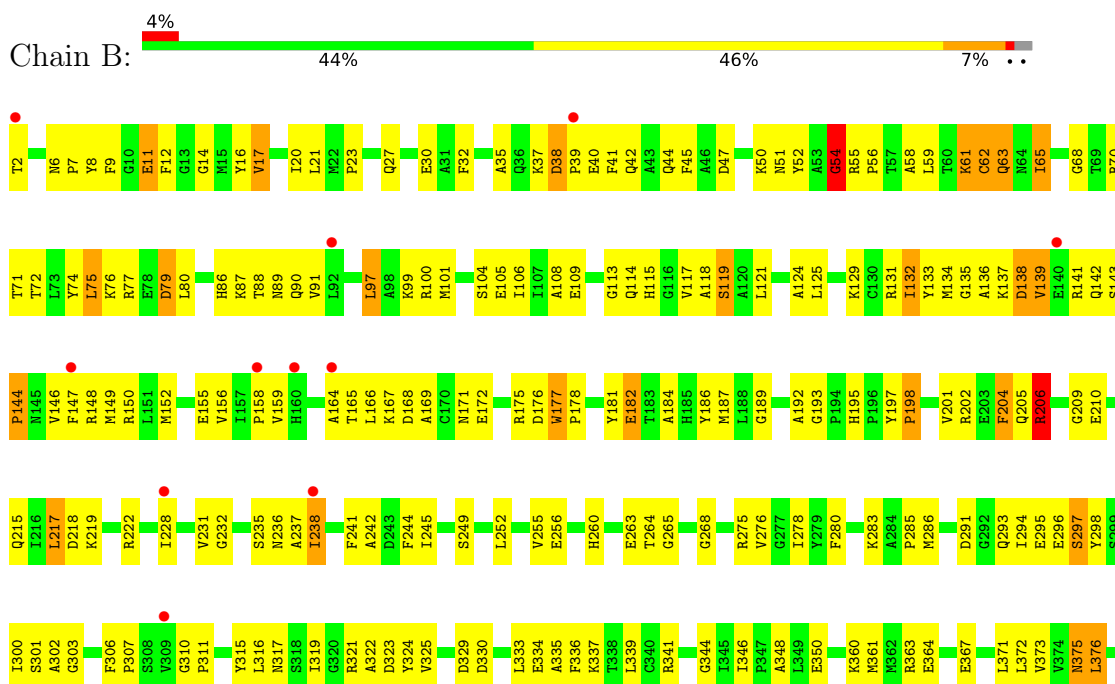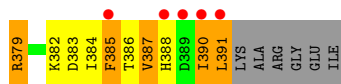
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	184.01Å 59.99Å 67.54Å 90.00° 94.65° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 29.16 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.8 (20.00-1.70) 96.8 (29.16-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 1.70Å)	Xtriage
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.187 , 0.238 0.184 , 0.230	Depositor DCC
R_{free} test set	3973 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	16.1	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 54.6	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5326	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	2.56	111/1955 (5.7%)	2.10	79/2656 (3.0%)
2	B	2.80	226/3035 (7.4%)	2.32	140/4101 (3.4%)
All	All	2.71	337/4990 (6.8%)	2.24	219/6757 (3.2%)

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
2	B	0	1

All (337) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	11	GLU	CD-OE2	15.02	1.42	1.25
1	A	102	TYR	CD1-CE1	14.04	1.60	1.39
2	B	32	PHE	CG-CD1	12.20	1.57	1.38
2	B	204	PHE	CD1-CE1	12.10	1.63	1.39
2	B	138	ASP	C-O	12.02	1.46	1.23
2	B	113	GLY	C-O	11.58	1.42	1.23
2	B	45	PHE	CE1-CZ	11.53	1.59	1.37
2	B	139	VAL	CB-CG2	11.30	1.76	1.52
1	A	82	PHE	CD2-CE2	11.03	1.61	1.39
1	A	152	PHE	CD1-CE1	10.76	1.60	1.39
1	A	140	ARG	CG-CD	10.71	1.78	1.51
2	B	390	ILE	CB-CG2	10.71	1.86	1.52
2	B	108	ALA	CA-CB	10.36	1.74	1.52
2	B	315	TYR	CD2-CE2	10.27	1.54	1.39
2	B	63	GLN	CG-CD	10.20	1.74	1.51
2	B	256	GLU	CD-OE1	10.20	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	11	GLU	CG-CD	10.08	1.67	1.51
1	A	18	ALA	CA-CB	10.05	1.73	1.52
2	B	295	GLU	CD-OE2	10.04	1.36	1.25
1	A	114	PHE	CE2-CZ	9.65	1.55	1.37
2	B	17	VAL	CB-CG2	9.51	1.72	1.52
1	A	117	ARG	CG-CD	9.48	1.75	1.51
1	A	83	GLU	CG-CD	9.45	1.66	1.51
2	B	117	VAL	CB-CG2	-9.44	1.33	1.52
2	B	124	ALA	CA-CB	9.40	1.72	1.52
2	B	295	GLU	CG-CD	9.35	1.66	1.51
1	A	121	VAL	CB-CG2	9.34	1.72	1.52
2	B	135	GLY	C-O	9.31	1.38	1.23
2	B	298	TYR	CE2-CZ	-9.20	1.26	1.38
1	A	111	ILE	CA-CB	9.13	1.75	1.54
2	B	164	ALA	C-O	9.06	1.40	1.23
1	A	83	GLU	CD-OE1	9.06	1.35	1.25
1	A	126	VAL	CB-CG1	9.04	1.71	1.52
2	B	298	TYR	CD2-CE2	9.03	1.52	1.39
2	B	387	VAL	CB-CG2	8.77	1.71	1.52
2	B	364	GLU	CD-OE2	-8.73	1.16	1.25
1	A	144	LEU	C-O	8.71	1.39	1.23
2	B	315	TYR	CG-CD1	8.65	1.50	1.39
2	B	235	SER	CB-OG	8.57	1.53	1.42
2	B	104	SER	CB-OG	8.56	1.53	1.42
2	B	324	TYR	CD2-CE2	8.42	1.51	1.39
1	A	107	PHE	CD2-CE2	8.40	1.56	1.39
2	B	319	ILE	C-O	-8.40	1.07	1.23
2	B	388	HIS	N-CA	8.39	1.63	1.46
2	B	302	ALA	C-O	-8.30	1.07	1.23
2	B	152	MET	SD-CE	-8.29	1.31	1.77
1	A	262	MET	CG-SD	8.27	2.02	1.81
2	B	311	PRO	N-CD	8.23	1.59	1.47
2	B	45	PHE	CG-CD1	8.20	1.51	1.38
2	B	280	PHE	CE1-CZ	8.15	1.52	1.37
1	A	227	GLY	C-O	8.14	1.36	1.23
1	A	259	VAL	CA-CB	8.12	1.71	1.54
2	B	263	GLU	CD-OE1	8.06	1.34	1.25
2	B	118	ALA	CA-CB	8.03	1.69	1.52
1	A	55	SER	N-CA	8.02	1.62	1.46
2	B	141	ARG	C-O	7.98	1.38	1.23
2	B	363	ARG	CB-CG	7.95	1.74	1.52
1	A	125	SER	CB-OG	7.93	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	PHE	CE2-CZ	7.90	1.52	1.37
2	B	295	GLU	CD-OE1	7.86	1.34	1.25
2	B	296	GLU	CB-CG	7.85	1.67	1.52
2	B	360	LYS	CB-CG	-7.83	1.31	1.52
2	B	76	LYS	CD-CE	7.82	1.70	1.51
2	B	61	LYS	N-CA	7.79	1.61	1.46
2	B	276	VAL	CB-CG1	7.76	1.69	1.52
2	B	39	PRO	C-O	7.76	1.38	1.23
1	A	198	GLU	CD-OE1	7.76	1.34	1.25
1	A	57	PRO	CA-CB	7.70	1.69	1.53
2	B	149	MET	CG-SD	7.65	2.01	1.81
2	B	61	LYS	CE-NZ	7.64	1.68	1.49
2	B	177	TRP	CE3-CZ3	-7.64	1.25	1.38
2	B	371	LEU	N-CA	7.60	1.61	1.46
1	A	114	PHE	CD1-CE1	7.60	1.54	1.39
2	B	298	TYR	CD1-CE1	7.56	1.50	1.39
2	B	100	ARG	CZ-NH1	-7.55	1.23	1.33
2	B	148	ARG	N-CA	7.54	1.61	1.46
2	B	325	VAL	CB-CG1	7.52	1.68	1.52
2	B	265	GLY	CA-C	7.51	1.63	1.51
2	B	165	THR	N-CA	7.50	1.61	1.46
2	B	379	ARG	CZ-NH1	-7.50	1.23	1.33
2	B	105	GLU	CD-OE2	7.47	1.33	1.25
2	B	294	ILE	C-O	7.44	1.37	1.23
1	A	173	TYR	CD1-CE1	-7.42	1.28	1.39
2	B	217	LEU	CG-CD2	7.40	1.79	1.51
1	A	135	GLU	CG-CD	7.40	1.63	1.51
1	A	17	GLY	C-O	7.38	1.35	1.23
1	A	49	GLU	CB-CG	7.33	1.66	1.52
2	B	39	PRO	N-CD	7.32	1.58	1.47
1	A	217	PRO	C-O	7.31	1.37	1.23
1	A	4	TYR	CE2-CZ	-7.26	1.29	1.38
2	B	37	LYS	CE-NZ	7.22	1.67	1.49
2	B	50	LYS	CE-NZ	7.14	1.66	1.49
1	A	175	TYR	CD1-CE1	-7.12	1.28	1.39
2	B	52	TYR	CG-CD2	-7.11	1.29	1.39
1	A	54	PHE	CG-CD2	7.11	1.49	1.38
1	A	205	ALA	CA-CB	7.07	1.67	1.52
2	B	256	GLU	CG-CD	7.07	1.62	1.51
2	B	62	CYS	CA-CB	7.06	1.69	1.53
1	A	4	TYR	CE1-CZ	7.02	1.47	1.38
2	B	100	ARG	C-O	6.99	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107	PHE	CG-CD2	6.99	1.49	1.38
2	B	8	TYR	CD2-CE2	6.97	1.49	1.39
1	A	54	PHE	CE1-CZ	-6.97	1.24	1.37
2	B	32	PHE	CE2-CZ	6.93	1.50	1.37
2	B	70	ARG	CA-CB	6.93	1.69	1.53
2	B	167	LYS	CE-NZ	6.92	1.66	1.49
2	B	59	LEU	N-CA	6.88	1.60	1.46
2	B	330	ASP	C-O	-6.88	1.10	1.23
1	A	155	PRO	CA-C	6.88	1.66	1.52
2	B	306	PHE	CD1-CE1	6.84	1.52	1.39
2	B	159	VAL	CB-CG1	6.84	1.67	1.52
2	B	97	LEU	CG-CD1	6.83	1.77	1.51
2	B	206	ARG	CB-CG	-6.83	1.34	1.52
2	B	231	VAL	CB-CG1	6.82	1.67	1.52
2	B	341	ARG	CZ-NH1	6.80	1.41	1.33
2	B	201	VAL	CB-CG2	6.80	1.67	1.52
2	B	310	GLY	N-CA	6.79	1.56	1.46
1	A	8	PHE	CE1-CZ	6.76	1.50	1.37
2	B	283	LYS	CE-NZ	6.76	1.66	1.49
2	B	40	GLU	CB-CG	6.75	1.65	1.52
2	B	181	TYR	CZ-OH	6.74	1.49	1.37
1	A	13	ASP	CB-CG	6.73	1.65	1.51
2	B	376	LEU	CG-CD2	6.70	1.76	1.51
2	B	244	PHE	CE1-CZ	6.68	1.50	1.37
1	A	175	TYR	CG-CD1	6.66	1.47	1.39
2	B	209	GLY	N-CA	6.62	1.55	1.46
1	A	26	GLY	CA-C	-6.62	1.41	1.51
2	B	307	PRO	CA-C	6.62	1.66	1.52
2	B	106	ILE	N-CA	6.60	1.59	1.46
2	B	205	GLN	CG-CD	6.54	1.66	1.51
2	B	283	LYS	N-CA	6.54	1.59	1.46
2	B	275	ARG	CG-CD	6.54	1.68	1.51
1	A	258	PHE	CB-CG	-6.52	1.40	1.51
2	B	350	GLU	CD-OE2	6.49	1.32	1.25
2	B	335	ALA	CA-CB	6.49	1.66	1.52
1	A	119	GLU	C-O	6.49	1.35	1.23
2	B	172	GLU	C-O	6.48	1.35	1.23
2	B	76	LYS	CA-CB	6.46	1.68	1.53
1	A	76	VAL	CB-CG1	6.43	1.66	1.52
2	B	206	ARG	CZ-NH2	6.43	1.41	1.33
2	B	133	TYR	CD1-CE1	6.42	1.49	1.39
1	A	129	ALA	CA-CB	6.40	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	35	ALA	CA-CB	6.38	1.65	1.52
1	A	152	PHE	CD2-CE2	6.37	1.51	1.39
2	B	231	VAL	CA-CB	-6.34	1.41	1.54
2	B	119	SER	CA-CB	6.33	1.62	1.52
2	B	249	SER	CB-OG	6.32	1.50	1.42
2	B	238	ILE	CB-CG2	6.29	1.72	1.52
2	B	202	ARG	CZ-NH2	6.28	1.41	1.33
1	A	214	ILE	N-CA	-6.26	1.33	1.46
1	A	84	MET	SD-CE	-6.26	1.42	1.77
2	B	150	ARG	CB-CG	6.21	1.69	1.52
2	B	285	PRO	CA-CB	6.21	1.66	1.53
1	A	79	ALA	CA-C	-6.20	1.36	1.52
1	A	135	GLU	CD-OE1	6.20	1.32	1.25
1	A	141	GLN	N-CA	-6.20	1.33	1.46
1	A	175	TYR	CE1-CZ	-6.19	1.30	1.38
2	B	344	GLY	CA-C	-6.19	1.42	1.51
2	B	215	GLN	N-CA	6.17	1.58	1.46
2	B	109	GLU	CB-CG	6.14	1.63	1.52
2	B	150	ARG	CZ-NH2	6.14	1.41	1.33
2	B	218	ASP	C-O	6.13	1.34	1.23
1	A	85	LEU	CG-CD1	6.12	1.74	1.51
2	B	88	THR	N-CA	6.12	1.58	1.46
2	B	16	TYR	CE2-CZ	6.12	1.46	1.38
2	B	264	THR	N-CA	6.12	1.58	1.46
1	A	83	GLU	N-CA	6.10	1.58	1.46
1	A	221	SER	CA-CB	6.06	1.62	1.52
2	B	186	TYR	CG-CD1	6.05	1.47	1.39
2	B	360	LYS	CD-CE	-6.04	1.36	1.51
1	A	12	ASN	CB-CG	6.04	1.65	1.51
2	B	382	LYS	CD-CE	6.03	1.66	1.51
1	A	70	ARG	CZ-NH1	6.03	1.40	1.33
2	B	150	ARG	CZ-NH1	6.03	1.40	1.33
1	A	38	ASP	N-CA	6.02	1.58	1.46
2	B	27	GLN	C-O	6.01	1.34	1.23
2	B	238	ILE	CA-C	5.98	1.68	1.52
1	A	115	TYR	CB-CG	5.98	1.60	1.51
2	B	14	GLY	CA-C	5.98	1.61	1.51
1	A	54	PHE	CD2-CE2	-5.97	1.27	1.39
1	A	55	SER	CA-CB	-5.97	1.44	1.52
2	B	156	VAL	CB-CG1	5.97	1.65	1.52
1	A	169	TYR	CD1-CE1	5.97	1.48	1.39
1	A	47	ALA	C-O	5.97	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	137	LYS	CA-CB	5.96	1.67	1.53
1	A	90	GLU	CD-OE2	5.96	1.32	1.25
2	B	37	LYS	CD-CE	5.96	1.66	1.51
2	B	316	LEU	C-O	5.95	1.34	1.23
2	B	175	ARG	CB-CG	5.95	1.68	1.52
2	B	373	VAL	N-CA	5.95	1.58	1.46
2	B	52	TYR	CD2-CE2	5.95	1.48	1.39
2	B	193	GLY	CA-C	5.94	1.61	1.51
1	A	132	PRO	CG-CD	5.92	1.70	1.50
1	A	218	GLU	CG-CD	5.90	1.60	1.51
2	B	363	ARG	NE-CZ	5.87	1.40	1.33
1	A	174	THR	C-O	5.87	1.34	1.23
1	A	160	ASP	C-O	5.86	1.34	1.23
1	A	90	GLU	CG-CD	5.86	1.60	1.51
2	B	344	GLY	C-O	5.85	1.33	1.23
2	B	181	TYR	CE2-CZ	5.84	1.46	1.38
1	A	62	PRO	N-CD	5.83	1.56	1.47
2	B	181	TYR	CG-CD2	-5.83	1.31	1.39
2	B	89	ASN	CG-ND2	5.83	1.47	1.32
2	B	235	SER	CA-CB	5.83	1.61	1.52
1	A	66	ASN	CB-CG	5.82	1.64	1.51
2	B	8	TYR	CB-CG	5.81	1.60	1.51
1	A	86	ALA	CA-CB	5.81	1.64	1.52
2	B	280	PHE	CD1-CE1	-5.77	1.27	1.39
2	B	41	PHE	CD1-CE1	5.76	1.50	1.39
1	A	4	TYR	CD1-CE1	5.75	1.48	1.39
1	A	20	VAL	CB-CG2	5.75	1.65	1.52
2	B	286	MET	CA-CB	5.73	1.66	1.53
2	B	8	TYR	CG-CD1	5.72	1.46	1.39
1	A	167	ALA	CA-C	-5.71	1.38	1.52
1	A	119	GLU	CA-C	5.71	1.67	1.52
2	B	303	GLY	C-O	-5.71	1.14	1.23
1	A	97	ILE	C-N	5.71	1.43	1.33
2	B	341	ARG	CG-CD	5.70	1.66	1.51
2	B	311	PRO	N-CA	-5.68	1.37	1.47
1	A	16	GLU	CB-CG	-5.67	1.41	1.52
2	B	133	TYR	CD2-CE2	5.67	1.47	1.39
2	B	148	ARG	CZ-NH2	5.66	1.40	1.33
2	B	232	GLY	C-O	-5.66	1.14	1.23
2	B	55	ARG	NE-CZ	5.65	1.40	1.33
2	B	9	PHE	CE1-CZ	5.65	1.48	1.37
2	B	52	TYR	CE2-CZ	5.65	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	341	ARG	CZ-NH2	5.64	1.40	1.33
2	B	74	TYR	CG-CD2	5.62	1.46	1.39
1	A	225	ARG	CZ-NH1	5.62	1.40	1.33
2	B	45	PHE	CG-CD2	5.62	1.47	1.38
2	B	298	TYR	CE1-CZ	5.62	1.45	1.38
1	A	216	SER	CB-OG	5.61	1.49	1.42
2	B	125	LEU	CG-CD2	5.61	1.72	1.51
2	B	158	PRO	C-O	5.58	1.34	1.23
1	A	77	THR	CB-CG2	5.57	1.70	1.52
1	A	143	ALA	CA-CB	5.57	1.64	1.52
2	B	168	ASP	CB-CG	5.56	1.63	1.51
2	B	70	ARG	CG-CD	5.54	1.65	1.51
2	B	341	ARG	CD-NE	5.54	1.55	1.46
1	A	23	VAL	CA-CB	5.54	1.66	1.54
1	A	131	VAL	C-O	5.53	1.33	1.23
2	B	192	ALA	CA-CB	5.52	1.64	1.52
1	A	31	GLU	CG-CD	5.51	1.60	1.51
2	B	41	PHE	C-O	5.50	1.33	1.23
1	A	102	TYR	CE2-CZ	5.50	1.45	1.38
2	B	268	GLY	C-O	5.49	1.32	1.23
2	B	142	GLN	CB-CG	5.49	1.67	1.52
2	B	346	ILE	N-CA	5.49	1.57	1.46
2	B	245	ILE	CA-CB	5.48	1.67	1.54
1	A	230	GLY	CA-C	5.48	1.60	1.51
2	B	68	GLY	C-O	5.47	1.32	1.23
2	B	260	HIS	C-O	5.46	1.33	1.23
2	B	386	THR	C-O	5.46	1.33	1.23
2	B	50	LYS	C-O	5.45	1.33	1.23
1	A	22	PHE	CE1-CZ	5.43	1.47	1.37
2	B	293	GLN	CB-CG	5.42	1.67	1.52
2	B	65	ILE	CB-CG2	5.42	1.69	1.52
2	B	255	VAL	C-O	5.42	1.33	1.23
2	B	32	PHE	CA-CB	5.41	1.65	1.53
1	A	62	PRO	CA-C	5.38	1.63	1.52
2	B	311	PRO	CA-CB	5.38	1.64	1.53
1	A	71	ALA	C-O	5.38	1.33	1.23
2	B	385	PHE	CG-CD1	5.37	1.46	1.38
2	B	324	TYR	CE2-CZ	5.36	1.45	1.38
2	B	195	HIS	N-CA	-5.36	1.35	1.46
2	B	237	ALA	CA-CB	5.36	1.63	1.52
2	B	275	ARG	CD-NE	5.35	1.55	1.46
2	B	45	PHE	CE2-CZ	5.35	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	72	THR	CA-CB	-5.35	1.39	1.53
1	A	250	GLN	CG-CD	5.35	1.63	1.51
2	B	30	GLU	CD-OE1	5.34	1.31	1.25
2	B	56	PRO	C-O	5.34	1.33	1.23
2	B	350	GLU	CB-CG	5.33	1.62	1.52
1	A	49	GLU	CG-CD	5.33	1.59	1.51
2	B	51	ASN	CG-ND2	5.33	1.46	1.32
1	A	102	TYR	CG-CD2	-5.33	1.32	1.39
1	A	210	GLN	C-O	5.31	1.33	1.23
1	A	73	ALA	CA-CB	-5.30	1.41	1.52
2	B	387	VAL	CB-CG1	-5.30	1.41	1.52
2	B	339	LEU	CB-CG	5.30	1.68	1.52
2	B	319	ILE	CA-CB	5.29	1.67	1.54
2	B	291	ASP	CB-CG	-5.28	1.40	1.51
1	A	70	ARG	NE-CZ	-5.28	1.26	1.33
2	B	361	MET	CB-CG	5.26	1.68	1.51
2	B	280	PHE	CG-CD2	5.25	1.46	1.38
1	A	239	LYS	CA-CB	5.25	1.65	1.53
2	B	391	LEU	C-O	5.25	1.33	1.23
2	B	101	MET	SD-CE	-5.24	1.48	1.77
2	B	375	ASN	N-CA	5.24	1.56	1.46
1	A	67	ALA	CA-CB	5.24	1.63	1.52
2	B	206	ARG	NE-CZ	5.23	1.39	1.33
2	B	166	LEU	CG-CD1	5.23	1.71	1.51
2	B	360	LYS	CE-NZ	5.23	1.62	1.49
2	B	334	GLU	CD-OE2	5.22	1.31	1.25
2	B	124	ALA	C-O	5.22	1.33	1.23
2	B	132	ILE	C-O	5.22	1.33	1.23
1	A	222	ALA	N-CA	-5.21	1.35	1.46
2	B	245	ILE	N-CA	5.21	1.56	1.46
2	B	42	GLN	CG-CD	5.21	1.63	1.51
1	A	225	ARG	CG-CD	5.20	1.65	1.51
2	B	241	PHE	CD1-CE1	5.20	1.49	1.39
2	B	6	ASN	CA-CB	5.20	1.66	1.53
2	B	136	ALA	CA-CB	5.19	1.63	1.52
1	A	145	ARG	NE-CZ	-5.19	1.26	1.33
2	B	155	GLU	CG-CD	5.18	1.59	1.51
1	A	164	ARG	N-CA	-5.16	1.36	1.46
2	B	298	TYR	CZ-OH	5.16	1.46	1.37
2	B	8	TYR	C-O	5.16	1.33	1.23
2	B	252	LEU	C-O	5.15	1.33	1.23
2	B	2	THR	N-CA	5.15	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	215	GLN	CG-CD	5.14	1.62	1.51
2	B	382	LYS	CB-CG	5.14	1.66	1.52
2	B	104	SER	CA-CB	5.13	1.60	1.52
2	B	244	PHE	CG-CD2	5.13	1.46	1.38
1	A	32	GLN	CG-CD	5.12	1.62	1.51
1	A	105	LEU	C-O	5.12	1.33	1.23
2	B	21	LEU	CG-CD2	5.12	1.70	1.51
1	A	50	LEU	CG-CD2	5.12	1.70	1.51
1	A	119	GLU	CG-CD	5.11	1.59	1.51
2	B	16	TYR	CG-CD1	5.11	1.45	1.39
2	B	317	ASN	CB-CG	5.10	1.62	1.51
2	B	99	LYS	N-CA	5.08	1.56	1.46
1	A	225	ARG	NE-CZ	5.07	1.39	1.33
2	B	206	ARG	CZ-NH1	5.07	1.39	1.33
2	B	171	ASN	N-CA	5.07	1.56	1.46
1	A	98	GLY	N-CA	5.06	1.53	1.46
2	B	186	TYR	CD2-CE2	5.06	1.47	1.39
2	B	382	LYS	N-CA	-5.06	1.36	1.46
1	A	17	GLY	CA-C	5.05	1.59	1.51
2	B	252	LEU	N-CA	5.04	1.56	1.46
1	A	128	VAL	CB-CG1	5.04	1.63	1.52
2	B	58	ALA	CA-CB	5.04	1.63	1.52
1	A	2	GLU	N-CA	5.01	1.56	1.46
2	B	144	PRO	CB-CG	5.01	1.75	1.50
2	B	301[A]	SER	CB-OG	-5.01	1.35	1.42
2	B	301[B]	SER	CB-OG	-5.01	1.35	1.42
1	A	106	VAL	CA-CB	5.00	1.65	1.54

All (219) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	206	ARG	NE-CZ-NH1	22.88	131.74	120.30
2	B	206	ARG	NE-CZ-NH2	-18.87	110.86	120.30
2	B	152	MET	CG-SD-CE	-16.83	73.28	100.20
1	A	225	ARG	NE-CZ-NH2	-14.90	112.85	120.30
2	B	176	ASP	CB-CG-OD2	13.76	130.68	118.30
2	B	100	ARG	NE-CZ-NH2	13.66	127.13	120.30
2	B	150	ARG	NE-CZ-NH1	-12.89	113.85	120.30
2	B	71	THR	CA-CB-CG2	-12.37	95.08	112.40
1	A	56	ASP	CB-CG-OD2	11.24	128.42	118.30
2	B	373	VAL	CA-CB-CG1	-11.15	94.17	110.90
2	B	321	ARG	NE-CZ-NH2	-11.05	114.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	376	LEU	CB-CG-CD2	-11.00	92.30	111.00
2	B	206	ARG	CD-NE-CZ	10.90	138.86	123.60
2	B	131	ARG	NE-CZ-NH1	10.47	125.54	120.30
1	A	117	ARG	NE-CZ-NH2	-10.33	115.13	120.30
2	B	291	ASP	CB-CG-OD2	10.29	127.56	118.30
2	B	363	ARG	NE-CZ-NH1	-10.23	115.19	120.30
2	B	47	ASP	CB-CG-OD2	10.07	127.36	118.30
2	B	41	PHE	CB-CG-CD1	-9.91	113.86	120.80
1	A	161	ASP	CB-CG-OD2	9.90	127.21	118.30
2	B	62	CYS	CA-CB-SG	-9.85	96.26	114.00
1	A	255	LEU	CB-CG-CD2	-9.63	94.63	111.00
1	A	256	ARG	NE-CZ-NH1	-9.55	115.52	120.30
1	A	117	ARG	NE-CZ-NH1	9.44	125.02	120.30
1	A	87	LEU	CA-CB-CG	9.40	136.92	115.30
2	B	38	ASP	CB-CG-OD1	-9.23	110.00	118.30
2	B	45	PHE	CD1-CE1-CZ	-9.22	109.03	120.10
1	A	115	TYR	CB-CG-CD2	-9.12	115.53	121.00
2	B	379	ARG	NE-CZ-NH2	8.95	124.78	120.30
2	B	315	TYR	CG-CD1-CE1	-8.92	114.16	121.30
2	B	169	ALA	N-CA-CB	-8.68	97.95	110.10
1	A	212	PHE	C-N-CA	-8.63	104.17	122.30
1	A	252	LEU	CB-CG-CD2	-8.61	96.37	111.00
1	A	196	LEU	CB-CG-CD1	8.57	125.57	111.00
2	B	325	VAL	CG1-CB-CG2	-8.49	97.32	110.90
2	B	45	PHE	CB-CG-CD2	-8.40	114.92	120.80
2	B	286	MET	CA-CB-CG	8.28	127.37	113.30
2	B	158	PRO	N-CD-CG	-8.19	90.91	103.20
1	A	89	ARG	NE-CZ-NH1	8.07	124.34	120.30
1	A	69	LEU	CB-CG-CD1	-7.98	97.43	111.00
1	A	82	PHE	CZ-CE2-CD2	-7.85	110.68	120.10
1	A	114	PHE	CB-CG-CD2	-7.84	115.31	120.80
2	B	204	PHE	CD1-CE1-CZ	-7.82	110.72	120.10
1	A	102	TYR	CD1-CE1-CZ	-7.81	112.77	119.80
2	B	159	VAL	CA-CB-CG2	-7.81	99.18	110.90
2	B	21	LEU	CA-CB-CG	7.79	133.21	115.30
2	B	222	ARG	NE-CZ-NH1	-7.78	116.41	120.30
1	A	124	ASP	CB-CG-OD1	7.73	125.26	118.30
2	B	150	ARG	NH1-CZ-NH2	7.71	127.89	119.40
2	B	65	ILE	CA-CB-CG1	-7.62	96.52	111.00
2	B	119	SER	N-CA-CB	-7.62	99.07	110.50
2	B	298	TYR	CA-CB-CG	-7.48	99.18	113.40
1	A	130	ASP	CB-CG-OD2	7.45	125.00	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	ASP	CB-CG-OD2	7.43	124.98	118.30
2	B	204	PHE	CB-CG-CD2	-7.41	115.61	120.80
1	A	109	ASN	N-CA-CB	-7.35	97.37	110.60
2	B	55	ARG	CD-NE-CZ	-7.33	113.34	123.60
1	A	84	MET	N-CA-CB	7.31	123.76	110.60
1	A	7	LEU	CB-CG-CD2	-7.27	98.65	111.00
2	B	77	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	A	16	GLU	N-CA-CB	-7.24	97.57	110.60
1	A	197	ILE	CG1-CB-CG2	-7.21	95.53	111.40
2	B	316	LEU	CB-CG-CD1	-7.13	98.87	111.00
2	B	298	TYR	CD1-CE1-CZ	-7.05	113.46	119.80
1	A	19	PHE	CB-CG-CD1	-7.04	115.88	120.80
1	A	27	ASP	CB-CG-OD2	6.94	124.55	118.30
2	B	152	MET	CB-CG-SD	-6.84	91.88	112.40
1	A	171	ARG	NE-CZ-NH2	-6.82	116.89	120.30
2	B	79	ASP	CB-CG-OD1	6.82	124.44	118.30
2	B	72	THR	OG1-CB-CG2	-6.78	94.42	110.00
1	A	159	ASP	CB-CG-OD2	6.77	124.39	118.30
2	B	367	GLU	OE1-CD-OE2	-6.77	115.18	123.30
1	A	225	ARG	NE-CZ-NH1	6.73	123.67	120.30
2	B	298	TYR	CE1-CZ-CE2	6.71	130.54	119.80
1	A	176	LEU	CB-CG-CD2	-6.70	99.62	111.00
2	B	80	LEU	CB-CG-CD2	-6.70	99.62	111.00
2	B	333	LEU	CB-CG-CD2	-6.68	99.64	111.00
2	B	321	ARG	NE-CZ-NH1	6.60	123.60	120.30
2	B	12	PHE	CB-CG-CD1	-6.59	116.19	120.80
2	B	175	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	A	118	CYS	N-CA-CB	-6.56	98.79	110.60
1	A	60	ASP	CB-CG-OD2	6.55	124.19	118.30
2	B	16	TYR	CB-CG-CD1	-6.50	117.10	121.00
1	A	72	PHE	CB-CG-CD1	-6.48	116.26	120.80
2	B	336	PHE	CB-CG-CD1	-6.48	116.27	120.80
2	B	315	TYR	CD1-CE1-CZ	6.47	125.63	119.80
2	B	295	GLU	CB-CA-C	-6.45	97.50	110.40
2	B	286	MET	N-CA-CB	-6.42	99.04	110.60
2	B	44	GLN	CA-CB-CG	-6.39	99.34	113.40
2	B	244	PHE	CB-CG-CD2	-6.39	116.33	120.80
1	A	238	VAL	CA-CB-CG2	-6.39	101.32	110.90
1	A	93	PRO	O-C-N	6.37	132.89	122.70
2	B	152	MET	CA-CB-CG	-6.36	102.49	113.30
2	B	364	GLU	OE1-CD-OE2	-6.36	115.67	123.30
2	B	383	ASP	CB-CG-OD2	6.32	123.99	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	219[A]	LYS	CA-CB-CG	-6.30	99.53	113.40
2	B	219[B]	LYS	CA-CB-CG	-6.30	99.53	113.40
1	A	138	PRO	N-CD-CG	-6.28	93.78	103.20
2	B	275	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	A	107	PHE	CG-CD2-CE2	-6.20	113.98	120.80
1	A	7	LEU	CD1-CG-CD2	-6.13	92.11	110.50
2	B	141	ARG	NE-CZ-NH2	-6.12	117.24	120.30
2	B	7	PRO	O-C-N	6.12	132.50	122.70
2	B	321	ARG	CB-CA-C	-6.12	98.17	110.40
2	B	215	GLN	CA-CB-CG	-6.11	99.96	113.40
2	B	121	LEU	CB-CG-CD2	-6.11	100.62	111.00
1	A	140	ARG	CG-CD-NE	-6.10	98.99	111.80
2	B	322	ALA	N-CA-CB	-6.10	101.56	110.10
2	B	184	ALA	CB-CA-C	-6.09	100.96	110.10
2	B	341	ARG	N-CA-CB	-6.09	99.64	110.60
1	A	54	PHE	CE1-CZ-CE2	6.08	130.94	120.00
2	B	55	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	A	58	LEU	CB-CG-CD1	-6.06	100.69	111.00
2	B	148	ARG	CG-CD-NE	6.06	124.53	111.80
2	B	97	LEU	CB-CA-C	-6.00	98.80	110.20
2	B	385	PHE	CB-CA-C	-5.99	98.43	110.40
1	A	102	TYR	CA-CB-CG	-5.97	102.06	113.40
2	B	12	PHE	CG-CD1-CE1	-5.96	114.25	120.80
1	A	11	LEU	CA-CB-CG	-5.95	101.61	115.30
1	A	151	ILE	CB-CA-C	-5.94	99.71	111.60
2	B	275	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	A	69	LEU	CA-CB-CG	-5.87	101.79	115.30
2	B	56	PRO	N-CA-CB	-5.84	96.17	102.60
2	B	99	LYS	CD-CE-NZ	-5.83	98.29	111.70
2	B	129	LYS	N-CA-CB	-5.81	100.14	110.60
2	B	323	ASP	CB-CG-OD2	5.81	123.53	118.30
2	B	321	ARG	CA-C-O	-5.81	107.91	120.10
2	B	348	ALA	O-C-N	5.80	131.97	122.70
2	B	263	GLU	CG-CD-OE2	-5.79	106.71	118.30
2	B	334	GLU	OE1-CD-OE2	-5.79	116.35	123.30
1	A	40	LEU	CB-CG-CD2	5.77	120.82	111.00
2	B	8	TYR	CG-CD2-CE2	-5.77	116.68	121.30
2	B	341	ARG	CG-CD-NE	5.76	123.91	111.80
2	B	361	MET	CA-CB-CG	-5.76	103.51	113.30
2	B	363	ARG	NH1-CZ-NH2	5.76	125.73	119.40
2	B	321	ARG	O-C-N	5.75	131.91	122.70
2	B	372	LEU	CB-CG-CD1	-5.74	101.24	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	100	ARG	NE-CZ-NH1	-5.73	117.44	120.30
2	B	367	GLU	CB-CA-C	5.73	121.85	110.40
1	A	87	LEU	CB-CG-CD1	5.72	120.72	111.00
2	B	228	ILE	CA-CB-CG1	-5.71	100.14	111.00
1	A	157	ASN	N-CA-CB	-5.71	100.32	110.60
1	A	177	LEU	N-CA-C	5.71	126.41	111.00
2	B	303	GLY	N-CA-C	5.70	127.35	113.10
2	B	58	ALA	O-C-N	5.69	131.81	122.70
1	A	54	PHE	N-CA-C	-5.68	95.66	111.00
2	B	65	ILE	CG1-CB-CG2	-5.68	98.90	111.40
2	B	75	LEU	CB-CG-CD2	-5.66	101.38	111.00
2	B	105	GLU	CB-CA-C	-5.66	99.09	110.40
2	B	182	GLU	OE1-CD-OE2	-5.65	116.52	123.30
1	A	127	LEU	N-CA-CB	-5.63	99.13	110.40
2	B	8	TYR	CG-CD1-CE1	5.61	125.79	121.30
2	B	198	PRO	CA-N-CD	5.61	119.55	111.70
1	A	140	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	A	59	ALA	CB-CA-C	-5.60	101.70	110.10
1	A	207	PRO	CB-CA-C	-5.58	98.04	112.00
2	B	252	LEU	CB-CG-CD2	5.56	120.45	111.00
2	B	138	ASP	O-C-N	-5.54	113.84	122.70
2	B	158	PRO	CA-CB-CG	-5.54	93.48	104.00
1	A	3	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	193	LEU	CB-CG-CD1	-5.53	101.59	111.00
2	B	315	TYR	CB-CG-CD1	-5.53	117.68	121.00
1	A	171	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	A	100	LEU	CB-CG-CD1	5.52	120.38	111.00
2	B	317	ASN	N-CA-CB	-5.51	100.69	110.60
2	B	367	GLU	N-CA-CB	-5.49	100.71	110.60
1	A	60	ASP	CB-CG-OD1	-5.48	113.36	118.30
2	B	9	PHE	CB-CG-CD2	-5.47	116.97	120.80
2	B	242	ALA	N-CA-CB	-5.47	102.44	110.10
1	A	46	ASP	CB-CG-OD2	5.45	123.20	118.30
2	B	52	TYR	CZ-CE2-CD2	-5.43	114.92	119.80
2	B	54	GLY	O-C-N	-5.43	114.02	122.70
2	B	371	LEU	CB-CG-CD1	-5.43	101.77	111.00
2	B	181	TYR	CB-CG-CD1	-5.39	117.76	121.00
1	A	106	VAL	O-C-N	-5.39	114.07	122.70
2	B	238	ILE	CG1-CB-CG2	-5.39	99.55	111.40
2	B	133	TYR	CZ-CE2-CD2	-5.39	114.95	119.80
2	B	23	PRO	O-C-N	5.38	131.31	122.70
2	B	132	ILE	CB-CG1-CD1	-5.38	98.85	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	229	ALA	C-N-CA	-5.34	111.08	122.30
1	A	49	GLU	CA-CB-CG	-5.33	101.68	113.40
1	A	109	ASN	CA-C-N	5.33	126.86	116.20
2	B	218	ASP	CB-CG-OD2	5.33	123.09	118.30
1	A	93	PRO	N-CD-CG	-5.32	95.22	103.20
2	B	298	TYR	CB-CG-CD2	-5.31	117.81	121.00
2	B	319	ILE	CA-C-N	-5.28	105.64	116.20
2	B	149	MET	CA-CB-CG	-5.27	104.34	113.30
2	B	291	ASP	OD1-CG-OD2	-5.26	113.31	123.30
2	B	297	SER	O-C-N	5.24	131.08	122.70
2	B	219[A]	LYS	CD-CE-NZ	-5.24	99.66	111.70
2	B	219[B]	LYS	CD-CE-NZ	-5.24	99.66	111.70
1	A	63	THR	OG1-CB-CG2	-5.23	97.96	110.00
2	B	106	ILE	CG1-CB-CG2	5.21	122.86	111.40
2	B	298	TYR	CD1-CG-CD2	5.19	123.61	117.90
2	B	91	VAL	CA-CB-CG1	-5.18	103.14	110.90
1	A	127	LEU	CA-CB-CG	-5.17	103.40	115.30
1	A	127	LEU	CB-CG-CD2	5.16	119.78	111.00
1	A	260	SER	CA-CB-OG	-5.16	97.26	111.20
1	A	4	TYR	CZ-CE2-CD2	5.14	124.43	119.80
1	A	256	ARG	NE-CZ-NH2	5.13	122.87	120.30
2	B	329	ASP	CB-CG-OD2	-5.13	113.68	118.30
2	B	319	ILE	CA-C-O	5.13	130.87	120.10
1	A	20	VAL	CA-CB-CG2	-5.12	103.22	110.90
1	A	52	VAL	CG1-CB-CG2	-5.11	102.72	110.90
2	B	280	PHE	CZ-CE2-CD2	-5.11	113.97	120.10
2	B	202	ARG	CD-NE-CZ	-5.10	116.46	123.60
2	B	134	MET	CB-CG-SD	-5.09	97.12	112.40
2	B	146	VAL	CA-CB-CG2	-5.09	103.26	110.90
2	B	11	GLU	CG-CD-OE2	5.06	128.42	118.30
2	B	198	PRO	N-CD-CG	-5.06	95.61	103.20
1	A	38	ASP	CB-CG-OD2	5.05	122.85	118.30
1	A	204	HIS	N-CA-CB	-5.05	101.51	110.60
2	B	177	TRP	CD1-NE1-CE2	-5.04	104.46	109.00
2	B	298	TYR	CE1-CZ-OH	-5.04	106.48	120.10
1	A	114	PHE	CD1-CG-CD2	5.04	124.85	118.30
1	A	69	LEU	CB-CG-CD2	5.02	119.54	111.00
1	A	152	PHE	CB-CG-CD2	-5.02	117.28	120.80
2	B	147	PHE	CB-CG-CD1	-5.01	117.29	120.80
2	B	47	ASP	CB-CG-OD1	-5.00	113.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	54	GLY	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1917	0	1927	45	0
2	B	2959	0	2933	65	0
3	B	1	0	0	0	0
4	B	15	0	7	1	0
5	A	139	0	0	2	0
5	B	295	0	0	2	0
All	All	5326	0	4867	108	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 11.

All (108) 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:240:ILE:CD1	1:A:240:ILE:CG1	1.76	1.64
1:A:111:ILE:CA	1:A:111:ILE:CB	1.75	1.62
2:B:217:LEU:CD2	2:B:217:LEU:CG	1.79	1.61
1:A:85:LEU:CG	1:A:85:LEU:CD1	1.74	1.59
1:A:140:ARG:CD	1:A:140:ARG:CG	1.78	1.58
1:A:117:ARG:CG	1:A:117:ARG:CD	1.75	1.58
2:B:376:LEU:CD2	2:B:376:LEU:CG	1.76	1.57
2:B:139:VAL:CB	2:B:139:VAL:CG2	1.76	1.57
2:B:97:LEU:CD1	2:B:97:LEU:CG	1.77	1.56
2:B:63:GLN:CD	2:B:63:GLN:CG	1.74	1.56
2:B:390:ILE:CG2	2:B:390:ILE:CB	1.86	1.52
2:B:61:LYS:CE	2:B:61:LYS:NZ	1.68	1.51
2:B:144:PRO:CG	2:B:144:PRO:CB	1.75	1.50
1:A:262:MET:CG	1:A:262:MET:SD	2.02	1.47
2:B:376:LEU:CD2	2:B:376:LEU:CB	2.37	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LEU:HG	1:A:197:ILE:HD12	1.54	0.86
2:B:97:LEU:CD1	2:B:97:LEU:CB	2.53	0.86
2:B:337:LYS:HE3	2:B:391:LEU:HD21	1.58	0.84
2:B:61:LYS:NZ	2:B:61:LYS:CD	2.44	0.80
1:A:211:GLY:O	1:A:212:PHE:CB	2.29	0.80
1:A:262:MET:SD	1:A:262:MET:CB	2.71	0.79
2:B:182:GLU:HG3	5:B:738:HOH:O	1.80	0.79
1:A:85:LEU:CD1	1:A:85:LEU:CD2	2.63	0.77
1:A:140:ARG:CG	1:A:140:ARG:NE	2.49	0.76
2:B:337:LYS:CE	2:B:391:LEU:HD21	2.15	0.75
2:B:376:LEU:CD2	2:B:376:LEU:CD1	2.65	0.74
1:A:85:LEU:CD1	1:A:85:LEU:CB	2.66	0.71
2:B:63:GLN:CD	2:B:63:GLN:CB	2.62	0.68
2:B:139:VAL:CG2	2:B:139:VAL:CG1	2.69	0.68
2:B:337:LYS:NZ	2:B:391:LEU:CD2	2.58	0.67
2:B:217:LEU:CD2	2:B:217:LEU:CD1	2.69	0.66
1:A:111:ILE:CB	1:A:111:ILE:C	2.61	0.66
1:A:111:ILE:CB	1:A:111:ILE:N	2.57	0.66
1:A:117:ARG:CD	1:A:117:ARG:CB	2.71	0.65
1:A:240:ILE:CD1	1:A:240:ILE:CB	2.72	0.65
2:B:54:GLY:O	5:B:777:HOH:O	2.14	0.64
2:B:337:LYS:NZ	2:B:391:LEU:HD21	2.14	0.63
1:A:203:TYR:O	1:A:204:HIS:HB2	1.99	0.62
2:B:337:LYS:HE3	2:B:391:LEU:HD11	1.80	0.62
1:A:117:ARG:NH1	1:A:120:GLN:OE1	2.31	0.61
2:B:337:LYS:CE	2:B:391:LEU:HD11	2.31	0.61
2:B:139:VAL:CG2	2:B:139:VAL:CA	2.77	0.60
1:A:111:ILE:CA	1:A:111:ILE:CG1	2.77	0.60
1:A:112:ASP:OD1	1:A:146:HIS:HE1	1.85	0.59
1:A:239:LYS:O	1:A:243:LYS:HG3	2.02	0.58
2:B:177:TRP:N	2:B:178:PRO:CD	2.65	0.58
2:B:206:ARG:HD3	2:B:210:GLU:OE2	2.03	0.57
2:B:337:LYS:NZ	2:B:391:LEU:HD22	2.19	0.57
2:B:337:LYS:HZ1	2:B:391:LEU:HD22	1.70	0.57
2:B:390:ILE:CG2	2:B:390:ILE:C	2.74	0.55
2:B:300:ILE:HD11	2:B:390:ILE:CD1	2.36	0.55
1:A:20:VAL:HB	1:A:232:ILE:HG12	1.87	0.55
2:B:20:ILE:HD13	2:B:178:PRO:HB3	1.88	0.55
1:A:15:ARG:O	1:A:268:ALA:HB2	2.08	0.54
2:B:390:ILE:CG2	2:B:390:ILE:CA	2.83	0.53
2:B:62:CYS:SG	2:B:75:LEU:HG	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:LYS:NZ	2:B:61:LYS:HD2	2.22	0.53
2:B:11:GLU:HG2	2:B:11:GLU:O	2.10	0.52
2:B:376:LEU:CD2	2:B:376:LEU:HB3	2.37	0.52
1:A:140:ARG:CD	1:A:140:ARG:CB	2.76	0.51
1:A:215:SER:N	1:A:219:GLN:OE1	2.26	0.51
1:A:213:GLY:N	5:A:281:HOH:O	2.43	0.51
2:B:206:ARG:CD	2:B:210:GLU:OE2	2.59	0.51
1:A:111:ILE:CA	1:A:111:ILE:CG2	2.82	0.50
2:B:115:HIS:CE1	2:B:189:GLY:HA2	2.47	0.49
2:B:38:ASP:OD1	2:B:38:ASP:C	2.51	0.49
2:B:337:LYS:CE	2:B:391:LEU:CD2	2.89	0.49
1:A:31:GLU:HA	1:A:31:GLU:OE1	2.12	0.49
1:A:58:LEU:C	1:A:58:LEU:HD12	2.32	0.49
2:B:217:LEU:CD2	2:B:217:LEU:CB	2.82	0.48
2:B:143:SER:HB2	2:B:144:PRO:HD3	1.94	0.48
1:A:1:MET:HG2	1:A:149:ALA:HB2	1.95	0.47
1:A:157:ASN:OD1	1:A:157:ASN:C	2.51	0.47
1:A:34:LEU:HD11	1:A:87:LEU:HD12	1.97	0.47
2:B:87:LYS:NZ	4:B:400:PLP:O3	2.47	0.47
1:A:262:MET:CG	1:A:262:MET:CE	2.92	0.46
1:A:117:ARG:CG	1:A:117:ARG:NE	2.66	0.45
2:B:61:LYS:HE3	2:B:63:GLN:CG	2.46	0.45
1:A:82:PHE:CE1	1:A:117:ARG:HG3	2.52	0.45
2:B:63:GLN:CG	2:B:63:GLN:NE2	2.64	0.45
2:B:384:ILE:HG13	2:B:385:PHE:N	2.30	0.45
2:B:300:ILE:HD11	2:B:390:ILE:HD13	1.98	0.45
1:A:69:LEU:HD22	1:A:69:LEU:HA	1.68	0.45
2:B:387:VAL:O	2:B:387:VAL:HG12	2.16	0.45
1:A:104:ASN:HB2	2:B:278:ILE:O	2.17	0.45
2:B:97:LEU:HA	2:B:97:LEU:HD23	1.60	0.45
2:B:390:ILE:O	2:B:391:LEU:C	2.55	0.44
2:B:379:ARG:HH11	2:B:379:ARG:HD3	1.56	0.44
2:B:390:ILE:CG2	2:B:390:ILE:CG1	2.81	0.44
2:B:337:LYS:HZ2	2:B:391:LEU:CD2	2.31	0.44
1:A:258:PHE:O	1:A:262:MET:HG2	2.18	0.44
2:B:87:LYS:HD2	2:B:114:GLN:HG3	1.98	0.44
2:B:61:LYS:HE3	2:B:63:GLN:HG3	1.99	0.43
1:A:64:ILE:HD11	1:A:234:GLY:O	2.18	0.43
2:B:132:ILE:HD13	2:B:132:ILE:HG21	1.77	0.43
1:A:132:PRO:HD3	2:B:17:VAL:O	2.19	0.42
2:B:86:HIS:CE1	2:B:236:ASN:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:ASP:O	2:B:139:VAL:C	2.58	0.42
1:A:11:LEU:HA	1:A:11:LEU:HD23	1.70	0.42
1:A:82:PHE:CD1	1:A:117:ARG:HG3	2.54	0.42
1:A:212:PHE:CA	5:A:281:HOH:O	2.67	0.42
2:B:119:SER:HA	2:B:187[A]:MET:HE3	2.01	0.41
2:B:238:ILE:HD12	2:B:238:ILE:HA	1.91	0.41
2:B:90:GLN:HA	2:B:204:PHE:HB3	2.02	0.41
1:A:115:TYR:CD1	1:A:143:ALA:HA	2.56	0.41
1:A:127:LEU:C	1:A:127:LEU:HD23	2.41	0.41
2:B:197:TYR:N	2:B:198:PRO:CD	2.84	0.41
2:B:79:ASP:HB2	2:B:379:ARG:HB3	2.03	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	250/268 (93%)	244 (98%)	3 (1%)	3 (1%)	13	3
2	B	391/396 (99%)	380 (97%)	11 (3%)	0	100	100
All	All	641/664 (96%)	624 (97%)	14 (2%)	3 (0%)	29	13

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	212	PHE
1	A	2	GLU

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	198/208 (95%)	191 (96%)	7 (4%)	36	17
2	B	309/310 (100%)	305 (99%)	4 (1%)	69	56
All	All	507/518 (98%)	496 (98%)	11 (2%)	52	34

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	PRO
1	A	69	LEU
1	A	132	PRO
1	A	196	LEU
1	A	247	SER
1	A	248	PRO
1	A	249	LYS
2	B	65	ILE
2	B	206	ARG
2	B	297	SER
2	B	375	ASN

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

Mol	Chain	Res	Type
1	A	80	GLN
2	B	27	GLN
2	B	44	GLN
2	B	236	ASN
2	B	375	ASN

5.3.3 RNA ⓘ

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	PLP	B	400	2	15,15,16	2.26	5 (33%)	20,22,23	2.66	7 (35%)

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	PLP	B	400	2	-	0/6/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	400	PLP	C2A-C2	5.23	1.59	1.50
4	B	400	PLP	C5A-C5	3.85	1.61	1.50
4	B	400	PLP	C4A-C4	-3.19	1.45	1.51
4	B	400	PLP	C6-C5	-2.52	1.32	1.37
4	B	400	PLP	O4P-C5A	2.07	1.52	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	400	PLP	C5A-C5-C6	6.39	129.88	119.37
4	B	400	PLP	O4P-C5A-C5	6.22	121.20	109.35
4	B	400	PLP	C6-C5-C4	-4.52	114.60	118.16
4	B	400	PLP	C5-C6-N1	3.29	129.29	123.82
4	B	400	PLP	C2A-C2-C3	2.49	123.97	120.89
4	B	400	PLP	C4A-C4-C5	-2.49	118.37	120.94
4	B	400	PLP	O4P-P-O1P	-2.07	100.67	106.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	400	PLP	1	0

5.7　Other polymers ⓘ

There are no such residues in this entry.

5.8　Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	254/268 (94%)	0.68	31 (12%)	4	4	13, 23, 44, 72	0
2	B	390/396 (98%)	0.23	16 (4%)	37	41	10, 16, 28, 49	0
All	All	644/664 (96%)	0.41	47 (7%)	15	17	10, 19, 38, 72	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	212	PHE	6.8
1	A	213	GLY	4.8
1	A	194	HIS	4.4
2	B	385	PHE	4.3
1	A	247	SER	4.3
2	B	391	LEU	4.0
2	B	390	ILE	3.9
2	B	388	HIS	3.9
1	A	13	ASP	3.9
2	B	389	ASP	3.8
2	B	140	GLU	3.7
2	B	2	THR	3.7
1	A	195	HIS	3.6
1	A	250	GLN	3.6
1	A	246	ALA	3.4
1	A	69	LEU	3.3
1	A	48	LEU	3.3
1	A	99	LEU	3.2
1	A	257	SER	3.1
1	A	268	ALA	3.0
2	B	160	HIS	2.9
1	A	161	ASP	2.8
2	B	39	PRO	2.8
2	B	147	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	203	TYR	2.7
1	A	2	GLU	2.7
2	B	228	ILE	2.6
1	A	100	LEU	2.6
1	A	12	ASN	2.6
2	B	92	LEU	2.5
2	B	238	ILE	2.5
2	B	309	VAL	2.5
1	A	73	ALA	2.4
1	A	198	GLU	2.4
2	B	158	PRO	2.4
1	A	6	ASN	2.4
1	A	193	LEU	2.3
1	A	109	ASN	2.3
1	A	15	ARG	2.3
1	A	9	ALA	2.2
1	A	66	ASN	2.2
1	A	216	SER	2.2
2	B	164	ALA	2.2
1	A	50	LEU	2.1
1	A	37	ILE	2.1
1	A	204	HIS	2.0
1	A	259	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\mathring{A}^2$)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\mathring{A}^2$)	Q<0.9
3	NA	B	500	1/1	0.99	0.06	14,14,14,14	0
4	PLP	B	400	15/16	0.99	0.08	9,14,27,31	0

6.5 Other polymers ⓘ

There are no such residues in this entry.