



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 6, 2016 – 03:53 PM EST

PDB ID : 5D0F
Title : Crystal Structure of the Candida Glabrata Glycogen Debranching Enzyme (E564Q) in complex with maltopentaose
Authors : Zhai, L.; Xiang, S.
Deposited on : 2015-08-03
Resolution : 3.30 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

<http://wwpdb.org/validation/2016/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
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

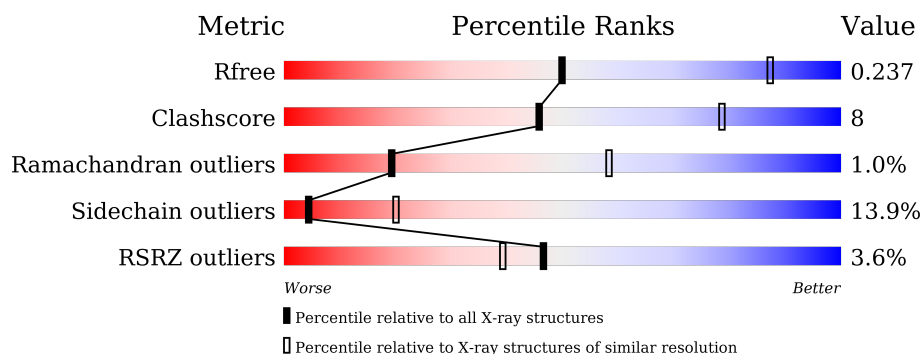
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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. 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	1528	<div> <div>3%</div> <div>72%</div> <div>25%</div> <div>.</div> </div>
1	B	1528	<div> <div>4%</div> <div>71%</div> <div>25%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MTT	A	2001	-	-	-	X
3	CEX	B	2002	-	-	-	X
3	CEX	B	2005	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 25070 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.

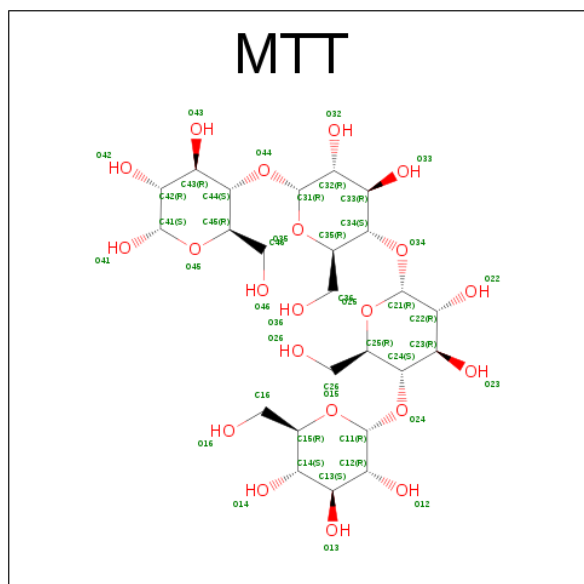
- Molecule 1 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1526	Total	C	N	O	S	0	0	0
			12278	7830	2066	2330	52			
1	B	1526	Total	C	N	O	S	0	0	0
			12278	7830	2066	2330	52			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	564	GLN	GLU	engineered mutation	UNP Q6FSK0
B	564	GLN	GLU	engineered mutation	UNP Q6FSK0

- Molecule 2 is MALTOTETRAOSE (three-letter code: MTT) (formula: $C_{24}H_{42}O_{21}$).



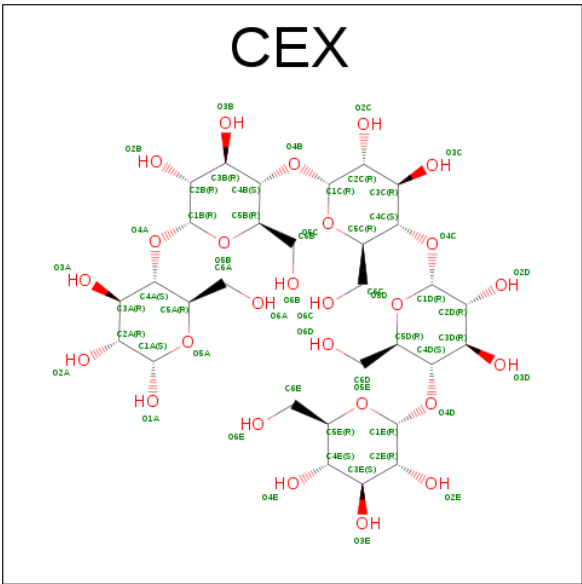
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			45	24	21		

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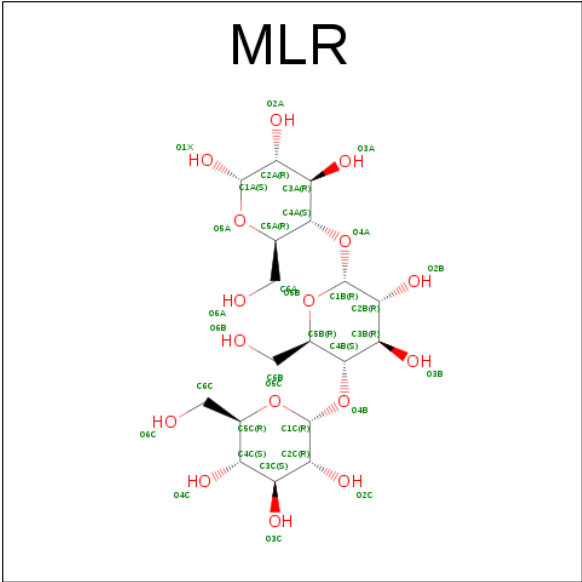
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			44	24	20		
2	A	1	Total	C	O	0	0
			44	24	20		
2	B	1	Total	C	O	0	0
			45	24	21		
2	B	1	Total	C	O	0	0
			44	24	20		

- Molecule 3 is alpha-D-glucopyranosyl-(1->4)-alpha-D-glucopyranosyl-(1->4)-alpha-D-glucopyranosyl-(1->4)-alpha-D-glucopyranosyl-(1->4)-alpha-D-glucopyranose (three-letter code: CEX) (formula: C₃₀H₅₂O₂₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			56	30	26		
3	A	1	Total	C	O	0	0
			56	30	26		
3	B	1	Total	C	O	0	0
			56	30	26		
3	B	1	Total	C	O	0	0
			56	30	26		

- Molecule 4 is MALTOTRIOSE (three-letter code: MLR) (formula: C₁₈H₃₂O₁₆).

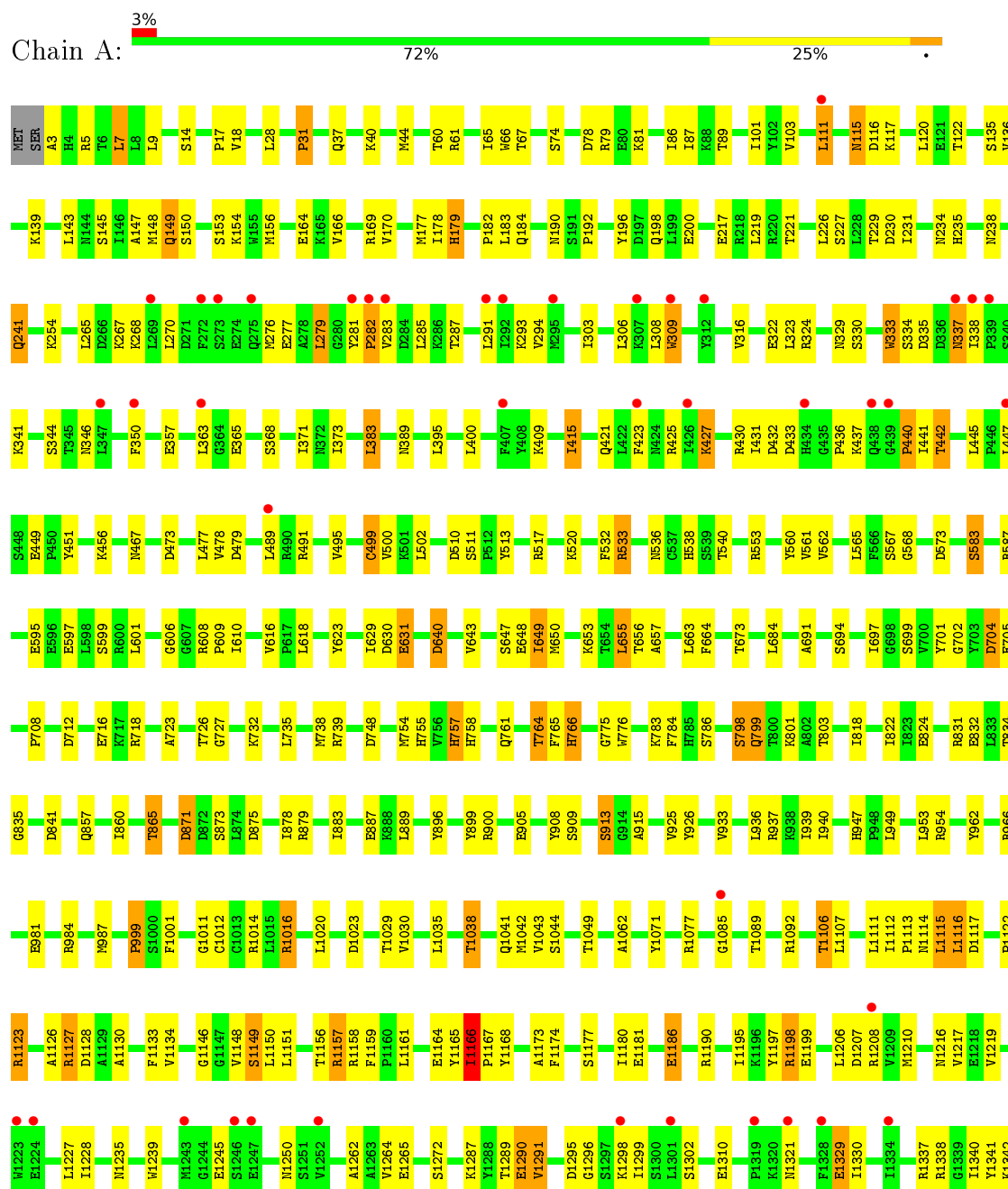


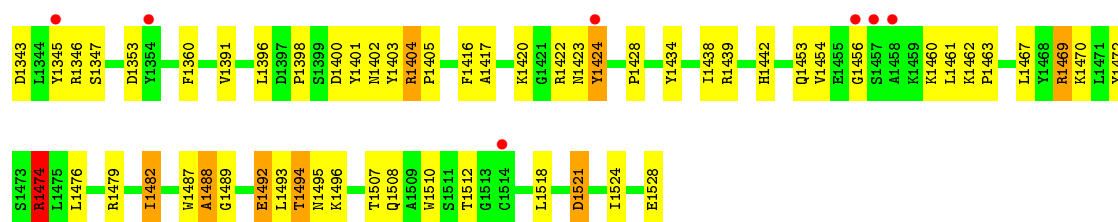
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			34	18	16		
4	B	1	Total	C	O	0	0
			34	18	16		

3 Residue-property plots

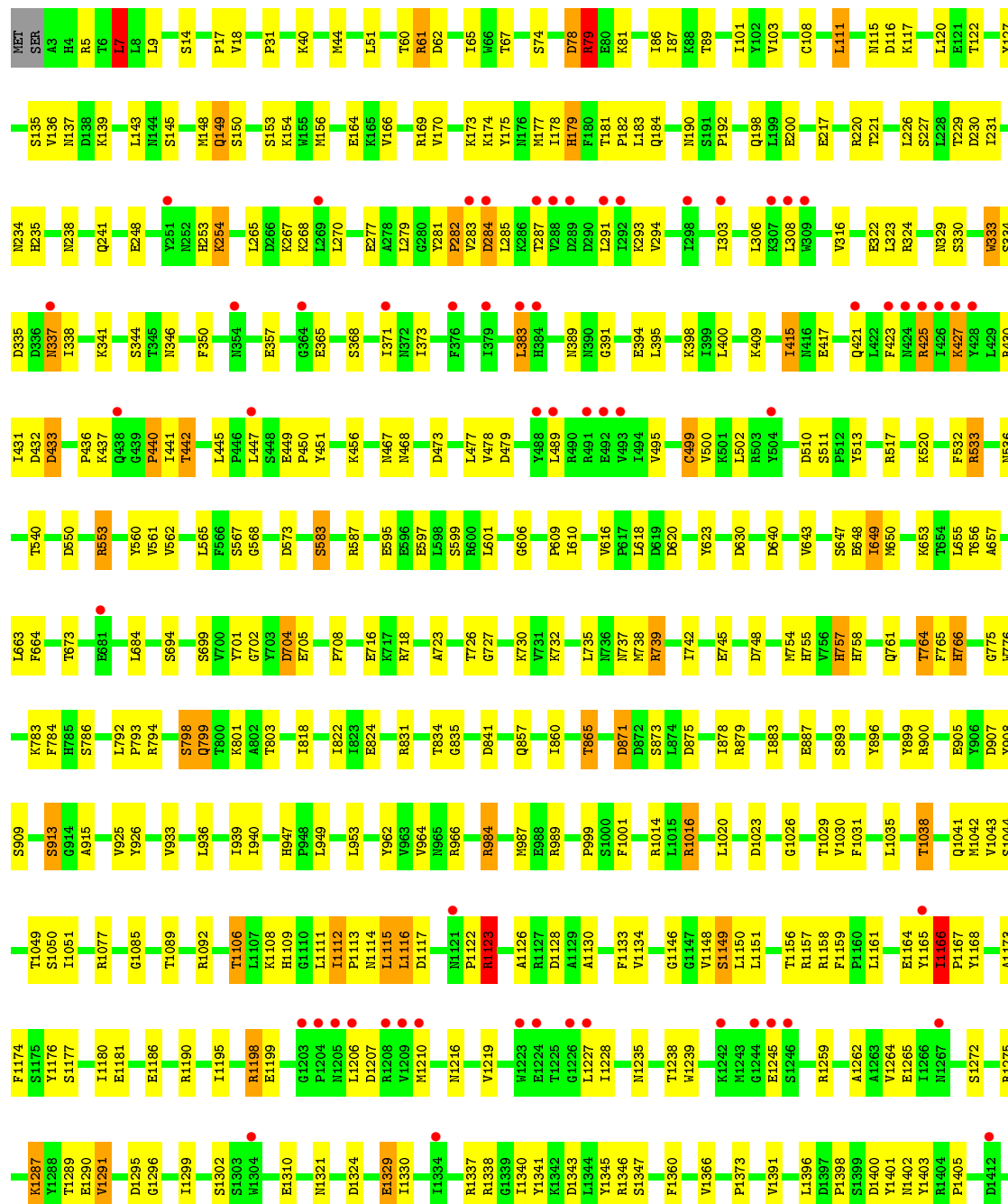
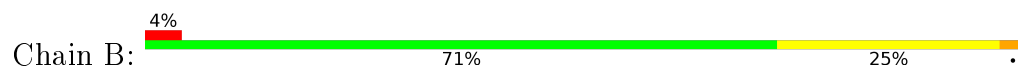
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

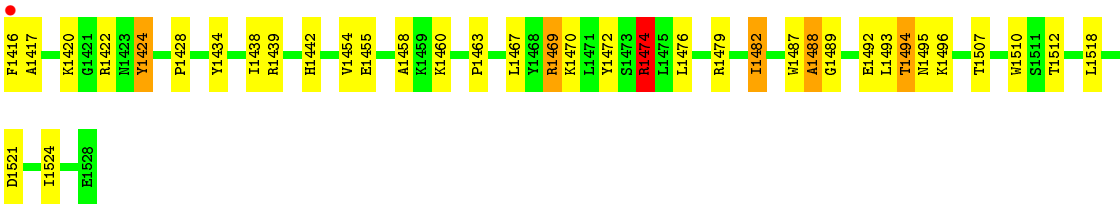
• Molecule 1: Uncharacterized protein





• Molecule 1: Uncharacterized protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.07Å 202.01Å 135.24Å 90.00° 101.32° 90.00°	Depositor
Resolution (Å)	49.05 – 3.30 49.05 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.8 (49.05-3.30) 95.9 (49.05-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.192 , 0.228 0.201 , 0.237	Depositor DCC
R_{free} test set	3072 reflections (5.41%)	DCC
Wilson B-factor (Å ²)	85.3	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 32.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	25070	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MLR, MTT, CEX

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	0.81	2/12589 (0.0%)	1.00	20/17071 (0.1%)
1	B	0.81	0/12589	1.00	26/17071 (0.2%)
All	All	0.81	2/25178 (0.0%)	1.00	46/34142 (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	3
1	B	0	4
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1071	TYR	CB-CG	5.10	1.59	1.51
1	A	832	GLU	CD-OE2	5.09	1.31	1.25

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1474	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	B	1469	ARG	NE-CZ-NH1	8.47	124.54	120.30
1	B	61	ARG	NE-CZ-NH1	7.97	124.29	120.30
1	B	1014	ARG	NE-CZ-NH2	-7.81	116.40	120.30
1	A	1469	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	A	1474	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	A	1014	ARG	NE-CZ-NH2	-7.18	116.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	640	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	A	533	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	B	533	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	B	79	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	A	61	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	B	1014	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	A	1488	ALA	N-CA-CB	6.30	118.91	110.10
1	B	984	ARG	N-CA-CB	6.25	121.86	110.60
1	B	1469	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	A	1014	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	B	553	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	A	954	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	B	1488	ALA	N-CA-CB	5.98	118.47	110.10
1	A	739	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	1127	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	A	640	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	5	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	1115	LEU	CA-CB-CG	5.59	128.15	115.30
1	B	841	ASP	CB-CG-OD2	5.57	123.31	118.30
1	B	1123	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	5	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	B	739	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	B	553	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	989	ARG	CG-CD-NE	-5.46	100.33	111.80
1	A	1115	LEU	CA-CB-CG	5.46	127.85	115.30
1	A	533	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	B	51	LEU	CA-CB-CG	-5.33	103.03	115.30
1	A	1127	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	1469	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	B	78	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	1127	ARG	CG-CD-NE	5.22	122.76	111.80
1	B	1489	GLY	N-CA-C	5.15	125.98	113.10
1	B	989	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	1489	GLY	N-CA-C	5.10	125.84	113.10
1	B	79	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	640	ASP	CB-CG-OD1	5.06	122.86	118.30
1	A	608	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	309	TRP	CA-CB-CG	-5.04	104.13	113.70
1	B	7	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1492	GLU	Peptide
1	A	306	LEU	Peptide
1	A	442	THR	Peptide
1	B	1492	GLU	Peptide
1	B	241	GLN	Peptide
1	B	306	LEU	Peptide
1	B	442	THR	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	12278	0	11962	192	0
1	B	12278	0	11962	192	0
2	A	133	0	122	0	0
2	B	89	0	82	0	0
3	A	112	0	104	0	0
3	B	112	0	104	1	0
4	A	34	0	32	0	0
4	B	34	0	32	1	0
All	All	25070	0	24400	383	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 8.

All (383) 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:1158:ARG:O	1:B:1159:PHE:HD2	1.38	1.04
1:B:1158:ARG:O	1:B:1159:PHE:CD2	2.17	0.97
1:A:1062:ALA:O	1:A:1508:GLN:OE1	1.92	0.86
1:A:230:ASP:OD1	1:A:533:ARG:HD3	1.77	0.84
1:B:230:ASP:OD1	1:B:533:ARG:HD3	1.79	0.83
1:B:757:HIS:HB3	1:B:764:THR:HG22	1.62	0.82
1:B:1482:ILE:HG12	1:B:1488:ALA:O	1.82	0.80
1:A:1482:ILE:HG12	1:A:1488:ALA:O	1.82	0.79
1:A:757:HIS:HB3	1:A:764:THR:HG22	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:871:ASP:N	1:B:871:ASP:OD1	2.20	0.75
1:B:1041:GLN:NE2	1:B:1488:ALA:HB3	2.07	0.70
1:A:1439:ARG:HD2	1:A:1521:ASP:OD2	1.91	0.69
1:A:282:PRO:HB3	1:A:294:VAL:HG22	1.74	0.69
1:B:1439:ARG:HD2	1:B:1521:ASP:OD2	1.94	0.68
1:B:282:PRO:HB3	1:B:294:VAL:HG22	1.75	0.68
1:B:964:VAL:HG11	1:B:984:ARG:HB3	1.75	0.68
1:A:1041:GLN:NE2	1:A:1488:ALA:HB3	2.09	0.67
1:A:1470:LYS:O	1:A:1474:ARG:HG3	1.94	0.67
1:A:629:ILE:HD13	1:A:631:GLU:HG2	1.76	0.67
1:A:871:ASP:N	1:A:871:ASP:OD1	2.28	0.66
1:B:1470:LYS:O	1:B:1474:ARG:HG3	1.97	0.65
1:A:3:ALA:HB3	1:A:640:ASP:HB3	1.77	0.65
1:B:783:LYS:HG2	1:B:857:GLN:HB3	1.80	0.64
1:A:1165:TYR:O	1:A:1167:PRO:CD	2.46	0.64
1:A:783:LYS:HG2	1:A:857:GLN:HB3	1.78	0.64
1:A:66:TRP:CZ3	1:B:1458:ALA:HB2	2.32	0.64
1:A:148:MET:HA	1:A:177:MET:O	1.98	0.63
1:A:705:GLU:N	1:A:705:GLU:OE1	2.31	0.63
1:B:1165:TYR:O	1:B:1167:PRO:CD	2.46	0.63
1:B:148:MET:HA	1:B:177:MET:O	1.98	0.63
1:A:704:ASP:OD2	1:A:732:LYS:HG3	1.99	0.63
1:B:115:ASN:HB3	1:B:117:LYS:H	1.64	0.63
1:B:1041:GLN:HE22	1:B:1488:ALA:HB3	1.64	0.63
1:B:656:THR:HG22	1:B:657:ALA:N	2.15	0.62
1:A:115:ASN:HB3	1:A:117:LYS:H	1.64	0.62
1:A:365:GLU:HB2	1:A:368:SER:HB3	1.82	0.61
1:B:704:ASP:OD2	1:B:732:LYS:HG3	2.01	0.61
1:A:915:ALA:HA	1:A:962:TYR:OH	2.00	0.61
1:B:365:GLU:HB2	1:B:368:SER:HB3	1.83	0.61
1:B:1085:GLY:O	1:B:1089:THR:HB	2.01	0.61
1:A:1041:GLN:HE22	1:A:1488:ALA:HB3	1.65	0.60
1:B:169:ARG:NH1	1:B:701:TYR:OH	2.34	0.60
1:B:1146:GLY:O	1:B:1149:SER:OG	2.20	0.60
1:B:684:LEU:HD11	1:B:860:ILE:HD12	1.83	0.60
1:B:1472:TYR:OH	1:B:1479:ARG:NH1	2.34	0.60
1:A:283:VAL:HA	1:A:441:ILE:HD11	1.85	0.59
1:A:9:LEU:HD11	1:A:17:PRO:HB3	1.83	0.59
1:B:757:HIS:HB3	1:B:764:THR:CG2	2.31	0.59
1:A:1085:GLY:O	1:A:1089:THR:HB	2.02	0.59
1:B:705:GLU:N	1:B:705:GLU:OE1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1165:TYR:O	1:A:1167:PRO:HD3	2.03	0.59
1:B:915:ALA:HA	1:B:962:TYR:OH	2.03	0.59
1:A:1157:ARG:NH2	1:A:1186:GLU:OE2	2.36	0.58
1:A:182:PRO:HG2	1:A:192:PRO:O	2.03	0.58
1:A:467:ASN:HB2	1:A:499:CYS:O	2.03	0.58
1:A:647:SER:OG	1:A:648:GLU:N	2.36	0.58
1:B:1038:THR:HG21	1:B:1512:THR:OG1	2.03	0.58
1:A:1038:THR:HG21	1:A:1512:THR:OG1	2.03	0.57
1:B:1396:LEU:HD21	1:B:1400:ASP:HB3	1.86	0.57
1:B:182:PRO:HG2	1:B:192:PRO:O	2.05	0.57
1:A:169:ARG:NH1	1:A:701:TYR:OH	2.34	0.57
1:B:432:ASP:HB2	1:B:436:PRO:HB3	1.86	0.57
1:B:1165:TYR:O	1:B:1167:PRO:HD3	2.04	0.57
1:B:283:VAL:HA	1:B:441:ILE:HD11	1.86	0.57
1:B:430:ARG:NH1	1:B:440:PRO:O	2.38	0.56
1:A:1158:ARG:O	1:A:1159:PHE:CD2	2.58	0.56
1:A:432:ASP:HB2	1:A:436:PRO:HB3	1.87	0.56
1:A:684:LEU:HD11	1:A:860:ILE:HD12	1.88	0.56
1:B:467:ASN:HB2	1:B:499:CYS:O	2.05	0.56
1:A:1146:GLY:O	1:A:1149:SER:OG	2.23	0.56
1:A:1493:LEU:HD23	1:A:1494:THR:N	2.21	0.56
1:A:1396:LEU:HD21	1:A:1400:ASP:HB3	1.88	0.56
1:A:1492:GLU:HG3	1:A:1508:GLN:HG3	1.88	0.56
1:B:1396:LEU:HD21	1:B:1400:ASP:CB	2.36	0.56
1:A:1472:TYR:OH	1:A:1479:ARG:NH1	2.39	0.55
1:A:1456:GLY:HA3	1:A:1462:LYS:HG3	1.88	0.55
1:A:1038:THR:HG21	1:A:1512:THR:CB	2.37	0.55
1:A:65:ILE:HG12	1:A:111:LEU:HD22	1.89	0.55
1:A:430:ARG:NH1	1:A:440:PRO:O	2.39	0.55
1:A:656:THR:HG22	1:A:657:ALA:N	2.22	0.55
1:B:925:VAL:CG1	1:B:1487:TRP:CE2	2.90	0.55
1:A:738:MET:HE2	1:A:776:TRP:CZ2	2.42	0.55
1:B:630:ASP:O	1:B:648:GLU:HG2	2.07	0.54
1:B:738:MET:HE3	1:B:776:TRP:CZ3	2.43	0.54
1:B:79:ARG:HH21	1:B:550:ASP:CG	2.10	0.54
1:A:1106:THR:HG21	1:A:1113:PRO:HG3	1.90	0.54
1:A:1123:ARG:NH2	1:A:1207:ASP:OD2	2.41	0.54
1:B:1493:LEU:HD23	1:B:1494:THR:N	2.22	0.54
1:A:630:ASP:O	1:A:648:GLU:HG2	2.06	0.54
1:B:65:ILE:HG12	1:B:111:LEU:HD22	1.90	0.54
1:B:1405:PRO:HA	1:B:1428:PRO:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:GLY:O	1:A:694:SER:HB3	2.08	0.54
1:A:303:ILE:HG13	1:A:415:ILE:HD11	1.90	0.54
1:B:647:SER:OG	1:B:648:GLU:N	2.41	0.53
1:A:1396:LEU:HD21	1:A:1400:ASP:CB	2.38	0.53
1:A:196:TYR:OH	1:A:241:GLN:NE2	2.42	0.53
1:B:303:ILE:HG13	1:B:415:ILE:HD11	1.91	0.53
1:B:1029:THR:HG22	1:B:1030:VAL:N	2.23	0.53
1:A:757:HIS:HB3	1:A:764:THR:CG2	2.37	0.53
1:B:1340:ILE:HG22	1:B:1341:TYR:C	2.29	0.53
1:B:1106:THR:HG21	1:B:1113:PRO:HG3	1.90	0.53
1:A:1156:THR:CG2	1:A:1174:PHE:HA	2.39	0.53
1:B:1123:ARG:NH2	1:B:1207:ASP:OD2	2.42	0.52
1:B:1108:LYS:HE2	1:B:1159:PHE:CD1	2.45	0.52
1:B:60:THR:HG22	1:B:87:ILE:HG21	1.91	0.52
1:A:1340:ILE:HG22	1:A:1341:TYR:C	2.30	0.52
1:A:738:MET:HB3	1:A:776:TRP:CH2	2.45	0.52
1:B:1038:THR:HG21	1:B:1512:THR:CB	2.40	0.52
1:B:606:GLY:O	1:B:694:SER:HB3	2.10	0.52
1:A:148:MET:HE3	1:A:663:LEU:HD21	1.92	0.52
1:B:560:TYR:CE2	1:B:562:VAL:CG2	2.93	0.52
1:A:60:THR:HG22	1:A:87:ILE:HG21	1.92	0.52
1:B:905:GLU:OE1	1:B:966:ARG:NH1	2.43	0.52
1:B:1128:ASP:OD2	1:B:1239:TRP:N	2.43	0.52
1:A:1114:ASN:HB2	1:A:1126:ALA:HB2	1.92	0.51
1:A:1029:THR:HG22	1:A:1030:VAL:N	2.26	0.51
1:B:925:VAL:CG1	1:B:1487:TRP:CD2	2.93	0.51
1:A:798:SER:O	1:A:799:GLN:C	2.47	0.51
1:A:281:TYR:N	1:A:282:PRO:HD3	2.25	0.51
1:B:798:SER:O	1:B:799:GLN:C	2.49	0.51
1:A:905:GLU:OE1	1:A:966:ARG:NH1	2.43	0.51
1:B:1156:THR:CG2	1:B:1174:PHE:HA	2.39	0.51
1:B:1262:ALA:HB3	1:B:1345:TYR:HB3	1.93	0.51
1:A:1041:GLN:OE1	1:A:1507:THR:HG21	2.11	0.51
1:A:287:THR:O	1:A:291:LEU:HG	2.11	0.51
1:B:1114:ASN:HB2	1:B:1126:ALA:HB2	1.92	0.51
1:B:9:LEU:HD11	1:B:17:PRO:HB3	1.92	0.51
1:A:1404:ARG:O	1:A:1423:ASN:OD1	2.29	0.51
1:A:909:SER:CB	1:A:913:SER:HB2	2.41	0.51
1:A:1195:ILE:HG12	1:A:1219:VAL:HB	1.93	0.50
1:B:1035:LEU:O	1:B:1038:THR:HG22	2.12	0.50
1:A:1405:PRO:HA	1:A:1428:PRO:HD3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1463:PRO:HB3	1:B:1467:LEU:HD23	1.94	0.50
1:B:177:MET:HA	1:B:226:LEU:O	2.12	0.50
1:B:925:VAL:HG11	1:B:1487:TRP:CD2	2.46	0.50
1:A:1264:VAL:HG11	1:A:1360:PHE:HA	1.93	0.50
1:A:282:PRO:CB	1:A:294:VAL:HG22	2.40	0.50
1:A:231:ILE:HD12	1:A:532:PHE:CD1	2.47	0.50
1:A:925:VAL:CG1	1:A:1487:TRP:CD2	2.95	0.50
1:A:1156:THR:HG21	1:A:1174:PHE:HA	1.94	0.50
1:A:1181:GLU:OE1	1:A:1287:LYS:HG3	2.12	0.50
1:A:1291:VAL:CG2	1:A:1299:ILE:O	2.60	0.50
1:B:1166:ILE:HD11	1:B:1168:TYR:HB2	1.94	0.50
1:A:1128:ASP:OD2	1:A:1239:TRP:N	2.44	0.50
1:B:834:THR:HG22	1:B:835:GLY:N	2.27	0.49
1:A:834:THR:HG22	1:A:835:GLY:N	2.28	0.49
1:B:775:GLY:O	1:B:776:TRP:HD1	1.94	0.49
1:A:1166:ILE:HD11	1:A:1168:TYR:HB2	1.94	0.49
1:A:761:GLN:NE2	1:A:857:GLN:OE1	2.44	0.49
1:A:925:VAL:HG11	1:A:1487:TRP:CD2	2.48	0.49
1:A:896:TYR:O	1:A:966:ARG:NH2	2.40	0.49
1:B:1195:ILE:HG12	1:B:1219:VAL:HB	1.93	0.49
1:A:1035:LEU:O	1:A:1038:THR:HG22	2.11	0.49
1:A:1463:PRO:HB3	1:A:1467:LEU:HD23	1.95	0.49
1:B:287:THR:O	1:B:291:LEU:HG	2.12	0.49
1:B:1041:GLN:OE1	1:B:1507:THR:HG21	2.13	0.49
1:B:282:PRO:CB	1:B:294:VAL:HG22	2.41	0.49
1:A:925:VAL:CG1	1:A:1487:TRP:CE2	2.95	0.49
1:B:148:MET:HE3	1:B:663:LEU:HD21	1.94	0.49
1:B:766:HIS:CE1	1:B:865:THR:HG21	2.48	0.49
1:A:441:ILE:HG22	1:A:442:THR:N	2.27	0.49
1:B:896:TYR:O	1:B:966:ARG:NH2	2.43	0.49
1:B:1198:ARG:HA	1:B:1216:ASN:HA	1.94	0.48
1:B:1434:TYR:OH	1:B:1474:ARG:HB3	2.13	0.48
1:B:909:SER:CB	1:B:913:SER:HB2	2.43	0.48
1:B:567:SER:OG	1:B:568:GLY:N	2.46	0.48
1:A:136:VAL:HG12	1:A:139:LYS:HB2	1.94	0.48
1:A:595:GLU:HG3	1:A:784:PHE:CD2	2.48	0.48
1:B:656:THR:CG2	1:B:657:ALA:N	2.77	0.48
1:A:467:ASN:HA	1:A:500:VAL:HA	1.95	0.48
1:A:513:TYR:CE2	1:A:517:ARG:HD2	2.48	0.48
1:B:101:ILE:HD12	1:B:101:ILE:N	2.29	0.48
1:B:253:HIS:CD2	1:B:254:LYS:N	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:MET:HA	1:A:226:LEU:O	2.13	0.48
1:B:1108:LYS:CE	1:B:1159:PHE:CD1	2.96	0.48
1:B:441:ILE:HG22	1:B:442:THR:N	2.29	0.48
1:A:1168:TYR:C	1:A:1168:TYR:CD1	2.86	0.48
1:A:1262:ALA:HB3	1:A:1345:TYR:HB3	1.96	0.48
1:B:899:TYR:CD1	1:B:1041:GLN:HG2	2.49	0.48
1:B:1156:THR:HG21	1:B:1174:PHE:HA	1.95	0.48
1:B:595:GLU:HG3	1:B:784:PHE:CD2	2.49	0.48
1:A:560:TYR:CE2	1:A:562:VAL:CG2	2.96	0.47
1:A:775:GLY:O	1:A:776:TRP:HD1	1.97	0.47
1:B:1108:LYS:HE2	1:B:1159:PHE:HD1	1.78	0.47
1:B:1291:VAL:CG2	1:B:1299:ILE:O	2.61	0.47
1:B:1416:PHE:CE2	1:B:1422:ARG:NH2	2.81	0.47
1:A:1398:PRO:HA	1:A:1403:TYR:CG	2.49	0.47
1:A:899:TYR:CD1	1:A:1041:GLN:HG2	2.49	0.47
1:B:1168:TYR:CD1	1:B:1168:TYR:O	2.67	0.47
1:B:1417:ALA:O	1:B:1422:ARG:HB2	2.15	0.47
1:A:427:LYS:HE2	1:A:433:ASP:OD2	2.14	0.47
1:A:610:ILE:HD12	1:A:755:HIS:HB2	1.95	0.47
1:B:7:LEU:HD22	1:B:643:VAL:HG21	1.96	0.47
1:A:28:LEU:HB3	1:A:655:LEU:HD11	1.96	0.47
1:A:567:SER:OG	1:A:568:GLY:N	2.48	0.47
1:A:766:HIS:CE1	1:A:865:THR:HG21	2.50	0.47
1:B:1165:TYR:O	1:B:1167:PRO:HD2	2.14	0.47
1:A:1295:ASP:OD1	1:A:1296:GLY:N	2.47	0.47
1:B:1198:ARG:O	1:B:1199:GLU:C	2.53	0.47
1:B:766:HIS:HE1	1:B:865:THR:HG21	1.79	0.47
1:A:101:ILE:N	1:A:101:ILE:HD12	2.29	0.47
1:B:150:SER:OG	1:B:179:HIS:HD2	1.98	0.47
1:B:757:HIS:CB	1:B:764:THR:HG22	2.39	0.47
1:B:136:VAL:HG12	1:B:139:LYS:HG3	1.97	0.47
1:B:234:ASN:OD1	1:B:540:THR:OG1	2.33	0.47
1:A:766:HIS:HE1	1:A:865:THR:HG21	1.79	0.47
1:A:1168:TYR:O	1:A:1168:TYR:CD1	2.67	0.46
1:B:1038:THR:O	1:B:1042:MET:HG2	2.15	0.46
1:B:1295:ASP:OD1	1:B:1296:GLY:N	2.48	0.46
1:B:1398:PRO:HA	1:B:1403:TYR:CG	2.50	0.46
1:B:648:GLU:HB3	1:B:883:ILE:HD12	1.98	0.46
1:A:1198:ARG:HA	1:A:1216:ASN:HA	1.97	0.46
1:B:1168:TYR:CD1	1:B:1168:TYR:C	2.87	0.46
1:A:1016:ARG:O	1:A:1020:LEU:HG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1165:TYR:O	1:A:1167:PRO:HD2	2.14	0.46
1:A:623:TYR:CD2	1:A:649:ILE:HD11	2.50	0.46
1:A:1038:THR:O	1:A:1042:MET:HG2	2.15	0.46
1:A:277:GLU:OE2	1:A:283:VAL:HG22	2.15	0.46
1:B:925:VAL:HG13	1:B:1487:TRP:CZ2	2.50	0.46
1:A:1077:ARG:NH1	1:A:1114:ASN:OD1	2.49	0.46
1:B:281:TYR:N	1:B:282:PRO:HD3	2.31	0.46
1:B:775:GLY:O	1:B:776:TRP:CD1	2.69	0.46
1:B:925:VAL:HG11	1:B:1487:TRP:CE2	2.50	0.46
1:A:154:LYS:NZ	1:A:190:ASN:O	2.49	0.46
1:B:1016:ARG:O	1:B:1020:LEU:HG	2.16	0.46
1:A:1106:THR:CG2	1:A:1113:PRO:HG3	2.46	0.46
1:A:1434:TYR:OH	1:A:1474:ARG:HB3	2.16	0.46
1:A:947:HIS:HD2	1:A:949:LEU:H	1.64	0.46
1:B:623:TYR:CD2	1:B:649:ILE:HD11	2.50	0.46
1:A:567:SER:HB3	1:A:573:ASP:OD1	2.16	0.46
1:B:1264:VAL:HG11	1:B:1360:PHE:HA	1.98	0.46
1:B:1077:ARG:NH1	1:B:1114:ASN:OD1	2.49	0.46
1:B:1438:ILE:HG23	1:B:1518:LEU:HD22	1.98	0.46
1:A:235:HIS:HA	1:A:502:LEU:HG	1.97	0.46
1:B:149:GLN:HA	1:B:699:SER:O	2.16	0.46
1:B:235:HIS:HA	1:B:502:LEU:HG	1.97	0.46
1:A:1417:ALA:O	1:A:1422:ARG:HB2	2.15	0.45
1:B:154:LYS:NZ	1:B:190:ASN:O	2.49	0.45
1:B:1405:PRO:HA	1:B:1428:PRO:CD	2.46	0.45
1:B:513:TYR:CE2	1:B:517:ARG:HD2	2.51	0.45
1:B:567:SER:HB3	1:B:573:ASP:OD1	2.17	0.45
1:A:648:GLU:HB3	1:A:883:ILE:HD12	1.98	0.45
1:A:936:LEU:O	1:A:940:ILE:HG13	2.16	0.45
1:B:427:LYS:HE2	1:B:433:ASP:OD2	2.16	0.45
1:A:1151:LEU:HA	1:A:1180:ILE:HG22	1.97	0.45
1:A:702:GLY:HA2	1:A:705:GLU:HB2	1.98	0.45
1:A:834:THR:HG22	1:A:835:GLY:H	1.81	0.45
1:B:1158:ARG:HD3	1:B:1173:ALA:HB1	1.99	0.45
1:B:561:VAL:H	1:B:583:SER:HG	1.65	0.45
1:A:1416:PHE:CE2	1:A:1422:ARG:NH2	2.85	0.45
1:A:1495:ASN:O	1:A:1496:LYS:C	2.53	0.45
1:A:231:ILE:HD12	1:A:532:PHE:CG	2.51	0.45
1:B:1106:THR:CG2	1:B:1113:PRO:HG3	2.47	0.45
1:A:1438:ILE:HG23	1:A:1518:LEU:HD22	1.98	0.45
1:A:7:LEU:HD22	1:A:643:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1107:LEU:O	1:A:1157:ARG:NH1	2.50	0.44
1:A:309:TRP:N	1:A:309:TRP:CD1	2.85	0.44
1:B:742:ILE:HD12	1:B:776:TRP:CH2	2.51	0.44
1:B:702:GLY:HA2	1:B:705:GLU:HB2	1.99	0.44
1:A:149:GLN:HA	1:A:699:SER:O	2.18	0.44
1:B:277:GLU:OE2	1:B:283:VAL:HG22	2.16	0.44
1:A:234:ASN:OD1	1:A:540:THR:OG1	2.33	0.44
1:B:1151:LEU:HA	1:B:1180:ILE:HG22	1.99	0.44
1:A:618:LEU:HD22	1:A:933:VAL:HG13	1.99	0.44
1:A:1043:VAL:HB	1:A:1092:ARG:HH22	1.82	0.44
1:A:1508:GLN:HA	1:A:1508:GLN:OE1	2.17	0.44
1:A:1116:LEU:HA	1:A:1122:PRO:HB3	1.99	0.44
1:A:1290:GLU:HG2	1:A:1298:LYS:NZ	2.33	0.44
1:B:338:ILE:HG21	1:B:383:LEU:HG	2.00	0.44
1:B:231:ILE:HD12	1:B:532:PHE:CD1	2.53	0.44
1:B:761:GLN:NE2	1:B:857:GLN:OE1	2.51	0.44
1:B:322:GLU:HB3	1:B:373:ILE:HD13	1.99	0.44
1:B:478:VAL:O	1:B:479:ASP:C	2.56	0.44
1:B:467:ASN:HA	1:B:500:VAL:HA	2.00	0.44
1:B:1219:VAL:HG13	1:B:1228:ILE:HG23	2.01	0.43
1:B:156:MET:HG2	1:B:166:VAL:HG21	2.00	0.43
1:B:738:MET:HB3	1:B:776:TRP:CH2	2.53	0.43
1:A:322:GLU:HB3	1:A:373:ILE:HD13	1.99	0.43
1:B:149:GLN:HG2	1:B:170:VAL:HG11	1.98	0.43
1:A:1492:GLU:HA	1:A:1508:GLN:CG	2.49	0.43
1:A:281:TYR:N	1:A:282:PRO:CD	2.82	0.43
1:A:738:MET:HE1	1:A:776:TRP:CE2	2.53	0.43
1:B:173:LYS:HE3	1:B:175:TYR:HE1	1.84	0.43
1:B:231:ILE:HD12	1:B:532:PHE:CG	2.53	0.43
1:B:716:GLU:OE2	1:B:718:ARG:NH1	2.51	0.43
1:B:899:TYR:O	1:B:926:TYR:HB3	2.18	0.43
1:A:656:THR:CG2	1:A:657:ALA:N	2.82	0.43
1:A:716:GLU:OE2	1:A:718:ARG:NH1	2.52	0.43
1:A:899:TYR:O	1:A:926:TYR:HB3	2.19	0.43
1:B:1043:VAL:HB	1:B:1092:ARG:HH22	1.83	0.43
1:A:338:ILE:HG21	1:A:383:LEU:HG	2.00	0.43
1:A:436:PRO:O	1:A:437:LYS:HG2	2.19	0.43
1:A:478:VAL:O	1:A:479:ASP:C	2.57	0.43
1:A:1405:PRO:HA	1:A:1428:PRO:CD	2.48	0.43
1:A:981:GLU:OE1	1:A:984:ARG:NH1	2.52	0.43
1:B:953:LEU:HD13	1:B:999:PRO:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LEU:N	1:A:111:LEU:HD23	2.33	0.43
1:A:561:VAL:H	1:A:583:SER:HG	1.65	0.43
1:B:1108:LYS:CE	1:B:1159:PHE:HD1	2.31	0.43
1:B:170:VAL:HG21	1:B:178:ILE:HD11	2.01	0.43
1:B:174:LYS:HG3	1:B:737:ASN:OD1	2.18	0.43
1:B:610:ILE:HD12	1:B:755:HIS:HB2	2.01	0.43
1:A:1011:GLY:O	1:A:1012:CYS:C	2.55	0.43
1:A:1198:ARG:O	1:A:1199:GLU:C	2.58	0.43
1:B:1116:LEU:HA	1:B:1122:PRO:HB3	1.99	0.43
1:B:1130:ALA:O	1:B:1133:PHE:HB3	2.19	0.43
1:A:1042:MET:CE	1:A:1507:THR:HG22	2.48	0.43
1:A:170:VAL:HG21	1:A:178:ILE:HD11	2.00	0.43
1:A:775:GLY:HA3	1:A:865:THR:CG2	2.49	0.43
1:B:618:LEU:HD22	1:B:933:VAL:HG13	2.00	0.42
1:B:1181:GLU:OE1	1:B:1287:LYS:HG3	2.19	0.42
1:B:893:SER:HA	1:B:896:TYR:CD2	2.54	0.42
1:A:939:ILE:HD11	1:A:947:HIS:CD2	2.54	0.42
1:B:1329:GLU:O	1:B:1330:ILE:HG23	2.20	0.42
1:A:451:TYR:CE1	1:A:495:VAL:HG21	2.55	0.42
1:A:925:VAL:HG11	1:A:1487:TRP:CE2	2.54	0.42
1:A:1158:ARG:HD3	1:A:1173:ALA:HB1	2.01	0.42
1:A:1329:GLU:O	1:A:1330:ILE:HG23	2.20	0.42
1:B:878:ILE:HD13	1:B:1001:PHE:HD1	1.85	0.42
1:B:1157:ARG:HG2	1:B:1176:TYR:OH	2.19	0.42
1:B:391:GLY:HA2	1:B:394:GLU:OE1	2.18	0.42
1:A:1130:ALA:O	1:A:1133:PHE:HB3	2.19	0.42
1:A:775:GLY:O	1:A:776:TRP:CD1	2.72	0.42
1:B:436:PRO:O	1:B:437:LYS:HG2	2.20	0.42
1:B:775:GLY:HA3	1:B:865:THR:CG2	2.50	0.42
1:A:149:GLN:HG2	1:A:170:VAL:HG11	2.02	0.42
1:A:436:PRO:O	1:A:437:LYS:CG	2.67	0.42
1:A:841:ASP:C	1:A:841:ASP:OD1	2.58	0.42
1:B:1495:ASN:O	1:B:1496:LYS:C	2.58	0.42
1:B:217:GLU:O	1:B:221:THR:HG23	2.19	0.42
1:B:834:THR:HG22	1:B:835:GLY:H	1.84	0.42
1:A:217:GLU:O	1:A:221:THR:HG23	2.19	0.42
1:B:875:ASP:OD2	1:B:879:ARG:HD2	2.19	0.42
1:B:1108:LYS:HD2	1:B:1109:HIS:CD2	2.55	0.42
1:A:147:ALA:HA	1:A:697:ILE:O	2.19	0.42
1:A:783:LYS:HG2	1:A:857:GLN:CB	2.46	0.42
1:B:148:MET:HG3	1:B:177:MET:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:939:ILE:HD11	1:B:947:HIS:CD2	2.55	0.42
1:A:1219:VAL:HG13	1:A:1228:ILE:HG23	2.01	0.41
1:B:1050:SER:OG	1:B:1051:ILE:N	2.52	0.41
1:B:1238:THR:HG21	1:B:1259:ARG:NH1	2.35	0.41
1:B:1275:ARG:NH2	1:B:1366:VAL:O	2.53	0.41
1:B:1112:ILE:HD13	1:B:1133:PHE:CG	2.55	0.41
1:B:108:CYS:HB3	1:B:127:TYR:CD2	2.55	0.41
1:A:618:LEU:HD12	1:A:937:ARG:HG3	2.03	0.41
1:B:1042:MET:CE	1:B:1507:THR:HG22	2.50	0.41
1:B:284:ASP:OD1	1:B:284:ASP:N	2.54	0.41
1:A:276:MET:O	1:A:279:LEU:O	2.38	0.41
1:A:1264:VAL:HG23	1:A:1343:ASP:O	2.20	0.41
1:A:937:ARG:HG2	1:A:937:ARG:NH1	2.36	0.41
1:A:691:ALA:HA	1:A:697:ILE:HD13	2.03	0.41
1:B:792:LEU:HA	1:B:793:PRO:HD3	1.91	0.41
1:A:150:SER:OG	1:A:179:HIS:HD2	2.04	0.41
1:A:230:ASP:OD1	1:A:533:ARG:CD	2.60	0.41
1:B:337:ASN:OD1	1:B:337:ASN:N	2.54	0.41
1:B:436:PRO:O	1:B:437:LYS:CG	2.69	0.41
1:A:1492:GLU:HB2	1:A:1508:GLN:HG2	2.03	0.41
1:A:149:GLN:OE1	1:A:701:TYR:HA	2.21	0.41
1:A:337:ASN:OD1	1:A:337:ASN:N	2.54	0.41
1:A:878:ILE:HD13	1:A:1001:PHE:HD1	1.85	0.41
1:B:1400:ASP:HA	4:B:2004:MLR:O6A	2.21	0.41
1:B:620:ASP:OD1	1:B:620:ASP:N	2.53	0.41
1:B:793:PRO:O	1:B:794:ARG:C	2.59	0.41
1:A:1453:GLN:NE2	1:A:1461:LEU:HD21	2.36	0.41
1:A:875:ASP:OD2	1:A:879:ARG:HD2	2.21	0.41
1:B:425:ARG:NE	3:B:2005:CEX:O6D	2.54	0.41
1:A:156:MET:HG2	1:A:166:VAL:HG21	2.03	0.40
1:A:333:TRP:CH2	1:A:350:PHE:HZ	2.38	0.40
1:B:1264:VAL:HG23	1:B:1343:ASP:O	2.21	0.40
1:B:451:TYR:CE1	1:B:495:VAL:HG21	2.55	0.40
1:A:1197:TYR:CE1	1:A:1217:VAL:HG23	2.56	0.40
1:A:1342:LYS:HB2	1:A:1353:ASP:O	2.21	0.40
1:B:1030:VAL:O	1:B:1031:PHE:C	2.60	0.40
1:B:136:VAL:HG13	1:B:137:ASN:N	2.35	0.40
1:B:230:ASP:OD1	1:B:533:ARG:CD	2.61	0.40
1:B:936:LEU:O	1:B:940:ILE:HG13	2.21	0.40
1:B:947:HIS:HD2	1:B:949:LEU:H	1.68	0.40
1:A:738:MET:CE	1:A:776:TRP:CE2	3.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:HIS:CD2	1:A:949:LEU:H	2.39	0.40
1:A:953:LEU:HD13	1:A:999:PRO:HA	2.03	0.40
1:B:181:THR:HB	1:B:182:PRO:HD2	2.03	0.40
1:B:333:TRP:CH2	1:B:350:PHE:HZ	2.39	0.40
1:B:111:LEU:HD23	1:B:111:LEU:N	2.36	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	1524/1528 (100%)	1314 (86%)	195 (13%)	15 (1%)	19	58
1	B	1524/1528 (100%)	1321 (87%)	188 (12%)	15 (1%)	19	58
All	All	3048/3056 (100%)	2635 (86%)	383 (13%)	30 (1%)	19	58

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	887	GLU
1	B	887	GLU
1	A	440	PRO
1	A	723	ALA
1	A	1424	TYR
1	B	440	PRO
1	B	1424	TYR
1	A	219	LEU
1	A	282	PRO
1	A	308	LEU
1	B	308	LEU
1	B	723	ALA
1	B	727	GLY

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Mol	Chain	Res	Type
1	B	745	GLU
1	B	1026	GLY
1	B	1166	ILE
1	A	31	PRO
1	A	538	HIS
1	A	708	PRO
1	A	1166	ILE
1	A	1521	ASP
1	B	31	PRO
1	B	282	PRO
1	A	115	ASN
1	A	727	GLY
1	B	708	PRO
1	A	511	SER
1	B	511	SER
1	B	450	PRO
1	B	1373	PRO

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	1344/1346 (100%)	1157 (86%)	187 (14%)	4	20
1	B	1344/1346 (100%)	1157 (86%)	187 (14%)	4	20
All	All	2688/2692 (100%)	2314 (86%)	374 (14%)	4	20

All (374) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	14	SER
1	A	18	VAL
1	A	31	PRO
1	A	37	GLN
1	A	40	LYS

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Mol	Chain	Res	Type
1	A	44	MET
1	A	67	THR
1	A	74	SER
1	A	78	ASP
1	A	79	ARG
1	A	81	LYS
1	A	86	ILE
1	A	89	THR
1	A	103	VAL
1	A	111	LEU
1	A	116	ASP
1	A	120	LEU
1	A	122	THR
1	A	135	SER
1	A	143	LEU
1	A	145	SER
1	A	149	GLN
1	A	153	SER
1	A	164	GLU
1	A	179	HIS
1	A	183	LEU
1	A	184	GLN
1	A	198	GLN
1	A	200	GLU
1	A	227	SER
1	A	229	THR
1	A	238	ASN
1	A	241	GLN
1	A	254	LYS
1	A	265	LEU
1	A	267	LYS
1	A	268	LYS
1	A	270	LEU
1	A	279	LEU
1	A	285	LEU
1	A	293	LYS
1	A	316	VAL
1	A	323	LEU
1	A	324	ARG
1	A	329	ASN
1	A	330	SER
1	A	333	TRP

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Mol	Chain	Res	Type
1	A	334	SER
1	A	335	ASP
1	A	337	ASN
1	A	341	LYS
1	A	344	SER
1	A	346	ASN
1	A	357	GLU
1	A	363	LEU
1	A	371	ILE
1	A	383	LEU
1	A	389	ASN
1	A	395	LEU
1	A	400	LEU
1	A	409	LYS
1	A	415	ILE
1	A	421	GLN
1	A	423	PHE
1	A	425	ARG
1	A	427	LYS
1	A	431	ILE
1	A	445	LEU
1	A	447	LEU
1	A	449	GLU
1	A	456	LYS
1	A	473	ASP
1	A	477	LEU
1	A	489	LEU
1	A	491	ARG
1	A	499	CYS
1	A	510	ASP
1	A	520	LYS
1	A	536	ASN
1	A	553	ARG
1	A	565	LEU
1	A	583	SER
1	A	587	ARG
1	A	597	GLU
1	A	599	SER
1	A	601	LEU
1	A	609	PRO
1	A	616	VAL
1	A	631	GLU

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Mol	Chain	Res	Type
1	A	649	ILE
1	A	650	MET
1	A	653	LYS
1	A	655	LEU
1	A	664	PHE
1	A	673	THR
1	A	704	ASP
1	A	712	ASP
1	A	726	THR
1	A	735	LEU
1	A	748	ASP
1	A	754	MET
1	A	757	HIS
1	A	758	HIS
1	A	764	THR
1	A	765	PHE
1	A	766	HIS
1	A	786	SER
1	A	798	SER
1	A	799	GLN
1	A	801	LYS
1	A	803	THR
1	A	818	ILE
1	A	822	ILE
1	A	824	GLU
1	A	831	ARG
1	A	865	THR
1	A	871	ASP
1	A	873	SER
1	A	889	LEU
1	A	900	ARG
1	A	908	TYR
1	A	913	SER
1	A	987	MET
1	A	999	PRO
1	A	1016	ARG
1	A	1023	ASP
1	A	1038	THR
1	A	1044	SER
1	A	1049	THR
1	A	1106	THR
1	A	1111	LEU

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Mol	Chain	Res	Type
1	A	1112	ILE
1	A	1115	LEU
1	A	1116	LEU
1	A	1117	ASP
1	A	1123	ARG
1	A	1127	ARG
1	A	1134	VAL
1	A	1148	VAL
1	A	1149	SER
1	A	1150	LEU
1	A	1157	ARG
1	A	1161	LEU
1	A	1164	GLU
1	A	1166	ILE
1	A	1177	SER
1	A	1186	GLU
1	A	1190	ARG
1	A	1198	ARG
1	A	1206	LEU
1	A	1208	ARG
1	A	1210	MET
1	A	1227	LEU
1	A	1235	ASN
1	A	1245	GLU
1	A	1250	ASN
1	A	1265	GLU
1	A	1272	SER
1	A	1289	THR
1	A	1290	GLU
1	A	1291	VAL
1	A	1302	SER
1	A	1310	GLU
1	A	1321	ASN
1	A	1329	GLU
1	A	1337	ARG
1	A	1338	ARG
1	A	1346	ARG
1	A	1347	SER
1	A	1391	VAL
1	A	1401	TYR
1	A	1402	ASN
1	A	1404	ARG

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Mol	Chain	Res	Type
1	A	1420	LYS
1	A	1424	TYR
1	A	1442	HIS
1	A	1454	VAL
1	A	1460	LYS
1	A	1469	ARG
1	A	1474	ARG
1	A	1476	LEU
1	A	1482	ILE
1	A	1494	THR
1	A	1510	TRP
1	A	1524	ILE
1	A	1528	GLU
1	B	7	LEU
1	B	14	SER
1	B	18	VAL
1	B	40	LYS
1	B	44	MET
1	B	61	ARG
1	B	62	ASP
1	B	67	THR
1	B	74	SER
1	B	78	ASP
1	B	79	ARG
1	B	81	LYS
1	B	86	ILE
1	B	89	THR
1	B	103	VAL
1	B	111	LEU
1	B	116	ASP
1	B	120	LEU
1	B	122	THR
1	B	135	SER
1	B	143	LEU
1	B	145	SER
1	B	149	GLN
1	B	153	SER
1	B	164	GLU
1	B	179	HIS
1	B	183	LEU
1	B	184	GLN
1	B	198	GLN

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Mol	Chain	Res	Type
1	B	200	GLU
1	B	220	ARG
1	B	227	SER
1	B	229	THR
1	B	238	ASN
1	B	248	GLU
1	B	254	LYS
1	B	265	LEU
1	B	267	LYS
1	B	268	LYS
1	B	270	LEU
1	B	279	LEU
1	B	284	ASP
1	B	285	LEU
1	B	293	LYS
1	B	316	VAL
1	B	323	LEU
1	B	324	ARG
1	B	329	ASN
1	B	330	SER
1	B	333	TRP
1	B	334	SER
1	B	335	ASP
1	B	337	ASN
1	B	341	LYS
1	B	344	SER
1	B	346	ASN
1	B	357	GLU
1	B	371	ILE
1	B	383	LEU
1	B	389	ASN
1	B	395	LEU
1	B	398	LYS
1	B	400	LEU
1	B	409	LYS
1	B	415	ILE
1	B	417	GLU
1	B	421	GLN
1	B	423	PHE
1	B	425	ARG
1	B	427	LYS
1	B	431	ILE

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Mol	Chain	Res	Type
1	B	433	ASP
1	B	445	LEU
1	B	447	LEU
1	B	449	GLU
1	B	456	LYS
1	B	468	ASN
1	B	473	ASP
1	B	477	LEU
1	B	489	LEU
1	B	499	CYS
1	B	510	ASP
1	B	520	LYS
1	B	536	ASN
1	B	553	ARG
1	B	565	LEU
1	B	583	SER
1	B	587	ARG
1	B	597	GLU
1	B	599	SER
1	B	601	LEU
1	B	609	PRO
1	B	616	VAL
1	B	649	ILE
1	B	650	MET
1	B	653	LYS
1	B	655	LEU
1	B	664	PHE
1	B	673	THR
1	B	704	ASP
1	B	726	THR
1	B	730	LYS
1	B	735	LEU
1	B	739	ARG
1	B	748	ASP
1	B	754	MET
1	B	757	HIS
1	B	758	HIS
1	B	764	THR
1	B	765	PHE
1	B	766	HIS
1	B	786	SER
1	B	798	SER

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Mol	Chain	Res	Type
1	B	799	GLN
1	B	801	LYS
1	B	803	THR
1	B	818	ILE
1	B	822	ILE
1	B	824	GLU
1	B	831	ARG
1	B	865	THR
1	B	871	ASP
1	B	873	SER
1	B	900	ARG
1	B	907	ASP
1	B	908	TYR
1	B	913	SER
1	B	987	MET
1	B	1016	ARG
1	B	1023	ASP
1	B	1038	THR
1	B	1044	SER
1	B	1049	THR
1	B	1106	THR
1	B	1111	LEU
1	B	1112	ILE
1	B	1115	LEU
1	B	1116	LEU
1	B	1117	ASP
1	B	1123	ARG
1	B	1134	VAL
1	B	1148	VAL
1	B	1149	SER
1	B	1150	LEU
1	B	1161	LEU
1	B	1164	GLU
1	B	1166	ILE
1	B	1177	SER
1	B	1186	GLU
1	B	1190	ARG
1	B	1198	ARG
1	B	1206	LEU
1	B	1210	MET
1	B	1227	LEU
1	B	1235	ASN

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Mol	Chain	Res	Type
1	B	1245	GLU
1	B	1265	GLU
1	B	1272	SER
1	B	1287	LYS
1	B	1289	THR
1	B	1290	GLU
1	B	1291	VAL
1	B	1302	SER
1	B	1310	GLU
1	B	1321	ASN
1	B	1324	ASP
1	B	1329	GLU
1	B	1337	ARG
1	B	1338	ARG
1	B	1346	ARG
1	B	1347	SER
1	B	1391	VAL
1	B	1401	TYR
1	B	1402	ASN
1	B	1420	LYS
1	B	1424	TYR
1	B	1442	HIS
1	B	1454	VAL
1	B	1455	GLU
1	B	1460	LYS
1	B	1469	ARG
1	B	1474	ARG
1	B	1476	LEU
1	B	1482	ILE
1	B	1494	THR
1	B	1510	TRP
1	B	1524	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	92	HIS
1	A	179	HIS
1	A	238	ASN
1	A	354	ASN
1	A	605	HIS

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Mol	Chain	Res	Type
1	A	766	HIS
1	A	790	GLN
1	A	866	GLN
1	A	876	HIS
1	A	947	HIS
1	A	1309	GLN
1	A	1355	GLN
1	A	1409	ASN
1	A	1442	HIS
1	A	1453	GLN
1	B	92	HIS
1	B	179	HIS
1	B	238	ASN
1	B	241	GLN
1	B	253	HIS
1	B	354	ASN
1	B	766	HIS
1	B	790	GLN
1	B	866	GLN
1	B	876	HIS
1	B	947	HIS
1	B	1250	ASN
1	B	1355	GLN
1	B	1409	ASN
1	B	1442	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

11 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	MTT	A	2001	-	48,48,48	1.12	4 (8%)	71,71,71	1.12	7 (9%)
3	CEX	A	2002	-	60,60,60	0.96	4 (6%)	89,89,89	1.04	4 (4%)
2	MTT	A	2003	-	47,47,48	0.95	2 (4%)	69,69,71	1.26	6 (8%)
4	MLR	A	2004	-	36,36,36	1.08	5 (13%)	53,53,53	1.35	6 (11%)
3	CEX	A	2005	-	60,60,60	0.96	5 (8%)	89,89,89	1.06	5 (5%)
2	MTT	A	2006	-	47,47,48	1.11	3 (6%)	69,69,71	1.16	6 (8%)
2	MTT	B	2001	-	48,48,48	1.10	2 (4%)	71,71,71	1.31	9 (12%)
3	CEX	B	2002	-	60,60,60	1.11	6 (10%)	89,89,89	1.19	6 (6%)
2	MTT	B	2003	-	47,47,48	1.13	7 (14%)	69,69,71	1.71	11 (15%)
4	MLR	B	2004	-	36,36,36	0.75	0	53,53,53	1.08	4 (7%)
3	CEX	B	2005	-	60,60,60	0.81	0	89,89,89	0.94	5 (5%)

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	MTT	A	2001	-	-	0/20/100/100	0/4/4/4
3	CEX	A	2002	-	-	0/26/126/126	0/5/5/5
2	MTT	A	2003	-	-	0/20/97/100	0/4/4/4
4	MLR	A	2004	-	-	0/14/74/74	0/3/3/3
3	CEX	A	2005	-	-	0/26/126/126	0/5/5/5
2	MTT	A	2006	-	-	0/20/97/100	0/4/4/4
2	MTT	B	2001	-	-	0/20/100/100	0/4/4/4
3	CEX	B	2002	-	-	0/26/126/126	0/5/5/5
2	MTT	B	2003	-	-	0/20/97/100	0/4/4/4
4	MLR	B	2004	-	-	0/14/74/74	0/3/3/3
3	CEX	B	2005	-	-	0/26/126/126	0/5/5/5

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2003	MTT	C43-C44	2.03	1.58	1.52
2	A	2006	MTT	O15-C11	2.03	1.47	1.41
2	A	2001	MTT	O34-C21	2.04	1.47	1.41
3	A	2005	CEX	C3E-C4E	2.05	1.57	1.52
2	A	2003	MTT	O44-C31	2.06	1.47	1.41
3	B	2002	CEX	C4B-C5B	2.09	1.58	1.52
3	A	2002	CEX	O4D-C1E	2.09	1.47	1.41
4	A	2004	MLR	O4A-C1B	2.11	1.47	1.41
3	A	2002	CEX	O4B-C1C	2.11	1.47	1.41
3	B	2002	CEX	O5E-C1E	2.13	1.47	1.41
4	A	2004	MLR	O5C-C1C	2.13	1.47	1.41
3	A	2005	CEX	O5A-C1A	2.14	1.47	1.43
3	A	2002	CEX	O4A-C1B	2.22	1.47	1.41
3	B	2002	CEX	O5D-C1D	2.22	1.47	1.41
3	A	2005	CEX	O5B-C1B	2.25	1.47	1.41
2	B	2003	MTT	C42-C43	2.26	1.55	1.52
2	B	2003	MTT	O44-C44	2.26	1.49	1.43
4	A	2004	MLR	O4B-C1C	2.27	1.47	1.41
4	A	2004	MLR	O5B-C1B	2.29	1.47	1.41
2	B	2003	MTT	O25-C21	2.30	1.47	1.41
2	B	2003	MTT	O15-C11	2.35	1.47	1.41
3	A	2005	CEX	O4A-C1B	2.38	1.48	1.41
2	B	2001	MTT	O24-C11	2.41	1.48	1.41
2	A	2001	MTT	O15-C15	2.48	1.50	1.44
2	A	2006	MTT	O35-C31	2.49	1.48	1.41
4	A	2004	MLR	O5B-C5B	2.52	1.50	1.44
2	A	2006	MTT	O25-C21	2.52	1.48	1.41
2	A	2003	MTT	O15-C11	2.58	1.48	1.41
3	A	2005	CEX	C4E-C5E	2.65	1.58	1.53
3	B	2002	CEX	O4A-C1B	2.73	1.49	1.41
3	B	2002	CEX	O5B-C5B	2.76	1.51	1.44
2	A	2001	MTT	O24-C11	2.79	1.49	1.41
2	B	2003	MTT	O44-C31	2.81	1.49	1.41
2	B	2003	MTT	O34-C21	2.90	1.49	1.41
2	A	2001	MTT	O15-C11	2.97	1.49	1.41
3	A	2002	CEX	O5B-C1B	3.04	1.49	1.41
2	B	2001	MTT	O15-C11	3.26	1.50	1.41
3	B	2002	CEX	O5B-C1B	3.38	1.50	1.41

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	MTT	C33-C34-C35	-3.00	104.00	110.85
3	B	2005	CEX	O4C-C1D-O5D	-2.82	103.35	110.69
2	A	2001	MTT	C23-C24-C25	-2.54	105.04	110.85
2	B	2003	MTT	O43-C43-C42	-2.50	105.42	110.01
4	B	2004	MLR	O6A-C6A-C5A	-2.42	103.23	111.30
2	B	2003	MTT	C23-C24-C25	-2.40	105.36	110.85
2	B	2003	MTT	C33-C34-C35	-2.32	105.54	110.85
3	A	2002	CEX	C3D-C4D-C5D	-2.30	105.59	110.85
2	B	2001	MTT	C33-C34-C35	-2.12	106.01	110.85
3	A	2005	CEX	O6E-C6E-C5E	-2.11	104.25	111.30
3	B	2002	CEX	C3E-C4E-C5E	-2.10	106.47	110.23
3	A	2005	CEX	O4C-C1D-O5D	-2.09	105.25	110.69
4	A	2004	MLR	C6B-C5B-C4B	-2.09	107.11	113.25
2	B	2001	MTT	O16-C16-C15	-2.06	104.41	111.30
3	A	2005	CEX	C6A-C5A-C4A	-2.04	107.27	113.25
2	A	2003	MTT	O16-C16-C15	-2.02	104.56	111.30
4	A	2004	MLR	O6C-C6C-C5C	-2.01	104.59	111.30
2	B	2001	MTT	O46-C46-C45	-2.00	104.61	111.30
2	A	2006	MTT	O34-C34-C35	2.01	114.67	109.33
3	B	2002	CEX	O5D-C5D-C6D	2.05	111.69	106.38
2	B	2001	MTT	C42-C43-C44	2.09	114.24	109.63
3	B	2005	CEX	C3E-C4E-C5E	2.12	114.00	110.23
2	A	2003	MTT	C42-C43-C44	2.12	114.96	110.56
2	A	2001	MTT	C21-C22-C23	2.13	114.20	109.98
3	B	2002	CEX	O4A-C1B-O5B	2.15	116.28	110.69
3	B	2005	CEX	O5E-C5E-C4E	2.15	113.78	109.67
2	B	2001	MTT	O25-C25-C24	2.16	114.38	109.78
2	B	2001	MTT	O24-C11-O15	2.22	116.46	110.69
2	B	2001	MTT	C31-O35-C35	2.22	118.10	113.74
2	A	2001	MTT	O34-C21-C22	2.27	113.77	108.12
2	A	2006	MTT	O35-C31-C32	2.29	115.03	110.28
2	A	2003	MTT	O25-C25-C26	2.29	112.31	106.38
2	A	2006	MTT	C21-O34-C34	2.37	124.31	118.00
3	B	2005	CEX	O5A-C5A-C6A	2.37	112.53	106.38
2	B	2003	MTT	O34-C21-O25	2.47	117.14	110.69
3	A	2002	CEX	C1A-O5A-C5A	2.52	118.36	113.54
3	A	2002	CEX	O4A-C1B-O5B	2.53	117.28	110.69
3	B	2002	CEX	O4A-C4A-C3A	2.56	113.85	107.18
4	A	2004	MLR	O5B-C5B-C4B	2.61	115.33	109.78
2	A	2001	MTT	O24-C11-O15	2.64	117.58	110.69
2	B	2003	MTT	O45-C41-C42	2.70	115.21	110.89
4	B	2004	MLR	O5B-C5B-C4B	2.74	115.63	109.78
4	A	2004	MLR	C1C-O5C-C5C	2.77	119.18	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2002	CEX	O5B-C5B-C6B	2.78	113.58	106.38
2	B	2001	MTT	C11-O15-C15	2.85	119.34	113.74
2	A	2006	MTT	C31-O35-C35	2.87	119.37	113.74
2	A	2001	MTT	O15-C15-C16	2.87	113.81	106.38
2	A	2001	MTT	O45-C45-C44	2.94	116.04	109.78
4	A	2004	MLR	O5B-C5B-C6B	2.94	114.00	106.38
3	B	2005	CEX	C1D-O5D-C5D	3.01	119.65	113.74
4	B	2004	MLR	C1C-O5C-C5C	3.14	119.90	113.74
3	B	2002	CEX	O5C-C5C-C6C	3.18	114.62	106.38
2	A	2003	MTT	C41-O45-C45	3.26	116.94	112.14
3	A	2005	CEX	O5E-C5E-C4E	3.29	115.94	109.67
2	B	2003	MTT	C11-O15-C15	3.35	120.31	113.74
4	B	2004	MLR	C1B-O5B-C5B	3.44	120.50	113.74
2	A	2006	MTT	O15-C15-C16	3.49	115.41	106.38
2	A	2006	MTT	C21-O25-C25	3.64	120.89	113.74
2	A	2003	MTT	O45-C45-C46	3.70	115.26	107.34
3	A	2005	CEX	C3E-C4E-C5E	3.73	116.88	110.23
2	B	2003	MTT	O25-C25-C26	3.74	116.08	106.38
2	B	2003	MTT	C42-C43-C44	3.85	118.53	110.56
2	A	2003	MTT	C11-O15-C15	4.04	121.67	113.74
2	B	2003	MTT	C41-C42-C43	4.24	114.69	109.55
2	B	2001	MTT	C21-O25-C25	5.11	123.77	113.74
2	B	2003	MTT	O45-C45-C46	5.12	118.29	107.34
4	A	2004	MLR	C1B-O5B-C5B	5.37	124.28	113.74
3	B	2002	CEX	C1B-O5B-C5B	5.84	125.20	113.74
2	B	2003	MTT	C41-O45-C45	6.16	121.20	112.14

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
4	B	2004	MLR	1	0
3	B	2005	CEX	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	1526/1528 (99%)	0.06	49 (3%)	51	44	50, 86, 144, 176	0
1	B	1526/1528 (99%)	0.07	60 (3%)	43	36	50, 83, 146, 191	0
All	All	3052/3056 (99%)	0.07	109 (3%)	46	39	50, 85, 145, 191	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	281	TYR	5.7
1	B	1245	GLU	5.7
1	A	1457	SER	5.5
1	A	1458	ALA	4.7
1	B	289	ASP	4.1
1	B	1244	GLY	4.1
1	B	427	LYS	4.1
1	B	288	VAL	4.0
1	B	488	TYR	3.8
1	B	1242	LYS	3.7
1	B	308	LEU	3.6
1	B	1206	LEU	3.5
1	A	363	LEU	3.5
1	B	1165	TYR	3.4
1	B	489	LEU	3.3
1	A	1334	ILE	3.3
1	B	379	ILE	3.3
1	B	364	GLY	3.2
1	B	1224	GLU	3.2
1	B	423	PHE	3.1
1	A	282	PRO	3.1
1	B	425	ARG	3.1
1	B	1210	MET	3.1
1	A	1246	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	338	ILE	3.1
1	A	1328	PHE	3.1
1	B	426	ILE	3.0
1	B	371	ILE	3.0
1	B	1208	ARG	3.0
1	B	291	LEU	3.0
1	A	1301	LEU	3.0
1	B	1226	GLY	2.9
1	B	1412	ASP	2.9
1	B	283	VAL	2.9
1	A	438	GLN	2.9
1	B	447	LEU	2.9
1	A	273	SER	2.8
1	B	1416	PHE	2.8
1	A	337	ASN	2.8
1	A	309	TRP	2.8
1	B	298	ILE	2.7
1	B	421	GLN	2.7
1	A	275	GLN	2.7
1	B	1205	ASN	2.7
1	A	307	LYS	2.7
1	B	491	ARG	2.7
1	B	1246	SER	2.7
1	A	1298	LYS	2.6
1	A	1224	GLU	2.6
1	B	1223	TRP	2.6
1	B	493	VAL	2.6
1	B	424	ASN	2.6
1	B	1209	VAL	2.6
1	B	309	TRP	2.6
1	B	1204	PRO	2.6
1	B	303	ILE	2.6
1	B	384	HIS	2.6
1	A	1424	TYR	2.5
1	B	438	GLN	2.5
1	A	1247	GLU	2.5
1	A	283	VAL	2.5
1	A	312	TYR	2.5
1	B	251	TYR	2.4
1	B	307	LYS	2.4
1	A	339	PRO	2.4
1	B	269	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	337	ASN	2.4
1	B	383	LEU	2.3
1	B	284	ASP	2.3
1	A	1243	MET	2.3
1	A	489	LEU	2.3
1	B	428	TYR	2.3
1	A	423	PHE	2.3
1	A	1223	TRP	2.3
1	B	1304	TRP	2.3
1	A	1514	CYS	2.3
1	A	1085	GLY	2.3
1	A	1456	GLY	2.3
1	A	447	LEU	2.2
1	B	292	ILE	2.2
1	A	1321	ASN	2.2
1	A	291	LEU	2.2
1	B	1267	ASN	2.2
1	B	681	GLU	2.2
1	A	350	PHE	2.2
1	A	1252	VAL	2.2
1	B	354	ASN	2.2
1	A	1345	TYR	2.2
1	B	504	TYR	2.2
1	A	407	PHE	2.2
1	A	439	GLY	2.2
1	A	426	ILE	2.2
1	A	434	HIS	2.2
1	A	1319	PRO	2.1
1	B	1334	ILE	2.1
1	B	376	PHE	2.1
1	A	1354	TYR	2.1
1	A	111	LEU	2.1
1	A	295	MET	2.1
1	B	1121	ASN	2.1
1	A	272	PHE	2.1
1	B	1227	LEU	2.1
1	A	292	ILE	2.0
1	B	287	THR	2.0
1	A	1208	ARG	2.0
1	B	1203	GLY	2.0
1	A	347	LEU	2.0
1	B	492	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	269	LEU	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 [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	MTT	A	2001	45/45	0.82	0.38	3.67	98,123,149,171	0
3	CEX	A	2005	56/56	0.69	0.38	1.66	131,176,203,208	0
3	CEX	A	2002	56/56	0.86	0.39	0.71	112,136,159,173	0
2	MTT	B	2001	45/45	0.82	0.27	0.69	102,127,153,162	0
3	CEX	B	2002	56/56	0.88	0.48	0.68	105,128,144,145	0
3	CEX	B	2005	56/56	0.48	0.43	0.53	137,177,205,211	0
4	MLR	A	2004	34/34	0.85	0.26	-0.08	129,164,179,185	0
2	MTT	A	2006	44/45	0.62	0.29	-0.13	113,158,188,196	0
4	MLR	B	2004	34/34	0.85	0.19	-0.36	114,134,162,190	0
2	MTT	A	2003	44/45	0.89	0.18	-0.52	71,114,131,135	0
2	MTT	B	2003	44/45	0.87	0.23	-0.71	91,116,130,136	0

6.5 Other polymers [i](#)

There are no such residues in this entry.