



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:45 AM GMT

PDB ID : 3FWL
Title : Crystal Structure of the Full-Length Transglycosylase PBP1b from Escherichia coli
Authors : Sung, M.T.; Lai, Y.T.; Huang, C.Y.; Chou, L.Y.; Wong, C.H.; Ma, C.
Deposited on : 2009-01-19
Resolution : 3.09 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

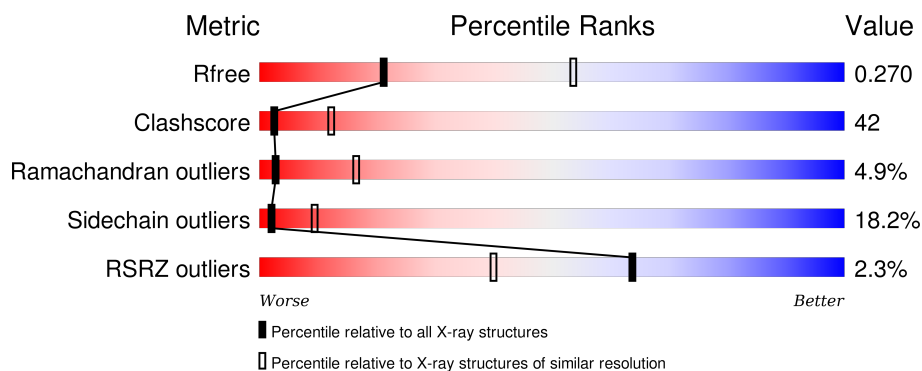
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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	1119 (3.12-3.04)
Clashscore	102246	1098 (3.10-3.06)
Ramachandran outliers	100387	1057 (3.10-3.06)
Sidechain outliers	100360	1057 (3.10-3.06)
RSRZ outliers	91569	1001 (3.10-3.06)

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	751	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 5641 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.

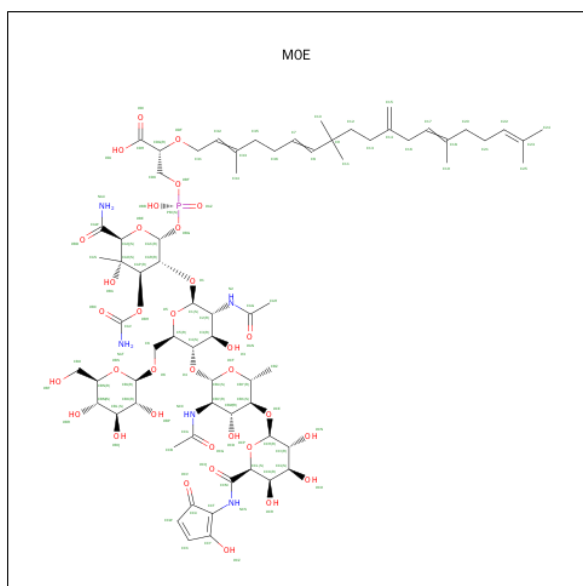
- Molecule 1 is a protein called Penicillin-binding protein 1B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	707	5564	3535	974	1029	2	24	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	GLY	-	EXPRESSION TAG	UNP P02919
A	55	SER	-	EXPRESSION TAG	UNP P02919
A	56	HIS	-	EXPRESSION TAG	UNP P02919
A	57	MSE	-	EXPRESSION TAG	UNP P02919

- Molecule 2 is MOENOMYCIN (three-letter code: M0E) (formula: $C_{69}H_{106}N_5O_{34}P$).

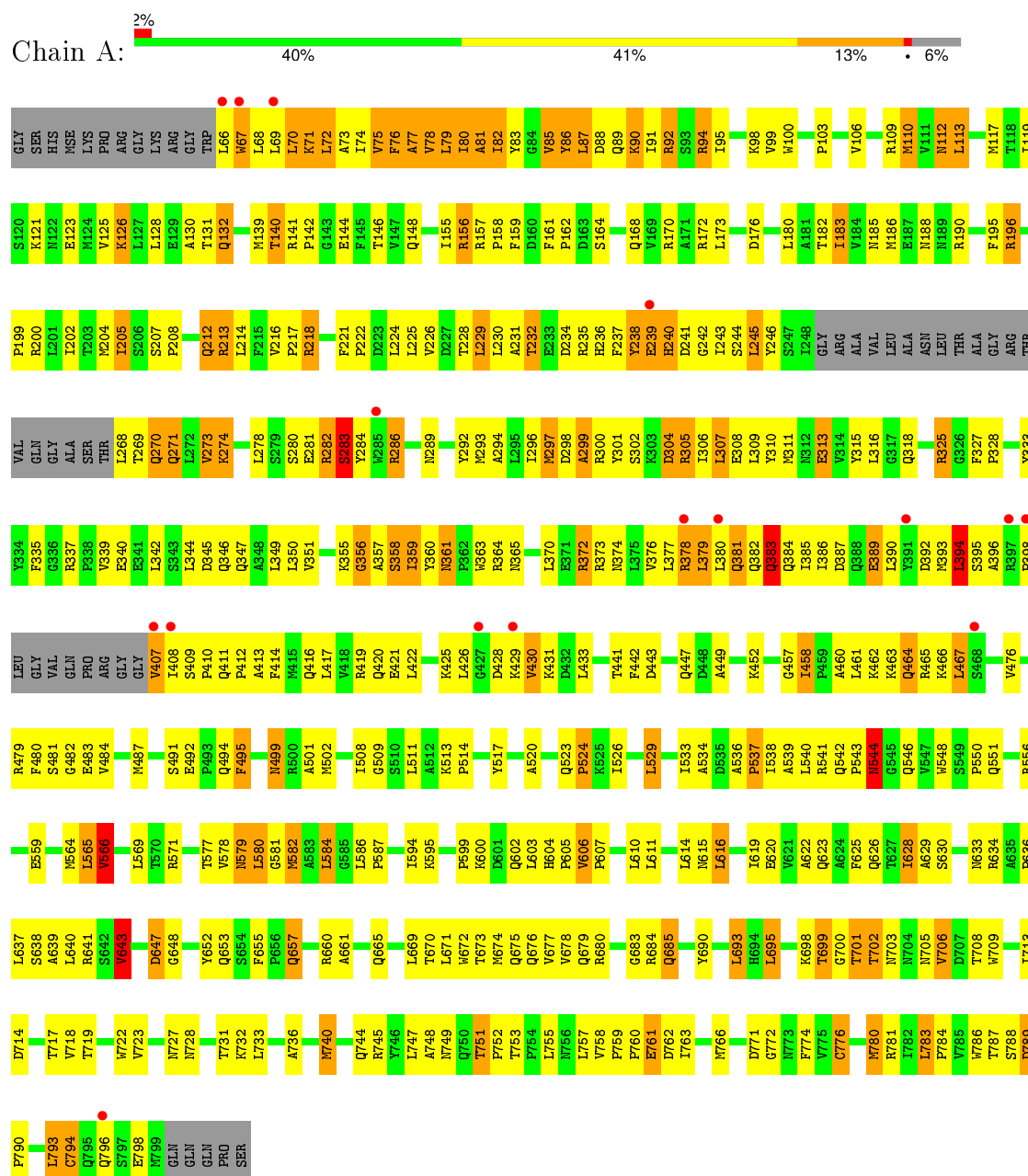


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	77	39	5	32	1	0	0

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: Penicillin-binding protein 1B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	63.24Å 297.00Å 62.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.26 – 3.09 29.26 – 3.09	Depositor EDS
% Data completeness (in resolution range)	95.5 (29.26-3.09) 95.6 (29.26-3.09)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 3.11Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.211 , 0.273 0.223 , 0.270	Depositor DCC
R_{free} test set	1112 reflections (5.41%)	DCC
Wilson B-factor (Å ²)	65.2	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 69.1	EDS
Estimated twinning fraction	0.046 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 21685 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5641	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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: M0E

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	0.31	0/5653	0.55	0/7632

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	5564	0	5610	472	0
2	A	77	0	59	8	0
All	All	5641	0	5669	472	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 42.

All (472) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:MSE:HE1	1:A:502:MSE:SE	2.13	0.99
1:A:700:GLY:HA3	1:A:709:TRP:HB2	1.45	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LYS:HZ3	1:A:91:ILE:H	1.13	0.94
1:A:77:ALA:HA	1:A:80:ILE:HD11	1.51	0.93
1:A:271:GLN:HE21	1:A:271:GLN:H	1.13	0.92
1:A:606:VAL:HG23	1:A:607:PRO:HD2	1.53	0.91
1:A:417:LEU:HA	1:A:502:MSE:HE1	1.49	0.90
1:A:282:ARG:H	1:A:282:ARG:HD3	1.37	0.89
1:A:430:VAL:HA	1:A:433:LEU:HD12	1.54	0.89
1:A:286:ARG:HH11	1:A:286:ARG:HG2	1.38	0.87
1:A:382:GLN:HA	1:A:383:GLN:HB3	1.56	0.87
1:A:146:THR:HG22	1:A:148:GLN:HE22	1.36	0.87
1:A:132:GLN:HE21	1:A:132:GLN:HA	1.40	0.86
1:A:90:LYS:NZ	1:A:91:ILE:H	1.72	0.85
1:A:304:ASP:O	1:A:307:LEU:HD22	1.76	0.85
1:A:776:CYS:HB3	1:A:793:LEU:HD21	1.57	0.85
1:A:110:MSE:HG3	1:A:199:PRO:HG3	1.59	0.84
1:A:92:ARG:HH11	1:A:92:ARG:HG3	1.43	0.84
1:A:283:SER:OG	1:A:284:TYR:HA	1.79	0.83
1:A:283:SER:CB	1:A:284:TYR:HA	2.08	0.83
1:A:188:ASN:OD1	1:A:190:ARG:HB2	1.79	0.82
1:A:224:LEU:HD12	1:A:224:LEU:H	1.47	0.79
1:A:556:ARG:NE	1:A:556:ARG:HA	1.96	0.79
1:A:441:THR:HG23	1:A:484:VAL:O	1.81	0.79
1:A:370:LEU:HD21	1:A:373:ARG:HH21	1.48	0.79
1:A:363:TRP:NE1	1:A:398:PRO:HD3	1.98	0.79
1:A:623:GLN:HE22	1:A:637:LEU:H	1.31	0.79
1:A:90:LYS:N	1:A:90:LYS:HZ3	1.81	0.78
1:A:586:LEU:HD13	1:A:605:PRO:O	1.83	0.78
1:A:78:VAL:HG23	1:A:79:LEU:HD23	1.65	0.78
1:A:344:LEU:HA	1:A:347:GLN:HB3	1.65	0.78
1:A:393:MSE:HA	1:A:393:MSE:HE2	1.66	0.77
1:A:236:HIS:CD2	1:A:237:PHE:H	2.03	0.77
1:A:281:GLU:HB3	1:A:282:ARG:HD3	1.66	0.76
1:A:92:ARG:HG3	1:A:92:ARG:NH1	1.97	0.76
1:A:282:ARG:CD	1:A:282:ARG:H	1.99	0.75
1:A:70:LEU:HD22	1:A:71:LYS:N	2.01	0.75
1:A:529:LEU:HG	1:A:566:VAL:HG13	1.69	0.75
1:A:274:LYS:HA	1:A:278:LEU:HD12	1.67	0.75
1:A:90:LYS:HZ3	1:A:91:ILE:N	1.85	0.74
1:A:85:VAL:O	1:A:89:GLN:HG2	1.88	0.74
1:A:569:LEU:HD23	1:A:673:THR:HG21	1.68	0.74
1:A:196:ARG:CG	1:A:196:ARG:HH11	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:ALA:O	1:A:523:GLN:HG2	1.88	0.74
1:A:75:VAL:O	1:A:79:LEU:HD21	1.88	0.73
1:A:442:PHE:CE1	1:A:447:GLN:HG3	2.23	0.73
1:A:196:ARG:HH11	1:A:196:ARG:HG2	1.52	0.72
1:A:271:GLN:H	1:A:271:GLN:NE2	1.88	0.72
1:A:87:LEU:HD11	1:A:292:TYR:HE2	1.53	0.72
1:A:447:GLN:HE21	1:A:487:MSE:H	1.38	0.72
1:A:441:THR:OG1	1:A:483:GLU:HB3	1.89	0.72
1:A:564:MSE:HE2	1:A:772:GLY:HA3	1.72	0.71
1:A:293:MSE:HA	1:A:296:ILE:HD12	1.71	0.71
1:A:82:ILE:O	1:A:85:VAL:HG12	1.91	0.70
1:A:225:LEU:HD13	1:A:347:GLN:HG3	1.72	0.70
1:A:318:GLN:NE2	2:A:901:M0E:HCL	2.06	0.70
1:A:780:MSE:HE3	1:A:781:ARG:HB2	1.72	0.70
1:A:628:ILE:HD11	1:A:671:LEU:HG	1.73	0.70
1:A:487:MSE:HE3	1:A:501:ALA:HB3	1.72	0.70
1:A:359:ILE:HG23	2:A:901:M0E:HCB1	1.74	0.70
1:A:110:MSE:CG	1:A:199:PRO:HG3	2.21	0.70
1:A:286:ARG:NH1	1:A:286:ARG:HG2	2.01	0.70
1:A:523:GLN:HB2	1:A:524:PRO:HA	1.72	0.70
1:A:690:TYR:HB3	1:A:693:LEU:HD22	1.73	0.70
1:A:229:LEU:HD12	1:A:311:MSE:HE3	1.73	0.70
1:A:229:LEU:O	1:A:232:THR:HG23	1.92	0.69
1:A:370:LEU:HD13	1:A:374:ASN:HD21	1.58	0.69
1:A:523:GLN:OE1	1:A:523:GLN:HA	1.93	0.68
1:A:126:LYS:HA	1:A:126:LYS:HE3	1.76	0.68
1:A:702:THR:HG21	1:A:706:VAL:HG22	1.76	0.68
1:A:109:ARG:HG2	1:A:442:PHE:O	1.93	0.68
1:A:442:PHE:CZ	1:A:447:GLN:HG3	2.29	0.68
1:A:72:LEU:HA	1:A:75:VAL:HG12	1.75	0.67
1:A:69:LEU:O	1:A:73:ALA:HB2	1.94	0.67
1:A:761:GLU:H	1:A:761:GLU:CD	1.98	0.67
1:A:271:GLN:HE21	1:A:271:GLN:N	1.91	0.66
1:A:180:LEU:HD21	1:A:183:ILE:HD11	1.78	0.66
1:A:487:MSE:HE2	1:A:499:ASN:OD1	1.95	0.66
1:A:556:ARG:NE	1:A:556:ARG:CA	2.57	0.66
1:A:776:CYS:HA	1:A:793:LEU:HG	1.76	0.66
1:A:774:PHE:HB2	1:A:796:GLN:HG3	1.78	0.66
1:A:447:GLN:NE2	1:A:487:MSE:H	1.93	0.66
1:A:581:GLY:HA3	1:A:610:LEU:HD21	1.78	0.66
1:A:373:ARG:O	1:A:377:LEU:HD13	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ARG:NE	1:A:300:ARG:HE	1.94	0.66
1:A:524:PRO:HG3	1:A:786:TRP:CD2	2.31	0.66
1:A:776:CYS:HA	1:A:793:LEU:CG	2.25	0.66
1:A:70:LEU:HD13	1:A:70:LEU:H	1.60	0.65
1:A:695:LEU:HD22	1:A:695:LEU:H	1.60	0.65
1:A:68:LEU:HA	1:A:71:LYS:HG3	1.77	0.65
1:A:373:ARG:O	1:A:373:ARG:HD2	1.97	0.65
1:A:603:LEU:HD22	1:A:603:LEU:H	1.61	0.65
1:A:713:ILE:HG12	1:A:718:VAL:HG22	1.79	0.64
1:A:88:ASP:HB3	1:A:300:ARG:HH22	1.61	0.64
1:A:655:PHE:O	1:A:657:GLN:HG3	1.96	0.64
1:A:533:ILE:HD11	1:A:565:LEU:HD22	1.78	0.64
1:A:83:TYR:O	1:A:87:LEU:HD12	1.98	0.64
1:A:67:TRP:CG	1:A:68:LEU:N	2.64	0.64
1:A:196:ARG:NH1	1:A:196:ARG:HG2	2.13	0.64
1:A:670:THR:O	1:A:674:MSE:HG3	1.97	0.64
1:A:218:ARG:HD3	1:A:307:LEU:HD21	1.80	0.63
1:A:92:ARG:HH11	1:A:92:ARG:CG	2.08	0.63
1:A:793:LEU:C	1:A:793:LEU:HD23	2.19	0.63
1:A:325:ARG:CG	1:A:325:ARG:HH11	2.11	0.63
1:A:776:CYS:HA	1:A:793:LEU:CD1	2.28	0.63
1:A:481:SER:OG	1:A:483:GLU:HG3	1.99	0.62
1:A:77:ALA:HA	1:A:80:ILE:CD1	2.27	0.62
1:A:110:MSE:HE1	1:A:162:PRO:HD3	1.81	0.62
1:A:580:LEU:HD22	1:A:584:LEU:HD22	1.82	0.62
1:A:389:GLU:CD	1:A:389:GLU:H	2.03	0.62
1:A:204:MSE:HB2	1:A:212:GLN:HE22	1.65	0.61
1:A:538:ILE:HB	1:A:550:PRO:HG2	1.81	0.61
1:A:117:MSE:HE2	1:A:119:ILE:CG2	2.30	0.61
1:A:499:ASN:HD22	1:A:499:ASN:C	2.03	0.61
1:A:556:ARG:CZ	1:A:556:ARG:HA	2.30	0.61
1:A:761:GLU:O	1:A:762:ASP:HB2	2.00	0.61
1:A:457:GLY:HA2	1:A:745:ARG:HE	1.64	0.61
1:A:208:PRO:HD3	1:A:431:LYS:HE2	1.81	0.61
1:A:90:LYS:NZ	1:A:90:LYS:H	1.98	0.61
1:A:67:TRP:HB2	1:A:70:LEU:HD11	1.82	0.61
1:A:236:HIS:CE1	1:A:269:THR:HG21	2.35	0.61
1:A:523:GLN:HG3	1:A:526:ILE:HB	1.82	0.61
1:A:457:GLY:HA2	1:A:745:ARG:NE	2.16	0.61
1:A:517:TYR:HD1	1:A:565:LEU:CD1	2.14	0.61
1:A:467:LEU:HD21	1:A:732:LYS:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:MSE:HB2	1:A:212:GLN:NE2	2.16	0.60
1:A:594:ILE:HG23	1:A:600:LYS:HD3	1.82	0.60
1:A:103:PRO:HB2	1:A:204:MSE:HE3	1.84	0.60
1:A:77:ALA:O	1:A:79:LEU:N	2.33	0.60
1:A:349:LEU:HD13	1:A:373:ARG:HB2	1.84	0.60
1:A:776:CYS:CB	1:A:793:LEU:HD21	2.31	0.60
1:A:286:ARG:HH12	2:A:901:M0E:HDK2	1.67	0.60
1:A:224:LEU:O	1:A:228:THR:HG22	2.01	0.59
1:A:226:VAL:HA	1:A:311:MSE:HE1	1.84	0.59
1:A:236:HIS:CG	1:A:237:PHE:H	2.17	0.59
1:A:103:PRO:HG3	1:A:207:SER:HB2	1.83	0.59
1:A:508:ILE:HG21	1:A:616:LEU:HD22	1.84	0.59
1:A:72:LEU:HD23	1:A:73:ALA:N	2.17	0.59
1:A:307:LEU:HD23	1:A:308:GLU:N	2.17	0.59
1:A:702:THR:CG2	1:A:703:ASN:N	2.66	0.59
1:A:278:LEU:HG	1:A:293:MSE:HE1	1.82	0.59
1:A:389:GLU:CD	1:A:389:GLU:N	2.56	0.59
1:A:685:GLN:HB3	1:A:740:MSE:HE2	1.84	0.59
1:A:582:MSE:CE	1:A:582:MSE:HA	2.33	0.59
1:A:72:LEU:O	1:A:76:PHE:N	2.35	0.59
1:A:243:ILE:HD12	1:A:244:SER:N	2.18	0.59
1:A:665:GLN:HG3	1:A:763:ILE:HD11	1.85	0.59
1:A:606:VAL:HG23	1:A:607:PRO:CD	2.32	0.58
1:A:325:ARG:HG2	1:A:325:ARG:HH11	1.67	0.58
1:A:714:ASP:HB2	1:A:753:THR:O	2.03	0.58
1:A:141:ARG:HB2	1:A:142:PRO:CD	2.33	0.58
1:A:170:ARG:HD3	1:A:186:MSE:HB2	1.86	0.58
1:A:482:GLY:O	1:A:637:LEU:HA	2.04	0.58
1:A:542:GLN:HB2	1:A:546:GLN:O	2.04	0.58
1:A:325:ARG:NH1	1:A:325:ARG:HG2	2.19	0.57
1:A:94:ARG:HH11	1:A:94:ARG:HG2	1.70	0.57
1:A:302:SER:O	1:A:306:ILE:HG12	2.04	0.57
1:A:411:GLN:N	1:A:412:PRO:HD3	2.18	0.57
1:A:786:TRP:C	1:A:786:TRP:CD1	2.78	0.57
1:A:381:GLN:HB2	1:A:382:GLN:OE1	2.05	0.57
1:A:327:PHE:CE1	1:A:350:LEU:HB3	2.39	0.57
1:A:370:LEU:CD1	1:A:374:ASN:HD21	2.18	0.57
1:A:216:VAL:HG13	1:A:328:PRO:HB3	1.87	0.56
1:A:776:CYS:HA	1:A:793:LEU:HD11	1.87	0.56
1:A:335:PHE:CE2	1:A:346:GLN:HB3	2.40	0.56
1:A:582:MSE:HA	1:A:582:MSE:HE2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:LEU:HD21	1:A:784:PRO:O	2.05	0.56
1:A:273:VAL:HB	1:A:293:MSE:HE3	1.86	0.56
1:A:541:ARG:HG2	1:A:541:ARG:O	2.05	0.56
1:A:92:ARG:HE	1:A:300:ARG:HE	1.54	0.56
1:A:92:ARG:HH21	1:A:300:ARG:HD2	1.71	0.55
1:A:72:LEU:HD11	1:A:76:PHE:CE2	2.40	0.55
1:A:359:ILE:HD12	2:A:901:M0E:HCB1	1.88	0.55
1:A:372:ARG:O	1:A:376:VAL:HG22	2.07	0.55
1:A:564:MSE:CE	1:A:772:GLY:HA3	2.35	0.55
1:A:356:GLY:O	1:A:359:ILE:HD13	2.06	0.55
1:A:736:ALA:O	1:A:740:MSE:HB2	2.06	0.55
1:A:386:ILE:O	1:A:386:ILE:HG22	2.07	0.55
1:A:376:VAL:HG23	1:A:377:LEU:H	1.72	0.55
1:A:318:GLN:CD	2:A:901:M0E:HCL	2.27	0.55
1:A:731:THR:O	1:A:732:LYS:HB2	2.07	0.55
1:A:87:LEU:HD11	1:A:292:TYR:CE2	2.39	0.54
1:A:316:LEU:HA	1:A:357:ALA:CB	2.37	0.54
1:A:673:THR:O	1:A:676:GLN:HB2	2.07	0.54
1:A:693:LEU:HB3	1:A:695:LEU:HD13	1.90	0.54
1:A:68:LEU:CD1	1:A:71:LYS:HD2	2.38	0.54
1:A:131:THR:O	1:A:132:GLN:HB2	2.08	0.54
1:A:327:PHE:HE1	1:A:350:LEU:HB3	1.71	0.54
1:A:110:MSE:HE2	1:A:161:PHE:CD1	2.43	0.54
1:A:619:ILE:O	1:A:622:ALA:HB3	2.07	0.54
1:A:578:VAL:HA	1:A:610:LEU:HD23	1.90	0.54
1:A:132:GLN:CA	1:A:132:GLN:HE21	2.17	0.54
1:A:363:TRP:CE2	1:A:398:PRO:HD3	2.42	0.54
1:A:780:MSE:CE	1:A:781:ARG:HB2	2.37	0.54
1:A:113:LEU:HD23	1:A:173:LEU:HD21	1.90	0.54
1:A:204:MSE:HE1	1:A:213:ARG:O	2.08	0.54
1:A:476:VAL:HG22	1:A:719:THR:HG23	1.89	0.54
1:A:271:GLN:NE2	1:A:271:GLN:N	2.53	0.54
1:A:236:HIS:CD2	1:A:239:GLU:N	2.77	0.53
1:A:86:TYR:CG	1:A:87:LEU:N	2.76	0.53
1:A:599:PRO:HB2	1:A:602:GLN:HG2	1.90	0.53
1:A:625:PHE:HA	1:A:628:ILE:HG23	1.90	0.53
1:A:543:PRO:C	1:A:544:ASN:HD22	2.12	0.53
1:A:643:VAL:CG1	1:A:652:TYR:HB3	2.38	0.53
1:A:196:ARG:CB	1:A:196:ARG:HH11	2.20	0.53
1:A:77:ALA:CA	1:A:80:ILE:HD11	2.33	0.53
1:A:333:TYR:CE1	1:A:363:TRP:HH2	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:GLU:HG2	1:A:425:LYS:HD2	1.90	0.53
1:A:196:ARG:HB3	1:A:196:ARG:HH11	1.74	0.53
1:A:302:SER:OG	1:A:305:ARG:HB3	2.08	0.52
1:A:529:LEU:O	1:A:566:VAL:HG22	2.09	0.52
1:A:340:GLU:O	1:A:340:GLU:HG2	2.09	0.52
1:A:499:ASN:ND2	1:A:499:ASN:C	2.62	0.52
1:A:81:ALA:O	1:A:83:TYR:N	2.42	0.52
1:A:68:LEU:HD13	1:A:71:LYS:HD2	1.90	0.52
1:A:499:ASN:ND2	1:A:501:ALA:H	2.07	0.52
1:A:140:THR:HG23	1:A:141:ARG:HG2	1.90	0.52
1:A:200:ARG:O	1:A:202:ILE:HD12	2.09	0.52
1:A:68:LEU:O	1:A:72:LEU:HB3	2.10	0.52
1:A:674:MSE:HE3	1:A:698:LYS:HB2	1.91	0.52
1:A:94:ARG:HH11	1:A:94:ARG:CG	2.23	0.52
1:A:305:ARG:HH21	1:A:309:LEU:HD21	1.75	0.52
1:A:347:GLN:O	1:A:351:VAL:HG23	2.10	0.52
1:A:508:ILE:HG23	1:A:614:LEU:O	2.10	0.52
1:A:72:LEU:HD21	1:A:76:PHE:HD2	1.75	0.52
1:A:78:VAL:CG2	1:A:79:LEU:HD23	2.36	0.52
1:A:328:PRO:HA	1:A:339:VAL:HB	1.92	0.52
1:A:683:GLY:HA2	1:A:740:MSE:HE1	1.92	0.51
1:A:582:MSE:HE3	1:A:610:LEU:HD22	1.92	0.51
1:A:693:LEU:HD21	1:A:752:PRO:HG2	1.93	0.51
1:A:87:LEU:C	1:A:90:LYS:HZ1	2.14	0.51
1:A:407:VAL:HB	1:A:410:PRO:HG3	1.93	0.51
1:A:110:MSE:HE3	1:A:159:PHE:HE2	1.76	0.51
1:A:594:ILE:HG12	1:A:600:LYS:HZ2	1.76	0.51
1:A:690:TYR:OH	1:A:748:ALA:HB2	2.11	0.51
1:A:393:MSE:HA	1:A:393:MSE:CE	2.40	0.51
1:A:517:TYR:HD1	1:A:565:LEU:HD13	1.76	0.51
1:A:289:ASN:O	1:A:293:MSE:HB2	2.11	0.50
1:A:460:ALA:HA	1:A:463:LYS:HE2	1.93	0.50
1:A:629:ALA:HB2	1:A:713:ILE:HD13	1.92	0.50
1:A:99:VAL:HG13	1:A:100:TRP:CE3	2.47	0.50
1:A:600:LYS:NZ	1:A:603:LEU:HD23	2.27	0.50
1:A:172:ARG:NH1	1:A:186:MSE:HE3	2.27	0.50
1:A:623:GLN:NE2	1:A:637:LEU:H	2.05	0.50
1:A:87:LEU:HA	1:A:90:LYS:HZ2	1.77	0.50
1:A:67:TRP:CE3	1:A:70:LEU:HD21	2.47	0.50
1:A:358:SER:HB2	2:A:901:M0E:OCG	2.11	0.50
1:A:594:ILE:HD11	1:A:600:LYS:HZ3	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:ASP:OD1	1:A:428:ASP:N	2.44	0.50
1:A:675:GLN:O	1:A:678:VAL:HG12	2.12	0.49
1:A:304:ASP:O	1:A:306:ILE:N	2.46	0.49
1:A:146:THR:CG2	1:A:148:GLN:HE22	2.14	0.49
1:A:88:ASP:HB3	1:A:300:ARG:NH2	2.26	0.49
1:A:113:LEU:HB3	1:A:183:ILE:CD1	2.43	0.49
1:A:243:ILE:HD12	1:A:244:SER:H	1.76	0.49
1:A:407:VAL:CG1	1:A:410:PRO:HG3	2.42	0.49
1:A:72:LEU:O	1:A:76:PHE:HB2	2.13	0.49
1:A:693:LEU:HB3	1:A:695:LEU:CD1	2.42	0.49
1:A:283:SER:HB3	1:A:284:TYR:CD1	2.48	0.49
1:A:705:ASN:O	1:A:731:THR:HG23	2.13	0.49
1:A:68:LEU:C	1:A:70:LEU:H	2.16	0.49
1:A:360:TYR:CZ	1:A:372:ARG:HG3	2.47	0.49
1:A:376:VAL:O	1:A:379:LEU:HB2	2.12	0.49
1:A:464:GLN:HE21	1:A:465:ARG:HH12	1.59	0.49
1:A:542:GLN:HE21	1:A:548:TRP:N	2.10	0.49
1:A:185:ASN:HB3	1:A:188:ASN:OD1	2.12	0.49
1:A:213:ARG:HH11	1:A:313:GLU:HA	1.77	0.49
1:A:270:GLN:C	1:A:270:GLN:HE21	2.15	0.49
1:A:494:GLN:O	1:A:495:PHE:HB2	2.13	0.49
1:A:709:TRP:CZ3	1:A:722:TRP:HB2	2.48	0.49
1:A:487:MSE:HE1	1:A:502:MSE:HB2	1.95	0.48
1:A:441:THR:CG2	1:A:639:ALA:HA	2.43	0.48
1:A:196:ARG:CG	1:A:196:ARG:NH1	2.68	0.48
1:A:202:ILE:HD12	1:A:202:ILE:N	2.28	0.48
1:A:83:TYR:CZ	1:A:87:LEU:HG	2.48	0.48
1:A:793:LEU:HD22	1:A:794:CYS:SG	2.53	0.48
1:A:283:SER:CB	1:A:284:TYR:CA	2.88	0.48
1:A:117:MSE:HE2	1:A:119:ILE:HG21	1.95	0.48
1:A:88:ASP:CB	1:A:300:ARG:HH22	2.26	0.48
1:A:224:LEU:HB2	1:A:347:GLN:OE1	2.12	0.48
1:A:315:TYR:CE2	1:A:357:ALA:HB3	2.49	0.48
1:A:327:PHE:N	1:A:328:PRO:HD2	2.29	0.48
1:A:325:ARG:CG	1:A:325:ARG:NH1	2.74	0.48
1:A:307:LEU:HD23	1:A:307:LEU:C	2.34	0.48
1:A:595:LYS:O	1:A:634:ARG:HD3	2.14	0.48
1:A:370:LEU:HD13	1:A:374:ASN:ND2	2.27	0.47
1:A:479:ARG:H	1:A:717:THR:HA	1.79	0.47
1:A:315:TYR:HE1	1:A:318:GLN:NE2	2.12	0.47
1:A:327:PHE:N	1:A:328:PRO:CD	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:VAL:HA	1:A:342:LEU:CD2	2.45	0.47
1:A:517:TYR:CD1	1:A:565:LEU:HD13	2.49	0.47
1:A:117:MSE:HE2	1:A:119:ILE:HG22	1.96	0.47
1:A:487:MSE:CE	1:A:502:MSE:HB2	2.44	0.47
1:A:70:LEU:N	1:A:70:LEU:HD13	2.30	0.47
1:A:110:MSE:HE3	1:A:159:PHE:CE2	2.49	0.47
1:A:236:HIS:HD2	1:A:239:GLU:N	2.13	0.47
1:A:239:GLU:HB2	1:A:240:HIS:H	1.45	0.47
1:A:449:ALA:HA	1:A:749:ASN:HB3	1.96	0.47
1:A:86:TYR:C	1:A:88:ASP:H	2.18	0.47
1:A:74:ILE:HG13	1:A:75:VAL:N	2.28	0.47
1:A:702:THR:HG23	1:A:703:ASN:N	2.30	0.47
1:A:236:HIS:CD2	1:A:238:TYR:N	2.83	0.47
1:A:119:ILE:HG13	1:A:123:GLU:HB3	1.97	0.47
1:A:793:LEU:C	1:A:793:LEU:CD2	2.84	0.47
1:A:517:TYR:HD1	1:A:565:LEU:HD11	1.79	0.47
1:A:294:ALA:O	1:A:297:MSE:HB3	2.14	0.47
1:A:513:LYS:O	1:A:517:TYR:HD2	1.99	0.46
1:A:342:LEU:HB3	1:A:347:GLN:HB2	1.98	0.46
1:A:204:MSE:HE3	1:A:204:MSE:HB3	1.80	0.46
1:A:747:LEU:HA	1:A:747:LEU:HD12	1.68	0.46
1:A:364:ARG:HG2	1:A:365:ASN:ND2	2.30	0.46
1:A:82:ILE:HG22	1:A:83:TYR:N	2.30	0.46
1:A:112:ASN:HD21	1:A:196:ARG:NH1	2.13	0.46
1:A:509:GLY:HA3	1:A:701:THR:O	2.15	0.46
1:A:87:LEU:C	1:A:90:LYS:NZ	2.68	0.46
1:A:381:GLN:CD	1:A:381:GLN:H	2.18	0.46
1:A:441:THR:HG21	1:A:639:ALA:HA	1.97	0.46
1:A:236:HIS:HD2	1:A:238:TYR:H	1.64	0.46
1:A:581:GLY:CA	1:A:610:LEU:HD21	2.45	0.46
1:A:755:LEU:HD11	1:A:757:LEU:CD1	2.45	0.46
1:A:511:LEU:HD22	1:A:709:TRP:CB	2.45	0.46
1:A:286:ARG:HH11	1:A:286:ARG:CG	2.17	0.46
1:A:382:GLN:CA	1:A:383:GLN:HB3	2.38	0.46
1:A:80:ILE:H	1:A:80:ILE:HG13	1.40	0.46
1:A:315:TYR:CE1	1:A:318:GLN:NE2	2.84	0.46
1:A:130:ALA:O	1:A:200:ARG:HD3	2.15	0.46
1:A:452:LYS:HD3	1:A:749:ASN:CG	2.35	0.46
1:A:176:ASP:OD1	1:A:176:ASP:C	2.54	0.46
1:A:67:TRP:O	1:A:68:LEU:HB3	2.16	0.46
1:A:242:GLY:O	1:A:245:LEU:HD13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ARG:HG3	1:A:195:PHE:CZ	2.50	0.46
1:A:271:GLN:NE2	1:A:310:TYR:HE1	2.14	0.46
1:A:361:ASN:OD1	1:A:363:TRP:HE3	1.99	0.46
1:A:582:MSE:HE3	1:A:610:LEU:CD2	2.46	0.46
1:A:731:THR:OG1	1:A:733:LEU:HB2	2.16	0.46
1:A:755:LEU:HD11	1:A:757:LEU:HD13	1.98	0.46
1:A:520:ALA:HB2	1:A:584:LEU:HD21	1.98	0.45
1:A:443:ASP:OD2	1:A:443:ASP:C	2.53	0.45
1:A:90:LYS:N	1:A:90:LYS:NZ	2.53	0.45
1:A:75:VAL:O	1:A:75:VAL:HG13	2.16	0.45
1:A:349:LEU:HB2	1:A:373:ARG:CG	2.46	0.45
1:A:541:ARG:O	1:A:541:ARG:CG	2.64	0.45
1:A:385:ILE:HG13	1:A:385:ILE:O	2.16	0.45
1:A:221:PHE:HA	1:A:222:PRO:HD2	1.81	0.45
1:A:335:PHE:O	1:A:337:ARG:HG3	2.16	0.45
1:A:349:LEU:HB2	1:A:373:ARG:HG2	1.99	0.45
1:A:106:VAL:HG21	1:A:205:ILE:HD12	1.98	0.45
1:A:214:LEU:O	1:A:328:PRO:HB2	2.17	0.45
1:A:121:LYS:O	1:A:125:VAL:HG23	2.17	0.45
1:A:70:LEU:HD22	1:A:71:LYS:H	1.75	0.45
1:A:72:LEU:HA	1:A:75:VAL:CG1	2.44	0.45
1:A:236:HIS:HD2	1:A:239:GLU:H	1.65	0.45
1:A:464:GLN:NE2	1:A:465:ARG:HH12	2.15	0.45
1:A:619:ILE:HG23	1:A:620:GLU:N	2.31	0.44
1:A:464:GLN:HE21	1:A:465:ARG:NH1	2.15	0.44
1:A:230:LEU:C	1:A:232:THR:H	2.21	0.44
1:A:413:ALA:O	1:A:416:GLN:HB3	2.17	0.44
1:A:383:GLN:HG3	1:A:384:GLN:HB2	1.99	0.44
1:A:776:CYS:CA	1:A:793:LEU:HG	2.45	0.44
1:A:569:LEU:HD23	1:A:673:THR:CG2	2.43	0.44
1:A:422:LEU:HD22	1:A:640:LEU:HD21	1.99	0.44
1:A:679:GLN:HG3	1:A:680:ARG:N	2.33	0.44
1:A:78:VAL:HG23	1:A:79:LEU:N	2.32	0.44
1:A:282:ARG:N	1:A:282:ARG:HD3	2.18	0.44
1:A:238:TYR:HA	1:A:298:ASP:OD2	2.18	0.44
1:A:702:THR:HG23	1:A:703:ASN:H	1.82	0.44
1:A:511:LEU:HD22	1:A:709:TRP:HB3	2.00	0.44
1:A:158:PRO:HG3	1:A:168:GLN:HB3	2.00	0.44
1:A:536:ALA:HB1	1:A:537:PRO:HD2	1.98	0.44
1:A:394:LEU:O	1:A:395:SER:HB3	2.16	0.44
1:A:685:GLN:HB3	1:A:740:MSE:CE	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:MSE:HE3	1:A:501:ALA:CB	2.47	0.44
1:A:131:THR:O	1:A:132:GLN:CB	2.65	0.44
1:A:90:LYS:NZ	1:A:91:ILE:N	2.51	0.43
1:A:236:HIS:HD2	1:A:238:TYR:N	2.16	0.43
1:A:603:LEU:HD22	1:A:603:LEU:N	2.28	0.43
1:A:683:GLY:HA2	1:A:740:MSE:CE	2.48	0.43
1:A:87:LEU:HA	1:A:90:LYS:NZ	2.32	0.43
1:A:407:VAL:HG11	1:A:410:PRO:HG3	2.00	0.43
1:A:458:ILE:HD13	1:A:491:SER:HB2	1.99	0.43
1:A:359:ILE:CD1	2:A:901:M0E:HCB1	2.47	0.43
1:A:333:TYR:CE1	1:A:363:TRP:CH2	3.06	0.43
1:A:88:ASP:O	1:A:300:ARG:NH2	2.52	0.43
1:A:131:THR:HG22	1:A:131:THR:O	2.18	0.43
1:A:600:LYS:HB3	1:A:600:LYS:HE3	1.76	0.43
1:A:239:GLU:C	1:A:240:HIS:CG	2.92	0.43
1:A:414:PHE:CE2	1:A:442:PHE:HB2	2.54	0.43
1:A:282:ARG:N	1:A:282:ARG:CD	2.76	0.42
1:A:240:HIS:HB2	1:A:241:ASP:H	1.73	0.42
1:A:534:ALA:HB3	1:A:579:ASN:OD1	2.19	0.42
1:A:79:LEU:H	1:A:79:LEU:HD23	1.85	0.42
1:A:222:PRO:HG2	1:A:225:LEU:CB	2.50	0.42
1:A:225:LEU:N	1:A:347:GLN:OE1	2.52	0.42
1:A:616:LEU:HD13	1:A:616:LEU:N	2.35	0.42
1:A:205:ILE:HG22	1:A:205:ILE:O	2.19	0.42
1:A:766:MSE:HE3	1:A:790:PRO:HB3	2.01	0.42
1:A:88:ASP:OD1	1:A:296:ILE:HD13	2.18	0.42
1:A:361:ASN:OD1	1:A:363:TRP:CE3	2.73	0.42
1:A:653:GLN:HG2	1:A:655:PHE:CZ	2.55	0.42
1:A:595:LYS:HB3	1:A:661:ALA:HB1	2.01	0.42
1:A:758:VAL:HA	1:A:759:PRO:HD3	1.74	0.42
1:A:586:LEU:N	1:A:587:PRO:CD	2.82	0.42
1:A:140:THR:HG22	1:A:144:GLU:OE1	2.20	0.42
1:A:235:ARG:HE	1:A:235:ARG:C	2.22	0.42
1:A:727:ASN:C	1:A:728:ASN:HD22	2.22	0.42
1:A:462:LYS:O	1:A:466:LYS:N	2.52	0.42
1:A:72:LEU:HD21	1:A:76:PHE:CD2	2.53	0.42
1:A:113:LEU:HB3	1:A:183:ILE:HD11	2.02	0.42
1:A:599:PRO:HB2	1:A:602:GLN:CG	2.48	0.42
1:A:759:PRO:HA	1:A:760:PRO:HD3	1.97	0.42
1:A:431:LYS:HD2	1:A:431:LYS:HA	1.86	0.42
1:A:672:TRP:CH2	1:A:783:LEU:HD12	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:TRP:CD1	1:A:398:PRO:HD3	2.53	0.42
1:A:70:LEU:HA	1:A:73:ALA:HB3	2.02	0.41
1:A:77:ALA:O	1:A:78:VAL:HG22	2.20	0.41
1:A:225:LEU:HG	1:A:311:MSE:HE2	2.00	0.41
1:A:286:ARG:NH1	2:A:901:M0E:HDK2	2.34	0.41
1:A:619:ILE:HD12	1:A:637:LEU:HD23	2.02	0.41
1:A:539:ALA:HA	1:A:548:TRP:O	2.18	0.41
1:A:633:ASN:HD22	1:A:660:ARG:HA	1.85	0.41
1:A:698:LYS:NZ	1:A:699:THR:HG22	2.35	0.41
1:A:94:ARG:NH1	1:A:94:ARG:CG	2.82	0.41
1:A:68:LEU:C	1:A:70:LEU:N	2.73	0.41
1:A:619:ILE:CD1	1:A:637:LEU:HD23	2.50	0.41
1:A:580:LEU:CD2	1:A:584:LEU:HD22	2.50	0.41
1:A:533:ILE:CD1	1:A:565:LEU:HD22	2.48	0.41
1:A:407:VAL:CB	1:A:410:PRO:HG3	2.50	0.41
1:A:626:GLN:NE2	1:A:630:SER:HB3	2.35	0.41
1:A:218:ARG:HD3	1:A:307:LEU:CD2	2.47	0.41
1:A:345:ASP:HB2	1:A:393:MSE:SE	2.70	0.41
1:A:674:MSE:O	1:A:677:VAL:HB	2.19	0.41
1:A:479:ARG:HD3	1:A:480:PHE:CE2	2.55	0.41
1:A:229:LEU:HD11	1:A:310:TYR:CE2	2.56	0.41
1:A:556:ARG:N	1:A:556:ARG:NE	2.68	0.41
1:A:586:LEU:HB2	1:A:587:PRO:HD3	2.03	0.41
1:A:604:HIS:HA	1:A:605:PRO:HD3	1.84	0.41
1:A:513:LYS:N	1:A:514:PRO:CD	2.84	0.41
1:A:383:GLN:HG3	1:A:384:GLN:N	2.35	0.41
1:A:94:ARG:HD2	1:A:95:ILE:HD12	2.03	0.41
1:A:76:PHE:C	1:A:77:ALA:O	2.59	0.41
1:A:280:SER:HA	1:A:281:GLU:HA	1.71	0.41
1:A:674:MSE:HA	1:A:677:VAL:HG23	2.02	0.41
1:A:85:VAL:O	1:A:88:ASP:HB2	2.21	0.41
1:A:85:VAL:HG22	1:A:89:GLN:HE21	1.85	0.41
1:A:77:ALA:HA	1:A:80:ILE:CG1	2.49	0.41
1:A:218:ARG:NH2	1:A:226:VAL:HG21	2.36	0.41
1:A:307:LEU:HA	1:A:310:TYR:HB3	2.03	0.41
1:A:132:GLN:HB2	1:A:157:ARG:NH2	2.36	0.41
1:A:615:ASN:C	1:A:616:LEU:HD13	2.41	0.41
1:A:299:ALA:C	1:A:301:TYR:H	2.23	0.41
1:A:139:MSE:SE	1:A:155:ILE:HG13	2.71	0.41
1:A:708:THR:OG1	1:A:723:VAL:HB	2.21	0.41
1:A:87:LEU:O	1:A:87:LEU:HD22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ASP:O	1:A:393:MSE:HG2	2.21	0.41
1:A:241:ASP:O	1:A:242:GLY:C	2.60	0.41
1:A:524:PRO:HD3	1:A:786:TRP:CZ3	2.56	0.41
1:A:83:TYR:CD2	1:A:83:TYR:C	2.94	0.40
1:A:417:LEU:O	1:A:420:GLN:HB3	2.21	0.40
1:A:67:TRP:C	1:A:69:LEU:H	2.24	0.40
1:A:218:ARG:HD2	1:A:218:ARG:HA	1.86	0.40
1:A:345:ASP:OD2	1:A:346:GLN:HG3	2.22	0.40
1:A:408:ILE:HG23	1:A:409:SER:H	1.87	0.40
1:A:623:GLN:HE22	1:A:636:PRO:HA	1.86	0.40
1:A:66:LEU:HA	1:A:66:LEU:HD12	1.92	0.40
1:A:292:TYR:O	1:A:296:ILE:HG13	2.21	0.40
1:A:304:ASP:O	1:A:305:ARG:C	2.60	0.40
1:A:751:THR:HA	1:A:752:PRO:HD3	1.81	0.40
1:A:685:GLN:CB	1:A:740:MSE:HE2	2.51	0.40
1:A:315:TYR:CD2	1:A:357:ALA:HB3	2.57	0.40
1:A:513:LYS:HD3	1:A:577:THR:OG1	2.22	0.40
1:A:313:GLU:O	1:A:325:ARG:HG2	2.21	0.40
1:A:386:ILE:O	1:A:386:ILE:CG2	2.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	701/751 (93%)	563 (80%)	104 (15%)	34 (5%)	3 16

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	305	ARG
1	A	430	VAL

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Mol	Chain	Res	Type
1	A	495	PHE
1	A	566	VAL
1	A	647	ASP
1	A	77	ALA
1	A	81	ALA
1	A	238	TYR
1	A	299	ALA
1	A	378	ARG
1	A	383	GLN
1	A	394	LEU
1	A	429	LYS
1	A	643	VAL
1	A	140	THR
1	A	164	SER
1	A	231	ALA
1	A	467	LEU
1	A	544	ASN
1	A	648	GLY
1	A	78	VAL
1	A	240	HIS
1	A	283	SER
1	A	297	MSE
1	A	396	ALA
1	A	234	ASP
1	A	274	LYS
1	A	356	GLY
1	A	82	ILE
1	A	361	ASN
1	A	380	LEU
1	A	789	ASP
1	A	217	PRO
1	A	537	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	599/605 (99%)	490 (82%)	109 (18%)	2 9

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	TRP
1	A	70	LEU
1	A	71	LYS
1	A	72	LEU
1	A	75	VAL
1	A	76	PHE
1	A	79	LEU
1	A	80	ILE
1	A	85	VAL
1	A	86	TYR
1	A	87	LEU
1	A	90	LYS
1	A	92	ARG
1	A	94	ARG
1	A	98	LYS
1	A	110	MSE
1	A	112	ASN
1	A	113	LEU
1	A	126	LYS
1	A	128	LEU
1	A	132	GLN
1	A	156	ARG
1	A	182	THR
1	A	183	ILE
1	A	196	ARG
1	A	205	ILE
1	A	212	GLN
1	A	213	ARG
1	A	218	ARG
1	A	229	LEU
1	A	232	THR
1	A	239	GLU
1	A	245	LEU
1	A	246	TYR
1	A	268	LEU
1	A	270	GLN
1	A	271	GLN
1	A	273	VAL

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Mol	Chain	Res	Type
1	A	282	ARG
1	A	283	SER
1	A	286	ARG
1	A	304	ASP
1	A	307	LEU
1	A	313	GLU
1	A	325	ARG
1	A	355	LYS
1	A	358	SER
1	A	359	ILE
1	A	372	ARG
1	A	378	ARG
1	A	379	LEU
1	A	381	GLN
1	A	383	GLN
1	A	387	ASP
1	A	389	GLU
1	A	390	LEU
1	A	394	LEU
1	A	407	VAL
1	A	419	ARG
1	A	426	LEU
1	A	458	ILE
1	A	461	LEU
1	A	464	GLN
1	A	492	GLU
1	A	499	ASN
1	A	524	PRO
1	A	529	LEU
1	A	540	LEU
1	A	544	ASN
1	A	551	GLN
1	A	559	GLU
1	A	565	LEU
1	A	566	VAL
1	A	571	ARG
1	A	579	ASN
1	A	580	LEU
1	A	582	MSE
1	A	584	LEU
1	A	606	VAL
1	A	611	LEU

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Mol	Chain	Res	Type
1	A	616	LEU
1	A	628	ILE
1	A	638	SER
1	A	641	ARG
1	A	643	VAL
1	A	647	ASP
1	A	657	GLN
1	A	684	ARG
1	A	685	GLN
1	A	693	LEU
1	A	695	LEU
1	A	699	THR
1	A	701	THR
1	A	702	THR
1	A	706	VAL
1	A	740	MSE
1	A	744	GLN
1	A	751	THR
1	A	761	GLU
1	A	771	ASP
1	A	776	CYS
1	A	780	MSE
1	A	783	LEU
1	A	787	THR
1	A	788	SER
1	A	789	ASP
1	A	793	LEU
1	A	794	CYS
1	A	798	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	112	ASN
1	A	132	GLN
1	A	148	GLN
1	A	179	HIS
1	A	191	GLN
1	A	209	ASN
1	A	270	GLN
1	A	271	GLN

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Mol	Chain	Res	Type
1	A	365	ASN
1	A	374	ASN
1	A	383	GLN
1	A	423	GLN
1	A	447	GLN
1	A	464	GLN
1	A	494	GLN
1	A	499	ASN
1	A	542	GLN
1	A	544	ASN
1	A	615	ASN
1	A	623	GLN
1	A	633	ASN
1	A	685	GLN
1	A	728	ASN
1	A	744	GLN
1	A	796	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	M0E	A	901	-	75,81,114	0.82	2 (2%)	94,122,166	1.15	8 (8%)

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	M0E	A	901	-	-	2/47/158/206	0/5/5/6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	M0E	CCM-NCS	-3.05	1.26	1.32
2	A	901	M0E	OCQ-CCM	5.16	1.33	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	M0E	CBU-CBV-NCC	-3.50	104.43	111.01
2	A	901	M0E	C3-C2-N2	-3.16	104.12	110.66
2	A	901	M0E	C1-O1-CAR	-3.07	109.98	118.01
2	A	901	M0E	CCH-OCE-CBX	-2.95	110.30	118.01
2	A	901	M0E	C1-C2-N2	-2.79	105.76	111.01
2	A	901	M0E	CBW-CBV-NCC	-2.45	105.60	110.66
2	A	901	M0E	OBS-CBN-CBM	2.35	114.09	109.68
2	A	901	M0E	CBL-CBM-CBN	2.50	114.56	110.20

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	M0E	CAP-OBH-CAV-OBC
2	A	901	M0E	CAP-OBH-CAV-NAT

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	M0E	8	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	683/751 (90%)	-0.12	16 (2%) 64 40	46, 79, 162, 228	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	67	TRP	3.6
1	A	378	ARG	2.9
1	A	468	SER	2.9
1	A	391	TYR	2.5
1	A	407	VAL	2.5
1	A	397	ARG	2.5
1	A	66	LEU	2.4
1	A	398	PRO	2.4
1	A	429	LYS	2.3
1	A	69	LEU	2.2
1	A	796	GLN	2.2
1	A	380	LEU	2.1
1	A	427	GLY	2.1
1	A	408	ILE	2.1
1	A	285	TRP	2.1
1	A	239	GLU	2.1

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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	M0E	A	901	77/109	0.89	0.19	-1.30	94,150,165,168	0

6.5 Other polymers [i](#)

There are no such residues in this entry.