



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:39 AM UTC

PDB ID : 5GGF / pdb_00005ggf
Title : Crystal structure of human protein O-mannose beta-1,2-N-acetylglucosaminyltransferase form II
Authors : Kuwabara, N.; Senda, T.; Kato, R.
Deposited on : 2016-06-15
Resolution : 2.49 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)	:	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

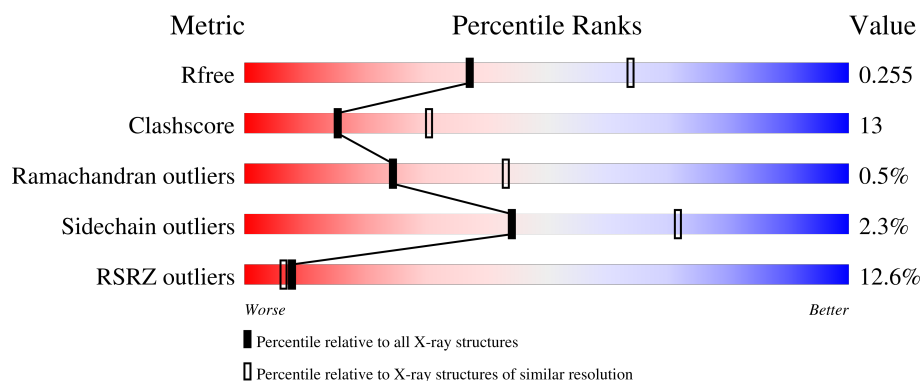
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	578	4% 73% 18% • 7%
1	B	578	22% 64% 26% •• 7%
1	C	578	9% 70% 21% • 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12790 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protein O-linked-mannose beta-1,2-N-acetylglucosaminyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	0	0
			4263	2723	737	783	20			
1	B	536	Total	C	N	O	S	0	2	0
			4244	2712	731	781	20			
1	C	536	Total	C	N	O	S	0	1	0
			4268	2726	736	786	20			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	623	VAL	MET	variant	UNP Q8WZA1
A	661	LEU	-	expression tag	UNP Q8WZA1
A	662	GLU	-	expression tag	UNP Q8WZA1
A	663	LEU	-	expression tag	UNP Q8WZA1
A	664	GLU	-	expression tag	UNP Q8WZA1
A	665	VAL	-	expression tag	UNP Q8WZA1
A	666	LEU	-	expression tag	UNP Q8WZA1
A	667	PHE	-	expression tag	UNP Q8WZA1
A	668	GLN	-	expression tag	UNP Q8WZA1
A	669	GLY	-	expression tag	UNP Q8WZA1
B	623	VAL	MET	variant	UNP Q8WZA1
B	661	LEU	-	expression tag	UNP Q8WZA1
B	662	GLU	-	expression tag	UNP Q8WZA1
B	663	LEU	-	expression tag	UNP Q8WZA1
B	664	GLU	-	expression tag	UNP Q8WZA1
B	665	VAL	-	expression tag	UNP Q8WZA1
B	666	LEU	-	expression tag	UNP Q8WZA1
B	667	PHE	-	expression tag	UNP Q8WZA1
B	668	GLN	-	expression tag	UNP Q8WZA1
B	669	GLY	-	expression tag	UNP Q8WZA1
C	623	VAL	MET	variant	UNP Q8WZA1
C	661	LEU	-	expression tag	UNP Q8WZA1

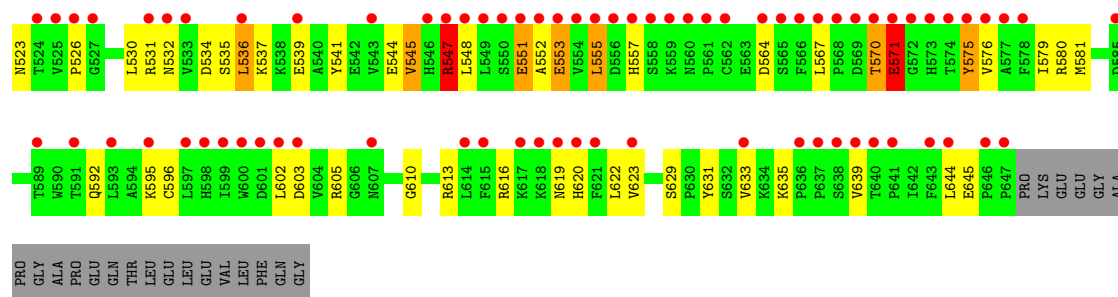
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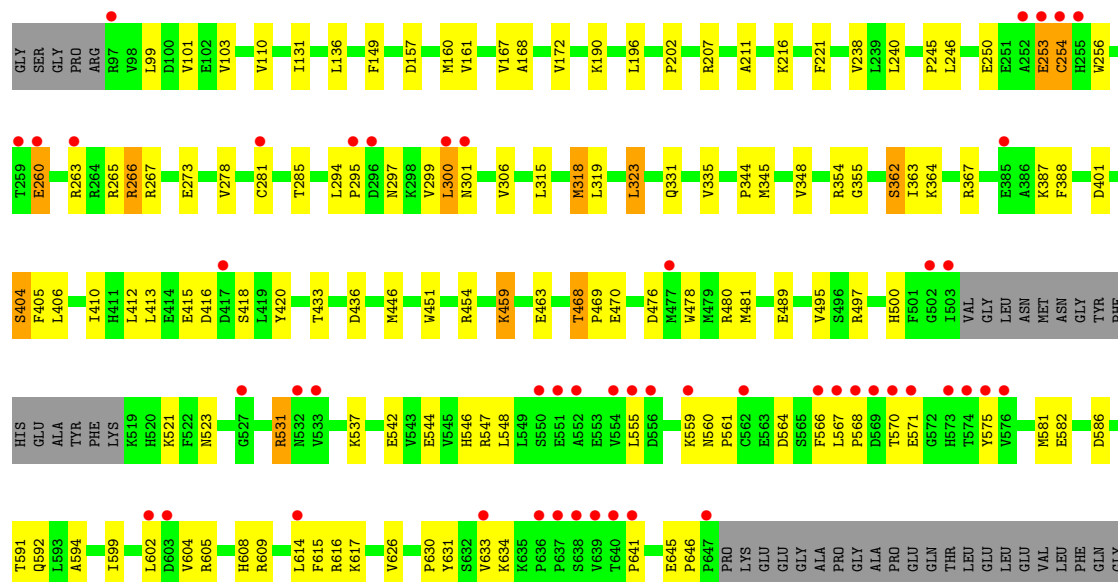
Chain	Residue	Modelled	Actual	Comment	Reference
C	662	GLU	-	expression tag	UNP Q8WZA1
C	663	LEU	-	expression tag	UNP Q8WZA1
C	664	GLU	-	expression tag	UNP Q8WZA1
C	665	VAL	-	expression tag	UNP Q8WZA1
C	666	LEU	-	expression tag	UNP Q8WZA1
C	667	PHE	-	expression tag	UNP Q8WZA1
C	668	GLN	-	expression tag	UNP Q8WZA1
C	669	GLY	-	expression tag	UNP Q8WZA1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	6	Total O 6 6	0	0
2	B	6	Total O 6 6	0	0
2	C	3	Total O 3 3	0	0



- Molecule 1: Protein O-linked-mannose beta-1,2-N-acetylglucosaminyltransferase 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	168.69Å 186.44Å 143.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.61 – 2.49 46.61 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.61-2.49) 92.6 (46.61-2.49)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.48Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.233 , 0.253 0.236 , 0.255	Depositor DCC
R_{free} test set	2000 reflections (2.52%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12790	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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	0.75	4/4379 (0.1%)	0.61	0/5955
1	B	0.65	1/4365 (0.0%)	0.75	13/5942 (0.2%)
1	C	0.61	1/4388 (0.0%)	0.63	2/5971 (0.0%)
All	All	0.67	6/13132 (0.0%)	0.67	15/17868 (0.1%)

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
1	B	0	5
1	C	0	1
All	All	0	7

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	547	ARG	NE-CZ	-15.04	1.16	1.33
1	A	547	ARG	CD-NE	-12.66	1.28	1.46
1	A	547	ARG	CZ-NH2	-12.00	1.17	1.33
1	A	547	ARG	CZ-NH1	-10.69	1.17	1.32
1	C	253	GLU	CB-CG	-6.23	1.33	1.52
1	B	547	ARG	CD-NE	5.49	1.53	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	547	ARG	CA-CB-CG	11.32	136.73	114.10
1	B	547	ARG	CG-CD-NE	-9.49	91.12	112.00
1	B	551	GLU	CG-CD-OE2	-8.55	98.73	118.40
1	B	250	GLU	N-CA-CB	-6.46	99.52	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	551	GLU	OE1-CD-OE2	5.90	137.07	122.90
1	B	251	GLU	CA-CB-CG	5.83	125.75	114.10
1	B	249	ALA	N-CA-C	-5.65	97.71	108.17
1	B	575	TYR	CA-CB-CG	-5.64	103.75	113.90
1	C	266	ARG	NE-CZ-NH1	-5.64	115.86	121.50
1	B	547	ARG	CB-CA-C	5.40	121.17	110.42
1	B	250	GLU	CA-C-N	5.32	131.28	121.70
1	B	250	GLU	C-N-CA	5.32	131.28	121.70
1	C	254	CYS	CA-CB-SG	-5.16	102.52	114.40
1	B	362	SER	CA-C-N	5.03	130.75	121.70
1	B	362	SER	C-N-CA	5.03	130.75	121.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	260	GLU	Peptide
1	B	249	ALA	Peptide
1	B	251	GLU	Peptide
1	B	361	ILE	Peptide
1	B	571	GLU	Peptide
1	B	619	ASN	Peptide
1	C	260	GLU	Peptide

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	4263	0	4160	93	0
1	B	4244	0	4117	143	0
1	C	4268	0	4151	106	0
2	A	6	0	0	1	0
2	B	6	0	0	0	0
2	C	3	0	0	0	0
All	All	12790	0	12428	339	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 13.

All (339) 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:547:ARG:HH21	1:B:548:LEU:HA	1.17	1.06
1:B:603:ASP:HB2	1:B:605:ARG:HE	1.31	0.96
1:C:260:GLU:HB3	1:C:263:ARG:HE	1.29	0.95
1:C:253:GLU:HG3	1:C:266:ARG:HH12	1.31	0.94
1:B:250:GLU:HG2	1:B:251:GLU:HA	1.50	0.90
1:B:329:SER:OG	1:B:331:GLN:NE2	2.05	0.90
1:B:97:ARG:NH1	1:B:247:SER:O	2.07	0.88
1:B:547:ARG:HH22	1:B:551:GLU:HB2	1.40	0.87
1:C:253:GLU:CG	1:C:266:ARG:HH12	1.87	0.86
1:B:281:CYS:SG	1:B:282:LYS:N	2.45	0.86
1:B:551:GLU:OE1	1:B:551:GLU:N	2.11	0.83
1:C:131:ILE:HD12	1:C:160:MET:HE1	1.62	0.82
1:C:413:LEU:O	1:C:454:ARG:NH1	2.13	0.81
1:B:102:GLU:OE1	1:B:241:LYS:NZ	2.13	0.80
1:B:294:LEU:HD23	1:B:297:ASN:HB2	1.64	0.80
1:A:306:VAL:HG13	1:A:318:MET:HE1	1.62	0.79
1:B:144:MET:HE1	1:B:171:ARG:HD3	1.63	0.79
1:B:292:ASP:OD1	1:C:301:ASN:ND2	2.16	0.79
1:C:436:ASP:OD2	1:C:531:ARG:NH1	2.16	0.79
1:C:468:THR:HG22	1:C:470:GLU:H	1.48	0.78
1:B:408:GLN:HE22	1:B:530:LEU:H	1.32	0.78
1:B:555:LEU:N	1:B:575:TYR:OH	2.17	0.77
1:B:250:GLU:OE2	1:B:255:HIS:NE2	2.18	0.77
1:A:103:VAL:HG23	1:A:211:ALA:HB1	1.66	0.76
1:A:158:GLU:OE1	1:A:186:LYS:NZ	2.14	0.76
1:A:260:GLU:CD	1:A:263:ARG:HH11	1.92	0.76
1:C:633:VAL:HG23	1:C:634:LYS:HD2	1.68	0.76
1:B:413:LEU:O	1:B:454:ARG:NH1	2.19	0.75
1:C:294:LEU:HB3	1:C:297:ASN:HD22	1.52	0.75
1:C:415:GLU:OE1	1:C:537:LYS:NZ	2.20	0.74
1:B:495:VAL:O	1:B:497:ARG:NH1	2.20	0.74
1:B:425:TRP:CH2	1:B:520:HIS:HD2	2.05	0.73
1:C:103:VAL:HG23	1:C:211:ALA:HB1	1.72	0.71
1:B:436:ASP:OD2	1:B:531:ARG:NH1	2.24	0.71
1:B:297:ASN:HB3	1:B:300:LEU:HD11	1.72	0.69
1:A:317:ARG:NH2	1:A:397:ASP:OD2	2.20	0.69
1:B:362:SER:HA	1:B:367:ARG:HB2	1.75	0.69
1:B:144:MET:CE	1:B:171:ARG:HD3	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:THR:HG23	1:B:262:ASN:H	1.58	0.68
1:B:465:LYS:NZ	1:B:484:GLN:HE21	1.92	0.68
1:B:411:HIS:NE2	1:B:534:ASP:OD1	2.20	0.67
1:A:599:ILE:HG22	1:A:600:TRP:H	1.58	0.67
1:B:555:LEU:HB2	1:B:575:TYR:OH	1.94	0.67
1:A:106:SER:HB3	1:A:109:LYS:O	1.96	0.66
1:C:331:GLN:O	1:C:354:ARG:NH2	2.27	0.66
1:A:645:GLU:HG2	1:A:646:PRO:HD2	1.77	0.66
1:C:478:TRP:HA	1:C:481:MET:HE2	1.78	0.66
1:B:581:MET:HE1	1:B:610:GLY:HA2	1.76	0.65
1:C:335:VAL:HG21	1:C:348:VAL:HG21	1.77	0.65
1:B:425:TRP:CH2	1:B:520:HIS:CD2	2.85	0.65
1:B:98:VAL:HG11	1:B:243:ASP:HB3	1.79	0.64
1:B:526:PRO:HG2	1:C:300:LEU:HG	1.79	0.64
1:C:335:VAL:HG21	1:C:348:VAL:CG2	2.27	0.64
1:A:306:VAL:CG1	1:A:318:MET:HE1	2.28	0.64
1:B:415:GLU:OE1	1:B:537:LYS:NZ	2.19	0.63
1:A:362:SER:HB3	1:A:363:ILE:HG22	1.79	0.63
1:A:589:THR:HG23	1:A:644:LEU:HD23	1.80	0.63
1:B:137:ASN:HD22	1:B:140:THR:H	1.47	0.63
1:B:103:VAL:HG23	1:B:211:ALA:HB1	1.81	0.63
1:C:167:VAL:O	1:C:216:LYS:NZ	2.30	0.63
1:C:253:GLU:HG3	1:C:266:ARG:NH1	2.09	0.62
1:B:289:PHE:O	1:B:291:PRO:HD3	1.99	0.62
1:A:555:LEU:HD21	1:A:575:TYR:HB3	1.80	0.62
1:C:614:LEU:HD12	1:C:615:PHE:N	2.15	0.62
1:C:265:ARG:NH1	1:C:278:VAL:O	2.31	0.62
1:C:345:MET:HE1	1:C:355:GLY:HA3	1.82	0.62
1:B:613:ARG:HH21	1:B:620:HIS:CE1	2.18	0.61
1:B:555:LEU:O	1:B:557:HIS:ND1	2.33	0.61
1:B:138:GLN:HE22	1:B:171:ARG:NH1	1.99	0.61
1:C:294:LEU:HD12	1:C:295:PRO:HD2	1.82	0.61
1:C:345:MET:HE3	1:C:345:MET:HA	1.82	0.60
1:B:298:LYS:HB2	1:B:410:ILE:HG21	1.84	0.60
1:A:595:LYS:HD3	1:A:601:ASP:CB	2.32	0.60
1:B:446:MET:HE1	1:B:451:TRP:CD2	2.36	0.60
1:B:547:ARG:NH2	1:B:551:GLU:HB2	2.12	0.60
1:B:144:MET:HE1	1:B:171:ARG:CD	2.31	0.59
1:A:136:LEU:HB2	1:A:172:VAL:HB	1.83	0.59
1:A:595:LYS:HD3	1:A:601:ASP:HB2	1.84	0.59
1:B:603:ASP:HB2	1:B:605:ARG:NE	2.13	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:SER:HB3	1:A:363:ILE:HA	1.84	0.59
1:A:587:PHE:CD2	1:A:604:VAL:HG21	2.37	0.59
1:B:331:GLN:CD	1:B:331:GLN:H	2.11	0.59
1:B:419:LEU:O	1:B:454:ARG:NH2	2.36	0.59
1:B:136:LEU:HB2	1:B:172:VAL:HB	1.85	0.59
1:B:322:LEU:HD21	1:B:333:ILE:HD13	1.83	0.59
1:A:301:ASN:HA	1:A:332:MET:HE2	1.85	0.58
1:B:592:GLN:NE2	1:B:645:GLU:O	2.32	0.58
1:C:103:VAL:HG22	1:C:240:LEU:HB3	1.84	0.58
1:B:635:LYS:HG3	1:B:639:VAL:HG21	1.85	0.58
1:B:547:ARG:HH22	1:B:551:GLU:CB	2.13	0.58
1:C:561:PRO:HA	1:C:566:PHE:CG	2.40	0.57
1:A:436:ASP:OD2	1:A:531:ARG:NH1	2.26	0.57
1:C:560:ASN:O	1:C:566:PHE:HB2	2.05	0.57
1:C:250:GLU:N	1:C:250:GLU:OE1	2.37	0.57
1:B:519:LYS:HD2	1:B:519:LYS:N	2.19	0.57
1:A:601:ASP:OD1	1:A:601:ASP:N	2.37	0.57
1:B:602:LEU:H	1:B:602:LEU:HD22	1.70	0.57
1:B:366:ALA:O	1:B:370:GLN:HG2	2.04	0.56
1:C:476:ASP:O	1:C:480:ARG:HG3	2.05	0.56
1:C:633:VAL:HG23	1:C:634:LYS:CD	2.35	0.56
1:B:635:LYS:HG3	1:B:639:VAL:CG2	2.34	0.56
1:A:446:MET:O	1:A:480:ARG:NH1	2.36	0.56
1:C:319:LEU:O	1:C:323:LEU:HD13	2.05	0.56
1:B:325:ALA:O	1:B:328:VAL:HG23	2.05	0.56
1:C:495:VAL:HG13	1:C:521:LYS:HG2	1.87	0.56
1:C:297:ASN:HB3	1:C:300:LEU:HD21	1.87	0.56
1:B:362:SER:HB3	1:B:363:ILE:HA	1.88	0.56
1:B:250:GLU:CG	1:B:251:GLU:HA	2.30	0.55
1:A:318:MET:CE	1:A:394:GLU:HA	2.36	0.55
1:B:157:ASP:OD2	1:B:186:LYS:N	2.31	0.55
1:C:103:VAL:CG2	1:C:211:ALA:HB1	2.37	0.55
1:A:362:SER:HA	1:A:367:ARG:HB2	1.87	0.55
1:A:459:LYS:NZ	2:A:702:HOH:O	2.38	0.55
1:B:483:GLU:OE1	1:B:483:GLU:N	2.33	0.55
1:A:299:VAL:HG21	1:A:406:LEU:HB3	1.89	0.55
1:A:103:VAL:CG2	1:A:211:ALA:HB1	2.37	0.54
1:B:532:ASN:HB3	1:B:535:SER:OG	2.07	0.54
1:B:603:ASP:CG	1:B:605:ARG:HH21	2.15	0.54
1:C:260:GLU:N	1:C:260:GLU:OE1	2.40	0.54
1:B:99:LEU:HG	1:B:246:LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:ARG:HH21	1:B:548:LEU:CA	2.07	0.54
1:A:322:LEU:O	1:A:328:VAL:HG11	2.08	0.54
1:B:103:VAL:CG2	1:B:211:ALA:HB1	2.38	0.54
1:B:438:ALA:HA	1:B:530:LEU:HD23	1.89	0.54
1:C:256:TRP:HE1	1:C:281:CYS:HA	1.73	0.54
1:B:135:VAL:HG11	1:B:273:GLU:HG2	1.90	0.54
1:B:547:ARG:HH12	1:B:551:GLU:HG2	1.72	0.54
1:C:446:MET:O	1:C:480:ARG:HD3	2.08	0.54
1:A:544:GLU:OE1	1:A:547:ARG:NH1	2.42	0.53
1:B:424:ALA:HB1	1:B:497:ARG:HB2	1.89	0.53
1:B:579:ILE:CD1	1:B:623:VAL:HG13	2.39	0.53
1:C:253:GLU:CG	1:C:266:ARG:NH1	2.66	0.53
1:B:545:VAL:O	1:B:548:LEU:N	2.42	0.52
1:B:592:GLN:HE21	1:B:644:LEU:HB3	1.73	0.52
1:C:594:ALA:HA	1:C:599:ILE:HD11	1.90	0.52
1:B:547:ARG:NH2	1:B:548:LEU:HA	2.03	0.52
1:B:392:LEU:HD23	1:B:450:GLY:HA2	1.91	0.52
1:A:338:ASP:HB2	1:A:371:HIS:CE1	2.45	0.52
1:A:362:SER:HB3	1:A:363:ILE:CG2	2.40	0.51
1:C:570:THR:HG21	1:C:575:TYR:OH	2.09	0.51
1:B:250:GLU:OE2	1:B:251:GLU:OE1	2.28	0.51
1:C:136:LEU:HB2	1:C:172:VAL:HB	1.91	0.51
1:C:387:LYS:O	1:C:454:ARG:HG3	2.11	0.51
1:B:405:PHE:HD1	1:B:530:LEU:HD11	1.74	0.51
1:B:579:ILE:HG22	1:B:580:ARG:H	1.75	0.51
1:B:592:GLN:NE2	1:B:644:LEU:HB3	2.25	0.51
1:C:344:PRO:O	1:C:348:VAL:HG23	2.11	0.50
1:B:122:ASP:OD2	1:B:128:GLY:HA3	2.11	0.50
1:B:579:ILE:HD11	1:B:623:VAL:HG13	1.94	0.50
1:A:318:MET:HE3	1:A:394:GLU:HA	1.93	0.50
1:B:541:TYR:O	1:B:545:VAL:HG23	2.12	0.50
1:B:579:ILE:HD12	1:B:579:ILE:N	2.27	0.50
1:C:433:THR:HA	1:C:615:PHE:O	2.11	0.50
1:B:495:VAL:HG23	1:B:497:ARG:NH1	2.27	0.50
1:A:420:TYR:CD2	1:A:485:ARG:HG3	2.47	0.49
1:B:465:LYS:HZ1	1:B:484:GLN:HE21	1.60	0.49
1:A:144:MET:HE3	1:A:273:GLU:HB2	1.92	0.49
1:A:260:GLU:HG2	1:A:263:ARG:HD3	1.95	0.49
1:C:265:ARG:NH2	1:C:285:THR:O	2.31	0.49
1:B:297:ASN:OD1	1:B:298:LYS:N	2.46	0.49
1:A:330:PRO:HA	1:A:333:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ASN:HB3	1:B:300:LEU:CD1	2.39	0.49
1:B:161:VAL:HG13	1:B:192:LEU:HD22	1.93	0.49
1:C:446:MET:HE2	1:C:451:TRP:CE3	2.48	0.48
1:A:425:TRP:CD2	1:A:449:LEU:HD23	2.48	0.48
1:B:448:GLY:HA2	1:B:451:TRP:CD1	2.48	0.48
1:C:260:GLU:HB3	1:C:263:ARG:NE	2.12	0.48
1:C:489:GLU:OE1	1:C:608:HIS:ND1	2.35	0.48
1:B:138:GLN:NE2	1:B:171:ARG:NH1	2.61	0.48
1:C:253:GLU:OE2	1:C:254:CYS:O	2.32	0.48
1:A:261:LEU:HD11	1:A:288:GLU:OE2	2.12	0.48
1:B:553:GLU:C	1:B:575:TYR:HE2	2.21	0.48
1:A:428:GLN:OE1	1:A:599:ILE:HG22	2.13	0.48
1:B:552:ALA:HB1	1:B:575:TYR:HA	1.96	0.48
1:A:366:ALA:O	1:A:370:GLN:HG2	2.13	0.47
1:A:595:LYS:HD3	1:A:601:ASP:OD2	2.14	0.47
1:B:432:HIS:CD2	1:B:433:THR:HG23	2.49	0.47
1:C:388:PHE:CD2	1:C:410:ILE:HD11	2.49	0.47
1:C:609:ARG:O	1:C:630:PRO:HD2	2.14	0.47
1:A:581:MET:HG3	1:A:586:ASP:O	2.14	0.47
1:B:443:VAL:O	1:B:489:GLU:HB2	2.14	0.47
1:A:338:ASP:HB2	1:A:371:HIS:ND1	2.30	0.47
1:A:180:GLU:OE1	1:A:182:SER:N	2.36	0.47
1:A:260:GLU:CG	1:A:263:ARG:HD3	2.45	0.47
1:B:451:TRP:CZ3	1:B:453:LEU:HB2	2.49	0.47
1:C:412:LEU:CD2	1:C:537:LYS:HG2	2.45	0.47
1:C:645:GLU:OE1	1:C:646:PRO:O	2.32	0.47
1:C:592:GLN:HE21	1:C:646:PRO:HD3	1.79	0.47
1:A:99:LEU:HB2	1:A:244:VAL:HG22	1.97	0.47
1:A:402:PHE:CE1	1:A:406:LEU:HD22	2.50	0.47
1:B:285:THR:HG23	1:B:286:PRO:HD2	1.96	0.47
1:C:263:ARG:O	1:C:267:ARG:N	2.27	0.47
1:C:335:VAL:HG23	1:C:335:VAL:O	2.14	0.47
1:A:167:VAL:O	1:A:216:LYS:NZ	2.47	0.46
1:A:413:LEU:HD22	1:A:454:ARG:HH21	1.79	0.46
1:A:362:SER:HB3	1:A:363:ILE:CA	2.46	0.46
1:B:425:TRP:CZ2	1:B:520:HIS:CD2	3.04	0.46
1:B:539:GLU:OE1	1:B:539:GLU:N	2.31	0.46
1:C:131:ILE:CD1	1:C:160:MET:HE1	2.41	0.46
1:B:446:MET:HB3	1:B:480:ARG:HG2	1.97	0.46
1:B:575:TYR:O	1:B:622:LEU:N	2.46	0.46
1:B:265:ARG:NH1	1:B:284:PRO:HB2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:ARG:NE	1:B:489:GLU:OE2	2.29	0.46
1:B:613:ARG:NH2	1:B:620:HIS:CE1	2.84	0.46
1:B:297:ASN:OD1	1:B:299:VAL:HG22	2.16	0.46
1:C:149:PHE:CD2	1:C:160:MET:HG3	2.51	0.46
1:C:401:ASP:OD1	1:C:523:ASN:ND2	2.49	0.46
1:A:319:LEU:HD23	1:A:319:LEU:HA	1.78	0.46
1:A:338:ASP:HB2	1:A:371:HIS:CG	2.51	0.46
1:C:420:TYR:N	1:C:489:GLU:O	2.32	0.46
1:A:402:PHE:CE1	1:A:406:LEU:CD2	2.99	0.45
1:C:592:GLN:NE2	1:C:646:PRO:HD3	2.31	0.45
1:A:186:LYS:O	1:A:190:LYS:HG3	2.15	0.45
1:A:633:VAL:HG12	1:A:634:LYS:HD2	1.97	0.45
1:C:362:SER:HA	1:C:367:ARG:HB2	1.97	0.45
1:C:405:PHE:CD2	1:C:406:LEU:HD23	2.51	0.45
1:C:446:MET:SD	1:C:446:MET:C	3.00	0.45
1:A:99:LEU:HG	1:A:246:LEU:HD21	1.98	0.45
1:A:607:ASN:OD1	1:A:607:ASN:N	2.47	0.45
1:B:425:TRP:CZ2	1:B:520:HIS:HD2	2.34	0.45
1:C:299:VAL:HG12	1:C:299:VAL:O	2.17	0.45
1:B:250:GLU:HA	1:B:252:ALA:H	1.82	0.45
1:C:604:VAL:C	1:C:605:ARG:HG2	2.42	0.45
1:A:570:THR:HG21	1:A:575:TYR:OH	2.17	0.45
1:B:173:LEU:HD11	1:B:216:LYS:HB2	1.99	0.45
1:C:500:HIS:C	1:C:500:HIS:CD2	2.95	0.45
1:C:555:LEU:HD11	1:C:575:TYR:HB3	1.98	0.45
1:A:428:GLN:OE1	1:A:600:TRP:HB3	2.16	0.44
1:A:599:ILE:HD12	1:A:599:ILE:HG23	1.57	0.44
1:B:401:ASP:OD1	1:B:401:ASP:N	2.39	0.44
1:C:559:LYS:HD3	1:C:566:PHE:HA	1.99	0.44
1:A:465:LYS:NZ	1:A:484:GLN:HE21	2.16	0.44
1:B:192:LEU:O	1:B:196:LEU:HD13	2.17	0.44
1:B:345:MET:HE2	1:B:355:GLY:HA3	1.99	0.44
1:B:456:SER:O	1:B:460:GLU:HG2	2.17	0.44
1:B:552:ALA:HB1	1:B:575:TYR:CA	2.48	0.44
1:B:564:ASP:HA	1:B:616:ARG:NH2	2.32	0.44
1:C:570:THR:OG1	1:C:571:GLU:N	2.50	0.44
1:A:144:MET:HE1	1:A:171:ARG:NE	2.32	0.44
1:B:144:MET:HE1	1:B:171:ARG:NE	2.33	0.44
1:C:495:VAL:O	1:C:497:ARG:NH1	2.49	0.44
1:B:312:PRO:HD3	1:B:344:PRO:HG3	1.99	0.44
1:B:579:ILE:HG22	1:B:580:ARG:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:547:ARG:HD3	1:C:548:LEU:N	2.32	0.44
1:C:631:TYR:C	1:C:633:VAL:H	2.25	0.44
1:C:362:SER:OG	1:C:363:ILE:HA	2.18	0.44
1:A:560:ASN:HD22	1:A:561:PRO:CD	2.31	0.44
1:A:425:TRP:CE2	1:A:449:LEU:HD23	2.53	0.43
1:B:294:LEU:CD2	1:B:297:ASN:HB2	2.42	0.43
1:B:437:PRO:HA	1:B:495:VAL:HG21	2.01	0.43
1:B:438:ALA:HB1	1:B:530:LEU:HA	2.00	0.43
1:B:603:ASP:CB	1:B:605:ARG:HE	2.17	0.43
1:A:157:ASP:OD1	1:A:158:GLU:N	2.50	0.43
1:C:555:LEU:HD21	1:C:567:LEU:HD13	2.00	0.43
1:A:317:ARG:HH21	1:A:397:ASP:CG	2.18	0.43
1:A:465:LYS:CE	1:A:484:GLN:HE21	2.32	0.43
1:B:298:LYS:HG2	1:B:407:SER:OG	2.18	0.43
1:B:610:GLY:HA3	1:B:629:SER:HB2	2.00	0.43
1:C:294:LEU:HD21	1:C:404:SER:HA	2.00	0.43
1:C:323:LEU:N	1:C:323:LEU:CD1	2.81	0.43
1:B:294:LEU:HA	1:B:295:PRO:HD3	1.88	0.43
1:B:171:ARG:HG2	1:B:171:ARG:HH11	1.82	0.43
1:B:303:PRO:HG3	1:B:383:PHE:CG	2.54	0.43
1:B:575:TYR:CD2	1:B:576:VAL:N	2.86	0.43
1:A:167:VAL:HG13	1:A:273:GLU:HG2	2.01	0.43
1:C:294:LEU:HD12	1:C:294:LEU:HA	1.85	0.43
1:C:614:LEU:HD12	1:C:615:PHE:C	2.44	0.43
1:C:614:LEU:HD11	1:C:616:ARG:HG3	2.01	0.43
1:A:556:ASP:HB3	1:A:559:LYS:HD2	2.01	0.43
1:C:542:GLU:OE2	1:C:631:TYR:OH	2.34	0.43
1:A:362:SER:CB	1:A:363:ILE:HA	2.48	0.42
1:B:635:LYS:NZ	1:B:639:VAL:HG23	2.34	0.42
1:C:168:ALA:N	1:C:273:GLU:OE1	2.47	0.42
1:C:546:HIS:ND1	1:C:634:LYS:HE2	2.34	0.42
1:A:476:ASP:O	1:A:480:ARG:HG3	2.19	0.42
1:C:315:LEU:HD12	1:C:318:MET:CE	2.50	0.42
1:A:318:MET:HE2	1:A:394:GLU:HA	2.01	0.42
1:C:626:VAL:CG2	1:C:641:PRO:HG2	2.49	0.42
1:B:567:LEU:HD21	1:B:571:GLU:OE2	2.19	0.42
1:A:260:GLU:CD	1:A:263:ARG:HD3	2.44	0.42
1:C:581:MET:HG3	1:C:586:ASP:O	2.20	0.42
1:C:446:MET:CE	1:C:451:TRP:CD2	3.03	0.42
1:B:544:GLU:O	1:B:548:LEU:HG	2.20	0.42
1:C:99:LEU:HG	1:C:246:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:VAL:HG11	1:B:174:ILE:HG23	2.02	0.42
1:C:221:PHE:CE1	1:C:245:PRO:HD2	2.55	0.42
1:C:306:VAL:HB	1:C:335:VAL:HG12	2.02	0.42
1:A:395:ASP:OD2	1:A:500:HIS:HE1	2.03	0.41
1:B:259:THR:HG23	1:B:262:ASN:N	2.32	0.41
1:B:401:ASP:OD2	1:B:523:ASN:ND2	2.53	0.41
1:B:405:PHE:CZ	1:B:493:PRO:HD3	2.55	0.41
1:B:595:LYS:HG3	1:B:596:CYS:N	2.34	0.41
1:B:631:TYR:C	1:B:633:VAL:N	2.76	0.41
1:C:459:LYS:HE3	1:C:463:GLU:OE1	2.20	0.41
1:A:643:PHE:CD1	1:A:643:PHE:C	2.98	0.41
1:B:190:LYS:HD3	1:B:202:PRO:O	2.20	0.41
1:C:364:LYS:HE3	1:C:364:LYS:HB3	1.91	0.41
1:C:599:ILE:HD12	1:C:599:ILE:C	2.45	0.41
1:A:560:ASN:HD22	1:A:561:PRO:HD2	1.85	0.41
1:B:301:ASN:OD1	1:B:301:ASN:N	2.52	0.41
1:B:378:ALA:O	1:B:382:LEU:HG	2.21	0.41
1:A:103:VAL:HG22	1:A:240:LEU:HB3	2.01	0.41
1:A:260:GLU:CD	1:A:263:ARG:NH1	2.72	0.41
1:A:474:ASP:HB2	1:A:477:MET:HB3	2.03	0.41
1:A:560:ASN:C	1:A:560:ASN:ND2	2.78	0.41
1:A:579:ILE:HB	1:A:589:THR:HG21	2.02	0.41
1:A:601:ASP:CG	1:A:602:LEU:HD13	2.46	0.41
1:B:570:THR:HG23	1:B:571:GLU:N	2.36	0.41
1:C:564:ASP:OD1	1:C:617:LYS:NZ	2.54	0.41
1:A:640:THR:HA	1:A:641:PRO:HD3	1.95	0.41
1:A:99:LEU:HD11	1:A:141:GLY:HA3	2.02	0.41
1:C:631:TYR:C	1:C:633:VAL:N	2.76	0.41
1:A:364:LYS:HE2	1:B:152:TYR:OH	2.20	0.41
1:B:250:GLU:OE2	1:B:251:GLU:HG2	2.19	0.41
1:B:419:LEU:HD23	1:B:419:LEU:HA	1.94	0.41
1:B:442:ARG:HD2	1:B:536:LEU:O	2.20	0.41
1:B:547:ARG:O	1:B:548:LEU:C	2.63	0.41
1:C:190:LYS:HD3	1:C:202:PRO:O	2.20	0.41
1:C:568:PRO:O	1:C:570:THR:HG22	2.21	0.41
1:A:426:ASN:HB2	1:A:493:PRO:O	2.20	0.41
1:A:584:ASP:OD1	1:A:584:ASP:N	2.53	0.41
1:A:599:ILE:HG22	1:A:600:TRP:N	2.32	0.41
1:B:437:PRO:HA	1:B:495:VAL:CG2	2.51	0.41
1:C:446:MET:CE	1:C:451:TRP:CE3	3.04	0.41
1:A:231:LEU:HD23	1:A:231:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:ASN:ND2	1:A:562:CYS:H	2.19	0.41
1:A:589:THR:HG23	1:A:644:LEU:CD2	2.49	0.41
1:C:362:SER:HB3	1:C:363:ILE:CG2	2.51	0.41
1:C:468:THR:HG23	1:C:469:PRO:HD2	2.02	0.41
1:A:419:LEU:HD23	1:A:419:LEU:HA	1.85	0.40
1:B:319:LEU:O	1:B:323:LEU:HD13	2.21	0.40
1:A:329:SER:HB2	1:A:332:MET:HG2	2.02	0.40
1:C:591:THR:O	1:C:594:ALA:HB3	2.22	0.40
1:A:420:TYR:CE2	1:A:485:ARG:HG3	2.57	0.40
1:C:446:MET:HE1	1:C:451:TRP:CD2	2.57	0.40
1:C:157:ASP:O	1:C:161:VAL:HG23	2.21	0.40
1:C:253:GLU:CD	1:C:266:ARG:NH1	2.80	0.40
1:C:416:ASP:OD2	1:C:418:SER:OG	2.30	0.40
1:C:544:GLU:HA	1:C:547:ARG:HB3	2.03	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	531/578 (92%)	517 (97%)	13 (2%)	1 (0%)	43 63
1	B	534/578 (92%)	495 (93%)	33 (6%)	6 (1%)	11 22
1	C	533/578 (92%)	508 (95%)	24 (4%)	1 (0%)	43 63
All	All	1598/1734 (92%)	1520 (95%)	70 (4%)	8 (0%)	24 43

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	553	GLU
1	B	547	ARG
1	B	571	GLU

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Mol	Chain	Res	Type
1	B	281	CYS
1	A	569	ASP
1	B	570	THR
1	C	531	ARG
1	B	545	VAL

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	465/504 (92%)	456 (98%)	9 (2%)	50	76
1	B	458/504 (91%)	449 (98%)	9 (2%)	48	75
1	C	465/504 (92%)	450 (97%)	15 (3%)	34	62
All	All	1388/1512 (92%)	1355 (98%)	33 (2%)	44	70

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	VAL
1	A	195	SER
1	A	238	VAL
1	A	323	LEU
1	A	329	SER
1	A	449	LEU
1	A	472	LEU
1	A	532	ASN
1	A	602	LEU
1	B	114	VAL
1	B	195	SER
1	B	238	VAL
1	B	323	LEU
1	B	446	MET
1	B	472	LEU
1	B	496	SER
1	B	536	LEU

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Mol	Chain	Res	Type
1	B	555	LEU
1	C	101	VAL
1	C	110	VAL
1	C	196	LEU
1	C	207	ARG
1	C	238	VAL
1	C	300	LEU
1	C	318	MET
1	C	323	LEU
1	C	362	SER
1	C	404	SER
1	C	459	LYS
1	C	468	THR
1	C	582[A]	GLU
1	C	582[B]	GLU
1	C	602	LEU

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	184	HIS
1	A	484	GLN
1	A	500	HIS
1	A	560	ASN
1	B	137	ASN
1	B	138	GLN
1	B	310	ASN
1	B	326	GLN
1	B	331	GLN
1	B	408	GLN
1	B	484	GLN
1	B	520	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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

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	535/578 (92%)	0.24	25 (4%) 36 32	32, 42, 85, 117	0
1	B	536/578 (92%)	1.03	127 (23%) 2 1	34, 58, 140, 217	2 (0%)
1	C	536/578 (92%)	0.60	50 (9%) 14 12	33, 49, 101, 134	1 (0%)
All	All	1607/1734 (92%)	0.62	202 (12%) 8 6	32, 47, 107, 217	3 (0%)

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	572	GLY	6.6
1	B	573	HIS	6.4
1	B	570	THR	6.0
1	B	561	PRO	5.9
1	B	568	PRO	5.8
1	B	503	ILE	5.7
1	B	555	LEU	5.6
1	B	550	SER	5.4
1	C	259	THR	5.4
1	B	647	PRO	5.3
1	C	254	CYS	5.2
1	B	574	THR	5.1
1	B	619	ASN	5.0
1	B	575	TYR	4.9
1	B	554	VAL	4.9
1	B	602	LEU	4.8
1	A	602	LEU	4.7
1	B	614	LEU	4.7
1	B	249	ALA	4.6
1	B	564	ASP	4.6
1	A	477	MET	4.6
1	C	554	VAL	4.6
1	B	549	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	562	CYS	4.4
1	A	646	PRO	4.4
1	A	503	ILE	4.3
1	B	431	GLU	4.3
1	B	557	HIS	4.2
1	C	503	ILE	4.2
1	B	553	GLU	4.2
1	B	435	GLU	4.1
1	B	571	GLU	4.0
1	B	552	ALA	4.0
1	C	638	SER	4.0
1	C	296	ASP	3.9
1	A	254	CYS	3.9
1	B	295	PRO	3.9
1	B	525	VAL	3.9
1	A	259	THR	3.9
1	B	291	PRO	3.9
1	B	560	ASN	3.8
1	B	432	HIS	3.8
1	B	556	ASP	3.8
1	B	567	LEU	3.8
1	B	548	LEU	3.7
1	C	477	MET	3.7
1	B	637	PRO	3.7
1	B	524	THR	3.7
1	C	640	THR	3.6
1	B	599	ILE	3.6
1	B	281	CYS	3.6
1	C	252	ALA	3.6
1	B	437	PRO	3.6
1	C	637	PRO	3.6
1	A	643	PHE	3.6
1	B	569	ASP	3.6
1	B	559	LYS	3.5
1	B	294	LEU	3.5
1	B	250	GLU	3.5
1	B	558	SER	3.5
1	C	570	THR	3.4
1	C	562	CYS	3.4
1	B	566	PHE	3.4
1	B	595	LYS	3.4
1	B	618	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	574	THR	3.4
1	C	603	ASP	3.4
1	C	568	PRO	3.4
1	C	301	ASN	3.3
1	B	490	CYS	3.3
1	C	575	TYR	3.3
1	B	597	LEU	3.2
1	B	598	HIS	3.2
1	B	617	LYS	3.2
1	B	501	PHE	3.2
1	B	293	PRO	3.2
1	B	520	HIS	3.2
1	B	621	PHE	3.2
1	C	260	GLU	3.2
1	C	602	LEU	3.2
1	A	249	ALA	3.1
1	B	519	LYS	3.1
1	A	257	ALA	3.1
1	B	633	VAL	3.1
1	C	263	ARG	3.1
1	B	436	ASP	3.0
1	B	623	VAL	3.0
1	B	434	ALA	3.0
1	B	292	ASP	3.0
1	B	638	SER	3.0
1	B	251	GLU	3.0
1	B	577	ALA	3.0
1	C	559	LYS	3.0
1	B	615	PHE	3.0
1	B	290	SER	3.0
1	B	526	PRO	2.9
1	B	324	SER	2.9
1	B	502	GLY	2.9
1	C	576	VAL	2.9
1	B	551	GLU	2.9
1	B	255	HIS	2.9
1	A	248	SER	2.8
1	C	573	HIS	2.8
1	B	300	LEU	2.8
1	B	439	LEU	2.8
1	B	536	LEU	2.8
1	B	494	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	362	SER	2.8
1	B	641	PRO	2.8
1	A	260	GLU	2.8
1	B	283	ASP	2.8
1	C	633	VAL	2.8
1	C	639	VAL	2.8
1	B	591	THR	2.8
1	B	405	PHE	2.8
1	C	566	PHE	2.7
1	B	532	ASN	2.7
1	C	636	PRO	2.7
1	C	567	LEU	2.7
1	C	614	LEU	2.7
1	B	607	ASN	2.7
1	C	253	GLU	2.7
1	C	502	GLY	2.6
1	B	643	PHE	2.6
1	B	646	PRO	2.6
1	B	296[A]	ASP	2.6
1	B	395	ASP	2.6
1	B	301	ASN	2.6
1	B	325	ALA	2.6
1	A	639	VAL	2.6
1	C	551	GLU	2.6
1	B	400	VAL	2.6
1	B	533	VAL	2.6
1	B	620	HIS	2.5
1	B	640	THR	2.5
1	B	429	GLY	2.5
1	C	647	PRO	2.5
1	B	297	ASN	2.5
1	B	527	GLY	2.5
1	B	547	ARG	2.5
1	A	638	SER	2.5
1	A	283	ASP	2.5
1	B	600	TRP	2.5
1	B	404	SER	2.5
1	B	565	SER	2.5
1	C	571	GLU	2.4
1	B	589	THR	2.4
1	C	641	PRO	2.4
1	B	421	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	417	ASP	2.4
1	C	550	SER	2.4
1	B	495	VAL	2.4
1	A	255	HIS	2.3
1	B	601	ASP	2.3
1	B	289	PHE	2.3
1	B	585	ASP	2.3
1	C	281	CYS	2.3
1	B	576	VAL	2.3
1	C	552	ALA	2.3
1	C	255	HIS	2.3
1	A	282	LYS	2.3
1	A	645	GLU	2.3
1	C	533	VAL	2.3
1	A	562	CYS	2.3
1	B	410	ILE	2.2
1	B	593	LEU	2.2
1	A	556	ASP	2.2
1	C	385	GLU	2.2
1	A	637	PRO	2.2
1	B	639	VAL	2.2
1	C	295	PRO	2.2
1	B	441	TYR	2.2
1	B	644	LEU	2.2
1	C	569	ASP	2.2
1	B	385	GLU	2.2
1	A	97	ARG	2.2
1	B	522	PHE	2.2
1	B	636	PRO	2.2
1	B	428	GLN	2.2
1	C	527	GLY	2.2
1	A	362	SER	2.2
1	B	539	GLU	2.2
1	C	97	ARG	2.2
1	B	438	ALA	2.1
1	B	543	VAL	2.1
1	B	477	MET	2.1
1	A	614	LEU	2.1
1	B	433	THR	2.1
1	C	300	LEU	2.1
1	C	555	LEU	2.1
1	B	298	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	217	GLY	2.1
1	B	603	ASP	2.1
1	C	556	ASP	2.1
1	B	578	PHE	2.1
1	B	546	HIS	2.1
1	C	532	ASN	2.0
1	A	250	GLU	2.0
1	B	531	ARG	2.0
1	B	252	ALA	2.0
1	B	257	ALA	2.0
1	A	218	GLY	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.