



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 02:43 PM UTC

PDB ID : 2ITM / pdb_00002itm
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

<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

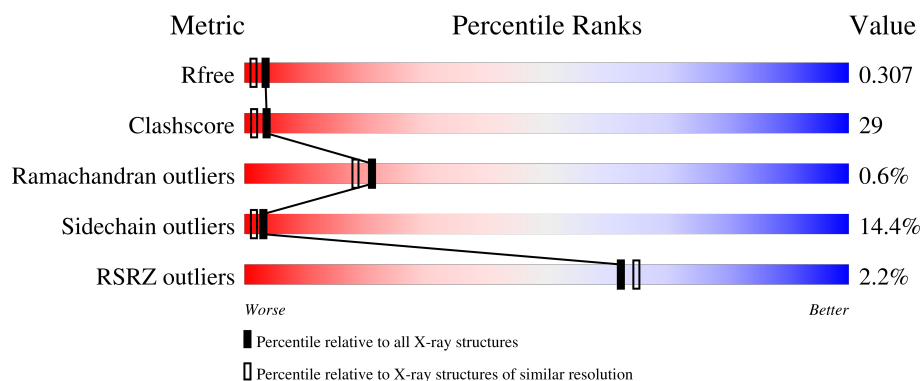
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 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	484	3% 67% 23% 7% ..
1	B	484	2% 57% 32% 8% ..

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	-

2 Entry composition [i](#)

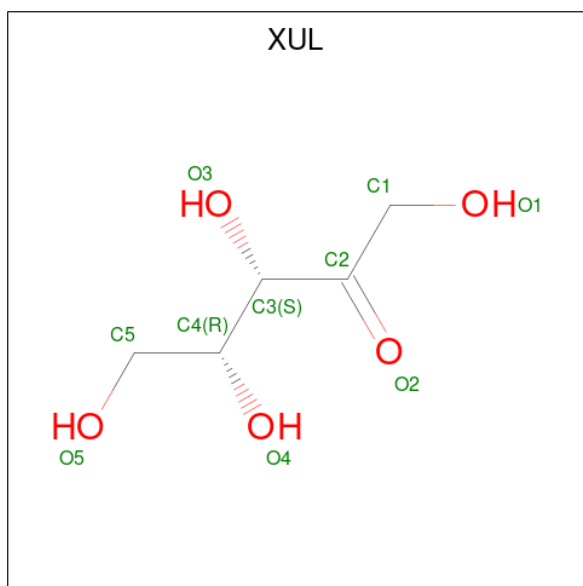
There are 5 unique types of molecules in this entry. The entry contains 7730 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-XYLULOSE (CCD ID: XUL) (formula: C₅H₁₀O₅).



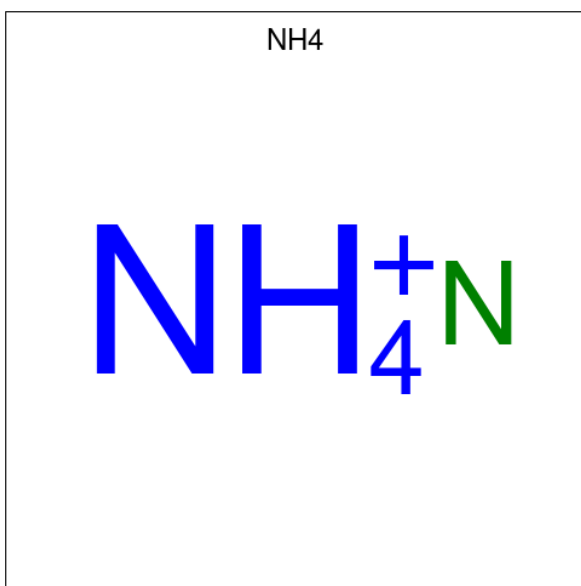
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	5	5		
2	B	1	Total	C	O	0	0
			10	5	5		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is AMMONIUM ION (CCD ID: NH4) (formula: H_4N).



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

Continued on next page...

Continued from previous page...

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	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
4	B	1	Total 1	N 1	0	0
4	B	1	Total 1	N 1	0	0
4	B	1	Total 1	N 1	0	0
4	B	1	Total 1	N 1	0	0

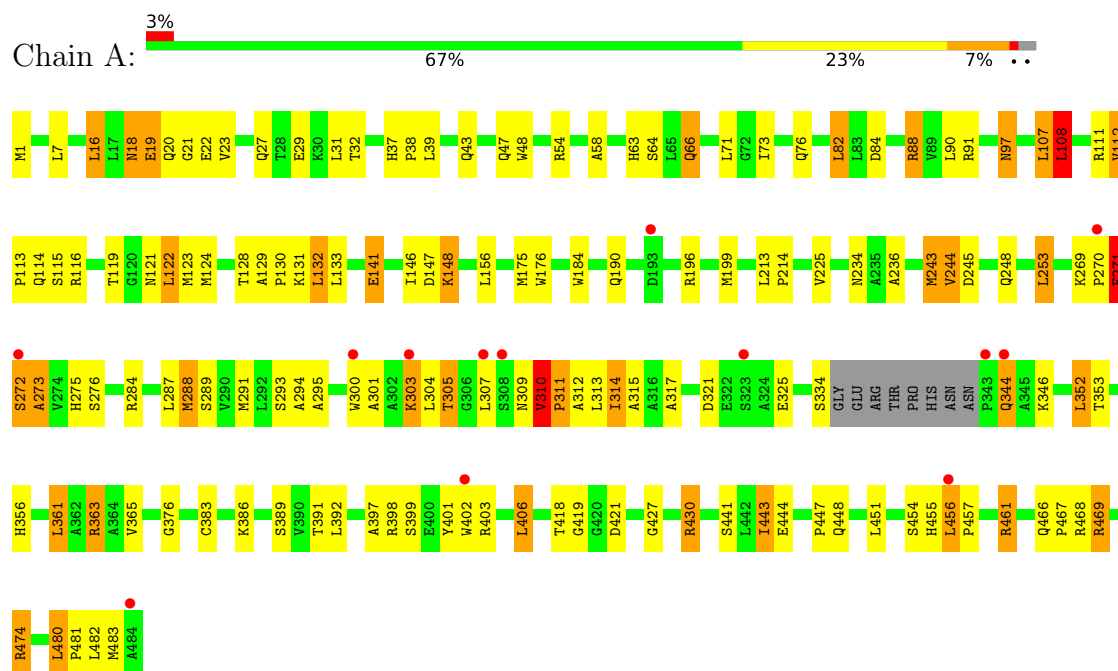
- Molecule 5 is water.

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

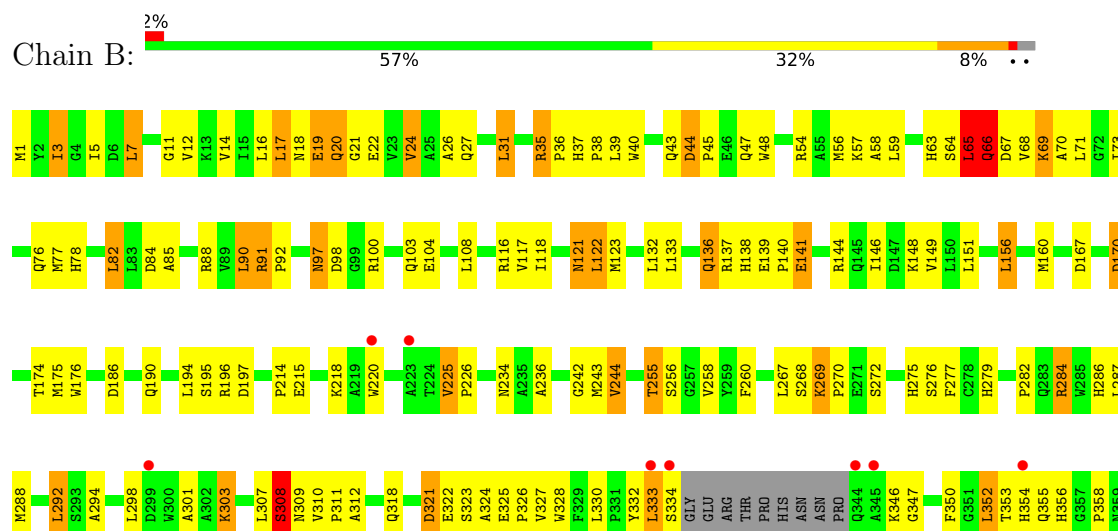
3 Residue-property plots

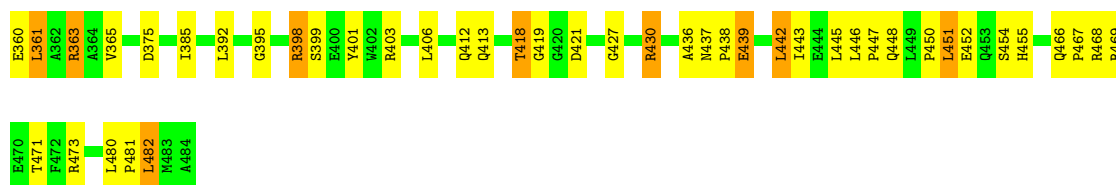
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 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 29.85 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.4 (29.85-2.10) 95.5 (29.85-2.10)	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 (Not available) , 0.307	Depositor DCC
R_{free} test set	2373 reflections (4.05%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NH4, XUL

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	0.99	4/3713 (0.1%)	0.95	7/5046 (0.1%)
1	B	0.97	4/3705 (0.1%)	0.95	11/5035 (0.2%)
All	All	0.98	8/7418 (0.1%)	0.95	18/10081 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
All	All	0	5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	333	LEU	C-O	-10.20	1.11	1.24
1	A	108	LEU	C-O	-6.42	1.16	1.24
1	B	118	ILE	C-O	-5.90	1.17	1.24
1	A	111	ARG	C-O	-5.64	1.17	1.24
1	A	23	VAL	C-O	-5.28	1.18	1.24
1	B	117	VAL	C-O	-5.21	1.18	1.24
1	B	26	ALA	C-O	-5.13	1.18	1.23
1	A	107	LEU	C-O	-5.12	1.18	1.24

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	ALA	N-CA-CB	13.14	132.69	110.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	GLN	CA-C-N	9.36	136.36	120.72
1	B	66	GLN	C-N-CA	9.36	136.36	120.72
1	A	272	SER	CB-CA-C	9.30	128.94	110.42
1	B	66	GLN	CB-CA-C	-7.78	94.93	110.42
1	B	308	SER	CB-CA-C	-7.20	96.09	110.42
1	A	305	THR	N-CA-C	-6.93	104.39	112.92
1	A	273	ALA	N-CA-C	-6.24	97.51	110.80
1	B	347	GLY	N-CA-C	5.81	120.20	110.56
1	B	324	ALA	CB-CA-C	-5.78	100.47	109.61
1	B	24	VAL	N-CA-C	5.64	116.29	110.82
1	B	66	GLN	N-CA-C	5.61	122.75	110.80
1	B	323	SER	N-CA-C	-5.53	107.18	114.04
1	B	333	LEU	CA-C-O	5.17	127.90	120.51
1	B	65	LEU	CB-CA-C	-5.16	105.06	113.37
1	A	272	SER	N-CA-C	-5.13	99.88	110.80
1	A	112	VAL	CA-C-N	5.02	125.29	119.47
1	A	112	VAL	C-N-CA	5.02	125.29	119.47

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 [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	3632	0	3607	174	0
1	B	3625	0	3599	249	0
2	A	10	0	10	3	0
2	B	10	0	10	10	0
3	A	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	19	0
5	B	206	0	0	15	0
All	All	7730	0	7226	422	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 29.

All (422) 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:H	1:A:443:ILE:CD1	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:B:77:MET:HE3	2:B:4931:XUL:H11	1.17	1.12
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
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:HG3	1:B:91:ARG:HH11	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:HH11	1:B:35:ARG:CG	1.70	1.04
1:A:334:SER:CB	1:A:344:GLN:HB3	1.86	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:ARG:HG2	1:A:469:ARG:HH11	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:309:ASN:HD22	1:A:311:PRO:HD2	1.21	1.01
1:A:443:ILE:HD12	1:A:443:ILE:N	1.73	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:A:293:SER:HB3	5:A:5154:HOH:O	1.61	0.98
1:B:292:LEU:HD23	1:B:333:LEU:CD2	1.93	0.98
1:B:398:ARG:HH11	1:B:398:ARG:CG	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:A:469:ARG:NH1	5:A:4940:HOH:O	1.98	0.96
1:B:292:LEU:CD2	1:B:333:LEU:HD21	1.95	0.96
1:B:35:ARG:NH1	1:B:35:ARG:HG2	1.53	0.94
1:B:77:MET:HE3	2:B:4931:XUL:C1	1.98	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:B:322:GLU:CD	1:B:363:ARG:HH22	1.82	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
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:A:19:GLU:CD	1:A:19:GLU:H	1.83	0.85
1:B:18:ASN:HD21	1:B:22:GLU:HB2	1.02	0.85
1:A:334:SER:OG	1:A:344:GLN:HB3	1.77	0.84
1:B:292:LEU:HD23	1:B:333:LEU:CG	2.07	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:293:SER:C	5:A:5154:HOH:O	2.22	0.81
1:B:322:GLU:CD	1:B:363:ARG:NH2	2.38	0.81
1:A:119:THR:HG21	1:A:175:MET:HE3	1.62	0.81
1:A:300:TRP:HA	5:A:5120:HOH:O	1.80	0.81
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:HH11	1:B:35:ARG:HG2	0.74	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:HD22	1:A:97:ASN:H	1.32	0.77
1:B:132:LEU:CD2	1:B:194:LEU:CD1	2.62	0.77
1:A:468:ARG:NH1	5:A:5096:HOH:O	2.17	0.76
1:B:132:LEU:HD22	1:B:176:TRP:CZ2	2.20	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:141:GLU:CD	1:B:141:GLU:H	1.96	0.72
1:A:91:ARG:HG3	1:A:91:ARG:HH11	1.54	0.72
1:A:18:ASN:C	1:A:18:ASN:HD22	1.98	0.71
1:A:253:LEU:HD12	1:A:397:ALA:HB2	1.72	0.71
1:B:18:ASN:OD1	1:B:20:GLN:HB2	1.91	0.71
1:B:480:LEU:C	1:B:480:LEU:HD13	2.16	0.71
1:B:333:LEU:O	1:B:334:SER:HB3	1.88	0.71
1:A:300:TRP:CZ2	1:A:304:LEU:HD22	2.25	0.71
1:B:18:ASN:ND2	1:B:22:GLU:CB	2.36	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:A:309:ASN:ND2	1:A:311:PRO:HD2	2.01	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:GLN:NE2	1:B:48:TRP:HE1	1.89	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:91:ARG:HG3	1:B:91:ARG:NH1	1.94	0.68
1:B:132:LEU:HD23	1:B:194:LEU:CD1	2.09	0.68
1:B:469:ARG:HD2	5:B:4941:HOH:O	1.93	0.68
1:B:303:LYS:HE2	1:B:308:SER:HA	1.76	0.68
1:B:269:LYS:CD	1:B:272:SER:OG	2.37	0.68
1:B:292:LEU:HD23	1:B:333:LEU:HD11	1.74	0.68
1:A:300:TRP:CH2	1:A:304:LEU:HD22	2.29	0.68
1:B:403:ARG:HE	1:B:455:HIS:HE2	1.43	0.67
1:B:332:TYR:C	1:B:334:SER:H	2.03	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:35:ARG:HH12	1:B:40:TRP:C	2.01	0.65
1:B:138:HIS:C	1:B:140:PRO:HD3	2.21	0.64
1:B:466:GLN:HB2	1:B:467:PRO:HD3	1.80	0.64
1:B:288:MET:HE2	5:B:5054:HOH:O	1.97	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:A:441:SER:OG	1:A:444:GLU:HG3	1.98	0.64
1:B:35:ARG:NH1	1:B:35:ARG:CG	2.39	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:B:18:ASN:OD1	1:B:20:GLN:C	2.42	0.63
1:A:97:ASN:H	1:A:97:ASN:ND2	1.97	0.63
1:A:474:ARG:HG3	1:A:474:ARG:HH11	1.64	0.63
1:B:84:ASP:OD2	1:B:88:ARG:HB3	1.98	0.62
1:A:66:GLN:HE21	1:A:66:GLN:HA	1.63	0.62
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:TRP:HZ3	1:B:468:ARG:O	1.82	0.61
1:A:97:ASN:HD22	1:A:97:ASN:N	1.93	0.61
1:A:141:GLU:CD	1:A:141:GLU:H	2.08	0.61
1:A:346:LYS:NZ	5:A:5032:HOH:O	2.32	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:360:GLU:CD	1:B:360:GLU:H	2.09	0.60
1:A:270:PRO:C	1:A:271:GLU:CG	2.74	0.60
1:B:437:ASN:HA	1:B:439:GLU:OE1	2.02	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:307:LEU:C	1:B:308:SER:OG	2.46	0.59
1:A:116:ARG:CZ	1:A:122:LEU:HD11	2.33	0.58
1:A:334:SER:OG	1:A:344:GLN:NE2	2.36	0.58
1:B:27:GLN:CD	1:B:58:ALA:HB1	2.27	0.58
1:B:445:LEU:C	1:B:447:PRO:HD3	2.29	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:HG3	1:A:430:ARG:HH11	1.68	0.57
1:A:304:LEU:O	1:B:358:PRO:HG3	2.05	0.57
1:A:234:ASN:HD21	2:A:4930:XUL:H3	1.69	0.57
1:B:27:GLN:CG	1:B:58:ALA:CB	2.76	0.57
1:A:317:ALA:HB1	1:A:363:ARG:HG2	1.85	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:B:63:HIS:HD2	1:B:64:SER:O	1.88	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:268:SER:C	1:B:270:PRO:HD3	2.31	0.56
1:B:27:GLN:HG2	1:B:58:ALA:HB1	1.82	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
1:B:54:ARG:NH2	4:B:4935:NH4:N	2.54	0.55
1:A:132:LEU:HD13	1:A:176:TRP:CH2	2.41	0.55
1:A:325:GLU:O	1:A:356:HIS:HE1	1.90	0.55
1:B:332:TYR:C	1:B:334:SER:N	2.64	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:141:GLU:CD	1:B:141:GLU:N	2.65	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:B:77:MET:CE	1:B:234:ASN:HD22	2.20	0.54
1:A:71:LEU:HD23	1:A:71:LEU:C	2.31	0.54
1:A:121:ASN:HD21	1:A:276:SER:H	1.56	0.54
1:A:245:ASP:N	1:A:248:GLN:OE1	2.34	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:B:121:ASN:HB2	1:B:175:MET:HE1	1.88	0.54
1:B:292:LEU:CB	1:B:333:LEU:HD11	2.34	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:77:MET:HE3	2:B:4931:XUL:C2	2.38	0.54
1:B:480:LEU:HB3	1:B:481:PRO:CD	2.37	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:1:MET:HE1	1:B:24:VAL:HG21	1.91	0.53
1:B:399:SER:O	1:B:403:ARG:HG3	2.09	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:N	1:B:97:ASN:HD22	2.05	0.53
1:A:270:PRO:O	1:A:271:GLU:CD	2.52	0.53
1:B:77:MET:HE2	1:B:234:ASN:HD22	1.74	0.52
1:B:91:ARG:NH1	1:B:91:ARG:CG	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:A:37:HIS:HB3	1:A:38:PRO:CD	2.40	0.52
1:B:18:ASN:OD1	1:B:20:GLN:CB	2.57	0.52
1:B:309:ASN:ND2	1:B:312:ALA:H	2.08	0.51
1:B:97:ASN:HD22	1:B:97:ASN:H	1.55	0.51
1:B:325:GLU:CB	1:B:326:PRO:HD2	2.35	0.51
1:B:269:LYS:N	1:B:270:PRO:HD3	2.25	0.51
1:B:436:ALA:C	1:B:438:PRO:HD3	2.36	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:17:LEU:HD21	1:B:21:GLY:C	2.35	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:A:43:GLN:HE22	1:A:76:GLN:HE22	1.58	0.50
1:B:292:LEU:CA	1:B:333:LEU:CD1	2.54	0.50
1:B:11:GLY:HA2	1:B:31:LEU:HD23	1.93	0.50
2:B:4931:XUL:O4	2:B:4931:XUL:O2	2.30	0.50
1:B:27:GLN:CG	1:B:58:ALA:HB1	2.40	0.50
1:B:418:THR:HG22	1:B:452:GLU:HB2	1.92	0.50
2:B:4931:XUL:H3	5:B:5058:HOH:O	2.11	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:A:288:MET:SD	1:A:288:MET:C	2.95	0.50
1:B:98:ASP:OD1	1:B:100:ARG:HG2	2.11	0.50
1:B:442:LEU:HD22	1:B:446:LEU:CD1	2.42	0.50
1:B:121:ASN:HD21	1:B:276:SER:H	1.60	0.50
1:B:18:ASN:C	1:B:20:GLN:N	2.67	0.49
1:B:480:LEU:C	1:B:480:LEU:CD1	2.85	0.49
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:108:LEU:HD23	1:B:108:LEU:C	2.37	0.49
1:B:108:LEU:HD23	1:B:108:LEU:O	2.13	0.49
1:B:328:TRP:CZ3	1:B:468:ARG:O	2.64	0.49
1:B:277:PHE:HB2	1:B:286:HIS:CE1	2.47	0.49
1:B:439:GLU:CD	1:B:439:GLU:H	2.20	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:A:119:THR:OG1	1:A:175:MET:HE1	2.12	0.49
1:B:301:ALA:CB	1:B:365:VAL:HG11	2.43	0.48
1:A:401:TYR:N	5:A:5056:HOH:O	2.31	0.48
1:A:430:ARG:HH11	1:A:430:ARG:CG	2.26	0.48
1:B:121:ASN:ND2	1:B:275:HIS:CD2	2.74	0.48
1:B:65:LEU:C	1:B:66:GLN:CG	2.79	0.48
1:A:66:GLN:HE21	1:A:66:GLN:CA	2.25	0.48
1:B:71:LEU:C	1:B:71:LEU:HD23	2.38	0.48
1:A:270:PRO:C	1:A:271:GLU:CD	2.82	0.48
1:B:5:ILE:HG12	1:B:14:VAL:HG12	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:VAL:N	1:B:311:PRO:CD	2.77	0.48
1:A:419:GLY:HA2	1:A:421:ASP:OD1	2.14	0.48
1:B:7:LEU:HG	1:B:156:LEU:HD22	1.96	0.48
1:A:18:ASN:ND2	1:A:21:GLY:N	2.62	0.48
1:A:119:THR:CG2	1:A:175:MET:HE3	2.38	0.48
1:B:234:ASN:ND2	2:B:4931:XUL:O2	2.43	0.48
1:B:419:GLY:C	1:B:421:ASP:H	2.21	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:A:18:ASN:ND2	1:A:18:ASN:C	2.70	0.47
1:A:82:LEU:HD13	1:A:146:ILE:CD1	2.44	0.47
1:B:38:PRO:O	1:B:39:LEU:HB2	2.14	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:A:38:PRO:O	1:A:39:LEU:CB	2.62	0.47
1:A:84:ASP:CG	1:A:88:ARG:HB2	2.39	0.47
1:A:403:ARG:HE	1:A:455:HIS:HE2	1.62	0.47
1:B:123:MET:SD	1:B:175:MET:HG3	2.54	0.47
1:A:253:LEU:HD12	1:A:397:ALA:CB	2.42	0.47
1:A:27:GLN:HG2	1:A:58:ALA:HB3	1.97	0.47
1:A:66:GLN:HA	1:A:66:GLN:NE2	2.27	0.47
1:B:310:VAL:HB	1:B:311:PRO:HD3	1.96	0.47
1:B:328:TRP:HH2	1:B:468:ARG:HA	1.79	0.47
1:A:19:GLU:CD	1:A:19:GLU:N	2.62	0.47
1:A:469:ARG:HG2	5:A:4940:HOH:O	2.14	0.47
1:A:1:MET:CE	1:A:16:LEU:CD1	2.93	0.47
1:A:295:ALA:N	5:A:5154:HOH:O	2.47	0.47
1:A:474:ARG:HH11	1:A:474:ARG:CG	2.28	0.47
1:A:112:VAL:HA	1:A:113:PRO:HD3	1.61	0.46
1:A:253:LEU:O	1:A:295:ALA:HB2	2.14	0.46
2:A:4930:XUL:O3	2:A:4930:XUL:O5	2.30	0.46
1:B:269:LYS:CE	1:B:272:SER:HB3	2.44	0.46
1:A:184:TRP:CZ2	1:A:199:MET:HB3	2.51	0.46
1:B:7:LEU:HG	1:B:156:LEU:CD2	2.46	0.46
1:A:91:ARG:HG3	1:A:91:ARG:NH1	2.27	0.46
1:B:122:LEU:HD22	1:B:122:LEU:HA	1.60	0.46
1:B:139:GLU:N	1:B:140:PRO:HD3	2.30	0.46
1:A:123:MET:SD	1:A:175:MET:HG3	2.55	0.46
1:B:43:GLN:HE21	1:B:48:TRP:HE1	1.61	0.46
1:B:18:ASN:O	1:B:19:GLU:C	2.57	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ILE:HG12	1:A:399:SER:OG	2.17	0.45
1:B:156:LEU:O	1:B:160:MET:HG3	2.16	0.45
1:B:12:VAL:O	1:B:12:VAL:HG23	2.16	0.45
1:B:328:TRP:CH2	1:B:471:THR:HB	2.51	0.45
1:A:269:LYS:HE2	1:A:383:CYS:HA	1.97	0.45
1:A:310:VAL:H	1:A:311:PRO:HD3	1.80	0.45
1:B:57:LYS:O	1:B:58:ALA:C	2.59	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:A:291:MET:HE1	1:A:376:GLY:HA3	1.99	0.45
1:B:70:ALA:HA	1:B:225:VAL:CG1	2.44	0.45
1:A:113:PRO:HD2	1:A:114:GLN:H	1.81	0.45
1:A:300:TRP:CZ2	1:A:304:LEU:CD2	2.98	0.45
1:B:309:ASN:HD22	1:B:311:PRO:HD2	1.82	0.45
1:B:108:LEU:HD22	1:B:123:MET:HE3	1.98	0.44
1:A:346:LYS:HE2	1:A:483:MET:HE3	1.99	0.44
1:B:334:SER:O	5:B:5121:HOH:O	2.21	0.44
1:B:123:MET:HE2	1:B:123:MET:HB2	1.86	0.44
1:B:136:GLN:HG3	1:B:137:ARG:N	2.31	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:288:MET:SD	1:A:289:SER:N	2.91	0.44
1:B:56:MET:HG3	1:B:220:TRP:CE2	2.53	0.44
1:B:132:LEU:HD22	1:B:176:TRP:CH2	2.53	0.44
1:B:186:ASP:OD1	1:B:196:ARG:HD2	2.17	0.44
1:A:300:TRP:CD1	1:B:354:HIS:HA	2.52	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:303:LYS:N	1:B:303:LYS:HD2	2.32	0.43
1:A:108:LEU:HD23	1:A:108:LEU:HA	1.85	0.43
1:A:128:THR:O	1:A:131:LYS:HB2	2.18	0.43
1:A:284:ARG:HD3	5:A:5083:HOH:O	2.18	0.43
1:A:313:LEU:C	1:A:315:ALA:N	2.76	0.43
1:A:305:THR:C	1:A:307:LEU:H	2.26	0.43
1:A:284:ARG:HA	5:A:5083:HOH:O	2.18	0.43
1:B:328:TRP:CD1	1:B:328:TRP:N	2.86	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:325:GLU:H	1:B:355:GLN:NE2	2.16	0.43
1:B:446:LEU:N	1:B:447:PRO:HD3	2.34	0.43

Continued on next page...

Continued from previous page...

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:B:451:LEU:HD11	1:B:454:SER:HB2	2.01	0.43
1:B:482:LEU:HD13	1:B:482:LEU:HA	1.65	0.43
1:B:255:THR:O	1:B:255:THR:CG2	2.64	0.43
1:A:121:ASN:HB2	1:A:175:MET:HE1	2.01	0.42
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:A:156:LEU:HD12	1:A:156:LEU:HA	1.91	0.42
1:B:45:PRO:O	1:B:48:TRP:HB2	2.19	0.42
1:A:108:LEU:HD13	1:A:123:MET:HE3	2.01	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:20:GLN:CD	1:A:20:GLN:N	2.77	0.42
1:A:129:ALA:N	1:A:130:PRO:HD2	2.34	0.42
1:A:213:LEU:HA	1:A:214:PRO:HD3	1.97	0.42
1:A:236:ALA:O	1:A:427:GLY:HA3	2.20	0.42
1:A:300:TRP:CA	5:A:5120:HOH:O	2.51	0.42
1:B:69:LYS:H	1:B:69:LYS:HG2	1.60	0.42
1:A:310:VAL:O	1:A:310:VAL:HG13	2.18	0.42
1:B:292:LEU:CD2	1:B:333:LEU:HD11	2.46	0.42
1:B:294:ALA:O	1:B:298:LEU:HG	2.18	0.42
1:A:402:TRP:CZ2	1:A:406:LEU:HD11	2.55	0.42
1:A:29:GLU:OE1	1:A:54:ARG:NE	2.53	0.42
1:B:442:LEU:HD23	1:B:442:LEU:HA	1.83	0.42
1:B:480:LEU:HD13	1:B:480:LEU:O	2.19	0.42
1:A:245:ASP:OD1	1:A:284:ARG:NH1	2.53	0.41
1:B:82:LEU:N	1:B:82:LEU:HD23	2.35	0.41
1:B:282:PRO:O	1:B:284:ARG:HD3	2.20	0.41
1:A:300:TRP:CE2	1:A:304:LEU:HD22	2.55	0.41
1:A:334:SER:HB2	1:A:344:GLN:C	2.42	0.41
1:A:456:LEU:HA	1:A:457:PRO:HD3	1.88	0.41
1:B:225:VAL:HG13	1:B:226:PRO:CD	2.50	0.41
1:B:292:LEU:CD2	1:B:333:LEU:CD2	2.73	0.41
1:B:327:VAL:HG11	1:B:352:LEU:HD13	2.01	0.41
1:B:480:LEU:N	1:B:481:PRO:HD2	2.35	0.41
1:A:18:ASN:HD22	1:A:21:GLY:H	1.68	0.41
1:B:63:HIS:CD2	1:B:63:HIS:C	2.98	0.41
1:B:174:THR:O	1:B:175:MET:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

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:119:THR:CB	1:A:175:MET:CE	2.99	0.41
1:A:352:LEU:HA	1:A:356:HIS:HD2	1.85	0.41
1:B:242:GLY:C	1:B:243:MET:HE2	2.45	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:360:GLU:CD	1:B:360:GLU:N	2.76	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:A:147:ASP:O	1:A:148:LYS:HD3	2.20	0.41
1:A:303:LYS:HD2	1:A:303:LYS:O	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:A:430:ARG:NH1	1:A:447:PRO:HD2	2.36	0.40
1:A:196:ARG:HG3	5:A:5082:HOH:O	2.20	0.40
1:B:328:TRP:CH2	1:B:468:ARG:HA	2.57	0.40
1:A:300:TRP:O	1:A:304:LEU:HB2	2.22	0.40
1:A:321:ASP:OD1	1:A:321:ASP:C	2.64	0.40
1:B:44:ASP:HA	1:B:45:PRO:HD3	1.87	0.40
1:B:151:LEU:HD13	1:B:170:ASP:CG	2.46	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%)	11 8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	471/484 (97%)	441 (94%)	29 (6%)	1 (0%)	43	44
All	All	943/968 (97%)	893 (95%)	44 (5%)	6 (1%)	21	18

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%)	326 (87%)	49 (13%)	4	2
1	B	374/382 (98%)	315 (84%)	59 (16%)	2	1
All	All	749/764 (98%)	641 (86%)	108 (14%)	3	1

All (108) 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	19	GLU
1	A	31	LEU
1	A	66	GLN
1	A	73	ILE
1	A	82	LEU
1	A	88	ARG
1	A	90	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	97	ASN
1	A	107	LEU
1	A	108	LEU
1	A	122	LEU
1	A	132	LEU
1	A	133	LEU
1	A	141	GLU
1	A	148	LYS
1	A	190	GLN
1	A	225	VAL
1	A	243	MET
1	A	244	VAL
1	A	253	LEU
1	A	287	LEU
1	A	288	MET
1	A	303	LYS
1	A	310	VAL
1	A	314	ILE
1	A	344	GLN
1	A	352	LEU
1	A	361	LEU
1	A	363	ARG
1	A	386	LYS
1	A	389	SER
1	A	391	THR
1	A	398	ARG
1	A	406	LEU
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	474	ARG
1	A	480	LEU
1	A	482	LEU
1	B	3	ILE
1	B	7	LEU
1	B	16	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	17	LEU
1	B	20	GLN
1	B	31	LEU
1	B	35	ARG
1	B	44	ASP
1	B	65	LEU
1	B	66	GLN
1	B	69	LYS
1	B	73	ILE
1	B	82	LEU
1	B	90	LEU
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	190	GLN
1	B	215	GLU
1	B	218	LYS
1	B	225	VAL
1	B	244	VAL
1	B	255	THR
1	B	256	SER
1	B	258	VAL
1	B	267	LEU
1	B	269	LYS
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	330	LEU
1	B	352	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	361	LEU
1	B	363	ARG
1	B	385	ILE
1	B	392	LEU
1	B	398	ARG
1	B	406	LEU
1	B	418	THR
1	B	430	ARG
1	B	439	GLU
1	B	442	LEU
1	B	443	ILE
1	B	448	GLN
1	B	451	LEU
1	B	482	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	20	GLN
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	275	HIS
1	A	286	HIS
1	A	309	ASN
1	A	344	GLN
1	A	356	HIS
1	A	404	GLN
1	A	477	GLN
1	B	43	GLN
1	B	63	HIS
1	B	97	ASN
1	B	121	ASN
1	B	145	GLN
1	B	190	GLN
1	B	234	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	275	HIS
1	B	286	HIS
1	B	309	ASN
1	B	355	GLN
1	B	356	HIS
1	B	388	GLN
1	B	404	GLN
1	B	412	GLN
1	B	437	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
3	SO4	B	4932	-	4,4,4	0.24	0	6,6,6	0.22	0
2	XUL	B	4931	-	9,9,9	3.92	1 (11%)	6,11,11	1.16	1 (16%)
2	XUL	A	4930	-	9,9,9	4.12	1 (11%)	6,11,11	1.59	1 (16%)
3	SO4	A	4931	-	4,4,4	0.23	0	6,6,6	0.14	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	B	4931	-	2/2/3/3	7/12/12/12	-
2	XUL	A	4930	-	-	4/12/12/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4930	XUL	O2-C2	12.07	1.41	1.21
2	B	4931	XUL	O2-C2	11.68	1.40	1.21

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4930	XUL	O4-C4-C3	-3.49	104.60	109.67
2	B	4931	XUL	O5-C5-C4	-2.05	106.84	111.16

All (2) chirality outliers are listed below:

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

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4930	XUL	O1-C1-C2-C3
2	A	4930	XUL	O1-C1-C2-O2
2	A	4930	XUL	C3-C4-C5-O5
2	A	4930	XUL	O4-C4-C5-O5
2	B	4931	XUL	O1-C1-C2-C3
2	B	4931	XUL	O1-C1-C2-O2
2	B	4931	XUL	O2-C2-C3-O3
2	B	4931	XUL	C2-C3-C4-C5
2	B	4931	XUL	C2-C3-C4-O4
2	B	4931	XUL	O3-C3-C4-C5
2	B	4931	XUL	O3-C3-C4-O4

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4931	XUL	10	0
2	A	4930	XUL	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	13 (2%) 56 59	16, 34, 59, 129	0
1	B	475/484 (98%)	0.28	8 (1%) 69 71	21, 37, 62, 108	0
All	All	951/968 (98%)	0.16	21 (2%) 62 65	16, 35, 61, 129	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	333	LEU	4.6
1	A	343	PRO	4.2
1	B	334	SER	4.2
1	B	223	ALA	3.4
1	B	220	TRP	3.2
1	B	345	ALA	2.9
1	B	344	GLN	2.7
1	A	193	ASP	2.7
1	A	270	PRO	2.6
1	A	323	SER	2.5
1	A	308	SER	2.4
1	A	307	LEU	2.4
1	A	344	GLN	2.4
1	A	300	TRP	2.4
1	A	303	LYS	2.4
1	B	299	ASP	2.4
1	B	354	HIS	2.4
1	A	272	SER	2.3
1	A	484	ALA	2.2
1	A	402	TRP	2.1
1	A	456	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 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($\text{\AA}^2$)	Q<0.9
2	XUL	B	4931	10/10	0.63	0.14	52,66,86,107	0
4	NH4	B	4934	1/1	0.65	0.12	47,47,47,47	0
4	NH4	B	4936	1/1	0.68	0.11	35,35,35,35	0
3	SO4	A	4931	5/5	0.69	0.10	51,62,114,151	0
4	NH4	A	4935	1/1	0.70	0.10	47,47,47,47	0
4	NH4	B	4935	1/1	0.77	0.12	40,40,40,40	0
4	NH4	A	4937	1/1	0.77	0.08	34,34,34,34	0
4	NH4	A	4932	1/1	0.79	0.07	40,40,40,40	0
2	XUL	A	4930	10/10	0.81	0.14	32,57,101,101	0
4	NH4	A	4936	1/1	0.82	0.08	42,42,42,42	0
4	NH4	A	4934	1/1	0.82	0.08	43,43,43,43	0
4	NH4	B	4933	1/1	0.82	0.07	49,49,49,49	0
3	SO4	B	4932	5/5	0.83	0.07	66,69,82,100	0
4	NH4	A	4938	1/1	0.86	0.13	34,34,34,34	0
4	NH4	B	4937	1/1	0.86	0.09	36,36,36,36	0
4	NH4	A	4933	1/1	0.96	0.04	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.