Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 11:41 AM EST

PDB ID	:	4W4H
Title	:	Escherichia coli tryptophanase in holo form
Authors	:	Goldgur, Y.
Deposited on	:	2014-08-14
Resolution	:	2.89 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 (i) 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 (i)) were used in the production of this report:

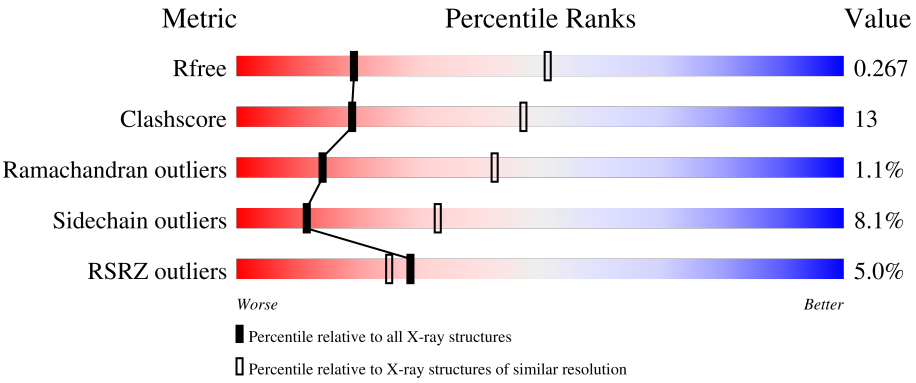
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.89 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	467	6% 65% 24% · 8%
1	B	467	4% 67% 23% · 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6832 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 Tryptophanase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	P	S	0	0	0
			3377	2146	567	641	1	22			
1	B	433	Total	C	N	O	P	S	0	0	0
			3413	2170	573	647	1	22			

- Molecule 2 is water.

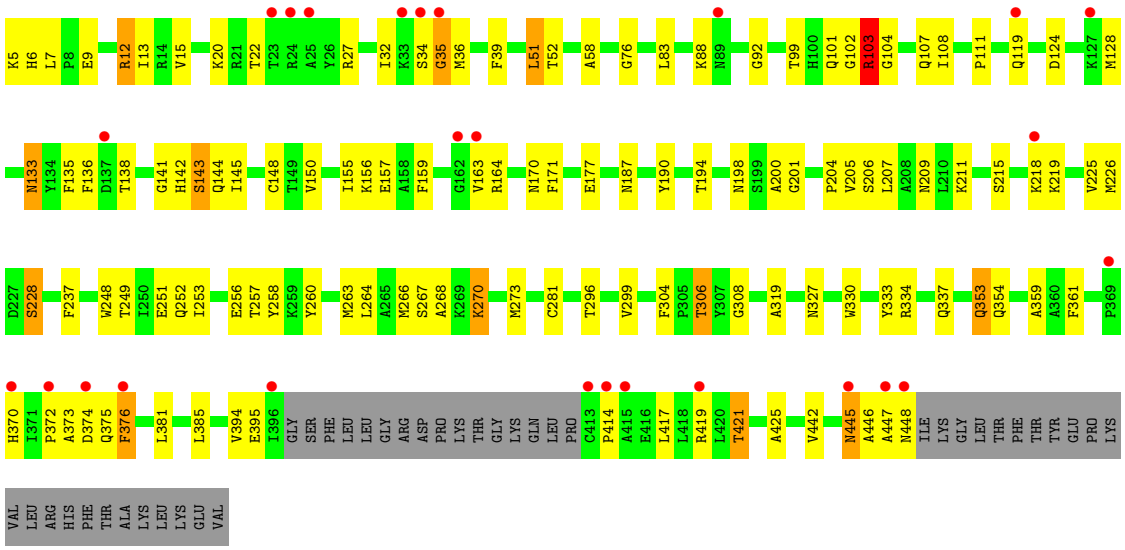
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	21	Total	O	0	0
			21	21		
2	B	21	Total	O	0	0
			21	21		

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.

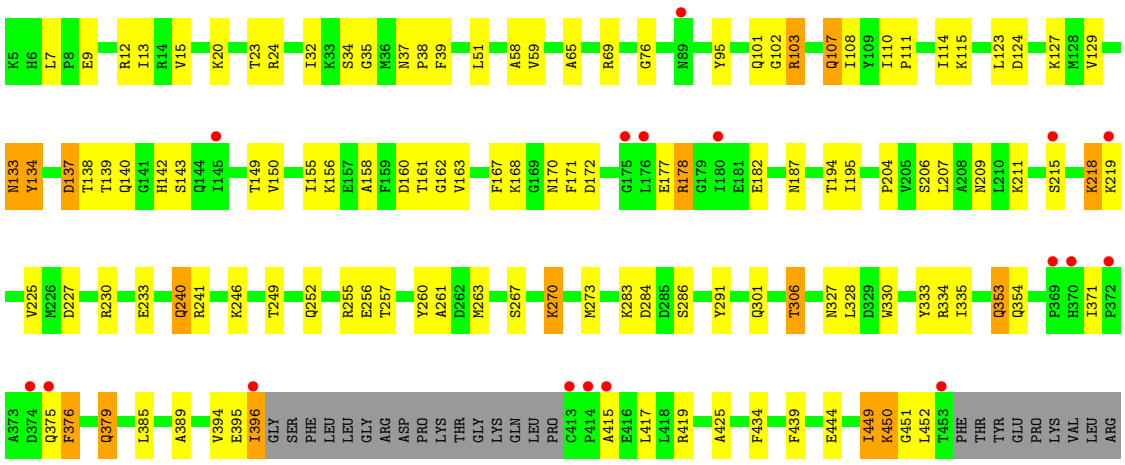
• Molecule 1: Tryptophanase

Chain A:



• Molecule 1: Tryptophanase

Chain B:



HIS
PHE
THR
ALA
LYS
LEU
LYS
GLU
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	112.44Å 112.44Å 232.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.97 – 2.89 14.97 – 2.89	Depositor EDS
% Data completeness (in resolution range)	100.0 (14.97-2.89) 98.6 (14.97-2.89)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.227 , 0.278 0.220 , 0.267	Depositor DCC
R_{free} test set	1687 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	64.3	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 48.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	6832	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 3.23% 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

Bond lengths and bond angles in the following residue types are not validated in this section: LLP

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	0.85	7/3421 (0.2%)	0.88	6/4624 (0.1%)
1	B	0.90	5/3457 (0.1%)	0.92	8/4672 (0.2%)
All	All	0.88	12/6878 (0.2%)	0.90	14/9296 (0.2%)

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	3
All	All	0	4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	103	ARG	CB-CG	15.22	1.93	1.52
1	A	103	ARG	CB-CG	11.83	1.84	1.52
1	B	103	ARG	CG-CD	10.12	1.77	1.51
1	B	103	ARG	CA-CB	9.30	1.74	1.53
1	A	103	ARG	CG-CD	8.83	1.74	1.51
1	B	103	ARG	CD-NE	8.43	1.60	1.46
1	B	103	ARG	NE-CZ	8.36	1.44	1.33
1	A	103	ARG	CD-NE	7.00	1.58	1.46
1	A	103	ARG	NE-CZ	6.87	1.42	1.33
1	A	103	ARG	CA-CB	6.35	1.68	1.53
1	A	251	GLU	CD-OE2	5.51	1.31	1.25
1	A	251	GLU	CG-CD	5.10	1.59	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	103	ARG	NE-CZ-NH1	11.27	125.93	120.30
1	B	103	ARG	NE-CZ-NH2	9.87	125.24	120.30
1	B	103	ARG	NH1-CZ-NH2	-9.71	108.72	119.40
1	A	103	ARG	NE-CZ-NH2	8.85	124.73	120.30
1	B	103	ARG	CB-CG-CD	8.19	132.91	111.60
1	A	103	ARG	CB-CG-CD	6.99	129.77	111.60
1	B	103	ARG	CG-CD-NE	6.68	125.82	111.80
1	A	103	ARG	NH1-CZ-NH2	-6.39	112.37	119.40
1	B	103	ARG	CB-CA-C	6.17	122.74	110.40
1	B	172	ASP	CB-CG-OD1	6.17	123.85	118.30
1	B	103	ARG	CD-NE-CZ	6.05	132.08	123.60
1	A	103	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	A	103	ARG	CG-CD-NE	5.17	122.67	111.80
1	A	103	ARG	CB-CA-C	5.13	120.66	110.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	34	SER	Peptide
1	B	34	SER	Peptide
1	B	415	ALA	Peptide
1	B	449	ILE	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	3377	0	3313	95	0
1	B	3413	0	3358	84	0
2	A	21	0	0	1	0
2	B	21	0	0	5	0
All	All	6832	0	6671	175	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 (175) 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:103:ARG:CD	1:B:103:ARG:CG	1.77	1.59
1:A:103:ARG:CB	1:A:103:ARG:CG	1.84	1.54
1:B:103:ARG:CG	1:B:103:ARG:CB	1.93	1.42
1:A:12:ARG:HG2	1:A:12:ARG:HH11	1.16	1.06
1:A:133:ASN:HD21	1:A:194:THR:H	1.04	0.98
1:B:133:ASN:HD21	1:B:194:THR:H	1.12	0.92
1:A:133:ASN:HD22	1:A:133:ASN:H	1.19	0.90
1:B:327:ASN:HD22	1:B:330:TRP:H	1.14	0.89
1:B:76:GLY:H	1:B:306:THR:HG21	1.36	0.89
1:B:371:ILE:HD11	1:B:449:ILE:O	1.75	0.85
1:B:133:ASN:ND2	1:B:194:THR:H	1.76	0.83
1:A:327:ASN:HD22	1:A:330:TRP:H	1.27	0.83
1:A:249:THR:OG1	1:A:252:GLN:HG3	1.81	0.81
1:B:249:THR:OG1	1:B:252:GLN:HG3	1.84	0.77
1:A:133:ASN:HD22	1:A:133:ASN:N	1.82	0.76
1:B:353:GLN:HE21	1:B:354:GLN:H	1.34	0.76
1:A:32:ILE:O	1:A:35:GLY:HA2	1.85	0.75
1:B:327:ASN:HB3	1:B:330:TRP:HB3	1.68	0.75
1:B:103:ARG:HG2	1:B:138:THR:HG21	1.67	0.75
1:B:233:GLU:HG2	1:B:335:ILE:HD11	1.66	0.75
1:B:240:GLN:HG2	1:B:241:ARG:HG3	1.68	0.73
1:B:65:ALA:O	2:B:501:HOH:O	2.06	0.73
1:B:76:GLY:N	1:B:306:THR:HG21	2.04	0.72
1:A:9:GLU:HG3	1:A:333:TYR:CZ	2.25	0.71
1:A:225:VAL:HG22	1:A:263:MET:HG3	1.72	0.71
1:B:107:GLN:HB3	1:B:301:GLN:OE1	1.90	0.71
1:B:69:ARG:HG3	2:B:501:HOH:O	1.90	0.71
1:A:12:ARG:HG2	1:A:12:ARG:NH1	1.94	0.70
1:B:9:GLU:HG3	1:B:333:TYR:CZ	2.27	0.70
1:B:133:ASN:HD21	1:B:194:THR:N	1.89	0.69
1:B:385:LEU:HD11	1:B:439:PHE:CE1	2.28	0.68
1:A:103:ARG:HG3	1:A:270:LLP:OP1	1.94	0.68
1:A:376:PHE:CD2	1:A:376:PHE:N	2.62	0.66
1:A:5:LYS:N	2:A:513:HOH:O	2.27	0.66
1:B:170:ASN:HD21	1:B:206:SER:H	1.43	0.66
1:B:171:PHE:H	1:B:209:ASN:HD21	1.42	0.65
1:A:170:ASN:HD21	1:A:206:SER:H	1.43	0.65
1:A:228:SER:HB3	1:A:258:TYR:OH	1.97	0.65
1:B:178:ARG:NH1	1:B:178:ARG:HG3	2.12	0.64
1:A:143:SER:OG	1:A:190:TYR:OH	2.15	0.64
1:A:51:LEU:O	1:A:419:ARG:NH2	2.31	0.64
1:B:110:ILE:O	1:B:114:ILE:HG13	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:ALA:HB1	1:B:434:PHE:CE1	2.34	0.63
1:B:58:ALA:HB3	1:B:425:ALA:HB3	1.81	0.62
1:B:171:PHE:HB2	1:B:209:ASN:HD21	1.64	0.62
1:A:101:GLN:HB2	1:A:270:LLP:OP2	2.01	0.61
1:B:38:PRO:HD2	1:B:379:GLN:HE22	1.65	0.61
1:A:124:ASP:H	1:A:187:ASN:HD22	1.48	0.60
1:B:178:ARG:HG3	1:B:178:ARG:HH11	1.65	0.60
1:B:101:GLN:HB2	1:B:270:LLP:OP2	2.00	0.60
1:B:218:LYS:HG3	2:B:518:HOH:O	2.01	0.60
1:A:381:LEU:CD1	1:A:442:VAL:HG11	2.31	0.60
1:B:124:ASP:H	1:B:187:ASN:HD22	1.48	0.59
1:B:103:ARG:HG3	1:B:270:LLP:OP1	2.03	0.59
1:A:171:PHE:H	1:A:209:ASN:HD21	1.50	0.59
1:A:141:GLY:O	1:A:145:ILE:HG12	2.03	0.57
1:A:327:ASN:ND2	1:A:330:TRP:H	2.01	0.57
1:A:353:GLN:HG3	1:A:354:GLN:N	2.18	0.57
1:B:124:ASP:HB3	1:B:127:LYS:HB2	1.87	0.57
1:A:359:ALA:HB2	1:A:421:THR:HG22	1.87	0.56
1:A:376:PHE:N	1:A:376:PHE:HD2	2.03	0.56
1:B:9:GLU:HG3	1:B:333:TYR:OH	2.05	0.56
1:B:171:PHE:H	1:B:209:ASN:ND2	2.03	0.56
1:A:376:PHE:HD2	1:A:376:PHE:H	1.53	0.56
1:A:133:ASN:H	1:A:133:ASN:ND2	1.98	0.56
1:A:133:ASN:HD21	1:A:194:THR:N	1.88	0.55
1:A:248:TRP:HZ3	1:A:256:GLU:HB2	1.72	0.55
1:A:108:ILE:O	1:A:111:PRO:HD2	2.07	0.55
1:A:133:ASN:ND2	1:A:194:THR:H	1.88	0.55
1:A:381:LEU:HD13	1:A:442:VAL:HG11	1.89	0.55
1:A:372:PRO:HD2	1:A:375:GLN:OE1	2.07	0.54
1:A:446:ALA:C	1:A:448:ASN:H	2.11	0.54
1:B:256:GLU:HA	1:B:256:GLU:OE2	2.08	0.54
1:A:13:ILE:HG23	1:B:13:ILE:HG23	1.90	0.53
1:B:267:SER:HB2	1:B:270:LLP:OP4	2.09	0.53
1:B:108:ILE:O	1:B:111:PRO:HD2	2.09	0.53
1:B:225:VAL:HG22	1:B:263:MET:HG3	1.92	0.52
1:B:178:ARG:HH11	1:B:178:ARG:CG	2.23	0.52
1:B:195:ILE:O	1:B:195:ILE:HG13	2.09	0.52
1:A:133:ASN:N	1:A:133:ASN:ND2	2.56	0.51
1:B:327:ASN:ND2	1:B:330:TRP:H	1.95	0.51
1:B:102:GLY:HA3	1:B:270:LLP:OP4	2.11	0.51
1:B:284:ASP:OD1	1:B:286:SER:OG	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LEU:HD21	1:A:257:THR:HA	1.93	0.51
1:A:6:HIS:CE1	1:A:337:GLN:HG3	2.46	0.50
1:B:133:ASN:O	1:B:134:TYR:HB2	2.11	0.50
1:B:261:ALA:O	1:B:283:LYS:HE3	2.11	0.50
1:A:135:PHE:CE2	1:A:150:VAL:HB	2.47	0.50
1:B:270:LLP:O3	1:B:270:LLP:NZ	2.43	0.50
1:A:201:GLY:HA2	1:A:361:PHE:CZ	2.47	0.49
1:A:39:PHE:CE1	1:A:51:LEU:HD21	2.47	0.49
1:A:267:SER:HB2	1:A:270:LLP:OP4	2.12	0.49
1:A:304:PHE:HD2	1:A:306:THR:HB	1.77	0.49
1:A:394:VAL:CG1	1:A:395:GLU:N	2.75	0.49
1:A:445:ASN:HD22	1:A:448:ASN:HD22	1.60	0.49
1:A:361:PHE:CZ	1:A:419:ARG:HG3	2.48	0.49
1:A:103:ARG:HG2	1:A:138:THR:HG21	1.95	0.49
1:A:171:PHE:HB2	1:A:209:ASN:HD21	1.77	0.48
1:A:226:MET:HG2	1:A:258:TYR:CE1	2.48	0.48
1:B:129:VAL:HG22	1:B:149:THR:HB	1.96	0.48
1:A:135:PHE:CD2	1:A:150:VAL:HB	2.48	0.48
1:A:136:PHE:CE1	1:A:198:ASN:ND2	2.82	0.48
1:A:228:SER:HB3	1:A:258:TYR:HH	1.79	0.48
1:A:15:VAL:HB	1:B:15:VAL:HG23	1.96	0.47
1:B:211:LYS:HG2	1:B:260:TYR:CE1	2.49	0.47
1:B:230:ARG:CZ	1:B:270:LLP:HG3	2.45	0.47
1:A:211:LYS:HG2	1:A:260:TYR:CZ	2.49	0.47
1:A:22:THR:O	1:A:27:ARG:NH1	2.47	0.47
1:A:159:PHE:CE2	1:A:200:ALA:HA	2.50	0.47
1:A:6:HIS:HD2	1:A:7:LEU:O	1.98	0.47
1:A:13:ILE:HD13	1:B:13:ILE:HG12	1.97	0.47
1:A:107:GLN:CG	1:A:142:HIS:NE2	2.77	0.47
1:A:306:THR:O	1:A:306:THR:CG2	2.62	0.47
1:B:233:GLU:HG2	1:B:335:ILE:CD1	2.40	0.47
1:B:207:LEU:HD21	1:B:257:THR:HA	1.96	0.46
1:A:304:PHE:CD2	1:A:306:THR:HB	2.50	0.46
1:A:306:THR:O	1:A:306:THR:HG23	2.15	0.46
1:A:249:THR:HG1	1:A:252:GLN:HG3	1.79	0.46
1:A:144:GLN:HE21	1:A:144:GLN:HB2	1.58	0.46
1:B:155:ILE:HD11	1:B:168:LYS:HA	1.98	0.46
1:A:51:LEU:O	1:A:52:THR:HB	2.16	0.46
1:B:124:ASP:H	1:B:187:ASN:ND2	2.13	0.46
1:A:76:GLY:N	1:A:306:THR:HG21	2.31	0.45
1:B:7:LEU:HD21	2:B:512:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:THR:HG22	1:B:353:GLN:HB2	1.99	0.45
1:B:194:THR:HA	1:B:227:ASP:HB3	1.97	0.45
1:A:15:VAL:HA	1:B:59:VAL:O	2.16	0.45
1:A:171:PHE:H	1:A:209:ASN:ND2	2.14	0.45
1:A:270:LLP:O3	1:A:270:LLP:NZ	2.49	0.45
1:A:211:LYS:HB3	1:A:211:LYS:HE2	1.62	0.45
1:B:142:HIS:O	1:B:143:SER:C	2.55	0.45
1:A:102:GLY:HA3	1:A:270:LLP:OP4	2.17	0.45
1:A:266:MET:HE3	1:A:268:ALA:HA	1.98	0.45
1:B:95:TYR:HB3	1:B:291:TYR:CD1	2.52	0.45
1:A:58:ALA:HB3	1:A:425:ALA:HB3	1.99	0.45
1:A:107:GLN:HG2	1:A:142:HIS:NE2	2.32	0.45
1:A:353:GLN:HG3	1:A:354:GLN:O	2.17	0.44
1:B:137:ASP:OD2	1:B:137:ASP:N	2.50	0.44
1:B:168:LYS:NZ	1:B:353:GLN:HE22	2.15	0.44
1:A:394:VAL:HG12	1:A:395:GLU:N	2.32	0.44
1:B:353:GLN:NE2	1:B:354:GLN:H	2.09	0.44
1:B:37:ASN:O	1:B:39:PHE:N	2.51	0.44
1:B:211:LYS:HG2	1:B:260:TYR:CZ	2.53	0.44
1:B:385:LEU:HD11	1:B:439:PHE:CZ	2.53	0.44
1:B:375:GLN:HB3	1:B:452:LEU:H	1.83	0.43
1:B:158:ALA:HA	1:B:168:LYS:HB3	1.99	0.43
1:A:102:GLY:O	1:A:104:GLY:N	2.51	0.43
1:A:155:ILE:HD12	1:A:157:GLU:OE2	2.18	0.43
1:A:88:LYS:O	1:A:92:GLY:HA2	2.19	0.43
1:A:264:LEU:HG	1:A:281:CYS:HB2	2.00	0.43
1:A:445:ASN:ND2	1:A:448:ASN:HD22	2.16	0.43
1:B:69:ARG:N	2:B:501:HOH:O	2.51	0.43
1:A:124:ASP:H	1:A:187:ASN:ND2	2.15	0.42
1:A:327:ASN:HB3	1:A:330:TRP:HB3	2.01	0.42
1:A:83:LEU:HA	1:A:319:ALA:HB2	2.00	0.42
1:B:123:LEU:HD12	1:B:187:ASN:HA	2.00	0.42
1:B:140:GLN:HG3	1:B:150:VAL:HG21	2.01	0.42
1:A:204:PRO:HG3	1:A:237:PHE:CG	2.54	0.42
1:A:128:MET:HE3	1:A:148:CYS:HB2	2.02	0.42
1:A:249:THR:O	1:A:253:ILE:HG13	2.20	0.42
1:B:160:ASP:C	1:B:162:GLY:H	2.24	0.41
1:B:133:ASN:H	1:B:133:ASN:HD22	1.67	0.41
1:B:396:ILE:O	1:B:419:ARG:NH1	2.53	0.41
1:B:451:GLY:O	1:B:452:LEU:HD23	2.20	0.41
1:A:102:GLY:C	1:A:104:GLY:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:THR:O	1:A:299:VAL:HB	2.21	0.41
1:B:379:GLN:HE21	1:B:379:GLN:HA	1.85	0.41
1:A:170:ASN:HD22	1:A:205:VAL:HG13	1.85	0.41
1:A:385:LEU:HD12	1:A:442:VAL:HG21	2.03	0.41
1:B:9:GLU:HA	1:B:333:TYR:CE1	2.56	0.41
1:B:23:THR:O	1:B:24:ARG:C	2.58	0.41
1:B:167:PHE:CD2	1:B:204:PRO:HB2	2.56	0.41
1:B:328:LEU:HA	1:B:328:LEU:HD12	1.82	0.40
1:A:99:THR:HA	1:A:308:GLY:O	2.21	0.40
1:A:201:GLY:HA2	1:A:361:PHE:CE2	2.57	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	423/467 (91%)	389 (92%)	29 (7%)	5 (1%)	13	40
1	B	428/467 (92%)	388 (91%)	36 (8%)	4 (1%)	17	48
All	All	851/934 (91%)	777 (91%)	65 (8%)	9 (1%)	14	42

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	35	GLY
1	A	373	ALA
1	A	447	ALA
1	B	450	LYS
1	A	35	GLY
1	A	414	PRO
1	B	376	PHE
1	A	103	ARG

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Mol	Chain	Res	Type
1	B	134	TYR

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	351/385 (91%)	326 (93%)	25 (7%)	14 40
1	B	355/385 (92%)	323 (91%)	32 (9%)	9 29
All	All	706/770 (92%)	649 (92%)	57 (8%)	11 33

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	20	LYS
1	A	36	MET
1	A	51	LEU
1	A	119	GLN
1	A	133	ASN
1	A	143	SER
1	A	156	LYS
1	A	163	VAL
1	A	164	ARG
1	A	177	GLU
1	A	215	SER
1	A	218	LYS
1	A	219	LYS
1	A	228	SER
1	A	273	MET
1	A	306	THR
1	A	334	ARG
1	A	353	GLN
1	A	370	HIS
1	A	374	ASP
1	A	376	PHE

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Mol	Chain	Res	Type
1	A	417	LEU
1	A	421	THR
1	A	445	ASN
1	B	12	ARG
1	B	20	LYS
1	B	32	ILE
1	B	51	LEU
1	B	107	GLN
1	B	115	LYS
1	B	133	ASN
1	B	137	ASP
1	B	139	THR
1	B	156	LYS
1	B	163	VAL
1	B	177	GLU
1	B	178	ARG
1	B	182	GLU
1	B	215	SER
1	B	218	LYS
1	B	219	LYS
1	B	240	GLN
1	B	246	LYS
1	B	255	ARG
1	B	273	MET
1	B	306	THR
1	B	334	ARG
1	B	353	GLN
1	B	376	PHE
1	B	379	GLN
1	B	394	VAL
1	B	395	GLU
1	B	396	ILE
1	B	417	LEU
1	B	444	GLU
1	B	450	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	64	GLN
1	A	119	GLN

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Mol	Chain	Res	Type
1	A	133	ASN
1	A	140	GLN
1	A	144	GLN
1	A	170	ASN
1	A	187	ASN
1	A	198	ASN
1	A	209	ASN
1	A	327	ASN
1	A	339	GLN
1	A	353	GLN
1	A	379	GLN
1	A	445	ASN
1	B	6	HIS
1	B	64	GLN
1	B	119	GLN
1	B	133	ASN
1	B	140	GLN
1	B	170	ASN
1	B	187	ASN
1	B	209	ASN
1	B	327	ASN
1	B	353	GLN
1	B	379	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	LLP	A	270	1	23,24,25	1.93	5 (21%)	25,32,34	2.15	5 (20%)
1	LLP	B	270	1	23,24,25	1.87	5 (21%)	25,32,34	2.15	3 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	A	270	1	-	5/16/17/19	0/1/1/1
1	LLP	B	270	1	-	6/16/17/19	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	270	LLP	O3-C3	-5.93	1.23	1.37
1	A	270	LLP	O3-C3	-5.58	1.24	1.37
1	A	270	LLP	C4-C4'	3.86	1.54	1.46
1	A	270	LLP	C6-N1	2.74	1.40	1.34
1	B	270	LLP	C3-C2	-2.56	1.38	1.40
1	A	270	LLP	C2-N1	2.50	1.38	1.33
1	B	270	LLP	C4'-NZ	2.46	1.35	1.27
1	B	270	LLP	C4-C4'	2.40	1.51	1.46
1	A	270	LLP	C4'-NZ	2.28	1.34	1.27
1	B	270	LLP	P-OP1	-2.27	1.43	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	270	LLP	OP4-C5'-C5	8.72	125.97	109.35
1	A	270	LLP	OP4-C5'-C5	8.33	125.22	109.35
1	A	270	LLP	OP2-P-OP4	-3.62	97.10	106.73
1	B	270	LLP	C4-C4'-NZ	-3.44	108.50	124.31
1	A	270	LLP	C4-C4'-NZ	-3.40	108.70	124.31
1	A	270	LLP	C4-C3-C2	2.83	121.94	120.19
1	B	270	LLP	OP3-P-OP2	2.71	118.01	107.64
1	A	270	LLP	OP3-P-OP2	2.13	115.78	107.64

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	270	LLP	O-C-CA-CB
1	B	270	LLP	C5'-OP4-P-OP1
1	B	270	LLP	O-C-CA-CB
1	B	270	LLP	CG-CD-CE-NZ
1	A	270	LLP	C4-C4'-NZ-CE
1	A	270	LLP	CG-CD-CE-NZ
1	A	270	LLP	C5'-OP4-P-OP1
1	A	270	LLP	CA-CB-CG-CD
1	B	270	LLP	C5'-OP4-P-OP2
1	B	270	LLP	C5'-OP4-P-OP3
1	B	270	LLP	C3-C4-C4'-NZ

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	270	LLP	5	0
1	B	270	LLP	6	0

5.5 Carbohydrates (i)

There are no monosaccharides 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, 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	427/467 (91%)	0.00	26 (6%)	21	17	32, 54, 108, 178	0
1	B	432/467 (92%)	-0.10	17 (3%)	39	35	29, 52, 87, 148	0
All	All	859/934 (91%)	-0.05	43 (5%)	28	25	29, 52, 103, 178	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	413	CYS	11.5
1	B	413	CYS	9.4
1	B	415	ALA	5.8
1	A	414	PRO	4.9
1	B	414	PRO	4.5
1	B	215	SER	4.4
1	A	35	GLY	4.2
1	A	415	ALA	4.1
1	A	119	GLN	3.9
1	A	23	THR	3.9
1	B	374	ASP	3.8
1	A	447	ALA	3.7
1	A	370	HIS	3.6
1	A	372	PRO	3.6
1	A	162	GLY	3.6
1	B	369	PRO	3.5
1	A	374	ASP	3.5
1	A	369	PRO	3.4
1	B	219	LYS	3.4
1	B	370	HIS	3.3
1	A	137	ASP	3.1
1	A	24	ARG	3.0
1	B	145	ILE	3.0
1	B	453	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	396	ILE	3.0
1	B	176	LEU	3.0
1	A	163	VAL	2.9
1	A	33	LYS	2.8
1	A	218	LYS	2.7
1	A	419	ARG	2.6
1	A	127	LYS	2.6
1	B	175	GLY	2.6
1	A	376	PHE	2.5
1	B	396	ILE	2.2
1	B	180	ILE	2.2
1	A	25	ALA	2.1
1	A	34	SER	2.1
1	A	89	ASN	2.1
1	A	445	ASN	2.1
1	A	448	ASN	2.1
1	B	89	ASN	2.1
1	B	375	GLN	2.0
1	B	372	PRO	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	LLP	A	270	24/25	0.95	0.15	37,50,52,53	0
1	LLP	B	270	24/25	0.98	0.10	35,41,45,47	0

6.3 Carbohydrates (i)

There are no monosaccharides 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.