Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2023 – 09:06 PM JST

PDB ID	:	8HCY
Title	:	Legionella glycosyltransferase
Authors	:	Chen, T.T.; Ouyang, S.Y.
Deposited on	:	2022-11-03
Resolution	:	2.64 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:

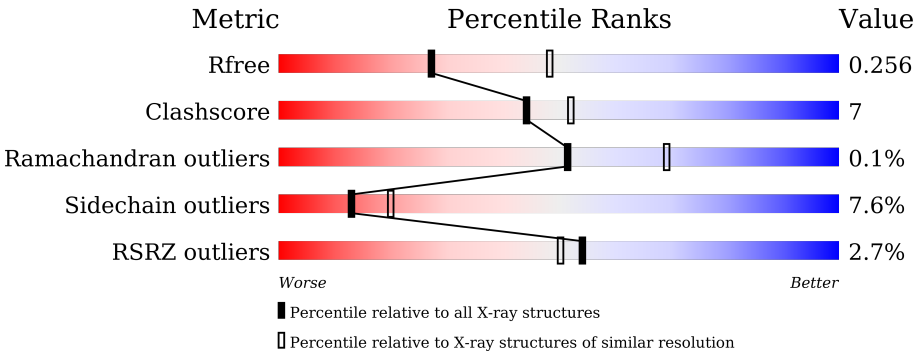
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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 <=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	865	2% 45% 11% 42%
1	B	865	48% 9% 42%
1	C	865	45% 12% 42%
1	D	865	2% 46% 10% 42%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 16216 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 Dot/Icm secretion system substrate.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	499	Total	C	N	O	S	0	0	0
			3956	2500	676	767	13			
1	A	499	Total	C	N	O	S	0	0	0
			3956	2500	676	767	13			
1	B	499	Total	C	N	O	S	0	0	0
			3956	2500	676	767	13			
1	D	499	Total	C	N	O	S	0	0	0
			3956	2500	676	767	13			

- Molecule 2 is water.

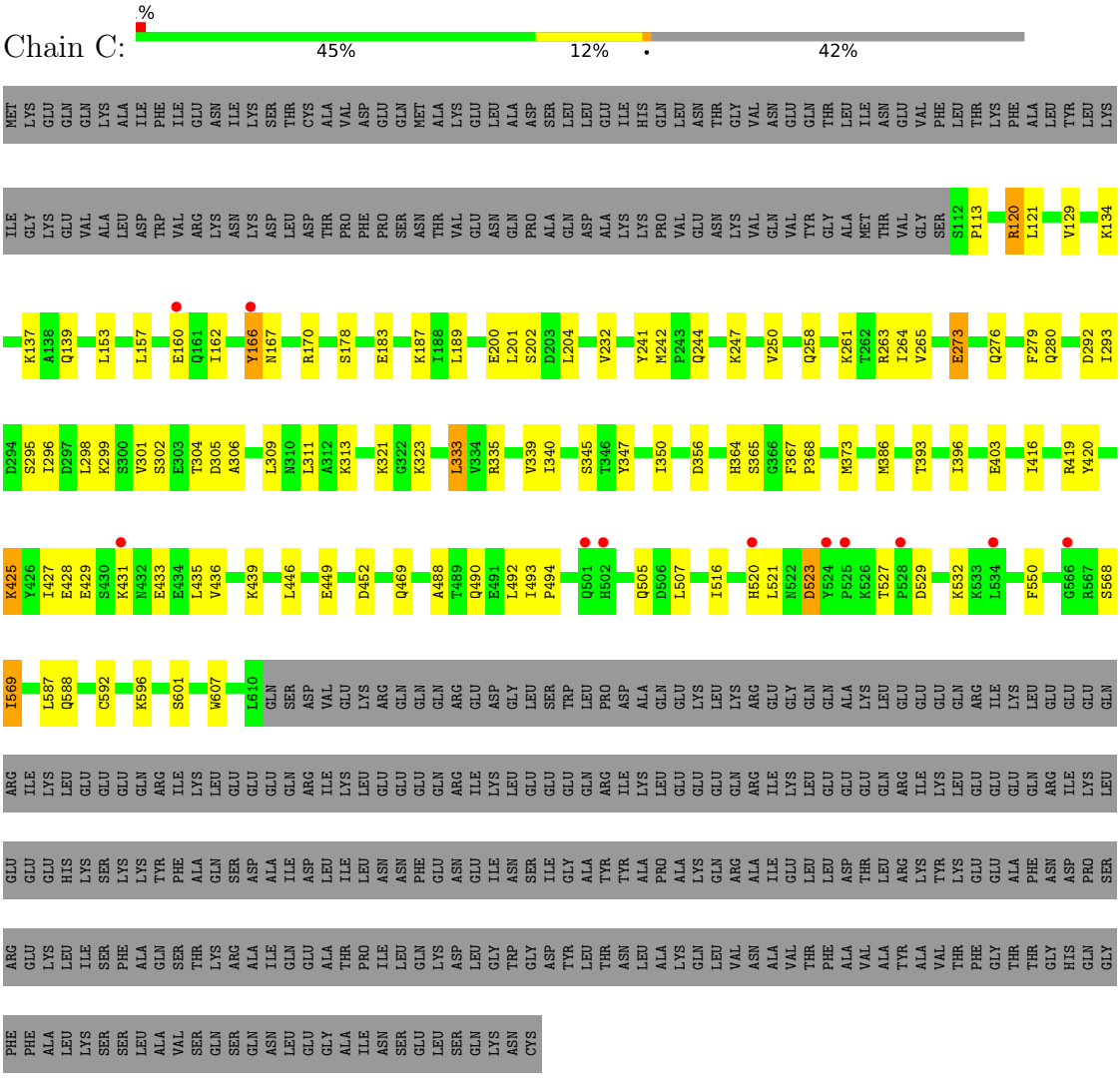
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	91	Total	O	0	0
			91	91		
2	A	83	Total	O	0	0
			83	83		
2	B	99	Total	O	0	0
			99	99		
2	D	119	Total	O	0	0
			119	119		

3 Residue-property plots (i)

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.

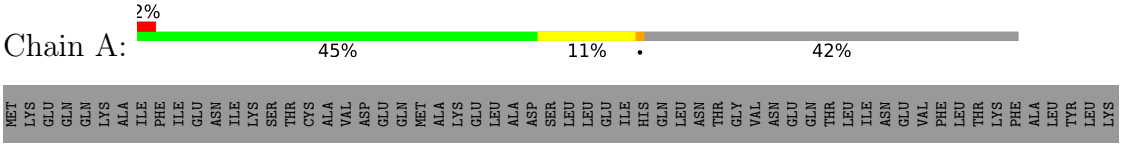
• Molecule 1: Dot/Icm secretion system substrate

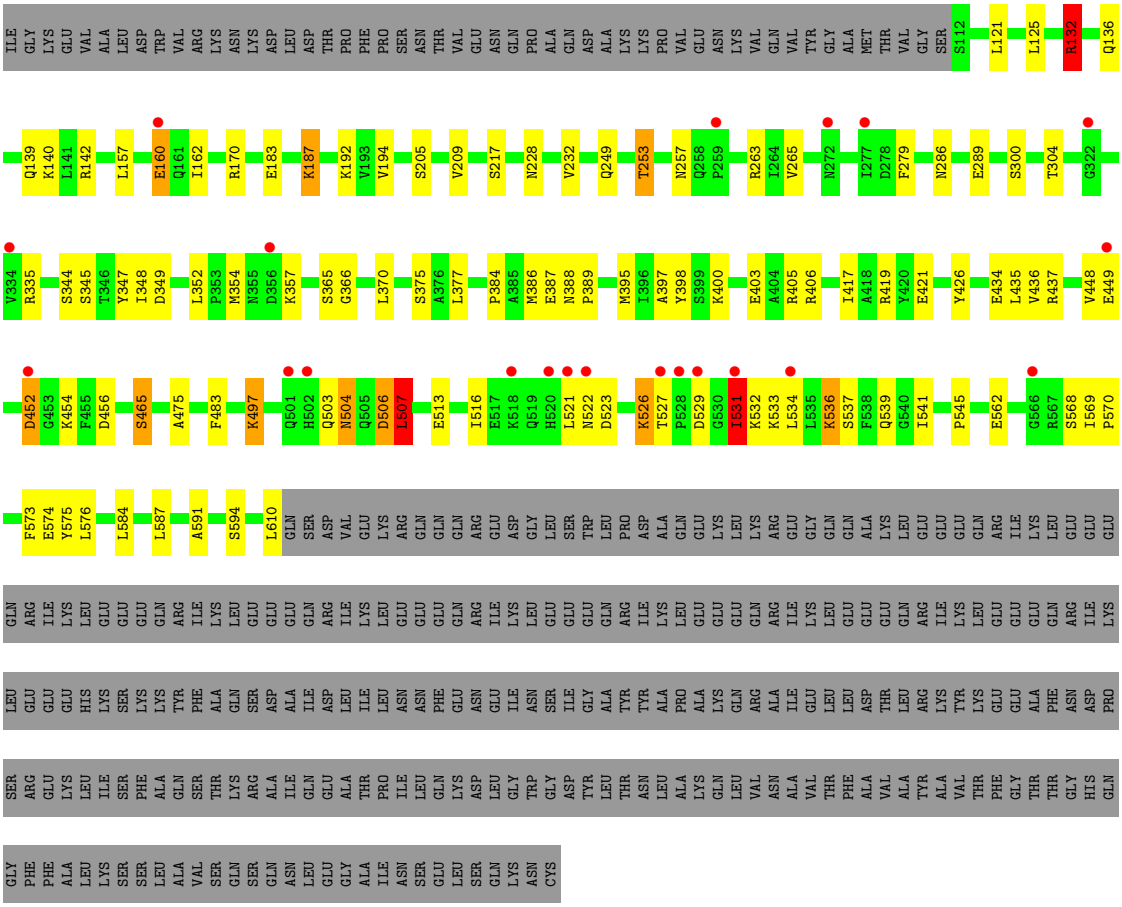
Chain C:



• Molecule 1: Dot/Icm secretion system substrate

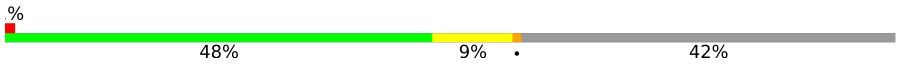
Chain A:

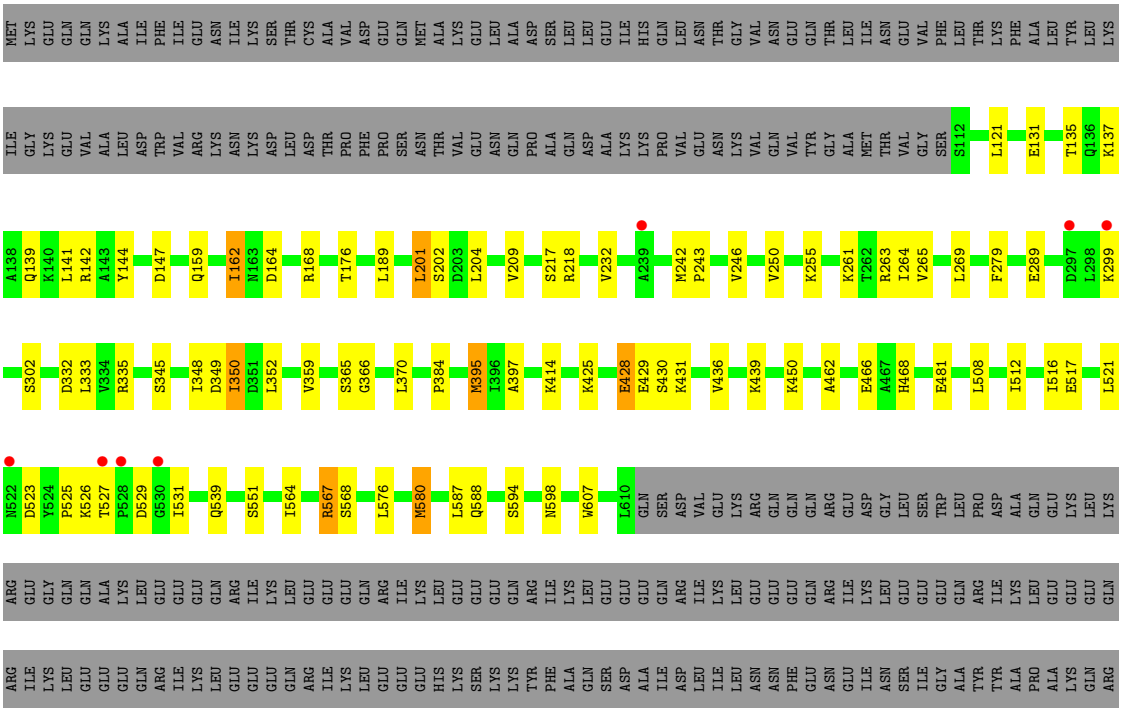


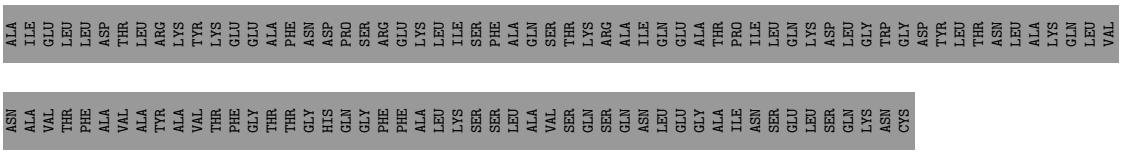


• Molecule 1: Dot/Icm secretion system substrate

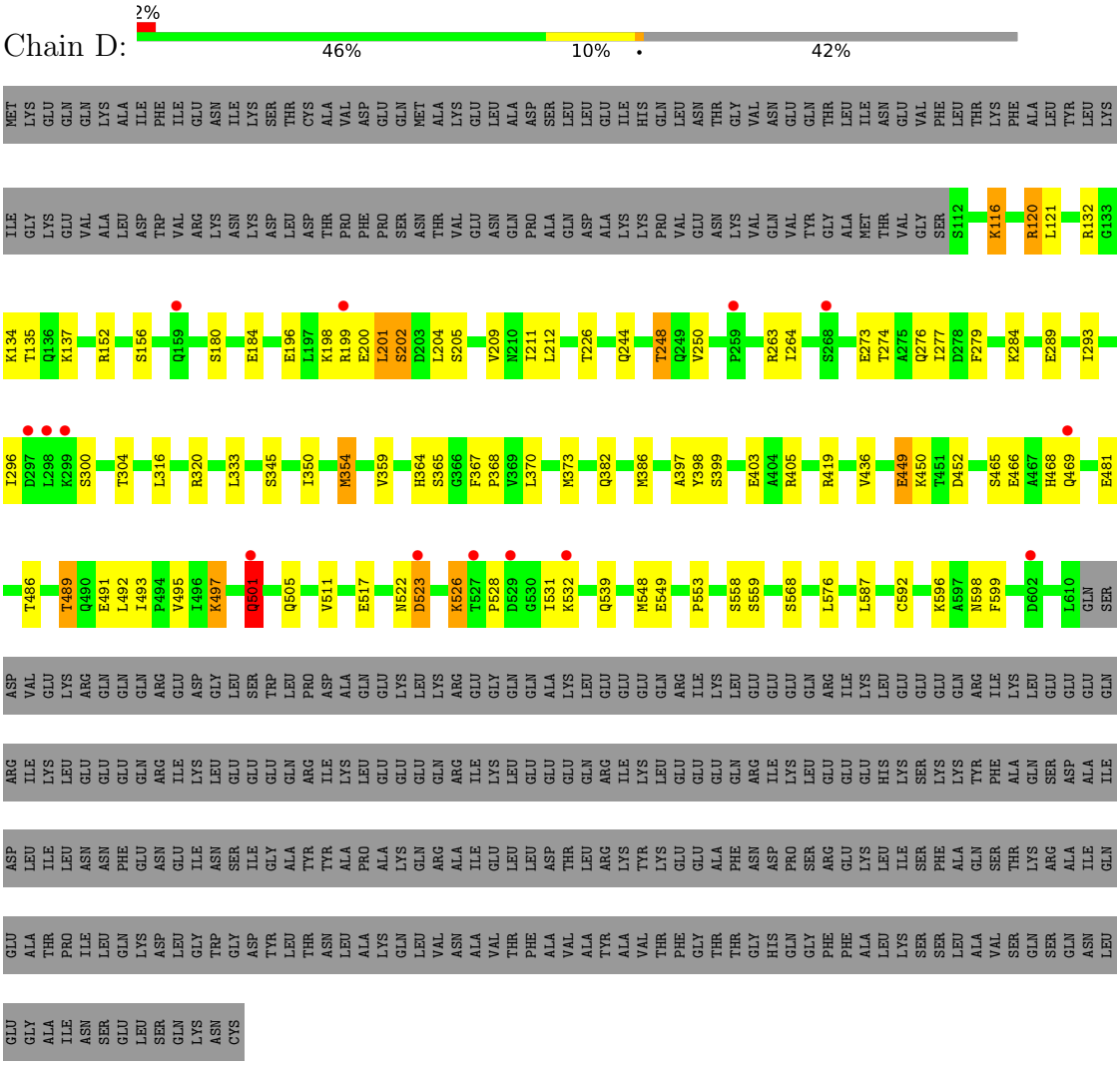
Chain B:







• Molecule 1: Dot/Icm secretion system substrate



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.36Å 112.61Å 125.80Å 90.00° 108.14° 90.00°	Depositor
Resolution (Å)	29.31 – 2.64 29.63 – 2.64	Depositor EDS
% Data completeness (in resolution range)	95.6 (29.31-2.64) 95.8 (29.63-2.64)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.64Å)	Xtriage
Refinement program	PHENIX 1.18_3845	Depositor
R, R_{free}	0.240 , 0.256 0.240 , 0.256	Depositor DCC
R_{free} test set	2001 reflections (2.90%)	wwPDB-VP
Wilson B-factor (Å^2)	28.3	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	16216	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.38 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.6758e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.37	2/4027 (0.0%)	0.59	6/5441 (0.1%)
1	B	0.37	0/4027	0.63	4/5441 (0.1%)
1	C	0.37	0/4027	0.71	7/5441 (0.1%)
1	D	0.36	0/4027	0.58	4/5441 (0.1%)
All	All	0.37	2/16108 (0.0%)	0.63	21/21764 (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	C	0	1
1	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	GLU	CD-OE2	7.43	1.33	1.25
1	A	526	LYS	CE-NZ	5.32	1.62	1.49

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	120	ARG	NE-CZ-NH2	-16.25	112.18	120.30
1	B	189	LEU	CB-CG-CD2	-15.63	84.43	111.00
1	C	120	ARG	NE-CZ-NH1	13.59	127.09	120.30
1	C	569	ILE	CG1-CB-CG2	-10.05	89.29	111.40
1	C	200	GLU	CB-CA-C	9.91	130.22	110.40
1	D	201	LEU	CB-CA-C	8.40	126.17	110.20
1	C	120	ARG	CG-CD-NE	-8.35	94.26	111.80
1	B	201	LEU	CB-CA-C	8.13	125.65	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	120	ARG	CB-CG-CD	-7.71	91.55	111.60
1	C	201	LEU	CB-CA-C	7.53	124.50	110.20
1	A	526	LYS	N-CA-CB	-7.34	97.38	110.60
1	A	526	LYS	CG-CD-CE	-7.13	90.52	111.90
1	A	507	LEU	CA-CB-CG	6.97	131.32	115.30
1	B	121	LEU	CB-CG-CD1	-6.59	99.79	111.00
1	D	501	GLN	CA-CB-CG	-6.21	99.74	113.40
1	A	132	ARG	CB-CA-C	5.94	122.28	110.40
1	A	531	ILE	CB-CG1-CD1	5.92	130.47	113.90
1	D	449	GLU	CB-CA-C	5.21	120.82	110.40
1	D	450	LYS	CB-CA-C	5.16	120.71	110.40
1	B	189	LEU	CB-CG-CD1	5.07	119.62	111.00
1	A	526	LYS	CB-CG-CD	-5.04	98.49	111.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	258	GLN	Peptide
1	D	120	ARG	Sidechain

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	3956	0	3964	58	0
1	B	3956	0	3964	42	0
1	C	3956	0	3964	67	0
1	D	3956	0	3964	45	0
2	A	83	0	0	2	0
2	B	99	0	0	3	0
2	C	91	0	0	2	0
2	D	119	0	0	2	0
All	All	16216	0	15856	210	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 7.

All (210) 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:C:166:TYR:HD2	1:C:167:ASN:N	1.39	1.20
1:C:166:TYR:HE2	1:C:167:ASN:CG	1.57	1.05
1:C:166:TYR:CD2	1:C:167:ASN:N	2.29	1.00
1:C:166:TYR:HE2	1:C:167:ASN:OD1	1.49	0.95
1:C:166:TYR:CE2	1:C:167:ASN:CG	2.41	0.93
1:A:527:THR:HG22	1:A:529:ASP:H	1.37	0.89
1:C:298:LEU:HD22	1:C:306:ALA:HA	1.56	0.86
1:C:166:TYR:CE2	1:C:170:ARG:NH1	2.45	0.82
1:C:166:TYR:CD2	1:C:166:TYR:C	2.56	0.78
1:C:166:TYR:CE2	1:C:167:ASN:OD1	2.36	0.76
1:C:166:TYR:CE2	1:C:167:ASN:ND2	2.54	0.76
1:D:359:VAL:H	1:D:598:ASN:HD21	1.34	0.76
1:D:489:THR:HG23	1:D:491:GLU:H	1.52	0.75
1:A:136:GLN:O	1:A:139:GLN:NE2	2.23	0.72
1:D:273:GLU:O	1:D:277:ILE:HG13	1.90	0.71
1:D:481:GLU:HA	1:D:493:ILE:HD11	1.72	0.71
1:C:166:TYR:HD2	1:C:167:ASN:H	1.37	0.70
1:C:419:ARG:NH1	2:C:902:HOH:O	2.24	0.70
1:B:255:LYS:NZ	2:B:902:HOH:O	2.25	0.69
1:C:166:TYR:CD2	1:C:170:ARG:NH1	2.60	0.69
1:A:506:ASP:OD1	1:A:506:ASP:N	2.26	0.69
1:C:527:THR:HG22	1:C:529:ASP:H	1.55	0.69
1:C:523:ASP:N	1:C:523:ASP:OD2	2.20	0.67
1:D:398:TYR:HB3	1:D:405:ARG:HD2	1.76	0.67
1:A:398:TYR:HB3	1:A:405:ARG:HD2	1.77	0.67
1:A:529:ASP:OD1	1:A:533:LYS:NZ	2.24	0.65
1:C:166:TYR:HE2	1:C:167:ASN:ND2	1.90	0.65
1:C:516:ILE:HA	1:C:521:LEU:HD12	1.78	0.64
1:C:250:VAL:HG11	1:C:264:ILE:HD11	1.78	0.64
1:B:348:ILE:HG22	1:B:349:ASP:O	1.99	0.63
1:C:241:TYR:OH	1:C:247:LYS:NZ	2.31	0.63
1:D:250:VAL:HG11	1:D:264:ILE:HD11	1.80	0.62
1:C:507:LEU:HD12	1:D:495:VAL:HG13	1.82	0.62
1:A:348:ILE:HG22	1:A:349:ASP:O	2.00	0.62
1:C:183:GLU:O	1:C:187:LYS:HG2	1.99	0.62
1:A:183:GLU:O	1:A:187:LYS:HE2	2.00	0.62
1:B:567:ARG:HD3	1:B:567:ARG:H	1.64	0.62
1:C:427:ILE:HG12	1:C:435:LEU:HD22	1.82	0.61
1:A:370:LEU:HB2	1:A:397:ALA:HB3	1.83	0.61
1:D:373:MET:HE2	1:D:592:CYS:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:MET:HE1	1:C:587:LEU:HB3	1.82	0.60
1:D:359:VAL:H	1:D:598:ASN:ND2	2.00	0.60
1:B:250:VAL:HG11	1:B:264:ILE:HD11	1.84	0.60
1:C:301:VAL:HG22	1:C:339:VAL:HG11	1.82	0.60
1:B:232:VAL:HG22	1:B:265:VAL:HB	1.84	0.59
1:A:516:ILE:HD11	1:A:534:LEU:HD22	1.83	0.59
1:A:386:MET:HE3	1:A:569:ILE:HG12	1.85	0.58
1:D:273:GLU:HA	1:D:276:GLN:HB2	1.85	0.58
1:B:462:ALA:O	1:B:466:GLU:HG2	2.04	0.58
1:D:152:ARG:NH2	1:D:200:GLU:OE2	2.33	0.58
1:A:531:ILE:HD12	1:A:532:LYS:N	2.19	0.57
1:C:129:VAL:HG12	1:C:202:SER:HB3	1.86	0.57
1:C:298:LEU:CD2	1:C:306:ALA:HA	2.31	0.57
1:A:232:VAL:HG22	1:A:265:VAL:HB	1.86	0.57
1:D:359:VAL:HG22	1:D:598:ASN:ND2	2.20	0.56
1:A:465:SER:HA	1:A:539:GLN:HE21	1.71	0.55
1:A:569:ILE:HG13	1:A:570:PRO:HD2	1.87	0.55
1:A:249:GLN:O	1:A:253:THR:HG23	2.07	0.55
1:A:344:SER:HB2	1:A:400:LYS:HG3	1.88	0.55
1:C:232:VAL:HG22	1:C:265:VAL:HB	1.88	0.54
1:A:532:LYS:HD2	1:A:536:LYS:HG2	1.90	0.54
1:D:359:VAL:HG22	1:D:598:ASN:HD21	1.71	0.54
1:B:564:ILE:O	1:B:567:ARG:HD2	2.06	0.54
1:B:428:GLU:HA	1:B:439:LYS:HD3	1.90	0.54
1:C:298:LEU:HD21	1:C:309:LEU:HB2	1.90	0.54
1:A:348:ILE:HG23	1:A:352:LEU:HD12	1.90	0.54
1:A:465:SER:HA	1:A:539:GLN:NE2	2.22	0.54
1:B:567:ARG:HG2	1:B:568:SER:O	2.08	0.54
1:D:209:VAL:HG11	1:D:587:LEU:HD21	1.91	0.53
1:D:481:GLU:HA	1:D:493:ILE:CD1	2.39	0.53
1:D:198:LYS:O	1:D:202:SER:OG	2.26	0.52
1:C:242:MET:HG2	1:C:247:LYS:HG3	1.90	0.52
1:C:373:MET:CE	1:C:587:LEU:HB3	2.40	0.52
1:C:490:GLN:O	1:C:493:ILE:HD12	2.09	0.52
1:D:419:ARG:NH1	1:D:549:GLU:O	2.42	0.52
1:D:250:VAL:HG11	1:D:264:ILE:CD1	2.41	0.51
1:D:548:MET:HG3	1:D:553:PRO:HD2	1.93	0.51
1:C:139:GLN:CD	1:C:139:GLN:H	2.14	0.51
1:C:276:GLN:O	1:C:280:GLN:HG2	2.10	0.51
1:A:132:ARG:H	1:A:132:ARG:HE	1.57	0.51
1:B:414:LYS:NZ	2:B:901:HOH:O	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:THR:HB	1:C:396:ILE:HD11	1.93	0.51
1:A:140:LYS:HB3	1:A:384:PRO:HD3	1.93	0.51
1:B:246:VAL:HG13	1:B:350:ILE:CD1	2.41	0.51
1:C:153:LEU:HD22	1:C:189:LEU:HD22	1.93	0.50
1:B:144:TYR:HB2	1:B:384:PRO:HD2	1.92	0.50
1:D:523:ASP:OD1	1:D:523:ASP:N	2.31	0.50
1:B:201:LEU:O	1:B:576:LEU:HD13	2.12	0.50
1:D:364:HIS:O	1:D:596:LYS:HE3	2.11	0.50
1:B:512:ILE:HG21	1:B:531:ILE:HG23	1.94	0.49
1:B:218:ARG:HD2	1:B:580:MET:HG3	1.94	0.49
1:D:528:PRO:O	1:D:531:ILE:HG13	2.12	0.49
1:C:493:ILE:HB	1:C:494:PRO:HD3	1.95	0.49
1:A:435:LEU:CD1	1:A:545:PRO:HB2	2.43	0.49
1:A:209:VAL:HG11	1:A:587:LEU:HD21	1.95	0.49
1:A:516:ILE:HA	1:A:521:LEU:HD12	1.95	0.49
1:B:348:ILE:HG23	1:B:352:LEU:HD12	1.93	0.49
1:D:468:HIS:CG	1:D:539:GLN:HB2	2.47	0.49
1:A:574:GLU:HB2	1:A:575:TYR:CD2	2.47	0.49
1:C:429:GLU:OE2	2:C:901:HOH:O	2.20	0.49
1:A:437:ARG:HG3	1:A:437:ARG:HH11	1.78	0.49
1:A:465:SER:HB2	1:A:539:GLN:HE22	1.78	0.49
1:B:527:THR:HG22	1:B:529:ASP:H	1.78	0.48
1:D:196:GLU:OE1	1:D:199:ARG:NH2	2.38	0.48
1:B:250:VAL:HG23	1:B:350:ILE:HD13	1.94	0.48
1:D:382:GLN:NE2	2:D:904:HOH:O	2.28	0.48
1:C:242:MET:HE3	1:C:247:LYS:HA	1.96	0.48
1:A:263:ARG:HG2	1:A:289:GLU:HB3	1.96	0.48
1:A:504:ASN:ND2	1:A:507:LEU:H	2.12	0.48
1:A:419:ARG:HG2	1:A:426:TYR:CD2	2.48	0.48
1:D:354:MET:HG2	1:D:599:PHE:CE2	2.49	0.47
1:B:567:ARG:HD3	1:B:567:ARG:N	2.24	0.47
1:D:120:ARG:NH2	2:D:916:HOH:O	2.47	0.47
1:C:364:HIS:O	1:C:596:LYS:HE3	2.14	0.47
1:A:526:LYS:HE3	1:A:526:LYS:HB2	1.49	0.47
1:B:425:LYS:O	1:B:429:GLU:HG3	2.14	0.47
1:D:293:ILE:O	1:D:296:ILE:HG22	2.15	0.47
1:C:293:ILE:HA	1:C:296:ILE:HD12	1.97	0.47
1:A:513:GLU:HG2	1:A:526:LYS:HG2	1.96	0.47
1:D:244:GLN:HE22	1:D:248:THR:HG23	1.78	0.47
1:D:116:LYS:HD3	1:D:116:LYS:HA	1.63	0.47
1:A:170:ARG:NH1	1:B:147:ASP:OD2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:LEU:HB2	1:B:397:ALA:HB3	1.96	0.47
1:D:501:GLN:O	1:D:501:GLN:HG3	2.15	0.47
1:B:164:ASP:O	1:B:168:ARG:HG3	2.15	0.46
1:B:359:VAL:HG22	1:B:598:ASN:OD1	2.15	0.46
1:B:516:ILE:HA	1:B:521:LEU:HD12	1.97	0.46
1:A:139:GLN:H	1:A:139:GLN:CD	2.18	0.46
1:D:201:LEU:O	1:D:576:LEU:HD13	2.14	0.46
1:A:125:LEU:HD22	1:A:194:VAL:HG13	1.98	0.46
1:B:468:HIS:CG	1:B:539:GLN:HB2	2.50	0.46
1:C:273:GLU:H	1:C:273:GLU:HG2	1.59	0.46
1:B:263:ARG:HG2	1:B:289:GLU:HB3	1.97	0.46
1:D:373:MET:CE	1:D:587:LEU:HB3	2.46	0.46
1:A:587:LEU:HA	1:A:591:ALA:HB3	1.97	0.46
1:C:469:GLN:O	1:C:532:LYS:NZ	2.48	0.46
1:B:139:GLN:OE1	1:B:142:ARG:NH1	2.49	0.46
1:C:469:GLN:O	1:C:532:LYS:HG2	2.16	0.46
1:D:211:ILE:HB	1:D:367:PHE:CZ	2.51	0.46
1:B:159:GLN:HA	1:B:162:ILE:HG12	1.98	0.45
1:C:431:LYS:HA	1:C:431:LYS:HD3	1.58	0.45
1:A:286:ASN:ND2	2:A:909:HOH:O	2.41	0.45
1:D:370:LEU:HB2	1:D:397:ALA:HB3	1.98	0.45
1:A:121:LEU:HD23	1:A:121:LEU:HA	1.85	0.45
1:C:446:LEU:HA	1:C:449:GLU:OE1	2.17	0.45
1:A:228:ASN:ND2	2:A:913:HOH:O	2.50	0.45
1:A:335:ARG:HG2	1:A:347:TYR:CD2	2.52	0.45
1:A:532:LYS:HB3	1:A:532:LYS:HE3	1.72	0.45
1:C:492:LEU:HD23	1:C:492:LEU:HA	1.84	0.45
1:C:157:LEU:HB2	1:C:162:ILE:HG13	1.97	0.45
1:C:311:LEU:HD21	1:C:420:TYR:CD2	2.52	0.45
1:A:348:ILE:HD13	1:A:395:MET:HG3	1.98	0.45
1:D:263:ARG:HG2	1:D:289:GLU:HB3	1.99	0.45
1:C:333:LEU:HD11	1:C:416:ILE:HG21	1.99	0.44
1:B:431:LYS:N	1:B:431:LYS:HD3	2.32	0.44
1:C:263:ARG:NH2	1:C:340:ILE:O	2.51	0.44
1:C:166:TYR:CZ	1:C:170:ARG:NH1	2.85	0.44
1:C:244:GLN:OE1	1:C:247:LYS:HE2	2.16	0.44
1:B:209:VAL:HG11	1:B:587:LEU:HD21	2.00	0.44
1:B:243:PRO:HD3	2:B:910:HOH:O	2.18	0.44
1:A:375:SER:HB2	1:A:387:GLU:HG3	2.00	0.43
1:A:497:LYS:HB3	1:A:497:LYS:HE3	1.56	0.43
1:D:497:LYS:HD2	1:D:497:LYS:HA	1.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:ASP:HB3	1:A:454:LYS:HE3	1.99	0.43
1:D:517:GLU:HG2	1:D:526:LYS:HD2	1.99	0.43
1:C:419:ARG:HD2	1:C:550:PHE:HA	2.00	0.43
1:B:332:ASP:HB3	1:B:551:SER:O	2.18	0.43
1:B:526:LYS:HE2	1:B:526:LYS:HB2	1.87	0.43
1:C:335:ARG:HG2	1:C:347:TYR:CD2	2.54	0.43
1:B:395:MET:HE2	1:B:395:MET:HB2	1.89	0.43
1:C:373:MET:HE2	1:C:592:CYS:HB3	2.00	0.43
1:B:517:GLU:CD	1:B:526:LYS:HD2	2.39	0.43
1:A:417:ILE:O	1:A:421:GLU:HG3	2.19	0.42
1:B:525:PRO:C	1:B:527:THR:H	2.22	0.42
1:D:212:LEU:HG	1:D:559:SER:HB3	2.02	0.42
1:D:316:LEU:O	1:D:320:ARG:HG3	2.19	0.42
1:C:301:VAL:HG13	1:C:305:ASP:CB	2.50	0.42
1:A:257:ASN:HB2	1:A:354:MET:HE1	2.01	0.42
1:A:573:PHE:HB3	1:A:576:LEU:HG	2.02	0.42
1:A:536:LYS:HA	1:A:536:LYS:HD2	1.54	0.42
1:D:373:MET:CE	1:D:592:CYS:HB3	2.49	0.42
1:C:436:VAL:HA	1:C:439:LYS:HE2	2.01	0.42
1:C:113:PRO:HG2	1:C:178:SER:O	2.20	0.42
1:C:321:LYS:O	1:C:323:LYS:HG2	2.20	0.42
1:C:425:LYS:HE2	1:C:425:LYS:HB2	1.88	0.42
1:B:588:GLN:HG3	1:B:607:TRP:CD1	2.54	0.42
1:C:309:LEU:O	1:C:313:LYS:HG3	2.19	0.42
1:A:157:LEU:HD12	1:A:162:ILE:HD13	2.01	0.42
1:A:475:ALA:HB2	1:A:483:PHE:CD1	2.54	0.42
1:A:534:LEU:O	1:A:537:SER:OG	2.35	0.42
1:A:532:LYS:O	1:A:536:LYS:HG2	2.20	0.41
1:C:137:LYS:HA	1:C:139:GLN:HE22	1.85	0.41
1:B:450:LYS:HD2	1:B:450:LYS:HA	1.92	0.41
1:D:386:MET:H	1:D:386:MET:HG2	1.72	0.41
1:C:367:PHE:CG	1:C:368:PRO:HD2	2.55	0.41
1:C:292:ASP:HB3	1:C:295:SER:HB2	2.02	0.41
1:A:403:GLU:HG2	1:A:406:ARG:HH21	1.85	0.41
1:B:242:MET:SD	1:B:246:VAL:HG12	2.60	0.41
1:A:217:SER:O	1:A:366:GLY:HA3	2.20	0.41
1:D:367:PHE:CG	1:D:368:PRO:HD2	2.55	0.41
1:A:388:ASN:HD22	1:A:389:PRO:HD2	1.85	0.41
1:D:373:MET:HE1	1:D:587:LEU:HB3	2.03	0.40
1:D:368:PRO:HA	1:D:399:SER:HB2	2.03	0.40
1:B:269:LEU:HD23	1:B:269:LEU:HA	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:MET:CE	1:C:592:CYS:HB3	2.52	0.40
1:A:377:LEU:HA	1:A:386:MET:O	2.22	0.40
1:A:434:GLU:HG3	1:A:541:ILE:O	2.21	0.40
1:B:217:SER:O	1:B:366:GLY:HA3	2.21	0.40
1:C:373:MET:HE2	1:C:373:MET:HB2	1.93	0.40
1:C:588:GLN:HG3	1:C:607:TRP:CD1	2.56	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	497/865 (58%)	482 (97%)	15 (3%)	0	100 100
1	B	497/865 (58%)	483 (97%)	14 (3%)	0	100 100
1	C	497/865 (58%)	484 (97%)	12 (2%)	1 (0%)	47 64
1	D	497/865 (58%)	480 (97%)	17 (3%)	0	100 100
All	All	1988/3460 (58%)	1929 (97%)	58 (3%)	1 (0%)	51 69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	488	ALA

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	439/763 (58%)	406 (92%)	33 (8%)	13 20
1	B	439/763 (58%)	412 (94%)	27 (6%)	18 28
1	C	439/763 (58%)	410 (93%)	29 (7%)	16 25
1	D	439/763 (58%)	395 (90%)	44 (10%)	7 10
All	All	1756/3052 (58%)	1623 (92%)	133 (8%)	13 20

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	120	ARG
1	C	121	LEU
1	C	134	LYS
1	C	160	GLU
1	C	166	TYR
1	C	204	LEU
1	C	261	LYS
1	C	273	GLU
1	C	279	PHE
1	C	299	LYS
1	C	302	SER
1	C	304	THR
1	C	333	LEU
1	C	345	SER
1	C	350	ILE
1	C	356	ASP
1	C	365	SER
1	C	386	MET
1	C	403	GLU
1	C	425	LYS
1	C	428	GLU
1	C	433	GLU
1	C	452	ASP
1	C	505	GLN
1	C	520	HIS
1	C	523	ASP
1	C	568	SER
1	C	569	ILE
1	C	601	SER
1	A	132	ARG
1	A	142	ARG

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Mol	Chain	Res	Type
1	A	160	GLU
1	A	187	LYS
1	A	192	LYS
1	A	205	SER
1	A	253	THR
1	A	279	PHE
1	A	300	SER
1	A	304	THR
1	A	345	SER
1	A	357	LYS
1	A	365	SER
1	A	436	VAL
1	A	448	VAL
1	A	449	GLU
1	A	452	ASP
1	A	456	ASP
1	A	465	SER
1	A	497	LYS
1	A	503	GLN
1	A	504	ASN
1	A	506	ASP
1	A	507	LEU
1	A	522	ASN
1	A	523	ASP
1	A	531	ILE
1	A	536	LYS
1	A	562	GLU
1	A	568	SER
1	A	584	LEU
1	A	594	SER
1	A	610	LEU
1	B	131	GLU
1	B	135	THR
1	B	137	LYS
1	B	141	LEU
1	B	162	ILE
1	B	176	THR
1	B	202	SER
1	B	204	LEU
1	B	261	LYS
1	B	279	PHE
1	B	299	LYS

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Mol	Chain	Res	Type
1	B	302	SER
1	B	333	LEU
1	B	335	ARG
1	B	345	SER
1	B	350	ILE
1	B	365	SER
1	B	395	MET
1	B	428	GLU
1	B	430	SER
1	B	436	VAL
1	B	481	GLU
1	B	508	LEU
1	B	523	ASP
1	B	567	ARG
1	B	580	MET
1	B	594	SER
1	D	116	LYS
1	D	121	LEU
1	D	132	ARG
1	D	134	LYS
1	D	135	THR
1	D	137	LYS
1	D	156	SER
1	D	180	SER
1	D	184	GLU
1	D	202	SER
1	D	204	LEU
1	D	205	SER
1	D	226	THR
1	D	248	THR
1	D	274	THR
1	D	279	PHE
1	D	284	LYS
1	D	300	SER
1	D	304	THR
1	D	333	LEU
1	D	345	SER
1	D	350	ILE
1	D	354	MET
1	D	365	SER
1	D	403	GLU
1	D	436	VAL

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Mol	Chain	Res	Type
1	D	449	GLU
1	D	452	ASP
1	D	465	SER
1	D	466	GLU
1	D	469	GLN
1	D	486	THR
1	D	489	THR
1	D	492	LEU
1	D	497	LYS
1	D	501	GLN
1	D	505	GLN
1	D	511	VAL
1	D	522	ASN
1	D	523	ASP
1	D	526	LYS
1	D	532	LYS
1	D	558	SER
1	D	568	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	286	ASN
1	C	432	ASN
1	C	519	GLN
1	A	272	ASN
1	A	388	ASN
1	A	504	ASN
1	A	505	GLN
1	A	539	GLN
1	B	281	GLN
1	B	382	GLN
1	B	407	GLN
1	D	244	GLN
1	D	257	ASN
1	D	258	GLN
1	D	287	ASN
1	D	598	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 monosaccharides 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	499/865 (57%)	0.21	21 (4%) 36 33	22, 34, 66, 103	0
1	B	499/865 (57%)	0.07	7 (1%) 75 73	21, 32, 53, 82	0
1	C	499/865 (57%)	0.15	11 (2%) 62 58	21, 33, 58, 116	0
1	D	499/865 (57%)	0.18	14 (2%) 53 49	23, 35, 56, 82	0
All	All	1996/3460 (57%)	0.15	53 (2%) 54 50	21, 34, 57, 116	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	528	PRO	6.0
1	A	160	GLU	5.4
1	A	527	THR	4.4
1	A	531	ILE	3.9
1	A	356	ASP	3.8
1	D	299	LYS	3.6
1	C	160	GLU	3.6
1	B	527	THR	3.2
1	C	166	TYR	3.1
1	D	298	LEU	3.0
1	D	532	LYS	2.8
1	B	299	LYS	2.8
1	C	524	TYR	2.8
1	A	521	LEU	2.8
1	C	431	LYS	2.8
1	A	529	ASP	2.7
1	D	529	ASP	2.7
1	A	452	ASP	2.7
1	D	501	GLN	2.7
1	D	527	THR	2.7
1	D	469	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	523	ASP	2.6
1	C	534	LEU	2.6
1	C	501	GLN	2.6
1	A	520	HIS	2.6
1	A	259	PRO	2.5
1	B	530	GLY	2.5
1	C	520	HIS	2.5
1	A	502	HIS	2.5
1	D	259	PRO	2.4
1	C	566	GLY	2.4
1	A	566	GLY	2.4
1	D	199	ARG	2.3
1	D	602	ASP	2.3
1	A	522	ASN	2.3
1	C	502	HIS	2.3
1	A	277	ILE	2.3
1	A	322	GLY	2.2
1	B	297	ASP	2.2
1	D	268	SER	2.2
1	C	528	PRO	2.2
1	A	272	ASN	2.2
1	B	522	ASN	2.2
1	A	518	LYS	2.1
1	A	449	GLU	2.1
1	A	334	VAL	2.1
1	D	159	GLN	2.1
1	A	501	GLN	2.1
1	A	534	LEU	2.0
1	B	528	PRO	2.0
1	D	297	ASP	2.0
1	C	525	PRO	2.0
1	B	239	ALA	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 monosaccharides 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.