



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:24 PM UTC

PDB ID : 4GXP / pdb_00004gxp
Title : Chimeric Family 1 beta-glucosidase made with non-contiguous SCHEMA
Authors : Smith, M.A.; Romero, P.A.; Wu, T.; Brustad, E.M.; Arnold, F.H.
Deposited on : 2012-09-04
Resolution : 3.00 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

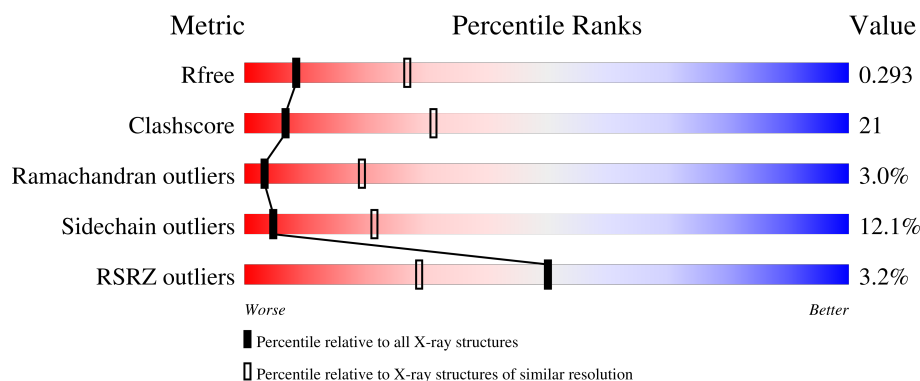
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	467	2% 61% 31% 5% .
1	B	467	% 56% 34% 6% . .
1	C	467	7% 55% 34% 8% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9869 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 Beta-glucosidase Chimeric protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	0	0
			3451	2206	592	644	9			
1	B	456	Total	C	N	O	S	0	0	0
			3288	2084	577	618	9			
1	C	454	Total	C	N	O	S	0	0	0
			3128	1957	554	609	8			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q08638
A	2	HIS	-	expression tag	UNP Q08638
A	3	HIS	-	expression tag	UNP Q08638
A	4	HIS	-	expression tag	UNP Q08638
A	5	HIS	-	expression tag	UNP Q08638
A	6	HIS	-	expression tag	UNP Q08638
A	7	HIS	-	expression tag	UNP Q08638
A	127	PHE	TYR	engineered mutation	UNP Q08638
A	141	LEU	TRP	engineered mutation	UNP Q08638
A	142	LEU	ALA	engineered mutation	UNP Q08638
A	398	TYR	HIS	engineered mutation	UNP Q08638
A	340	ALA	GLN	engineered mutation	UNP O93785
A	341	MET	SER	engineered mutation	UNP O93785
B	1	MET	-	expression tag	UNP Q08638
B	2	HIS	-	expression tag	UNP Q08638
B	3	HIS	-	expression tag	UNP Q08638
B	4	HIS	-	expression tag	UNP Q08638
B	5	HIS	-	expression tag	UNP Q08638
B	6	HIS	-	expression tag	UNP Q08638
B	7	HIS	-	expression tag	UNP Q08638
B	127	PHE	TYR	engineered mutation	UNP Q08638
B	141	LEU	TRP	engineered mutation	UNP Q08638
B	142	LEU	ALA	engineered mutation	UNP Q08638

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Chain	Residue	Modelled	Actual	Comment	Reference
B	398	TYR	HIS	engineered mutation	UNP Q08638
B	340	ALA	GLN	engineered mutation	UNP O93785
B	341	MET	SER	engineered mutation	UNP O93785
C	1	MET	-	expression tag	UNP Q08638
C	2	HIS	-	expression tag	UNP Q08638
C	3	HIS	-	expression tag	UNP Q08638
C	4	HIS	-	expression tag	UNP Q08638
C	5	HIS	-	expression tag	UNP Q08638
C	6	HIS	-	expression tag	UNP Q08638
C	7	HIS	-	expression tag	UNP Q08638
C	127	PHE	TYR	engineered mutation	UNP Q08638
C	141	LEU	TRP	engineered mutation	UNP Q08638
C	142	LEU	ALA	engineered mutation	UNP Q08638
C	398	TYR	HIS	engineered mutation	UNP Q08638
C	340	ALA	GLN	engineered mutation	UNP O93785
C	341	MET	SER	engineered mutation	UNP O93785

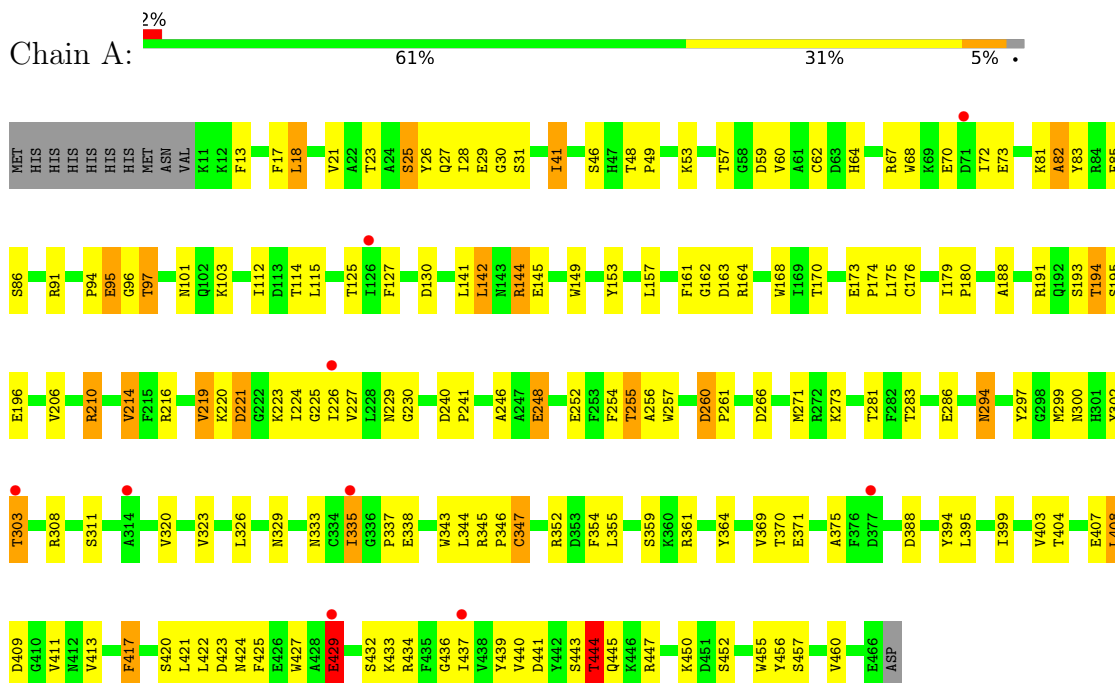
- Molecule 2 is water.

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

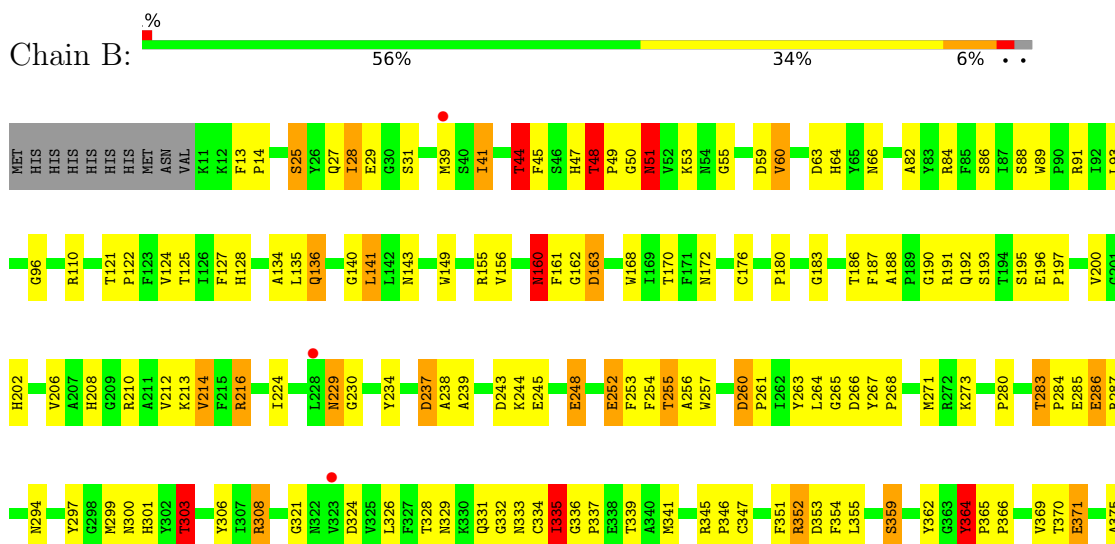
3 Residue-property plots

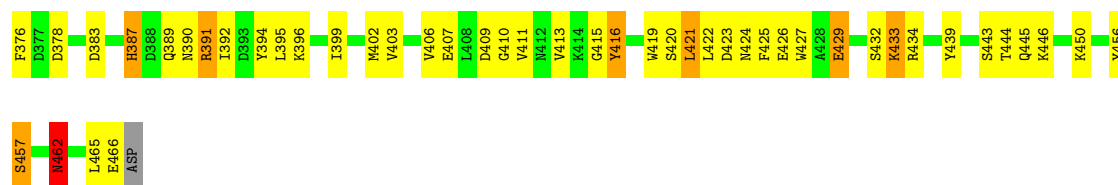
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Beta-glucosidase Chimeric protein

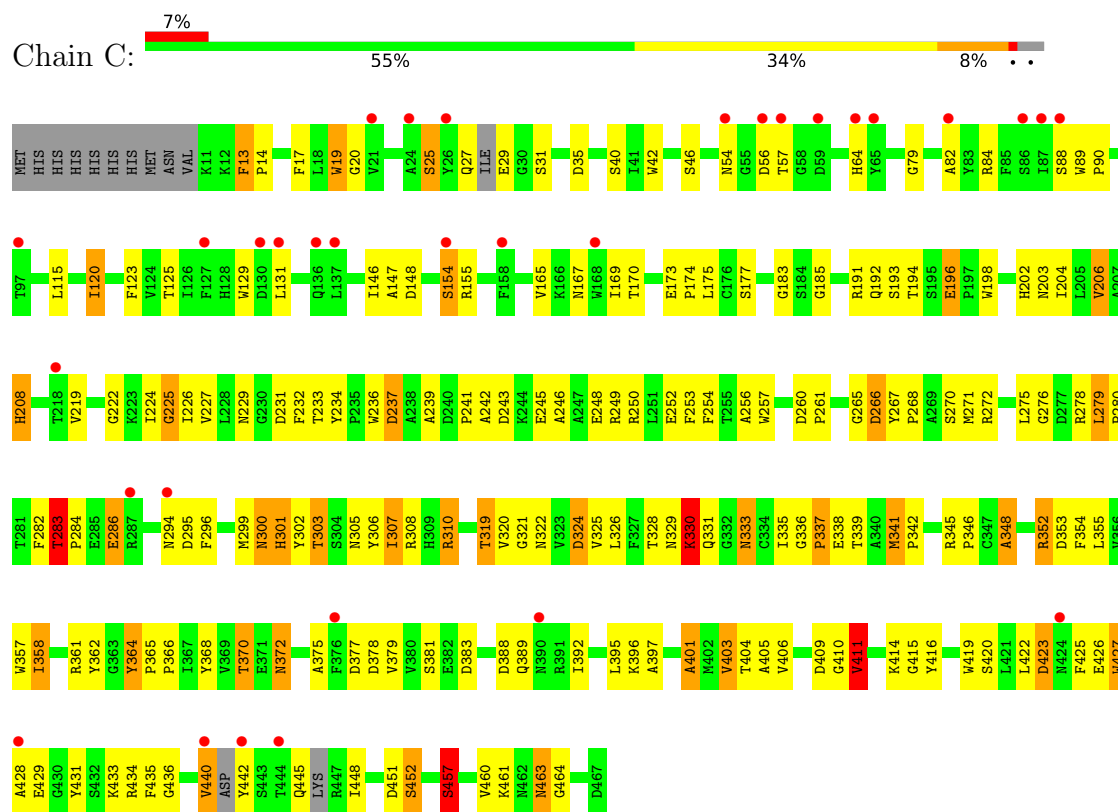


• Molecule 1: Beta-glucosidase Chimeric protein





• Molecule 1: Beta-glucosidase Chimeric protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	115.38Å 115.38Å 282.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.43 – 3.00 37.43 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (37.43-3.00) 99.5 (37.43-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.239 , 0.294 0.238 , 0.293	Depositor DCC
R_{free} test set	2188 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	92.2	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 125.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9869	wwPDB-VP
Average B, all atoms (Å ²)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.96	0/3563	1.19	18/4871 (0.4%)
1	B	1.15	10/3398 (0.3%)	1.28	35/4665 (0.8%)
1	C	1.17	12/3220 (0.4%)	1.20	34/4418 (0.8%)
All	All	1.09	22/10181 (0.2%)	1.23	87/13954 (0.6%)

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	B	0	1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	401	ALA	C-O	15.82	1.42	1.24
1	C	404	THR	CB-OG1	11.64	1.62	1.43
1	C	301	HIS	ND1-CE1	9.87	1.42	1.32
1	C	348	ALA	C-O	7.40	1.32	1.24
1	C	457	SER	CB-OG	7.35	1.56	1.42
1	C	301	HIS	CG-CD2	6.83	1.43	1.35
1	C	415	GLY	N-CA	6.33	1.51	1.45
1	B	366	PRO	CA-C	6.22	1.59	1.52
1	C	463	ASN	C-O	6.08	1.31	1.23
1	B	364	TYR	CA-C	5.99	1.58	1.53
1	B	301	HIS	CG-CD2	5.94	1.42	1.35
1	B	208	HIS	CG-CD2	5.84	1.42	1.35
1	B	303	THR	CA-C	-5.83	1.46	1.53
1	C	330	LYS	CA-CB	5.50	1.62	1.53
1	C	463	ASN	C-N	5.44	1.39	1.32
1	B	301	HIS	ND1-CE1	5.44	1.38	1.32
1	C	464	GLY	C-N	5.33	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	387	HIS	CG-CD2	5.20	1.41	1.35
1	B	208	HIS	ND1-CE1	5.20	1.37	1.32
1	B	216	ARG	NE-CZ	5.18	1.38	1.33
1	C	348	ALA	C-N	5.12	1.40	1.33
1	B	264	LEU	CA-C	5.11	1.59	1.53

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	267	TYR	CA-C-N	8.45	128.95	119.83
1	B	267	TYR	C-N-CA	8.45	128.95	119.83
1	B	89	TRP	CA-C-N	-7.92	112.75	120.83
1	B	89	TRP	C-N-CA	-7.92	112.75	120.83
1	B	48	THR	CA-C-N	7.69	129.45	119.84
1	B	48	THR	C-N-CA	7.69	129.45	119.84
1	C	20	GLY	N-CA-C	7.68	121.29	110.38
1	A	82	ALA	N-CA-C	7.58	120.89	108.99
1	C	279	LEU	CA-C-N	7.32	127.08	119.76
1	C	279	LEU	C-N-CA	7.32	127.08	119.76
1	C	303	THR	N-CA-C	7.23	117.56	108.45
1	A	345	ARG	CA-C-N	-7.12	112.60	120.14
1	A	345	ARG	C-N-CA	-7.12	112.60	120.14
1	A	260	ASP	CA-C-N	-7.03	111.24	119.05
1	A	260	ASP	C-N-CA	-7.03	111.24	119.05
1	C	82	ALA	N-CA-C	6.98	119.77	108.32
1	B	336	GLY	CA-C-N	6.75	127.15	119.92
1	B	336	GLY	C-N-CA	6.75	127.15	119.92
1	B	28	ILE	N-CA-C	6.74	117.78	112.12
1	B	260	ASP	CA-C-N	-6.73	111.97	118.97
1	B	260	ASP	C-N-CA	-6.73	111.97	118.97
1	C	305	ASN	N-CA-C	6.70	120.45	109.06
1	B	433	LYS	N-CA-C	6.70	119.39	107.80
1	B	51	ASN	N-CA-C	6.67	121.08	112.41
1	A	144	ARG	N-CA-C	-6.61	104.11	111.71
1	A	326	LEU	N-CA-C	6.45	118.98	109.69
1	B	55	GLY	N-CA-C	-6.37	106.89	115.36
1	B	60	VAL	N-CA-C	6.31	117.66	111.67
1	A	194	THR	N-CA-C	-6.21	103.37	113.19
1	C	31	SER	CA-C-N	6.20	125.42	118.97
1	C	31	SER	C-N-CA	6.20	125.42	118.97
1	C	245	GLU	N-CA-C	-6.18	103.86	111.33
1	B	335	ILE	N-CA-C	-6.10	106.86	112.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	ARG	N-CA-C	6.10	118.90	111.82
1	A	444	THR	N-CA-C	-6.10	101.26	110.28
1	A	266	ASP	N-CA-C	6.08	117.81	109.18
1	B	93	LEU	CB-CA-C	6.06	116.95	110.65
1	C	326	LEU	N-CA-C	6.03	118.23	109.07
1	C	404	THR	CB-CA-C	6.01	120.48	110.92
1	B	50	GLY	CA-C-N	-6.00	113.07	122.49
1	B	50	GLY	C-N-CA	-6.00	113.07	122.49
1	C	225	GLY	N-CA-C	5.97	119.02	111.09
1	C	364	TYR	CA-C-N	-5.96	114.24	120.38
1	C	364	TYR	C-N-CA	-5.96	114.24	120.38
1	B	365	PRO	CA-C-N	-5.92	113.44	120.13
1	B	365	PRO	C-N-CA	-5.92	113.44	120.13
1	C	320	VAL	N-CA-C	-5.84	106.62	112.17
1	C	283	THR	CA-C-N	5.83	127.13	119.84
1	C	283	THR	C-N-CA	5.83	127.13	119.84
1	A	127	PHE	N-CA-C	5.81	117.86	107.80
1	B	347	CYS	N-CA-C	-5.79	98.47	110.80
1	A	429	GLU	N-CA-C	-5.78	106.21	113.72
1	C	196	GLU	CA-C-N	-5.77	113.73	119.56
1	C	196	GLU	C-N-CA	-5.77	113.73	119.56
1	C	404	THR	CA-CB-CG2	5.77	120.31	110.50
1	B	294	ASN	N-CA-C	5.76	118.28	108.02
1	C	404	THR	N-CA-C	-5.73	104.03	111.02
1	B	303	THR	CB-CA-C	-5.70	102.07	114.10
1	B	371	GLU	N-CA-C	5.64	117.83	108.13
1	C	196	GLU	N-CA-C	5.51	121.11	113.45
1	B	416	TYR	N-CA-C	5.46	117.10	107.61
1	A	294	ASN	CB-CA-C	5.44	119.14	109.72
1	B	127	PHE	N-CA-C	5.42	116.29	107.23
1	A	408	LEU	N-CA-C	5.38	118.17	111.24
1	B	286	GLU	N-CA-C	5.37	116.94	111.14
1	B	66	ASN	N-CA-C	5.34	120.07	113.50
1	C	336	GLY	CA-C-N	5.34	126.52	119.84
1	C	336	GLY	C-N-CA	5.34	126.52	119.84
1	B	415	GLY	N-CA-C	5.32	119.39	110.56
1	B	429	GLU	N-CA-C	-5.27	106.89	113.38
1	C	370	THR	N-CA-C	5.24	119.15	112.34
1	B	190	GLY	N-CA-C	5.23	121.12	113.48
1	C	404	THR	N-CA-CB	5.21	117.73	109.82
1	A	81	LYS	N-CA-C	5.18	119.07	112.34
1	C	406	VAL	N-CA-C	-5.16	105.47	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	84	ARG	N-CA-C	-5.15	98.87	107.99
1	B	396	LYS	N-CA-C	-5.13	104.75	111.02
1	C	222	GLY	N-CA-C	5.13	121.73	112.54
1	C	452	SER	CA-C-N	5.10	125.60	119.94
1	C	452	SER	C-N-CA	5.10	125.60	119.94
1	B	160	ASN	N-CA-C	5.09	119.36	113.20
1	A	437	ILE	N-CA-C	-5.06	106.98	112.80
1	C	358	ILE	CB-CA-C	-5.06	103.00	111.29
1	A	95	GLU	N-CA-C	-5.05	107.14	113.15
1	B	413	VAL	CB-CA-C	-5.05	105.77	111.23
1	C	415	GLY	N-CA-C	5.01	118.42	111.10
1	C	410	GLY	N-CA-C	-5.00	108.42	115.32

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	364	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	3451	0	3027	106	0
1	B	3288	0	2645	140	0
1	C	3128	0	2393	141	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	9869	0	8065	384	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 21.

All (384) 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:299:MET:HE1	1:B:355:LEU:HD21	1.11	1.06
1:B:299:MET:HE1	1:B:355:LEU:CD2	1.84	1.06
1:B:303:THR:HG21	1:B:345:ARG:H	1.26	1.00
1:B:303:THR:HG22	1:B:345:ARG:O	1.66	0.95
1:B:283:THR:HG22	1:B:286:GLU:H	1.32	0.93
1:B:186:THR:O	1:B:187:PHE:HD1	1.55	0.90
1:B:303:THR:HG21	1:B:345:ARG:N	1.86	0.90
1:C:123:PHE:HA	1:C:167:ASN:O	1.72	0.89
1:B:41:ILE:HG12	1:B:136:GLN:HG3	1.57	0.87
1:C:202:HIS:HD2	1:C:267:TYR:OH	1.55	0.87
1:C:375:ALA:HA	1:C:434:ARG:O	1.77	0.85
1:B:41:ILE:HG12	1:B:136:GLN:CG	2.07	0.85
1:A:299:MET:HE1	1:A:355:LEU:CD2	2.07	0.85
1:B:84:ARG:HH22	1:B:172:ASN:ND2	1.74	0.85
1:A:41:ILE:HG13	1:A:188:ALA:HB1	1.60	0.83
1:B:96:GLY:HA3	1:B:135:LEU:HD21	1.61	0.82
1:C:378:ASP:HB2	1:C:434:ARG:HD2	1.60	0.82
1:A:299:MET:HE3	1:A:369:VAL:HG22	1.62	0.82
1:A:299:MET:HE1	1:A:355:LEU:HD23	1.62	0.82
1:C:252:GLU:HA	1:C:256:ALA:HB3	1.61	0.80
1:A:41:ILE:HD12	1:A:41:ILE:O	1.82	0.80
1:B:253:PHE:CE2	1:B:321:GLY:HA2	2.16	0.80
1:B:444:THR:O	1:B:446:LYS:N	2.14	0.80
1:C:202:HIS:CD2	1:C:267:TYR:OH	2.36	0.79
1:A:337:PRO:HD2	1:A:346:PRO:HD2	1.65	0.78
1:B:389:GLN:O	1:B:392:ILE:HG13	1.84	0.78
1:C:366:PRO:HB3	1:C:414:LYS:HE2	1.66	0.77
1:A:225:GLY:HA2	1:A:294:ASN:HB2	1.65	0.76
1:B:248:GLU:HA	1:B:248:GLU:OE2	1.85	0.76
1:B:300:ASN:CG	1:B:371:GLU:HB2	2.10	0.76
1:B:299:MET:CE	1:B:355:LEU:HD21	2.05	0.75
1:C:19:TRP:HE1	1:C:463:ASN:HA	1.51	0.75
1:C:310:ARG:HG3	1:C:322:ASN:O	1.86	0.75
1:A:219:VAL:O	1:A:221:ASP:N	2.19	0.74
1:C:13:PHE:HB3	1:C:14:PRO:CD	2.18	0.74
1:B:253:PHE:CD1	1:B:271:MET:HG2	2.22	0.74
1:B:253:PHE:CE1	1:B:271:MET:HG2	2.23	0.73
1:B:44:THR:O	1:B:48:THR:HG22	1.88	0.73
1:C:173:GLU:HG2	1:C:229:ASN:HB3	1.69	0.73
1:C:310:ARG:CG	1:C:322:ASN:O	2.38	0.71
1:B:306:TYR:CD1	1:B:329:ASN:HB3	2.25	0.71
1:C:231:ASP:HB3	1:C:303:THR:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:MET:HE2	1:C:301:HIS:HB2	1.72	0.70
1:C:13:PHE:HB3	1:C:14:PRO:HD2	1.74	0.70
1:A:29:GLU:OE1	1:A:91:ARG:NH1	2.25	0.69
1:B:25:SER:H	1:B:86:SER:HB3	1.58	0.69
1:C:339:THR:HB	1:C:375:ALA:O	1.94	0.68
1:A:399:ILE:O	1:A:403:VAL:HG23	1.94	0.68
1:C:389:GLN:HA	1:C:392:ILE:HG12	1.76	0.68
1:B:84:ARG:HH22	1:B:172:ASN:HD22	1.41	0.67
1:C:308:ARG:HG2	1:C:324:ASP:OD2	1.94	0.67
1:C:335:ILE:O	1:C:335:ILE:HG22	1.93	0.67
1:A:441:ASP:O	1:A:444:THR:O	2.12	0.67
1:A:173:GLU:OE1	1:A:300:ASN:ND2	2.27	0.67
1:B:210:ARG:O	1:B:214:VAL:HG13	1.93	0.67
1:A:226:ILE:H	1:A:294:ASN:HD22	1.43	0.67
1:B:427:TRP:C	1:B:429:GLU:H	2.03	0.66
1:B:462:ASN:HD22	1:B:462:ASN:H	1.41	0.66
1:B:300:ASN:OD1	1:B:371:GLU:HB2	1.96	0.66
1:B:402:MET:HE1	1:B:416:TYR:CD1	2.31	0.66
1:C:420:SER:O	1:C:436:GLY:HA2	1.95	0.66
1:A:225:GLY:CA	1:A:294:ASN:HB2	2.26	0.66
1:A:210:ARG:HG3	1:A:210:ARG:HH11	1.60	0.65
1:A:163:ASP:OD2	1:A:164:ARG:HG3	1.95	0.65
1:C:265:GLY:O	1:C:266:ASP:HB2	1.95	0.65
1:B:13:PHE:CZ	1:B:403:VAL:HG13	2.32	0.65
1:C:232:PHE:CE2	1:C:353:ASP:HB3	2.32	0.65
1:C:257:TRP:CD1	1:C:271:MET:HE1	2.32	0.65
1:C:392:ILE:HG22	1:C:452:SER:HA	1.79	0.65
1:C:352:ARG:NH1	1:C:409:ASP:OD2	2.29	0.65
1:B:253:PHE:HD1	1:B:271:MET:HE3	1.62	0.65
1:B:257:TRP:HB2	1:B:271:MET:SD	2.37	0.65
1:A:153:TYR:HE1	1:A:157:LEU:HD21	1.62	0.64
1:B:27:GLN:HB3	1:B:424:ASN:HD22	1.62	0.64
1:C:296:PHE:CD1	1:C:368:TYR:HD2	2.16	0.64
1:C:426:GLU:HA	1:C:426:GLU:OE1	1.96	0.64
1:B:29:GLU:HA	1:B:64:HIS:HB3	1.79	0.64
1:C:341:MET:HE2	1:C:435:PHE:HE1	1.63	0.64
1:C:225:GLY:HA2	1:C:294:ASN:HB2	1.79	0.63
1:A:255:THR:HG21	1:A:354:PHE:HZ	1.63	0.63
1:C:341:MET:HE2	1:C:435:PHE:CE1	2.33	0.63
1:A:283:THR:HG22	1:A:286:GLU:H	1.64	0.63
1:C:261:PRO:HA	1:C:266:ASP:H	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:PHE:CZ	1:A:403:VAL:HG22	2.34	0.62
1:A:153:TYR:CE1	1:A:157:LEU:HD21	2.35	0.62
1:A:421:LEU:HD23	1:A:422:LEU:HG	1.82	0.62
1:B:41:ILE:HG12	1:B:136:GLN:HG2	1.80	0.62
1:C:429:GLU:HG2	1:C:433:LYS:HE3	1.82	0.61
1:C:377:ASP:OD1	1:C:379:VAL:HG23	2.00	0.61
1:A:427:TRP:C	1:A:429:GLU:H	2.07	0.61
1:A:329:ASN:HD21	1:A:333:ASN:HB2	1.66	0.61
1:B:253:PHE:CD2	1:B:321:GLY:CA	2.84	0.60
1:B:352:ARG:NH1	1:B:409:ASP:OD2	2.34	0.60
1:C:362:TYR:O	1:C:365:PRO:HD3	2.01	0.60
1:B:329:ASN:OD1	1:B:331:GLN:N	2.35	0.60
1:B:375:ALA:HA	1:B:434:ARG:O	2.02	0.60
1:B:212:VAL:O	1:B:216:ARG:HG2	2.02	0.60
1:C:310:ARG:HD2	1:C:322:ASN:O	2.02	0.60
1:A:179:ILE:HB	1:A:180:PRO:HD3	1.84	0.59
1:A:252:GLU:HA	1:A:256:ALA:HB3	1.84	0.59
1:B:255:THR:HG21	1:B:354:PHE:HZ	1.67	0.59
1:C:239:ALA:O	1:C:241:PRO:HD3	2.03	0.59
1:C:392:ILE:O	1:C:396:LYS:HB2	2.03	0.59
1:B:432:SER:OG	1:B:433:LYS:HG2	2.02	0.59
1:C:388:ASP:OD2	1:C:452:SER:HB3	2.01	0.59
1:B:283:THR:HG22	1:B:283:THR:O	2.03	0.58
1:C:260:ASP:HB2	1:C:268:PRO:HD3	1.85	0.58
1:B:329:ASN:HD21	1:B:333:ASN:HB2	1.68	0.58
1:C:306:TYR:CE1	1:C:329:ASN:HB3	2.37	0.58
1:A:248:GLU:O	1:A:252:GLU:HG3	2.04	0.58
1:B:196:GLU:O	1:B:200:VAL:HG23	2.02	0.58
1:C:231:ASP:CB	1:C:303:THR:O	2.51	0.58
1:C:249:ARG:HA	1:C:252:GLU:OE1	2.03	0.58
1:C:146:ILE:C	1:C:148:ASP:H	2.12	0.58
1:A:225:GLY:HA2	1:A:294:ASN:CB	2.33	0.58
1:B:439:TYR:HB2	1:B:450:LYS:HE3	1.84	0.58
1:C:257:TRP:CG	1:C:271:MET:HE1	2.40	0.57
1:A:176:CYS:O	1:A:180:PRO:HD2	2.05	0.56
1:B:254:PHE:HB3	1:B:255:THR:HG22	1.87	0.56
1:B:186:THR:O	1:B:187:PHE:CD1	2.47	0.56
1:C:13:PHE:CE1	1:C:403:VAL:HG13	2.40	0.56
1:B:306:TYR:CE1	1:B:329:ASN:HB3	2.41	0.56
1:C:310:ARG:CD	1:C:322:ASN:O	2.54	0.56
1:A:18:LEU:HD23	1:A:82:ALA:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:PHE:HZ	1:B:369:VAL:HG21	1.71	0.56
1:C:79:GLY:O	1:C:460:VAL:HG11	2.05	0.56
1:A:210:ARG:HG3	1:A:210:ARG:NH1	2.18	0.56
1:C:303:THR:HG22	1:C:345:ARG:O	2.05	0.55
1:B:376:PHE:HD2	1:B:391:ARG:HH11	1.54	0.55
1:C:225:GLY:CA	1:C:294:ASN:HB2	2.36	0.55
1:C:260:ASP:HB2	1:C:261:PRO:HD3	1.88	0.55
1:C:115:LEU:O	1:C:120:ILE:HG13	2.07	0.55
1:B:257:TRP:CG	1:B:271:MET:HE1	2.42	0.55
1:C:299:MET:HE2	1:C:301:HIS:CB	2.36	0.55
1:C:335:ILE:O	1:C:335:ILE:CG2	2.54	0.55
1:C:348:ALA:HB2	1:C:397:ALA:HB1	1.88	0.54
1:B:82:ALA:HA	1:B:121:THR:O	2.07	0.54
1:B:353:ASP:OD1	1:C:352:ARG:NH2	2.38	0.54
1:C:352:ARG:O	1:C:355:LEU:N	2.39	0.54
1:A:101:ASN:OD1	1:A:103:LYS:N	2.40	0.54
1:A:28:ILE:HG22	1:A:424:ASN:HB3	1.87	0.54
1:B:45:PHE:O	1:B:51:ASN:ND2	2.41	0.54
1:C:27:GLN:O	1:C:425:PHE:HB3	2.08	0.54
1:A:193:SER:HB3	1:A:196:GLU:HB2	1.89	0.53
1:A:404:THR:HG23	1:A:408:LEU:HD12	1.90	0.53
1:C:256:ALA:HB1	1:C:260:ASP:OD1	2.08	0.53
1:A:83:TYR:CE2	1:A:85:PHE:HB3	2.44	0.53
1:C:299:MET:CE	1:C:301:HIS:HB2	2.37	0.53
1:A:302:TYR:C	1:A:303:THR:HG22	2.33	0.53
1:B:253:PHE:CE1	1:B:271:MET:HA	2.43	0.53
1:A:174:PRO:O	1:A:175:LEU:C	2.52	0.53
1:C:268:PRO:HB2	1:C:271:MET:HG3	1.89	0.53
1:A:68:TRP:O	1:A:72:ILE:HG13	2.09	0.53
1:B:202:HIS:ND1	1:B:280:PRO:HB2	2.24	0.53
1:C:208:HIS:C	1:C:208:HIS:CD2	2.85	0.53
1:A:302:TYR:C	1:A:303:THR:CG2	2.82	0.52
1:C:329:ASN:O	1:C:330:LYS:C	2.52	0.52
1:A:370:THR:O	1:A:371:GLU:HG3	2.09	0.52
1:B:253:PHE:CD2	1:B:321:GLY:HA2	2.45	0.52
1:C:260:ASP:HB2	1:C:261:PRO:CD	2.40	0.52
1:A:404:THR:CG2	1:A:408:LEU:HD12	2.40	0.52
1:C:242:ALA:O	1:C:246:ALA:N	2.43	0.52
1:B:44:THR:HG22	1:B:45:PHE:N	2.23	0.52
1:C:265:GLY:O	1:C:266:ASP:CB	2.57	0.52
1:C:427:TRP:O	1:C:429:GLU:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:ASN:O	1:C:331:GLN:N	2.44	0.51
1:A:352:ARG:NH1	1:A:409:ASP:OD2	2.42	0.51
1:B:263:TYR:HB2	1:B:362:TYR:HD1	1.75	0.51
1:B:303:THR:CG2	1:B:345:ARG:N	2.68	0.51
1:C:254:PHE:HD1	1:C:254:PHE:O	1.93	0.51
1:A:359:SER:HB3	1:A:364:TYR:CE2	2.46	0.51
1:C:198:TRP:CH2	1:C:319:THR:HG22	2.46	0.51
1:B:351:PHE:O	1:B:355:LEU:HD12	2.12	0.50
1:C:275:LEU:HA	1:C:278:ARG:HH21	1.76	0.50
1:B:427:TRP:C	1:B:429:GLU:N	2.69	0.50
1:C:237:ASP:OD1	1:C:239:ALA:HB3	2.11	0.50
1:A:417:PHE:N	1:A:417:PHE:CD1	2.80	0.50
1:A:456:TYR:O	1:A:460:VAL:HG23	2.11	0.50
1:C:185:GLY:HA3	1:C:192:GLN:HG2	1.94	0.50
1:B:141:LEU:O	1:B:200:VAL:HG13	2.12	0.50
1:B:168:TRP:O	1:B:224:ILE:HA	2.11	0.50
1:C:429:GLU:HG2	1:C:433:LYS:CE	2.42	0.50
1:C:337:PRO:O	1:C:346:PRO:HD2	2.11	0.49
1:B:84:ARG:NH2	1:B:172:ASN:HD22	2.08	0.49
1:C:306:TYR:CZ	1:C:329:ASN:HB3	2.47	0.49
1:A:441:ASP:OD1	1:A:443:SER:HB2	2.12	0.49
1:C:183:GLY:O	1:C:192:GLN:HA	2.11	0.49
1:B:27:GLN:O	1:B:424:ASN:HB2	2.12	0.49
1:B:334:CYS:SG	1:B:335:ILE:N	2.84	0.49
1:C:89:TRP:N	1:C:90:PRO:HD2	2.28	0.49
1:A:210:ARG:O	1:A:214:VAL:HG13	2.13	0.49
1:B:253:PHE:CE2	1:B:321:GLY:CA	2.94	0.49
1:B:329:ASN:OD1	1:B:329:ASN:C	2.56	0.49
1:C:392:ILE:CG2	1:C:452:SER:HA	2.42	0.49
1:B:303:THR:CG2	1:B:345:ARG:O	2.51	0.49
1:C:193:SER:OG	1:C:196:GLU:HB2	2.12	0.49
1:A:62:CYS:SG	1:A:423:ASP:O	2.71	0.49
1:B:394:TYR:HD1	1:B:395:LEU:HD23	1.78	0.48
1:C:328:THR:HA	1:C:333:ASN:O	2.13	0.48
1:A:257:TRP:CG	1:A:271:MET:HE1	2.47	0.48
1:A:436:GLY:O	1:A:450:LYS:HD2	2.13	0.48
1:C:14:PRO:HD2	1:C:17:PHE:HB2	1.95	0.48
1:A:18:LEU:HD23	1:A:82:ALA:CB	2.44	0.48
1:B:297:TYR:CD1	1:B:297:TYR:C	2.91	0.48
1:C:226:ILE:H	1:C:294:ASN:HD22	1.61	0.48
1:A:359:SER:HB3	1:A:364:TYR:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:ASN:ND2	1:B:333:ASN:HB2	2.29	0.48
1:B:156:VAL:O	1:B:160:ASN:HB2	2.13	0.48
1:B:176:CYS:HA	1:B:180:PRO:HG2	1.96	0.48
1:B:299:MET:O	1:B:370:THR:N	2.46	0.48
1:B:303:THR:CG2	1:B:345:ARG:H	2.12	0.48
1:A:230:GLY:HA2	1:A:254:PHE:CE1	2.49	0.48
1:A:94:PRO:C	1:A:96:GLY:H	2.20	0.47
1:A:206:VAL:HG11	1:A:286:GLU:HG2	1.95	0.47
1:B:283:THR:O	1:B:284:PRO:C	2.57	0.47
1:B:406:VAL:O	1:B:410:GLY:HA2	2.14	0.47
1:B:253:PHE:CD2	1:B:321:GLY:HA3	2.49	0.47
1:B:238:ALA:HB1	1:C:364:TYR:OH	2.14	0.47
1:C:261:PRO:HA	1:C:266:ASP:N	2.28	0.47
1:A:70:GLU:O	1:A:73:GLU:HB2	2.15	0.47
1:B:88:SER:O	1:B:91:ARG:HB2	2.14	0.47
1:B:399:ILE:HA	1:B:402:MET:HE2	1.95	0.47
1:C:282:PHE:CB	1:C:286:GLU:OE1	2.62	0.47
1:C:433:LYS:HA	1:C:433:LYS:HD3	1.73	0.47
1:C:203:ASN:HA	1:C:206:VAL:CG2	2.45	0.47
1:C:354:PHE:O	1:C:357:TRP:N	2.47	0.47
1:C:405:ALA:HB1	1:C:411:VAL:CG2	2.44	0.47
1:A:175:LEU:C	1:A:175:LEU:HD23	2.40	0.47
1:A:283:THR:HB	1:A:286:GLU:HB2	1.96	0.47
1:A:427:TRP:O	1:A:429:GLU:N	2.47	0.47
1:B:39:MET:HB3	1:B:39:MET:HE2	1.31	0.47
1:B:265:GLY:O	1:B:287:ARG:NH1	2.48	0.47
1:A:347:CYS:O	1:A:347:CYS:SG	2.72	0.46
1:A:403:VAL:HG12	1:A:407:GLU:HG3	1.96	0.46
1:A:142:LEU:HD11	1:A:196:GLU:HG2	1.97	0.46
1:A:254:PHE:HB3	1:A:255:THR:HG22	1.96	0.46
1:B:328:THR:HG22	1:B:334:CYS:HA	1.96	0.46
1:B:378:ASP:OD2	1:B:450:LYS:HE2	2.15	0.46
1:B:183:GLY:O	1:B:192:GLN:HG2	2.15	0.46
1:C:29:GLU:HA	1:C:64:HIS:HB3	1.97	0.46
1:C:253:PHE:CD2	1:C:321:GLY:HA3	2.50	0.46
1:A:29:GLU:HA	1:A:64:HIS:HB3	1.97	0.46
1:C:272:ARG:NH1	1:C:280:PRO:O	2.40	0.46
1:A:25:SER:HB3	1:A:86:SER:HB2	1.97	0.46
1:C:303:THR:HG21	1:C:345:ARG:N	2.29	0.46
1:C:372:ASN:HD22	1:C:416:TYR:HE1	1.64	0.46
1:B:420:SER:OG	1:B:421:LEU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLU:C	1:A:97:THR:H	2.24	0.46
1:A:145:GLU:HB3	1:A:149:TRP:CZ2	2.51	0.46
1:B:47:HIS:HE2	1:B:59:ASP:CG	2.24	0.46
1:B:352:ARG:HH22	1:C:353:ASP:CG	2.24	0.45
1:C:88:SER:O	1:C:89:TRP:C	2.58	0.45
1:A:67:ARG:CZ	1:A:445:GLN:HB2	2.46	0.45
1:B:47:HIS:CE1	1:B:59:ASP:OD2	2.69	0.45
1:B:260:ASP:HB2	1:B:268:PRO:HD3	1.98	0.45
1:A:452:SER:HA	1:A:455:TRP:HB3	1.98	0.45
1:B:229:ASN:C	1:B:229:ASN:HD22	2.25	0.45
1:B:257:TRP:O	1:B:257:TRP:CD1	2.69	0.45
1:C:42:TRP:CH2	1:C:427:TRP:HB3	2.52	0.45
1:C:234:TYR:OH	1:C:353:ASP:OD2	2.28	0.45
1:B:196:GLU:O	1:B:197:PRO:C	2.57	0.45
1:B:229:ASN:C	1:B:229:ASN:ND2	2.75	0.45
1:C:352:ARG:HG2	1:C:353:ASP:N	2.31	0.45
1:A:27:GLN:HB3	1:A:424:ASN:HB2	1.99	0.45
1:A:68:TRP:H	1:A:68:TRP:CD1	2.33	0.45
1:B:143:ASN:OD1	1:B:143:ASN:C	2.59	0.45
1:B:332:GLY:O	1:B:333:ASN:C	2.60	0.45
1:C:13:PHE:HB2	1:C:463:ASN:OD1	2.17	0.45
1:C:337:PRO:HG2	1:C:346:PRO:CG	2.47	0.45
1:B:260:ASP:HB3	1:B:266:ASP:O	2.17	0.45
1:A:394:TYR:HD1	1:A:395:LEU:HD23	1.81	0.44
1:A:30:GLY:HA3	1:A:60:VAL:O	2.17	0.44
1:A:31:SER:N	1:A:59:ASP:O	2.46	0.44
1:B:44:THR:O	1:B:48:THR:CG2	2.63	0.44
1:B:253:PHE:CD1	1:B:271:MET:HE3	2.48	0.44
1:C:457:SER:O	1:C:461:LYS:HG3	2.17	0.44
1:B:308:ARG:HG2	1:B:324:ASP:OD2	2.17	0.44
1:C:440:VAL:HG12	1:C:442:TYR:CE1	2.53	0.44
1:C:381:SER:OG	1:C:383:ASP:OD1	2.36	0.44
1:A:427:TRP:C	1:A:429:GLU:N	2.73	0.44
1:B:390:ASN:OD1	1:B:390:ASN:N	2.48	0.44
1:C:146:ILE:C	1:C:148:ASP:N	2.75	0.44
1:C:300:ASN:HD22	1:C:302:TYR:HE2	1.66	0.44
1:B:283:THR:HG23	1:B:285:GLU:H	1.82	0.44
1:C:303:THR:CG2	1:C:345:ARG:O	2.66	0.44
1:C:405:ALA:HB1	1:C:411:VAL:HG21	1.99	0.44
1:A:246:ALA:HB1	1:A:323:VAL:HG12	2.00	0.44
1:B:27:GLN:HA	1:B:425:PHE:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:THR:O	1:C:278:ARG:HD2	2.17	0.44
1:C:261:PRO:O	1:C:265:GLY:N	2.48	0.44
1:A:168:TRP:O	1:A:224:ILE:HA	2.18	0.43
1:A:206:VAL:CG1	1:A:286:GLU:HG2	2.48	0.43
1:B:96:GLY:HA3	1:B:135:LEU:CD2	2.40	0.43
1:C:40:SER:HA	1:C:131:LEU:O	2.18	0.43
1:C:249:ARG:O	1:C:250:ARG:C	2.59	0.43
1:C:397:ALA:O	1:C:401:ALA:N	2.48	0.43
1:B:427:TRP:O	1:B:429:GLU:N	2.52	0.43
1:B:456:TYR:O	1:B:457:SER:C	2.62	0.43
1:B:86:SER:HB2	1:B:128:HIS:HB2	2.01	0.43
1:B:63:ASP:CG	1:B:63:ASP:O	2.60	0.43
1:B:339:THR:HB	1:B:375:ALA:O	2.19	0.43
1:A:23:THR:HB	1:A:28:ILE:HD13	1.99	0.43
1:B:230:GLY:HA2	1:B:254:PHE:CZ	2.54	0.43
1:B:419:TRP:HA	1:B:420:SER:HA	1.82	0.43
1:A:27:GLN:HA	1:A:425:PHE:HB3	2.00	0.43
1:B:260:ASP:O	1:B:261:PRO:C	2.60	0.43
1:B:383:ASP:OD2	1:B:387:HIS:NE2	2.49	0.43
1:B:162:GLY:O	1:B:163:ASP:C	2.62	0.43
1:B:403:VAL:O	1:B:407:GLU:N	2.37	0.43
1:A:343:TRP:CE3	1:A:344:LEU:HB2	2.54	0.43
1:B:341:MET:HE2	1:B:433:LYS:HD2	2.01	0.43
1:C:243:ASP:HA	1:C:246:ALA:HB3	2.00	0.43
1:C:352:ARG:HB2	1:C:401:ALA:O	2.19	0.43
1:B:237:ASP:OD2	1:B:239:ALA:HB3	2.19	0.42
1:A:114:THR:O	1:A:115:LEU:C	2.62	0.42
1:B:193:SER:C	1:B:195:SER:H	2.27	0.42
1:B:229:ASN:HD22	1:B:230:GLY:N	2.17	0.42
1:C:283:THR:HG23	1:C:286:GLU:OE2	2.18	0.42
1:A:429:GLU:HG3	1:A:433:LYS:HG3	2.01	0.42
1:A:173:GLU:HG2	1:A:229:ASN:ND2	2.33	0.42
1:A:439:TYR:N	1:A:450:LYS:HG3	2.34	0.42
1:B:41:ILE:O	1:B:44:THR:HB	2.20	0.42
1:B:426:GLU:O	1:B:429:GLU:CB	2.67	0.42
1:C:231:ASP:O	1:C:354:PHE:HE2	2.02	0.42
1:C:306:TYR:CD1	1:C:329:ASN:HB3	2.53	0.42
1:C:337:PRO:HG2	1:C:346:PRO:HG3	2.02	0.42
1:A:335:ILE:HD13	1:A:335:ILE:HA	1.74	0.42
1:C:88:SER:C	1:C:90:PRO:HD2	2.44	0.42
1:C:174:PRO:HB3	1:C:204:ILE:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:TYR:C	1:A:297:TYR:CD2	2.97	0.42
1:B:41:ILE:HD12	1:B:188:ALA:HB1	2.02	0.42
1:C:169:ILE:HG22	1:C:170:THR:N	2.35	0.42
1:C:232:PHE:CG	1:C:233:THR:N	2.88	0.42
1:C:249:ARG:O	1:C:252:GLU:N	2.53	0.42
1:C:236:TRP:N	1:C:307:ILE:O	2.40	0.42
1:A:101:ASN:OD1	1:A:101:ASN:C	2.62	0.42
1:A:240:ASP:HA	1:A:241:PRO:HD3	1.83	0.42
1:C:25:SER:O	1:C:29:GLU:N	2.52	0.42
1:C:427:TRP:C	1:C:429:GLU:H	2.27	0.42
1:B:47:HIS:NE2	1:B:59:ASP:OD2	2.53	0.42
1:C:46:SER:HB2	1:C:57:THR:HA	2.01	0.42
1:C:416:TYR:O	1:C:416:TYR:CD2	2.73	0.42
1:A:17:PHE:HE1	1:A:413:VAL:HG12	1.85	0.41
1:B:243:ASP:C	1:B:245:GLU:N	2.78	0.41
1:A:440:VAL:HG22	1:A:447:ARG:HD3	2.02	0.41
1:B:234:TYR:O	1:B:306:TYR:HA	2.20	0.41
1:B:376:PHE:HD2	1:B:391:ARG:NH1	2.18	0.41
1:C:405:ALA:C	1:C:411:VAL:HG22	2.45	0.41
1:C:419:TRP:HA	1:C:420:SER:HA	1.70	0.41
1:A:164:ARG:HG3	1:A:164:ARG:HH11	1.85	0.41
1:A:420:SER:O	1:A:436:GLY:HA2	2.20	0.41
1:B:422:LEU:C	1:B:423:ASP:O	2.61	0.41
1:C:54:ASN:C	1:C:56:ASP:N	2.79	0.41
1:C:175:LEU:C	1:C:177:SER:H	2.29	0.41
1:C:341:MET:HA	1:C:342:PRO:HD3	1.89	0.41
1:B:252:GLU:HA	1:B:256:ALA:HB3	2.03	0.41
1:B:429:GLU:HG2	1:B:433:LYS:HG3	2.02	0.41
1:C:422:LEU:O	1:C:423:ASP:C	2.63	0.41
1:A:46:SER:HB2	1:A:57:THR:HA	2.01	0.41
1:A:246:ALA:HB1	1:A:323:VAL:CG1	2.51	0.41
1:C:431:TYR:C	1:C:433:LYS:H	2.29	0.41
1:B:299:MET:HE3	1:B:369:VAL:HG22	2.02	0.41
1:B:359:SER:HB3	1:B:364:TYR:CD2	2.56	0.41
1:B:399:ILE:HG23	1:B:402:MET:CE	2.51	0.41
1:C:224:ILE:O	1:C:295:ASP:HB2	2.21	0.41
1:C:279:LEU:HA	1:C:280:PRO:HD3	1.75	0.41
1:A:48:THR:HG23	1:A:49:PRO:HD2	2.02	0.41
1:A:21:VAL:HG21	1:A:421:LEU:HD13	2.03	0.40
1:A:260:ASP:O	1:A:261:PRO:C	2.61	0.40
1:B:283:THR:O	1:B:286:GLU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:PRO:HG2	1:B:346:PRO:HD2	2.03	0.40
1:B:389:GLN:O	1:B:392:ILE:N	2.55	0.40
1:A:144:ARG:HG3	1:A:144:ARG:HH11	1.87	0.40
1:A:375:ALA:HA	1:A:434:ARG:O	2.21	0.40
1:A:388:ASP:OD1	1:A:388:ASP:N	2.54	0.40
1:C:324:ASP:O	1:C:325:VAL:C	2.64	0.40
1:B:13:PHE:HB3	1:B:14:PRO:HD2	2.02	0.40
1:C:329:ASN:O	1:C:329:ASN:OD1	2.39	0.40
1:A:343:TRP:CZ3	1:A:344:LEU:HB2	2.57	0.40
1:A:25:SER:OG	1:A:26:TYR:N	2.55	0.40
1:A:161:PHE:O	1:A:162:GLY:C	2.64	0.40
1:A:329:ASN:ND2	1:A:333:ASN:HB2	2.34	0.40
1:B:465:LEU:O	1:B:466:GLU:C	2.64	0.40
1:C:154:SER:O	1:C:155:ARG:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	454/467 (97%)	393 (87%)	56 (12%)	5 (1%)	11	43
1	B	454/467 (97%)	390 (86%)	48 (11%)	16 (4%)	3	16
1	C	446/467 (96%)	338 (76%)	88 (20%)	20 (4%)	2	12
All	All	1354/1401 (97%)	1121 (83%)	192 (14%)	41 (3%)	3	19

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	LYS
1	B	445	GLN
1	B	462	ASN

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Mol	Chain	Res	Type
1	C	35	ASP
1	C	266	ASP
1	C	270	SER
1	C	428	ALA
1	B	53	LYS
1	C	276	GLY
1	C	330	LYS
1	C	333	ASN
1	A	25	SER
1	A	53	LYS
1	A	170	THR
1	B	122	PRO
1	B	161	PHE
1	B	163	ASP
1	B	213	LYS
1	B	244	LYS
1	B	421	LEU
1	C	147	ALA
1	C	165	VAL
1	C	337	PRO
1	C	427	TRP
1	A	432	SER
1	B	25	SER
1	B	141	LEU
1	C	19	TRP
1	C	154	SER
1	C	372	ASN
1	B	44	THR
1	B	110	ARG
1	B	134	ALA
1	B	149	TRP
1	C	370	THR
1	C	411	VAL
1	C	423	ASP
1	B	140	GLY
1	C	13	PHE
1	C	284	PRO
1	C	358	ILE

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	321/391 (82%)	287 (89%)	34 (11%)	6	27
1	B	268/391 (68%)	233 (87%)	35 (13%)	4	19
1	C	232/391 (59%)	202 (87%)	30 (13%)	4	19
All	All	821/1173 (70%)	722 (88%)	99 (12%)	5	21

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	41	ILE
1	A	97	THR
1	A	112	ILE
1	A	125	THR
1	A	130	ASP
1	A	141	LEU
1	A	142	LEU
1	A	191	ARG
1	A	194	THR
1	A	195	SER
1	A	210	ARG
1	A	214	VAL
1	A	216	ARG
1	A	219	VAL
1	A	221	ASP
1	A	223	LYS
1	A	227	VAL
1	A	248	GLU
1	A	255	THR
1	A	273	LYS
1	A	281	THR
1	A	303	THR
1	A	308	ARG
1	A	311	SER
1	A	320	VAL

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Mol	Chain	Res	Type
1	A	335	ILE
1	A	338	GLU
1	A	347	CYS
1	A	411	VAL
1	A	417	PHE
1	A	429	GLU
1	A	444	THR
1	A	457	SER
1	B	28	ILE
1	B	31	SER
1	B	41	ILE
1	B	44	THR
1	B	48	THR
1	B	49	PRO
1	B	51	ASN
1	B	60	VAL
1	B	124	VAL
1	B	125	THR
1	B	136	GLN
1	B	155	ARG
1	B	160	ASN
1	B	170	THR
1	B	191	ARG
1	B	206	VAL
1	B	214	VAL
1	B	229	ASN
1	B	237	ASP
1	B	248	GLU
1	B	252	GLU
1	B	255	THR
1	B	273	LYS
1	B	283	THR
1	B	303	THR
1	B	308	ARG
1	B	326	LEU
1	B	335	ILE
1	B	352	ARG
1	B	359	SER
1	B	391	ARG
1	B	411	VAL
1	B	443	SER
1	B	457	SER

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Mol	Chain	Res	Type
1	B	462	ASN
1	C	25	SER
1	C	120	ILE
1	C	125	THR
1	C	129	TRP
1	C	191	ARG
1	C	206	VAL
1	C	208	HIS
1	C	219	VAL
1	C	227	VAL
1	C	237	ASP
1	C	248	GLU
1	C	283	THR
1	C	286	GLU
1	C	300	ASN
1	C	307	ILE
1	C	310	ARG
1	C	319	THR
1	C	324	ASP
1	C	338	GLU
1	C	341	MET
1	C	352	ARG
1	C	361	ARG
1	C	395	LEU
1	C	403	VAL
1	C	411	VAL
1	C	440	VAL
1	C	445	GLN
1	C	448	ILE
1	C	451	ASP
1	C	457	SER

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	27	GLN
1	A	43	HIS
1	A	128	HIS
1	A	291	HIS
1	A	294	ASN
1	A	305	ASN
1	A	458	ASN

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Mol	Chain	Res	Type
1	B	128	HIS
1	B	136	GLN
1	B	172	ASN
1	B	229	ASN
1	B	294	ASN
1	B	300	ASN
1	B	305	ASN
1	B	372	ASN
1	B	412	ASN
1	B	424	ASN
1	B	462	ASN
1	C	43	HIS
1	C	64	HIS
1	C	172	ASN
1	C	202	HIS
1	C	294	ASN
1	C	300	ASN
1	C	372	ASN
1	C	412	ASN
1	C	462	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	456/467 (97%)	0.34	9 (1%) 65 41	93, 112, 124, 136	6 (1%)
1	B	456/467 (97%)	0.15	3 (0%) 84 66	94, 112, 129, 150	2 (0%)
1	C	454/467 (97%)	0.52	32 (7%) 22 12	94, 171, 225, 249	1 (0%)
All	All	1366/1401 (97%)	0.33	44 (3%) 50 29	93, 116, 208, 249	9 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	130	ASP	6.6
1	C	26	TYR	5.3
1	C	82	ALA	3.8
1	B	323	VAL	3.3
1	A	437	ILE	3.1
1	A	71	ASP	3.0
1	C	65	TYR	3.0
1	C	56	ASP	3.0
1	A	126	ILE	2.9
1	C	444	THR	2.9
1	C	428	ALA	2.8
1	C	97	THR	2.8
1	C	287	ARG	2.7
1	C	390	ASN	2.7
1	C	424	ASN	2.7
1	C	218	THR	2.6
1	C	24	ALA	2.6
1	C	168	TRP	2.5
1	C	136	GLN	2.5
1	A	314	ALA	2.5
1	A	429	GLU	2.5
1	C	376	PHE	2.5
1	C	442	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	127	PHE	2.4
1	C	57	THR	2.4
1	C	88	SER	2.4
1	C	137	LEU	2.4
1	C	154	SER	2.4
1	C	21	VAL	2.4
1	C	131	LEU	2.3
1	C	158	PHE	2.3
1	C	54	ASN	2.3
1	C	64	HIS	2.3
1	A	303	THR	2.2
1	B	39	MET	2.2
1	C	59	ASP	2.2
1	A	226	ILE	2.2
1	C	440	VAL	2.2
1	B	228	LEU	2.2
1	C	294	ASN	2.1
1	A	335	ILE	2.1
1	A	377	ASP	2.0
1	C	86	SER	2.0
1	C	87	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.