Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 11:29 am BST

PDB ID	:	5GGF
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 following versions of software and data (see references ⓘ) were used in the production of this report:

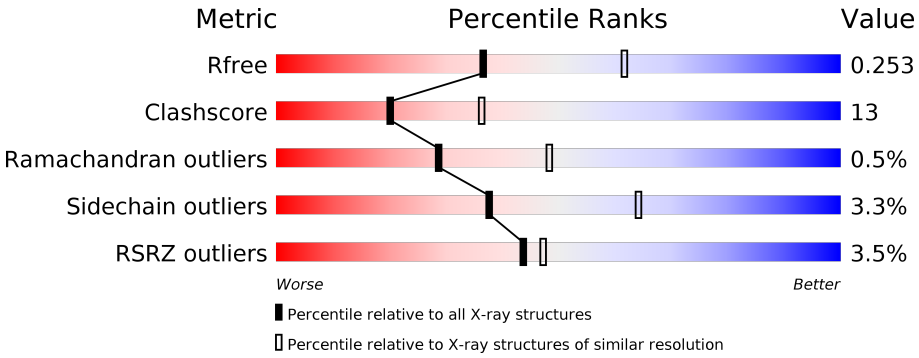
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 on 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 <=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	73% 18% • 7%
1	B	578	7% 64% 26% • • 7%
1	C	578	2% 69% 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.

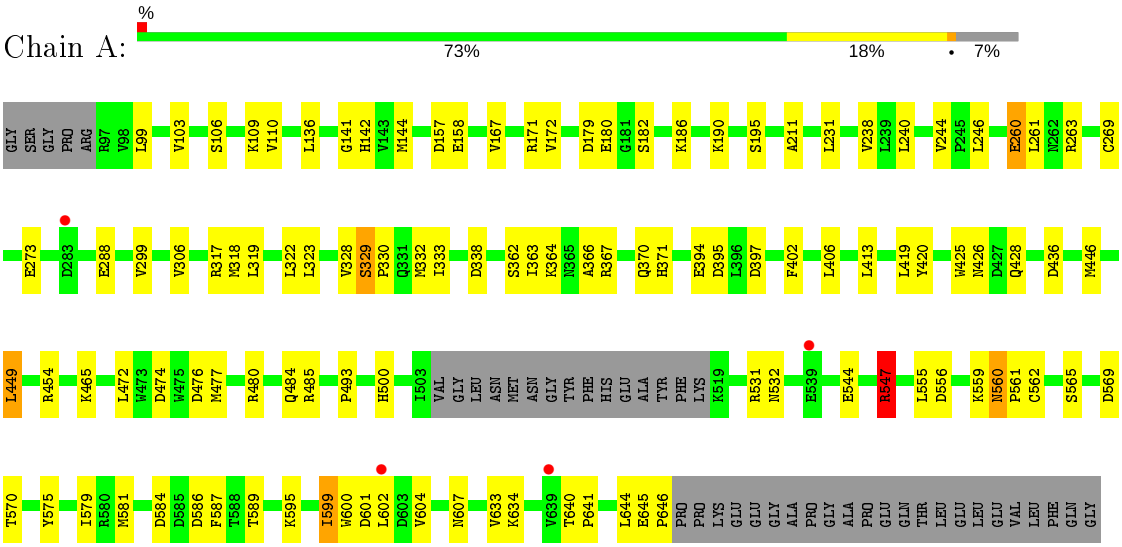
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	6	Total O 6 6	0	0
2	B	6	Total O 6 6	0	0
2	C	3	Total O 3 3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

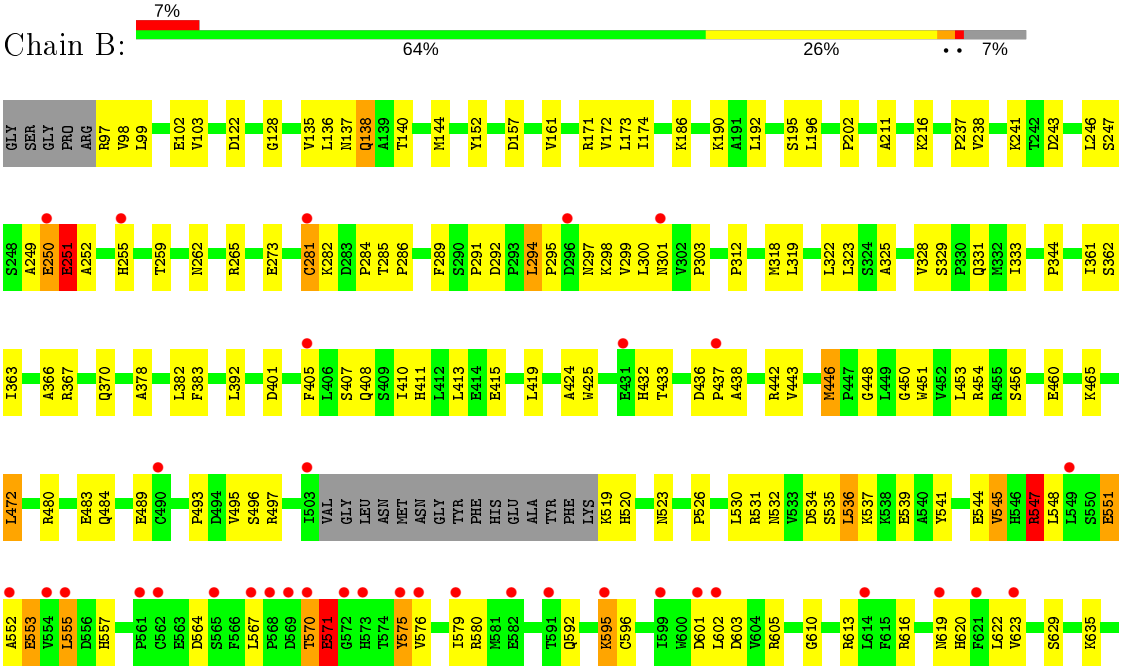
• Molecule 1: Protein O-linked-mannose beta-1,2-N-acetylglucosaminyltransferase 1

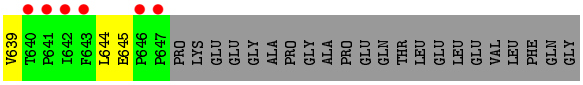
Chain A:



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

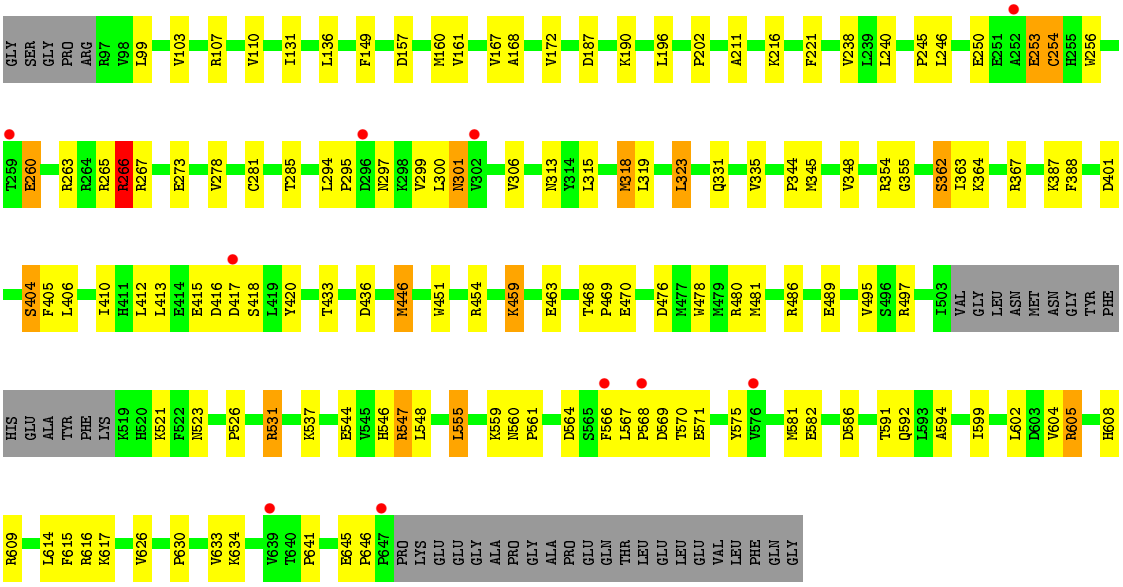
Chain B:





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

Chain C:



4 Data and refinement statistics (i)

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 47.20 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.61-2.49) 92.6 (47.20-2.49)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.48Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.233 , 0.253 0.233 , 0.253	Depositor DCC
R_{free} test set	2000 reflections (2.53%)	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)	0.34 , 32.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.78	6/4379 (0.1%)	0.64	2/5955 (0.0%)
1	B	0.68	2/4365 (0.0%)	0.76	10/5942 (0.2%)
1	C	0.67	1/4388 (0.0%)	0.66	3/5971 (0.1%)
All	All	0.71	9/13132 (0.1%)	0.68	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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	547	ARG	NE-CZ	-12.73	1.16	1.33
1	A	547	ARG	CZ-NH1	-11.74	1.17	1.33
1	A	547	ARG	CZ-NH2	-11.69	1.17	1.33
1	A	547	ARG	CD-NE	-10.55	1.28	1.46
1	C	253	GLU	CB-CG	-9.68	1.33	1.52
1	B	250	GLU	CB-CG	-5.81	1.41	1.52
1	B	547	ARG	CG-CD	-5.64	1.37	1.51
1	A	238	VAL	CB-CG1	-5.15	1.42	1.52
1	A	269	CYS	CB-SG	-5.15	1.73	1.81

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	551	GLU	OE1-CD-OE2	11.47	137.07	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	547	ARG	CA-CB-CG	10.61	136.73	113.40
1	B	547	ARG	CG-CD-NE	-9.85	91.12	111.80
1	B	551	GLU	CG-CD-OE2	-9.78	98.73	118.30
1	C	266	ARG	NE-CZ-NH1	-8.87	115.86	120.30
1	B	575	TYR	CB-CG-CD2	-6.46	117.12	121.00
1	C	254	CYS	CA-CB-SG	-6.38	102.52	114.00
1	B	250	GLU	N-CA-CB	-6.16	99.52	110.60
1	B	251	GLU	CA-CB-CG	5.62	125.75	113.40
1	A	599	ILE	CG1-CB-CG2	-5.52	99.25	111.40
1	B	547	ARG	CB-CA-C	5.39	121.17	110.40
1	A	179	ASP	CB-CG-OD2	5.18	122.96	118.30
1	C	107	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	B	472	LEU	CB-CG-CD2	-5.08	102.36	111.00
1	B	575	TYR	CA-CB-CG	-5.08	103.75	113.40

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 (i)

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	82	0
1	B	4244	0	4117	138	0
1	C	4268	0	4151	99	0
2	A	6	0	0	0	0
2	B	6	0	0	0	0
2	C	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12790	0	12428	316	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 (316) 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:A:318:MET:HE2	1:A:394:GLU:HA	1.54	0.89
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: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:C:131:ILE:HD12	1:C:160:MET:HE1	1.64	0.80
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:144:MET:HE1	1:B:171:ARG:HD3	1.64	0.78
1:A:158:GLU:OE1	1:A:186:LYS:NZ	2.14	0.77
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: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:A:260:GLU:CD	1:A:263:ARG:HH11	1.92	0.72
1:C:103:VAL:HG23	1:C:211:ALA:HB1	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:259:THR:HG23	1:B:262:ASN:H	1.58	0.68
1:C:478:TRP:HA	1:C:481:MET:HE2	1.74	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: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:C:345:MET:HA	1:C:345:MET:HE3	1.79	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:A:306:VAL:HG13	1:A:318:MET:HE1	1.80	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: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: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:547:ARG:NH2	1:B:551:GLU:HB2	2.12	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603:ASP:HB2	1:B:605:ARG:NE	2.13	0.59
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: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:B:592:GLN:NE2	1:B:645:GLU:O	2.32	0.58
1:C:345:MET:HE1	1:C:355:GLY:HA3	1.86	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:OE1	1:C:250:GLU:N	2.37	0.57
1:B:519:LYS:N	1:B:519:LYS:HD2	2.19	0.57
1:A:601:ASP:N	1:A:601:ASP:OD1	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:A:144:MET:HE1	1:A:171:ARG:NE	2.20	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: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: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:C:446:MET:HE2	1:C:451:TRP:CD2	2.42	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: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
1:B:547:ARG:HH21	1:B:548:LEU:CA	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:LEU:O	1:A:328:VAL:HG11	2.08	0.54
1:B:331:GLN:CD	1:B:331:GLN:H	2.11	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: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: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
1:B:603:ASP:CG	1:B:605:ARG:HH21	2.15	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:318:MET:CE	1:A:394:GLU:HA	2.36	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:C:446:MET:HE2	1:C:451:TRP:CE3	2.49	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:B:451:TRP:CZ3	1:B:453:LEU:HB2	2.49	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: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:402:PHE:CE1	1:A:406:LEU:HD22	2.50	0.47
1:A:99:LEU:HB2	1:A:244:VAL:HG22	1.97	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: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:N	1:B:539:GLU:OE1	2.31	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:416:ASP:OD2	1:C:418:SER:OG	2.30	0.45
1:A:607:ASN:N	1:A:607:ASN:OD1	2.47	0.45
1:A:99:LEU:HG	1:A:246:LEU:HD21	1.98	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: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:570:THR:OG1	1:C:571:GLU:N	2.50	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:HG23	1:A:599:ILE:HD12	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: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: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
1:C:547:ARG:HD3	1:C:548:LEU:N	2.32	0.44
1:B:318:MET:HE1	1:B:322:LEU:HD22	2.00	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:C:306:VAL:HG11	1:C:318:MET:HE1	2.00	0.43
1:B:438:ALA:HB1	1:B:530:LEU:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:553:GLU:C	1:B:575:TYR:HE2	2.21	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: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:323:LEU:N	1:C:323:LEU:CD1	2.81	0.43
1:C:294:LEU:HD21	1:C:404:SER:HA	2.00	0.43
1:B:294:LEU:HA	1:B:295:PRO:HD3	1.88	0.43
1:B:171:ARG:HH11	1:B:171:ARG:HG2	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: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: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:306:VAL:HG13	1:A:318:MET:CE	2.48	0.42
1:A:476:ASP:O	1:A:480:ARG:HG3	2.19	0.42
1:B:465:LYS:HZ1	1:B:484:GLN:HE21	1.67	0.42
1:C:315:LEU:HD12	1:C:318:MET:CE	2.50	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:B:301:ASN:OD1	1:B:301:ASN:N	2.52	0.42
1:C:581:MET:HG3	1:C:586:ASP:O	2.20	0.42
1:B:544:GLU:O	1:B:548:LEU:HG	2.20	0.42
1:C:446:MET:CE	1:C:451:TRP:CD2	3.03	0.42
1:C:99:LEU:HG	1:C:246:LEU:HD21	2.02	0.42
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:465:LYS:HZ2	1:B:484:GLN:HE21	1.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:459:LYS:HE3	1:C:463:GLU:OE1	2.20	0.41
1:B:190:LYS:HD3	1:B:202:PRO:O	2.20	0.41
1:C:364:LYS:HB3	1:C:364:LYS:HE3	1.91	0.41
1:A:560:ASN:HD22	1:A:561:PRO:HD2	1.85	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:474:ASP:HB2	1:A:477:MET:HB3	2.03	0.41
1:A:579:ILE:HB	1:A:589:THR:HG21	2.02	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: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:HA	1:B:419:LEU:HD23	1.94	0.41
1:B:442:ARG:HD2	1:B:536:LEU:O	2.20	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:HA	1:A:231:LEU:HD23	1.91	0.41
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:446:MET:SD	1:C:446:MET:C	3.00	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:C:604:VAL:C	1:C:605:ARG:HG2	2.42	0.40
1:A:420:TYR:CE2	1:A:485:ARG:HG3	2.57	0.40
1:C:157:ASP:O	1:C:161:VAL:HG23	2.21	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%)	47	68
1	B	534/578 (92%)	495 (93%)	33 (6%)	6 (1%)	14	26
1	C	533/578 (92%)	508 (95%)	24 (4%)	1 (0%)	47	68
All	All	1598/1734 (92%)	1520 (95%)	70 (4%)	8 (0%)	29	48

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	553	GLU
1	B	547	ARG
1	B	571	GLU
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 (i)

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%)	453 (97%)	12 (3%)	46	72
1	B	458/504 (91%)	446 (97%)	12 (3%)	46	72
1	C	465/504 (92%)	442 (95%)	23 (5%)	25	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1388/1512 (92%)	1341 (97%)	47 (3%)	38 63

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	VAL
1	A	142	HIS
1	A	195	SER
1	A	323	LEU
1	A	329	SER
1	A	449	LEU
1	A	472	LEU
1	A	532	ASN
1	A	547	ARG
1	A	560	ASN
1	A	565	SER
1	A	602	LEU
1	B	138	GLN
1	B	195	SER
1	B	237	PRO
1	B	238	VAL
1	B	294	LEU
1	B	446	MET
1	B	472	LEU
1	B	496	SER
1	B	536	LEU
1	B	555	LEU
1	B	595	LYS
1	B	601	ASP
1	C	110	VAL
1	C	187	ASP
1	C	196	LEU
1	C	238	VAL
1	C	266	ARG
1	C	301	ASN
1	C	313	ASN
1	C	318	MET
1	C	323	LEU
1	C	362	SER
1	C	404	SER
1	C	417	ASP
1	C	446	MET

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Mol	Chain	Res	Type
1	C	459	LYS
1	C	486	ARG
1	C	526	PRO
1	C	547	ARG
1	C	555	LEU
1	C	569	ASP
1	C	582[A]	GLU
1	C	582[B]	GLU
1	C	602	LEU
1	C	605	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) 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	326	GLN
1	B	331	GLN
1	B	408	GLN
1	B	484	GLN
1	B	520	HIS

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 carbohydrates 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, 95^{th} 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%)	-0.03	4 (0%) 87 89	32, 42, 85, 117	0
1	B	536/578 (92%)	0.40	42 (7%) 13 13	34, 58, 140, 217	0
1	C	536/578 (92%)	0.12	10 (1%) 66 69	33, 50, 101, 134	0
All	All	1607/1734 (92%)	0.16	56 (3%) 44 47	32, 47, 108, 217	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	619	ASN	9.1
1	B	602	LEU	6.0
1	B	621	PHE	4.6
1	B	614	LEU	4.5
1	B	569	ASP	4.2
1	B	552	ALA	4.1
1	B	568	PRO	4.1
1	B	570	THR	4.0
1	B	647	PRO	3.6
1	B	575	TYR	3.5
1	B	296[A]	ASP	3.5
1	B	643	PHE	3.3
1	C	259	THR	3.3
1	B	565	SER	3.2
1	B	549	LEU	3.2
1	B	431	GLU	3.1
1	A	639	VAL	3.0
1	B	576	VAL	3.0
1	B	623	VAL	3.0
1	B	640	THR	3.0
1	B	582[A]	GLU	2.9
1	B	561	PRO	2.9
1	B	642	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	554	VAL	2.8
1	B	503	ILE	2.8
1	B	591	THR	2.7
1	B	250	GLU	2.7
1	A	602	LEU	2.7
1	B	562	CYS	2.6
1	B	599	ILE	2.6
1	B	555	LEU	2.6
1	B	579	ILE	2.6
1	C	576	VAL	2.6
1	B	572	GLY	2.5
1	B	281	CYS	2.5
1	B	595	LYS	2.4
1	C	252	ALA	2.4
1	B	255	HIS	2.4
1	C	566	PHE	2.4
1	A	539	GLU	2.3
1	C	568	PRO	2.3
1	B	646	PRO	2.3
1	B	405	PHE	2.3
1	B	567	LEU	2.2
1	C	647	PRO	2.2
1	A	283	ASP	2.2
1	B	301	ASN	2.2
1	B	641	PRO	2.2
1	B	573	HIS	2.2
1	B	490	CYS	2.1
1	B	437	PRO	2.1
1	B	601	ASP	2.0
1	C	302	VAL	2.0
1	C	296	ASP	2.0
1	C	417	ASP	2.0
1	C	639	VAL	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 carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.