



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:03 AM UTC

PDB ID : 1GGT / pdb_00001ggt
Title : THREE-DIMENSIONAL STRUCTURE OF A TRANSGLUTAMINASE:
HUMAN BLOOD COAGULATION FACTOR XIII
Authors : Yee, V.C.; Pedersen, L.C.; Trong, I.L.; Bishop, P.D.; Stenkamp, R.E.; Teller,
D.C.
Deposited on : 1994-01-25
Resolution : 2.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
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

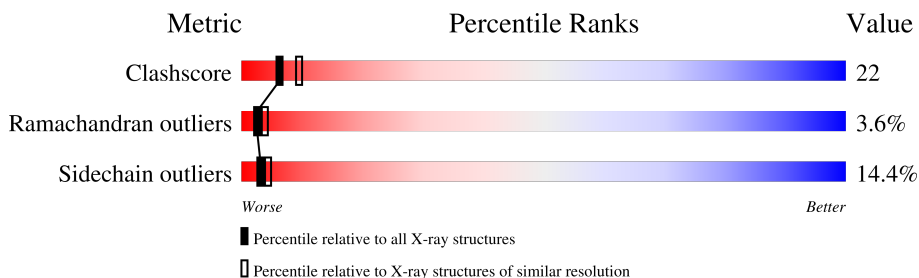
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

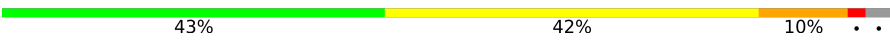
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)

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	731	
1	B	731	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11382 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 COAGULATION FACTOR XIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	710	Total	C	N	O	S	0	0	0
			5700	3614	983	1076	27			
1	B	708	Total	C	N	O	S	0	0	0
			5682	3603	978	1074	27			

There are 2 discrepancies between the modelled and reference sequences:

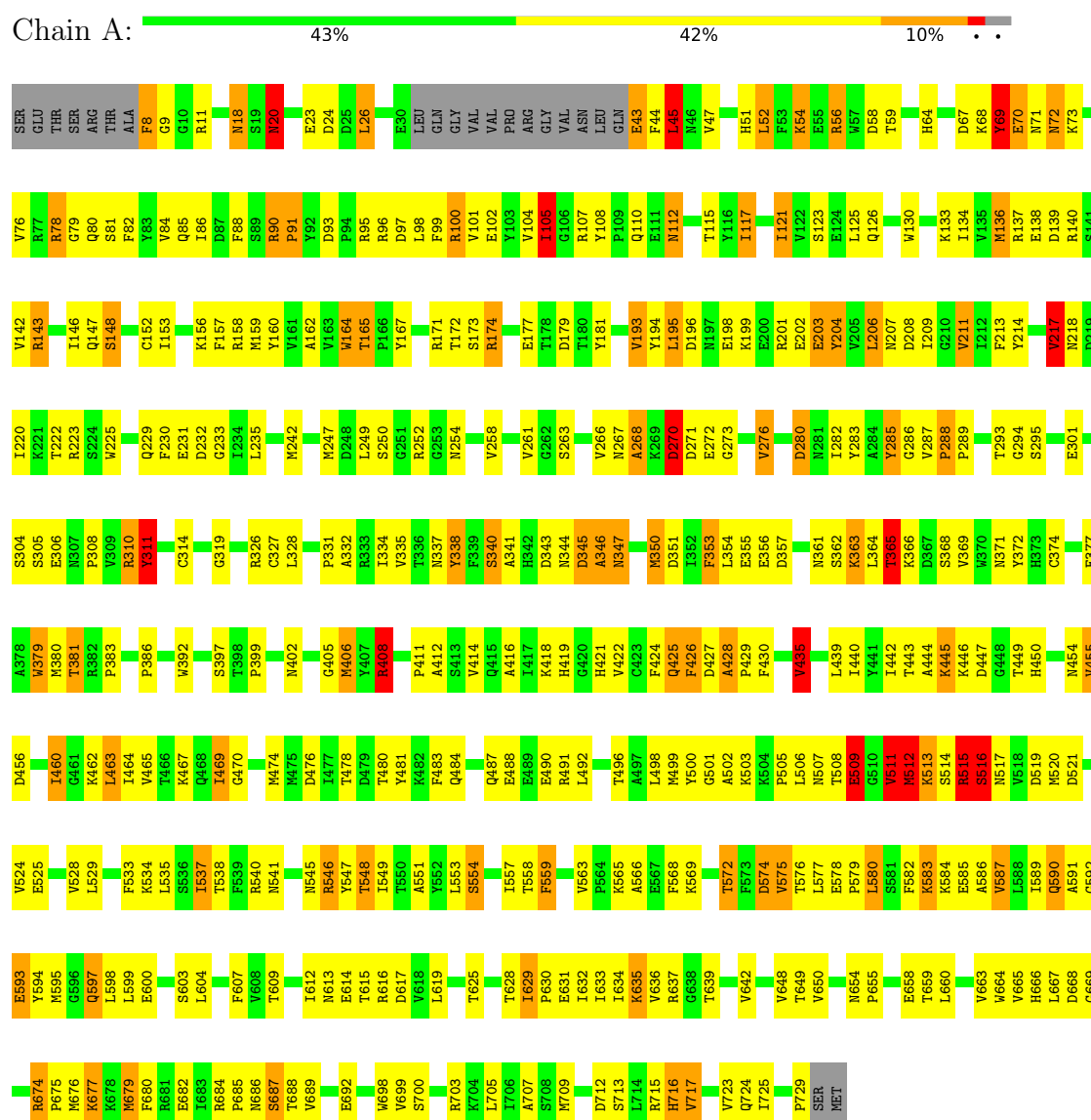
Chain	Residue	Modelled	Actual	Comment	Reference
A	651	GLU	GLN	conflict	UNP P00488
B	651	GLU	GLN	conflict	UNP P00488

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: COAGULATION FACTOR XIII



• Molecule 1: COAGULATION FACTOR XIII



Q724	T639	K570	K504	F424	N337	L235	L144	V76	SER
I725	Q640	E571	P505	Q425	Y338	D236	S145	R77	GLU
Q726	V641	T572	L506	F426	F339	T237	I146	R78	THR
	V642	F573	N507	D427	S340	C238	Q147	G79	SER
		D574	T508	A428	A341	L239	S148	Q80	ARG
	H646	V575	E509	P429	H342	Y240	S149	S81	THR
		T576	G510	F430	D343		P150	F82	ALA
	T649	L577	V511	V431	N344	M247			F8
	V650	E578	M512			D248	I153	Q85	G9
	E651	P579	K513	E434	N347	L249		I86	G10
		L580	S514	V435		S250	F157	D87	R11
	N654	S581	S515	E436	N350	G251	R158		N17
	P655	F582	S516	S437	D351	R252	A162	R90	N18
	L656	K583	N517	D438	F352	G253		P91	S19
	K657	A584	V518	L439	F353	N254	V163	Y92	N20
	T659	E585	D519	I440	L354	P255	W164	D93	
		A586	M520	Y441		I256	T165	P94	
		V587	D521	I442	N359	K257		R95	D24
	V663	L588	F522	T443	V360	V258	L170	R96	D25
		T589	E523	A444	N361		R171	D97	L26
	H666	Q590	V524	K445	S362	S263	T172	L98	P27
	L667	A591	E525	K446	K363		S173	F99	T28
	D668	G592	N526	D447	L364	A268	R174	R100	V29
	G669	E593	A527	G448	T365	K269		V101	E30
	P670	Y594	V528		K366	D270	F184	E102	LEU
		M595	L529	V451		D271	M185	Y103	GLN
	R674	G596	G530	V452	Y372	E272	P186	V104	GLY
	P675	Q597	K531	E453		G273	W187	I105	VAL
	H676	L598	D532	N454	W379	V274	C188	G106	VAL
		L599	F533	V455	K380	L275	E189	R107	PRO
	H679	E600	K534	D456	T381	V276		Y108	ARG
			L535		R382		V193	P109	GLY
	E682	L604	S536		P383	D280	Y194	Q110	VAL
	T683	H605	T537	I460	D384	N281	L195	E111	ASN
	R684	P606	T538	L463	L385	I282			LEU
	P685	F607	F539	I464	P386	Y283	R201	T115	GLN
	N686	V608	R540		V387	A284	E202	Y116	E43
			N541	K467		Y285	E203	I117	P44
		I612	N542		S397	G286	Y204	P118	L45
		N613	S543			V287	V205	V119	
	E614	T615	R546	D472	E401	P288	L206	P120	T48
	R616	Y547	M474	M474	S403	W292		I121	H51
	P617	T548	T480		D404		V211	V122	L52
	V618	L549		F483	G405	I298	F212	S123	F53
	L619			Q487	M406	E301	F213	K54	K54
	A620	L553		E488	R408	Y302	V217	E55	R56
	K621	S554		E489	G409	R303		W57	R57
		I557	T586		G410		I220	D58	
	S624	F599	P599	L494	P411	R310	K133	K133	
				E495	A412	Y311	I134	I134	K61
					S413	G312	V135	V135	
							M136	M136	
					I417	Q313	R137	R137	H64
					L498	G314	E138	E138	H65
					M499		D139	D139	T66
					Y500	T323	R140	R140	
					G501		S141	S141	N71
					A502		V142	V142	
					K503		R143	R143	I75

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	101.20 Å 182.70 Å 93.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.65	Depositor
% Data completeness (in resolution range)	97.6 (10.00-2.65)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.216 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11382	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.79	2/5835 (0.0%)	1.24	69/7917 (0.9%)
1	B	0.83	3/5816 (0.1%)	1.26	71/7891 (0.9%)
All	All	0.81	5/11651 (0.0%)	1.25	140/15808 (0.9%)

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	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	460	ILE	CA-CB	-6.75	1.45	1.54
1	A	266	VAL	CA-CB	-5.57	1.47	1.54
1	B	380	MET	SD-CE	-5.25	1.66	1.79
1	A	424	PHE	CA-C	-5.06	1.46	1.52
1	B	651	GLU	CD-OE2	5.04	1.34	1.25

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	THR	N-CA-C	-12.51	84.15	110.80
1	B	460	ILE	N-CA-C	11.44	133.12	109.34
1	B	363	LYS	N-CA-C	-10.45	99.43	111.03
1	A	310	ARG	N-CA-C	9.98	124.59	108.63
1	B	44	PHE	N-CA-C	9.31	123.66	109.23
1	B	365	THR	N-CA-C	-9.26	91.07	110.80
1	A	559	PHE	N-CA-C	-9.08	95.89	110.32
1	B	274	VAL	N-CA-C	8.99	118.98	110.53
1	B	425	GLN	N-CA-C	8.99	129.94	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	674	ARG	N-CA-C	-8.64	97.62	110.24
1	B	674	ARG	N-CA-C	-8.62	99.24	109.93
1	A	285	TYR	N-CA-C	8.62	121.51	110.65
1	B	574	ASP	N-CA-C	-8.29	95.72	109.07
1	A	631	GLU	N-CA-C	8.19	121.34	110.53
1	B	134	ILE	N-CA-C	-7.97	95.95	107.98
1	A	280	ASP	N-CA-C	7.79	122.63	113.20
1	A	363	LYS	N-CA-C	-7.79	102.74	111.07
1	B	632	ILE	N-CA-C	-7.72	97.00	108.97
1	B	417	ILE	N-CA-C	-7.66	103.06	110.42
1	B	298	ILE	N-CA-C	7.66	117.73	110.53
1	B	314	CYS	N-CA-C	7.65	120.35	111.02
1	A	117	ILE	N-CA-C	7.58	115.65	108.15
1	B	559	PHE	N-CA-C	-7.58	100.32	110.55
1	A	314	CYS	N-CA-C	7.52	120.19	111.02
1	B	52	LEU	N-CA-C	-7.46	97.43	109.96
1	A	18	ASN	N-CA-C	7.35	123.30	112.94
1	B	239	LEU	N-CA-C	-7.30	103.41	111.36
1	B	705	LEU	N-CA-C	-7.28	98.45	110.17
1	B	141	SER	N-CA-C	7.26	120.75	109.07
1	A	425	GLN	N-CA-C	7.23	126.21	110.80
1	B	194	TYR	N-CA-C	7.13	120.17	109.25
1	B	501	GLY	N-CA-C	7.12	123.17	114.69
1	A	20	ASN	N-CA-C	-7.10	104.09	112.89
1	A	345	ASP	N-CA-C	-7.09	101.94	110.44
1	A	512	MET	N-CA-C	-7.08	95.72	110.80
1	B	344	ASN	N-CA-C	7.05	121.63	112.89
1	A	355	GLU	N-CA-C	-7.04	99.81	109.95
1	A	340	SER	N-CA-C	6.84	119.88	108.73
1	A	480	THR	N-CA-C	-6.82	105.11	113.50
1	A	24	ASP	N-CA-C	-6.70	100.55	110.46
1	B	532	ASP	N-CA-C	-6.68	100.90	110.59
1	B	284	ALA	N-CA-C	6.68	119.41	111.33
1	A	338	TYR	CA-C-N	-6.64	112.65	122.41
1	A	338	TYR	C-N-CA	-6.64	112.65	122.41
1	A	500	TYR	N-CA-C	6.58	120.71	111.30
1	A	435	VAL	N-CA-CB	-6.58	103.77	112.26
1	B	268	ALA	N-CA-C	6.56	119.23	109.59
1	A	446	LYS	N-CA-C	6.51	120.68	112.87
1	B	206	LEU	N-CA-C	6.47	120.43	112.54
1	A	351	ASP	N-CA-C	6.46	119.14	109.25
1	A	597	GLN	N-CA-C	6.45	118.68	110.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	310	ARG	N-CA-C	6.41	119.05	109.25
1	B	516	SER	N-CA-C	-6.40	102.83	111.54
1	A	344	ASN	N-CA-C	-6.38	101.54	110.35
1	A	288	PRO	CA-C-N	6.36	127.78	119.84
1	A	288	PRO	C-N-CA	6.36	127.78	119.84
1	A	408	ARG	N-CA-C	-6.19	102.36	110.53
1	A	428	ALA	N-CA-C	6.18	121.16	112.75
1	B	75	ILE	N-CA-C	-6.14	99.64	108.48
1	B	503	LYS	N-CA-C	6.11	119.44	109.24
1	A	24	ASP	CA-C-N	-6.09	114.59	123.00
1	A	24	ASP	C-N-CA	-6.09	114.59	123.00
1	B	24	ASP	N-CA-C	-6.05	101.04	110.42
1	A	311	TYR	N-CA-C	5.96	123.49	110.80
1	B	287	VAL	CA-C-N	-5.91	114.29	120.38
1	B	287	VAL	C-N-CA	-5.91	114.29	120.38
1	A	483	PHE	N-CA-C	-5.89	102.93	110.53
1	A	217	VAL	N-CA-C	5.88	121.58	109.34
1	A	90	ARG	CA-C-N	5.85	127.15	119.84
1	A	90	ARG	C-N-CA	5.85	127.15	119.84
1	A	73	LYS	N-CA-C	5.85	117.87	110.33
1	A	287	VAL	CA-C-N	-5.80	114.40	120.38
1	A	287	VAL	C-N-CA	-5.80	114.40	120.38
1	B	26	LEU	CA-C-N	5.80	126.00	119.90
1	B	26	LEU	C-N-CA	5.80	126.00	119.90
1	B	568	PHE	N-CA-C	5.79	120.62	113.50
1	B	323	THR	N-CA-C	-5.78	104.89	111.14
1	A	26	LEU	CA-C-N	5.77	126.06	119.83
1	A	26	LEU	C-N-CA	5.77	126.06	119.83
1	A	69	TYR	N-CA-C	-5.76	98.53	110.80
1	A	233	GLY	N-CA-C	5.71	122.64	115.21
1	B	538	THR	N-CA-C	5.68	117.66	108.34
1	A	503	LYS	N-CA-C	5.67	118.46	109.50
1	A	196	ASP	N-CA-C	5.65	119.87	113.15
1	A	45	LEU	N-CA-C	-5.64	105.61	112.88
1	A	717	VAL	N-CA-C	-5.63	100.36	108.53
1	A	427	ASP	N-CA-C	5.61	119.17	111.54
1	B	285	TYR	N-CA-C	5.60	120.11	112.88
1	A	558	THR	N-CA-C	5.59	118.69	109.85
1	A	511	VAL	N-CA-C	5.55	117.91	108.86
1	B	185	ASN	CA-C-N	5.53	125.20	119.56
1	B	185	ASN	C-N-CA	5.53	125.20	119.56
1	B	57	TRP	N-CA-C	-5.53	106.53	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	GLN	CA-C-N	5.49	132.03	121.54
1	A	425	GLN	C-N-CA	5.49	132.03	121.54
1	B	472	ASP	N-CA-C	5.46	119.57	113.02
1	A	9	GLY	N-CA-C	-5.45	100.27	113.18
1	B	583	LYS	N-CA-C	5.44	117.39	108.52
1	A	52	LEU	N-CA-C	-5.43	100.33	109.07
1	B	93	ASP	CA-C-N	5.41	126.61	119.84
1	B	93	ASP	C-N-CA	5.41	126.61	119.84
1	B	165	THR	CA-C-N	5.40	126.59	119.84
1	B	165	THR	C-N-CA	5.40	126.59	119.84
1	B	634	ILE	CB-CA-C	-5.40	102.64	110.63
1	B	227	TYR	N-CA-C	-5.38	105.50	111.36
1	A	554	SER	N-CA-C	-5.34	100.47	109.07
1	B	273	GLY	CA-C-N	5.34	127.39	120.56
1	B	273	GLY	C-N-CA	5.34	127.39	120.56
1	A	460	ILE	N-CA-C	5.30	115.93	109.30
1	B	274	VAL	CB-CA-C	-5.29	105.09	112.02
1	A	574	ASP	N-CA-C	-5.28	99.67	108.34
1	A	295	SER	N-CA-C	5.27	118.87	112.23
1	A	204	TYR	N-CA-C	5.27	119.33	113.01
1	B	18	ASN	N-CA-C	5.26	120.35	112.94
1	B	557	ILE	N-CA-C	-5.25	100.20	108.23
1	A	546	ARG	N-CA-C	-5.25	101.91	110.20
1	A	614	GLU	N-CA-C	5.24	116.80	111.14
1	B	412	ALA	N-CA-C	-5.23	100.37	108.90
1	B	288	PRO	CA-C-N	5.21	126.36	119.84
1	B	288	PRO	C-N-CA	5.21	126.36	119.84
1	B	650	VAL	N-CA-C	-5.20	100.90	108.17
1	A	416	ALA	N-CA-C	-5.17	105.53	111.07
1	A	353	PHE	N-CA-C	5.17	117.05	108.20
1	B	110	GLN	N-CA-C	-5.17	98.49	107.49
1	B	508	THR	N-CA-C	-5.16	104.38	111.81
1	B	366	LYS	N-CA-C	-5.16	107.12	113.41
1	B	124	GLU	N-CA-C	5.15	116.79	108.34
1	B	600	GLU	N-CA-C	5.14	119.86	111.37
1	B	351	ASP	N-CA-C	5.12	118.15	109.76
1	A	501	GLY	N-CA-C	5.10	120.80	114.37
1	B	204	TYR	N-CA-C	5.09	119.12	113.01
1	B	596	GLY	N-CA-C	5.09	119.29	112.77
1	B	312	GLY	N-CA-C	-5.09	103.67	111.10
1	A	346	ALA	N-CA-C	-5.08	106.49	113.56
1	B	425	GLN	CA-C-N	5.08	131.25	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	425	GLN	C-N-CA	5.08	131.25	121.54
1	B	117	ILE	CB-CA-C	-5.08	102.11	111.36
1	B	408	ARG	N-CA-C	-5.07	103.79	110.43
1	A	105	ILE	CB-CA-C	-5.06	102.28	110.28
1	A	54	LYS	N-CA-C	5.05	119.59	111.81

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	214	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5700	0	5557	263	0
1	B	5682	0	5537	237	0
All	All	11382	0	11094	499	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 22.

All (499) 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:659:THR:HG22	1:B:685:PRO:HD3	1.43	0.98
1:A:538:THR:HG22	1:A:584:LYS:HG2	1.50	0.92
1:A:100:ARG:HD2	1:A:164:TRP:HZ3	1.34	0.91
1:A:381:THR:HG23	1:A:383:PRO:HD3	1.51	0.91
1:B:527:ALA:HB2	1:B:533:PHE:HB3	1.55	0.88
1:A:231:GLU:HB3	1:A:674:ARG:HH22	1.39	0.87
1:A:363:LYS:HG3	1:A:364:LEU:N	1.87	0.87
1:A:363:LYS:HG3	1:A:364:LEU:H	1.40	0.85
1:A:356:GLU:HG2	1:A:445:LYS:NZ	1.92	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ARG:HD2	1:A:67:ASP:O	1.80	0.81
1:B:247:MET:HE3	1:B:257:LYS:HG2	1.63	0.81
1:B:43:GLU:HB2	1:B:165:THR:HG21	1.60	0.81
1:B:521:ASP:O	1:B:522:PHE:HB3	1.81	0.80
1:B:111:GLU:HB3	1:B:116:TYR:HD2	1.46	0.80
1:B:541:ASN:HB2	1:B:577:LEU:HD23	1.65	0.79
1:B:220:ILE:HD13	1:B:474:MET:HE1	1.65	0.79
1:B:411:PRO:O	1:B:426:PHE:HB2	1.83	0.77
1:A:110:GLN:H	1:A:115:THR:HG23	1.49	0.76
1:A:578:GLU:CD	1:A:578:GLU:H	1.93	0.76
1:A:211:VAL:HG13	1:A:467:LYS:HD2	1.66	0.75
1:A:516:SER:HB3	1:A:615:THR:HG21	1.67	0.75
1:A:217:VAL:HG22	1:A:338:TYR:HB3	1.69	0.75
1:B:331:PRO:HB2	1:B:379:TRP:HB3	1.69	0.74
1:A:356:GLU:HG2	1:A:445:LYS:HZ3	1.49	0.74
1:B:233:GLY:O	1:B:237:THR:HG23	1.86	0.74
1:A:439:LEU:HB2	1:A:456:ASP:HB3	1.70	0.74
1:A:520:MET:HE2	1:A:619:LEU:HB3	1.70	0.74
1:B:43:GLU:HA	1:B:165:THR:HB	1.67	0.74
1:A:559:PHE:HD1	1:A:563:VAL:O	1.71	0.74
1:B:520:MET:HA	1:B:538:THR:O	1.87	0.73
1:A:549:ILE:HB	1:A:575:VAL:HG23	1.72	0.72
1:A:492:LEU:O	1:A:496:THR:HG23	1.91	0.71
1:A:537:ILE:H	1:A:537:ILE:HD12	1.55	0.71
1:B:514:SER:O	1:B:515:ARG:HG2	1.90	0.71
1:A:285:TYR:O	1:A:310:ARG:HD3	1.91	0.71
1:A:698:TRP:CD1	1:A:699:VAL:HG23	2.25	0.71
1:B:51:HIS:HB2	1:B:85:GLN:HB3	1.71	0.71
1:B:385:LEU:HD22	1:B:424:PHE:HB3	1.74	0.70
1:B:520:MET:HE1	1:B:608:VAL:HG12	1.73	0.70
1:B:136:MET:HE3	1:B:138:GLU:HG2	1.75	0.69
1:B:211:VAL:HG22	1:B:467:LYS:HB2	1.75	0.69
1:A:650:VAL:HG11	1:A:665:VAL:HG11	1.73	0.68
1:A:529:LEU:HD12	1:A:595:MET:HE1	1.75	0.68
1:A:110:GLN:N	1:A:115:THR:HG23	2.09	0.68
1:A:347:ASN:HD21	1:A:505:PRO:HG2	1.57	0.68
1:A:242:MET:HB3	1:A:247:MET:HE3	1.74	0.68
1:A:636:VAL:HG11	1:A:723:VAL:HG11	1.74	0.68
1:A:668:ASP:OD2	1:A:675:PRO:HB3	1.94	0.68
1:B:632:ILE:HG13	1:B:717:VAL:HG12	1.76	0.68
1:A:136:MET:HG3	1:A:143:ARG:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:LEU:O	1:A:682:GLU:HA	1.95	0.67
1:B:363:LYS:HG2	1:B:364:LEU:N	2.08	0.67
1:A:529:LEU:HD22	1:A:529:LEU:H	1.59	0.66
1:A:440:ILE:HD13	1:A:455:VAL:HB	1.77	0.66
1:B:29:VAL:HG23	1:B:170:LEU:HD22	1.77	0.66
1:B:353:PHE:HB2	1:B:364:LEU:O	1.96	0.65
1:B:254:ASN:O	1:B:258:VAL:HG23	1.97	0.64
1:A:454:ASN:OD1	1:A:512:MET:SD	2.56	0.64
1:A:254:ASN:O	1:A:258:VAL:HG23	1.96	0.64
1:B:439:LEU:HB2	1:B:456:ASP:HB3	1.79	0.63
1:A:276:VAL:O	1:A:311:TYR:HA	1.98	0.63
1:A:648:VAL:O	1:A:692:GLU:HA	1.97	0.63
1:A:91:PRO:HD3	1:A:140:ARG:HG2	1.79	0.63
1:B:539:PHE:HB3	1:B:577:LEU:HD21	1.80	0.63
1:A:397:SER:HA	1:A:408:ARG:HB2	1.80	0.62
1:A:666:HIS:O	1:A:707:ALA:HA	1.98	0.62
1:B:90:ARG:HG3	1:B:90:ARG:HH11	1.64	0.62
1:A:709:MET:HB3	1:A:717:VAL:CG2	2.30	0.62
1:B:670:PRO:O	1:B:703:ARG:NH1	2.32	0.62
1:A:535:LEU:HB2	1:A:587:VAL:HG13	1.80	0.62
1:B:43:GLU:HG3	1:B:170:LEU:HD11	1.81	0.62
1:B:303:ARG:HG2	1:B:303:ARG:HH11	1.64	0.61
1:B:582:PHE:N	1:B:582:PHE:HD1	1.99	0.61
1:A:411:PRO:O	1:A:426:PHE:HB2	2.00	0.61
1:B:594:TYR:CD1	1:B:595:MET:N	2.69	0.61
1:A:100:ARG:HD2	1:A:164:TRP:CZ3	2.26	0.61
1:A:100:ARG:HB3	1:A:100:ARG:HH11	1.65	0.61
1:A:193:VAL:HG13	1:A:331:PRO:HD3	1.81	0.61
1:A:419:HIS:O	1:B:387:VAL:HG11	2.00	0.60
1:B:66:THR:HG21	1:B:75:ILE:HG22	1.83	0.60
1:B:445:LYS:NZ	1:B:445:LYS:HB3	2.16	0.60
1:B:437:SER:HB2	1:B:460:ILE:HG12	1.83	0.60
1:B:636:VAL:HG11	1:B:646:MET:HE3	1.84	0.60
1:A:435:VAL:CG2	1:A:464:ILE:HD11	2.32	0.60
1:A:379:TRP:HD1	1:A:392:TRP:CE2	2.20	0.60
1:A:443:THR:O	1:A:450:HIS:HA	2.02	0.60
1:A:529:LEU:HD21	1:A:629:ILE:HG23	1.83	0.60
1:A:213:PHE:CD2	1:A:222:THR:HG22	2.37	0.60
1:A:361:ASN:ND2	1:A:363:LYS:HG2	2.17	0.60
1:B:109:PRO:HB3	1:B:116:TYR:HB2	1.84	0.60
1:B:185:ASN:OD1	1:B:187:TRP:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:GLY:O	1:B:406:MET:HB3	2.02	0.60
1:B:634:ILE:HA	1:B:649:THR:O	2.02	0.60
1:A:463:LEU:HD21	1:A:476:ASP:OD2	2.02	0.59
1:A:207:ASN:HD22	1:A:208:ASP:N	2.01	0.59
1:A:528:VAL:HG13	1:A:628:THR:O	2.02	0.59
1:B:105:ILE:HG23	1:B:157:PHE:CD2	2.37	0.59
1:B:512:MET:SD	1:B:512:MET:N	2.75	0.59
1:A:51:HIS:HB2	1:A:85:GLN:HB3	1.84	0.59
1:B:698:TRP:CD1	1:B:699:VAL:HG23	2.37	0.59
1:A:488:GLU:CD	1:A:491:ARG:HH12	2.10	0.59
1:B:217:VAL:HG22	1:B:338:TYR:HB3	1.85	0.59
1:B:657:LYS:C	1:B:685:PRO:HB3	2.28	0.59
1:A:595:MET:HE3	1:A:598:LEU:HD12	1.83	0.59
1:A:549:ILE:HB	1:A:575:VAL:CG2	2.32	0.58
1:A:679:MET:HG3	1:A:680:PHE:N	2.17	0.58
1:B:657:LYS:O	1:B:685:PRO:HB3	2.03	0.58
1:B:582:PHE:N	1:B:582:PHE:CD1	2.70	0.58
1:B:642:VAL:HG13	1:B:698:TRP:HA	1.85	0.58
1:B:518:VAL:HG21	1:B:612:ILE:HD12	1.85	0.58
1:B:435:VAL:HG21	1:B:464:ILE:HD11	1.86	0.58
1:A:247:MET:HE2	1:A:261:VAL:HG11	1.86	0.57
1:B:64:HIS:CE1	1:B:76:VAL:HG22	2.40	0.57
1:B:122:VAL:HG12	1:B:123:SER:N	2.19	0.57
1:A:353:PHE:CD2	1:A:364:LEU:O	2.57	0.57
1:A:554:SER:HB3	1:A:607:PHE:HB2	1.87	0.57
1:A:231:GLU:HB3	1:A:674:ARG:NH2	2.16	0.57
1:A:654:ASN:ND2	1:A:660:LEU:HG	2.19	0.56
1:B:615:THR:O	1:B:616:ARG:HG2	2.04	0.56
1:B:43:GLU:O	1:B:44:PHE:HD1	1.87	0.56
1:A:100:ARG:CD	1:A:164:TRP:HZ3	2.13	0.56
1:A:537:ILE:O	1:A:584:LYS:HA	2.05	0.56
1:B:211:VAL:HG22	1:B:467:LYS:HD2	1.87	0.56
1:A:379:TRP:HD1	1:A:392:TRP:CD2	2.23	0.56
1:B:220:ILE:HG21	1:B:474:MET:HE1	1.88	0.56
1:A:529:LEU:HD22	1:A:529:LEU:N	2.20	0.56
1:A:541:ASN:HB2	1:A:577:LEU:HD23	1.87	0.56
1:B:573:PHE:CD1	1:B:573:PHE:N	2.72	0.56
1:A:174:ARG:NH2	1:A:179:ASP:OD1	2.39	0.56
1:A:220:ILE:HD12	1:A:220:ILE:H	1.70	0.56
1:A:565:LYS:HD3	1:A:599:LEU:HD21	1.88	0.55
1:A:577:LEU:HA	1:A:583:LYS:HE3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:SER:HB2	1:A:408:ARG:HG3	1.89	0.55
1:B:410:GLY:C	1:B:426:PHE:HB3	2.32	0.55
1:B:516:SER:HB2	1:B:547:TYR:CZ	2.41	0.55
1:A:363:LYS:CG	1:A:364:LEU:N	2.66	0.55
1:A:364:LEU:HA	1:A:366:LYS:HG2	1.88	0.55
1:B:382:ARG:NH1	1:B:384:ASP:OD2	2.39	0.55
1:A:78:ARG:HG2	1:A:152:CYS:HB3	1.88	0.55
1:B:598:LEU:HD11	1:B:627:LEU:HD12	1.89	0.55
1:A:207:ASN:ND2	1:A:209:ILE:H	2.05	0.55
1:A:356:GLU:HG2	1:A:445:LYS:HZ2	1.70	0.55
1:A:551:ALA:O	1:A:572:THR:HA	2.06	0.55
1:B:363:LYS:CG	1:B:364:LEU:N	2.70	0.54
1:A:156:LYS:HE2	1:A:181:TYR:CZ	2.41	0.54
1:B:303:ARG:HG2	1:B:303:ARG:NH1	2.21	0.54
1:B:541:ASN:HB2	1:B:577:LEU:HB3	1.89	0.54
1:B:554:SER:HB3	1:B:567:GLU:OE2	2.07	0.54
1:B:659:THR:HG22	1:B:685:PRO:CD	2.29	0.54
1:A:642:VAL:CG2	1:A:700:SER:HB3	2.38	0.54
1:A:107:ARG:HG2	1:A:108:TYR:CE2	2.43	0.54
1:B:43:GLU:O	1:B:43:GLU:HG2	2.06	0.54
1:A:663:VAL:O	1:A:679:MET:HA	2.08	0.53
1:B:516:SER:OG	1:B:612:ILE:HG21	2.07	0.53
1:A:123:SER:O	1:A:133:LYS:NZ	2.42	0.53
1:B:109:PRO:CB	1:B:116:TYR:HB2	2.39	0.53
1:B:153:ILE:HD11	1:B:250:SER:HA	1.90	0.53
1:A:591:ALA:O	1:A:595:MET:HB2	2.08	0.53
1:A:591:ALA:HA	1:A:594:TYR:CE2	2.44	0.53
1:B:51:HIS:CD2	1:B:85:GLN:HE21	2.27	0.53
1:A:363:LYS:CG	1:A:364:LEU:H	2.19	0.53
1:B:263:SER:OG	1:B:408:ARG:HD3	2.08	0.53
1:B:530:GLY:HA2	1:B:595:MET:SD	2.49	0.53
1:A:52:LEU:HD23	1:A:84:VAL:HG22	1.90	0.53
1:A:435:VAL:HG21	1:A:464:ILE:HD11	1.91	0.53
1:A:629:ILE:HD12	1:A:629:ILE:H	1.74	0.53
1:A:454:ASN:HA	1:A:512:MET:SD	2.49	0.52
1:A:455:VAL:HG13	1:A:512:MET:HG2	1.91	0.52
1:B:100:ARG:HB2	1:B:119:VAL:O	2.09	0.52
1:A:455:VAL:HG11	1:A:508:THR:HG21	1.91	0.52
1:B:524:VAL:HG22	1:B:535:LEU:HG	1.92	0.52
1:A:229:GLN:HB2	1:A:327:CYS:HB2	1.90	0.52
1:A:578:GLU:CD	1:A:578:GLU:N	2.64	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:GLU:HG3	1:A:469:ILE:HA	1.91	0.52
1:A:529:LEU:H	1:A:529:LEU:CD2	2.23	0.52
1:B:90:ARG:HG3	1:B:90:ARG:NH1	2.25	0.52
1:B:443:THR:HG22	1:B:445:LYS:HG3	1.92	0.52
1:A:484:GLN:O	1:A:487:GLN:HG2	2.09	0.52
1:A:524:VAL:HG12	1:A:525:GLU:O	2.10	0.52
1:A:345:ASP:O	1:A:346:ALA:HB3	2.10	0.52
1:B:573:PHE:N	1:B:573:PHE:HD1	2.08	0.51
1:B:632:ILE:HD11	1:B:709:MET:HB2	1.91	0.51
1:A:674:ARG:HE	1:A:674:ARG:HA	1.75	0.51
1:A:207:ASN:HD22	1:A:207:ASN:C	2.19	0.51
1:B:105:ILE:CD1	1:B:115:THR:HG22	2.41	0.51
1:B:515:ARG:HG3	1:B:518:VAL:O	2.11	0.51
1:A:353:PHE:HB2	1:A:365:THR:HG1	1.75	0.51
1:B:77:ARG:HB3	1:B:185:ASN:HB2	1.92	0.51
1:B:213:PHE:CD2	1:B:222:THR:HG22	2.45	0.51
1:A:43:GLU:N	1:A:165:THR:HG1	2.08	0.51
1:A:213:PHE:CE2	1:A:474:MET:HB2	2.46	0.51
1:A:418:LYS:HA	1:A:481:TYR:O	2.11	0.51
1:A:455:VAL:HG13	1:A:512:MET:CG	2.41	0.51
1:B:247:MET:CE	1:B:257:LYS:HG2	2.37	0.51
1:A:45:LEU:HD22	1:A:45:LEU:O	2.11	0.50
1:A:270:ASP:O	1:A:271:ASP:HB2	2.10	0.50
1:A:513:LYS:O	1:A:515:ARG:HD2	2.11	0.50
1:B:418:LYS:HD2	1:B:480:THR:O	2.11	0.50
1:B:428:ALA:N	1:B:429:PRO:HD2	2.26	0.50
1:A:509:GLU:OE1	1:A:511:VAL:HG12	2.11	0.50
1:A:537:ILE:HD12	1:A:537:ILE:N	2.23	0.50
1:A:338:TYR:O	1:A:371:ASN:O	2.29	0.50
1:B:337:ASN:O	1:B:372:TYR:HA	2.12	0.50
1:B:520:MET:O	1:B:520:MET:HG3	2.11	0.50
1:B:568:PHE:HD2	1:B:593:GLU:HG2	1.75	0.50
1:A:81:SER:HA	1:A:146:ILE:O	2.12	0.50
1:A:341:ALA:HB2	1:A:460:ILE:HD13	1.93	0.50
1:A:64:HIS:CE1	1:A:76:VAL:HG22	2.47	0.50
1:A:525:GLU:HG3	1:A:533:PHE:HB2	1.94	0.50
1:A:548:THR:HB	1:A:613:ASN:HD22	1.76	0.50
1:A:633:ILE:HG22	1:A:635:LYS:HD3	1.94	0.50
1:A:557:ILE:CD1	1:A:597:GLN:HG3	2.42	0.50
1:B:256:ILE:HD12	1:B:256:ILE:N	2.27	0.50
1:B:363:LYS:HE3	1:B:364:LEU:CB	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:MET:HG3	1:A:143:ARG:CB	2.42	0.50
1:B:283:TYR:HE2	1:B:600:GLU:OE1	1.94	0.50
1:B:578:GLU:O	1:B:579:PRO:C	2.53	0.50
1:A:659:THR:HG22	1:A:682:GLU:HB2	1.93	0.50
1:B:54:LYS:O	1:B:55:GLU:O	2.30	0.50
1:B:559:PHE:HD1	1:B:563:VAL:O	1.95	0.50
1:B:714:LEU:HG	1:B:715:ARG:N	2.27	0.50
1:A:634:ILE:HA	1:A:649:THR:O	2.12	0.49
1:B:24:ASP:O	1:B:158:ARG:NH2	2.45	0.49
1:B:119:VAL:HG11	1:B:146:ILE:HG23	1.94	0.49
1:A:521:ASP:HB2	1:A:540:ARG:HH22	1.78	0.49
1:B:445:LYS:HB3	1:B:445:LYS:HZ3	1.77	0.49
1:B:516:SER:HB2	1:B:547:TYR:CE2	2.47	0.49
1:A:445:LYS:HB3	1:A:447:ASP:OD1	2.12	0.49
1:A:93:ASP:O	1:A:97:ASP:HB2	2.12	0.49
1:A:220:ILE:HD12	1:A:220:ILE:N	2.26	0.49
1:B:513:LYS:HE3	1:B:618:VAL:H	1.77	0.49
1:B:529:LEU:HD13	1:B:656:LEU:HD21	1.93	0.49
1:B:541:ASN:HB2	1:B:577:LEU:CD2	2.40	0.49
1:A:595:MET:CE	1:A:598:LEU:HD12	2.43	0.49
1:B:440:ILE:HG22	1:B:442:ILE:HG13	1.95	0.49
1:B:446:LYS:C	1:B:448:GLY:H	2.20	0.49
1:A:211:VAL:HG22	1:A:467:LYS:HB2	1.93	0.49
1:A:402:ASN:HA	1:A:430:PHE:CZ	2.47	0.49
1:A:594:TYR:CD1	1:A:595:MET:N	2.81	0.49
1:B:594:TYR:O	1:B:596:GLY:N	2.46	0.49
1:A:381:THR:CG2	1:A:383:PRO:HD3	2.34	0.49
1:B:515:ARG:HH12	1:B:519:ASP:CG	2.21	0.49
1:A:283:TYR:HE2	1:A:600:GLU:OE1	1.96	0.48
1:A:498:LEU:HD23	1:A:502:ALA:O	2.12	0.48
1:B:93:ASP:O	1:B:97:ASP:HB2	2.13	0.48
1:B:237:THR:HA	1:B:240:TYR:HB3	1.95	0.48
1:B:270:ASP:O	1:B:271:ASP:HB2	2.13	0.48
1:B:521:ASP:HB2	1:B:540:ARG:HH21	1.77	0.48
1:A:469:ILE:CG2	1:A:470:GLY:N	2.75	0.48
1:B:419:HIS:HD2	1:B:483:PHE:HZ	1.60	0.48
1:B:587:VAL:HG12	1:B:588:LEU:H	1.78	0.48
1:A:64:HIS:CE1	1:A:80:GLN:HB3	2.48	0.48
1:B:522:PHE:CD1	1:B:535:LEU:HD21	2.48	0.48
1:A:198:GLU:OE1	1:A:201:ARG:NH1	2.46	0.48
1:B:220:ILE:HG21	1:B:474:MET:CE	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:LYS:HB2	1:B:480:THR:O	2.13	0.48
1:A:442:ILE:CG2	1:A:450:HIS:HB3	2.44	0.48
1:A:165:THR:HG22	1:A:167:TYR:H	1.79	0.48
1:A:247:MET:HE2	1:A:261:VAL:CG1	2.43	0.48
1:A:541:ASN:HB2	1:A:577:LEU:HB3	1.96	0.48
1:B:133:LYS:O	1:B:144:LEU:HA	2.13	0.48
1:A:568:PHE:O	1:A:593:GLU:HG3	2.14	0.48
1:B:61:LYS:NZ	1:B:71:ASN:O	2.47	0.48
1:B:455:VAL:CG2	1:B:512:MET:HE2	2.44	0.48
1:B:455:VAL:HG22	1:B:512:MET:HE2	1.95	0.48
1:A:204:TYR:O	1:A:326:ARG:HG2	2.14	0.47
1:A:405:GLY:O	1:A:406:MET:HB3	2.14	0.47
1:A:20:ASN:C	1:A:20:ASN:HD22	2.22	0.47
1:A:449:THR:HG22	1:A:450:HIS:N	2.30	0.47
1:B:285:TYR:CB	1:B:310:ARG:HH11	2.28	0.47
1:B:405:GLY:O	1:B:406:MET:CB	2.63	0.47
1:B:573:PHE:HZ	1:B:587:VAL:HG22	1.78	0.47
1:B:95:ARG:NH2	1:B:96:ARG:HB2	2.30	0.47
1:B:654:ASN:O	1:B:686:ASN:HA	2.14	0.47
1:B:549:ILE:HD12	1:B:577:LEU:HD13	1.96	0.47
1:A:217:VAL:O	1:A:220:ILE:HD11	2.15	0.47
1:B:51:HIS:HD2	1:B:85:GLN:HE21	1.62	0.47
1:B:435:VAL:CG2	1:B:464:ILE:HD11	2.44	0.47
1:B:546:ARG:HE	1:B:578:GLU:HG3	1.78	0.47
1:B:705:LEU:HD23	1:B:705:LEU:HA	1.74	0.47
1:A:267:ASN:ND2	1:A:399:PRO:HG2	2.30	0.47
1:A:630:PRO:HG3	1:A:655:PRO:HB3	1.96	0.47
1:B:64:HIS:CE1	1:B:80:GLN:HB3	2.50	0.47
1:A:98:LEU:HD12	1:A:121:ILE:HD11	1.97	0.46
1:A:206:LEU:O	1:A:230:PHE:HE2	1.98	0.46
1:A:280:ASP:O	1:A:282:ILE:HD12	2.15	0.46
1:B:193:VAL:HG13	1:B:193:VAL:O	2.16	0.46
1:A:153:ILE:N	1:A:153:ILE:HD12	2.30	0.46
1:A:548:THR:HA	1:A:575:VAL:O	2.15	0.46
1:B:26:LEU:HD11	1:B:104:VAL:HG11	1.96	0.46
1:B:95:ARG:CZ	1:B:96:ARG:HB2	2.46	0.46
1:B:122:VAL:CG1	1:B:123:SER:N	2.77	0.46
1:B:422:VAL:HG23	1:B:500:TYR:HB2	1.95	0.46
1:B:506:LEU:HD23	1:B:506:LEU:HA	1.71	0.46
1:B:570:LYS:O	1:B:570:LYS:HG2	2.14	0.46
1:B:78:ARG:HG3	1:B:150:PRO:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:PHE:CZ	1:B:474:MET:HA	2.51	0.46
1:B:528:VAL:HG12	1:B:529:LEU:N	2.30	0.46
1:A:95:ARG:HE	1:A:95:ARG:HB2	1.63	0.46
1:B:546:ARG:HE	1:B:578:GLU:CG	2.28	0.46
1:A:76:VAL:HG21	1:A:82:PHE:CD1	2.51	0.46
1:A:350:MET:HB3	1:A:439:LEU:HD23	1.97	0.46
1:A:549:ILE:HG23	1:A:612:ILE:HD13	1.98	0.46
1:B:111:GLU:HB3	1:B:116:TYR:CD2	2.38	0.46
1:B:347:ASN:HD21	1:B:505:PRO:HG3	1.81	0.46
1:B:549:ILE:CD1	1:B:577:LEU:HD13	2.46	0.46
1:A:102:GLU:CD	1:A:171:ARG:HH21	2.24	0.46
1:B:98:LEU:HD23	1:B:164:TRP:HB2	1.98	0.46
1:B:547:TYR:HD1	1:B:614:GLU:CG	2.29	0.46
1:A:165:THR:HG22	1:A:167:TYR:N	2.30	0.46
1:A:664:TRP:CE2	1:A:679:MET:HE3	2.51	0.46
1:A:700:SER:HA	1:A:725:ILE:HB	1.98	0.46
1:B:359:ASN:HD21	1:B:570:LYS:HE3	1.81	0.46
1:B:554:SER:HB2	1:B:607:PHE:HB2	1.96	0.46
1:A:86:ILE:N	1:A:86:ILE:HD12	2.30	0.46
1:B:632:ILE:CG2	1:B:650:VAL:HG13	2.46	0.46
1:B:539:PHE:CB	1:B:577:LEU:HD21	2.45	0.46
1:B:202:GLU:HA	1:B:206:LEU:HB2	1.97	0.45
1:A:23:GLU:HG2	1:A:158:ARG:HD2	1.98	0.45
1:A:26:LEU:HD12	1:A:160:TYR:CE2	2.51	0.45
1:A:515:ARG:HB3	1:A:617:ASP:HB3	1.98	0.45
1:A:463:LEU:HD23	1:A:478:THR:OG1	2.16	0.45
1:A:105:ILE:HG12	1:A:157:PHE:CE2	2.52	0.45
1:A:537:ILE:HD12	1:A:585:GLU:O	2.16	0.45
1:A:546:ARG:HD3	1:A:578:GLU:HA	1.98	0.45
1:B:51:HIS:N	1:B:85:GLN:O	2.48	0.45
1:A:428:ALA:N	1:A:429:PRO:HD2	2.32	0.45
1:A:549:ILE:O	1:A:574:ASP:HA	2.17	0.45
1:B:51:HIS:HD2	1:B:85:GLN:NE2	2.14	0.45
1:B:666:HIS:O	1:B:707:ALA:HA	2.17	0.45
1:A:64:HIS:CE1	1:A:80:GLN:OE1	2.70	0.45
1:A:56:ARG:NH2	1:A:70:GLU:OE2	2.49	0.45
1:A:112:ASN:N	1:A:112:ASN:HD22	2.13	0.45
1:A:125:LEU:HD23	1:A:125:LEU:HA	1.79	0.45
1:A:520:MET:HE2	1:A:520:MET:HB3	1.84	0.45
1:A:685:PRO:C	1:A:687:SER:H	2.24	0.45
1:B:133:LYS:HB3	1:B:133:LYS:HE3	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:ARG:O	1:B:518:VAL:HG23	2.17	0.45
1:B:528:VAL:CG1	1:B:529:LEU:N	2.80	0.45
1:B:546:ARG:HH21	1:B:578:GLU:HG2	1.82	0.45
1:B:663:VAL:O	1:B:679:MET:HA	2.17	0.45
1:A:225:TRP:CE2	1:A:294:GLY:HA2	2.52	0.45
1:A:332:ALA:HA	1:A:377:GLU:O	2.17	0.45
1:A:665:VAL:O	1:A:677:LYS:HA	2.17	0.45
1:B:43:GLU:HB2	1:B:165:THR:CG2	2.39	0.45
1:B:453:GLU:O	1:B:512:MET:HB2	2.17	0.45
1:B:605:HIS:HE1	1:B:607:PHE:CZ	2.35	0.45
1:A:663:VAL:HB	1:A:680:PHE:HB2	1.99	0.44
1:B:105:ILE:HD11	1:B:115:THR:HG22	2.00	0.44
1:B:634:ILE:HD13	1:B:650:VAL:HG22	1.99	0.44
1:A:331:PRO:HB2	1:A:379:TRP:HB2	2.00	0.44
1:B:220:ILE:CD1	1:B:474:MET:HE1	2.42	0.44
1:B:640:GLN:O	1:B:726:GLN:OE1	2.35	0.44
1:A:361:ASN:CG	1:A:363:LYS:HG2	2.42	0.44
1:A:529:LEU:HD12	1:A:598:LEU:CD1	2.48	0.44
1:B:276:VAL:O	1:B:311:TYR:HA	2.18	0.44
1:B:460:ILE:HA	1:B:460:ILE:HD12	1.68	0.44
1:B:511:VAL:HG22	1:B:512:MET:H	1.83	0.44
1:A:337:ASN:O	1:A:372:TYR:HA	2.18	0.44
1:A:379:TRP:CD1	1:A:392:TRP:CE2	3.04	0.44
1:B:443:THR:HB	1:B:451:VAL:HG13	1.98	0.44
1:A:99:PHE:HA	1:A:162:ALA:O	2.18	0.44
1:A:547:TYR:O	1:A:576:THR:HA	2.17	0.44
1:A:674:ARG:HG3	1:A:675:PRO:HD2	1.99	0.44
1:A:705:LEU:HD23	1:A:705:LEU:HA	1.74	0.44
1:A:402:ASN:HA	1:A:430:PHE:CE1	2.52	0.44
1:A:565:LYS:O	1:A:566:ALA:HB2	2.18	0.44
1:A:577:LEU:HG	1:A:583:LYS:HE3	1.99	0.44
1:B:107:ARG:NH1	1:B:107:ARG:HG3	2.31	0.44
1:B:636:VAL:HG11	1:B:646:MET:CE	2.47	0.44
1:A:107:ARG:HG2	1:A:108:TYR:CD2	2.53	0.44
1:A:249:LEU:HA	1:A:252:ARG:HG3	2.00	0.44
1:A:506:LEU:HD23	1:A:506:LEU:HA	1.83	0.43
1:A:594:TYR:CD1	1:A:594:TYR:C	2.96	0.43
1:A:405:GLY:O	1:A:406:MET:CB	2.65	0.43
1:A:157:PHE:CD1	1:A:157:PHE:N	2.87	0.43
1:B:541:ASN:O	1:B:580:LEU:HA	2.18	0.43
1:A:79:GLY:HA2	1:A:148:SER:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:GLY:C	1:B:11:ARG:H	2.27	0.43
1:B:195:LEU:O	1:B:201:ARG:NE	2.51	0.43
1:A:444:ALA:HA	1:A:450:HIS:ND1	2.33	0.43
1:B:385:LEU:CD2	1:B:424:PHE:HB3	2.47	0.43
1:B:527:ALA:HB2	1:B:533:PHE:CB	2.38	0.43
1:B:547:TYR:HD1	1:B:614:GLU:HG2	1.82	0.43
1:B:620:ALA:O	1:B:621:LYS:HG2	2.18	0.43
1:A:69:TYR:O	1:A:71:ASN:N	2.52	0.43
1:B:17:ASN:OD1	1:B:106:GLY:HA3	2.18	0.43
1:A:26:LEU:HD12	1:A:160:TYR:CD2	2.54	0.43
1:A:268:ALA:HB2	1:A:308:PRO:HB3	2.01	0.43
1:B:82:PHE:CD1	1:B:82:PHE:N	2.86	0.43
1:B:587:VAL:HG12	1:B:588:LEU:N	2.33	0.43
1:A:194:TYR:HE1	1:A:201:ARG:HH21	1.66	0.43
1:A:353:PHE:HB2	1:A:365:THR:OG1	2.18	0.43
1:A:513:LYS:NZ	1:A:516:SER:H	2.15	0.43
1:A:684:ARG:HD3	1:A:684:ARG:HA	1.73	0.43
1:A:703:ARG:HA	1:A:703:ARG:NE	2.33	0.43
1:B:543:SER:O	1:B:580:LEU:HD12	2.19	0.43
1:A:283:TYR:CD2	1:A:288:PRO:HB3	2.53	0.43
1:A:535:LEU:O	1:A:586:ALA:HA	2.18	0.43
1:B:666:HIS:HA	1:B:676:MET:O	2.18	0.43
1:A:286:GLY:HA3	1:A:310:ARG:HB3	2.00	0.43
1:B:135:VAL:HG12	1:B:143:ARG:O	2.19	0.43
1:B:447:ASP:OD1	1:B:447:ASP:N	2.52	0.43
1:B:573:PHE:HZ	1:B:587:VAL:CG2	2.32	0.43
1:A:335:VAL:O	1:A:374:CYS:HA	2.19	0.42
1:B:153:ILE:HD13	1:B:249:LEU:O	2.19	0.42
1:A:535:LEU:N	1:A:535:LEU:HD12	2.35	0.42
1:B:213:PHE:CE2	1:B:474:MET:HB3	2.54	0.42
1:A:72:ASN:OD1	1:A:72:ASN:N	2.52	0.42
1:A:519:ASP:HB2	1:A:540:ARG:CG	2.49	0.42
1:A:534:LYS:HB2	1:A:587:VAL:O	2.19	0.42
1:A:582:PHE:O	1:A:583:LYS:HE2	2.19	0.42
1:B:633:ILE:HD13	1:B:633:ILE:HA	1.90	0.42
1:A:134:ILE:HD12	1:A:134:ILE:H	1.85	0.42
1:A:288:PRO:HA	1:A:289:PRO:HD3	1.74	0.42
1:A:455:VAL:HG11	1:A:508:THR:CG2	2.49	0.42
1:B:206:LEU:HD12	1:B:230:PHE:HZ	1.84	0.42
1:B:361:ASN:OD1	1:B:362:SER:N	2.53	0.42
1:A:43:GLU:OE1	1:A:43:GLU:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:PHE:HE2	1:A:142:VAL:CG2	2.33	0.42
1:A:676:MET:HB2	1:A:676:MET:HE3	1.82	0.42
1:B:99:PHE:HB2	1:B:162:ALA:O	2.19	0.42
1:B:363:LYS:HE3	1:B:364:LEU:HB3	2.00	0.42
1:B:489:GLU:H	1:B:489:GLU:HG2	1.60	0.42
1:A:535:LEU:CD1	1:A:589:ILE:HD11	2.50	0.42
1:A:90:ARG:HA	1:A:91:PRO:HD2	1.77	0.42
1:B:605:HIS:HD2	1:B:624:SER:OG	2.03	0.42
1:A:414:VAL:O	1:A:414:VAL:HG12	2.19	0.42
1:B:256:ILE:H	1:B:256:ILE:CD1	2.32	0.42
1:B:578:GLU:HB3	1:B:579:PRO:HD2	2.00	0.42
1:B:580:LEU:HD12	1:B:580:LEU:N	2.35	0.42
1:B:598:LEU:HD11	1:B:627:LEU:CD1	2.50	0.42
1:A:195:LEU:HA	1:A:195:LEU:HD23	1.77	0.42
1:B:48:THR:N	1:B:87:ASP:O	2.50	0.42
1:B:342:HIS:ND1	1:B:434:GLU:OE2	2.48	0.42
1:B:413:SER:O	1:B:417:ILE:HG12	2.19	0.42
1:A:419:HIS:HB3	1:A:421:HIS:CD2	2.54	0.42
1:A:629:ILE:H	1:A:629:ILE:CD1	2.32	0.42
1:B:280:ASP:O	1:B:282:ILE:N	2.53	0.42
1:B:668:ASP:HB3	1:B:706:ILE:HB	2.01	0.42
1:B:43:GLU:O	1:B:44:PHE:CD1	2.71	0.41
1:B:575:VAL:HG22	1:B:585:GLU:OE2	2.20	0.41
1:A:8:PHE:N	1:A:8:PHE:CD1	2.88	0.41
1:A:45:LEU:HD22	1:A:88:PHE:HB3	2.02	0.41
1:B:269:LYS:O	1:B:272:GLU:HB2	2.19	0.41
1:B:353:PHE:HE2	1:B:364:LEU:HD22	1.85	0.41
1:B:530:GLY:O	1:B:591:ALA:CB	2.68	0.41
1:A:206:LEU:HD12	1:A:230:PHE:HZ	1.85	0.41
1:A:568:PHE:HB2	1:A:593:GLU:OE1	2.20	0.41
1:B:287:VAL:HB	1:B:292:TRP:CZ2	2.55	0.41
1:B:347:ASN:ND2	1:B:505:PRO:HG3	2.35	0.41
1:A:633:ILE:CG2	1:A:635:LYS:HD3	2.50	0.41
1:B:20:ASN:O	1:B:20:ASN:ND2	2.43	0.41
1:B:90:ARG:O	1:B:91:PRO:C	2.63	0.41
1:A:513:LYS:NZ	1:A:514:SER:O	2.40	0.41
1:B:153:ILE:HG23	1:B:252:ARG:HB2	2.03	0.41
1:B:401:GLU:HA	1:B:406:MET:H	1.84	0.41
1:A:268:ALA:HA	1:A:272:GLU:O	2.20	0.41
1:B:101:VAL:HG12	1:B:102:GLU:N	2.36	0.41
1:B:684:ARG:HD3	1:B:684:ARG:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:VAL:HG11	1:A:159:MET:HE2	2.03	0.41
1:A:117:ILE:HG21	1:A:130:TRP:CE2	2.56	0.41
1:A:134:ILE:HD12	1:A:134:ILE:N	2.35	0.41
1:B:93:ASP:HA	1:B:94:PRO:HD2	1.73	0.41
1:B:634:ILE:HD11	1:B:707:ALA:CB	2.51	0.41
1:A:105:ILE:HG12	1:A:157:PHE:CD2	2.56	0.41
1:A:199:LYS:HA	1:A:202:GLU:HG3	2.03	0.41
1:A:380:MET:HE2	1:A:380:MET:HB3	1.80	0.41
1:A:90:ARG:HH11	1:A:90:ARG:HD2	1.73	0.41
1:A:319:GLY:HA2	1:A:334:ILE:HD11	2.02	0.41
1:A:412:ALA:HB2	1:A:426:PHE:O	2.21	0.41
1:B:8:PHE:O	1:B:9:GLY:C	2.64	0.41
1:B:9:GLY:C	1:B:11:ARG:N	2.78	0.41
1:B:446:LYS:HD3	1:B:446:LYS:HA	1.67	0.41
1:A:353:PHE:HD2	1:A:364:LEU:O	2.02	0.41
1:A:516:SER:O	1:A:517:ASN:HB2	2.21	0.41
1:A:579:PRO:O	1:A:580:LEU:C	2.63	0.41
1:B:127:SER:O	1:B:128:GLY:C	2.64	0.41
1:A:559:PHE:CD1	1:A:563:VAL:O	2.63	0.40
1:A:715:ARG:O	1:A:716:HIS:CB	2.69	0.40
1:B:117:ILE:HA	1:B:118:PRO:HD2	1.92	0.40
1:B:338:TYR:O	1:B:339:PHE:HB2	2.21	0.40
1:A:268:ALA:HA	1:A:273:GLY:HA3	2.03	0.40
1:B:134:ILE:H	1:B:134:ILE:HD12	1.87	0.40
1:B:513:LYS:HB3	1:B:514:SER:H	1.70	0.40
1:A:86:ILE:HD12	1:A:86:ILE:H	1.86	0.40
1:A:172:THR:HG22	1:A:173:SER:H	1.86	0.40
1:A:283:TYR:CE2	1:A:600:GLU:OE1	2.75	0.40
1:A:305:SER:O	1:A:306:GLU:HB2	2.21	0.40
1:A:590:GLN:C	1:A:592:GLY:N	2.79	0.40
1:A:590:GLN:C	1:A:592:GLY:H	2.29	0.40
1:B:64:HIS:HE1	1:B:80:GLN:HB3	1.87	0.40
1:B:184:PHE:CE2	1:B:255:PRO:HG3	2.56	0.40
1:B:71:ASN:HB3	1:B:75:ILE:HD11	2.03	0.40
1:B:515:ARG:CB	1:B:619:LEU:HD21	2.50	0.40
1:B:515:ARG:HB2	1:B:619:LEU:HD21	2.03	0.40
1:A:541:ASN:ND2	1:A:545:ASN:O	2.54	0.40
1:B:55:GLU:OE1	1:B:55:GLU:HA	2.21	0.40
1:B:563:VAL:HA	1:B:564:PRO:HD3	1.93	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	706/731 (97%)	633 (90%)	49 (7%)	24 (3%)	3	4
1	B	704/731 (96%)	607 (86%)	70 (10%)	27 (4%)	2	3
All	All	1410/1462 (96%)	1240 (88%)	119 (8%)	51 (4%)	2	4

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	PHE
1	A	91	PRO
1	A	139	ASP
1	A	426	PHE
1	A	509	GLU
1	B	54	LYS
1	B	55	GLU
1	B	270	ASP
1	B	272	GLU
1	B	365	THR
1	B	509	GLU
1	B	522	PHE
1	A	69	TYR
1	A	217	VAL
1	A	512	MET
1	A	513	LYS
1	A	515	ARG
1	A	580	LEU
1	B	45	LEU
1	B	128	GLY
1	B	273	GLY
1	B	460	ILE
1	B	595	MET
1	B	716	HIS
1	A	78	ARG

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Mol	Chain	Res	Type
1	A	138	GLU
1	A	406	MET
1	A	516	SER
1	B	136	MET
1	B	139	ASP
1	B	189	GLU
1	B	252	ARG
1	B	514	SER
1	B	631	GLU
1	A	268	ALA
1	A	270	ASP
1	A	70	GLU
1	A	311	TYR
1	A	425	GLN
1	A	687	SER
1	B	232	ASP
1	B	311	TYR
1	B	406	MET
1	B	425	GLN
1	B	447	ASP
1	A	686	ASN
1	A	716	HIS
1	B	445	LYS
1	B	697	PRO
1	A	669	GLY
1	B	9	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	626/644 (97%)	521 (83%)	105 (17%)	2	2
1	B	624/644 (97%)	549 (88%)	75 (12%)	5	7
All	All	1250/1288 (97%)	1070 (86%)	180 (14%)	3	4

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	PHE
1	A	11	ARG
1	A	18	ASN
1	A	20	ASN
1	A	43	GLU
1	A	45	LEU
1	A	47	VAL
1	A	54	LYS
1	A	56	ARG
1	A	58	ASP
1	A	59	THR
1	A	68	LYS
1	A	72	ASN
1	A	96	ARG
1	A	100	ARG
1	A	104	VAL
1	A	105	ILE
1	A	112	ASN
1	A	121	ILE
1	A	126	GLN
1	A	136	MET
1	A	137	ARG
1	A	143	ARG
1	A	147	GLN
1	A	148	SER
1	A	164	TRP
1	A	165	THR
1	A	174	ARG
1	A	177	GLU
1	A	193	VAL
1	A	195	LEU
1	A	203	GLU
1	A	206	LEU
1	A	211	VAL
1	A	217	VAL
1	A	218	ASN
1	A	223	ARG
1	A	232	ASP
1	A	235	LEU
1	A	250	SER
1	A	270	ASP
1	A	276	VAL
1	A	293	THR

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Mol	Chain	Res	Type
1	A	301	GLU
1	A	304	SER
1	A	328	LEU
1	A	340	SER
1	A	343	ASP
1	A	347	ASN
1	A	350	MET
1	A	354	LEU
1	A	357	ASP
1	A	362	SER
1	A	365	THR
1	A	368	SER
1	A	369	VAL
1	A	379	TRP
1	A	381	THR
1	A	386	PRO
1	A	408	ARG
1	A	422	VAL
1	A	435	VAL
1	A	445	LYS
1	A	455	VAL
1	A	462	LYS
1	A	463	LEU
1	A	465	VAL
1	A	469	ILE
1	A	490	GLU
1	A	499	MET
1	A	507	ASN
1	A	509	GLU
1	A	511	VAL
1	A	515	ARG
1	A	516	SER
1	A	537	ILE
1	A	548	THR
1	A	553	LEU
1	A	569	LYS
1	A	572	THR
1	A	575	VAL
1	A	583	LYS
1	A	587	VAL
1	A	590	GLN
1	A	593	GLU

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Mol	Chain	Res	Type
1	A	603	SER
1	A	604	LEU
1	A	609	THR
1	A	616	ARG
1	A	625	THR
1	A	629	ILE
1	A	632	ILE
1	A	635	LYS
1	A	637	ARG
1	A	639	THR
1	A	658	GLU
1	A	667	LEU
1	A	677	LYS
1	A	679	MET
1	A	688	THR
1	A	689	VAL
1	A	712	ASP
1	A	713	SER
1	A	724	GLN
1	A	729	PRO
1	B	28	THR
1	B	30	GLU
1	B	44	PHE
1	B	48	THR
1	B	58	ASP
1	B	95	ARG
1	B	96	ARG
1	B	104	VAL
1	B	110	GLN
1	B	121	ILE
1	B	135	VAL
1	B	143	ARG
1	B	148	SER
1	B	165	THR
1	B	172	THR
1	B	174	ARG
1	B	193	VAL
1	B	206	LEU
1	B	217	VAL
1	B	221	LYS
1	B	223	ARG
1	B	235	LEU

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Mol	Chain	Res	Type
1	B	237	THR
1	B	270	ASP
1	B	272	GLU
1	B	301	GLU
1	B	314	CYS
1	B	340	SER
1	B	350	MET
1	B	354	LEU
1	B	363	LYS
1	B	386	PRO
1	B	397	SER
1	B	403	SER
1	B	427	ASP
1	B	431	VAL
1	B	446	LYS
1	B	452	VAL
1	B	460	ILE
1	B	463	LEU
1	B	487	GLN
1	B	489	GLU
1	B	494	LEU
1	B	495	GLU
1	B	498	LEU
1	B	499	MET
1	B	504	LYS
1	B	509	GLU
1	B	516	SER
1	B	517	ASN
1	B	520	MET
1	B	523	GLU
1	B	526	ASN
1	B	529	LEU
1	B	536	SER
1	B	553	LEU
1	B	565	LYS
1	B	571	GLU
1	B	572	THR
1	B	573	PHE
1	B	582	PHE
1	B	583	LYS
1	B	588	LEU
1	B	590	GLN

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Mol	Chain	Res	Type
1	B	593	GLU
1	B	597	GLN
1	B	604	LEU
1	B	639	THR
1	B	640	GLN
1	B	682	GLU
1	B	690	GLN
1	B	713	SER
1	B	721	LEU
1	B	724	GLN
1	B	725	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	112	ASN
1	A	126	GLN
1	A	175	ASN
1	A	207	ASN
1	A	218	ASN
1	A	267	ASN
1	A	347	ASN
1	A	419	HIS
1	A	459	HIS
1	A	484	GLN
1	A	487	GLN
1	A	545	ASN
1	A	613	ASN
1	A	666	HIS
1	B	51	HIS
1	B	71	ASN
1	B	313	GLN
1	B	322	ASN
1	B	337	ASN
1	B	347	ASN
1	B	415	GLN
1	B	419	HIS
1	B	454	ASN
1	B	545	ASN
1	B	556	ASN
1	B	640	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](#)

There are no ligands in this entry.

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.