



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:26 PM GMT

PDB ID : 1FLG
Title : CRYSTAL STRUCTURE OF THE QUINOPROTEIN ETHANOL DEHYDROGENASE FROM PSEUDOMONAS AERUGINOSA
Authors : Keitel, T.; Diehl, A.; Knaute, T.; Stezowski, J.J.; Hohne, W.; Gorisch, H.
Deposited on : 2000-08-14
Resolution : 2.60 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

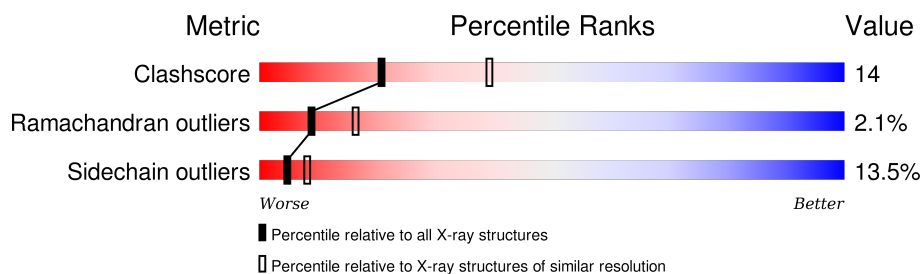
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	582	 48% 34% 15% •
1	B	582	 50% 34% 13% •

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9232 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.

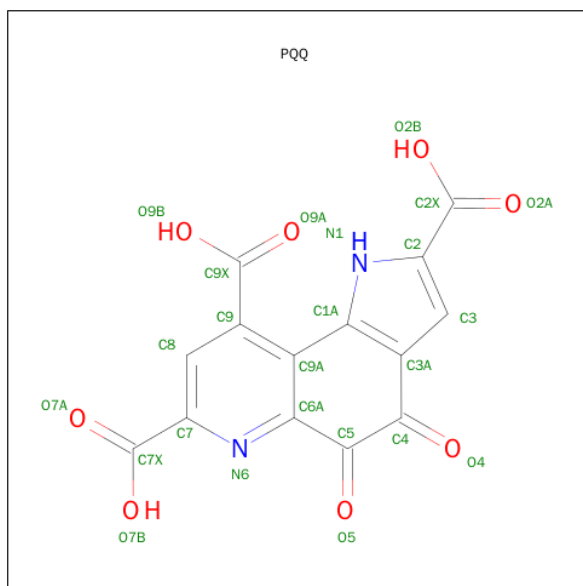
- Molecule 1 is a protein called PROTEIN (QUINOPROTEIN ETHANOL DEHYDROGENASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	0	0	0
			4537	2891	783	852	11			
1	B	582	Total	C	N	O	S	0	0	0
			4537	2891	783	852	11			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is PYRROLOQUINOLINE QUINONE (three-letter code: PQQ) (formula: C₁₄H₆N₂O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			24	14	2	8		
3	B	1	Total	C	N	O	0	0
			24	14	2	8		

- Molecule 4 is water.

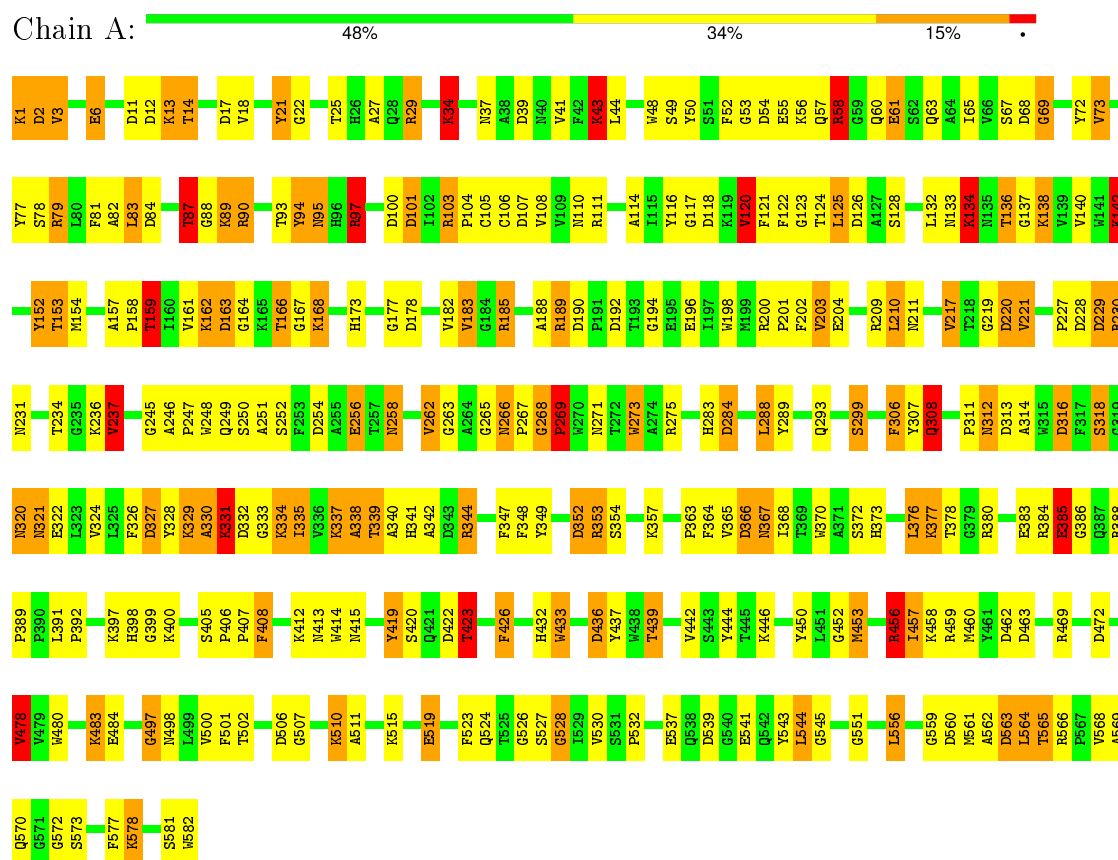
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	73	Total	O	0	0
			73	73		
4	B	33	Total	O	0	0
			33	33		

3 Residue-property plots [i](#)

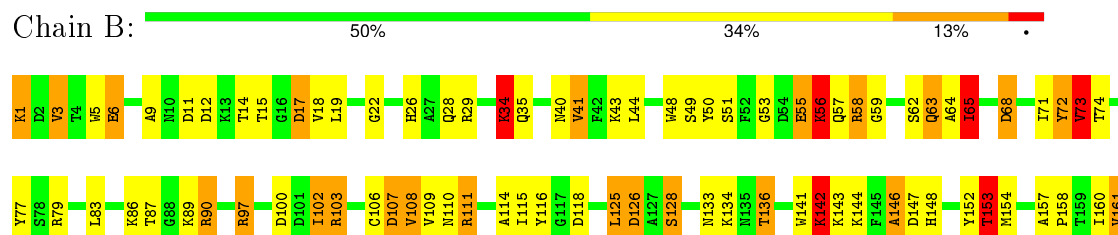
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: PROTEIN (QUINOPROTEIN ETHANOL DEHYDROGENASE)



• Molecule 1: PROTEIN (QUINOPROTEIN ETHANOL DEHYDROGENASE)





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	159.40 Å 159.40 Å 130.95 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	12.50 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (12.50-2.60)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.192 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9232	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.05	8/4679 (0.2%)	2.69	315/6366 (4.9%)
1	B	0.82	0/4679	2.19	175/6366 (2.7%)
All	All	0.95	8/9358 (0.1%)	2.45	490/12732 (3.8%)

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	36
1	B	0	21
All	All	0	57

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	367	ASN	N-CA	11.72	1.69	1.46
1	A	386	GLY	N-CA	7.77	1.57	1.46
1	A	299	SER	CB-OG	-6.44	1.33	1.42
1	A	312	ASN	N-CA	6.12	1.58	1.46
1	A	88	GLY	N-CA	5.66	1.54	1.46
1	A	414	TRP	CD2-CE3	5.34	1.48	1.40
1	A	414	TRP	CA-CB	5.15	1.65	1.53
1	A	366	ASP	C-O	5.07	1.32	1.23

All (490) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	ARG	NE-CZ-NH2	-36.92	101.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	29	ARG	NE-CZ-NH2	29.67	135.14	120.30
1	A	29	ARG	CD-NE-CZ	27.13	161.58	123.60
1	A	348	PHE	CB-CG-CD1	24.74	138.12	120.80
1	A	469	ARG	NE-CZ-NH1	-23.27	108.67	120.30
1	A	348	PHE	CB-CG-CD2	-23.15	104.59	120.80
1	A	288	LEU	C-N-CA	21.98	176.66	121.70
1	A	459	ARG	NE-CZ-NH2	-19.29	110.66	120.30
1	B	288	LEU	C-N-CA	19.22	169.76	121.70
1	A	209	ARG	NE-CZ-NH1	-18.55	111.02	120.30
1	A	118	ASP	CB-CG-OD1	18.54	134.98	118.30
1	A	537	GLU	OE1-CD-OE2	18.28	145.24	123.30
1	A	385	GLU	CA-C-N	16.86	149.92	116.20
1	A	103	ARG	NE-CZ-NH2	-16.64	111.98	120.30
1	A	79	ARG	NE-CZ-NH2	16.30	128.45	120.30
1	A	469	ARG	NE-CZ-NH2	16.08	128.34	120.30
1	A	472	ASP	CB-CG-OD1	16.04	132.73	118.30
1	A	366	ASP	O-C-N	-15.40	98.06	122.70
1	A	29	ARG	NE-CZ-NH2	-15.39	112.60	120.30
1	A	29	ARG	NE-CZ-NH1	14.43	127.51	120.30
1	A	103	ARG	CD-NE-CZ	14.40	143.76	123.60
1	A	77	TYR	CB-CG-CD2	-14.25	112.45	121.00
1	A	307	TYR	CB-CG-CD1	14.19	129.51	121.00
1	A	353	ARG	NH1-CZ-NH2	13.78	134.55	119.40
1	A	185	ARG	NE-CZ-NH2	13.58	127.09	120.30
1	A	307	TYR	CB-CG-CD2	-13.58	112.85	121.00
1	A	90	ARG	NE-CZ-NH2	-13.53	113.53	120.30
1	B	97	ARG	CD-NE-CZ	13.43	142.40	123.60
1	B	268	GLY	CA-C-O	-13.38	96.51	120.60
1	B	436	ASP	CB-CG-OD1	13.38	130.34	118.30
1	B	189	ARG	NE-CZ-NH2	-13.35	113.63	120.30
1	A	126	ASP	CB-CG-OD1	13.24	130.21	118.30
1	A	384	ARG	NE-CZ-NH2	13.17	126.89	120.30
1	A	61	GLU	OE1-CD-OE2	-13.14	107.53	123.30
1	A	87	THR	CA-C-N	12.93	142.06	116.20
1	B	11	ASP	CB-CG-OD2	12.73	129.76	118.30
1	A	284	ASP	CB-CG-OD1	-12.72	106.85	118.30
1	B	153	THR	CA-CB-CG2	12.64	130.09	112.40
1	B	209	ARG	CD-NE-CZ	12.61	141.26	123.60
1	A	103	ARG	NE-CZ-NH1	12.36	126.48	120.30
1	B	343	ASP	CB-CG-OD2	12.30	129.37	118.30
1	B	209	ARG	NE-CZ-NH1	12.20	126.40	120.30
1	B	483	LYS	CA-CB-CG	12.05	139.92	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	ARG	NE-CZ-NH1	11.95	126.27	120.30
1	B	469	ARG	CD-NE-CZ	11.44	139.62	123.60
1	B	185	ARG	NE-CZ-NH1	-11.37	114.61	120.30
1	A	68	ASP	C-N-CA	-11.26	98.65	122.30
1	B	29	ARG	NE-CZ-NH1	-11.22	114.69	120.30
1	A	275	ARG	NE-CZ-NH2	11.20	125.90	120.30
1	A	366	ASP	CB-CA-C	-11.15	88.11	110.40
1	A	433	TRP	CA-CB-CG	10.99	134.58	113.70
1	B	12	ASP	CB-CG-OD2	-10.91	108.48	118.30
1	A	14	THR	O-C-N	-10.87	105.31	122.70
1	A	469	ARG	CD-NE-CZ	10.86	138.81	123.60
1	A	288	LEU	CA-C-O	10.76	142.70	120.10
1	A	228	ASP	CB-CG-OD1	10.73	127.96	118.30
1	B	79	ARG	NE-CZ-NH1	10.73	125.66	120.30
1	B	437	TYR	CB-CG-CD2	-10.72	114.57	121.00
1	B	273	TRP	CA-CB-CG	-10.65	93.46	113.70
1	A	209	ARG	NE-CZ-NH2	10.57	125.59	120.30
1	A	388	ARG	NE-CZ-NH2	-10.45	115.07	120.30
1	A	288	LEU	O-C-N	-10.44	106.00	122.70
1	B	384	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	A	17	ASP	CB-CG-OD1	10.40	127.66	118.30
1	A	269	PRO	CA-N-CD	-10.36	96.99	111.50
1	B	456	ARG	CD-NE-CZ	10.35	138.09	123.60
1	B	87	THR	CA-C-N	10.34	136.87	116.20
1	A	385	GLU	O-C-N	-10.31	105.67	123.20
1	A	506	ASP	CB-CG-OD1	10.20	127.48	118.30
1	A	352	ASP	CB-CG-OD2	-10.20	109.12	118.30
1	B	344	ARG	CD-NE-CZ	10.10	137.74	123.60
1	A	111	ARG	NE-CZ-NH1	10.06	125.33	120.30
1	B	544	LEU	CA-CB-CG	10.06	138.43	115.30
1	A	311	PRO	CA-C-N	10.00	139.20	117.20
1	A	283	HIS	CA-C-O	9.96	141.01	120.10
1	A	366	ASP	CA-C-O	9.95	140.99	120.10
1	A	77	TYR	CB-CG-CD1	9.90	126.94	121.00
1	B	437	TYR	CB-CG-CD1	9.84	126.90	121.00
1	B	100	ASP	CB-CG-OD1	-9.80	109.48	118.30
1	A	190	ASP	CB-CG-OD1	9.73	127.06	118.30
1	B	17	ASP	CB-CG-OD2	9.68	127.01	118.30
1	A	136	THR	CA-CB-OG1	-9.64	88.76	109.00
1	A	337	LYS	CD-CE-NZ	9.59	133.76	111.70
1	A	426	PHE	CB-CG-CD2	9.53	127.47	120.80
1	B	252	SER	CA-CB-OG	9.51	136.88	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	90	ARG	NE-CZ-NH2	-9.50	115.55	120.30
1	B	269	PRO	CA-N-CD	-9.48	98.23	111.50
1	A	12	ASP	CB-CG-OD1	9.41	126.77	118.30
1	A	344	ARG	NE-CZ-NH2	9.40	125.00	120.30
1	B	12	ASP	CB-CG-OD1	9.40	126.76	118.30
1	A	460	MET	CA-CB-CG	9.39	129.26	113.30
1	B	288	LEU	O-C-N	-9.34	107.76	122.70
1	A	178	ASP	CB-CG-OD1	9.31	126.68	118.30
1	A	116	TYR	CB-CG-CD1	-9.25	115.45	121.00
1	A	419	TYR	CB-CG-CD2	9.23	126.54	121.00
1	A	79	ARG	CD-NE-CZ	9.22	136.51	123.60
1	B	65	ILE	CA-CB-CG2	9.17	129.25	110.90
1	B	262	VAL	CB-CA-C	-9.15	94.01	111.40
1	A	101	ASP	CB-CG-OD1	-9.11	110.10	118.30
1	A	198	TRP	CA-CB-CG	9.09	130.97	113.70
1	A	543	TYR	CB-CG-CD1	9.09	126.45	121.00
1	A	340	ALA	N-CA-CB	9.08	122.81	110.10
1	B	190	ASP	CB-CG-OD1	9.07	126.47	118.30
1	A	72	TYR	CG-CD1-CE1	9.06	128.55	121.30
1	A	188	ALA	N-CA-CB	9.05	122.77	110.10
1	A	87	THR	N-CA-CB	-8.99	93.21	110.30
1	A	322	GLU	OE1-CD-OE2	-8.99	112.51	123.30
1	B	111	ARG	NE-CZ-NH1	-8.99	115.80	120.30
1	A	539	ASP	CB-CG-OD1	8.96	126.37	118.30
1	B	97	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	A	268	GLY	CA-C-O	-8.87	104.64	120.60
1	A	189	ARG	NE-CZ-NH2	-8.87	115.87	120.30
1	A	456	ARG	NE-CZ-NH2	8.85	124.72	120.30
1	A	388	ARG	NE-CZ-NH1	8.83	124.71	120.30
1	A	185	ARG	NE-CZ-NH1	-8.78	115.91	120.30
1	A	56	LYS	CA-CB-CG	8.75	132.66	113.40
1	A	142	LYS	O-C-N	-8.68	108.81	122.70
1	A	54	ASP	CB-CG-OD2	8.62	126.06	118.30
1	A	364	PHE	CB-CG-CD2	8.58	126.81	120.80
1	A	311	PRO	O-C-N	-8.45	109.19	122.70
1	B	29	ARG	NH1-CZ-NH2	-8.38	110.18	119.40
1	A	111	ARG	NE-CZ-NH2	-8.37	116.12	120.30
1	B	311	PRO	CA-C-N	8.35	135.58	117.20
1	A	116	TYR	CB-CG-CD2	8.34	126.00	121.00
1	A	34	LYS	CA-CB-CG	8.30	131.67	113.40
1	A	330	ALA	N-CA-CB	8.30	121.73	110.10
1	B	352	ASP	CB-CG-OD1	8.26	125.73	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	539	ASP	CB-CG-OD2	8.25	125.73	118.30
1	A	284	ASP	C-N-CA	8.15	142.08	121.70
1	A	539	ASP	OD1-CG-OD2	-8.11	107.89	123.30
1	B	483	LYS	CB-CG-CD	8.10	132.66	111.60
1	A	221	VAL	CB-CA-C	-8.09	96.03	111.40
1	A	283	HIS	O-C-N	-8.06	109.80	122.70
1	B	72	TYR	CB-CG-CD2	-8.05	116.17	121.00
1	A	262	VAL	CB-CA-C	-8.03	96.15	111.40
1	A	209	ARG	CD-NE-CZ	8.03	134.84	123.60
1	A	352	ASP	CB-CG-OD1	8.00	125.50	118.30
1	A	480	TRP	CA-CB-CG	7.99	128.89	113.70
1	A	367	ASN	CA-CB-CG	7.95	130.88	113.40
1	A	190	ASP	OD1-CG-OD2	-7.93	108.23	123.30
1	B	456	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	B	288	LEU	CA-C-O	7.90	136.69	120.10
1	A	273	TRP	CA-CB-CG	-7.85	98.78	113.70
1	A	385	GLU	CA-C-O	-7.84	103.64	120.10
1	B	56	LYS	CB-CG-CD	7.83	131.95	111.60
1	B	68	ASP	CB-CG-OD2	7.80	125.32	118.30
1	A	544	LEU	CA-CB-CG	7.80	133.23	115.30
1	A	419	TYR	CB-CG-CD1	-7.79	116.33	121.00
1	B	327	ASP	CB-CG-OD2	-7.78	111.30	118.30
1	A	101	ASP	OD1-CG-OD2	7.75	138.02	123.30
1	A	327	ASP	CB-CG-OD2	-7.63	111.43	118.30
1	B	313	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	A	426	PHE	CD1-CE1-CZ	-7.61	110.97	120.10
1	B	284	ASP	CB-CA-C	7.57	125.54	110.40
1	A	250	SER	N-CA-CB	-7.52	99.23	110.50
1	B	284	ASP	CA-C-O	7.49	135.83	120.10
1	B	274	ALA	CB-CA-C	7.49	121.34	110.10
1	B	126	ASP	CB-CG-OD1	7.49	125.04	118.30
1	A	6	GLU	OE1-CD-OE2	-7.45	114.36	123.30
1	B	187	PHE	CA-CB-CG	7.44	131.75	113.90
1	A	501	PHE	CB-CG-CD2	-7.44	115.59	120.80
1	A	49	SER	N-CA-CB	-7.41	99.39	110.50
1	A	21	TYR	CG-CD2-CE2	7.39	127.22	121.30
1	A	456	ARG	CG-CD-NE	7.39	127.32	111.80
1	A	118	ASP	OD1-CG-OD2	-7.37	109.29	123.30
1	B	507	GLY	N-CA-C	7.37	131.53	113.10
1	B	142	LYS	CA-CB-CG	7.31	129.49	113.40
1	A	211	ASN	O-C-N	-7.31	110.77	123.20
1	B	339	THR	CA-CB-CG2	7.27	122.58	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	THR	N-CA-CB	-7.27	96.49	110.30
1	B	352	ASP	CB-CG-OD2	-7.26	111.77	118.30
1	A	123	GLY	C-N-CA	7.26	139.84	121.70
1	A	192	ASP	CB-CG-OD1	7.24	124.81	118.30
1	A	426	PHE	CG-CD1-CE1	7.21	128.73	120.80
1	B	34	LYS	CA-CB-CG	7.20	129.24	113.40
1	B	490	ALA	N-CA-CB	7.20	120.18	110.10
1	A	368	ILE	CB-CG1-CD1	7.16	133.95	113.90
1	A	101	ASP	CB-CG-OD2	-7.14	111.87	118.30
1	A	537	GLU	CG-CD-OE2	-7.14	104.02	118.30
1	A	313	ASP	CB-CG-OD2	-7.14	111.88	118.30
1	A	73	VAL	CB-CA-C	-7.13	97.85	111.40
1	A	72	TYR	CB-CG-CD1	7.10	125.26	121.00
1	A	190	ASP	CB-CG-OD2	7.09	124.68	118.30
1	A	88	GLY	O-C-N	-7.07	111.38	122.70
1	B	353	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	B	109	VAL	C-N-CA	7.05	139.33	121.70
1	B	79	ARG	CD-NE-CZ	7.02	133.43	123.60
1	B	228	ASP	CB-CG-OD1	6.99	124.59	118.30
1	B	73	VAL	CA-CB-CG2	6.99	121.38	110.90
1	A	163	ASP	CB-CG-OD1	6.98	124.58	118.30
1	A	501	PHE	CB-CG-CD1	6.97	125.68	120.80
1	A	100	ASP	CB-CG-OD1	6.96	124.57	118.30
1	A	87	THR	O-C-N	-6.91	111.45	123.20
1	B	273	TRP	NE1-CE2-CZ2	-6.91	122.80	130.40
1	A	383	GLU	OE1-CD-OE2	-6.89	115.03	123.30
1	B	383	GLU	OE1-CD-OE2	-6.89	115.04	123.30
1	B	11	ASP	CA-C-N	6.86	132.29	117.20
1	B	539	ASP	C-N-CA	6.84	136.67	122.30
1	A	415	ASN	CB-CA-C	6.84	124.08	110.40
1	A	81	PHE	CB-CG-CD2	6.83	125.58	120.80
1	B	285	TYR	CB-CG-CD2	-6.82	116.91	121.00
1	B	241	SER	O-C-N	-6.81	111.80	122.70
1	B	422	ASP	CB-CG-OD1	6.81	124.43	118.30
1	B	483	LYS	CB-CA-C	6.80	124.01	110.40
1	A	365	VAL	CA-CB-CG1	-6.80	100.70	110.90
1	A	565	THR	CA-CB-CG2	6.79	121.90	112.40
1	A	426	PHE	CB-CG-CD1	-6.77	116.06	120.80
1	A	342	ALA	N-CA-CB	6.76	119.57	110.10
1	A	231	ASN	N-CA-CB	6.76	122.77	110.60
1	A	545	GLY	CA-C-O	6.76	132.76	120.60
1	A	2	ASP	O-C-N	-6.75	111.90	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	189	ARG	CD-NE-CZ	6.74	133.04	123.60
1	B	377	LYS	CA-CB-CG	6.73	128.21	113.40
1	B	459	ARG	NE-CZ-NH2	6.73	123.67	120.30
1	A	462	ASP	CB-CG-OD1	6.72	124.34	118.30
1	B	385	GLU	OE1-CD-OE2	-6.72	115.24	123.30
1	A	385	GLU	C-N-CA	-6.70	108.23	122.30
1	B	539	ASP	CA-CB-CG	6.69	128.12	113.40
1	B	196	GLU	OE1-CD-OE2	-6.68	115.28	123.30
1	A	539	ASP	O-C-N	-6.68	111.85	123.20
1	B	237	VAL	CA-CB-CG1	6.67	120.90	110.90
1	B	273	TRP	CE3-CZ3-CH2	6.65	128.51	121.20
1	A	125	LEU	CA-CB-CG	6.64	130.58	115.30
1	A	556	LEU	O-C-N	-6.64	112.07	122.70
1	A	273	TRP	CD2-CE3-CZ3	-6.62	110.19	118.80
1	A	569	ALA	CB-CA-C	-6.62	100.18	110.10
1	A	189	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	A	353	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	A	444	TYR	O-C-N	-6.59	112.16	122.70
1	A	284	ASP	O-C-N	-6.58	112.17	122.70
1	B	384	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	A	14	THR	CA-C-N	6.55	131.62	117.20
1	A	67	SER	N-CA-CB	-6.55	100.68	110.50
1	A	82	ALA	CA-C-O	6.55	133.85	120.10
1	A	383	GLU	CG-CD-OE1	6.54	131.38	118.30
1	A	27	ALA	N-CA-CB	-6.54	100.95	110.10
1	A	110	ASN	CB-CG-ND2	6.52	132.34	116.70
1	A	312	ASN	CA-CB-CG	6.51	127.73	113.40
1	A	87	THR	CA-C-O	-6.51	106.43	120.10
1	A	105	CYS	CA-CB-SG	6.51	125.71	114.00
1	A	256	GLU	OE1-CD-OE2	6.50	131.10	123.30
1	A	269	PRO	N-CD-CG	6.50	112.94	103.20
1	A	384	ARG	C-N-CA	6.50	137.94	121.70
1	B	14	THR	CA-C-N	6.49	131.49	117.20
1	A	196	GLU	O-C-N	-6.49	112.31	122.70
1	B	324	VAL	CA-CB-CG2	6.49	120.64	110.90
1	A	192	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	B	511	ALA	N-CA-CB	6.46	119.14	110.10
1	A	87	THR	C-N-CA	-6.46	108.73	122.30
1	A	79	ARG	NH1-CZ-NH2	-6.44	112.32	119.40
1	A	52	PHE	CB-CG-CD2	6.44	125.31	120.80
1	A	230	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	B	557	TRP	CA-CB-CG	6.42	125.90	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	283	HIS	N-CA-CB	6.42	122.15	110.60
1	A	353	ARG	CA-CB-CG	6.41	127.50	113.40
1	A	321	ASN	CB-CG-ND2	6.39	132.04	116.70
1	B	543	TYR	CB-CG-CD1	6.38	124.83	121.00
1	A	562	ALA	N-CA-CB	6.37	119.02	110.10
1	A	506	ASP	OD1-CG-OD2	-6.37	111.21	123.30
1	B	388	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	B	575	TRP	CA-CB-CG	6.36	125.79	113.70
1	A	422	ASP	CB-CG-OD1	-6.36	112.58	118.30
1	A	497	GLY	CA-C-O	-6.35	109.17	120.60
1	B	125	LEU	O-C-N	-6.33	112.56	122.70
1	A	433	TRP	CD1-CG-CD2	-6.33	101.24	106.30
1	B	209	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	273	TRP	CE3-CZ3-CH2	6.32	128.15	121.20
1	B	11	ASP	O-C-N	-6.32	112.59	122.70
1	A	273	TRP	CH2-CZ2-CE2	-6.31	111.09	117.40
1	B	469	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	B	316	ASP	O-C-N	-6.29	112.64	122.70
1	B	417	MET	CA-CB-CG	6.28	123.97	113.30
1	B	185	ARG	CG-CD-NE	-6.26	98.65	111.80
1	B	314	ALA	C-N-CA	6.26	137.34	121.70
1	B	541	GLU	N-CA-CB	-6.26	99.34	110.60
1	A	366	ASP	N-CA-C	6.24	127.84	111.00
1	B	494	ALA	C-N-CA	6.23	137.28	121.70
1	A	368	ILE	O-C-N	6.19	132.61	122.70
1	B	107	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	B	416	PRO	C-N-CA	6.18	137.16	121.70
1	A	299	SER	CA-CB-OG	6.18	127.89	111.20
1	A	72	TYR	CD1-CE1-CZ	-6.17	114.25	119.80
1	A	44	LEU	CB-CA-C	6.16	121.89	110.20
1	A	254	ASP	CB-CG-OD1	6.13	123.82	118.30
1	B	313	ASP	CB-CG-OD1	6.13	123.82	118.30
1	A	136	THR	C-N-CA	-6.13	109.43	122.30
1	A	459	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	237	VAL	N-CA-CB	-6.12	98.03	111.50
1	A	338	ALA	N-CA-CB	-6.10	101.56	110.10
1	B	147	ASP	CB-CG-OD1	6.10	123.79	118.30
1	B	403	GLU	OE1-CD-OE2	-6.09	115.99	123.30
1	A	437	TYR	CA-CB-CG	6.09	124.97	113.40
1	A	73	VAL	O-C-N	-6.07	112.98	122.70
1	A	341	HIS	CA-CB-CG	6.05	123.88	113.60
1	A	436	ASP	CB-CG-OD2	6.05	123.74	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	311	PRO	CA-C-O	-6.05	105.69	120.20
1	B	351	VAL	CG1-CB-CG2	-6.04	101.23	110.90
1	B	125	LEU	CA-CB-CG	6.04	129.19	115.30
1	A	189	ARG	CG-CD-NE	-6.04	99.11	111.80
1	A	21	TYR	OH-CZ-CE2	6.03	136.38	120.10
1	A	106	CYS	N-CA-CB	-6.03	99.75	110.60
1	A	366	ASP	C-N-CA	-6.03	106.63	121.70
1	A	539	ASP	C-N-CA	6.03	134.96	122.30
1	A	82	ALA	O-C-N	-6.02	113.08	122.70
1	B	258	ASN	CB-CG-OD1	6.01	133.62	121.60
1	B	125	LEU	CA-C-N	6.00	130.40	117.20
1	B	284	ASP	O-C-N	-6.00	113.10	122.70
1	B	50	TYR	CA-CB-CG	-5.99	102.03	113.40
1	A	459	ARG	NH1-CZ-NH2	5.97	125.97	119.40
1	B	55	GLU	OE1-CD-OE2	-5.97	116.14	123.30
1	A	307	TYR	N-CA-CB	5.93	121.28	110.60
1	A	220	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	453	MET	CA-CB-CG	5.92	123.36	113.30
1	B	343	ASP	N-CA-CB	-5.92	99.95	110.60
1	A	182	VAL	N-CA-CB	-5.91	98.50	111.50
1	B	496	ALA	CA-C-N	5.91	128.01	116.20
1	A	231	ASN	CA-CB-CG	5.90	126.38	113.40
1	B	102	ILE	CA-CB-CG2	5.90	122.70	110.90
1	A	12	ASP	OD1-CG-OD2	-5.89	112.10	123.30
1	B	237	VAL	CB-CA-C	5.88	122.57	111.40
1	B	309	HIS	O-C-N	-5.87	113.30	122.70
1	B	323	LEU	CA-CB-CG	-5.87	101.79	115.30
1	A	314	ALA	CB-CA-C	-5.87	101.30	110.10
1	A	79	ARG	CA-CB-CG	5.87	126.31	113.40
1	B	65	ILE	CA-CB-CG1	-5.86	99.87	111.00
1	A	284	ASP	CA-C-N	-5.86	104.31	117.20
1	B	146	ALA	N-CA-CB	5.86	118.30	110.10
1	A	329	LYS	C-N-CA	5.85	136.33	121.70
1	A	331	LYS	N-CA-C	-5.85	95.20	111.00
1	B	225	SER	O-C-N	-5.83	113.36	122.70
1	A	120	VAL	O-C-N	-5.81	113.40	122.70
1	A	423	THR	CA-C-N	5.81	127.82	116.20
1	A	204	GLU	OE1-CD-OE2	-5.80	116.34	123.30
1	A	563	ASP	CB-CA-C	5.80	122.00	110.40
1	A	97	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	312	ASN	N-CA-C	-5.79	95.36	111.00
1	A	128	SER	N-CA-CB	5.79	119.19	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	279	GLY	N-CA-C	-5.78	98.64	113.10
1	A	104	PRO	O-C-N	-5.76	113.48	122.70
1	B	108	VAL	O-C-N	-5.76	113.48	122.70
1	B	192	ASP	CB-CG-OD1	5.76	123.49	118.30
1	A	523	PHE	CB-CG-CD1	5.75	124.83	120.80
1	A	68	ASP	CA-CB-CG	5.75	126.04	113.40
1	B	275	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	A	422	ASP	CB-CG-OD2	5.71	123.44	118.30
1	B	436	ASP	OD1-CG-OD2	-5.71	112.46	123.30
1	A	500	VAL	N-CA-CB	5.70	124.05	111.50
1	B	289	TYR	CB-CA-C	5.70	121.80	110.40
1	A	263	GLY	O-C-N	5.70	131.81	122.70
1	B	106	CYS	N-CA-CB	-5.69	100.36	110.60
1	A	330	ALA	O-C-N	5.67	131.78	122.70
1	A	153	THR	CB-CA-C	-5.67	96.29	111.60
1	A	316	ASP	CB-CG-OD2	5.67	123.40	118.30
1	B	287	SER	CB-CA-C	5.65	120.83	110.10
1	A	519	GLU	OE1-CD-OE2	-5.64	116.53	123.30
1	A	578	LYS	CA-CB-CG	5.63	125.80	113.40
1	B	333	GLY	N-CA-C	5.63	127.17	113.10
1	B	462	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	463	ASP	CB-CG-OD1	5.62	123.36	118.30
1	B	362	PHE	CB-CG-CD1	-5.62	116.87	120.80
1	A	414	TRP	CA-CB-CG	-5.61	103.04	113.70
1	A	472	ASP	OD1-CG-OD2	-5.61	112.65	123.30
1	A	515	LYS	CD-CE-NZ	5.61	124.59	111.70
1	A	306	PHE	O-C-N	-5.59	113.76	122.70
1	A	229	ASP	CB-CG-OD2	5.58	123.33	118.30
1	A	556	LEU	CA-CB-CG	5.57	128.11	115.30
1	A	570	GLN	C-N-CA	5.57	133.99	122.30
1	B	216	THR	N-CA-C	5.56	126.01	111.00
1	A	566	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	121	PHE	CB-CG-CD1	5.54	124.68	120.80
1	A	273	TRP	NE1-CE2-CZ2	-5.54	124.30	130.40
1	A	560	ASP	N-CA-CB	5.53	120.56	110.60
1	A	153	THR	CA-CB-CG2	5.53	120.14	112.40
1	B	470	ALA	C-N-CA	5.53	135.52	121.70
1	B	87	THR	CA-C-O	-5.52	108.51	120.10
1	A	252	SER	O-C-N	-5.51	113.89	122.70
1	A	284	ASP	OD1-CG-OD2	5.51	133.76	123.30
1	A	94	TYR	CB-CG-CD1	-5.50	117.70	121.00
1	A	25	THR	CA-CB-CG2	5.50	120.10	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	SER	N-CA-CB	5.50	118.75	110.50
1	B	64	ALA	N-CA-CB	-5.49	102.41	110.10
1	A	433	TRP	CG-CD1-NE1	5.49	115.59	110.10
1	B	489	TRP	CB-CA-C	5.48	121.36	110.40
1	B	221	VAL	CB-CA-C	-5.48	100.99	111.40
1	A	568	VAL	C-N-CA	5.48	135.39	121.70
1	A	530	VAL	O-C-N	-5.47	113.95	122.70
1	A	450	TYR	N-CA-CB	-5.46	100.77	110.60
1	A	60	GLN	CA-CB-CG	5.46	125.41	113.40
1	B	100	ASP	OD1-CG-OD2	5.46	133.67	123.30
1	A	54	ASP	OD1-CG-OD2	-5.46	112.93	123.30
1	B	480	TRP	CA-CB-CG	5.46	124.07	113.70
1	A	510	LYS	CD-CE-NZ	5.45	124.24	111.70
1	B	251	ALA	N-CA-CB	-5.45	102.47	110.10
1	A	543	TYR	CG-CD2-CE2	5.43	125.64	121.30
1	B	496	ALA	C-N-CA	5.43	133.69	122.30
1	A	69	GLY	O-C-N	-5.42	114.02	122.70
1	A	121	PHE	CB-CG-CD2	-5.42	117.01	120.80
1	A	236	LYS	CA-CB-CG	5.42	125.32	113.40
1	A	564	LEU	CA-CB-CG	5.42	127.76	115.30
1	A	83	LEU	CB-CG-CD1	5.41	120.19	111.00
1	B	249	GLN	CB-CA-C	5.41	121.21	110.40
1	B	58	ARG	NE-CZ-NH2	5.40	123.00	120.30
1	A	266	ASN	CB-CG-OD1	-5.40	110.81	121.60
1	A	262	VAL	CG1-CB-CG2	5.39	119.53	110.90
1	A	528	GLY	O-C-N	-5.39	114.08	122.70
1	A	498	ASN	CB-CG-OD1	-5.37	110.87	121.60
1	B	185	ARG	NH1-CZ-NH2	5.36	125.30	119.40
1	B	462	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	B	72	TYR	CG-CD2-CE2	-5.36	117.01	121.30
1	A	419	TYR	CZ-CE2-CD2	-5.36	114.98	119.80
1	B	236	LYS	CA-C-O	-5.36	108.85	120.10
1	B	340	ALA	N-CA-CB	5.36	117.60	110.10
1	A	2	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	A	484	GLU	CA-CB-CG	5.35	125.16	113.40
1	B	35	GLN	CB-CA-C	5.35	121.09	110.40
1	B	182	VAL	CG1-CB-CG2	5.35	119.45	110.90
1	B	141	TRP	NE1-CE2-CZ2	5.34	136.27	130.40
1	A	478	VAL	CA-CB-CG1	5.33	118.90	110.90
1	B	6	GLU	CA-CB-CG	5.32	125.10	113.40
1	A	408	PHE	CB-CG-CD1	-5.32	117.08	120.80
1	B	565	THR	N-CA-CB	-5.29	100.24	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	GLU	OE1-CD-OE2	-5.29	116.95	123.30
1	B	513	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	452	GLY	CA-C-O	-5.28	111.10	120.60
1	A	364	PHE	O-C-N	-5.28	114.25	122.70
1	A	159	THR	O-C-N	-5.28	114.26	122.70
1	A	308	GLN	N-CA-CB	5.27	120.09	110.60
1	A	478	VAL	CB-CA-C	5.27	121.42	111.40
1	B	141	TRP	CH2-CZ2-CE2	5.27	122.67	117.40
1	A	348	PHE	CG-CD1-CE1	-5.27	115.01	120.80
1	A	58	ARG	CG-CD-NE	-5.26	100.75	111.80
1	A	183	VAL	O-C-N	5.26	132.14	123.20
1	A	376	LEU	CA-C-O	-5.25	109.07	120.10
1	B	114	ALA	O-C-N	-5.25	114.30	122.70
1	A	152	TYR	CB-CG-CD1	-5.25	117.85	121.00
1	A	13	LYS	N-CA-C	5.25	125.16	111.00
1	A	210	LEU	CA-C-N	5.24	128.73	117.20
1	A	140	VAL	O-C-N	-5.24	114.32	122.70
1	B	562	ALA	N-CA-CB	5.24	117.44	110.10
1	A	211	ASN	C-N-CA	5.24	133.30	122.30
1	B	128	SER	CB-CA-C	-5.24	100.15	110.10
1	A	459	ARG	O-C-N	-5.23	114.33	122.70
1	A	114	ALA	N-CA-CB	5.23	117.42	110.10
1	A	370	TRP	CA-CB-CG	-5.23	103.77	113.70
1	A	288	LEU	N-CA-CB	5.22	120.85	110.40
1	B	458	LYS	CA-CB-CG	5.22	124.89	113.40
1	B	345	ASN	CA-C-N	5.22	126.65	116.20
1	A	43	LYS	CA-CB-CG	5.22	124.88	113.40
1	A	565	THR	N-CA-CB	-5.22	100.38	110.30
1	A	307	TYR	CA-CB-CG	-5.21	103.50	113.40
1	B	388	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	110	ASN	CA-CB-CG	-5.19	101.97	113.40
1	B	546	VAL	CA-CB-CG2	5.18	118.67	110.90
1	A	58	ARG	CB-CG-CD	5.18	125.06	111.60
1	A	41	VAL	CA-CB-CG1	5.17	118.66	110.90
1	A	527	SER	N-CA-CB	-5.17	102.75	110.50
1	B	312	ASN	N-CA-CB	5.16	119.89	110.60
1	A	228	ASP	CB-CA-C	-5.15	100.09	110.40
1	B	380	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	216	THR	CA-C-N	5.13	128.50	117.20
1	A	88	GLY	CA-C-N	5.13	128.49	117.20
1	A	326	PHE	N-CA-CB	-5.13	101.36	110.60
1	B	180	PHE	CB-CG-CD1	-5.13	117.21	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	412	LYS	CA-CB-CG	-5.12	102.12	113.40
1	A	262	VAL	CA-C-O	5.12	130.86	120.10
1	A	511	ALA	C-N-CA	5.12	134.50	121.70
1	B	280	GLY	N-CA-C	5.12	125.90	113.10
1	A	39	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	134	LYS	CA-CB-CG	5.11	124.63	113.40
1	A	551	GLY	CA-C-O	-5.09	111.43	120.60
1	B	319	GLY	C-N-CA	5.09	134.43	121.70
1	B	220	ASP	CB-CG-OD1	5.08	122.88	118.30
1	B	416	PRO	O-C-N	-5.08	114.56	122.70
1	A	159	THR	CA-CB-CG2	5.08	119.52	112.40
1	A	237	VAL	O-C-N	-5.08	114.56	122.70
1	A	348	PHE	CD1-CE1-CZ	5.08	126.20	120.10
1	A	412	LYS	CG-CD-CE	5.08	127.15	111.90
1	A	331	LYS	N-CA-CB	5.08	119.74	110.60
1	A	126	ASP	C-N-CA	5.06	134.34	121.70
1	A	577	PHE	CB-CG-CD2	5.06	124.34	120.80
1	A	510	LYS	CB-CA-C	-5.05	100.30	110.40
1	B	87	THR	O-C-N	-5.05	114.62	123.20
1	A	69	GLY	CA-C-N	5.04	128.30	117.20
1	A	450	TYR	CB-CG-CD1	-5.04	117.97	121.00
1	A	105	CYS	CB-CA-C	-5.04	100.32	110.40
1	A	271	ASN	OD1-CG-ND2	-5.04	110.30	121.90
1	A	48	TRP	CA-CB-CG	5.03	123.25	113.70
1	A	326	PHE	CG-CD2-CE2	-5.01	115.29	120.80
1	B	29	ARG	CA-CB-CG	5.01	124.42	113.40
1	B	200	ARG	CA-CB-CG	5.01	124.43	113.40

There are no chirality outliers.

All (57) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	ASP	Mainchain
1	A	120	VAL	Mainchain
1	A	13	LYS	Mainchain
1	A	14	THR	Mainchain
1	A	142	LYS	Mainchain
1	A	157	ALA	Mainchain
1	A	158	PRO	Mainchain
1	A	177	GLY	Mainchain
1	A	210	LEU	Mainchain
1	A	220	ASP	Mainchain

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Mol	Chain	Res	Type	Group
1	A	234	THR	Mainchain
1	A	248	TRP	Mainchain
1	A	251	ALA	Mainchain
1	A	268	GLY	Mainchain,Peptide
1	A	284	ASP	Mainchain,Peptide
1	A	288	LEU	Peptide
1	A	316	ASP	Mainchain
1	A	328	TYR	Mainchain
1	A	331	LYS	Mainchain
1	A	338	ALA	Mainchain
1	A	347	PHE	Mainchain
1	A	353	ARG	Mainchain
1	A	363	PRO	Mainchain
1	A	385	GLU	Mainchain
1	A	413	ASN	Mainchain
1	A	423	THR	Mainchain
1	A	478	VAL	Mainchain
1	A	528	GLY	Mainchain
1	A	559	GLY	Mainchain
1	A	563	ASP	Mainchain
1	A	58	ARG	Mainchain
1	A	6	GLU	Mainchain
1	A	69	GLY	Mainchain
1	A	95	ASN	Mainchain
1	B	103	ARG	Mainchain
1	B	142	LYS	Mainchain
1	B	218	THR	Mainchain
1	B	234	THR	Mainchain
1	B	262	VAL	Mainchain
1	B	268	GLY	Mainchain,Peptide
1	B	284	ASP	Peptide
1	B	285	TYR	Mainchain
1	B	287	SER	Mainchain
1	B	288	LEU	Peptide
1	B	289	TYR	Mainchain
1	B	351	VAL	Mainchain
1	B	356	GLY	Mainchain
1	B	366	ASP	Mainchain
1	B	390	PRO	Mainchain
1	B	40	ASN	Mainchain
1	B	459	ARG	Mainchain
1	B	49	SER	Mainchain

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Mol	Chain	Res	Type	Group
1	B	496	ALA	Mainchain
1	B	65	ILE	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	4537	0	4311	123	6
1	B	4537	0	4311	143	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	24	0	3	1	0
3	B	24	0	3	0	0
4	A	73	0	0	4	0
4	B	33	0	0	1	0
All	All	9232	0	8628	255	6

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 14.

All (255) 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:367:ASN:CA	1:A:367:ASN:N	1.69	1.51
1:A:366:ASP:O	1:A:367:ASN:HA	1.37	1.21
1:A:293:GLN:HE22	1:A:339:THR:HG21	0.95	1.06
1:A:366:ASP:O	1:A:367:ASN:CA	2.02	1.02
1:A:293:GLN:NE2	1:A:339:THR:HG21	1.77	0.98
1:B:329:LYS:HE3	1:B:333:GLY:H	1.29	0.97
1:A:79:ARG:HG2	1:A:95:ASN:HD22	1.30	0.94
1:A:29:ARG:HH22	1:A:63:GLN:HE21	1.13	0.92
1:A:366:ASP:H	1:A:432:HIS:HE1	1.19	0.91
1:A:456:ARG:HD2	1:A:458:LYS:HE3	1.50	0.90
1:A:183:VAL:HB	1:A:185:ARG:HH12	1.37	0.88
1:A:366:ASP:C	1:A:367:ASN:CA	2.43	0.88
1:B:125:LEU:O	1:B:153:THR:HG22	1.74	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:LEU:HA	1:B:439:THR:HG21	1.57	0.87
1:B:442:VAL:HG22	1:B:452:GLY:HA3	1.58	0.85
1:A:392:PRO:HD3	1:A:439:THR:HG21	1.58	0.85
1:B:293:GLN:OE1	1:B:339:THR:HG21	1.78	0.84
1:B:339:THR:HG22	1:B:351:VAL:HB	1.62	0.82
1:B:65:ILE:HG22	1:B:72:TYR:HB2	1.60	0.81
1:B:118:ASP:HA	1:B:134:LYS:HD2	1.62	0.81
1:A:456:ARG:CD	1:A:458:LYS:HE3	2.10	0.79
1:B:456:ARG:HH11	1:B:456:ARG:HB3	1.46	0.79
1:A:87:THR:HG22	1:A:89:LYS:H	1.48	0.79
1:A:166:THR:HG23	1:A:168:LYS:HB2	1.63	0.78
1:A:22:GLY:H	1:A:63:GLN:HE22	1.31	0.77
1:A:97:ARG:HH11	1:A:97:ARG:HG2	1.49	0.77
1:A:392:PRO:HD3	1:A:439:THR:CG2	2.14	0.77
1:A:366:ASP:H	1:A:432:HIS:CE1	2.03	0.76
1:A:183:VAL:HB	1:A:185:ARG:NH1	2.01	0.75
1:B:216:THR:O	1:B:217:VAL:HB	1.87	0.73
1:B:22:GLY:H	1:B:63:GLN:HE22	1.37	0.72
1:B:28:GLN:HG3	1:B:419:TYR:HB3	1.73	0.71
1:A:29:ARG:HH22	1:A:63:GLN:NE2	1.87	0.69
1:A:339:THR:HG22	4:A:775:HOH:O	1.92	0.69
1:A:334:LYS:HA	1:A:334:LYS:HE3	1.75	0.69
1:A:524:GLN:HE21	1:A:526:GLY:H	1.41	0.69
1:B:378:THR:HG23	1:B:380:ARG:HB2	1.76	0.68
1:B:366:ASP:H	1:B:432:HIS:HE1	1.41	0.68
1:A:436:ASP:OD2	1:A:458:LYS:NZ	2.28	0.66
1:B:325:LEU:HD22	1:B:353:ARG:HD2	1.76	0.66
1:B:102:ILE:HD11	1:B:126:ASP:HA	1.77	0.66
1:A:327:ASP:HB3	1:A:335:ILE:HD13	1.79	0.65
1:B:405:SER:HB2	1:B:434:LYS:HB3	1.79	0.65
1:B:249:GLN:HE22	1:B:321:ASN:HA	1.60	0.65
1:A:136:THR:OG1	1:A:137:GLY:N	2.28	0.65
1:A:133:ASN:O	1:A:136:THR:O	2.16	0.64
1:A:57:GLN:NE2	1:B:55:GLU:H	1.96	0.64
1:A:273:TRP:HZ3	1:A:389:PRO:O	1.80	0.64
1:A:266:ASN:HB2	1:A:267:PRO:HD2	1.78	0.64
1:A:378:THR:HG22	1:A:380:ARG:H	1.62	0.64
1:A:391:LEU:HA	1:A:439:THR:HG21	1.80	0.63
1:B:392:PRO:HD3	1:B:439:THR:HG22	1.81	0.63
1:A:173:HIS:HE1	1:A:189:ARG:HE	1.46	0.63
1:A:87:THR:CG2	1:A:89:LYS:HB3	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:TRP:HZ3	1:B:389:PRO:O	1.81	0.63
1:A:53:GLY:HA2	1:B:57:GLN:HE22	1.64	0.62
1:B:329:LYS:HE3	1:B:333:GLY:N	2.10	0.62
1:B:372:SER:OG	1:B:373:HIS:HD2	1.83	0.61
1:B:541:GLU:OE2	1:B:578:LYS:HE3	1.99	0.61
1:B:133:ASN:HB3	1:B:136:THR:HG23	1.82	0.61
1:B:366:ASP:H	1:B:432:HIS:CE1	2.17	0.61
1:B:3:VAL:HG21	1:B:115:ILE:HG13	1.81	0.60
1:A:162:LYS:HD2	1:A:167:GLY:O	2.01	0.60
1:B:34:LYS:HE3	1:B:497:GLY:HA2	1.83	0.60
1:B:538:GLN:O	1:B:539:ASP:C	2.40	0.59
1:B:468:LEU:HB3	1:B:482:HIS:HB3	1.84	0.59
1:A:408:PHE:CE1	1:A:457:ILE:HD11	2.38	0.59
1:A:152:TYR:OH	1:A:185:ARG:NH1	2.36	0.59
1:A:79:ARG:CG	1:A:95:ASN:HD22	2.11	0.59
1:A:457:ILE:HD13	4:A:807:HOH:O	2.02	0.58
1:B:281:ASN:OD1	1:B:283:HIS:HB2	2.02	0.58
1:B:328:TYR:CE2	1:B:330:ALA:HA	2.39	0.58
1:A:57:GLN:HE21	1:B:55:GLU:H	1.52	0.57
1:B:56:LYS:CB	1:B:56:LYS:NZ	2.66	0.57
1:B:434:LYS:NZ	1:B:458:LYS:HE2	2.19	0.57
1:A:183:VAL:HG13	1:A:203:VAL:CG1	2.34	0.57
1:A:329:LYS:HE2	1:A:333:GLY:O	2.04	0.57
1:A:166:THR:HG23	1:A:168:LYS:H	1.68	0.57
1:B:116:TYR:CZ	1:B:169:VAL:HG11	2.39	0.57
1:A:510:LYS:HE2	1:A:519:GLU:OE1	2.05	0.57
1:B:210:LEU:HD12	1:B:211:ASN:H	1.68	0.57
1:B:144:LYS:NZ	1:B:148:HIS:HD2	2.03	0.56
1:A:378:THR:HG22	1:A:380:ARG:HB2	1.88	0.55
1:A:582:TRP:CH2	1:B:43:LYS:HD2	2.41	0.55
1:B:17:ASP:CG	1:B:19:LEU:HD11	2.26	0.55
1:A:329:LYS:HD2	1:A:335:ILE:HG22	1.88	0.55
1:A:245:GLY:HA2	1:A:265:GLY:O	2.06	0.55
1:A:136:THR:HG23	1:A:138:LYS:H	1.71	0.55
1:B:362:PHE:CZ	1:B:476:GLY:HA2	2.42	0.55
1:A:189:ARG:HD3	1:A:194:GLY:O	2.07	0.55
1:A:456:ARG:HH11	1:A:456:ARG:HB3	1.72	0.55
1:A:483:LYS:O	1:A:483:LYS:HD3	2.06	0.55
1:B:153:THR:HG23	4:B:795:HOH:O	2.07	0.54
1:B:59:GLY:CA	1:B:551:GLY:HA3	2.37	0.54
1:B:490:ALA:HB1	1:B:531:SER:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:ARG:CB	1:B:456:ARG:HH11	2.18	0.54
1:B:173:HIS:HE1	1:B:189:ARG:HE	1.54	0.54
1:B:245:GLY:HA2	1:B:265:GLY:O	2.06	0.54
1:B:56:LYS:CB	1:B:56:LYS:HZ3	2.20	0.54
1:A:84:ASP:OD1	1:A:87:THR:HB	2.08	0.54
1:A:320:ASN:H	1:A:320:ASN:HD22	1.54	0.54
1:A:164:GLY:H	1:A:258:ASN:ND2	2.04	0.54
1:B:256:GLU:OE2	1:B:353:ARG:NH2	2.40	0.54
1:A:372:SER:OG	1:A:373:HIS:HD2	1.90	0.54
1:A:163:ASP:HB3	1:A:166:THR:HG22	1.90	0.54
1:B:392:PRO:HD3	1:B:439:THR:CG2	2.37	0.54
1:A:55:GLU:O	1:B:55:GLU:HG2	2.08	0.53
1:A:456:ARG:HD2	1:A:458:LYS:CE	2.30	0.53
1:A:524:GLN:NE2	1:A:526:GLY:H	2.05	0.53
1:A:57:GLN:HE22	1:B:53:GLY:HA2	1.74	0.53
1:A:524:GLN:HE21	1:A:526:GLY:N	2.05	0.52
1:B:133:ASN:OD1	1:B:136:THR:HG22	2.09	0.52
1:A:1:LYS:O	1:A:1:LYS:HE3	2.08	0.52
1:A:29:ARG:NH2	1:A:63:GLN:HE21	1.95	0.52
1:B:102:ILE:HD11	1:B:126:ASP:CA	2.40	0.52
1:B:456:ARG:NH1	1:B:456:ARG:HB3	2.20	0.51
1:B:133:ASN:CG	1:B:136:THR:HG22	2.31	0.51
1:B:56:LYS:HG2	1:B:77:TYR:CD2	2.45	0.51
1:A:93:THR:HG22	1:A:94:TYR:N	2.26	0.51
1:A:87:THR:HG22	1:A:89:LYS:HB3	1.93	0.51
1:A:327:ASP:HB3	1:A:335:ILE:CD1	2.41	0.51
1:A:97:ARG:HH11	1:A:97:ARG:CG	2.21	0.51
1:A:378:THR:CG2	1:A:380:ARG:HB2	2.41	0.51
1:A:405:SER:HA	1:A:406:PRO:C	2.29	0.51
1:A:510:LYS:HE2	1:A:519:GLU:CD	2.31	0.50
1:A:43:LYS:HD2	1:B:582:TRP:CZ3	2.47	0.50
1:A:164:GLY:H	1:A:258:ASN:HD21	1.58	0.50
1:A:200:ARG:HD3	1:A:201:PRO:HD2	1.93	0.50
1:A:2:ASP:O	1:A:3:VAL:HB	2.11	0.50
1:A:256:GLU:OE1	1:A:337:LYS:HE2	2.11	0.50
1:B:3:VAL:HG21	1:B:115:ILE:CG1	2.42	0.50
1:A:159:THR:HG21	4:A:789:HOH:O	2.12	0.50
1:A:18:VAL:O	1:A:65:ILE:HB	2.11	0.49
1:A:34:LYS:HE3	1:A:37:ASN:HD22	1.76	0.49
1:B:226:TRP:O	1:B:236:LYS:NZ	2.30	0.49
1:A:456:ARG:HH11	1:A:456:ARG:CB	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:LYS:HD2	1:B:579:LEU:O	2.13	0.49
1:B:300:SER:OG	1:B:302:GLU:HG3	2.12	0.49
1:A:377:LYS:HG3	1:A:378:THR:N	2.28	0.49
1:B:34:LYS:NZ	1:B:496:ALA:O	2.33	0.49
1:B:17:ASP:OD1	1:B:19:LEU:HD11	2.13	0.48
1:B:164:GLY:H	1:B:258:ASN:ND2	2.11	0.48
1:B:133:ASN:HB3	1:B:136:THR:CG2	2.43	0.48
1:B:111:ARG:HD3	1:B:414:TRP:CE3	2.48	0.48
1:A:217:VAL:HG12	1:A:219:GLY:O	2.14	0.48
1:B:392:PRO:HB2	1:B:396:GLN:O	2.13	0.48
1:B:1:LYS:O	1:B:1:LYS:HE2	2.13	0.48
1:B:412:LYS:HD2	1:B:429:PRO:HG2	1.96	0.48
1:B:19:LEU:HD12	1:B:19:LEU:N	2.29	0.48
1:B:216:THR:O	1:B:217:VAL:CB	2.58	0.47
1:B:201:PRO:HD3	1:B:208:GLY:HA2	1.97	0.47
1:B:362:PHE:HB2	1:B:363:PRO:HD2	1.96	0.47
1:B:28:GLN:CG	1:B:419:TYR:HB3	2.43	0.47
1:B:200:ARG:NE	1:B:301:GLY:O	2.36	0.47
1:B:555:PRO:HB2	1:B:556:LEU:HD23	1.97	0.47
1:B:406:PRO:CB	1:B:407:PRO:HD2	2.44	0.47
1:A:101:ASP:OD1	1:A:101:ASP:N	2.40	0.47
1:B:56:LYS:HB2	1:B:56:LYS:HZ2	1.80	0.47
1:B:556:LEU:N	1:B:556:LEU:HD23	2.30	0.47
1:A:269:PRO:HG3	1:A:442:VAL:HG21	1.97	0.47
1:B:348:PHE:O	1:B:361:ALA:HA	2.14	0.47
1:B:286:ASP:CG	1:B:380:ARG:HH22	2.18	0.46
1:B:357:LYS:HA	1:B:357:LYS:HD2	1.64	0.46
1:A:229:ASP:OD1	1:A:230:ARG:O	2.32	0.46
1:A:352:ASP:OD1	1:A:354:SER:OG	2.28	0.46
1:B:210:LEU:O	1:B:211:ASN:C	2.54	0.46
1:B:118:ASP:CA	1:B:134:LYS:HD2	2.40	0.46
1:B:286:ASP:OD2	1:B:380:ARG:NH2	2.49	0.46
1:B:538:GLN:HB3	1:B:543:TYR:CE1	2.51	0.46
1:A:78:SER:HB3	1:A:124:THR:HG22	1.97	0.46
1:B:337:LYS:HZ3	1:B:353:ARG:NH2	2.13	0.45
1:B:57:GLN:O	1:B:58:ARG:HB2	2.15	0.45
1:B:283:HIS:O	1:B:284:ASP:C	2.54	0.45
1:B:164:GLY:H	1:B:258:ASN:HD21	1.64	0.45
1:A:419:TYR:HB2	1:A:426:PHE:CE1	2.51	0.45
1:B:220:ASP:HB3	1:B:224:PRO:HD2	1.97	0.45
1:A:61:GLU:OE2	3:A:701:PQQ:O2A	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:GLY:O	1:A:573:SER:HB3	2.15	0.45
1:B:116:TYR:HB2	1:B:160:ILE:HG13	1.98	0.45
1:B:146:ALA:HB1	1:B:152:TYR:CD2	2.52	0.45
1:A:117:GLY:O	1:A:134:LYS:NZ	2.49	0.45
1:B:56:LYS:NZ	1:B:56:LYS:HB2	2.31	0.44
1:B:564:LEU:O	1:B:567:PRO:HD2	2.16	0.44
1:A:200:ARG:HA	1:A:201:PRO:HD3	1.86	0.44
1:A:34:LYS:HD2	1:A:497:GLY:HA2	2.00	0.44
1:A:43:LYS:HD2	1:B:582:TRP:CE3	2.52	0.44
1:B:44:LEU:HD23	1:B:521:TRP:CH2	2.53	0.44
1:A:120:VAL:HG23	1:A:132:LEU:HB2	1.98	0.44
1:B:202:PHE:O	1:B:289:TYR:HB2	2.18	0.44
1:A:21:TYR:HA	1:A:63:GLN:NE2	2.32	0.44
1:A:227:PRO:O	1:A:237:VAL:HB	2.18	0.44
1:B:420:SER:HB2	1:B:427:TYR:HE2	1.83	0.44
1:A:55:GLU:H	1:B:57:GLN:HE21	1.66	0.43
1:A:202:PHE:O	1:A:289:TYR:HB2	2.17	0.43
1:A:43:LYS:HB3	1:B:582:TRP:CZ2	2.53	0.43
1:B:414:TRP:O	1:B:415:ASN:C	2.55	0.43
1:B:383:GLU:OE2	1:B:388:ARG:NH2	2.32	0.43
1:A:397:LYS:O	1:A:398:HIS:HB3	2.18	0.43
1:B:560:ASP:O	1:B:563:ASP:HB2	2.17	0.43
1:B:6:GLU:HA	1:B:9:ALA:HB3	2.00	0.43
1:B:405:SER:HB2	1:B:434:LYS:CB	2.47	0.43
1:B:405:SER:HA	1:B:406:PRO:C	2.38	0.43
1:B:210:LEU:HD12	1:B:211:ASN:N	2.34	0.43
1:A:453:MET:HB3	1:A:453:MET:HE3	1.79	0.43
1:B:157:ALA:HA	1:B:158:PRO:HD3	1.81	0.43
1:B:163:ASP:OD2	1:B:299:SER:HB3	2.18	0.43
1:A:136:THR:CG2	1:A:138:LYS:HG3	2.48	0.43
1:B:41:VAL:HG11	1:B:520:LEU:HB3	2.00	0.43
1:B:393:GLU:HB3	1:B:394:PRO:CD	2.48	0.43
1:B:292:GLY:HA2	1:B:309:HIS:ND1	2.34	0.43
1:B:561:MET:O	1:B:565:THR:HB	2.18	0.42
1:A:420:SER:HB3	1:A:423:THR:OG1	2.18	0.42
1:A:318:SER:O	1:A:344:ARG:HG3	2.19	0.42
1:B:544:LEU:O	1:B:576:VAL:HA	2.20	0.42
1:B:48:TRP:CZ2	1:B:576:VAL:HG21	2.54	0.42
1:A:249:GLN:HE22	1:A:321:ASN:HA	1.84	0.42
1:B:18:VAL:O	1:B:65:ILE:HG13	2.19	0.42
1:A:398:HIS:HD2	1:A:399:GLY:O	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ALA:HA	1:B:247:PRO:HD3	1.90	0.42
1:B:63:GLN:HB2	1:B:532:PRO:HG2	2.01	0.42
1:B:406:PRO:HB2	1:B:407:PRO:HD2	2.01	0.42
1:B:389:PRO:HA	1:B:390:PRO:HD3	1.83	0.42
1:B:370:TRP:CE3	1:B:371:ALA:HB2	2.55	0.42
1:A:84:ASP:O	1:A:87:THR:O	2.38	0.42
1:B:543:TYR:CZ	1:B:578:LYS:NZ	2.87	0.42
1:A:349:TYR:CD1	1:A:349:TYR:N	2.88	0.42
1:B:509:PHE:O	1:B:522:LYS:HA	2.20	0.42
1:A:55:GLU:H	1:B:57:GLN:NE2	2.17	0.42
1:A:50:TYR:OH	1:A:90:ARG:HD3	2.20	0.42
1:A:306:PHE:CZ	1:A:308:GLN:HG3	2.54	0.42
1:B:442:VAL:CG2	1:B:452:GLY:HA3	2.41	0.41
1:A:266:ASN:HB2	1:A:267:PRO:CD	2.47	0.41
1:A:507:GLY:HA3	1:A:524:GLN:HE22	1.85	0.41
1:B:317:PHE:O	1:B:318:SER:C	2.58	0.41
1:B:222:LYS:HE2	1:B:222:LYS:HB3	1.93	0.41
1:A:246:ALA:HA	1:A:247:PRO:HD3	1.83	0.41
1:B:163:ASP:HB3	1:B:166:THR:HG22	2.02	0.41
1:B:288:LEU:HD23	1:B:288:LEU:HA	1.85	0.41
1:B:312:ASN:C	1:B:312:ASN:HD22	2.24	0.41
1:A:339:THR:CG2	4:A:775:HOH:O	2.62	0.41
1:B:190:ASP:HA	1:B:191:PRO:HD3	1.90	0.41
1:A:63:GLN:HB2	1:A:532:PRO:HG2	2.03	0.41
1:B:306:PHE:CE2	1:B:308:GLN:HB2	2.56	0.41
1:B:144:LYS:NZ	1:B:148:HIS:CD2	2.87	0.41
1:A:2:ASP:O	1:A:3:VAL:CB	2.69	0.41
1:B:62:SER:HB2	1:B:74:THR:OG1	2.20	0.41
1:B:203:VAL:HG22	1:B:206:HIS:ND1	2.36	0.41
1:B:152:TYR:CZ	1:B:182:VAL:HG22	2.56	0.40
1:B:71:ILE:HG22	1:B:73:VAL:HG22	2.04	0.40
1:B:5:TRP:CZ3	1:B:161:VAL:HA	2.56	0.40
1:A:457:ILE:N	1:A:457:ILE:CD1	2.84	0.40
1:B:128:SER:HA	1:B:144:LYS:HA	2.04	0.40
1:A:200:ARG:HD3	1:A:201:PRO:CD	2.50	0.40
1:A:334:LYS:CA	1:A:334:LYS:HE3	2.47	0.40
1:B:59:GLY:HA3	1:B:551:GLY:HA3	2.03	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:HIS:CD2	1:A:456:ARG:NH2[2_665]	1.57	0.63
1:A:372:SER:OG	1:A:456:ARG:NH2[2_665]	1.92	0.28
1:A:372:SER:OG	1:A:456:ARG:NH1[2_665]	2.04	0.16
1:A:373:HIS:CG	1:A:456:ARG:NH2[2_665]	2.08	0.12
1:A:373:HIS:CD2	1:A:456:ARG:CZ[2_665]	2.13	0.07
1:A:372:SER:OG	1:A:456:ARG:CZ[2_665]	2.18	0.02

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	580/582 (100%)	530 (91%)	45 (8%)	5 (1%)	21	42
1	B	580/582 (100%)	514 (89%)	47 (8%)	19 (3%)	5	7
All	All	1160/1164 (100%)	1044 (90%)	92 (8%)	24 (2%)	9	16

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	ALA
1	A	385	GLU
1	B	217	VAL
1	B	289	TYR
1	B	330	ALA
1	B	332	ASP
1	B	366	ASP
1	B	385	GLU
1	B	107	ASP
1	B	280	GLY
1	B	331	LYS
1	A	107	ASP
1	B	313	ASP
1	B	3	VAL
1	B	15	THR

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Mol	Chain	Res	Type
1	B	211	ASN
1	B	269	PRO
1	B	496	ALA
1	A	108	VAL
1	B	375	ASP
1	B	459	ARG
1	A	3	VAL
1	B	108	VAL
1	B	572	GLY

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	469/469 (100%)	409 (87%)	60 (13%)	5	10
1	B	469/469 (100%)	402 (86%)	67 (14%)	4	7
All	All	938/938 (100%)	811 (86%)	127 (14%)	5	8

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LYS
1	A	34	LYS
1	A	43	LYS
1	A	58	ARG
1	A	73	VAL
1	A	83	LEU
1	A	87	THR
1	A	89	LYS
1	A	97	ARG
1	A	103	ARG
1	A	122	PHE
1	A	125	LEU
1	A	134	LYS
1	A	138	LYS

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Mol	Chain	Res	Type
1	A	142	LYS
1	A	153	THR
1	A	154	MET
1	A	159	THR
1	A	161	VAL
1	A	162	LYS
1	A	166	THR
1	A	168	LYS
1	A	203	VAL
1	A	217	VAL
1	A	221	VAL
1	A	237	VAL
1	A	258	ASN
1	A	262	VAL
1	A	269	PRO
1	A	299	SER
1	A	308	GLN
1	A	312	ASN
1	A	320	ASN
1	A	324	VAL
1	A	331	LYS
1	A	332	ASP
1	A	334	LYS
1	A	335	ILE
1	A	339	THR
1	A	357	LYS
1	A	376	LEU
1	A	377	LYS
1	A	400	LYS
1	A	407	PRO
1	A	433	TRP
1	A	439	THR
1	A	446	LYS
1	A	456	ARG
1	A	457	ILE
1	A	478	VAL
1	A	483	LYS
1	A	502	THR
1	A	541	GLU
1	A	544	LEU
1	A	556	LEU
1	A	561	MET

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Mol	Chain	Res	Type
1	A	564	LEU
1	A	565	THR
1	A	578	LYS
1	A	581	SER
1	B	1	LYS
1	B	26	HIS
1	B	34	LYS
1	B	41	VAL
1	B	51	SER
1	B	56	LYS
1	B	63	GLN
1	B	65	ILE
1	B	68	ASP
1	B	73	VAL
1	B	83	LEU
1	B	86	LYS
1	B	89	LYS
1	B	90	ARG
1	B	97	ARG
1	B	103	ARG
1	B	136	THR
1	B	142	LYS
1	B	143	LYS
1	B	153	THR
1	B	154	MET
1	B	161	VAL
1	B	166	THR
1	B	182	VAL
1	B	195	GLU
1	B	203	VAL
1	B	213	LYS
1	B	218	THR
1	B	221	VAL
1	B	222	LYS
1	B	230	ARG
1	B	256	GLU
1	B	262	VAL
1	B	269	PRO
1	B	299	SER
1	B	312	ASN
1	B	320	ASN
1	B	324	VAL

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Mol	Chain	Res	Type
1	B	326	PHE
1	B	329	LYS
1	B	334	LYS
1	B	339	THR
1	B	377	LYS
1	B	378	THR
1	B	397	LYS
1	B	398	HIS
1	B	402	VAL
1	B	433	TRP
1	B	434	LYS
1	B	437	TYR
1	B	445	THR
1	B	456	ARG
1	B	458	LYS
1	B	460	MET
1	B	472	ASP
1	B	477	LYS
1	B	483	LYS
1	B	493	LEU
1	B	495	THR
1	B	513	ASP
1	B	538	GLN
1	B	556	LEU
1	B	563	ASP
1	B	564	LEU
1	B	565	THR
1	B	566	ARG
1	B	578	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	28	GLN
1	A	57	GLN
1	A	63	GLN
1	A	95	ASN
1	A	96	HIS
1	A	173	HIS
1	A	206	HIS
1	A	249	GLN

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Mol	Chain	Res	Type
1	A	258	ASN
1	A	293	GLN
1	A	308	GLN
1	A	312	ASN
1	A	320	ASN
1	A	373	HIS
1	A	398	HIS
1	A	421	GLN
1	A	432	HIS
1	A	464	HIS
1	A	524	GLN
1	B	28	GLN
1	B	57	GLN
1	B	63	GLN
1	B	96	HIS
1	B	148	HIS
1	B	173	HIS
1	B	249	GLN
1	B	258	ASN
1	B	312	ASN
1	B	320	ASN
1	B	373	HIS
1	B	421	GLN
1	B	432	HIS
1	B	464	HIS

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

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	PQQ	A	701	2	16,26,26	4.22	7 (43%)	17,40,40	6.29	13 (76%)
3	PQQ	B	702	2	16,26,26	3.61	6 (37%)	17,40,40	5.17	13 (76%)

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	PQQ	A	701	2	-	0/0/28/28	0/3/3/3
3	PQQ	B	702	2	-	0/0/28/28	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	PQQ	C6A-C5	-8.75	1.39	1.49
3	B	702	PQQ	C6A-C5	-6.18	1.42	1.49
3	B	702	PQQ	C5-C4	-4.14	1.40	1.53
3	A	701	PQQ	C3A-C4	-3.98	1.40	1.48
3	A	701	PQQ	C5-C4	-3.82	1.41	1.53
3	B	702	PQQ	C3A-C4	-3.02	1.42	1.48
3	A	701	PQQ	C3-C3A	-2.32	1.35	1.40
3	B	702	PQQ	C9A-C6A	3.30	1.43	1.40
3	A	701	PQQ	C9A-C6A	5.13	1.45	1.40
3	B	702	PQQ	O4-C4	7.40	1.39	1.23
3	A	701	PQQ	O5-C5	7.60	1.39	1.23
3	B	702	PQQ	O5-C5	8.27	1.40	1.23
3	A	701	PQQ	O4-C4	8.84	1.42	1.23

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	PQQ	C8-C7-N6	-14.01	106.05	122.39
3	B	702	PQQ	C8-C7-N6	-11.66	108.79	122.39
3	B	702	PQQ	O5-C5-C4	-9.01	105.53	119.29
3	A	701	PQQ	C9A-C6A-C5	-7.70	113.75	120.85
3	A	701	PQQ	O4-C4-C5	-7.41	107.97	119.29
3	A	701	PQQ	O5-C5-C4	-7.31	108.12	119.29
3	A	701	PQQ	C3A-C4-C5	-3.96	112.98	118.08
3	B	702	PQQ	C3A-C4-C5	-3.93	113.01	118.08
3	B	702	PQQ	C9A-C6A-C5	-3.27	117.83	120.85
3	A	701	PQQ	C6A-C9A-C1A	-2.85	114.10	118.21
3	B	702	PQQ	C3A-C3-C2	-2.66	104.17	105.98
3	A	701	PQQ	O4-C4-C3A	-2.12	117.99	121.55
3	A	701	PQQ	C3-C3A-C1A	2.02	109.28	106.49
3	B	702	PQQ	C8-C9-C9A	2.04	121.87	118.95
3	A	701	PQQ	C9A-C6A-N6	2.21	126.54	123.35
3	A	701	PQQ	C6A-N6-C7	2.56	122.08	118.38
3	B	702	PQQ	O4-C4-C3A	3.29	127.08	121.55
3	B	702	PQQ	C9-C8-C7	3.86	124.16	120.34
3	B	702	PQQ	C9A-C1A-N1	4.07	132.20	124.29
3	B	702	PQQ	C6A-C5-C4	4.36	124.45	119.16
3	B	702	PQQ	C9-C9A-C1A	5.87	128.33	123.27
3	B	702	PQQ	C6A-N6-C7	6.72	128.09	118.38
3	A	701	PQQ	C6A-C5-C4	6.82	127.44	119.16
3	B	702	PQQ	O5-C5-C6A	7.03	129.91	122.10
3	A	701	PQQ	C9-C9A-C1A	9.91	131.82	123.27
3	A	701	PQQ	C9-C8-C7	10.67	130.93	120.34

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
3	A	701	PQQ	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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.