



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2014 – 07:32 PM EDT

PDB ID : 4O7P
Title : Crystal structure of Mycobacterium tuberculosis maltose kinase MaK complexed with maltose
Authors : Li, J.; Guan, X.T.; Rao, Z.H.
Deposited on : 2013-12-26
Resolution : 2.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

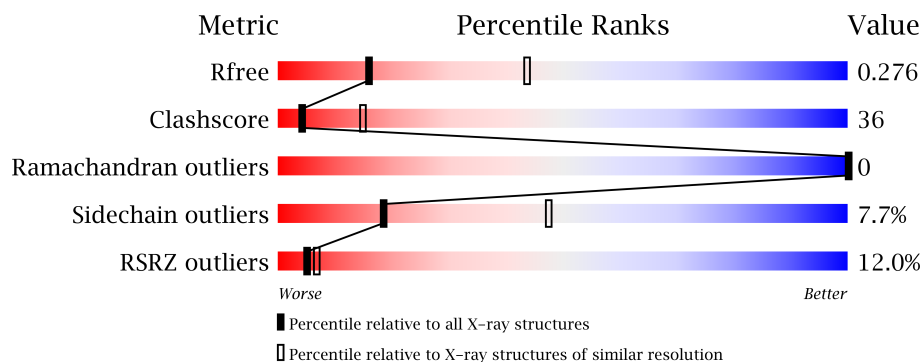
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23828
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23828

1 Overall quality at a glance



The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	455	
1	B	455	

2 Entry composition ⓘ

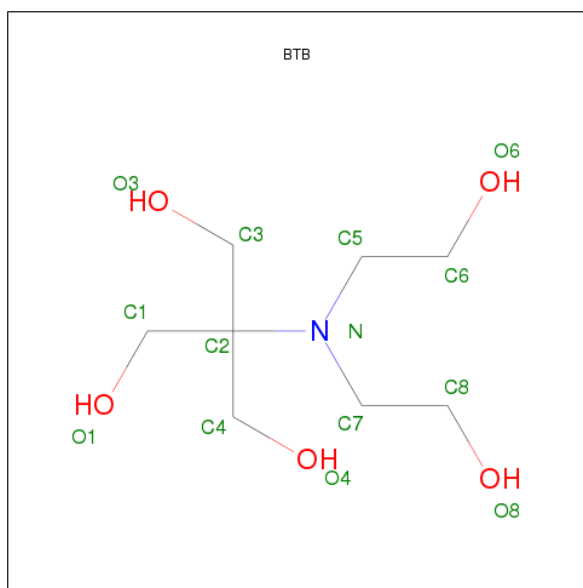
There are 4 unique types of molecules in this entry. The entry contains 6895 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Maltokinase.

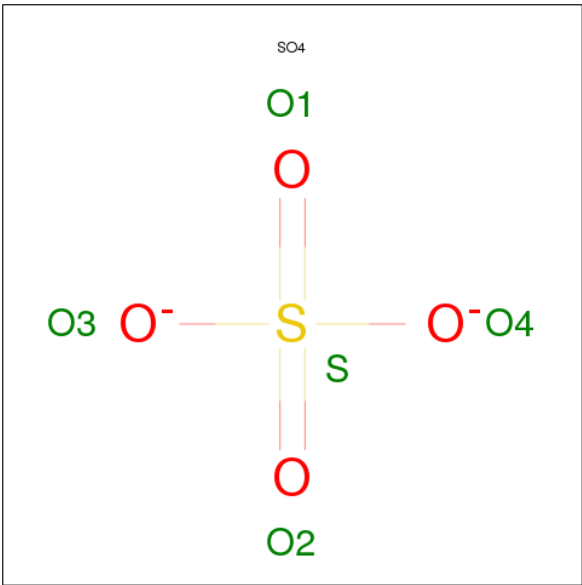
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	0	0
			3349	2114	593	636	6			
1	B	451	Total	C	N	O	S	0	0	0
			3490	2199	618	667	6			

- Molecule 2 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).



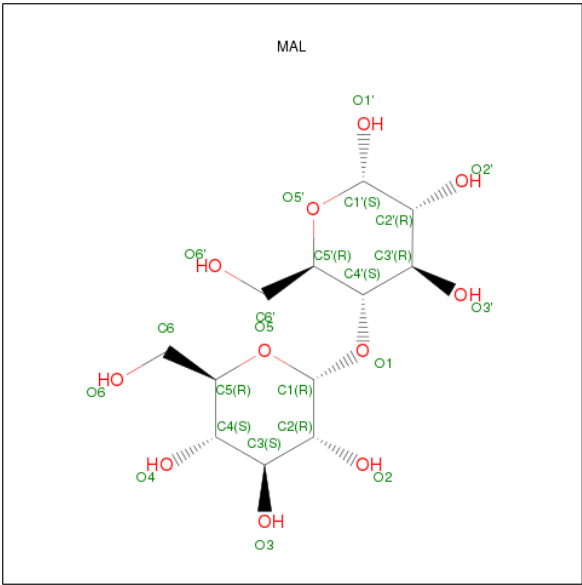
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is SUGAR (MALTOSE) (three-letter code: MAL) (formula: C₁₂H₂₂O₁₁).

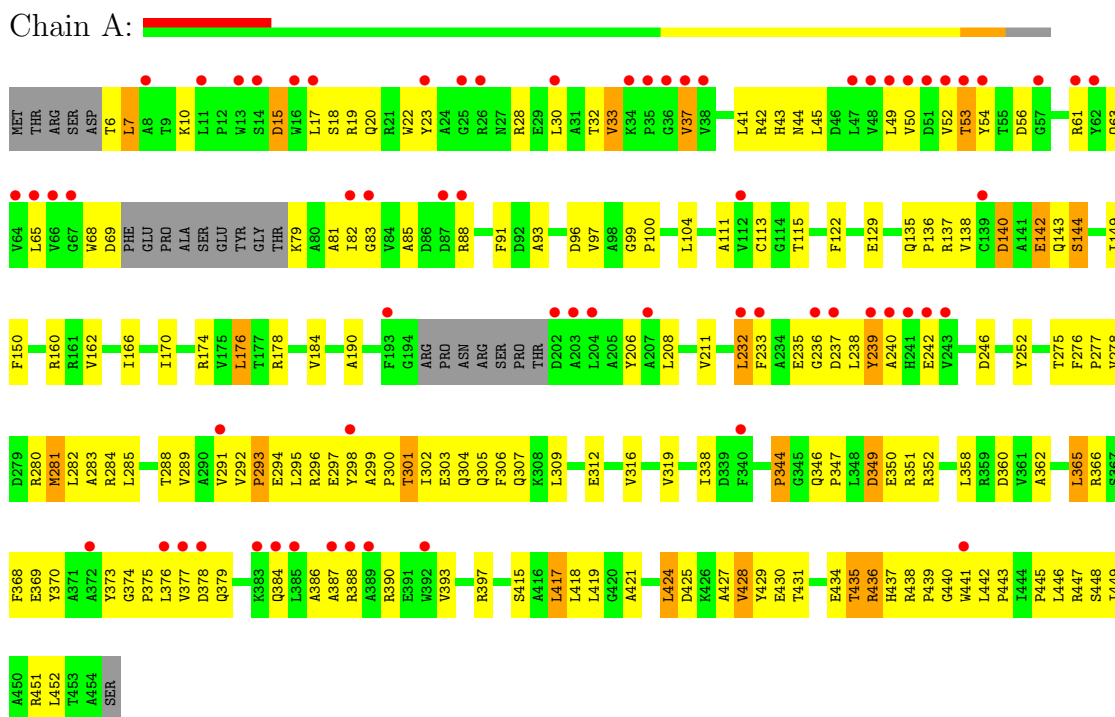


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			23	12	11		

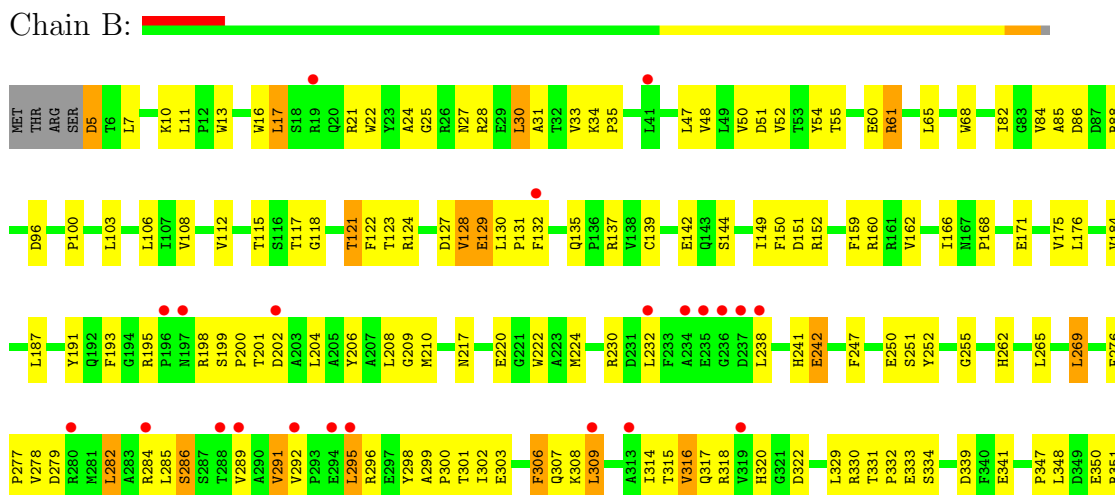
3 Residue-property plots

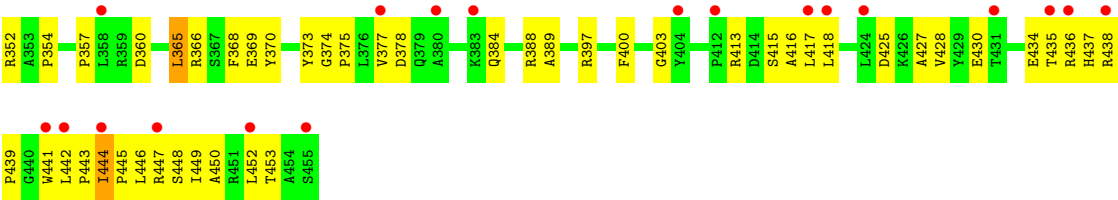
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



• Molecule 1: Maltokinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	96.73Å 96.73Å 461.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.60 – 2.90 48.36 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.2 (44.60-2.90) 99.7 (48.36-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.239 , 0.281 0.230 , 0.276	Depositor DCC
R_{free} test set	1492 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	98.7	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 74.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 29570 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6895	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.66	0/3420	0.86	1/4661 (0.0%)
1	B	0.66	0/3568	0.84	2/4867 (0.0%)
All	All	0.66	0/6988	0.85	3/9528 (0.0%)

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	1
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	265	LEU	CB-CG-CD1	-8.29	96.90	111.00
1	A	138	VAL	N-CA-C	-5.93	95.00	111.00
1	B	329	LEU	CB-CG-CD1	-5.33	101.94	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	GLU	Peptide
1	A	293	PRO	Peptide
1	A	344	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	B	115	THR	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3349	0	3283	241	0
1	B	3490	0	3409	253	0
2	A	28	0	38	7	0
3	A	5	0	0	0	0
4	B	23	0	20	0	0
All	All	6895	0	6750	494	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 36.

All (494) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:198:ARG:HG2	1:B:204:LEU:HD13	1.25	1.17
1:A:10:LYS:NZ	1:A:85:ALA:HB1	1.56	1.17
1:B:303:GLU:HA	1:B:306:PHE:CE2	1.87	1.10
1:A:302:ILE:HG22	1:A:306:PHE:HE2	1.10	1.10
1:A:7:LEU:HG	1:A:10:LYS:HE3	1.26	1.09
1:A:295:LEU:HD23	1:A:298:TYR:HE2	0.96	1.09
1:A:295:LEU:HD23	1:A:298:TYR:CE2	1.87	1.07
1:A:446:LEU:HA	1:A:449:ILE:HD12	1.36	1.05
1:B:289:VAL:HG23	1:B:295:LEU:HD21	1.07	1.05
1:B:289:VAL:HA	1:B:295:LEU:HD11	1.29	1.04
1:B:306:PHE:CE1	1:B:307:GLN:HG2	1.92	1.04
1:A:302:ILE:CG2	1:A:306:PHE:HE2	1.72	1.03
1:A:431:THR:O	1:A:435:THR:HB	1.57	1.01
1:A:442:LEU:O	1:A:446:LEU:HD13	1.61	1.01
1:B:289:VAL:HG21	1:B:296:ARG:HH12	1.24	1.00
1:A:96:ASP:O	1:A:100:PRO:HD3	1.62	0.99
1:A:18:SER:HA	1:A:23:TYR:CD2	1.99	0.98

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:65:LEU:HD11	1:B:103:LEU:HD11	1.44	0.98
1:A:238:LEU:HD12	1:A:239:TYR:N	1.79	0.97
1:A:285:LEU:O	1:A:288:THR:HG22	1.64	0.97
1:B:96:ASP:O	1:B:100:PRO:HD2	1.63	0.97
1:B:198:ARG:HG2	1:B:204:LEU:CD1	1.94	0.97
1:B:289:VAL:CG2	1:B:295:LEU:HD21	1.95	0.96
1:A:302:ILE:HG22	1:A:306:PHE:CE2	2.00	0.96
1:B:306:PHE:HD1	1:B:307:GLN:N	1.63	0.96
1:A:295:LEU:CD2	1:A:298:TYR:HE2	1.79	0.95
1:B:306:PHE:CD1	1:B:307:GLN:N	2.35	0.95
1:A:424:LEU:HD12	1:A:425:ASP:H	1.30	0.95
1:B:303:GLU:HA	1:B:306:PHE:CD2	2.04	0.93
1:B:10:LYS:NZ	1:B:86:ASP:H	1.67	0.91
1:B:306:PHE:HE1	1:B:307:GLN:HG2	1.24	0.91
1:A:10:LYS:HZ3	1:A:85:ALA:HB1	1.34	0.91
1:A:135:GLN:NE2	1:A:136:PRO:HD3	1.84	0.91
1:A:424:LEU:HD12	1:A:425:ASP:N	1.85	0.91
1:A:135:GLN:HG3	1:A:136:PRO:CD	2.00	0.90
1:A:365:LEU:HD12	1:A:397:ARG:HG2	1.51	0.90
1:A:135:GLN:HG3	1:A:136:PRO:HD2	1.52	0.90
1:A:417:LEU:HD13	1:A:418:LEU:HD12	1.54	0.90
1:A:7:LEU:HG	1:A:10:LYS:CE	2.01	0.90
1:A:10:LYS:HZ2	1:A:85:ALA:HB1	1.35	0.90
1:A:69:ASP:C	1:A:88:ARG:HG2	1.90	0.90
1:B:195:ARG:HG3	1:B:198:ARG:NH1	1.87	0.90
1:A:238:LEU:HD12	1:A:239:TYR:H	1.34	0.89
1:B:10:LYS:HZ2	1:B:86:ASP:H	0.89	0.89
1:A:346:GLN:HE21	1:A:350:GLU:HG2	1.39	0.87
1:B:289:VAL:HG23	1:B:295:LEU:CD2	1.99	0.87
1:A:373:TYR:OH	1:A:390:ARG:HG2	1.74	0.87
1:B:301:THR:HG21	1:B:453:THR:HG21	1.55	0.86
1:B:106:LEU:HB3	1:B:122:PHE:CD2	2.11	0.86
1:A:347:PRO:HG2	1:A:350:GLU:HB2	1.57	0.85
1:A:7:LEU:HD21	1:A:68:TRP:CH2	2.12	0.85
1:B:11:LEU:HD12	1:B:85:ALA:HB2	1.58	0.85
1:A:7:LEU:CD2	1:A:68:TRP:CH2	2.60	0.84
1:B:289:VAL:HG21	1:B:296:ARG:NH1	1.91	0.84
1:B:30:LEU:HD11	1:B:33:VAL:HG23	1.57	0.84
1:B:306:PHE:HE1	1:B:307:GLN:CG	1.90	0.84
1:A:451:ARG:NH1	1:A:451:ARG:HB2	1.92	0.84
1:B:436:ARG:O	1:B:436:ARG:HD2	1.78	0.84
1:B:11:LEU:HD11	1:B:68:TRP:HH2	1.42	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:301:THR:O	1:A:305:GLN:HG3	1.79	0.83
1:A:438:ARG:HH22	2:A:501:BTB:H12	1.44	0.83
1:A:10:LYS:NZ	1:A:85:ALA:CB	2.41	0.83
1:B:296:ARG:HH21	1:B:299:ALA:CB	1.90	0.82
1:B:308:LYS:HD2	1:B:308:LYS:O	1.79	0.82
1:A:417:LEU:HD13	1:A:418:LEU:CD1	2.09	0.82
1:A:280:ARG:NH1	1:A:284:ARG:HH12	1.77	0.82
1:B:299:ALA:O	1:B:302:ILE:HG12	1.79	0.82
1:B:370:TYR:CE1	1:B:444:ILE:HD11	2.14	0.81
1:B:445:PRO:O	1:B:449:ILE:HG23	1.81	0.81
1:B:10:LYS:HZ2	1:B:86:ASP:N	1.75	0.81
1:B:276:PHE:HD2	1:B:278:VAL:HG13	1.46	0.81
1:A:302:ILE:CG2	1:A:306:PHE:CE2	2.63	0.80
1:B:296:ARG:NH2	1:B:299:ALA:CB	2.44	0.80
1:B:238:LEU:O	1:B:388:ARG:NH1	2.13	0.80
1:B:286:SER:O	1:B:289:VAL:HG12	1.82	0.80
1:A:451:ARG:HB2	1:A:451:ARG:CZ	2.13	0.79
1:A:346:GLN:NE2	1:A:350:GLU:HG2	1.98	0.79
1:B:198:ARG:CG	1:B:204:LEU:HD13	2.09	0.79
1:B:300:PRO:HA	1:B:303:GLU:OE1	1.82	0.79
1:A:390:ARG:HH22	1:A:447:ARG:HD3	1.46	0.79
1:B:303:GLU:CA	1:B:306:PHE:CE2	2.67	0.78
1:A:7:LEU:CG	1:A:10:LYS:HE3	2.13	0.77
1:A:142:GLU:HA	1:A:143:GLN:C	2.05	0.77
1:B:444:ILE:HG13	1:B:445:PRO:CD	2.14	0.77
1:B:298:TYR:O	1:B:301:THR:HG22	1.84	0.77
1:B:252:TYR:CE1	1:B:403:GLY:HA2	2.19	0.77
1:A:232:LEU:C	1:A:232:LEU:HD13	2.05	0.76
1:B:28:ARG:HG3	1:B:54:TYR:HE2	1.51	0.76
1:A:79:LYS:HE3	1:A:81:ALA:CB	2.14	0.76
1:A:135:GLN:NE2	1:A:136:PRO:CD	2.48	0.76
1:A:417:LEU:N	1:A:417:LEU:HD12	2.01	0.75
1:B:299:ALA:O	1:B:303:GLU:OE1	2.04	0.75
1:B:441:TRP:O	1:B:444:ILE:HG13	1.86	0.75
1:A:96:ASP:O	1:A:100:PRO:CD	2.34	0.75
1:B:427:ALA:HA	1:B:430:GLU:OE1	1.86	0.75
1:B:108:VAL:HG13	1:B:124:ARG:NH1	2.02	0.75
1:B:278:VAL:O	1:B:282:LEU:HD13	1.87	0.75
1:B:384:GLN:OE1	1:B:388:ARG:HG2	1.87	0.74
1:A:79:LYS:HE3	1:A:81:ALA:HB2	1.69	0.74
1:B:296:ARG:HH21	1:B:299:ALA:HB3	1.52	0.74
1:A:421:ALA:O	1:A:424:LEU:HD12	1.87	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:304:GLN:HA	1:A:307:GLN:HG2	1.68	0.74
1:A:82:ILE:HG22	1:A:91:PHE:HA	1.68	0.74
1:A:295:LEU:CD2	1:A:298:TYR:CE2	2.61	0.74
1:B:299:ALA:O	1:B:302:ILE:CG1	2.36	0.74
1:A:277:PRO:HG2	1:A:281:MET:CE	2.19	0.73
1:A:370:TYR:OH	1:A:430:GLU:HB3	1.88	0.73
1:A:135:GLN:HE21	1:A:136:PRO:CD	2.02	0.73
1:A:45:LEU:HD21	1:A:99:GLY:HA2	1.71	0.72
1:A:7:LEU:O	1:A:7:LEU:HD23	1.89	0.72
1:A:439:PRO:O	1:A:442:LEU:HD13	1.89	0.72
1:A:135:GLN:CD	1:A:136:PRO:HD3	2.10	0.72
1:A:285:LEU:O	1:A:289:VAL:HG13	1.90	0.72
1:A:280:ARG:HH12	1:A:284:ARG:HH12	1.35	0.71
1:A:428:VAL:CG2	1:A:429:TYR:N	2.53	0.71
1:B:303:GLU:HG3	1:B:306:PHE:HE2	1.56	0.71
1:B:439:PRO:HA	1:B:442:LEU:HD13	1.72	0.71
1:B:106:LEU:HD13	1:B:122:PHE:CE2	2.26	0.70
1:B:307:GLN:OE1	1:B:307:GLN:HA	1.91	0.70
1:A:174:ARG:HD3	1:A:178:ARG:HH21	1.57	0.70
1:B:446:LEU:O	1:B:449:ILE:HG12	1.92	0.70
1:B:13:TRP:O	1:B:17:LEU:HB2	1.92	0.70
1:B:128:VAL:O	1:B:130:LEU:HD13	1.89	0.70
1:A:7:LEU:HD23	1:A:7:LEU:C	2.13	0.69
1:B:369:GLU:HG2	1:B:448:SER:OG	1.93	0.69
1:A:232:LEU:O	1:A:232:LEU:HD13	1.91	0.69
1:B:415:SER:HB3	1:B:418:LEU:HD13	1.72	0.69
1:A:7:LEU:O	1:A:10:LYS:HG2	1.93	0.69
1:A:135:GLN:CG	1:A:136:PRO:CD	2.71	0.69
1:B:122:PHE:HD1	1:B:191:TYR:CB	2.05	0.69
1:B:295:LEU:HD23	1:B:296:ARG:N	2.06	0.69
1:B:65:LEU:HD11	1:B:103:LEU:CD1	2.22	0.69
1:A:97:VAL:C	1:A:100:PRO:HD2	2.12	0.69
1:B:52:VAL:HG22	1:B:54:TYR:CE1	2.28	0.69
1:B:52:VAL:HG22	1:B:54:TYR:HE1	1.58	0.69
1:A:115:THR:HG22	1:A:122:PHE:HB2	1.75	0.69
1:B:106:LEU:HD13	1:B:122:PHE:HE2	1.57	0.68
1:B:122:PHE:HD1	1:B:191:TYR:HB2	1.58	0.68
1:B:301:THR:CG2	1:B:453:THR:HG21	2.23	0.68
1:B:220:GLU:OE2	1:B:222:TRP:HB3	1.93	0.68
1:B:448:SER:O	1:B:452:LEU:HD13	1.93	0.68
1:A:28:ARG:NH1	1:A:54:TYR:CD2	2.62	0.67
1:A:7:LEU:HD22	1:A:68:TRP:CZ2	2.30	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:10:LYS:HZ2	1:A:85:ALA:CB	2.03	0.67
1:B:374:GLY:N	1:B:375:PRO:HD2	2.10	0.67
1:A:417:LEU:CD1	1:A:417:LEU:H	2.07	0.67
1:B:106:LEU:HB3	1:B:122:PHE:CE2	2.29	0.67
1:B:449:ILE:HG13	1:B:450:ALA:N	2.09	0.67
1:A:63:GLN:OE1	1:A:208:LEU:HD22	1.95	0.67
1:B:52:VAL:CG2	1:B:54:TYR:HE1	2.08	0.66
1:B:65:LEU:CD1	1:B:103:LEU:HD11	2.21	0.66
1:B:292:VAL:O	1:B:295:LEU:HD13	1.95	0.66
1:B:347:PRO:HG2	1:B:350:GLU:OE1	1.95	0.66
1:B:373:TYR:HE2	1:B:447:ARG:HD3	1.61	0.66
1:A:424:LEU:O	1:A:428:VAL:HG13	1.96	0.65
1:B:436:ARG:HG3	1:B:437:HIS:CE1	2.32	0.65
1:A:17:LEU:C	1:A:17:LEU:HD23	2.17	0.64
1:A:18:SER:HA	1:A:23:TYR:HD2	1.60	0.64
1:A:97:VAL:O	1:A:100:PRO:HD2	1.97	0.64
1:B:444:ILE:HG13	1:B:445:PRO:HD2	1.78	0.64
1:A:166:ILE:O	1:A:352:ARG:HD2	1.97	0.64
1:A:276:PHE:CD1	1:A:277:PRO:HD2	2.32	0.64
1:B:171:GLU:OE1	1:B:352:ARG:NH1	2.31	0.64
1:B:373:TYR:CE2	1:B:447:ARG:HD3	2.33	0.64
1:B:299:ALA:HA	1:B:302:ILE:HG12	1.80	0.64
1:B:442:LEU:O	1:B:446:LEU:HD13	1.99	0.63
1:A:282:LEU:O	1:A:285:LEU:HB3	1.99	0.63
1:B:195:ARG:HG3	1:B:198:ARG:HH12	1.63	0.63
1:B:295:LEU:CD2	1:B:296:ARG:N	2.62	0.63
1:A:7:LEU:HD22	1:A:68:TRP:CH2	2.33	0.63
1:B:276:PHE:CD2	1:B:278:VAL:HG13	2.31	0.63
1:A:390:ARG:NH2	1:A:447:ARG:HD3	2.14	0.62
1:B:30:LEU:HD13	1:B:31:ALA:N	2.14	0.62
1:A:96:ASP:HB2	1:B:132:PHE:CE1	2.34	0.62
1:A:434:GLU:O	1:A:442:LEU:HD11	2.00	0.62
1:B:300:PRO:CA	1:B:303:GLU:OE1	2.47	0.62
1:B:122:PHE:CD1	1:B:191:TYR:HB2	2.34	0.62
1:B:162:VAL:HG13	1:B:206:TYR:HD1	1.65	0.62
1:B:10:LYS:HB3	1:B:85:ALA:HB1	1.81	0.62
1:B:27:ASN:OD1	1:B:28:ARG:HD2	1.98	0.62
1:B:299:ALA:HB3	1:B:300:PRO:CD	2.30	0.62
1:B:252:TYR:CE1	1:B:403:GLY:CA	2.83	0.61
1:A:309:LEU:HD23	1:A:312:GLU:OE1	2.00	0.61
1:A:428:VAL:HG23	1:A:429:TYR:N	2.16	0.61
1:A:421:ALA:O	1:A:424:LEU:CD1	2.48	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:140:ASP:HB3	1:B:21:ARG:HD2	1.80	0.61
1:B:306:PHE:CE1	1:B:307:GLN:CG	2.71	0.61
1:B:316:VAL:HG13	1:B:354:PRO:HB2	1.83	0.61
1:A:280:ARG:NH1	1:A:284:ARG:NH1	2.46	0.61
1:A:238:LEU:HD12	1:A:239:TYR:HB2	1.83	0.61
1:A:430:GLU:O	1:A:434:GLU:HG2	2.01	0.60
1:A:82:ILE:HG23	1:A:83:GLY:H	1.65	0.60
1:B:298:TYR:O	1:B:301:THR:CG2	2.49	0.60
1:B:96:ASP:O	1:B:100:PRO:CD	2.44	0.60
1:A:424:LEU:CD1	1:A:425:ASP:N	2.62	0.60
1:A:10:LYS:CE	1:A:85:ALA:HB1	2.30	0.60
1:A:282:LEU:CD2	1:A:303:GLU:HG3	2.31	0.60
1:A:10:LYS:HZ3	1:A:85:ALA:CB	2.07	0.60
1:B:444:ILE:HG13	1:B:445:PRO:HD3	1.82	0.60
1:A:232:LEU:CD1	1:A:232:LEU:C	2.70	0.60
1:A:417:LEU:HD12	1:A:417:LEU:H	1.62	0.60
2:A:501:BTB:O1	2:A:501:BTB:H52	2.00	0.60
1:A:425:ASP:O	1:A:428:VAL:HG22	2.01	0.60
1:A:346:GLN:HG3	1:A:347:PRO:HD2	1.84	0.59
1:B:291:VAL:CG2	1:B:435:THR:HG21	2.32	0.59
1:B:299:ALA:HB3	1:B:300:PRO:HD3	1.84	0.59
1:A:282:LEU:HD22	1:A:303:GLU:HG3	1.84	0.59
1:A:278:VAL:HA	1:A:281:MET:HG3	1.83	0.59
1:B:269:LEU:HD23	1:B:318:ARG:HG3	1.84	0.59
1:B:303:GLU:HG3	1:B:306:PHE:CE2	2.36	0.59
1:A:386:ALA:O	1:A:390:ARG:HG3	2.01	0.59
1:A:104:LEU:HD22	1:B:150:PHE:CE2	2.37	0.59
1:B:289:VAL:CG2	1:B:296:ARG:NH1	2.65	0.59
1:B:11:LEU:HD11	1:B:68:TRP:CH2	2.30	0.59
1:A:142:GLU:HA	1:A:144:SER:HA	1.85	0.59
2:A:501:BTB:H42	2:A:501:BTB:O8	2.02	0.58
1:A:17:LEU:HD21	1:A:23:TYR:CD1	2.37	0.58
1:A:288:THR:HG23	1:A:289:VAL:N	2.18	0.58
1:A:277:PRO:HG2	1:A:281:MET:HE1	1.86	0.58
1:B:30:LEU:HD11	1:B:33:VAL:CG2	2.32	0.58
1:B:444:ILE:CD1	1:B:445:PRO:HD3	2.34	0.58
1:A:427:ALA:O	1:A:431:THR:HG23	2.04	0.58
1:B:370:TYR:CE1	1:B:444:ILE:CD1	2.85	0.58
1:B:28:ARG:HG3	1:B:54:TYR:CE2	2.36	0.58
1:B:441:TRP:O	1:B:444:ILE:CG1	2.51	0.58
1:A:362:ALA:O	1:A:366:ARG:HG2	2.03	0.58
1:A:275:THR:HG22	1:A:276:PHE:O	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:28:ARG:NH1	1:A:54:TYR:CG	2.73	0.57
1:A:276:PHE:CD2	1:A:309:LEU:HB2	2.39	0.57
1:A:37:VAL:HG13	1:A:49:LEU:HB2	1.85	0.57
1:B:373:TYR:CE1	1:B:389:ALA:HB1	2.40	0.57
1:A:42:ARG:HE	1:A:45:LEU:HD13	1.69	0.57
1:B:299:ALA:C	1:B:303:GLU:OE1	2.43	0.57
1:A:111:ALA:HB2	2:A:502:BTB:H62	1.87	0.57
1:A:292:VAL:O	1:A:292:VAL:HG13	2.04	0.57
1:B:122:PHE:CD1	1:B:191:TYR:CB	2.88	0.57
1:A:232:LEU:HD12	1:A:233:PHE:CD1	2.40	0.56
1:B:339:ASP:OD1	1:B:341:GLU:HG2	2.05	0.56
1:A:104:LEU:HD12	1:A:211:VAL:HG21	1.88	0.56
1:A:309:LEU:CD2	1:A:312:GLU:OE1	2.53	0.56
1:B:47:LEU:HD23	1:B:47:LEU:C	2.26	0.56
1:A:174:ARG:HD3	1:A:178:ARG:NH2	2.19	0.56
1:B:47:LEU:HD23	1:B:48:VAL:N	2.20	0.56
1:B:16:TRP:CD1	1:B:82:ILE:HA	2.40	0.56
1:B:65:LEU:CD1	1:B:103:LEU:CD1	2.83	0.56
1:B:199:SER:OG	1:B:201:THR:HG23	2.06	0.56
1:B:308:LYS:HG3	1:B:309:LEU:HD23	1.86	0.56
1:A:277:PRO:O	1:A:281:MET:HG2	2.05	0.56
1:B:434:GLU:OE1	1:B:438:ARG:HB2	2.05	0.56
1:A:79:LYS:HE3	1:A:81:ALA:HB3	1.86	0.56
1:B:306:PHE:HE1	1:B:307:GLN:CD	2.09	0.56
1:A:434:GLU:HB2	1:A:438:ARG:HB3	1.88	0.55
1:A:15:ASP:OD1	1:A:15:ASP:N	2.39	0.55
1:A:293:PRO:O	1:A:296:ARG:HG3	2.07	0.55
1:B:302:ILE:HG13	1:B:303:GLU:N	2.20	0.55
1:A:440:GLY:O	1:A:443:PRO:HD2	2.06	0.55
1:A:393:VAL:O	1:A:397:ARG:HG3	2.07	0.55
1:B:303:GLU:CG	1:B:306:PHE:CE2	2.90	0.55
1:B:30:LEU:HD21	1:B:52:VAL:HG23	1.89	0.55
1:A:347:PRO:HG2	1:A:350:GLU:CB	2.32	0.54
1:A:302:ILE:O	1:A:306:PHE:CD2	2.61	0.54
1:A:438:ARG:HG2	1:A:441:TRP:CD1	2.42	0.54
1:B:303:GLU:O	1:B:306:PHE:CD1	2.61	0.54
1:A:295:LEU:HG	1:A:297:GLU:HG3	1.89	0.54
1:A:435:THR:CG2	1:A:436:ARG:N	2.70	0.54
1:B:54:TYR:HD1	1:B:54:TYR:N	2.04	0.54
1:A:435:THR:HG22	1:A:436:ARG:N	2.23	0.54
1:A:441:TRP:CD1	1:A:441:TRP:N	2.76	0.54
1:B:159:PHE:HD2	1:B:208:LEU:C	2.11	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:291:VAL:CG2	1:B:291:VAL:O	2.56	0.54
1:B:373:TYR:HE1	1:B:389:ALA:CB	2.20	0.54
1:B:370:TYR:CZ	1:B:444:ILE:HD11	2.42	0.54
1:A:238:LEU:CD1	1:A:239:TYR:H	2.13	0.54
1:A:415:SER:C	1:A:417:LEU:HD12	2.28	0.54
1:B:333:GLU:HG2	1:B:334:SER:H	1.72	0.54
1:A:162:VAL:CG1	1:A:206:TYR:HD1	2.21	0.54
2:A:501:BTB:H42	2:A:501:BTB:C8	2.35	0.53
1:B:201:THR:O	1:B:202:ASP:HB2	2.08	0.53
1:B:30:LEU:HD21	1:B:33:VAL:HG22	1.89	0.53
1:A:150:PHE:HZ	1:B:100:PRO:HB2	1.74	0.53
1:B:282:LEU:N	1:B:282:LEU:HD13	2.23	0.53
1:B:5:ASP:OD1	1:B:5:ASP:N	2.41	0.53
1:B:296:ARG:O	1:B:300:PRO:HD2	2.09	0.53
1:B:278:VAL:O	1:B:282:LEU:HD22	2.08	0.53
1:B:282:LEU:CD1	1:B:282:LEU:N	2.71	0.53
1:B:320:HIS:HE1	1:B:322:ASP:O	1.92	0.53
1:B:373:TYR:CE1	1:B:389:ALA:CB	2.92	0.53
1:B:54:TYR:N	1:B:54:TYR:CD1	2.73	0.53
1:A:232:LEU:HD11	1:A:388:ARG:HB3	1.91	0.53
1:A:43:HIS:O	1:A:44:ASN:HB2	2.09	0.53
1:A:135:GLN:CG	1:A:136:PRO:HD3	2.39	0.52
1:A:349:ASP:N	1:A:349:ASP:OD1	2.38	0.52
1:B:128:VAL:O	1:B:130:LEU:CD1	2.56	0.52
1:B:317:GLN:O	1:B:354:PRO:HA	2.08	0.52
1:A:446:LEU:CA	1:A:449:ILE:HD12	2.24	0.52
1:A:377:VAL:O	1:A:379:GLN:OE1	2.27	0.52
1:A:280:ARG:O	1:A:283:ALA:HB3	2.10	0.52
1:A:427:ALA:HA	1:A:430:GLU:OE2	2.10	0.52
1:A:7:LEU:CD2	1:A:7:LEU:C	2.78	0.52
1:B:370:TYR:OH	1:B:430:GLU:HB3	2.11	0.51
1:B:295:LEU:HD23	1:B:295:LEU:C	2.30	0.51
1:A:295:LEU:HD11	1:A:297:GLU:OE2	2.10	0.51
1:A:451:ARG:NH1	1:A:451:ARG:CB	2.71	0.51
1:B:444:ILE:CG1	1:B:445:PRO:HD3	2.40	0.51
1:A:428:VAL:HG22	1:A:429:TYR:H	1.74	0.51
1:A:445:PRO:O	1:A:449:ILE:HG13	2.11	0.51
1:A:302:ILE:HG23	1:A:306:PHE:CE2	2.45	0.51
1:A:49:LEU:HB3	1:A:61:ARG:HD3	1.92	0.51
1:B:303:GLU:CB	1:B:306:PHE:CE2	2.94	0.51
1:B:425:ASP:O	1:B:428:VAL:HB	2.11	0.51
1:A:140:ASP:CB	1:B:21:ARG:HD2	2.41	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:276:PHE:CD2	1:B:278:VAL:CG1	2.94	0.50
1:A:174:ARG:HG2	1:A:178:ARG:HD2	1.94	0.50
1:B:137:ARG:HB2	1:B:149:ILE:HB	1.93	0.50
1:B:142:GLU:HG3	1:B:144:SER:H	1.75	0.50
1:B:122:PHE:HE1	1:B:191:TYR:CD1	2.29	0.50
1:B:296:ARG:NH2	1:B:299:ALA:HB2	2.26	0.50
1:B:130:LEU:HB3	1:B:131:PRO:HD2	1.93	0.50
1:B:299:ALA:C	1:B:302:ILE:HG12	2.33	0.50
1:A:442:LEU:N	1:A:442:LEU:CD1	2.75	0.49
1:A:297:GLU:O	1:A:300:PRO:HD2	2.12	0.49
1:A:418:LEU:H	1:A:418:LEU:HD12	1.76	0.49
1:A:93:ALA:HB1	1:A:99:GLY:HA3	1.93	0.49
1:B:48:VAL:HG12	1:B:50:VAL:HG23	1.92	0.49
1:B:377:VAL:HG22	1:B:378:ASP:H	1.76	0.49
1:B:436:ARG:C	1:B:436:ARG:HD2	2.32	0.49
1:B:51:ASP:OD2	1:B:61:ARG:HD2	2.13	0.49
1:B:370:TYR:CZ	1:B:444:ILE:CD1	2.96	0.49
1:A:135:GLN:CG	1:A:136:PRO:HD2	2.34	0.49
1:A:142:GLU:HG3	1:A:144:SER:HB3	1.95	0.49
1:A:238:LEU:HD12	1:A:239:TYR:CB	2.42	0.49
1:A:447:ARG:HG2	1:A:451:ARG:HH12	1.77	0.49
1:B:108:VAL:CG1	1:B:124:ARG:NH1	2.74	0.48
1:B:444:ILE:CG1	1:B:445:PRO:CD	2.89	0.48
1:B:84:VAL:HA	1:B:88:ARG:O	2.13	0.48
1:A:288:THR:CG2	1:A:289:VAL:N	2.76	0.48
1:B:129:GLU:CD	1:B:129:GLU:H	2.17	0.48
1:B:299:ALA:O	1:B:302:ILE:HG13	2.11	0.48
1:A:278:VAL:O	1:A:281:MET:HG3	2.13	0.48
1:B:250:GLU:OE1	1:B:330:ARG:NH1	2.43	0.48
1:A:428:VAL:CG2	1:A:429:TYR:H	2.26	0.48
1:A:142:GLU:HA	1:A:144:SER:N	2.28	0.48
1:A:174:ARG:CD	1:A:178:ARG:HH21	2.25	0.47
1:B:118:GLY:HA3	1:B:193:PHE:CZ	2.49	0.47
1:B:162:VAL:HG13	1:B:206:TYR:CD1	2.47	0.47
1:A:30:LEU:HD22	1:A:33:VAL:HG12	1.94	0.47
1:B:299:ALA:CA	1:B:302:ILE:HG12	2.41	0.47
1:B:52:VAL:CG2	1:B:54:TYR:CE1	2.91	0.47
1:B:252:TYR:CD1	1:B:403:GLY:CA	2.97	0.47
1:B:373:TYR:HE1	1:B:389:ALA:HB1	1.77	0.47
1:A:344:PRO:HA	1:A:351:ARG:HH21	1.79	0.47
1:B:384:GLN:O	1:B:384:GLN:OE1	2.32	0.47
1:A:162:VAL:HG12	1:A:206:TYR:HD1	1.80	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:346:GLN:HG3	1:A:347:PRO:CD	2.43	0.47
1:B:309:LEU:HD22	1:B:417:LEU:HG	1.95	0.47
1:A:242:GLU:HA	1:A:242:GLU:OE1	2.14	0.47
1:B:314:ILE:HG22	1:B:315:THR:O	2.14	0.47
1:B:444:ILE:HD12	1:B:445:PRO:HD3	1.97	0.47
1:A:276:PHE:CE2	1:A:309:LEU:HB2	2.50	0.47
1:A:319:VAL:HB	1:A:360:ASP:OD2	2.14	0.47
1:A:33:VAL:O	1:A:33:VAL:CG2	2.63	0.47
1:B:112:VAL:HG22	1:B:121:THR:HG23	1.96	0.47
1:B:441:TRP:C	1:B:443:PRO:HD2	2.36	0.47
1:A:281:MET:HG2	1:A:281:MET:H	1.35	0.47
1:B:306:PHE:C	1:B:306:PHE:CD1	2.88	0.47
1:B:442:LEU:N	1:B:443:PRO:CD	2.78	0.47
1:A:439:PRO:C	1:A:442:LEU:HD13	2.34	0.47
1:B:176:LEU:HD13	1:B:184:VAL:HG11	1.98	0.46
1:B:199:SER:HA	1:B:200:PRO:HD3	1.64	0.46
1:B:159:PHE:CE2	1:B:209:GLY:HA2	2.50	0.46
1:B:175:VAL:HG21	1:B:269:LEU:HD11	1.97	0.46
1:B:198:ARG:O	1:B:199:SER:HB3	2.15	0.46
1:B:230:ARG:HG2	1:B:230:ARG:HH21	1.79	0.46
1:B:350:GLU:OE1	1:B:350:GLU:N	2.48	0.46
1:A:174:ARG:CG	1:A:178:ARG:HD2	2.45	0.46
1:A:20:GLN:HG3	1:A:22:TRP:CZ2	2.51	0.46
1:A:237:ASP:HA	1:A:240:ALA:CB	2.45	0.46
1:A:415:SER:O	1:A:417:LEU:HD12	2.16	0.46
1:A:32:THR:CG2	1:A:53:THR:OG1	2.64	0.46
1:A:82:ILE:HG23	1:A:83:GLY:N	2.30	0.46
1:B:34:LYS:HA	1:B:35:PRO:HD3	1.79	0.46
1:B:159:PHE:CD2	1:B:209:GLY:HA2	2.51	0.46
1:B:434:GLU:CB	1:B:442:LEU:HD12	2.46	0.45
1:A:390:ARG:HH12	1:A:447:ARG:HD3	1.80	0.45
1:B:139:CYS:SG	1:B:149:ILE:HD11	2.57	0.45
1:A:113:CYS:O	1:A:113:CYS:SG	2.74	0.45
1:A:377:VAL:O	1:A:378:ASP:HB2	2.15	0.45
1:A:436:ARG:HG3	1:A:437:HIS:CE1	2.51	0.45
1:B:10:LYS:O	1:B:10:LYS:HG2	2.16	0.45
1:B:241:HIS:CE1	1:B:242:GLU:HG2	2.51	0.45
1:B:252:TYR:CD1	1:B:403:GLY:N	2.84	0.45
1:A:170:ILE:HD13	1:A:190:ALA:HB1	1.97	0.45
1:B:166:ILE:HD12	1:B:352:ARG:NH2	2.31	0.45
1:B:286:SER:HA	1:B:289:VAL:HG12	1.99	0.45
1:A:142:GLU:HA	1:A:144:SER:CA	2.44	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:276:PHE:CE1	1:A:281:MET:SD	3.10	0.45
1:B:276:PHE:CD2	1:B:276:PHE:C	2.90	0.45
1:B:374:GLY:N	1:B:375:PRO:CD	2.77	0.45
1:B:436:ARG:HG3	1:B:437:HIS:ND1	2.31	0.45
1:B:276:PHE:HA	1:B:277:PRO:HD3	1.61	0.45
1:A:365:LEU:CD1	1:A:397:ARG:HG2	2.37	0.45
1:B:269:LEU:N	1:B:269:LEU:CD1	2.80	0.45
1:A:137:ARG:HB3	1:A:149:ILE:HD12	1.99	0.44
1:A:358:LEU:HD23	1:A:419:LEU:HB2	1.99	0.44
1:A:252:TYR:CD1	1:A:252:TYR:C	2.91	0.44
1:A:434:GLU:HG3	1:A:442:LEU:HD12	2.00	0.44
1:A:446:LEU:HA	1:A:449:ILE:CD1	2.26	0.44
1:B:262:HIS:ND1	1:B:357:PRO:HB3	2.32	0.44
1:A:15:ASP:O	1:A:19:ARG:HG3	2.17	0.44
1:B:295:LEU:C	1:B:295:LEU:CD2	2.85	0.44
1:A:235:GLU:HG3	1:A:236:GLY:O	2.17	0.44
1:A:278:VAL:CA	1:A:281:MET:HG3	2.48	0.44
1:A:304:GLN:CA	1:A:307:GLN:HG2	2.45	0.44
1:B:292:VAL:O	1:B:292:VAL:HG12	2.17	0.44
1:B:306:PHE:CE1	1:B:307:GLN:CD	2.90	0.44
1:A:135:GLN:HE21	1:A:136:PRO:HD2	1.78	0.44
1:A:176:LEU:HG	1:A:184:VAL:HG11	1.99	0.44
1:B:276:PHE:HB2	1:B:314:ILE:HD11	2.00	0.44
1:B:317:GLN:O	1:B:354:PRO:CA	2.66	0.44
1:A:338:ILE:O	1:A:338:ILE:HG13	2.18	0.44
1:B:122:PHE:HD1	1:B:191:TYR:HB3	1.79	0.44
1:B:24:ALA:HA	1:B:25:GLY:HA2	1.73	0.44
1:B:320:HIS:CE1	1:B:322:ASP:O	2.71	0.44
1:B:300:PRO:O	1:B:303:GLU:HB2	2.18	0.44
1:B:331:THR:HB	1:B:332:PRO:CD	2.48	0.44
1:B:446:LEU:O	1:B:449:ILE:CG1	2.65	0.44
1:B:162:VAL:CG1	1:B:206:TYR:CD1	3.01	0.43
1:A:384:GLN:O	1:A:387:ALA:HB3	2.18	0.43
2:A:502:BTB:H72	2:A:502:BTB:O6	2.18	0.43
1:B:187:LEU:HD13	1:B:210:MET:HE3	2.00	0.43
1:A:30:LEU:HD22	1:A:33:VAL:CG1	2.48	0.43
1:B:224:MET:HE2	1:B:247:PHE:HE1	1.83	0.43
1:B:262:HIS:CE1	1:B:360:ASP:HB2	2.53	0.43
1:B:397:ARG:HH21	1:B:397:ARG:HD2	1.69	0.43
1:B:434:GLU:HB2	1:B:442:LEU:HD12	2.00	0.43
1:B:447:ARG:O	1:B:450:ALA:HB3	2.19	0.43
1:A:365:LEU:HD11	1:A:397:ARG:HA	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:333:GLU:HG2	1:B:334:SER:N	2.33	0.43
1:B:168:PRO:HD3	1:B:348:LEU:CD1	2.48	0.43
1:A:65:LEU:HD23	1:A:93:ALA:HB3	2.00	0.43
1:A:136:PRO:HG2	1:A:149:ILE:O	2.18	0.43
1:B:166:ILE:O	1:B:348:LEU:HD11	2.19	0.43
1:B:279:ASP:HA	1:B:282:LEU:HD22	2.00	0.42
1:B:306:PHE:C	1:B:306:PHE:HD1	2.21	0.42
1:B:365:LEU:O	1:B:368:PHE:HB2	2.19	0.42
1:A:276:PHE:CD2	1:A:309:LEU:CB	3.01	0.42
1:A:52:VAL:HG12	1:A:54:TYR:CE2	2.54	0.42
1:B:341:GLU:O	1:B:351:ARG:HD2	2.19	0.42
1:B:10:LYS:NZ	1:B:86:ASP:N	2.49	0.42
1:B:22:TRP:CG	1:B:160:ARG:HG3	2.55	0.42
1:A:373:TYR:HD1	1:A:376:LEU:HD12	1.85	0.42
1:B:255:GLY:HA2	1:B:400:PHE:CE1	2.54	0.42
1:B:285:LEU:HD11	1:B:302:ILE:HD11	2.01	0.42
1:A:17:LEU:C	1:A:17:LEU:CD2	2.87	0.42
1:B:306:PHE:HD1	1:B:307:GLN:CA	2.30	0.42
1:B:30:LEU:CD2	1:B:52:VAL:HG23	2.49	0.42
1:A:22:TRP:CG	1:A:160:ARG:HG3	2.54	0.42
2:A:502:BTB:H31	2:A:502:BTB:H52	1.95	0.42
1:A:277:PRO:O	1:A:281:MET:CG	2.68	0.42
1:A:299:ALA:N	1:A:300:PRO:HD2	2.35	0.42
1:A:278:VAL:C	1:A:281:MET:HG3	2.40	0.42
1:A:427:ALA:O	1:A:430:GLU:HB2	2.19	0.42
1:A:365:LEU:O	1:A:368:PHE:HB2	2.20	0.42
1:A:442:LEU:N	1:A:442:LEU:HD12	2.35	0.42
1:B:366:ARG:HH12	1:B:448:SER:CB	2.33	0.42
1:A:291:VAL:O	1:A:291:VAL:HG12	2.20	0.41
1:B:417:LEU:O	1:B:417:LEU:HD12	2.20	0.41
1:A:17:LEU:CD2	1:A:23:TYR:CD1	3.04	0.41
1:A:442:LEU:O	1:A:446:LEU:CD1	2.51	0.41
1:A:10:LYS:HZ3	1:A:85:ALA:C	2.23	0.41
1:A:285:LEU:O	1:A:289:VAL:CG1	2.65	0.41
1:A:435:THR:HG22	1:A:436:ARG:H	1.85	0.41
1:B:298:TYR:O	1:B:299:ALA:C	2.58	0.41
1:B:413:ARG:O	1:B:416:ALA:HB2	2.20	0.41
1:A:233:PHE:CZ	1:A:376:LEU:HD21	2.56	0.41
1:B:151:ASP:C	1:B:152:ARG:HG2	2.40	0.41
1:B:370:TYR:CD1	1:B:444:ILE:CD1	3.04	0.41
1:B:28:ARG:HB2	1:B:54:TYR:CD2	2.56	0.41
1:A:294:GLU:OE1	1:A:295:LEU:N	2.54	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:424:LEU:HB3	1:A:452:LEU:HD13	2.03	0.41
1:B:285:LEU:CD1	1:B:302:ILE:HD11	2.51	0.41
1:A:302:ILE:HG21	1:A:302:ILE:HD13	1.84	0.41
1:B:7:LEU:HA	1:B:7:LEU:HD12	1.93	0.41
1:A:374:GLY:N	1:A:375:PRO:CD	2.83	0.41
1:A:417:LEU:CD1	1:A:418:LEU:CD1	2.91	0.41
1:A:442:LEU:H	1:A:442:LEU:CD1	2.34	0.40
1:A:208:LEU:HD23	1:A:208:LEU:HA	1.83	0.40
1:A:294:GLU:OE1	1:A:294:GLU:C	2.59	0.40
1:A:418:LEU:H	1:A:418:LEU:CD1	2.34	0.40
1:B:52:VAL:CG1	1:B:60:GLU:HB2	2.52	0.40
1:B:251:SER:O	1:B:400:PHE:HA	2.21	0.40
1:B:331:THR:HB	1:B:332:PRO:HD2	2.03	0.40
1:A:346:GLN:HG3	1:A:350:GLU:HB3	2.03	0.40
1:B:373:TYR:CD1	1:B:373:TYR:N	2.89	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	427/455 (94%)	409 (96%)	18 (4%)	0	100	100
1	B	449/455 (99%)	433 (96%)	16 (4%)	0	100	100
All	All	876/910 (96%)	842 (96%)	34 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	342/362 (94%)	314 (92%)	28 (8%)	17	44
1	B	358/362 (99%)	332 (93%)	26 (7%)	20	51
All	All	700/724 (97%)	646 (92%)	54 (8%)	18	47

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	7	LEU
1	A	15	ASP
1	A	33	VAL
1	A	37	VAL
1	A	41	LEU
1	A	50	VAL
1	A	53	THR
1	A	56	ASP
1	A	129	GLU
1	A	140	ASP
1	A	144	SER
1	A	176	LEU
1	A	232	LEU
1	A	239	TYR
1	A	246	ASP
1	A	281	MET
1	A	301	THR
1	A	316	VAL
1	A	349	ASP
1	A	365	LEU
1	A	369	GLU
1	A	417	LEU
1	A	424	LEU
1	A	428	VAL
1	A	435	THR
1	A	436	ARG
1	A	448	SER
1	B	5	ASP
1	B	17	LEU
1	B	30	LEU
1	B	55	THR
1	B	61	ARG

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Mol	Chain	Res	Type
1	B	117	THR
1	B	121	THR
1	B	123	THR
1	B	127	ASP
1	B	128	VAL
1	B	129	GLU
1	B	135	GLN
1	B	217	ASN
1	B	232	LEU
1	B	242	GLU
1	B	269	LEU
1	B	282	LEU
1	B	284	ARG
1	B	286	SER
1	B	291	VAL
1	B	295	LEU
1	B	306	PHE
1	B	309	LEU
1	B	316	VAL
1	B	365	LEU
1	B	444	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	346	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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

4 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	BTB	A	501	-	13,13,13	0.57	0	16,16,16	2.50	6 (37%)
2	BTB	A	502	-	13,13,13	1.50	3 (23%)	16,16,16	2.19	5 (31%)
3	SO4	A	503	-	4,4,4	0.28	0	6,6,6	0.36	0
4	MAL	B	501	-	24,24,24	1.92	6 (25%)	35,35,35	1.35	6 (17%)

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	BTB	A	501	-	-	0/21/21/21	0/0/0/0
2	BTB	A	502	-	-	0/21/21/21	0/0/0/0
3	SO4	A	503	-	-	0/0/0/0	0/0/0/0
4	MAL	B	501	-	-	0/8/48/48	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	MAL	C3'-C2'	-4.14	1.41	1.52
4	B	501	MAL	O5'-C1'	3.99	1.51	1.43
4	B	501	MAL	C3-C2	-3.76	1.42	1.52
4	B	501	MAL	C4-C3	-3.08	1.44	1.52
2	A	502	BTB	C3-C2	-2.58	1.50	1.53
2	A	502	BTB	C1-C2	-2.46	1.50	1.53
2	A	502	BTB	C4-C2	-2.36	1.50	1.53
4	B	501	MAL	O5'-C5'	-2.23	1.38	1.44
4	B	501	MAL	O3'-C3'	-2.22	1.37	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	BTB	O3-C3-C2	5.02	123.45	111.08
2	A	501	BTB	O4-C4-C2	4.90	123.17	111.08
2	A	501	BTB	C7-N-C5	4.24	114.51	111.22
2	A	502	BTB	C7-N-C5	-4.05	108.08	111.22
2	A	501	BTB	O1-C1-C2	3.95	120.82	111.08
2	A	502	BTB	O4-C4-C2	3.81	120.46	111.08
2	A	502	BTB	O1-C1-C2	3.76	120.36	111.08
4	B	501	MAL	O3'-C3'-C4'	-2.82	103.25	109.86
4	B	501	MAL	O2-C2-C3	-2.79	104.13	110.36
2	A	502	BTB	C4-C2-C3	-2.59	105.62	110.39
2	A	502	BTB	C4-C2-C1	-2.58	105.64	110.39
4	B	501	MAL	O2-C2-C1	2.55	115.57	110.03
4	B	501	MAL	C1-O1-C4'	-2.43	111.83	118.00
4	B	501	MAL	C1-O5-C5	-2.18	109.51	113.73
2	A	501	BTB	C6-C5-N	2.12	120.31	111.55
2	A	501	BTB	O6-C6-C5	2.10	120.75	111.27
4	B	501	MAL	O1-C1-O5	-2.06	105.57	110.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	433/455 (95%)	0.79	65 (15%) 3 4	68, 113, 168, 196	0
1	B	451/455 (99%)	0.64	41 (9%) 9 12	60, 107, 177, 205	0
All	All	884/910 (97%)	0.71	106 (11%) 5 7	60, 110, 174, 205	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	197	ASN	10.4
1	A	241	HIS	10.4
1	A	240	ALA	9.6
1	B	380	ALA	7.7
1	A	13	TRP	7.6
1	B	196	PRO	6.1
1	B	235	GLU	6.0
1	B	435	THR	6.0
1	A	36	GLY	5.9
1	A	62	TYR	5.9
1	A	30	LEU	5.6
1	A	376	LEU	5.5
1	B	288	THR	5.2
1	A	203	ALA	5.0
1	A	26	ARG	4.9
1	B	418	LEU	4.9
1	B	358	LEU	4.8
1	B	295	LEU	4.8
1	A	50	VAL	4.7
1	A	243	VAL	4.6
1	A	48	VAL	4.4
1	B	132	PHE	4.2
1	A	54	TYR	4.2
1	A	37	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	51	ASP	4.1
1	A	52	VAL	4.1
1	A	35	PRO	4.1
1	B	289	VAL	4.1
1	A	8	ALA	4.1
1	A	17	LEU	3.9
1	A	204	LEU	3.6
1	B	319	VAL	3.6
1	A	83	GLY	3.6
1	A	49	LEU	3.5
1	A	14	SER	3.5
1	A	82	ILE	3.5
1	A	64	VAL	3.5
1	A	16	TRP	3.5
1	B	280	ARG	3.5
1	A	61	ARG	3.5
1	B	292	VAL	3.4
1	A	378	ASP	3.4
1	B	424	LEU	3.4
1	A	57	GLY	3.4
1	B	237	ASP	3.3
1	B	313	ALA	3.3
1	B	238	LEU	3.3
1	B	441	TRP	3.3
1	A	11	LEU	3.3
1	A	38	VAL	3.3
1	B	383	LYS	3.2
1	B	442	LEU	3.1
1	A	237	ASP	3.1
1	B	234	ALA	3.1
1	A	34	LYS	3.1
1	A	388	ARG	3.0
1	A	23	TYR	3.0
1	A	291	VAL	3.0
1	A	372	ALA	3.0
1	B	404	TYR	2.9
1	A	387	ALA	2.8
1	B	417	LEU	2.8
1	B	455	SER	2.7
1	A	193	PHE	2.7
1	A	202	ASP	2.7
1	A	384	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	25	GLY	2.7
1	B	294	GLU	2.6
1	A	53	THR	2.6
1	B	284	ARG	2.6
1	A	65	LEU	2.6
1	A	239	TYR	2.6
1	B	41	LEU	2.6
1	B	236	GLY	2.6
1	A	392	TRP	2.5
1	B	436	ARG	2.5
1	A	383	LYS	2.5
1	A	87	ASP	2.5
1	A	385	LEU	2.5
1	A	88	ARG	2.5
1	B	412	PRO	2.5
1	A	236	GLY	2.5
1	A	340	PHE	2.4
1	B	447	ARG	2.4
1	B	202	ASP	2.3
1	A	47	LEU	2.3
1	B	431	THR	2.3
1	A	377	VAL	2.2
1	B	444	ILE	2.2
1	A	139	CYS	2.2
1	A	66	VAL	2.2
1	B	309	LEU	2.2
1	B	438	ARG	2.1
1	A	112	VAL	2.1
1	B	377	VAL	2.1
1	A	242	GLU	2.1
1	A	441	TRP	2.1
1	A	298	TYR	2.1
1	B	232	LEU	2.1
1	A	389	ALA	2.0
1	B	19	ARG	2.0
1	A	233	PHE	2.0
1	A	67	GLY	2.0
1	A	232	LEU	2.0
1	A	207	ALA	2.0
1	B	452	LEU	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	BTB	A	501	14/14	0.32	1.25	94,111,131,137	0
2	BTB	A	502	14/14	0.22	0.35	128,134,141,143	0
4	MAL	B	501	23/23	0.19	-0.96	87,96,113,115	0
3	SO4	A	503	5/5	0.10	-2.00	96,98,113,123	0

6.5 Other polymers

There are no such residues in this entry.