



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:33 PM UTC

PDB ID : 1TPL / pdb_00001tpl
Title : THE THREE-DIMENSIONAL STRUCTURE OF TYROSINE PHENOL-
LYASE
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Deposited on : 1992-11-25
Resolution : 2.30 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

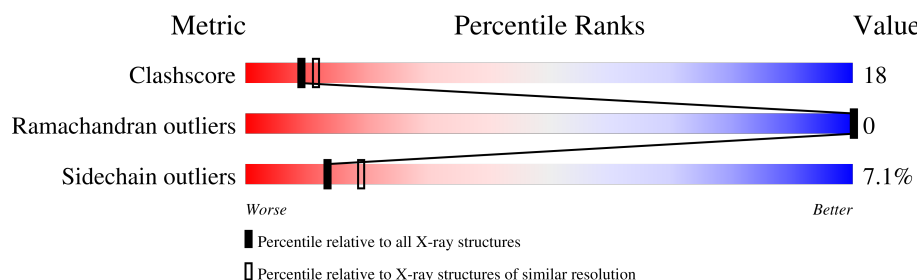
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	456	
1	B	456	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	458	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7194 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 TYROSINE PHENOL-LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	0	0
			3361	2134	572	629	26			
1	B	426	Total	C	N	O	S	0	0	0
			3363	2136	573	628	26			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is water.

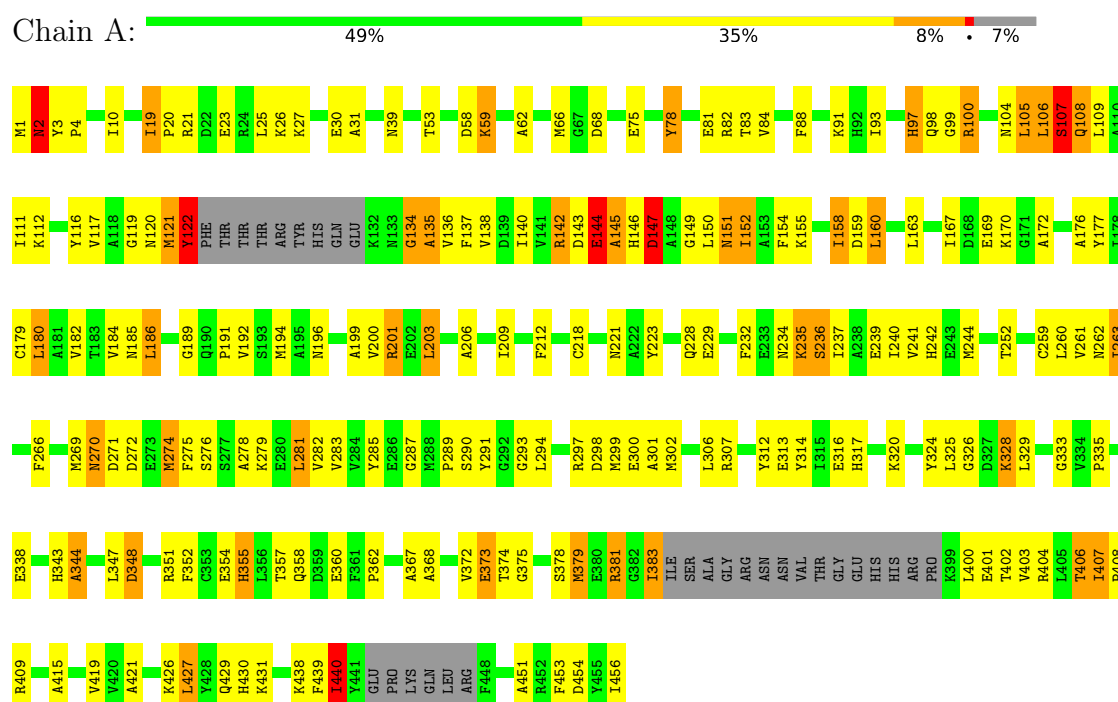
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	244	Total 244	O 244	0	0
3	B	206	Total 206	O 206	0	0

3 Residue-property plots

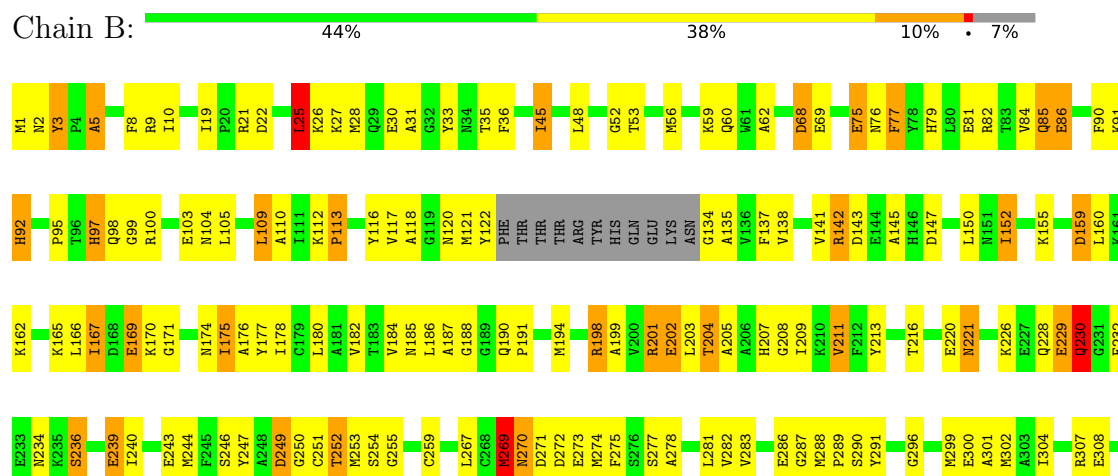
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: TYROSINE PHENOL-LYASE



• Molecule 1: TYROSINE PHENOL-LYASE



VAL	THR	GLY	HIS	HIS	ARG	PRO	K399	L400	E401	T402	V403	R404	L405	T406	I407	P408	R409	R410	A415	H416	V419	V420	A421	D422	I425	K426	Q429	H430	K431	F439	I440	Y441	GLU	PRO	LYS	GLN	I446	R447	F448	F449	T450	D454	Y455	I456									
H317	R318	Q321	V322	L325	G326	D327	K328	L329	K330	E338	P339	V340	G341	G342	H343	A344	V345	F346	L347	D348	A349	R350	R351	F352	C353	E354	H355	L356	T357	Q358	D359	E360	A363	Q364	S369	E373	T374	G375	V376	R377	S378	M379	E380	R381	G382	I383	ILE	SER	ALA	GLY	ARG	ASN	ASN

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	76.02Å 138.27Å 93.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.162 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7194	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.98	1/3423 (0.0%)	2.14	143/4603 (3.1%)
1	B	0.99	0/3425	2.22	172/4606 (3.7%)
All	All	0.98	1/6848 (0.0%)	2.18	315/9209 (3.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	407	ILE	CA-CB	5.74	1.59	1.53

All (315) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	358	GLN	CA-C-N	11.48	135.66	120.28
1	B	358	GLN	C-N-CA	11.48	135.66	120.28
1	B	440	ILE	CA-C-N	11.46	142.33	121.70
1	B	440	ILE	C-N-CA	11.46	142.33	121.70
1	B	159	ASP	CA-CB-CG	11.02	123.62	112.60
1	B	232	PHE	CA-CB-CG	-10.37	103.43	113.80
1	B	137	PHE	CA-CB-CG	-10.06	103.74	113.80
1	A	270	ASN	OD1-CG-ND2	9.88	132.49	122.60
1	B	2	ASN	CA-CB-CG	9.84	122.44	112.60
1	A	407	ILE	N-CA-C	9.29	117.55	107.60
1	A	2	ASN	CA-CB-CG	9.11	121.70	112.60
1	B	198	ARG	CD-NE-CZ	8.92	136.89	124.40
1	B	97	HIS	CA-CB-CG	-8.91	104.89	113.80
1	B	354	GLU	CB-CG-CD	8.91	127.74	112.60
1	A	266	PHE	CA-CB-CG	8.59	122.39	113.80
1	B	75	GLU	CA-CB-CG	8.58	131.26	114.10
1	A	223	TYR	CA-C-N	8.55	131.74	120.28
1	A	223	TYR	C-N-CA	8.55	131.74	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	269	MET	N-CA-CB	8.42	124.87	111.56
1	A	88	PHE	CA-CB-CG	8.32	122.12	113.80
1	B	407	ILE	N-CA-C	8.24	117.12	107.73
1	A	97	HIS	CA-CB-CG	-8.20	105.60	113.80
1	A	407	ILE	O-C-N	8.15	128.42	120.92
1	A	147	ASP	CA-CB-CG	8.14	120.74	112.60
1	A	146	HIS	CA-C-N	8.01	133.51	120.94
1	A	146	HIS	C-N-CA	8.01	133.51	120.94
1	B	448	PHE	CA-CB-CG	7.84	121.64	113.80
1	B	325	LEU	CA-C-N	7.70	128.69	119.99
1	B	325	LEU	C-N-CA	7.70	128.69	119.99
1	B	52	GLY	N-CA-C	7.70	125.60	115.36
1	A	58	ASP	CA-C-N	7.66	131.16	120.29
1	A	58	ASP	C-N-CA	7.66	131.16	120.29
1	B	201	ARG	O-C-N	7.61	129.94	122.03
1	A	206	ALA	N-CA-C	-7.59	103.09	111.36
1	B	169	GLU	CA-CB-CG	7.51	129.12	114.10
1	B	234	ASN	CA-CB-CG	-7.48	105.12	112.60
1	A	112	LYS	N-CA-C	-7.47	100.66	110.07
1	A	281	LEU	CA-C-O	-7.44	112.94	120.90
1	A	136	VAL	O-C-N	7.36	131.21	123.26
1	A	379	MET	N-CA-CB	-7.28	98.57	110.43
1	A	105	LEU	O-C-N	7.26	129.55	122.07
1	B	322	VAL	CA-C-N	7.24	129.98	120.28
1	B	322	VAL	C-N-CA	7.24	129.98	120.28
1	B	291	TYR	N-CA-C	-7.22	103.78	112.59
1	B	229	GLU	CB-CG-CD	7.19	124.83	112.60
1	B	211	VAL	CA-C-O	7.16	127.95	120.36
1	B	186	LEU	CB-CA-C	7.13	122.42	109.37
1	A	151	ASN	N-CA-C	7.13	120.71	108.02
1	B	400	LEU	N-CA-CB	-7.11	98.72	110.23
1	B	92	HIS	CA-CB-CG	-7.10	106.70	113.80
1	A	152	ILE	N-CA-C	-7.09	97.28	107.77
1	A	221	ASN	CA-CB-CG	-7.07	105.53	112.60
1	B	271	ASP	CA-CB-CG	-7.00	105.60	112.60
1	A	108	GLN	CB-CG-CD	-6.99	100.71	112.60
1	A	81	GLU	CA-C-O	-6.98	113.67	121.00
1	B	271	ASP	CA-C-N	6.96	129.91	120.38
1	B	271	ASP	C-N-CA	6.96	129.91	120.38
1	B	171	GLY	CA-C-N	6.95	134.82	121.54
1	B	171	GLY	C-N-CA	6.95	134.82	121.54
1	A	312	TYR	O-C-N	6.93	129.30	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	329	LEU	CA-C-N	6.91	132.17	121.19
1	B	329	LEU	C-N-CA	6.91	132.17	121.19
1	B	77	PHE	CA-CB-CG	-6.88	106.92	113.80
1	B	317	HIS	CA-CB-CG	-6.81	106.99	113.80
1	B	19	ILE	CA-C-N	6.79	126.76	120.03
1	B	19	ILE	C-N-CA	6.79	126.76	120.03
1	B	203	LEU	CB-CA-C	6.75	121.66	110.92
1	A	300	GLU	CA-C-N	6.75	129.88	120.29
1	A	300	GLU	C-N-CA	6.75	129.88	120.29
1	B	205	ALA	CA-C-N	6.75	129.62	120.44
1	B	205	ALA	C-N-CA	6.75	129.62	120.44
1	B	375	GLY	N-CA-C	-6.67	106.02	115.43
1	B	150	LEU	N-CA-C	6.64	119.40	109.25
1	A	120	ASN	CA-C-N	6.61	132.07	122.16
1	A	120	ASN	C-N-CA	6.61	132.07	122.16
1	A	348	ASP	CB-CA-C	6.59	121.69	110.81
1	B	399	LYS	CA-C-N	6.58	131.82	122.09
1	B	399	LYS	C-N-CA	6.58	131.82	122.09
1	B	340	VAL	CA-C-O	-6.56	114.14	121.36
1	B	21	ARG	O-C-N	6.54	129.63	122.11
1	B	220	GLU	N-CA-C	-6.54	104.23	111.36
1	A	186	LEU	CB-CA-C	6.50	122.57	109.38
1	A	172	ALA	CA-C-N	6.49	130.18	120.31
1	A	172	ALA	C-N-CA	6.49	130.18	120.31
1	B	440	ILE	CA-C-O	6.49	128.89	120.78
1	A	297	ARG	CD-NE-CZ	-6.47	115.35	124.40
1	A	206	ALA	CA-C-O	-6.46	113.57	120.42
1	B	304	ILE	CA-C-N	6.46	127.11	120.00
1	B	304	ILE	C-N-CA	6.46	127.11	120.00
1	B	117	VAL	CB-CA-C	6.45	120.43	110.50
1	A	262	ASN	CA-C-N	6.42	129.30	122.11
1	A	262	ASN	C-N-CA	6.42	129.30	122.11
1	B	143	ASP	N-CA-C	6.39	119.94	111.75
1	B	439	PHE	CA-CB-CG	6.37	120.17	113.80
1	A	151	ASN	CA-C-N	6.37	132.02	122.98
1	A	151	ASN	C-N-CA	6.37	132.02	122.98
1	B	221	ASN	CA-C-N	6.34	129.10	120.54
1	B	221	ASN	C-N-CA	6.34	129.10	120.54
1	A	100	ARG	CD-NE-CZ	6.33	133.26	124.40
1	A	312	TYR	CA-C-O	-6.31	114.15	120.90
1	A	241	VAL	O-C-N	6.31	128.09	121.91
1	B	31	ALA	CA-C-O	6.29	127.17	119.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	VAL	CA-C-O	-6.26	114.54	121.17
1	B	45	ILE	CA-C-O	-6.26	113.60	120.48
1	B	229	GLU	CA-C-O	6.21	127.69	120.98
1	A	134	GLY	CA-C-N	6.19	134.31	121.32
1	A	134	GLY	C-N-CA	6.19	134.31	121.32
1	A	373	GLU	N-CA-C	6.19	120.03	112.23
1	A	375	GLY	N-CA-C	-6.16	106.21	115.32
1	B	174	ASN	N-CA-C	-6.14	105.43	113.17
1	B	277	SER	CA-C-N	6.14	128.83	120.54
1	B	277	SER	C-N-CA	6.14	128.83	120.54
1	B	147	ASP	CA-C-N	6.13	128.49	120.28
1	B	147	ASP	C-N-CA	6.13	128.49	120.28
1	A	354	GLU	CA-C-N	6.11	129.08	120.28
1	A	354	GLU	C-N-CA	6.11	129.08	120.28
1	A	143	ASP	N-CA-C	6.08	120.25	112.34
1	B	342	GLY	CA-C-O	-6.08	112.32	119.50
1	A	147	ASP	N-CA-C	6.08	119.07	110.50
1	B	62	ALA	CB-CA-C	6.07	120.86	110.79
1	A	335	PRO	O-C-N	6.05	127.03	122.73
1	A	122	TYR	CA-CB-CG	6.05	124.79	113.90
1	B	207	HIS	CA-CB-CG	-6.04	107.75	113.80
1	B	202	GLU	CB-CG-CD	6.04	122.87	112.60
1	A	62	ALA	CA-C-N	6.04	127.89	120.22
1	A	62	ALA	C-N-CA	6.04	127.89	120.22
1	B	449	PHE	CB-CA-C	6.03	121.79	109.55
1	B	3	TYR	N-CA-C	6.00	118.16	109.04
1	B	374	THR	CA-CB-OG1	-5.94	100.69	109.60
1	A	429	GLN	CA-C-N	5.93	132.12	121.15
1	A	429	GLN	C-N-CA	5.93	132.12	121.15
1	A	203	LEU	CB-CA-C	5.87	120.00	110.96
1	A	135	ALA	CA-C-O	5.86	128.73	121.81
1	B	86	GLU	N-CA-C	5.86	117.67	111.28
1	B	169	GLU	N-CA-CB	5.85	118.72	110.12
1	A	149	GLY	CA-C-N	5.84	131.09	121.39
1	A	149	GLY	C-N-CA	5.84	131.09	121.39
1	A	151	ASN	CA-C-O	5.84	126.64	120.33
1	B	186	LEU	N-CA-C	-5.83	100.69	109.95
1	A	298	ASP	CA-CB-CG	-5.82	106.78	112.60
1	B	69	GLU	N-CA-C	5.82	119.45	112.93
1	B	85	GLN	O-C-N	5.81	128.06	122.07
1	A	301	ALA	CA-C-N	5.81	128.54	120.29
1	A	301	ALA	C-N-CA	5.81	128.54	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	GLU	CB-CA-C	-5.79	101.79	110.88
1	B	112	LYS	N-CA-C	-5.79	102.32	110.31
1	A	419	VAL	CA-C-N	5.78	127.85	120.56
1	A	419	VAL	C-N-CA	5.78	127.85	120.56
1	B	410	ARG	NE-CZ-NH1	5.78	127.28	121.50
1	A	453	PHE	CA-CB-CG	5.78	119.58	113.80
1	B	220	GLU	CA-CB-CG	5.77	125.64	114.10
1	B	252	THR	N-CA-C	-5.77	99.61	109.24
1	B	255	GLY	CA-C-N	5.76	131.70	120.99
1	B	255	GLY	C-N-CA	5.76	131.70	120.99
1	A	355	HIS	CA-CB-CG	5.75	119.56	113.80
1	A	145	ALA	CA-C-N	5.75	128.55	120.28
1	A	145	ALA	C-N-CA	5.75	128.55	120.28
1	A	151	ASN	CA-CB-CG	5.74	118.34	112.60
1	B	416	HIS	N-CA-CB	5.74	118.66	110.16
1	A	144	GLU	N-CA-CB	5.73	119.97	110.91
1	A	236	SER	CB-CA-C	-5.73	97.93	109.68
1	B	216	THR	N-CA-C	5.73	118.27	111.33
1	B	142	ARG	CA-C-N	5.73	128.74	120.38
1	B	142	ARG	C-N-CA	5.73	128.74	120.38
1	B	357	THR	CA-C-O	-5.72	114.64	121.11
1	A	358	GLN	CA-C-N	5.72	129.75	120.60
1	A	358	GLN	C-N-CA	5.72	129.75	120.60
1	B	228	GLN	N-CA-C	5.71	120.90	113.88
1	B	415	ALA	CA-C-N	5.70	128.38	120.29
1	B	415	ALA	C-N-CA	5.70	128.38	120.29
1	B	299	MET	N-CA-C	-5.68	105.17	111.36
1	B	230	GLN	CB-CA-C	5.67	117.95	110.06
1	A	234	ASN	CA-CB-CG	-5.67	106.93	112.60
1	A	374	THR	CA-CB-CG2	5.65	120.11	110.50
1	A	325	LEU	CA-C-N	5.64	126.37	119.99
1	A	325	LEU	C-N-CA	5.64	126.37	119.99
1	B	249	ASP	CA-CB-CG	-5.64	106.96	112.60
1	B	448	PHE	CA-C-O	5.64	128.58	120.51
1	B	287	GLY	CA-C-O	5.64	124.47	119.56
1	A	59	LYS	CA-C-N	5.63	128.28	120.29
1	A	59	LYS	C-N-CA	5.63	128.28	120.29
1	B	402	THR	N-CA-CB	-5.62	102.62	111.05
1	B	296	GLY	N-CA-C	-5.61	106.00	112.73
1	B	187	ALA	CA-C-O	5.60	127.76	120.81
1	B	25	LEU	CA-C-N	5.59	127.70	120.44
1	B	25	LEU	C-N-CA	5.59	127.70	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	335	PRO	N-CA-CB	5.57	106.04	102.92
1	B	431	LYS	CA-C-N	5.56	132.16	121.54
1	B	431	LYS	C-N-CA	5.56	132.16	121.54
1	A	83	THR	CA-CB-OG1	-5.56	101.26	109.60
1	B	410	ARG	CD-NE-CZ	5.54	132.16	124.40
1	A	228	GLN	N-CA-C	5.52	121.79	114.12
1	A	291	TYR	CA-C-N	5.51	128.43	120.11
1	A	291	TYR	C-N-CA	5.51	128.43	120.11
1	B	308	GLU	CA-C-N	5.51	128.21	120.28
1	B	308	GLU	C-N-CA	5.51	128.21	120.28
1	B	8	PHE	CA-CB-CG	5.51	119.31	113.80
1	B	401	GLU	CA-C-O	5.51	126.98	120.70
1	A	121	MET	N-CA-CB	-5.50	103.14	110.57
1	B	81	GLU	CA-C-O	-5.49	115.05	120.82
1	B	351	ARG	CD-NE-CZ	5.49	132.09	124.40
1	B	326	GLY	CA-C-N	5.49	127.57	120.44
1	B	326	GLY	C-N-CA	5.49	127.57	120.44
1	B	239	GLU	N-CA-CB	5.48	117.96	110.01
1	B	204	THR	N-CA-C	5.48	117.25	111.28
1	B	383	ILE	N-CA-CB	5.46	120.79	111.50
1	B	2	ASN	CA-C-N	5.46	130.35	121.83
1	B	2	ASN	C-N-CA	5.46	130.35	121.83
1	A	317	HIS	CA-CB-CG	-5.46	108.34	113.80
1	A	329	LEU	CA-C-N	5.46	127.91	120.54
1	A	329	LEU	C-N-CA	5.46	127.91	120.54
1	A	31	ALA	N-CA-C	-5.45	106.58	113.18
1	B	84	VAL	O-C-N	5.45	127.45	121.83
1	B	68	ASP	CB-CA-C	5.41	120.52	111.22
1	B	185	ASN	N-CA-C	5.40	120.54	113.20
1	B	338	GLU	CA-C-O	5.40	125.99	120.64
1	B	2	ASN	N-CA-C	-5.40	107.34	114.31
1	A	68	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	81	GLU	CA-C-N	5.39	127.51	120.28
1	A	81	GLU	C-N-CA	5.39	127.51	120.28
1	A	201	ARG	NE-CZ-NH1	-5.38	116.12	121.50
1	B	103	GLU	O-C-N	5.38	127.62	122.07
1	A	290	SER	CA-C-N	5.37	131.79	121.54
1	A	290	SER	C-N-CA	5.37	131.79	121.54
1	A	19	ILE	CB-CA-C	5.36	116.25	111.00
1	A	351	ARG	NE-CZ-NH2	-5.36	114.38	119.20
1	A	66	MET	CA-CB-CG	-5.36	103.39	114.10
1	B	27	LYS	CG-CD-CE	5.36	123.62	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	288	MET	O-C-N	5.35	127.56	121.94
1	A	78	TYR	N-CA-C	-5.35	105.36	111.14
1	A	194	MET	N-CA-C	-5.34	105.46	111.28
1	B	142	ARG	CD-NE-CZ	-5.34	116.92	124.40
1	B	177	TYR	CA-C-O	5.34	127.07	121.25
1	B	402	THR	N-CA-C	5.34	117.97	109.81
1	B	273	GLU	CA-C-N	5.33	127.69	120.38
1	B	273	GLU	C-N-CA	5.33	127.69	120.38
1	B	201	ARG	CA-C-O	-5.32	115.41	121.00
1	B	426	LYS	CA-CB-CG	-5.32	103.46	114.10
1	A	152	ILE	N-CA-CB	5.32	119.05	111.82
1	A	403	VAL	N-CA-C	-5.31	100.10	107.80
1	B	416	HIS	N-CA-C	-5.31	105.57	111.36
1	A	451	ALA	N-CA-C	5.29	117.99	110.10
1	B	113	PRO	CB-CA-C	5.29	118.28	111.56
1	A	107	SER	CA-C-O	5.28	126.37	120.82
1	A	146	HIS	CA-CB-CG	5.28	119.08	113.80
1	A	440	ILE	CA-C-N	5.28	131.20	121.70
1	A	440	ILE	C-N-CA	5.28	131.20	121.70
1	A	326	GLY	CA-C-N	5.28	127.62	120.65
1	A	326	GLY	C-N-CA	5.28	127.62	120.65
1	B	201	ARG	N-CA-C	-5.27	105.22	110.97
1	B	21	ARG	CA-C-O	-5.27	115.02	120.92
1	A	407	ILE	CB-CA-C	-5.25	105.14	111.18
1	A	427	LEU	N-CA-C	-5.25	105.45	111.07
1	A	58	ASP	CA-CB-CG	5.25	117.85	112.60
1	A	307	ARG	NE-CZ-NH2	-5.24	114.48	119.20
1	A	2	ASN	N-CA-C	-5.23	106.74	113.23
1	A	99	GLY	CA-C-N	5.22	127.54	120.38
1	A	99	GLY	C-N-CA	5.22	127.54	120.38
1	B	135	ALA	N-CA-C	5.22	117.19	108.99
1	A	313	GLU	CA-C-O	-5.22	114.20	120.10
1	B	62	ALA	CA-C-N	5.22	126.85	120.22
1	B	62	ALA	C-N-CA	5.22	126.85	120.22
1	B	354	GLU	CA-C-N	5.22	129.44	120.72
1	B	354	GLU	C-N-CA	5.22	129.44	120.72
1	B	112	LYS	N-CA-CB	5.20	118.69	110.11
1	A	39	ASN	OD1-CG-ND2	5.20	127.80	122.60
1	A	262	ASN	OD1-CG-ND2	-5.20	117.40	122.60
1	B	82	ARG	CD-NE-CZ	5.19	131.67	124.40
1	A	228	GLN	OE1-CD-NE2	5.18	127.78	122.60
1	B	246	SER	N-CA-C	-5.18	106.47	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	ILE	CB-CA-C	-5.18	104.10	111.40
1	A	426	LYS	N-CA-CB	5.17	117.72	110.12
1	B	92	HIS	CB-CA-C	-5.16	99.17	109.33
1	A	260	LEU	N-CA-CB	-5.15	104.16	111.84
1	B	35	THR	CA-CB-OG1	-5.15	101.87	109.60
1	B	350	ARG	N-CA-CB	5.15	117.47	110.01
1	B	419	VAL	N-CA-C	-5.13	105.49	110.42
1	A	136	VAL	N-CA-C	-5.13	100.92	108.11
1	B	270	ASN	N-CA-C	-5.12	107.58	113.88
1	B	363	ALA	CA-C-N	5.12	127.14	120.28
1	B	363	ALA	C-N-CA	5.12	127.14	120.28
1	A	427	LEU	N-CA-CB	5.11	117.42	110.01
1	A	263	ILE	N-CA-CB	5.11	119.39	110.96
1	B	321	GLN	N-CA-C	-5.11	105.79	111.36
1	B	300	GLU	CA-C-N	5.10	127.12	120.28
1	B	300	GLU	C-N-CA	5.10	127.12	120.28
1	A	344	ALA	CA-C-N	5.10	129.82	123.14
1	A	344	ALA	C-N-CA	5.10	129.82	123.14
1	A	367	ALA	CA-C-N	5.09	127.11	120.28
1	A	367	ALA	C-N-CA	5.09	127.11	120.28
1	B	301	ALA	CA-C-N	5.09	127.52	120.29
1	B	301	ALA	C-N-CA	5.09	127.52	120.29
1	A	145	ALA	N-CA-C	-5.08	105.39	112.45
1	B	25	LEU	CA-C-O	5.08	125.94	120.55
1	B	5	ALA	N-CA-C	-5.07	103.84	110.53
1	A	229	GLU	N-CA-CB	5.07	118.68	110.42
1	B	117	VAL	N-CA-C	-5.07	100.91	108.46
1	B	201	ARG	CA-CB-CG	5.05	124.20	114.10
1	A	136	VAL	CA-C-O	-5.05	115.09	120.39
1	B	82	ARG	CA-C-O	5.05	126.62	121.07
1	B	208	GLY	CA-C-N	5.05	127.92	120.91
1	B	208	GLY	C-N-CA	5.05	127.92	120.91
1	A	218	CYS	CA-C-O	-5.04	114.17	119.97
1	A	252	THR	CA-CB-OG1	-5.04	102.04	109.60
1	B	360	GLU	CA-C-N	5.04	134.09	121.80
1	B	360	GLU	C-N-CA	5.04	134.09	121.80
1	A	237	ILE	N-CA-C	-5.02	105.50	110.62
1	A	68	ASP	N-CA-C	-5.02	98.42	107.75
1	B	68	ASP	N-CA-C	-5.02	97.74	107.62
1	B	234	ASN	OD1-CG-ND2	5.02	127.62	122.60
1	B	318	ARG	NE-CZ-NH2	-5.02	114.69	119.20
1	A	378	SER	CA-C-N	5.00	129.62	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	378	SER	C-N-CA	5.00	129.62	122.72
1	B	45	ILE	CA-C-N	5.00	129.80	122.85
1	B	45	ILE	C-N-CA	5.00	129.80	122.85

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3361	0	3319	119	0
1	B	3363	0	3324	127	0
2	A	10	0	0	2	0
2	B	10	0	0	0	0
3	A	244	0	0	13	0
3	B	206	0	0	25	2
All	All	7194	0	6643	244	2

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 18.

All (244) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:TYR:CA	3:B:618:HOH:O	1.99	1.10
1:B:441:TYR:CB	3:B:618:HOH:O	1.97	1.09
1:B:441:TYR:HA	3:B:618:HOH:O	1.57	1.03
1:B:441:TYR:HB3	3:B:618:HOH:O	1.59	1.00
1:A:379:MET:HA	3:A:497:HOH:O	1.62	0.97
1:B:68:ASP:H	1:B:76:ASN:HD21	0.95	0.94
1:B:68:ASP:H	1:B:76:ASN:ND2	1.65	0.94
1:B:259:CYS:HB3	3:B:649:HOH:O	1.68	0.94
1:B:160:LEU:HD11	1:B:199:ALA:HB1	1.49	0.93
1:A:100:ARG:HH21	1:A:104:ASN:HB2	1.40	0.87
1:B:121:MET:HB2	1:B:184:VAL:HG23	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ASP:N	1:B:76:ASN:HD21	1.76	0.84
1:A:134:GLY:HA3	3:A:668:HOH:O	1.77	0.83
1:A:150:LEU:HD22	1:A:151:ASN:H	1.47	0.78
1:A:2:ASN:HB2	3:A:678:HOH:O	1.84	0.77
1:A:145:ALA:HA	1:A:155:LYS:HG2	1.66	0.77
1:B:374:THR:O	3:B:552:HOH:O	2.02	0.77
1:B:75:GLU:HG3	3:B:522:HOH:O	1.86	0.75
1:A:271:ASP:HB3	1:A:274:MET:HB3	1.69	0.74
1:B:36:PHE:HB2	1:B:379:MET:HE3	1.69	0.73
1:A:368:ALA:O	1:A:372:VAL:HG23	1.91	0.71
1:B:404:ARG:O	3:B:655:HOH:O	2.09	0.69
1:A:236:SER:HB2	1:A:239:GLU:HG3	1.73	0.69
1:B:178:ILE:HB	1:B:211:VAL:HG22	1.73	0.69
1:A:117:VAL:HG23	1:A:176:ALA:HB3	1.75	0.68
1:B:116:TYR:CZ	1:B:170:LYS:HG2	2.28	0.68
1:A:84:VAL:HG21	1:A:93:ILE:HD12	1.74	0.68
1:A:109:LEU:HD11	1:A:278:ALA:HB2	1.75	0.68
1:B:99:GLY:HA3	1:B:254:SER:HB2	1.75	0.68
1:B:357:THR:HB	1:B:360:GLU:HG3	1.75	0.68
1:B:338:GLU:HB3	1:B:339:PRO:HA	1.77	0.67
1:B:48:LEU:HD12	1:B:379:MET:HB2	1.75	0.67
1:B:59:LYS:HD3	3:B:594:HOH:O	1.93	0.67
1:B:204:THR:HB	1:B:209:ILE:HG22	1.77	0.66
1:A:151:ASN:HA	3:A:700:HOH:O	1.95	0.66
1:B:226:LYS:HB2	1:B:240:ILE:CD1	2.26	0.65
1:A:381:ARG:HG3	1:A:383:ILE:HD11	1.79	0.64
1:A:100:ARG:NH2	1:A:104:ASN:HB2	2.11	0.64
1:A:373:GLU:HB3	3:A:549:HOH:O	1.97	0.63
1:B:382:GLY:HA2	1:B:400:LEU:O	1.98	0.62
1:B:430:HIS:O	1:B:431:LYS:C	2.42	0.62
1:A:147:ASP:OD1	1:A:150:LEU:HB3	1.99	0.62
1:A:21:ARG:N	2:A:458:SO4:O3	2.31	0.62
1:A:106:LEU:HD23	1:A:107:SER:N	2.15	0.62
1:B:97:HIS:HD1	1:B:97:HIS:H	1.48	0.62
1:B:122:TYR:N	3:B:635:HOH:O	2.32	0.62
1:B:160:LEU:HD11	1:B:199:ALA:CB	2.27	0.62
1:B:383:ILE:HB	3:B:508:HOH:O	1.99	0.62
1:B:348:ASP:O	1:B:352:PHE:HB2	1.99	0.61
1:A:23:GLU:HG2	1:A:26:LYS:NZ	2.16	0.60
1:A:78:TYR:HB3	1:A:82:ARG:CZ	2.31	0.60
1:A:155:LYS:HD2	3:A:700:HOH:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:PHE:CZ	1:A:279:LYS:HD2	2.37	0.60
1:A:184:VAL:O	1:A:189:GLY:HA2	2.02	0.59
1:B:344:ALA:HB2	1:B:406:THR:HG23	1.83	0.59
1:A:383:ILE:HD12	3:A:664:HOH:O	2.02	0.59
1:A:294:LEU:HD23	1:A:299:MET:HG2	1.83	0.59
1:B:188:GLY:HA3	1:B:346:PHE:HE1	1.67	0.58
1:A:269:MET:HG3	1:A:274:MET:HG2	1.85	0.58
1:A:344:ALA:HB2	1:A:406:THR:HG23	1.86	0.58
1:B:118:ALA:HB3	1:B:178:ILE:HD12	1.85	0.58
1:A:242:HIS:HE1	3:A:610:HOH:O	1.85	0.57
1:B:100:ARG:HB2	3:B:533:HOH:O	2.04	0.57
1:A:116:TYR:O	1:A:176:ALA:N	2.33	0.57
1:A:232:PHE:HA	1:A:235:LYS:HG3	1.87	0.57
1:B:166:LEU:HG	1:B:175:ILE:HD11	1.86	0.57
1:A:105:LEU:O	1:A:109:LEU:HB2	2.04	0.56
1:B:431:LYS:HD2	3:B:646:HOH:O	2.04	0.56
1:B:353:CYS:HA	1:B:355:HIS:CE1	2.40	0.56
1:A:408:PRO:HB3	3:A:698:HOH:O	2.05	0.56
1:A:122:TYR:H	1:A:122:TYR:HD1	1.54	0.56
1:B:404:ARG:HB3	3:B:655:HOH:O	2.05	0.56
1:B:198:ARG:O	1:B:202:GLU:HG2	2.06	0.56
1:A:348:ASP:O	1:A:352:PHE:HB2	2.07	0.55
1:A:106:LEU:HD23	1:A:106:LEU:C	2.31	0.55
1:A:272:ASP:O	1:A:275:PHE:HB3	2.06	0.55
1:A:373:GLU:HG3	1:A:427:LEU:HD21	1.87	0.55
1:B:116:TYR:OH	1:B:170:LYS:HG2	2.06	0.55
1:A:163:LEU:O	1:A:167:ILE:HG13	2.06	0.55
1:B:121:MET:HB2	1:B:184:VAL:CG2	2.34	0.55
1:B:376:VAL:HG21	1:B:420:VAL:HG22	1.89	0.54
1:A:106:LEU:HD21	1:A:177:TYR:OH	2.07	0.54
1:B:155:LYS:NZ	1:B:338:GLU:O	2.40	0.54
1:B:448:PHE:HB3	1:B:449:PHE:CD2	2.42	0.54
1:B:201:ARG:HE	1:B:201:ARG:HA	1.72	0.54
1:A:144:GLU:O	1:A:155:LYS:HE3	2.07	0.54
1:A:440:ILE:HG21	1:A:454:ASP:HB3	1.89	0.54
1:B:441:TYR:CD1	1:B:441:TYR:N	2.76	0.54
1:A:186:LEU:HD11	3:A:634:HOH:O	2.08	0.54
1:A:236:SER:HB2	1:A:239:GLU:CG	2.38	0.53
1:B:357:THR:HG22	1:B:359:ASP:H	1.73	0.53
1:A:150:LEU:HD22	1:A:151:ASN:N	2.20	0.53
1:B:45:ILE:HB	1:B:376:VAL:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:THR:HG23	1:A:408:PRO:HB3	1.89	0.53
1:B:48:LEU:CD1	1:B:379:MET:HB2	2.37	0.53
1:A:180:LEU:HD21	1:A:192:VAL:HG11	1.89	0.53
1:B:383:ILE:N	1:B:383:ILE:HD12	2.24	0.53
1:B:269:MET:HG2	1:B:274:MET:SD	2.49	0.52
1:A:333:GLY:C	3:A:683:HOH:O	2.52	0.52
1:A:23:GLU:O	1:A:27:LYS:HG2	2.10	0.52
1:A:362:PRO:HG2	1:A:401:GLU:OE1	2.10	0.52
1:A:142:ARG:HA	1:A:159:ASP:HB2	1.92	0.52
1:A:381:ARG:HB3	1:A:383:ILE:HG12	1.91	0.52
1:A:23:GLU:HG2	1:A:26:LYS:HZ1	1.75	0.51
1:A:201:ARG:HE	1:A:201:ARG:HA	1.74	0.51
1:A:106:LEU:HD21	1:A:177:TYR:CZ	2.45	0.51
1:A:167:ILE:HD13	1:A:209:ILE:HD12	1.93	0.51
1:B:105:LEU:O	1:B:109:LEU:HB2	2.11	0.51
1:A:373:GLU:CG	1:A:427:LEU:HD21	2.41	0.51
1:B:378:SER:HB3	1:B:405:LEU:HD23	1.93	0.51
1:B:77:PHE:HE1	1:B:95:PRO:HG3	1.76	0.51
1:A:121:MET:HG3	1:A:137:PHE:CZ	2.46	0.50
1:B:142:ARG:NH2	1:B:152:ILE:HD12	2.26	0.50
1:A:400:LEU:HD12	1:A:401:GLU:H	1.75	0.50
1:B:118:ALA:HB3	1:B:178:ILE:CD1	2.42	0.50
1:B:26:LYS:O	1:B:30:GLU:HG3	2.11	0.50
1:A:196:ASN:O	1:A:200:VAL:HG23	2.12	0.50
1:B:201:ARG:HE	1:B:201:ARG:CA	2.24	0.50
1:A:348:ASP:OD1	1:A:400:LEU:HD11	2.12	0.50
1:A:109:LEU:HD13	1:A:274:MET:HE3	1.93	0.50
1:B:317:HIS:HD2	3:B:461:HOH:O	1.95	0.50
1:B:159:ASP:OD2	1:B:162:LYS:HG3	2.12	0.50
1:A:59:LYS:HD3	3:A:574:HOH:O	2.12	0.49
1:B:283:VAL:HG22	1:B:289:PRO:HD3	1.94	0.49
1:B:25:LEU:HD12	1:B:25:LEU:O	2.11	0.49
1:B:120:ASN:HA	1:B:141:VAL:HB	1.95	0.49
1:A:240:ILE:O	1:A:244:MET:HG3	2.12	0.49
1:B:155:LYS:HB2	3:B:525:HOH:O	2.12	0.49
1:B:440:ILE:HG12	1:B:454:ASP:HB2	1.93	0.49
1:A:121:MET:SD	1:A:179:CYS:SG	3.10	0.49
1:A:316:GLU:OE2	1:A:320:LYS:NZ	2.46	0.48
1:B:302:MET:HG3	3:B:649:HOH:O	2.13	0.48
1:A:355:HIS:NE2	1:A:431:LYS:O	2.47	0.48
1:B:90:PHE:CE1	1:B:250:GLY:HA2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:ILE:O	1:B:429:GLN:HG3	2.11	0.48
1:A:121:MET:H	1:A:121:MET:HG2	1.26	0.48
1:A:294:LEU:HD21	1:A:302:MET:CE	2.43	0.48
1:B:175:ILE:HD13	3:B:657:HOH:O	2.13	0.48
1:A:10:ILE:HG12	1:B:10:ILE:HG12	1.95	0.48
1:B:91:LYS:HG3	1:B:270:ASN:OD1	2.13	0.48
1:A:91:LYS:HD3	1:A:270:ASN:O	2.13	0.48
1:A:179:CYS:HA	1:A:212:PHE:O	2.14	0.48
1:B:190:GLN:HA	1:B:190:GLN:OE1	2.14	0.48
1:A:201:ARG:HA	1:A:201:ARG:NE	2.29	0.48
1:B:178:ILE:HB	1:B:211:VAL:CG2	2.43	0.47
1:A:283:VAL:HG22	1:A:289:PRO:HD3	1.96	0.47
1:B:145:ALA:HA	1:B:155:LYS:HG2	1.96	0.47
1:A:104:ASN:O	1:A:108:GLN:HG3	2.15	0.47
1:B:236:SER:HB3	1:B:239:GLU:H	1.80	0.47
1:B:357:THR:O	1:B:358:GLN:C	2.57	0.47
1:A:109:LEU:HD11	1:A:278:ALA:CB	2.43	0.46
1:A:261:VAL:HG21	1:A:302:MET:HG3	1.97	0.46
1:A:169:GLU:HG3	1:A:170:LYS:HD2	1.97	0.46
1:B:109:LEU:HD21	1:B:278:ALA:HB2	1.97	0.46
1:B:213:TYR:O	1:B:251:CYS:HA	2.14	0.46
1:B:155:LYS:NZ	3:B:634:HOH:O	2.48	0.46
1:B:28:MET:HE3	1:B:28:MET:HA	1.97	0.46
1:B:28:MET:HE2	1:B:33:TYR:HA	1.98	0.46
1:B:363:ALA:HB1	1:B:380:GLU:HB2	1.98	0.46
1:B:138:VAL:HG11	1:B:166:LEU:HD13	1.98	0.46
1:A:117:VAL:CG2	1:A:176:ALA:HB3	2.45	0.46
1:A:119:GLY:HA3	1:A:179:CYS:O	2.15	0.46
1:B:198:ARG:HG3	1:B:247:TYR:CE1	2.51	0.46
1:A:121:MET:SD	1:A:179:CYS:HB3	2.55	0.45
1:A:78:TYR:O	1:A:82:ARG:HD2	2.16	0.45
1:A:177:TYR:HE1	1:A:179:CYS:HB2	1.81	0.45
1:A:185:ASN:OD1	1:A:343:HIS:NE2	2.48	0.45
1:A:111:ILE:HG21	1:A:135:ALA:HB2	1.98	0.45
1:B:85:GLN:NE2	1:B:91:LYS:O	2.46	0.45
1:A:328:LYS:HD3	1:A:421:ALA:CB	2.47	0.45
1:A:201:ARG:HE	1:A:201:ARG:CA	2.29	0.45
1:B:253:MET:HE2	1:B:259:CYS:SG	2.57	0.45
1:B:259:CYS:CB	3:B:649:HOH:O	2.45	0.45
1:B:211:VAL:O	1:B:249:ASP:HB2	2.17	0.45
1:B:364:GLN:CD	1:B:380:GLU:HG2	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:GLN:HB2	3:A:673:HOH:O	2.17	0.45
1:B:369:SER:O	1:B:373:GLU:HG2	2.17	0.45
1:A:20:PRO:HA	2:A:458:SO4:O3	2.17	0.44
1:A:415:ALA:HB1	1:B:5:ALA:HA	1.99	0.44
1:B:53:THR:HG23	1:B:408:PRO:HB3	1.99	0.44
1:A:281:LEU:O	1:A:285:TYR:HD1	2.00	0.44
1:B:79:HIS:HB3	3:B:516:HOH:O	2.18	0.44
1:B:352:PHE:O	1:B:431:LYS:HD2	2.17	0.44
1:A:154:PHE:CD2	1:A:191:PRO:HB2	2.53	0.44
1:A:381:ARG:HD2	1:A:381:ARG:HA	1.77	0.44
1:A:108:GLN:NE2	1:A:285:TYR:OH	2.51	0.44
1:B:116:TYR:CE1	1:B:170:LYS:HG2	2.51	0.44
1:B:3:TYR:OH	1:B:327:ASP:OD2	2.31	0.44
1:B:338:GLU:HA	1:B:339:PRO:C	2.43	0.44
1:A:160:LEU:HD21	1:A:199:ALA:HB1	1.99	0.43
1:B:97:HIS:NE2	1:B:98:GLN:NE2	2.57	0.43
1:A:324:TYR:CD1	1:A:324:TYR:C	2.96	0.43
1:B:188:GLY:CA	1:B:346:PHE:HE1	2.30	0.43
1:B:379:MET:HB3	3:B:523:HOH:O	2.17	0.43
1:A:26:LYS:O	1:A:30:GLU:HG3	2.18	0.43
1:B:194:MET:HE3	1:B:243:GLU:CD	2.44	0.43
1:B:252:THR:HG22	1:B:267:LEU:CD1	2.48	0.43
1:B:142:ARG:HA	1:B:159:ASP:HB2	1.99	0.43
1:B:191:PRO:HA	1:B:221:ASN:OD1	2.19	0.43
1:A:379:MET:HE2	1:A:404:ARG:NH2	2.34	0.43
1:B:182:VAL:HG23	1:B:182:VAL:O	2.18	0.43
1:B:407:ILE:HA	1:B:408:PRO:HD3	1.76	0.43
1:A:182:VAL:HG23	1:A:182:VAL:O	2.19	0.43
1:A:381:ARG:HB2	1:A:402:THR:OG1	2.19	0.43
1:A:440:ILE:O	1:A:440:ILE:HG13	2.18	0.43
1:A:283:VAL:O	1:A:287:GLY:N	2.52	0.42
1:B:167:ILE:HA	3:B:657:HOH:O	2.19	0.42
1:A:381:ARG:CG	1:A:383:ILE:HD11	2.46	0.42
1:A:314:TYR:OH	1:A:409:ARG:HD3	2.19	0.42
1:A:438:LYS:HB3	1:A:456:ILE:HG22	2.01	0.42
1:B:338:GLU:HB3	1:B:339:PRO:CA	2.48	0.42
1:A:269:MET:HE2	1:A:274:MET:CG	2.50	0.42
1:B:56:MET:HA	1:B:60:GLN:OE1	2.20	0.42
1:A:347:LEU:O	1:A:402:THR:HA	2.20	0.42
1:B:353:CYS:HA	1:B:355:HIS:HE1	1.85	0.42
1:A:19:ILE:HA	1:A:20:PRO:HD3	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:HIS:HB3	1:A:293:GLY:O	2.20	0.42
1:A:121:MET:HE2	1:A:137:PHE:CE1	2.55	0.41
1:A:236:SER:CB	1:A:239:GLU:H	2.32	0.41
1:A:269:MET:HE2	1:A:274:MET:HG2	2.02	0.41
1:A:3:TYR:HA	1:A:4:PRO:HD2	1.84	0.41
1:B:229:GLU:O	1:B:230:GLN:C	2.63	0.41
1:B:86:GLU:CD	1:B:307:ARG:HH22	2.28	0.41
1:B:110:ALA:O	1:B:176:ALA:HB1	2.21	0.41
1:A:294:LEU:HD21	1:A:302:MET:HE1	2.03	0.41
1:B:282:VAL:O	1:B:286:GLU:HB2	2.21	0.41
1:A:140:ILE:HG13	1:A:158:ILE:HG12	2.03	0.41
1:B:165:LYS:O	1:B:165:LYS:HG2	2.20	0.41
1:B:243:GLU:O	1:B:244:MET:C	2.63	0.41
1:A:25:LEU:HD13	1:A:372:VAL:HG11	2.03	0.41
1:A:282:VAL:HG12	1:A:289:PRO:HA	2.03	0.41
1:B:282:VAL:HG12	1:B:289:PRO:HA	2.02	0.41
1:A:430:HIS:O	1:A:431:LYS:C	2.64	0.41
1:B:113:PRO:HB3	1:B:134:GLY:N	2.36	0.41
1:B:180:LEU:HA	1:B:180:LEU:HD23	1.89	0.41
1:B:381:ARG:HD2	1:B:381:ARG:HA	1.88	0.41
1:A:259:CYS:SG	1:A:306:LEU:HD13	2.62	0.40
1:B:166:LEU:CG	1:B:175:ILE:HD11	2.50	0.40
1:B:9:ARG:HD2	3:B:652:HOH:O	2.22	0.40
1:B:77:PHE:CE1	1:B:95:PRO:HG3	2.56	0.40
1:B:92:HIS:HB3	1:B:275:PHE:CD1	2.56	0.40
1:B:422:ASP:O	1:B:426:LYS:HD2	2.20	0.40
1:B:350:ARG:NE	3:B:661:HOH:O	2.54	0.40
1:B:440:ILE:O	1:B:440:ILE:HD12	2.21	0.40

All (2) 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)
3:B:503:HOH:O	3:B:503:HOH:O[2_655]	0.62	1.58
3:B:471:HOH:O	3:B:471:HOH:O[2_655]	0.78	1.42

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	418/456 (92%)	396 (95%)	22 (5%)	0	100	100
1	B	418/456 (92%)	395 (94%)	23 (6%)	0	100	100
All	All	836/912 (92%)	791 (95%)	45 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	351/378 (93%)	322 (92%)	29 (8%)	10	14
1	B	351/378 (93%)	330 (94%)	21 (6%)	17	25
All	All	702/756 (93%)	652 (93%)	50 (7%)	13	19

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	ASN
1	A	75	GLU
1	A	106	LEU
1	A	107	SER
1	A	122	TYR
1	A	138	VAL
1	A	142	ARG

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Mol	Chain	Res	Type
1	A	144	GLU
1	A	147	ASP
1	A	152	ILE
1	A	158	ILE
1	A	160	LEU
1	A	180	LEU
1	A	203	LEU
1	A	235	LYS
1	A	263	ILE
1	A	274	MET
1	A	276	SER
1	A	328	LYS
1	A	338	GLU
1	A	357	THR
1	A	360	GLU
1	A	381	ARG
1	A	383	ILE
1	A	406	THR
1	A	407	ILE
1	A	439	PHE
1	A	440	ILE
1	B	1	MET
1	B	22	ASP
1	B	25	LEU
1	B	104	ASN
1	B	109	LEU
1	B	152	ILE
1	B	167	ILE
1	B	169	GLU
1	B	175	ILE
1	B	230	GLN
1	B	236	SER
1	B	269	MET
1	B	272	ASP
1	B	281	LEU
1	B	290	SER
1	B	330	LYS
1	B	383	ILE
1	B	406	THR
1	B	440	ILE
1	B	441	TYR
1	B	450	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	A	108	GLN
1	A	190	GLN
1	A	311	GLN
1	B	39	ASN
1	B	76	ASN
1	B	92	HIS
1	B	98	GLN
1	B	228	GLN
1	B	230	GLN
1	B	317	HIS
1	B	321	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	458	-	4,4,4	0.84	0	6,6,6	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	457	-	4,4,4	0.67	0	6,6,6	0.34	0
2	SO4	B	458	-	4,4,4	0.87	0	6,6,6	0.34	0
2	SO4	B	457	-	4,4,4	0.81	0	6,6,6	0.49	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	458	SO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.