



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:48 AM GMT

PDB ID : 2ITM
Title : Crystal structure of the E. coli xylulose kinase complexed with xylulose
Authors : di Luccio, E.; Voegtli, J.; Wilson, D.K.
Deposited on : 2006-10-19
Resolution : 2.10 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

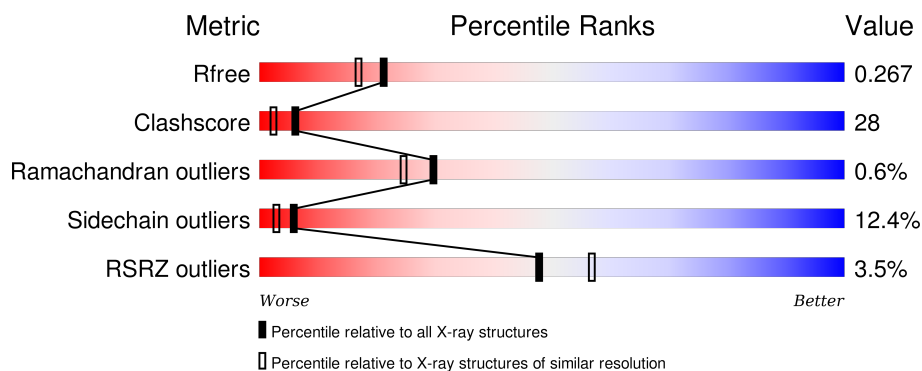
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	484	<div> <div>4%</div> <div>66%</div> <div>26%</div> <div>6%</div> <div>.</div> </div>
1	B	484	<div> <div>3%</div> <div>59%</div> <div>31%</div> <div>7%</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	XUL	B	4931	X	-	X	X

2 Entry composition [i](#)

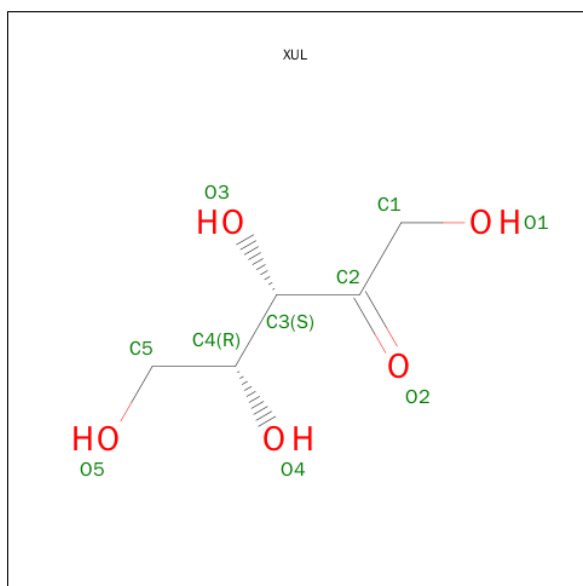
There are 5 unique types of molecules in this entry. The entry contains 7730 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Xylulose kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	0	0	0
			3632	2297	637	674	24			
1	B	475	Total	C	N	O	S	0	0	0
			3625	2292	636	673	24			

- Molecule 2 is SUGAR (D-XYLULOSE) (three-letter code: XUL) (formula: C₅H₁₀O₅).



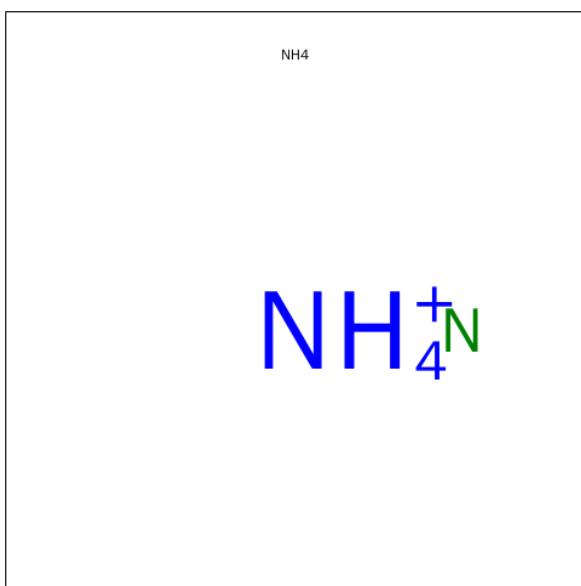
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	5	5		
2	B	1	Total	C	O	0	0
			10	5	5		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is AMMONIUM ION (three-letter code: NH4) (formula: H₄N).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	N	0	0
			1	1		
4	B	1	Total	N	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	N 1	0	0
4	A	1	Total 1	N 1	0	0
4	B	1	Total 1	N 1	0	0
4	A	1	Total 1	N 1	0	0
4	A	1	Total 1	N 1	0	0
4	B	1	Total 1	N 1	0	0
4	A	1	Total 1	N 1	0	0
4	A	1	Total 1	N 1	0	0
4	A	1	Total 1	N 1	0	0
4	B	1	Total 1	N 1	0	0

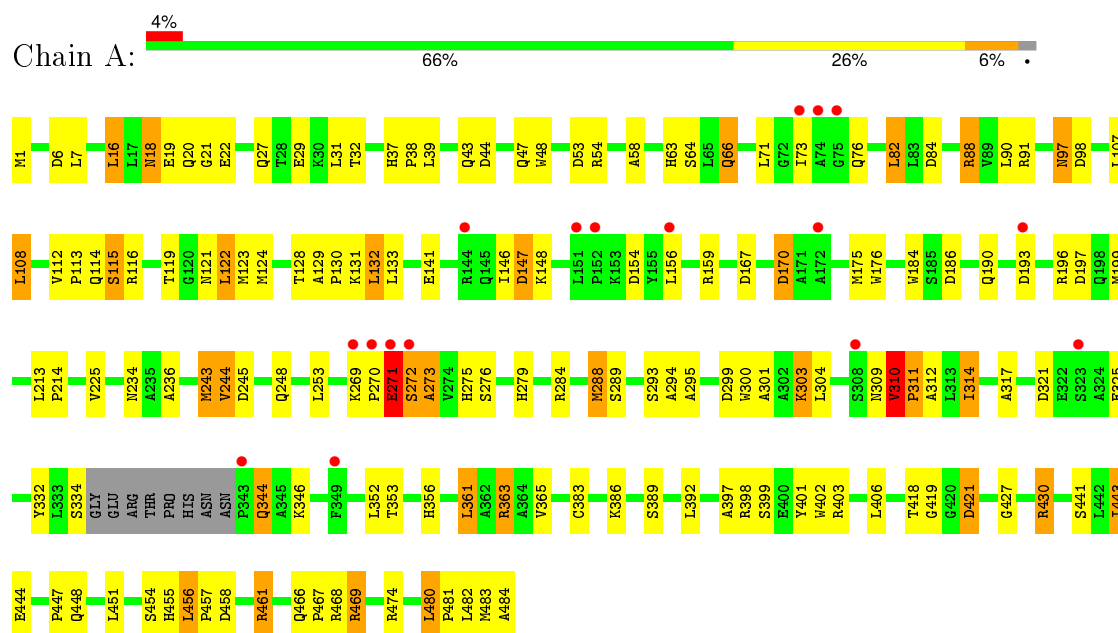
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	225	Total 225	O 225	0	0
5	B	206	Total 206	O 206	0	0

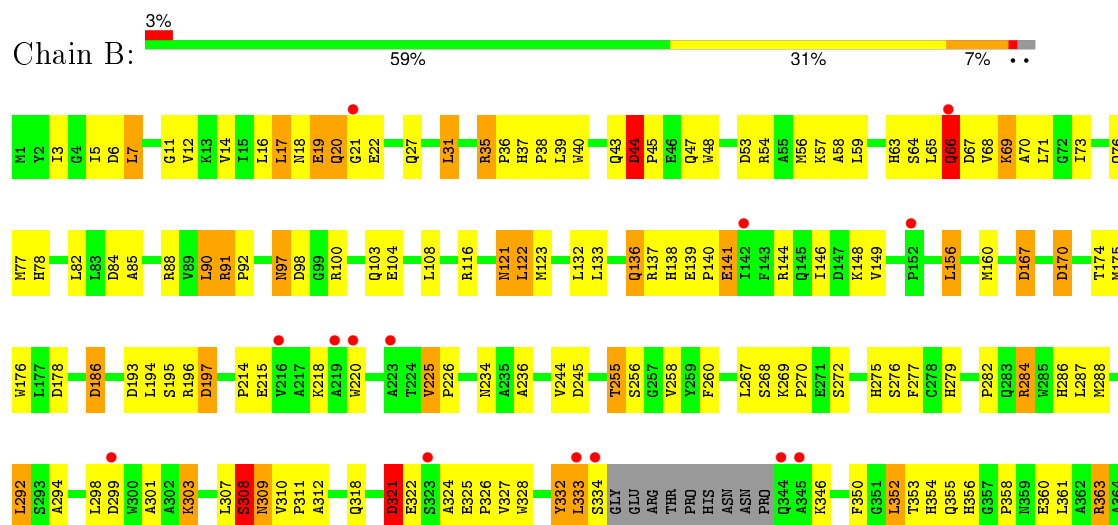
3 Residue-property plots

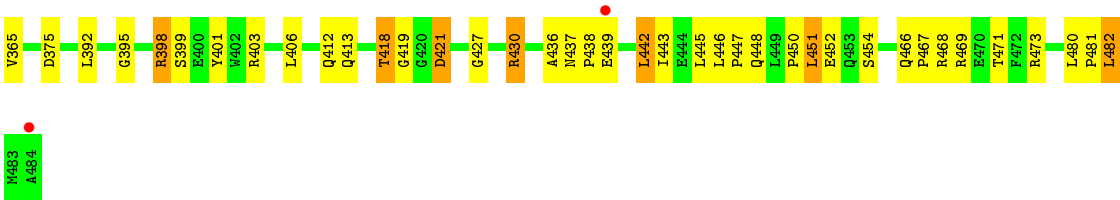
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



• Molecule 1: Xylulose kinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.88Å 112.61Å 143.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.85 – 2.10 29.86 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.4 (29.85-2.10) 95.6 (29.86-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.201 , 0.263 0.207 , 0.267	Depositor DCC
R_{free} test set	2373 reflections (4.37%)	DCC
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 59.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 58658 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7730	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: XUL, NH4, SO4

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	0.74	2/3713 (0.1%)	0.78	17/5046 (0.3%)
1	B	0.71	2/3705 (0.1%)	0.76	17/5035 (0.3%)
All	All	0.72	4/7418 (0.1%)	0.77	34/10081 (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	2
1	B	0	3
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	333	LEU	C-O	-6.43	1.11	1.23
1	A	332	TYR	CD2-CE2	-5.29	1.31	1.39
1	A	484	ALA	C-OXT	5.09	1.33	1.23
1	B	332	TYR	CD2-CE2	-5.04	1.31	1.39

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	ALA	N-CA-CB	16.14	132.69	110.10
1	A	272	SER	CB-CA-C	9.91	128.94	110.10
1	B	66	GLN	CB-CA-C	-7.74	94.93	110.40
1	B	308	SER	CB-CA-C	-7.37	96.09	110.10
1	A	170	ASP	CB-CG-OD2	7.11	124.70	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	ASP	CB-CG-OD2	6.74	124.36	118.30
1	A	310	VAL	C-N-CD	-6.59	106.09	120.60
1	B	324	ALA	CB-CA-C	-6.42	100.47	110.10
1	A	6	ASP	CB-CG-OD2	6.34	124.01	118.30
1	A	53	ASP	CB-CG-OD2	6.19	123.87	118.30
1	B	299	ASP	CB-CG-OD2	6.13	123.81	118.30
1	B	309	ASN	N-CA-CB	6.07	121.52	110.60
1	B	66	GLN	C-N-CA	5.86	136.36	121.70
1	A	299	ASP	CB-CG-OD2	5.86	123.57	118.30
1	B	421	ASP	CB-CG-OD2	5.83	123.55	118.30
1	B	193	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	197	ASP	CB-CG-OD2	5.61	123.35	118.30
1	B	170	ASP	CB-CG-OD2	5.61	123.34	118.30
1	B	321	ASP	CB-CG-OD2	5.56	123.31	118.30
1	A	147	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	6	ASP	CB-CG-OD2	5.47	123.22	118.30
1	B	245	ASP	CB-CG-OD2	5.44	123.19	118.30
1	B	167	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	167	ASP	CB-CG-OD2	5.37	123.14	118.30
1	A	421	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	458	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	178	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	154	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	44	ASP	CB-CG-OD2	5.12	122.90	118.30
1	A	186	ASP	CB-CG-OD2	5.11	122.89	118.30
1	A	321	ASP	CB-CG-OD2	5.05	122.84	118.30
1	B	53	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	98	ASP	CB-CG-OD2	5.02	122.82	118.30
1	B	186	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	243	MET	Peptide
1	A	271	GLU	Peptide
1	B	121	ASN	Peptide
1	B	321	ASP	Peptide
1	B	66	GLN	Peptide

5.2 Too-close contacts ⓘ

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	3632	0	3607	167	0
1	B	3625	0	3599	243	0
2	A	10	0	10	3	0
2	B	10	0	10	12	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	7	0	0	0	0
4	B	5	0	0	1	0
5	A	225	0	0	18	0
5	B	206	0	0	15	0
All	All	7730	0	7226	409	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 28.

All (409) 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:44:ASP:HB2	5:B:5089:HOH:O	1.23	1.33
1:B:18:ASN:ND2	1:B:22:GLU:HB2	1.40	1.33
1:B:35:ARG:NH1	1:B:40:TRP:O	1.65	1.26
1:B:292:LEU:CA	1:B:333:LEU:HD11	1.68	1.22
1:B:322:GLU:OE1	1:B:363:ARG:NH2	1.71	1.21
1:B:269:LYS:HD3	1:B:272:SER:CB	1.70	1.21
1:A:270:PRO:O	1:A:271:GLU:HG3	1.39	1.20
1:B:292:LEU:HA	1:B:333:LEU:CD1	1.72	1.20
1:A:461:ARG:HD3	5:A:5119:HOH:O	1.41	1.16
1:A:443:ILE:CD1	1:A:443:ILE:H	1.57	1.16
1:B:65:LEU:O	1:B:66:GLN:CG	1.95	1.15
1:A:443:ILE:H	1:A:443:ILE:HD12	1.00	1.14
1:A:271:GLU:H	1:A:272:SER:CB	1.60	1.14
1:A:271:GLU:N	1:A:272:SER:HB3	1.60	1.13
1:A:288:MET:HG2	5:A:5156:HOH:O	1.44	1.12
1:B:132:LEU:HD23	1:B:194:LEU:HD11	1.16	1.11
1:B:438:PRO:HD2	1:B:439:GLU:OE1	1.49	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:LEU:CD2	1:B:194:LEU:HD11	1.84	1.07
1:B:35:ARG:HD2	5:B:5109:HOH:O	1.54	1.07
1:B:269:LYS:HD3	1:B:272:SER:HB3	1.33	1.07
1:B:91:ARG:HH11	1:B:91:ARG:HG3	1.17	1.07
1:B:27:GLN:HG2	1:B:58:ALA:HB3	1.31	1.06
1:B:292:LEU:HD23	1:B:333:LEU:HD21	1.29	1.06
1:B:65:LEU:O	1:B:66:GLN:HG3	1.52	1.06
1:B:398:ARG:HH11	1:B:398:ARG:HG2	0.91	1.06
1:B:35:ARG:CG	1:B:35:ARG:HH11	1.70	1.04
1:A:334:SER:CB	1:A:344:GLN:HB3	1.86	1.03
1:A:469:ARG:HH11	1:A:469:ARG:HG2	0.92	1.03
1:B:269:LYS:HD3	1:B:272:SER:OG	1.57	1.01
1:B:27:GLN:HG2	1:B:58:ALA:CB	1.90	1.01
1:B:395:GLY:O	1:B:398:ARG:HG3	1.56	1.01
1:A:443:ILE:N	1:A:443:ILE:HD12	1.73	1.01
1:A:309:ASN:HD22	1:A:311:PRO:HD2	1.21	1.01
1:B:82:LEU:HD13	1:B:146:ILE:HD11	1.40	1.00
1:B:140:PRO:HD2	1:B:141:GLU:OE2	1.61	1.00
1:A:469:ARG:HG2	1:A:469:ARG:NH1	1.71	0.99
1:B:292:LEU:HD23	1:B:333:LEU:CD2	1.93	0.98
1:A:293:SER:HB3	5:A:5154:HOH:O	1.61	0.98
1:B:398:ARG:CG	1:B:398:ARG:HH11	1.77	0.97
1:B:398:ARG:HG2	1:B:398:ARG:NH1	1.72	0.97
1:B:214:PRO:HD2	5:B:4983:HOH:O	1.64	0.96
1:B:292:LEU:CD2	1:B:333:LEU:HD21	1.95	0.96
1:A:469:ARG:NH1	5:A:4940:HOH:O	1.98	0.96
1:B:35:ARG:HG2	1:B:35:ARG:NH1	1.53	0.94
1:B:82:LEU:HD13	1:B:146:ILE:CD1	1.97	0.94
1:A:270:PRO:O	1:A:271:GLU:CG	2.15	0.93
1:B:353:THR:H	1:B:356:HIS:HD2	1.11	0.93
1:B:353:THR:H	1:B:356:HIS:CD2	1.87	0.93
1:B:121:ASN:HD22	1:B:275:HIS:HD2	1.18	0.92
1:B:18:ASN:O	1:B:20:GLN:O	1.88	0.91
1:B:77:MET:CE	2:B:4931:XUL:H11	2.01	0.91
1:A:271:GLU:H	1:A:272:SER:HB3	0.75	0.91
1:A:334:SER:HB2	1:A:344:GLN:O	1.71	0.90
1:A:253:LEU:HD11	1:A:392:LEU:HD11	1.52	0.90
1:B:18:ASN:HD21	1:B:22:GLU:CB	1.85	0.89
1:A:469:ARG:HH11	1:A:469:ARG:CG	1.83	0.87
1:A:32:THR:H	1:A:47:GLN:HE22	1.23	0.87
1:A:310:VAL:N	1:A:311:PRO:CD	2.38	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:LEU:HA	1:B:333:LEU:HD11	0.88	0.86
1:B:121:ASN:HD22	1:B:275:HIS:CD2	1.94	0.85
1:B:18:ASN:HD21	1:B:22:GLU:HB2	1.02	0.85
1:B:292:LEU:HD23	1:B:333:LEU:CG	2.07	0.84
1:A:334:SER:OG	1:A:344:GLN:HB3	1.77	0.84
1:A:88:ARG:HG3	1:A:88:ARG:HH11	1.43	0.83
1:A:353:THR:H	1:A:356:HIS:HD2	1.24	0.83
1:A:119:THR:HG21	1:A:175:MET:HE3	1.59	0.83
1:A:353:THR:H	1:A:356:HIS:CD2	1.97	0.83
1:B:65:LEU:O	1:B:66:GLN:HG2	1.77	0.83
1:B:82:LEU:CD1	1:B:146:ILE:HD11	2.09	0.82
1:B:322:GLU:CD	1:B:363:ARG:HH22	1.82	0.82
1:A:300:TRP:HA	5:A:5120:HOH:O	1.80	0.81
1:A:19:GLU:H	1:A:19:GLU:CD	1.83	0.81
1:B:77:MET:HE3	2:B:4931:XUL:H11	1.64	0.80
1:B:140:PRO:CD	1:B:141:GLU:OE2	2.30	0.80
1:B:269:LYS:CD	1:B:272:SER:HB3	2.12	0.79
1:A:18:ASN:ND2	1:A:22:GLU:H	1.80	0.79
1:B:353:THR:OG1	1:B:355:GLN:HG2	1.82	0.79
1:B:35:ARG:HG2	1:B:35:ARG:HH11	0.74	0.79
1:B:77:MET:HE2	1:B:234:ASN:HD22	1.48	0.79
1:B:63:HIS:CD2	1:B:64:SER:N	2.52	0.78
1:B:91:ARG:NH1	1:B:92:PRO:HD2	1.97	0.78
1:A:97:ASN:H	1:A:97:ASN:HD22	1.32	0.77
1:B:132:LEU:CD2	1:B:194:LEU:CD1	2.62	0.77
1:A:293:SER:C	5:A:5154:HOH:O	2.22	0.77
1:B:322:GLU:CD	1:B:363:ARG:NH2	2.38	0.77
1:B:132:LEU:HD22	1:B:176:TRP:CZ2	2.20	0.76
1:A:468:ARG:NH1	5:A:5096:HOH:O	2.17	0.76
1:A:253:LEU:HB3	1:A:294:ALA:HB3	1.66	0.76
1:A:310:VAL:N	1:A:311:PRO:HD3	1.99	0.76
1:A:293:SER:CB	5:A:5154:HOH:O	2.24	0.76
1:B:438:PRO:CD	1:B:439:GLU:OE1	2.31	0.75
1:A:113:PRO:HD2	5:A:5153:HOH:O	1.85	0.75
1:B:325:GLU:HB3	1:B:326:PRO:HD2	1.70	0.74
1:B:413:GLN:NE2	5:B:5079:HOH:O	2.19	0.74
1:B:69:LYS:O	1:B:226:PRO:HD2	1.88	0.73
2:B:4931:XUL:O4	5:B:5113:HOH:O	2.05	0.73
1:B:77:MET:HE1	2:B:4931:XUL:H11	1.71	0.72
1:A:91:ARG:HH11	1:A:91:ARG:HG3	1.54	0.72
1:A:253:LEU:HD12	1:A:397:ALA:HB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ASN:OD1	1:B:20:GLN:HB2	1.91	0.71
1:B:333:LEU:O	1:B:334:SER:HB3	1.88	0.71
1:B:18:ASN:ND2	1:B:22:GLU:CB	2.36	0.71
1:A:300:TRP:CZ2	1:A:304:LEU:HD22	2.25	0.71
1:A:18:ASN:HD21	1:A:22:GLU:H	1.39	0.70
1:B:395:GLY:O	1:B:398:ARG:CG	2.38	0.70
1:A:38:PRO:O	1:A:39:LEU:HB2	1.91	0.70
1:A:334:SER:HB2	1:A:344:GLN:HB3	1.73	0.69
1:B:43:GLN:NE2	1:B:48:TRP:HE1	1.89	0.69
1:A:309:ASN:ND2	1:A:311:PRO:HD2	2.01	0.69
1:B:122:LEU:HD23	1:B:270:PRO:O	1.92	0.68
1:B:70:ALA:HA	1:B:225:VAL:HG13	1.76	0.68
1:B:132:LEU:HD23	1:B:194:LEU:CD1	2.09	0.68
1:B:91:ARG:HG3	1:B:91:ARG:NH1	1.94	0.68
1:B:469:ARG:HD2	5:B:4941:HOH:O	1.93	0.68
1:B:141:GLU:CD	1:B:141:GLU:H	1.96	0.68
1:B:303:LYS:HE2	1:B:308:SER:HA	1.76	0.68
1:B:292:LEU:HD23	1:B:333:LEU:HD11	1.74	0.68
1:B:269:LYS:CD	1:B:272:SER:OG	2.37	0.68
1:A:300:TRP:CH2	1:A:304:LEU:HD22	2.29	0.68
1:A:18:ASN:C	1:A:18:ASN:HD22	1.98	0.67
1:B:480:LEU:C	1:B:480:LEU:HD13	2.16	0.66
1:B:292:LEU:HD23	1:B:333:LEU:CD1	2.26	0.66
1:B:17:LEU:HD23	1:B:22:GLU:O	1.96	0.66
1:A:353:THR:HG22	1:B:346:LYS:HG2	1.77	0.66
1:B:269:LYS:CD	1:B:272:SER:CB	2.61	0.66
1:B:36:PRO:O	1:B:37:HIS:ND1	2.30	0.65
1:B:11:GLY:HA2	1:B:31:LEU:CD2	2.26	0.65
1:B:466:GLN:HB2	1:B:467:PRO:HD3	1.80	0.64
1:A:334:SER:CB	1:A:344:GLN:CB	2.73	0.64
1:A:443:ILE:CD1	1:A:443:ILE:N	2.36	0.64
1:A:293:SER:CA	5:A:5154:HOH:O	2.46	0.64
1:B:63:HIS:CD2	1:B:64:SER:H	2.15	0.64
1:B:35:ARG:NH1	1:B:35:ARG:CG	2.39	0.64
1:A:441:SER:OG	1:A:444:GLU:HG3	1.98	0.64
1:A:37:HIS:HB3	1:A:38:PRO:HD2	1.81	0.63
1:A:63:HIS:HD2	1:A:64:SER:O	1.81	0.63
1:A:97:ASN:H	1:A:97:ASN:ND2	1.97	0.63
1:A:474:ARG:HH11	1:A:474:ARG:HG3	1.64	0.63
1:B:84:ASP:OD2	1:B:88:ARG:HB3	1.98	0.62
1:A:66:GLN:HA	1:A:66:GLN:HE21	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ARG:HG3	1:A:88:ARG:NH1	2.11	0.62
1:B:333:LEU:O	1:B:334:SER:CB	2.47	0.62
1:B:332:TYR:C	1:B:334:SER:H	2.03	0.62
1:B:398:ARG:CG	1:B:398:ARG:NH1	2.44	0.62
1:B:11:GLY:HA2	1:B:31:LEU:HD22	1.82	0.62
1:B:279:HIS:HB3	1:B:284:ARG:HB2	1.82	0.62
1:A:19:GLU:OE2	1:A:20:GLN:NE2	2.33	0.61
1:B:328:TRP:HZ3	1:B:468:ARG:O	1.82	0.61
1:A:97:ASN:N	1:A:97:ASN:HD22	1.93	0.61
1:A:334:SER:CB	1:A:344:GLN:O	2.48	0.60
1:A:124:MET:HB3	5:A:5003:HOH:O	2.01	0.60
1:B:195:SER:OG	1:B:197:ASP:HB2	2.00	0.60
1:B:437:ASN:HA	1:B:439:GLU:OE1	2.02	0.60
1:B:138:HIS:C	1:B:140:PRO:HD3	2.21	0.60
1:A:301:ALA:HB2	1:A:365:VAL:HG11	1.83	0.59
1:B:244:VAL:HG11	1:B:446:LEU:HD13	1.84	0.59
1:B:18:ASN:OD1	1:B:20:GLN:C	2.42	0.58
1:A:334:SER:OG	1:A:344:GLN:NE2	2.36	0.58
1:A:116:ARG:CZ	1:A:122:LEU:HD11	2.33	0.58
1:A:310:VAL:CG1	1:A:310:VAL:O	2.51	0.58
1:B:37:HIS:HB3	1:B:38:PRO:CD	2.32	0.58
1:B:18:ASN:OD1	1:B:20:GLN:CA	2.52	0.58
1:B:27:GLN:OE1	1:B:58:ALA:HB1	2.04	0.57
1:B:132:LEU:HD22	1:B:176:TRP:HZ2	1.66	0.57
1:A:430:ARG:HH11	1:A:430:ARG:HG3	1.68	0.57
1:A:304:LEU:O	1:B:358:PRO:HG3	2.05	0.57
1:B:27:GLN:CG	1:B:58:ALA:CB	2.76	0.57
1:A:119:THR:CG2	1:A:175:MET:HE3	2.33	0.57
1:A:234:ASN:HD21	2:A:4930:XUL:H3	1.69	0.57
1:B:43:GLN:HE22	1:B:76:GLN:HE22	1.51	0.57
1:B:78:HIS:CD2	2:B:4931:XUL:H12	2.40	0.57
1:B:466:GLN:HG2	5:B:4949:HOH:O	2.04	0.57
1:A:317:ALA:HB1	1:A:363:ARG:HG2	1.85	0.57
1:B:63:HIS:HD2	1:B:64:SER:O	1.88	0.56
1:A:141:GLU:CD	1:A:141:GLU:H	2.08	0.56
1:A:43:GLN:NE2	1:A:48:TRP:HE1	2.03	0.56
1:A:116:ARG:CZ	1:A:122:LEU:CD1	2.83	0.56
1:B:27:GLN:HG2	1:B:58:ALA:HB1	1.82	0.56
1:B:288:MET:HE2	5:B:5054:HOH:O	2.06	0.56
1:B:236:ALA:O	1:B:427:GLY:HA3	2.07	0.56
1:B:44:ASP:O	1:B:47:GLN:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:ARG:NH2	4:B:4935:NH4:N	2.54	0.55
1:A:325:GLU:O	1:A:356:HIS:HE1	1.90	0.55
1:A:132:LEU:HD13	1:A:176:TRP:CH2	2.41	0.55
1:A:294:ALA:HB1	1:A:402:TRP:CH2	2.41	0.55
1:A:300:TRP:CH2	1:A:304:LEU:CD2	2.90	0.55
1:B:360:GLU:H	1:B:360:GLU:CD	2.09	0.55
1:B:121:ASN:HB2	1:B:175:MET:HE1	1.87	0.55
1:A:270:PRO:C	1:A:271:GLU:CG	2.74	0.55
1:A:234:ASN:ND2	2:A:4930:XUL:H3	2.22	0.55
1:A:309:ASN:HD22	1:A:311:PRO:CD	2.07	0.55
1:B:56:MET:HG3	1:B:220:TRP:CZ2	2.43	0.54
1:A:121:ASN:HD21	1:A:276:SER:H	1.56	0.54
1:B:140:PRO:N	1:B:141:GLU:OE2	2.41	0.54
1:B:442:LEU:HD22	1:B:446:LEU:HD11	1.90	0.54
1:A:245:ASP:N	1:A:248:GLN:OE1	2.34	0.54
1:B:292:LEU:CB	1:B:333:LEU:HD11	2.34	0.54
1:B:307:LEU:C	1:B:308:SER:OG	2.46	0.54
1:B:3:ILE:HG21	1:B:71:LEU:HD12	1.90	0.54
1:B:412:GLN:NE2	5:B:5073:HOH:O	2.41	0.54
1:B:480:LEU:HB3	1:B:481:PRO:CD	2.37	0.53
1:B:27:GLN:CD	1:B:58:ALA:HB1	2.27	0.53
1:B:77:MET:HE3	2:B:4931:XUL:C1	2.36	0.53
1:B:279:HIS:CB	1:B:284:ARG:HB2	2.38	0.53
1:B:18:ASN:OD1	1:B:20:GLN:N	2.40	0.53
1:A:84:ASP:OD2	1:A:88:ARG:HB2	2.09	0.53
1:B:445:LEU:C	1:B:447:PRO:HD3	2.29	0.53
1:B:399:SER:O	1:B:403:ARG:HG3	2.09	0.53
1:A:346:LYS:HE2	1:A:483:MET:HE3	1.90	0.53
1:B:307:LEU:O	1:B:309:ASN:N	2.42	0.53
1:A:346:LYS:HE2	1:A:483:MET:CE	2.39	0.53
1:B:97:ASN:HD22	1:B:97:ASN:N	2.05	0.53
1:B:91:ARG:CG	1:B:91:ARG:NH1	2.65	0.52
1:A:121:ASN:HD22	1:A:275:HIS:HD2	1.56	0.52
1:A:480:LEU:HB3	1:A:481:PRO:HD3	1.92	0.52
1:A:132:LEU:HD13	1:A:176:TRP:HH2	1.74	0.52
1:B:286:HIS:HE1	5:B:5015:HOH:O	1.92	0.52
1:B:353:THR:N	1:B:356:HIS:HD2	1.92	0.52
1:B:18:ASN:OD1	1:B:20:GLN:CB	2.57	0.52
1:A:37:HIS:HB3	1:A:38:PRO:CD	2.40	0.52
1:B:309:ASN:ND2	1:B:312:ALA:H	2.08	0.51
1:B:325:GLU:CB	1:B:326:PRO:HD2	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:MET:CE	1:B:234:ASN:HD22	2.20	0.51
1:B:97:ASN:HD22	1:B:97:ASN:H	1.55	0.51
1:B:332:TYR:C	1:B:334:SER:N	2.64	0.51
1:B:269:LYS:N	1:B:270:PRO:HD3	2.25	0.51
1:B:268:SER:C	1:B:270:PRO:HD3	2.31	0.51
1:A:271:GLU:N	1:A:272:SER:CB	2.42	0.51
1:A:334:SER:HB2	1:A:344:GLN:CB	2.38	0.51
1:B:63:HIS:HD2	1:B:64:SER:N	2.08	0.51
1:B:132:LEU:HD21	1:B:149:VAL:HG21	1.93	0.51
1:B:292:LEU:CA	1:B:333:LEU:CD1	2.54	0.50
1:A:43:GLN:HE22	1:A:76:GLN:HE22	1.58	0.50
2:B:4931:XUL:O2	2:B:4931:XUL:O4	2.30	0.50
1:B:11:GLY:HA2	1:B:31:LEU:HD23	1.93	0.50
1:B:27:GLN:CG	1:B:58:ALA:HB1	2.40	0.50
1:B:141:GLU:CD	1:B:141:GLU:N	2.65	0.50
2:B:4931:XUL:H3	5:B:5058:HOH:O	2.11	0.50
1:A:71:LEU:HD23	1:A:71:LEU:C	2.31	0.50
1:B:418:THR:HG22	1:B:452:GLU:HB2	1.92	0.50
1:A:469:ARG:NH1	1:A:469:ARG:CG	2.52	0.50
1:B:308:SER:O	1:B:309:ASN:HB3	2.12	0.50
1:B:97:ASN:H	1:B:97:ASN:ND2	2.10	0.50
1:B:442:LEU:HD22	1:B:446:LEU:CD1	2.42	0.50
1:B:98:ASP:OD1	1:B:100:ARG:HG2	2.11	0.50
1:B:121:ASN:HD21	1:B:276:SER:H	1.60	0.50
1:A:32:THR:H	1:A:47:GLN:NE2	2.01	0.49
1:A:309:ASN:ND2	1:A:312:ALA:H	2.10	0.49
1:B:328:TRP:CZ3	1:B:468:ARG:O	2.64	0.49
1:B:108:LEU:O	1:B:108:LEU:HD23	2.13	0.49
1:B:277:PHE:HB2	1:B:286:HIS:CE1	2.47	0.49
1:B:375:ASP:OD2	1:B:473:ARG:HD3	2.12	0.49
1:A:466:GLN:N	1:A:467:PRO:HD2	2.27	0.49
1:A:1:MET:CE	1:A:16:LEU:HD13	2.42	0.49
1:B:301:ALA:CB	1:B:365:VAL:HG11	2.43	0.48
1:B:121:ASN:ND2	1:B:275:HIS:CD2	2.74	0.48
1:A:430:ARG:HH11	1:A:430:ARG:CG	2.26	0.48
1:A:401:TYR:N	5:A:5056:HOH:O	2.31	0.48
1:A:66:GLN:HE21	1:A:66:GLN:CA	2.25	0.48
1:A:270:PRO:O	1:A:271:GLU:CD	2.52	0.48
1:B:310:VAL:N	1:B:311:PRO:CD	2.77	0.48
1:B:5:ILE:HG12	1:B:14:VAL:HG12	1.95	0.48
1:A:419:GLY:HA2	1:A:421:ASP:OD1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LEU:HG	1:B:156:LEU:HD22	1.96	0.48
1:B:234:ASN:ND2	2:B:4931:XUL:O2	2.43	0.48
1:A:18:ASN:ND2	1:A:21:GLY:N	2.62	0.48
1:A:121:ASN:HD22	1:A:275:HIS:CD2	2.32	0.48
1:B:68:VAL:HG12	1:B:225:VAL:HG21	1.95	0.48
1:B:38:PRO:O	1:B:39:LEU:HB2	2.14	0.47
1:A:82:LEU:HD13	1:A:146:ILE:CD1	2.44	0.47
1:B:437:ASN:N	1:B:438:PRO:HD3	2.29	0.47
1:B:84:ASP:N	1:B:90:LEU:HD22	2.29	0.47
1:B:418:THR:HG23	1:B:450:PRO:HB2	1.96	0.47
1:B:123:MET:SD	1:B:175:MET:HG3	2.54	0.47
1:A:38:PRO:O	1:A:39:LEU:CB	2.62	0.47
1:A:403:ARG:HE	1:A:455:HIS:HE2	1.62	0.47
1:A:253:LEU:HD12	1:A:397:ALA:CB	2.42	0.47
1:B:310:VAL:HB	1:B:311:PRO:HD3	1.96	0.47
1:A:66:GLN:HA	1:A:66:GLN:NE2	2.27	0.47
1:B:328:TRP:HH2	1:B:468:ARG:HA	1.79	0.47
1:A:27:GLN:HG2	1:A:58:ALA:HB3	1.97	0.47
1:A:469:ARG:HG2	5:A:4940:HOH:O	2.14	0.47
1:A:295:ALA:N	5:A:5154:HOH:O	2.47	0.47
1:A:474:ARG:CG	1:A:474:ARG:HH11	2.28	0.47
1:A:1:MET:CE	1:A:16:LEU:CD1	2.93	0.47
1:B:436:ALA:C	1:B:438:PRO:HD3	2.36	0.47
1:B:17:LEU:HD21	1:B:21:GLY:C	2.35	0.46
1:A:253:LEU:O	1:A:295:ALA:HB2	2.14	0.46
1:A:112:VAL:HA	1:A:113:PRO:HD3	1.61	0.46
1:B:269:LYS:CE	1:B:272:SER:HB3	2.44	0.46
2:A:4930:XUL:O3	2:A:4930:XUL:O5	2.30	0.46
1:B:7:LEU:HG	1:B:156:LEU:CD2	2.46	0.46
1:A:184:TRP:CZ2	1:A:199:MET:HB3	2.51	0.46
1:B:122:LEU:HD22	1:B:122:LEU:HA	1.60	0.46
1:A:91:ARG:NH1	1:A:91:ARG:HG3	2.27	0.46
1:B:139:GLU:N	1:B:140:PRO:HD3	2.30	0.46
1:B:43:GLN:HE21	1:B:48:TRP:HE1	1.61	0.46
1:A:123:MET:SD	1:A:175:MET:HG3	2.55	0.46
1:A:19:GLU:N	1:A:19:GLU:CD	2.62	0.46
1:B:35:ARG:HH12	1:B:40:TRP:C	2.01	0.45
1:B:156:LEU:O	1:B:160:MET:HG3	2.16	0.45
1:A:314:ILE:HG12	1:A:399:SER:OG	2.17	0.45
1:B:328:TRP:CH2	1:B:471:THR:HB	2.51	0.45
1:B:12:VAL:O	1:B:12:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:VAL:H	1:A:311:PRO:HD3	1.80	0.45
1:A:269:LYS:HE2	1:A:383:CYS:HA	1.97	0.45
1:A:288:MET:C	1:A:288:MET:SD	2.95	0.45
1:B:225:VAL:HG13	1:B:226:PRO:HD2	1.97	0.45
1:A:480:LEU:N	1:A:481:PRO:CD	2.80	0.45
1:A:353:THR:N	1:A:356:HIS:HD2	2.02	0.45
1:B:70:ALA:HA	1:B:225:VAL:CG1	2.44	0.45
1:A:300:TRP:CZ2	1:A:304:LEU:CD2	2.98	0.45
1:A:121:ASN:HB2	1:A:175:MET:HE1	1.98	0.45
1:A:113:PRO:HD2	1:A:114:GLN:H	1.81	0.45
1:B:309:ASN:HD22	1:B:311:PRO:HD2	1.82	0.45
1:B:18:ASN:C	1:B:20:GLN:N	2.67	0.44
1:B:334:SER:O	5:B:5121:HOH:O	2.21	0.44
1:B:480:LEU:C	1:B:480:LEU:CD1	2.85	0.44
1:B:439:GLU:CD	1:B:439:GLU:H	2.20	0.44
1:B:136:GLN:HG3	1:B:137:ARG:N	2.31	0.44
1:B:108:LEU:C	1:B:108:LEU:HD23	2.37	0.44
1:A:430:ARG:HD3	1:A:430:ARG:HA	1.63	0.44
1:A:483:MET:SD	1:B:350:PHE:CZ	3.11	0.44
1:A:119:THR:OG1	1:A:175:MET:HE1	2.17	0.44
1:A:288:MET:SD	1:A:289:SER:N	2.91	0.44
1:B:132:LEU:HD22	1:B:176:TRP:CH2	2.53	0.44
1:B:56:MET:HG3	1:B:220:TRP:CE2	2.53	0.44
1:B:186:ASP:OD1	1:B:196:ARG:HD2	2.17	0.44
1:B:65:LEU:C	1:B:66:GLN:CG	2.79	0.43
1:A:300:TRP:CD1	1:B:354:HIS:HA	2.52	0.43
1:B:303:LYS:HD2	1:B:303:LYS:N	2.32	0.43
1:B:37:HIS:CB	1:B:38:PRO:CD	2.95	0.43
1:B:56:MET:O	1:B:59:LEU:HB3	2.17	0.43
1:B:71:LEU:HD23	1:B:71:LEU:C	2.38	0.43
1:A:284:ARG:HD3	5:A:5083:HOH:O	2.18	0.43
1:A:128:THR:O	1:A:131:LYS:HB2	2.18	0.43
1:A:108:LEU:HD23	1:A:108:LEU:HA	1.85	0.43
1:B:328:TRP:CD1	1:B:328:TRP:N	2.86	0.43
1:A:284:ARG:HA	5:A:5083:HOH:O	2.18	0.43
1:A:19:GLU:HB2	1:A:20:GLN:NE2	2.33	0.43
1:A:361:LEU:HD12	1:A:361:LEU:HA	1.79	0.43
1:B:419:GLY:C	1:B:421:ASP:H	2.21	0.43
1:B:325:GLU:H	1:B:355:GLN:NE2	2.16	0.43
1:B:77:MET:HE3	2:B:4931:XUL:C2	2.49	0.43
1:B:446:LEU:N	1:B:447:PRO:HD3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:PHE:CE1	1:B:286:HIS:CD2	3.07	0.43
1:B:361:LEU:O	1:B:365:VAL:HG23	2.18	0.43
1:A:18:ASN:C	1:A:18:ASN:ND2	2.70	0.43
1:B:482:LEU:HD13	1:B:482:LEU:HA	1.65	0.43
1:B:451:LEU:HD11	1:B:454:SER:HB2	2.01	0.43
1:B:255:THR:O	1:B:255:THR:CG2	2.64	0.43
1:A:304:LEU:HD13	1:B:356:HIS:O	2.19	0.42
1:A:352:LEU:HA	1:A:356:HIS:CD2	2.54	0.42
1:B:45:PRO:O	1:B:48:TRP:HB2	2.19	0.42
1:A:156:LEU:HD12	1:A:156:LEU:HA	1.91	0.42
1:A:112:VAL:O	1:A:115:SER:HB3	2.19	0.42
1:B:67:ASP:OD2	5:B:5135:HOH:O	2.22	0.42
1:B:85:ALA:N	5:B:5057:HOH:O	2.51	0.42
1:B:78:HIS:NE2	2:B:4931:XUL:H12	2.34	0.42
1:A:300:TRP:CA	5:A:5120:HOH:O	2.51	0.42
1:A:119:THR:CB	1:A:175:MET:HE3	2.49	0.42
1:B:69:LYS:H	1:B:69:LYS:HG2	1.60	0.42
1:A:129:ALA:N	1:A:130:PRO:HD2	2.34	0.42
1:A:236:ALA:O	1:A:427:GLY:HA3	2.20	0.42
1:A:213:LEU:HA	1:A:214:PRO:HD3	1.97	0.42
1:B:292:LEU:CD2	1:B:333:LEU:HD11	2.46	0.42
1:A:310:VAL:HG13	1:A:310:VAL:O	2.18	0.42
1:B:294:ALA:O	1:B:298:LEU:HG	2.18	0.42
1:A:84:ASP:CG	1:A:88:ARG:HB2	2.39	0.42
1:A:402:TRP:CZ2	1:A:406:LEU:HD11	2.55	0.42
1:B:480:LEU:O	1:B:480:LEU:HD13	2.19	0.42
1:B:442:LEU:HA	1:B:442:LEU:HD23	1.83	0.42
1:A:1:MET:HE3	1:A:16:LEU:HD13	2.02	0.42
1:A:29:GLU:OE1	1:A:54:ARG:NE	2.53	0.42
1:B:82:LEU:HD23	1:B:82:LEU:N	2.35	0.41
1:B:282:PRO:O	1:B:284:ARG:HD3	2.20	0.41
1:A:245:ASP:OD1	1:A:284:ARG:NH1	2.53	0.41
1:B:292:LEU:CD2	1:B:333:LEU:CD2	2.73	0.41
1:A:300:TRP:CE2	1:A:304:LEU:HD22	2.55	0.41
1:B:225:VAL:HG13	1:B:226:PRO:CD	2.50	0.41
1:B:480:LEU:N	1:B:481:PRO:HD2	2.35	0.41
1:A:456:LEU:HA	1:A:457:PRO:HD3	1.88	0.41
1:B:327:VAL:HG11	1:B:352:LEU:HD13	2.01	0.41
1:B:174:THR:O	1:B:175:MET:HB2	2.20	0.41
1:B:77:MET:CE	2:B:4931:XUL:C1	2.85	0.41
1:A:18:ASN:HD22	1:A:21:GLY:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:LEU:HB3	1:B:481:PRO:HD3	2.02	0.41
1:A:352:LEU:HA	1:A:356:HIS:HD2	1.85	0.41
1:A:119:THR:CB	1:A:175:MET:CE	2.99	0.41
1:B:310:VAL:N	1:B:311:PRO:HD2	2.36	0.41
1:B:141:GLU:OE2	1:B:141:GLU:N	2.44	0.41
1:B:18:ASN:HD21	1:B:22:GLU:CG	2.33	0.41
1:B:17:LEU:HD21	1:B:21:GLY:O	2.21	0.41
1:B:91:ARG:HB2	1:B:92:PRO:CD	2.50	0.41
1:B:18:ASN:O	1:B:19:GLU:C	2.57	0.41
1:A:147:ASP:O	1:A:148:LYS:HD3	2.20	0.41
1:A:303:LYS:O	1:A:303:LYS:HD2	2.21	0.41
1:B:318:GLN:HG2	1:B:401:TYR:CD1	2.56	0.41
1:A:121:ASN:ND2	1:A:276:SER:H	2.17	0.41
1:B:430:ARG:HD3	5:B:5038:HOH:O	2.21	0.41
1:B:57:LYS:O	1:B:58:ALA:C	2.59	0.40
1:A:430:ARG:NH1	1:A:447:PRO:HD2	2.36	0.40
1:B:328:TRP:CH2	1:B:468:ARG:HA	2.57	0.40
1:A:196:ARG:HG3	5:A:5082:HOH:O	2.20	0.40
1:B:44:ASP:HA	1:B:45:PRO:HD3	1.87	0.40
1:A:300:TRP:O	1:A:304:LEU:HB2	2.22	0.40
1:B:18:ASN:ND2	1:B:22:GLU:OE2	2.53	0.40
1:B:104:GLU:OE2	1:B:137:ARG:NE	2.46	0.40
1:B:91:ARG:CB	1:B:92:PRO:CD	2.99	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	472/484 (98%)	452 (96%)	15 (3%)	5 (1%)	17	11
1	B	471/484 (97%)	441 (94%)	29 (6%)	1 (0%)	52	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	943/968 (97%)	893 (95%)	44 (5%)	6 (1%)	30	24

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	271	GLU
1	A	311	PRO
1	B	19	GLU
1	A	273	ALA
1	A	310	VAL
1	A	244	VAL

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	375/382 (98%)	331 (88%)	44 (12%)	7	3
1	B	374/382 (98%)	325 (87%)	49 (13%)	5	2
All	All	749/764 (98%)	656 (88%)	93 (12%)	6	3

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	16	LEU
1	A	18	ASN
1	A	31	LEU
1	A	66	GLN
1	A	73	ILE
1	A	82	LEU
1	A	88	ARG
1	A	90	LEU
1	A	97	ASN
1	A	107	LEU
1	A	108	LEU

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Mol	Chain	Res	Type
1	A	115	SER
1	A	122	LEU
1	A	132	LEU
1	A	133	LEU
1	A	159	ARG
1	A	170	ASP
1	A	190	GLN
1	A	193	ASP
1	A	225	VAL
1	A	243	MET
1	A	244	VAL
1	A	279	HIS
1	A	288	MET
1	A	303	LYS
1	A	314	ILE
1	A	344	GLN
1	A	361	LEU
1	A	363	ARG
1	A	386	LYS
1	A	389	SER
1	A	398	ARG
1	A	418	THR
1	A	430	ARG
1	A	443	ILE
1	A	448	GLN
1	A	451	LEU
1	A	454	SER
1	A	456	LEU
1	A	461	ARG
1	A	469	ARG
1	A	480	LEU
1	A	482	LEU
1	B	7	LEU
1	B	16	LEU
1	B	17	LEU
1	B	20	GLN
1	B	31	LEU
1	B	35	ARG
1	B	44	ASP
1	B	69	LYS
1	B	73	ILE
1	B	90	LEU

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Mol	Chain	Res	Type
1	B	91	ARG
1	B	97	ASN
1	B	103	GLN
1	B	116	ARG
1	B	122	LEU
1	B	133	LEU
1	B	136	GLN
1	B	141	GLU
1	B	144	ARG
1	B	148	LYS
1	B	156	LEU
1	B	167	ASP
1	B	170	ASP
1	B	197	ASP
1	B	215	GLU
1	B	218	LYS
1	B	225	VAL
1	B	255	THR
1	B	256	SER
1	B	258	VAL
1	B	267	LEU
1	B	284	ARG
1	B	287	LEU
1	B	292	LEU
1	B	303	LYS
1	B	308	SER
1	B	321	ASP
1	B	352	LEU
1	B	363	ARG
1	B	392	LEU
1	B	398	ARG
1	B	406	LEU
1	B	418	THR
1	B	430	ARG
1	B	442	LEU
1	B	443	ILE
1	B	448	GLN
1	B	451	LEU
1	B	482	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	43	GLN
1	A	47	GLN
1	A	50	GLN
1	A	63	HIS
1	A	66	GLN
1	A	97	ASN
1	A	121	ASN
1	A	136	GLN
1	A	234	ASN
1	A	275	HIS
1	A	286	HIS
1	A	309	ASN
1	A	344	GLN
1	A	356	HIS
1	A	404	GLN
1	B	43	GLN
1	B	63	HIS
1	B	97	ASN
1	B	121	ASN
1	B	138	HIS
1	B	190	GLN
1	B	234	ASN
1	B	275	HIS
1	B	286	HIS
1	B	309	ASN
1	B	355	GLN
1	B	356	HIS
1	B	404	GLN
1	B	412	GLN
1	B	437	ASN
1	B	448	GLN

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

Of 16 ligands modelled in this entry, 12 are modelled with single atom - leaving 4 for Mogul analysis.

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	XUL	A	4930	-	9,9,9	3.91	2 (22%)	6,11,11	1.25	1 (16%)
3	SO4	A	4931	-	4,4,4	0.30	0	6,6,6	0.12	0
2	XUL	B	4931	-	9,9,9	3.66	1 (11%)	6,11,11	1.04	0
3	SO4	B	4932	-	4,4,4	0.55	0	6,6,6	0.18	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	XUL	A	4930	-	-	1/12/12/12	0/0/0/0
3	SO4	A	4931	-	-	0/0/0/0	0/0/0/0
2	XUL	B	4931	-	2/2/3/3	0/12/12/12	0/0/0/0
3	SO4	B	4932	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4930	XUL	C4-C3	-2.70	1.51	1.53
2	B	4931	XUL	O2-C2	10.87	1.40	1.21
2	A	4930	XUL	O2-C2	11.22	1.41	1.21

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	4930	XUL	O3-C3-C2	-2.66	106.09	111.01

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	4931	XUL	C3
2	B	4931	XUL	C4

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4930	XUL	O2-C2-C1-O1

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4930	XUL	3	0
2	B	4931	XUL	12	0

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, 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	476/484 (98%)	-0.04	17 (3%) 46 55	16, 34, 59, 129	0
1	B	475/484 (98%)	0.03	16 (3%) 49 58	21, 37, 62, 108	0
All	All	951/968 (98%)	-0.00	33 (3%) 48 57	16, 35, 61, 129	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	334	SER	6.6
1	B	333	LEU	6.1
1	A	270	PRO	4.2
1	B	345	ALA	3.9
1	B	344	GLN	3.9
1	B	223	ALA	3.8
1	A	151	LEU	3.4
1	B	439	GLU	3.3
1	A	308	SER	3.2
1	A	323	SER	3.1
1	A	343	PRO	3.1
1	B	484	ALA	3.1
1	A	74	ALA	2.9
1	B	220	TRP	2.8
1	B	216	VAL	2.8
1	A	271	GLU	2.7
1	B	219	ALA	2.7
1	A	349	PHE	2.7
1	A	73	ILE	2.6
1	B	21	GLY	2.5
1	A	144	ARG	2.4
1	A	193	ASP	2.4
1	A	75	GLY	2.3
1	B	152	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	142	ILE	2.3
1	A	156	LEU	2.3
1	A	172	ALA	2.3
1	B	66	GLN	2.1
1	A	269	LYS	2.1
1	A	272	SER	2.1
1	B	299	ASP	2.1
1	B	323	SER	2.1
1	A	152	PRO	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(Å ²)	Q<0.9
2	XUL	B	4931	10/10	0.72	0.26	3.84	52,66,86,107	0
3	SO4	B	4932	5/5	0.92	0.18	1.64	66,69,82,100	0
2	XUL	A	4930	10/10	0.90	0.20	0.73	32,57,101,101	0
4	NH4	B	4937	1/1	0.78	0.21	-	36,36,36,36	0
4	NH4	B	4936	1/1	0.74	0.29	-	35,35,35,35	0
4	NH4	B	4933	1/1	0.85	0.14	-	49,49,49,49	0
4	NH4	A	4933	1/1	0.93	0.15	-	31,31,31,31	0
4	NH4	A	4934	1/1	0.90	0.11	-	43,43,43,43	0
4	NH4	A	4938	1/1	0.87	0.16	-	34,34,34,34	0
4	NH4	A	4937	1/1	0.94	0.34	-	34,34,34,34	0
4	NH4	A	4935	1/1	0.46	0.28	-	47,47,47,47	0
4	NH4	B	4935	1/1	0.74	0.11	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NH4	A	4936	1/1	0.82	0.09	-	42,42,42,42	0
4	NH4	A	4932	1/1	0.76	0.23	-	40,40,40,40	0
3	SO4	A	4931	5/5	0.62	0.45	-	51,62,114,151	0
4	NH4	B	4934	1/1	0.58	0.34	-	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.