



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:50 PM UTC

PDB ID : 1ZYZ / pdb_00001zyz
Title : Structures of Yeast Ribonucleotide Reductase I
Authors : Xu, H.; Faber, C.; Uchiki, T.; Fairman, J.W.; Racca, J.; Dealwis, C.
Deposited on : 2005-06-13
Resolution : 2.90 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

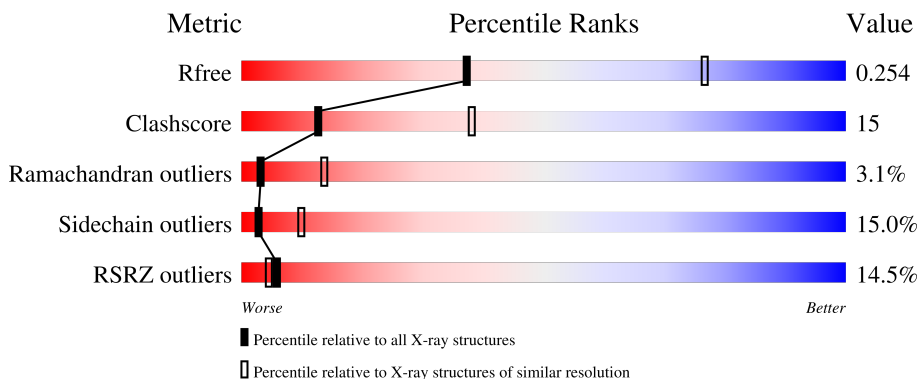
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 $\leq 5\%$. 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	888	11% 57% 21% 7% • 13%
1	B	888	14% 58% 22% 7% • 13%

2 Entry composition [i](#)

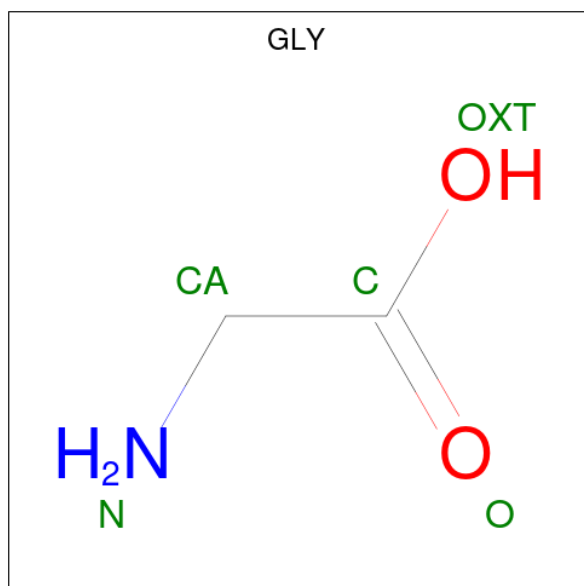
There are 2 unique types of molecules in this entry. The entry contains 12275 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ribonucleoside-diphosphate reductase large chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	776	Total	C	N	O	S	0	0	0
			6159	3913	1049	1162	35			
1	B	769	Total	C	N	O	S	0	0	0
			6108	3882	1040	1151	35			

- Molecule 2 is GLYCINE (CCD ID: GLY) (formula: C₂H₅NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			4	2	1	1		
2	A	1	Total	C	N	O	0	0
			4	2	1	1		



4 Data and refinement statistics

Property	Value	Source
Space group	F 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	433.70 Å 433.70 Å 433.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 50.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (50.00-2.90) 98.4 (50.00-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.21 (at 2.69 Å)	Xtriage
Refinement program	REFMAC 5.2.0007	Depositor
R, R_{free}	0.217 , 0.257 0.215 , 0.254	Depositor DCC
R_{free} test set	4547 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12275	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% 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	0.79	3/6296 (0.0%)	1.14	30/8531 (0.4%)
1	B	0.76	0/6244	1.07	14/8459 (0.2%)
All	All	0.78	3/12540 (0.0%)	1.11	44/16990 (0.3%)

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	7
1	B	0	5
All	All	0	12

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	389	TRP	C-N	10.82	1.47	1.33
1	A	664	ILE	CA-CB	5.60	1.61	1.54
1	A	633	VAL	CA-CB	5.37	1.61	1.54

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	675	ASN	OD1-CG-ND2	-13.54	109.06	122.60
1	A	34	ILE	O-C-N	-10.88	108.97	122.57
1	A	675	ASN	CB-CG-ND2	-10.55	100.57	116.40
1	A	638	PHE	N-CA-C	8.69	122.39	108.41
1	B	19	THR	N-CA-C	-8.31	102.57	114.12
1	B	428	CYS	N-CA-C	-8.19	97.80	110.17
1	A	389	TRP	CA-C-N	7.83	130.62	120.44
1	A	389	TRP	C-N-CA	7.83	130.62	120.44
1	A	390	TYR	N-CA-CB	7.75	121.25	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	ILE	N-CA-C	7.41	116.79	108.05
1	A	28	GLY	N-CA-C	-7.40	104.37	115.32
1	B	428	CYS	CA-C-N	-6.89	108.37	121.54
1	B	428	CYS	C-N-CA	-6.89	108.37	121.54
1	A	211	PRO	CA-C-N	-6.77	114.83	123.16
1	A	211	PRO	C-N-CA	-6.77	114.83	123.16
1	A	291	ASN	N-CA-C	6.76	119.03	110.24
1	A	428	CYS	CA-C-N	-6.59	108.94	121.54
1	A	428	CYS	C-N-CA	-6.59	108.94	121.54
1	B	334	ILE	N-CA-C	6.33	114.86	107.77
1	B	721	MET	N-CA-C	-6.22	101.21	110.23
1	A	657	GLU	N-CA-C	-6.21	100.46	109.59
1	A	389	TRP	O-C-N	6.07	130.66	122.59
1	B	699	ALA	N-CA-C	-6.05	104.77	111.36
1	A	249	GLY	N-CA-C	-5.90	101.68	110.71
1	B	607	PRO	N-CA-C	-5.86	102.06	111.38
1	A	675	ASN	N-CA-C	5.74	123.03	110.80
1	A	344	GLU	CA-C-N	-5.69	114.68	122.87
1	A	344	GLU	C-N-CA	-5.69	114.68	122.87
1	A	775	LYS	N-CA-C	5.65	118.75	109.72
1	A	654	ILE	N-CA-C	5.60	120.99	109.34
1	A	655	TRP	N-CA-C	5.48	117.17	108.67
1	B	753	GLN	N-CA-C	-5.48	99.14	110.80
1	B	292	LYS	N-CA-C	5.38	120.25	111.37
1	B	365	ASP	N-CA-C	5.34	119.67	113.20
1	A	721	MET	N-CA-C	-5.34	102.39	110.24
1	A	428	CYS	N-CA-C	-5.34	102.09	110.36
1	A	264	GLY	N-CA-C	-5.31	106.37	115.08
1	A	265	THR	N-CA-C	5.21	117.25	109.59
1	B	466	ASN	N-CA-C	5.12	117.90	108.58
1	B	771	ILE	CB-CA-C	-5.11	105.34	111.88
1	A	664	ILE	CB-CA-C	5.09	119.01	112.14
1	B	631	ARG	N-CA-C	5.07	115.69	107.23
1	A	390	TYR	N-CA-C	-5.06	105.65	111.07
1	A	266	ASN	N-CA-C	-5.01	100.12	110.80

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	ASP	Peptide
1	A	265	THR	Peptide

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Mol	Chain	Res	Type	Group
1	A	292	LYS	Peptide
1	A	34	ILE	Mainchain
1	A	656	ASP	Peptide
1	A	674	PRO	Peptide
1	A	675	ASN	Sidechain
1	B	265	THR	Peptide
1	B	266	ASN	Peptide
1	B	293	ARG	Peptide
1	B	321	GLU	Peptide
1	B	322	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	6159	0	6095	199	0
1	B	6108	0	6041	171	0
2	A	8	0	4	2	0
All	All	12275	0	12140	370	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 15.

All (370) 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:A:220:LEU:CD2	1:A:431:ILE:HD11	1.79	1.13
1:A:220:LEU:HD21	1:A:431:ILE:CD1	1.84	1.07
1:B:464:THR:HG21	1:B:789:SER:HB3	1.43	0.99
1:A:179:HIS:HD2	1:A:483:ARG:HH11	1.06	0.98
1:A:220:LEU:HD21	1:A:431:ILE:HD11	0.98	0.97
1:B:464:THR:CG2	1:B:789:SER:HB3	1.96	0.96
1:A:447:SER:HB3	1:A:606:MET:CE	1.97	0.95
1:A:179:HIS:CD2	1:A:483:ARG:HH11	1.86	0.94
1:A:393:LEU:HD22	1:A:724:LEU:HD13	1.50	0.91
1:A:153:ARG:HH22	1:A:632:ARG:HH11	1.01	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ASP:HB3	1:A:85:ASN:HD21	1.37	0.90
1:B:467:PHE:CG	1:B:582:MET:HE1	2.06	0.89
1:B:277:ARG:HH11	1:B:277:ARG:HB2	1.36	0.89
1:B:316:LYS:O	1:B:324:ARG:HD3	1.73	0.88
1:B:95:SER:H	1:B:132:ASN:HD21	1.22	0.86
1:A:717:ARG:O	1:A:719:PRO:HD3	1.75	0.86
1:A:179:HIS:HD2	1:A:483:ARG:NH1	1.73	0.85
1:B:277:ARG:HD2	1:B:322:GLU:CD	2.03	0.83
1:B:467:PHE:CB	1:B:582:MET:HE1	2.09	0.82
1:B:377:GLU:HG3	1:B:379:ARG:HD3	1.61	0.82
1:A:334:ILE:HD12	1:A:404:VAL:HG13	1.62	0.81
1:A:538:THR:HB	1:A:583:TRP:NE1	1.96	0.81
1:A:505:ILE:HG22	1:A:602:THR:HA	1.61	0.81
1:A:445:LEU:HD22	1:A:506:ALA:HB3	1.63	0.80
1:A:57:ASP:HB3	1:A:85:ASN:ND2	1.97	0.80
1:B:557:TYR:HE1	1:B:559:THR:HG22	1.46	0.79
1:A:90:THR:CG2	1:A:166:ARG:HE	1.96	0.79
1:A:787:ALA:O	1:A:788:ALA:HB2	1.84	0.77
1:A:368:GLU:O	1:A:372:THR:HB	1.84	0.77
1:A:538:THR:HB	1:A:583:TRP:HE1	1.48	0.77
1:B:277:ARG:HB2	1:B:277:ARG:NH1	1.98	0.77
1:B:332:LEU:HD11	1:B:392:ILE:HD12	1.65	0.77
1:A:447:SER:HB3	1:A:606:MET:HE3	1.66	0.76
1:B:277:ARG:HD2	1:B:322:GLU:OE2	1.87	0.74
1:A:71:HIS:HD2	1:A:73:ASP:HB2	1.52	0.74
1:B:776:ARG:HG3	1:B:776:ARG:HH11	1.53	0.74
1:B:520:ARG:HG3	1:B:520:ARG:HH11	1.51	0.74
1:A:153:ARG:HH22	1:A:632:ARG:NH1	1.84	0.73
1:A:57:ASP:CB	1:A:85:ASN:HD21	2.01	0.73
1:A:317:ASN:HA	1:A:326:ARG:HH21	1.54	0.72
1:A:426:ASN:HB3	1:A:431:ILE:CD1	2.21	0.71
1:B:39:VAL:HG13	1:B:67:MET:HE1	1.73	0.71
1:B:538:THR:HB	1:B:583:TRP:NE1	2.06	0.71
1:A:320:LYS:HD2	1:A:320:LYS:H	1.56	0.70
1:B:320:LYS:HG3	1:B:323:ILE:HD13	1.74	0.70
1:A:95:SER:H	1:A:132:ASN:HD21	1.39	0.70
1:A:517:MET:HE1	1:A:624:VAL:HG11	1.74	0.70
1:A:179:HIS:CD2	1:A:483:ARG:NH1	2.54	0.69
1:A:481:LEU:HB3	1:A:505:ILE:HG12	1.75	0.69
1:A:81:ILE:O	1:A:85:ASN:HB2	1.94	0.67
1:A:277:ARG:HG3	1:A:277:ARG:HH11	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:SER:H	1:B:269:SER:HB3	1.59	0.67
1:A:534:GLN:O	1:A:538:THR:HG22	1.95	0.67
1:A:26:CYS:HB2	1:A:29:LEU:HD23	1.77	0.67
1:B:618:ASN:O	1:B:619:GLU:O	2.12	0.67
1:B:714:LEU:HG	1:B:727:MET:HE3	1.77	0.66
1:A:293:ARG:O	1:A:294:PRO:C	2.39	0.66
1:B:447:SER:HB3	1:B:606:MET:HE1	1.78	0.66
1:A:571:GLN:HE21	1:A:571:GLN:HA	1.60	0.66
1:B:365:ASP:HA	1:B:368:GLU:HB2	1.78	0.66
1:B:675:ASN:ND2	1:B:675:ASN:H	1.93	0.66
1:A:153:ARG:NH2	1:A:632:ARG:HH11	1.85	0.66
1:B:94:PHE:HB3	1:B:132:ASN:HD22	1.61	0.66
1:A:444:ASN:C	1:A:445:LEU:HD23	2.21	0.65
1:B:538:THR:HB	1:B:583:TRP:HE1	1.60	0.65
1:A:454:ILE:HD12	1:A:519:LEU:CD1	2.27	0.65
1:B:170:LEU:HD22	1:B:173:ARG:NH2	2.12	0.65
1:B:211:PRO:O	1:B:213:PRO:HD3	1.96	0.65
1:A:66:TYR:HA	1:A:638:PHE:CZ	2.32	0.65
1:B:586:ASP:O	1:B:590:LYS:HG2	1.97	0.65
1:A:717:ARG:NH1	1:A:746:GLN:OE1	2.30	0.64
1:A:393:LEU:HD22	1:A:724:LEU:CD1	2.26	0.64
1:A:602:THR:N	1:A:707:ASP:OD2	2.26	0.64
1:A:632:ARG:HG2	1:A:633:VAL:N	2.12	0.64
1:B:776:ARG:HG3	1:B:776:ARG:NH1	2.11	0.64
1:B:316:LYS:HE2	1:B:398:GLU:OE2	1.98	0.64
1:A:454:ILE:HD12	1:A:519:LEU:HD11	1.80	0.64
1:A:770:ASP:O	1:A:771:ILE:HB	1.96	0.64
1:A:787:ALA:O	1:A:788:ALA:CB	2.46	0.64
1:A:389:TRP:HA	1:A:389:TRP:CE3	2.31	0.64
1:A:223:MET:HG2	1:A:255:ILE:HD11	1.80	0.63
1:B:220:LEU:HD11	1:B:431:ILE:HD11	1.80	0.63
1:A:312:ILE:CD1	1:A:332:LEU:HD21	2.29	0.63
1:A:771:ILE:C	1:A:773:ASN:H	2.07	0.63
1:A:458:GLU:HA	1:A:458:GLU:OE2	1.99	0.62
1:B:447:SER:HB3	1:B:606:MET:CE	2.29	0.62
1:A:87:HIS:HE1	1:A:140:ASP:OD1	1.82	0.62
1:B:18:ILE:O	1:B:22:ILE:HD13	1.99	0.62
1:A:534:GLN:O	1:A:538:THR:CG2	2.48	0.61
1:A:654:ILE:HD11	1:A:769:ALA:HB2	1.83	0.61
1:B:671:GLN:O	1:B:672:GLY:C	2.43	0.61
1:A:481:LEU:C	1:A:505:ILE:HD11	2.24	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:SER:HB3	1:A:606:MET:HE1	1.80	0.60
1:B:94:PHE:HB3	1:B:132:ASN:ND2	2.16	0.60
1:B:467:PHE:HB3	1:B:582:MET:HE1	1.82	0.60
1:B:16:ASP:HB3	1:B:18:ILE:HG23	1.83	0.60
1:A:389:TRP:O	1:A:392:ILE:HB	2.02	0.60
1:B:431:ILE:C	1:B:431:ILE:HD12	2.26	0.60
1:B:520:ARG:HH11	1:B:520:ARG:CG	2.14	0.60
1:A:277:ARG:HH11	1:A:277:ARG:CG	2.14	0.60
2:A:890:GLY:N	1:B:745:THR:HG1	1.99	0.60
1:B:288:GLN:HE22	1:B:293:ARG:NH1	1.99	0.60
1:B:90:THR:CG2	1:B:166:ARG:HE	2.15	0.60
1:B:159:ILE:HG23	1:B:160:ASN:H	1.68	0.59
1:B:401:THR:HB	1:B:402:PRO:HA	1.84	0.59
1:B:663:LEU:HD22	1:B:668:GLY:HA2	1.83	0.59
1:A:447:SER:HA	1:A:508:GLY:O	2.01	0.59
1:A:69:THR:O	1:A:655:TRP:CZ3	2.55	0.59
1:A:255:ILE:HD13	1:A:275:MET:SD	2.43	0.59
1:A:153:ARG:NH2	1:A:632:ARG:HD3	2.17	0.58
1:B:464:THR:HG23	1:B:789:SER:HB3	1.84	0.58
1:A:779:TYR:O	1:A:781:PRO:HD3	2.04	0.58
1:A:770:ASP:O	1:A:771:ILE:CB	2.51	0.58
1:A:94:PHE:HB3	1:A:132:ASN:ND2	2.19	0.57
1:B:520:ARG:NH2	1:B:648:ASP:OD2	2.36	0.57
1:B:140:ASP:OD2	1:B:168:GLN:HG2	2.03	0.57
1:B:30:ASP:HB3	1:B:33:HIS:CE1	2.40	0.57
1:B:67:MET:C	1:B:69:THR:H	2.13	0.57
1:B:179:HIS:HE1	1:B:189:THR:HG21	1.70	0.57
1:B:557:TYR:CE1	1:B:559:THR:HG22	2.34	0.57
1:B:467:PHE:CB	1:B:582:MET:CE	2.83	0.56
1:B:588:LEU:O	1:B:592:ILE:HG12	2.05	0.56
1:B:71:HIS:CG	1:B:72:PRO:HD2	2.40	0.56
1:B:471:HIS:HE1	1:B:541:HIS:ND1	2.03	0.56
1:A:388:LEU:O	1:A:389:TRP:C	2.45	0.56
1:A:467:PHE:HD2	1:A:538:THR:HG21	1.70	0.56
1:B:26:CYS:O	1:B:29:LEU:HG	2.05	0.56
1:A:69:THR:HG23	1:A:655:TRP:HH2	1.70	0.56
1:B:288:GLN:HE22	1:B:293:ARG:CZ	2.19	0.56
1:A:71:HIS:CG	1:A:72:PRO:HD2	2.41	0.56
1:A:223:MET:HG2	1:A:255:ILE:CD1	2.36	0.56
1:B:388:LEU:O	1:B:392:ILE:HG12	2.04	0.56
1:B:179:HIS:CE1	1:B:189:THR:HG21	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:LEU:HD21	1:A:559:THR:HG21	1.88	0.55
1:B:686:THR:HG22	1:B:688:TRP:H	1.71	0.55
1:B:220:LEU:N	1:B:220:LEU:HD23	2.21	0.55
1:A:71:HIS:CD2	1:A:73:ASP:HB2	2.38	0.55
1:B:80:ARG:O	1:B:84:SER:HB2	2.07	0.55
1:B:482:ASN:OD1	1:B:503:ARG:NH1	2.39	0.55
1:A:76:THR:O	1:A:80:ARG:HG2	2.07	0.54
1:B:342:VAL:HG22	1:B:729:PHE:HZ	1.71	0.54
1:B:293:ARG:HB3	1:B:295:GLY:N	2.23	0.54
1:A:445:LEU:CD2	1:A:506:ALA:HB3	2.37	0.54
1:A:557:TYR:HE1	1:A:559:THR:HG22	1.73	0.54
1:A:656:ASP:HB2	1:A:659:MET:H	1.73	0.54
1:A:571:GLN:HA	1:A:571:GLN:NE2	2.23	0.54
1:A:482:ASN:OD1	1:A:503:ARG:NH1	2.41	0.53
1:A:511:GLY:O	1:A:515:THR:HG23	2.09	0.53
1:A:66:TYR:HA	1:A:638:PHE:CE2	2.43	0.53
1:B:607:PRO:HD3	1:B:711:SER:OG	2.09	0.53
1:B:561:GLN:H	1:B:561:GLN:CD	2.16	0.53
1:A:633:VAL:O	1:A:634:LEU:HB2	2.08	0.53
1:B:658:GLY:HA2	1:B:661:GLN:HB2	1.91	0.53
1:B:675:ASN:H	1:B:675:ASN:HD22	1.55	0.53
1:A:34:ILE:HG23	1:A:35:ASP:N	2.25	0.52
1:A:71:HIS:CD2	1:A:73:ASP:H	2.28	0.52
1:A:629:TYR:CE1	1:A:640:VAL:HG12	2.44	0.52
1:A:159:ILE:HG22	1:A:160:ASN:N	2.23	0.52
1:A:661:GLN:HE22	1:A:757:ASP:H	1.57	0.52
1:A:686:THR:HG22	1:A:688:TRP:H	1.74	0.52
1:B:292:LYS:HB2	1:B:293:ARG:HH21	1.74	0.52
1:A:426:ASN:HB3	1:A:431:ILE:HD12	1.91	0.52
1:A:318:HIS:O	1:A:324:ARG:NH1	2.40	0.52
1:B:467:PHE:HB3	1:B:582:MET:CE	2.39	0.52
1:B:673:LEU:HD23	1:B:674:PRO:HD2	1.91	0.52
1:A:771:ILE:C	1:A:773:ASN:N	2.68	0.52
1:B:686:THR:HG21	1:B:688:TRP:HD1	1.74	0.52
1:A:172:MET:HE3	1:A:175:ALA:HB3	1.92	0.52
1:A:60:ALA:O	1:A:64:CYS:HB2	2.09	0.51
1:B:628:MET:CE	1:B:639:GLN:HG2	2.41	0.51
1:A:293:ARG:O	1:A:293:ARG:HG3	2.10	0.51
1:B:159:ILE:HG23	1:B:160:ASN:N	2.25	0.51
1:B:334:ILE:HD12	1:B:404:VAL:HG13	1.92	0.51
1:B:662:TYR:CE2	1:B:673:LEU:HG	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ILE:O	1:A:35:ASP:CB	2.58	0.51
1:A:639:GLN:HE21	1:A:639:GLN:HA	1.75	0.51
1:A:190:TYR:C	1:A:190:TYR:CD2	2.87	0.50
1:A:482:ASN:N	1:A:505:ILE:HD11	2.26	0.50
1:B:486:ASP:OD2	1:B:503:ARG:NH2	2.44	0.50
1:B:511:GLY:O	1:B:515:THR:HG23	2.10	0.50
1:A:94:PHE:HB3	1:A:132:ASN:HD22	1.76	0.50
1:B:630:SER:HA	1:B:639:GLN:HB2	1.92	0.50
1:A:351:PHE:HE1	1:A:371:TYR:CE1	2.30	0.50
1:B:606:MET:HB2	1:B:607:PRO:HD2	1.93	0.50
1:A:471:HIS:HE1	1:A:541:HIS:ND1	2.09	0.50
1:A:64:CYS:SG	1:A:77:LEU:HB3	2.51	0.50
1:A:42:ARG:HD2	1:A:67:MET:HE2	1.94	0.49
1:A:433:GLU:OE1	1:A:441:ALA:HB1	2.12	0.49
1:A:220:LEU:N	1:A:220:LEU:HD23	2.27	0.49
1:A:312:ILE:HD11	1:A:332:LEU:HD21	1.94	0.49
1:A:661:GLN:HA	1:A:664:ILE:CG2	2.42	0.49
1:A:17:LYS:HA	1:A:17:LYS:HE3	1.92	0.49
1:B:190:TYR:O	1:B:194:SER:HB2	2.12	0.49
1:A:342:VAL:HG22	1:A:729:PHE:HZ	1.78	0.49
1:A:660:LYS:O	1:A:664:ILE:HG22	2.13	0.49
1:B:224:LYS:HD3	1:B:233:ASP:HB3	1.95	0.49
1:A:270:ASN:HB3	1:A:274:PRO:HG2	1.95	0.49
1:A:383:ILE:HG12	1:A:384:LYS:N	2.27	0.49
1:A:511:GLY:O	1:A:515:THR:CG2	2.61	0.49
1:B:79:ALA:O	1:B:83:ILE:HG12	2.13	0.49
1:B:345:ASN:O	1:B:346:GLY:O	2.31	0.49
1:A:661:GLN:HA	1:A:664:ILE:HG22	1.95	0.48
1:A:296:ALA:C	1:A:297:PHE:HD2	2.21	0.48
1:A:316:LYS:O	1:A:324:ARG:HD3	2.14	0.48
1:A:663:LEU:HD21	1:A:670:ILE:CD1	2.44	0.48
1:B:293:ARG:H	1:B:293:ARG:HE	1.62	0.48
1:B:766:GLU:OE2	1:B:766:GLU:HA	2.13	0.48
1:A:608:THR:OG1	1:A:612:SER:HB3	2.14	0.48
1:B:37:VAL:HG23	1:B:38:LYS:H	1.77	0.48
1:B:288:GLN:NE2	1:B:293:ARG:NH1	2.62	0.48
1:B:538:THR:CB	1:B:583:TRP:HE1	2.26	0.48
1:A:146:PHE:HD1	1:A:632:ARG:NH2	2.12	0.48
1:B:450:LEU:CB	1:B:515:THR:HG21	2.43	0.48
1:B:520:ARG:HG3	1:B:520:ARG:NH1	2.25	0.48
1:B:589:ARG:O	1:B:593:MET:HG3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:TYR:O	1:B:194:SER:CB	2.62	0.48
1:B:662:TYR:O	1:B:666:GLN:HB2	2.14	0.48
1:A:745:THR:H	2:A:889:GLY:N	2.12	0.47
1:B:450:LEU:HB2	1:B:515:THR:HG21	1.94	0.47
1:A:273:ILE:HB	1:A:274:PRO:HD3	1.97	0.47
1:A:393:LEU:HB3	1:A:724:LEU:HD12	1.96	0.47
1:A:481:LEU:HB3	1:A:505:ILE:CG1	2.42	0.47
1:A:656:ASP:OD2	1:A:767:ASN:OD1	2.32	0.47
1:B:688:TRP:HB3	1:B:717:ARG:HG3	1.95	0.47
1:B:39:VAL:HG22	1:B:67:MET:SD	2.55	0.47
1:A:312:ILE:CD1	1:A:402:PRO:HG3	2.45	0.47
1:A:436:ALA:HB1	1:A:437:PRO:HD2	1.95	0.47
1:B:211:PRO:C	1:B:213:PRO:HD3	2.39	0.47
1:B:775:LYS:HD3	1:B:775:LYS:HA	1.69	0.47
1:A:160:ASN:C	1:A:162:GLN:H	2.22	0.47
1:A:686:THR:HG21	1:A:688:TRP:HD1	1.80	0.47
1:A:503:ARG:N	1:A:504:PRO:HD3	2.30	0.47
1:B:296:ALA:C	1:B:297:PHE:HD1	2.23	0.47
1:B:766:GLU:HG3	1:B:767:ASN:H	1.80	0.47
1:A:632:ARG:HG2	1:A:633:VAL:H	1.78	0.46
1:A:560:PHE:CZ	1:A:596:GLY:HA2	2.51	0.46
1:A:605:PRO:HD2	1:A:710:HIS:HB3	1.97	0.46
1:A:627:ASN:HB2	1:A:668:GLY:O	2.14	0.46
1:A:656:ASP:CB	1:A:659:MET:H	2.29	0.46
1:B:60:ALA:O	1:B:64:CYS:HB2	2.13	0.46
1:B:511:GLY:O	1:B:515:THR:CG2	2.63	0.46
1:A:306:ALA:HA	1:A:350:LEU:HB3	1.97	0.46
1:A:343:GLU:C	1:A:344:GLU:O	2.57	0.46
1:A:606:MET:HB2	1:A:607:PRO:HD2	1.97	0.46
1:B:356:ALA:HB1	1:B:374:TYR:CD1	2.51	0.46
1:B:560:PHE:CZ	1:B:596:GLY:HA2	2.50	0.46
1:A:454:ILE:HD13	1:A:465:TYR:HD1	1.79	0.46
1:B:64:CYS:SG	1:B:77:LEU:HD12	2.56	0.46
1:A:419:LEU:HD21	1:A:559:THR:CG2	2.46	0.46
1:B:534:GLN:O	1:B:538:THR:HG23	2.16	0.46
1:B:660:LYS:HD3	1:B:664:ILE:HD11	1.98	0.46
1:B:77:LEU:HD13	1:B:81:ILE:HD11	1.98	0.46
1:B:464:THR:HG21	1:B:789:SER:CB	2.32	0.46
1:B:212:LYS:H	1:B:212:LYS:HG3	1.58	0.46
1:B:213:PRO:HD2	1:B:489:TYR:HB2	1.97	0.46
1:A:217:SER:O	1:A:246:GLY:HA2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:ILE:HD13	1:A:465:TYR:CD1	2.51	0.45
1:A:464:THR:HG23	1:A:789:SER:OG	2.16	0.45
1:B:293:ARG:HB3	1:B:295:GLY:H	1.81	0.45
1:B:332:LEU:CD1	1:B:392:ILE:HD12	2.39	0.45
1:A:273:ILE:HG21	1:A:323:ILE:HG13	1.97	0.45
1:A:654:ILE:CD1	1:A:769:ALA:HB2	2.45	0.45
1:B:605:PRO:HD2	1:B:710:HIS:HB3	1.98	0.45
1:B:634:LEU:O	1:B:635:SER:HB2	2.16	0.45
1:B:642:ASN:C	1:B:642:ASN:OD1	2.59	0.45
1:A:458:GLU:O	1:A:459:ASP:HB3	2.15	0.45
1:A:678:GLN:OE1	1:A:678:GLN:HA	2.15	0.45
1:B:215:MET:HE3	1:B:484:VAL:HG13	1.98	0.45
1:A:297:PHE:N	1:A:297:PHE:CD2	2.83	0.45
1:B:139:ARG:HD3	1:B:194:SER:OG	2.16	0.45
1:B:444:ASN:C	1:B:445:LEU:HD23	2.42	0.45
1:A:95:SER:N	1:A:132:ASN:HD21	2.11	0.45
1:A:459:ASP:C	1:A:459:ASP:OD1	2.60	0.45
1:B:64:CYS:SG	1:B:77:LEU:CD1	3.04	0.45
1:B:172:MET:HE3	1:B:175:ALA:HB3	1.99	0.45
1:A:304:TRP:O	1:A:350:LEU:HA	2.16	0.45
1:A:401:THR:HB	1:A:402:PRO:HA	1.99	0.45
1:A:628:MET:HE1	1:A:664:ILE:HB	1.98	0.45
1:A:758:GLN:NE2	1:A:758:GLN:O	2.50	0.45
1:B:445:LEU:HD22	1:B:506:ALA:HB3	1.98	0.45
1:B:686:THR:CG2	1:B:688:TRP:CD1	2.99	0.45
1:A:453:PHE:CE2	1:A:470:LEU:HA	2.51	0.45
1:A:458:GLU:OE2	1:A:458:GLU:CA	2.63	0.45
1:B:120:VAL:HG21	1:B:209:GLY:HA2	1.97	0.45
1:B:652:LEU:HD23	1:B:652:LEU:HA	1.89	0.45
1:B:716:LEU:O	1:B:745:THR:HA	2.16	0.45
1:B:19:THR:HG22	1:B:23:SER:HB3	1.98	0.45
1:B:670:ILE:HD13	1:B:670:ILE:HA	1.58	0.44
1:A:467:PHE:CD2	1:A:538:THR:HG21	2.51	0.44
1:A:664:ILE:C	1:A:664:ILE:HD13	2.42	0.44
1:B:25:LEU:O	1:B:80:ARG:HD3	2.17	0.44
1:B:251:HIS:HB3	1:B:424:SER:HB3	1.99	0.44
1:A:717:ARG:O	1:A:746:GLN:O	2.36	0.44
1:B:603:MET:HB2	1:B:707:ASP:HB2	1.98	0.44
1:B:95:SER:N	1:B:132:ASN:HD21	2.02	0.44
1:B:227:SER:O	1:B:231:ILE:HG13	2.17	0.44
1:B:359:LEU:HD12	1:B:359:LEU:HA	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:766:GLU:CG	1:B:767:ASN:H	2.31	0.44
1:A:454:ILE:HD12	1:A:519:LEU:HD13	2.00	0.44
1:A:702:ARG:HD2	1:A:710:HIS:CE1	2.52	0.44
1:B:390:TYR:HD2	1:B:721:MET:HE3	1.83	0.44
1:A:291:ASN:O	1:A:292:LYS:CG	2.67	0.43
1:A:481:LEU:CB	1:A:505:ILE:HG12	2.47	0.43
1:B:519:LEU:HG	1:B:779:TYR:CD1	2.53	0.43
1:A:34:ILE:HG23	1:A:35:ASP:H	1.83	0.43
1:B:713:ASN:ND2	1:B:742:TYR:H	2.15	0.43
1:B:156:LEU:HG	1:B:165:GLU:O	2.19	0.43
1:A:277:ARG:CG	1:A:277:ARG:NH1	2.82	0.43
1:B:490:TYR:HA	1:B:491:PRO:HD3	1.92	0.43
1:B:639:GLN:N	1:B:639:GLN:CD	2.77	0.43
1:B:641:VAL:HG13	1:B:646:LEU:HD22	2.00	0.43
1:A:628:MET:HB3	1:A:628:MET:HE2	1.67	0.43
1:A:115:MET:HE1	1:A:159:ILE:HD13	1.99	0.43
1:A:425:SER:OG	1:A:426:ASN:N	2.52	0.43
1:B:447:SER:OG	1:B:510:GLN:NE2	2.51	0.43
1:A:334:ILE:HA	1:A:335:PRO:HD3	1.84	0.42
1:A:680:LEU:HD22	1:A:680:LEU:HA	1.87	0.42
1:B:673:LEU:H	1:B:681:LYS:NZ	2.17	0.42
1:A:607:PRO:HD3	1:A:711:SER:OG	2.19	0.42
1:B:713:ASN:ND2	1:B:742:TYR:HB2	2.35	0.42
1:B:199:THR:HG21	1:B:611:THR:HB	2.00	0.42
1:A:630:SER:HA	1:A:638:PHE:O	2.19	0.42
1:B:390:TYR:HD2	1:B:721:MET:CE	2.32	0.42
1:B:447:SER:HA	1:B:508:GLY:O	2.19	0.42
1:B:603:MET:H	1:B:707:ASP:HB2	1.84	0.42
1:A:215:MET:HE3	1:A:484:VAL:HG13	2.00	0.42
1:A:297:PHE:HD2	1:A:297:PHE:N	2.17	0.42
1:A:539:ILE:HG22	1:A:603:MET:SD	2.60	0.42
1:B:220:LEU:HD21	1:B:431:ILE:CG1	2.49	0.42
1:A:458:GLU:O	1:A:459:ASP:CB	2.67	0.42
1:A:654:ILE:O	1:A:654:ILE:CG2	2.67	0.42
1:A:670:ILE:HG13	1:A:673:LEU:HD12	2.02	0.42
1:A:686:THR:CG2	1:A:688:TRP:CD1	3.03	0.42
1:B:277:ARG:HH11	1:B:277:ARG:CB	2.19	0.42
1:B:326:ARG:HB2	1:B:326:ARG:NH1	2.35	0.42
1:A:451:PRO:HG3	1:A:515:THR:HG22	2.02	0.42
1:A:312:ILE:HD11	1:A:402:PRO:HG3	2.01	0.42
1:A:312:ILE:HD13	1:A:332:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:VAL:HG13	1:A:646:LEU:HD22	2.01	0.42
1:B:251:HIS:HB2	1:B:253:HIS:NE2	2.35	0.42
1:B:713:ASN:HD22	1:B:742:TYR:H	1.68	0.42
1:A:86:LEU:O	1:A:90:THR:HB	2.20	0.42
1:A:663:LEU:HD23	1:A:663:LEU:HA	1.83	0.41
1:B:71:HIS:ND1	1:B:72:PRO:HD2	2.34	0.41
1:B:256:ARG:HG3	1:B:269:SER:OG	2.20	0.41
1:A:621:PHE:CD2	1:A:621:PHE:N	2.87	0.41
1:A:667:ASN:C	1:A:667:ASN:HD22	2.29	0.41
1:A:140:ASP:OD2	1:A:168:GLN:HG2	2.20	0.41
1:B:699:ALA:HA	1:B:702:ARG:NH1	2.36	0.41
1:A:160:ASN:C	1:A:162:GLN:N	2.78	0.41
1:A:713:ASN:HD22	1:A:742:TYR:H	1.67	0.41
1:B:243:LYS:HD2	1:B:293:ARG:HH12	1.84	0.41
1:A:314:ILE:HA	1:A:314:ILE:HD13	1.67	0.41
1:A:714:LEU:HD23	1:A:727:MET:HE3	2.03	0.41
1:B:220:LEU:CD1	1:B:431:ILE:HD11	2.49	0.41
1:B:593:MET:HE2	1:B:593:MET:HB3	1.95	0.41
1:A:604:ALA:HB2	1:A:708:GLN:HB2	2.03	0.41
1:A:702:ARG:HH11	1:A:710:HIS:CE1	2.39	0.41
1:B:71:HIS:HD2	1:B:73:ASP:HB2	1.86	0.41
1:B:179:HIS:CE1	1:B:189:THR:CG2	3.04	0.41
1:B:714:LEU:HD12	1:B:714:LEU:HA	1.90	0.41
1:A:30:ASP:HB3	1:A:33:HIS:HB2	2.03	0.40
1:A:661:GLN:HE21	1:A:755:THR:CG2	2.34	0.40
1:B:559:THR:O	1:B:559:THR:CG2	2.69	0.40
1:A:775:LYS:HD2	1:A:775:LYS:HA	1.87	0.40
1:B:220:LEU:HD11	1:B:431:ILE:CD1	2.48	0.40
1:A:21:ARG:NH2	1:A:57:ASP:OD2	2.55	0.40
1:A:52:THR:N	1:A:55:GLU:HG2	2.36	0.40
1:B:557:TYR:CZ	1:B:600:SER:HB3	2.57	0.40
1:B:683:LEU:HD12	1:B:683:LEU:HA	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	772/888 (87%)	694 (90%)	54 (7%)	24 (3%)	3	14
1	B	763/888 (86%)	685 (90%)	55 (7%)	23 (3%)	3	14
All	All	1535/1776 (86%)	1379 (90%)	109 (7%)	47 (3%)	3	14

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	PRO
1	A	314	ILE
1	A	633	VAL
1	A	654	ILE
1	A	675	ASN
1	A	770	ASP
1	A	771	ILE
1	A	787	ALA
1	B	37	VAL
1	B	265	THR
1	B	346	GLY
1	B	417	LYS
1	B	619	GLU
1	B	634	LEU
1	B	635	SER
1	A	290	GLY
1	A	459	ASP
1	A	632	ARG
1	A	788	ALA
1	B	36	ALA
1	B	290	GLY
1	B	314	ILE
1	B	672	GLY
1	B	741	TYR
1	B	773	ASN
1	B	774	LEU
1	A	620	CYS
1	A	634	LEU
1	A	741	TYR
1	B	35	ASP
1	B	287	ASP

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Mol	Chain	Res	Type
1	A	144	SER
1	A	159	ILE
1	A	292	LYS
1	A	344	GLU
1	B	325	ALA
1	B	768	VAL
1	A	29	LEU
1	A	717	ARG
1	A	795	ALA
1	B	29	LEU
1	B	266	ASN
1	B	753	GLN
1	B	253	HIS
1	A	293	ARG
1	A	43	ILE
1	B	18	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	667/761 (88%)	563 (84%)	104 (16%)	2	9
1	B	662/761 (87%)	567 (86%)	95 (14%)	3	11
All	All	1329/1522 (87%)	1130 (85%)	199 (15%)	3	10

All (199) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASP
1	A	17	LYS
1	A	22	ILE
1	A	26	CYS
1	A	29	LEU
1	A	34	ILE
1	A	40	THR

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Mol	Chain	Res	Type
1	A	44	ILE
1	A	54	ILE
1	A	69	THR
1	A	77	LEU
1	A	80	ARG
1	A	85	ASN
1	A	86	LEU
1	A	90	THR
1	A	128	LYS
1	A	131	LEU
1	A	135	ILE
1	A	142	GLN
1	A	144	SER
1	A	153	ARG
1	A	156	LEU
1	A	158	ARG
1	A	163	VAL
1	A	170	LEU
1	A	176	LEU
1	A	187	LEU
1	A	189	THR
1	A	196	LYS
1	A	211	PRO
1	A	214	GLN
1	A	220	LEU
1	A	243	LYS
1	A	265	THR
1	A	268	THR
1	A	277	ARG
1	A	282	THR
1	A	293	ARG
1	A	297	PHE
1	A	301	LEU
1	A	312	ILE
1	A	314	ILE
1	A	320	LYS
1	A	323	ILE
1	A	324	ARG
1	A	328	LEU
1	A	337	LEU
1	A	340	LYS
1	A	342	VAL

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Mol	Chain	Res	Type
1	A	359	LEU
1	A	368	GLU
1	A	372	THR
1	A	383	ILE
1	A	384	LYS
1	A	388	LEU
1	A	398	GLU
1	A	407	LYS
1	A	431	ILE
1	A	432	VAL
1	A	445	LEU
1	A	458	GLU
1	A	462	THR
1	A	464	THR
1	A	505	ILE
1	A	512	LEU
1	A	515	THR
1	A	518	LEU
1	A	519	LEU
1	A	530	LEU
1	A	538	THR
1	A	553	LYS
1	A	559	THR
1	A	577	GLN
1	A	606	MET
1	A	610	SER
1	A	624	VAL
1	A	625	THR
1	A	628	MET
1	A	632	ARG
1	A	639	GLN
1	A	640	VAL
1	A	641	VAL
1	A	655	TRP
1	A	659	MET
1	A	660	LYS
1	A	664	ILE
1	A	670	ILE
1	A	675	ASN
1	A	678	GLN
1	A	680	LEU
1	A	686	THR

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Mol	Chain	Res	Type
1	A	693	LYS
1	A	694	THR
1	A	712	LEU
1	A	714	LEU
1	A	717	ARG
1	A	723	LYS
1	A	724	LEU
1	A	743	LEU
1	A	744	ARG
1	A	753	GLN
1	A	758	GLN
1	A	768	VAL
1	A	775	LYS
1	B	15	PHE
1	B	18	ILE
1	B	29	LEU
1	B	38	LYS
1	B	56	LEU
1	B	64	CYS
1	B	77	LEU
1	B	86	LEU
1	B	90	THR
1	B	116	ILE
1	B	131	LEU
1	B	144	SER
1	B	149	LYS
1	B	154	SER
1	B	156	LEU
1	B	159	ILE
1	B	170	LEU
1	B	176	LEU
1	B	187	LEU
1	B	189	THR
1	B	191	ASN
1	B	212	LYS
1	B	214	GLN
1	B	220	LEU
1	B	233	ASP
1	B	258	THR
1	B	265	THR
1	B	277	ARG
1	B	282	THR

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Mol	Chain	Res	Type
1	B	288	GLN
1	B	291	ASN
1	B	292	LYS
1	B	293	ARG
1	B	301	LEU
1	B	314	ILE
1	B	320	LYS
1	B	323	ILE
1	B	324	ARG
1	B	326	ARG
1	B	327	ASP
1	B	328	LEU
1	B	337	LEU
1	B	340	LYS
1	B	342	VAL
1	B	345	ASN
1	B	359	LEU
1	B	365	ASP
1	B	368	GLU
1	B	372	THR
1	B	376	LYS
1	B	379	ARG
1	B	388	LEU
1	B	392	ILE
1	B	397	THR
1	B	431	ILE
1	B	432	VAL
1	B	445	LEU
1	B	448	VAL
1	B	462	THR
1	B	464	THR
1	B	512	LEU
1	B	515	THR
1	B	518	LEU
1	B	519	LEU
1	B	520	ARG
1	B	526	GLU
1	B	530	LEU
1	B	538	THR
1	B	558	GLU
1	B	559	THR
1	B	578	LYS

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Mol	Chain	Res	Type
1	B	625	THR
1	B	626	SER
1	B	632	ARG
1	B	637	GLU
1	B	638	PHE
1	B	639	GLN
1	B	654	ILE
1	B	655	TRP
1	B	670	ILE
1	B	673	LEU
1	B	675	ASN
1	B	681	LYS
1	B	686	THR
1	B	693	LYS
1	B	712	LEU
1	B	714	LEU
1	B	743	LEU
1	B	744	ARG
1	B	749	SER
1	B	752	ILE
1	B	758	GLN
1	B	771	ILE
1	B	775	LYS
1	B	776	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	85	ASN
1	A	87	HIS
1	A	106	ASN
1	A	132	ASN
1	A	142	GLN
1	A	179	HIS
1	A	251	HIS
1	A	266	ASN
1	A	270	ASN
1	A	291	ASN
1	A	444	ASN
1	A	471	HIS
1	A	567	GLN

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Mol	Chain	Res	Type
1	A	571	GLN
1	A	618	ASN
1	A	639	GLN
1	A	661	GLN
1	A	667	ASN
1	A	675	ASN
1	A	710	HIS
1	A	713	ASN
1	A	758	GLN
1	A	767	ASN
1	B	33	HIS
1	B	87	HIS
1	B	93	GLN
1	B	132	ASN
1	B	179	HIS
1	B	207	ASN
1	B	251	HIS
1	B	266	ASN
1	B	288	GLN
1	B	471	HIS
1	B	510	GLN
1	B	552	GLN
1	B	618	ASN
1	B	666	GLN
1	B	667	ASN
1	B	675	ASN
1	B	710	HIS
1	B	713	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands 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	$\# Z > 2$
2	GLY	A	889	-	3,3,4	0.95	0	1,2,4	0.23	0
2	GLY	A	890	-	3,3,4	0.92	0	1,2,4	0.34	0

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
2	GLY	A	889	-	-	0/0/1/2	-
2	GLY	A	890	-	-	0/0/1/2	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	889	GLY	1	0
2	A	890	GLY	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	776/888 (87%)	0.54	101 (13%) 7 6	27, 43, 101, 130	0
1	B	769/888 (86%)	0.54	123 (15%) 5 4	25, 42, 115, 135	0
All	All	1545/1776 (86%)	0.54	224 (14%) 6 4	25, 43, 113, 135	0

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	633	VAL	12.5
1	B	634	LEU	9.5
1	B	54	ILE	8.6
1	B	15	PHE	8.4
1	A	15	PHE	8.1
1	A	52	THR	7.7
1	A	44	ILE	7.0
1	A	632	ARG	7.0
1	B	52	THR	7.0
1	A	634	LEU	6.6
1	A	107	ALA	6.5
1	B	633	VAL	6.4
1	B	796	VAL	6.1
1	B	769	ALA	5.9
1	B	37	VAL	5.9
1	B	17	LYS	5.8
1	B	18	ILE	5.8
1	B	29	LEU	5.8
1	A	638	PHE	5.8
1	B	38	LYS	5.7
1	B	66	TYR	5.6
1	A	108	ALA	5.6
1	B	45	SER	5.6
1	A	265	THR	5.6

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Mol	Chain	Res	Type	RSRZ
1	B	323	ILE	5.5
1	A	29	LEU	5.5
1	A	796	VAL	5.5
1	A	636	GLY	5.4
1	A	294	PRO	5.4
1	A	111	LYS	5.4
1	B	768	VAL	5.4
1	B	21	ARG	5.3
1	B	320	LYS	5.2
1	B	33	HIS	5.1
1	B	53	THR	5.1
1	B	638	PHE	5.1
1	B	32	LYS	5.1
1	B	771	ILE	5.0
1	B	20	ALA	5.0
1	A	28	GLY	4.9
1	B	322	GLU	4.9
1	A	32	LYS	4.8
1	A	17	LYS	4.8
1	A	45	SER	4.8
1	B	70	VAL	4.7
1	A	33	HIS	4.6
1	A	106	ASN	4.6
1	A	290	GLY	4.5
1	A	27	TYR	4.5
1	B	72	PRO	4.4
1	A	31	PRO	4.4
1	B	69	THR	4.3
1	A	38	LYS	4.3
1	B	267	GLY	4.3
1	B	42	ARG	4.3
1	A	264	GLY	4.3
1	A	320	LYS	4.3
1	A	16	ASP	4.2
1	A	54	ILE	4.2
1	A	53	THR	4.2
1	B	639	GLN	4.1
1	B	289	GLY	4.1
1	A	37	VAL	4.1
1	A	36	ALA	4.1
1	A	18	ILE	4.1
1	B	265	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	635	SER	4.0
1	B	766	GLU	3.9
1	A	291	ASN	3.9
1	A	70	VAL	3.9
1	B	263	ALA	3.9
1	B	631	ARG	3.9
1	B	56	LEU	3.9
1	A	69	THR	3.9
1	A	57	ASP	3.8
1	B	290	GLY	3.8
1	A	637	GLU	3.8
1	B	26	CYS	3.8
1	B	64	CYS	3.8
1	A	66	TYR	3.8
1	A	56	LEU	3.8
1	B	16	ASP	3.8
1	B	44	ILE	3.8
1	B	31	PRO	3.8
1	B	637	GLU	3.7
1	B	295	GLY	3.7
1	A	42	ARG	3.7
1	A	43	ILE	3.7
1	B	318	HIS	3.6
1	B	767	ASN	3.6
1	B	636	GLY	3.6
1	A	109	THR	3.6
1	A	635	SER	3.6
1	A	295	GLY	3.6
1	B	772	SER	3.6
1	A	458	GLU	3.6
1	B	212	LYS	3.5
1	B	41	GLN	3.5
1	A	34	ILE	3.5
1	B	658	GLY	3.5
1	A	112	PRO	3.5
1	A	323	ILE	3.5
1	B	27	TYR	3.4
1	B	68	THR	3.4
1	B	264	GLY	3.4
1	A	21	ARG	3.4
1	A	261	TYR	3.4
1	B	672	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	770	ASP	3.4
1	A	266	ASN	3.3
1	B	319	GLY	3.3
1	A	40	THR	3.3
1	B	294	PRO	3.2
1	B	19	THR	3.2
1	A	39	VAL	3.2
1	B	28	GLY	3.2
1	B	39	VAL	3.2
1	A	322	GLU	3.2
1	B	34	ILE	3.2
1	A	639	GLN	3.1
1	A	658	GLY	3.1
1	B	655	TRP	3.1
1	B	36	ALA	3.1
1	B	71	HIS	3.1
1	A	84	SER	3.1
1	B	73	ASP	3.1
1	B	43	ILE	3.1
1	B	63	THR	3.1
1	A	655	TRP	3.0
1	A	768	VAL	3.0
1	A	105	VAL	3.0
1	B	58	ASN	3.0
1	B	35	ASP	2.9
1	B	629	TYR	2.9
1	B	675	ASN	2.9
1	A	775	LYS	2.9
1	A	289	GLY	2.9
1	B	458	GLU	2.9
1	B	630	SER	2.9
1	A	41	GLN	2.8
1	B	59	LEU	2.8
1	B	266	ASN	2.8
1	B	261	TYR	2.8
1	B	107	ALA	2.8
1	B	270	ASN	2.8
1	A	19	THR	2.8
1	B	268	THR	2.8
1	B	665	THR	2.8
1	A	319	GLY	2.8
1	A	26	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	721	MET	2.7
1	B	674	PRO	2.7
1	A	113	ALA	2.7
1	B	40	THR	2.7
1	A	35	ASP	2.7
1	B	670	ILE	2.7
1	A	160	ASN	2.7
1	B	657	GLU	2.7
1	B	67	MET	2.6
1	B	160	ASN	2.6
1	B	345	ASN	2.6
1	A	59	LEU	2.6
1	A	389	TRP	2.6
1	A	64	CYS	2.5
1	B	22	ILE	2.5
1	A	647	ARG	2.5
1	A	30	ASP	2.5
1	B	74	TYR	2.5
1	B	159	ILE	2.5
1	B	60	ALA	2.5
1	A	25	LEU	2.4
1	A	24	ARG	2.4
1	A	288	GLN	2.4
1	A	793	PRO	2.4
1	B	654	ILE	2.4
1	A	110	GLY	2.4
1	A	161	GLY	2.4
1	B	30	ASP	2.4
1	B	292	LYS	2.4
1	B	775	LYS	2.4
1	A	63	THR	2.4
1	B	659	MET	2.4
1	B	752	ILE	2.4
1	A	527	GLU	2.3
1	A	769	ALA	2.3
1	A	22	ILE	2.3
1	A	55	GLU	2.3
1	B	55	GLU	2.3
1	A	640	VAL	2.3
1	B	146	PHE	2.3
1	A	693	LYS	2.3
1	B	748	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	327	ASP	2.2
1	B	493	GLU	2.2
1	B	293	ARG	2.2
1	B	656	ASP	2.2
1	A	268	THR	2.2
1	A	631	ARG	2.2
1	B	326	ARG	2.2
1	B	632	ARG	2.2
1	A	318	HIS	2.2
1	B	23	SER	2.2
1	B	277	ARG	2.2
1	B	652	LEU	2.2
1	B	65	ALA	2.2
1	B	773	ASN	2.1
1	A	376	LYS	2.1
1	B	647	ARG	2.1
1	B	662	TYR	2.1
1	A	675	ASN	2.1
1	B	109	THR	2.1
1	B	296	ALA	2.1
1	B	619	GLU	2.1
1	B	418	ASN	2.1
1	A	20	ALA	2.1
1	A	159	ILE	2.1
1	A	368	GLU	2.1
1	A	418	ASN	2.0
1	B	25	LEU	2.0
1	A	267	GLY	2.0
1	B	62	GLU	2.0
1	B	321	GLU	2.0
1	B	758	GLN	2.0
1	A	344	GLU	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](#)

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, 95th 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
2	GLY	A	889	4/5	0.73	0.26	66,66,66,66	0
2	GLY	A	890	4/5	0.73	0.25	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.