



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:17 PM GMT

PDB ID : 1GKU
Title : REVERSE GYRASE FROM ARCHAEoglobus fulgidus
Authors : Rodriguez, A.C.; Stock, D.
Deposited on : 2001-08-21
Resolution : 2.70 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>

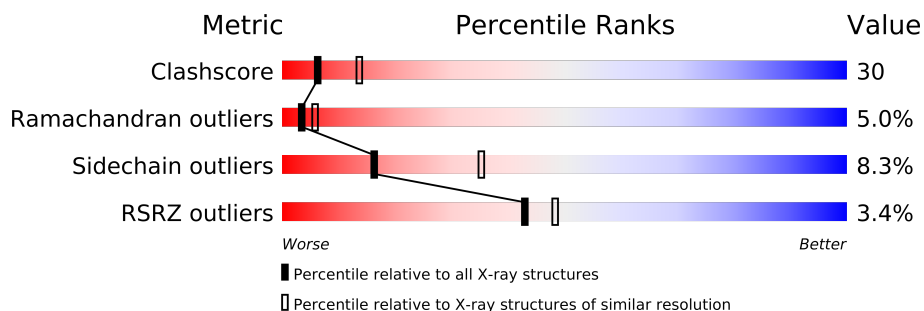
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
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) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.70 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))
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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	B	1054	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8308 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 REVERSE GYRASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1011	Total	C	N	O	S	0	0	0
			8151	5196	1437	1493	25			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	719	LEU	PRO	ENGINEERED MUTATION	UNP O29238
B	1046	MET	LEU	ENGINEERED MUTATION	UNP O29238

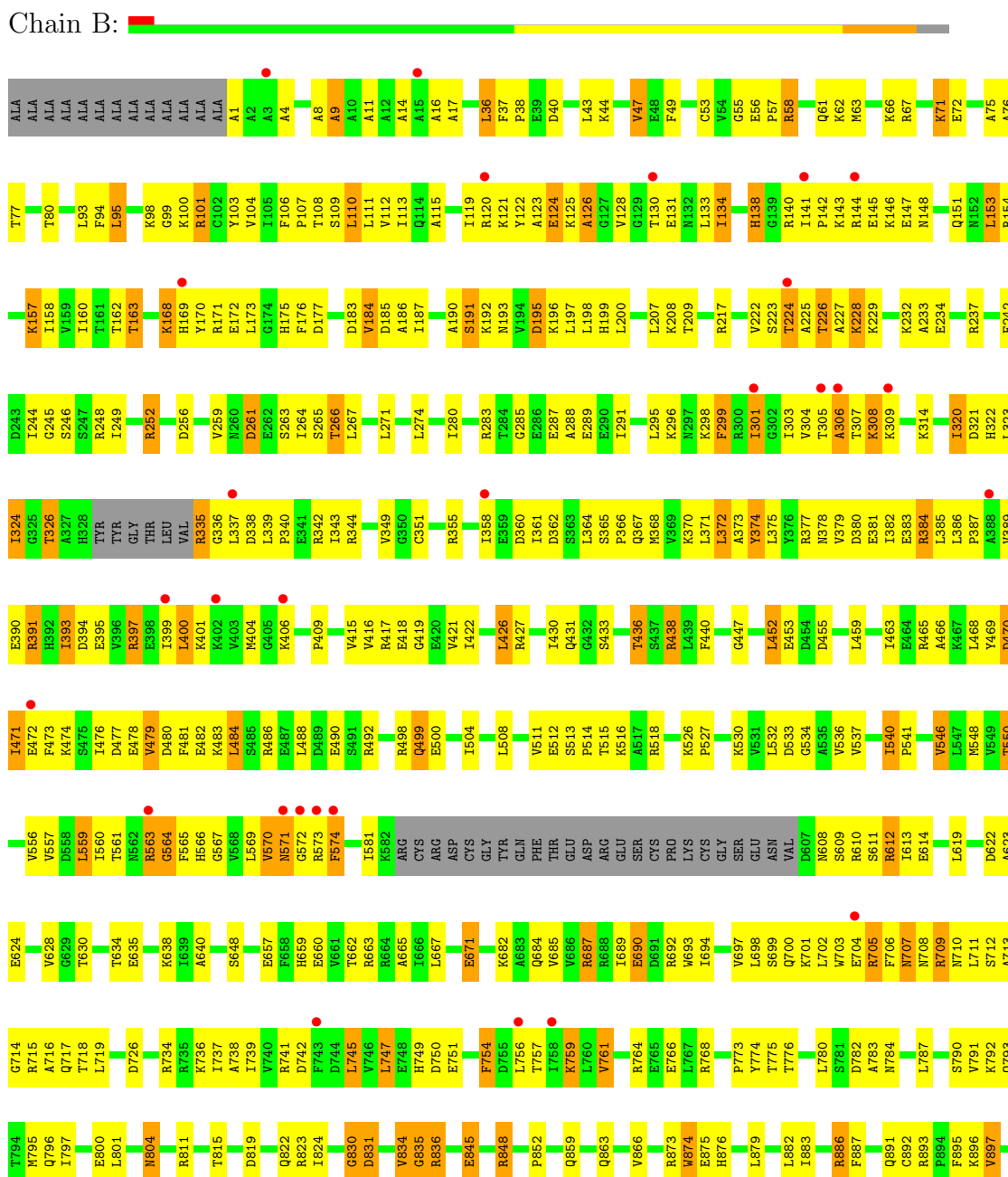
- Molecule 2 is water.

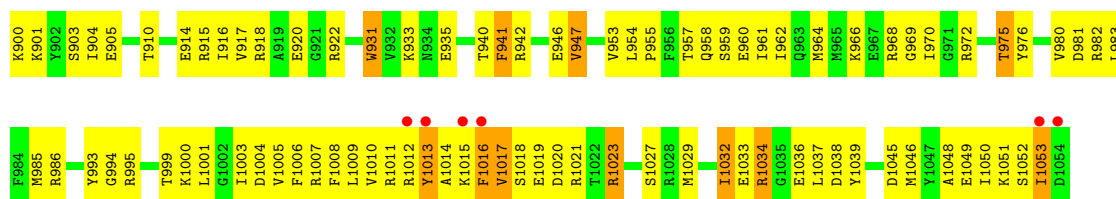
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	157	Total	O	0	0
			157	157		

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: REVERSE GYRASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.20Å 67.98Å 129.73Å 90.00° 104.01° 90.00°	Depositor
Resolution (Å)	41.00 – 2.70 46.20 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (41.00-2.70) 99.3 (46.20-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.69Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.226 , 0.295 0.230 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	54.0	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.8	EDS
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 30333 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8308	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	B	0.38	0/8293	0.64	4/11159 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	546	VAL	N-CA-C	-5.74	95.50	111.00
1	B	478	GLU	N-CA-C	-5.53	96.08	111.00
1	B	775	THR	N-CA-C	-5.16	97.07	111.00
1	B	374	TYR	N-CA-C	-5.07	97.32	111.00

There are no chirality outliers.

There are no planarity outliers.

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	B	8151	0	8285	498	0
2	B	157	0	0	8	0
All	All	8308	0	8285	498	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 30.

All (498) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:208:LYS:HG3	1:B:209:THR:H	1.20	1.06
1:B:436:THR:HG23	1:B:447:GLY:HA3	1.41	1.02
1:B:305:THR:HG21	1:B:326:THR:HB	1.41	1.01
1:B:130:THR:HG22	1:B:131:GLU:H	1.31	0.94
1:B:113:ILE:HD11	1:B:138:HIS:ND1	1.87	0.90
1:B:610:ARG:HH11	1:B:610:ARG:HB3	1.36	0.89
1:B:148:ASN:HA	1:B:151:GLN:HE21	1.37	0.87
1:B:208:LYS:HG3	1:B:209:THR:N	1.91	0.85
1:B:738:ALA:HB3	1:B:747:LEU:HD12	1.59	0.84
1:B:737:ILE:O	1:B:947:VAL:HA	1.81	0.80
1:B:757:THR:HB	1:B:905:GLU:HB2	1.65	0.79
1:B:190:ALA:HB3	1:B:193:ASN:ND2	1.99	0.78
1:B:109:SER:OG	1:B:138:HIS:HB2	1.85	0.76
1:B:1011:ARG:HD2	2:B:2152:HOH:O	1.85	0.76
1:B:1010:VAL:HA	1:B:1014:ALA:HB2	1.66	0.76
1:B:824:ILE:HG23	1:B:852:PRO:HG3	1.68	0.75
1:B:108:THR:HG22	1:B:111:LEU:H	1.51	0.75
1:B:532:LEU:O	1:B:534:GLY:N	2.20	0.75
1:B:374:TYR:O	1:B:375:LEU:HB2	1.87	0.74
1:B:101:ARG:HA	1:B:157:LYS:O	1.86	0.74
1:B:897:VAL:HG22	1:B:916:ILE:HG23	1.68	0.74
1:B:395:GLU:O	1:B:399:ILE:HG12	1.87	0.74
1:B:124:GLU:C	1:B:125:LYS:HD2	2.09	0.73
1:B:958:GLN:O	1:B:961:ILE:HG22	1.88	0.73
1:B:1023:ARG:CZ	1:B:1027:SER:HB2	2.19	0.73
1:B:108:THR:HB	1:B:111:LEU:HD12	1.70	0.73
1:B:536:VAL:O	1:B:550:THR:HG23	1.89	0.72
1:B:1023:ARG:NH1	1:B:1027:SER:HB2	2.04	0.72
1:B:572:GLY:O	1:B:573:ARG:HG3	1.90	0.72
1:B:466:ALA:HB1	1:B:472:GLU:HB3	1.71	0.72
1:B:256:ASP:HB3	1:B:474:LYS:HD3	1.70	0.72
1:B:704:GLU:HG3	1:B:705:ARG:H	1.53	0.71
1:B:486:ARG:O	1:B:490:GLU:HG3	1.90	0.71
1:B:288:ALA:O	1:B:324:ILE:HD11	1.91	0.71
1:B:143:LYS:O	1:B:147:GLU:HG3	1.90	0.71
1:B:335:ARG:NH2	1:B:338:ASP:H	1.88	0.71
1:B:44:LYS:O	1:B:47:VAL:HG13	1.90	0.70
1:B:183:ASP:HB2	1:B:186:ALA:HB3	1.72	0.70
1:B:609:SER:O	1:B:613:ILE:HG12	1.92	0.70
1:B:703:TRP:CD1	1:B:709:ARG:HA	2.27	0.69
1:B:190:ALA:HB3	1:B:193:ASN:HD21	1.57	0.69
1:B:610:ARG:NH1	1:B:610:ARG:HB3	2.08	0.69
1:B:694:ILE:HD12	1:B:1050:ILE:HD11	1.75	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:662:THR:HG23	1:B:665:ALA:H	1.57	0.69
1:B:1034:ARG:HB3	1:B:1036:GLU:HG3	1.74	0.69
1:B:358:ILE:HB	1:B:419:GLY:HA2	1.74	0.69
1:B:415:VAL:O	1:B:421:VAL:HA	1.92	0.69
1:B:291:ILE:HD11	1:B:349:VAL:HG11	1.75	0.68
1:B:704:GLU:HG3	1:B:705:ARG:N	2.08	0.68
1:B:559:LEU:HD12	1:B:692:ARG:NH1	2.08	0.68
1:B:469:TYR:O	1:B:471:ILE:N	2.27	0.68
1:B:830:GLY:O	1:B:831:ASP:HB2	1.92	0.68
1:B:1016:PHE:HA	1:B:1021:ARG:HD2	1.73	0.67
1:B:361:ILE:HD12	1:B:361:ILE:H	1.58	0.67
1:B:304:VAL:HG23	1:B:323:LEU:HD11	1.75	0.67
1:B:1029:MET:O	1:B:1032:ILE:HG22	1.94	0.67
1:B:610:ARG:O	1:B:614:GLU:HG3	1.94	0.67
1:B:368:MET:HE1	1:B:371:LEU:HD23	1.76	0.67
1:B:374:TYR:O	1:B:375:LEU:CB	2.41	0.66
1:B:130:THR:HG22	1:B:131:GLU:N	2.10	0.66
1:B:784:ASN:ND2	1:B:959:SER:H	1.92	0.66
1:B:386:LEU:HB3	1:B:389:VAL:HG22	1.78	0.65
1:B:804:ASN:HD22	1:B:804:ASN:N	1.93	0.65
1:B:784:ASN:HD22	1:B:959:SER:H	1.44	0.65
1:B:834:VAL:HG21	1:B:893:ARG:HA	1.78	0.65
1:B:999:THR:O	1:B:1003:ILE:HG22	1.95	0.65
1:B:361:ILE:HG23	1:B:364:LEU:HD12	1.78	0.65
1:B:476:ILE:HG23	1:B:476:ILE:O	1.95	0.65
1:B:131:GLU:HA	1:B:131:GLU:OE1	1.95	0.65
1:B:466:ALA:HB1	1:B:472:GLU:CB	2.26	0.65
1:B:163:THR:HB	1:B:187:ILE:CD1	2.27	0.64
1:B:367:GLN:HG3	1:B:368:MET:N	2.12	0.64
1:B:283:ARG:HB2	1:B:287:GLU:OE2	1.98	0.64
1:B:252:ARG:HD2	2:B:2032:HOH:O	1.97	0.64
1:B:274:LEU:O	1:B:344:ARG:NH2	2.31	0.64
1:B:504:ILE:HG22	1:B:546:VAL:HG23	1.79	0.64
1:B:774:TYR:CZ	1:B:886:ARG:HG3	2.32	0.64
1:B:972:ARG:HH22	1:B:1029:MET:HB2	1.63	0.64
1:B:427:ARG:O	1:B:431:GLN:HG3	1.98	0.63
1:B:321:ASP:HA	1:B:342:ARG:NH2	2.13	0.63
1:B:690:GLU:OE2	1:B:715:ARG:HD3	1.97	0.63
1:B:738:ALA:HB3	1:B:747:LEU:CD1	2.27	0.63
1:B:774:TYR:CE1	1:B:886:ARG:HG3	2.33	0.63
1:B:222:VAL:HG12	1:B:224:THR:H	1.63	0.63
1:B:793:GLN:O	1:B:797:ILE:HG12	1.98	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1017:VAL:O	1:B:1017:VAL:HG12	1.98	0.63
1:B:124:GLU:O	1:B:125:LYS:HD2	1.99	0.62
1:B:113:ILE:HD11	1:B:138:HIS:CE1	2.33	0.62
1:B:717:GLN:HG2	1:B:983:LEU:HD21	1.81	0.62
1:B:43:LEU:O	1:B:47:VAL:HG12	1.98	0.62
1:B:873:ARG:H	1:B:876:HIS:CD2	2.17	0.62
1:B:222:VAL:HG12	1:B:224:THR:N	2.14	0.62
1:B:918:ARG:HG2	1:B:918:ARG:HH11	1.65	0.62
1:B:184:VAL:HG22	1:B:222:VAL:HG13	1.82	0.62
1:B:512:GLU:HG3	1:B:630:THR:HG22	1.82	0.62
1:B:1052:SER:O	1:B:1053:ILE:HG23	2.00	0.62
1:B:515:THR:HG21	1:B:804:ASN:HD21	1.65	0.61
1:B:367:GLN:HG3	1:B:368:MET:H	1.65	0.61
1:B:58:ARG:NH1	2:B:2005:HOH:O	2.29	0.61
1:B:242:PHE:CE1	1:B:244:ILE:HG23	2.34	0.61
1:B:170:TYR:HB3	1:B:196:LYS:HB3	1.82	0.61
1:B:530:LYS:HB3	1:B:537:VAL:HG13	1.83	0.61
1:B:99:GLY:HA2	1:B:157:LYS:HZ3	1.66	0.61
1:B:107:PRO:HD3	1:B:183:ASP:HB3	1.83	0.61
1:B:836:ARG:NH2	1:B:892:CYS:O	2.33	0.61
1:B:556:VAL:HB	1:B:613:ILE:HD11	1.82	0.60
1:B:739:ILE:HD12	1:B:739:ILE:N	2.15	0.60
1:B:499:GLN:HG2	1:B:500:GLU:OE2	2.01	0.60
1:B:171:ARG:O	1:B:172:GLU:HB2	2.00	0.60
1:B:351:CYS:N	1:B:453:GLU:OE1	2.31	0.60
1:B:873:ARG:H	1:B:876:HIS:HD2	1.50	0.60
1:B:957:THR:H	1:B:960:GLU:CG	2.14	0.60
1:B:433:SER:O	1:B:436:THR:HG22	2.02	0.60
1:B:635:GLU:HG3	1:B:811:ARG:HH22	1.67	0.60
1:B:718:THR:HG21	1:B:1017:VAL:HG11	1.83	0.60
1:B:901:LYS:HB3	1:B:914:GLU:HG2	1.83	0.60
1:B:261:ASP:OD2	1:B:267:LEU:HG	2.01	0.60
1:B:791:VAL:HG23	1:B:792:LYS:N	2.16	0.60
1:B:314:LYS:HD3	1:B:320:ILE:HD13	1.84	0.60
1:B:662:THR:CG2	1:B:665:ALA:H	2.15	0.59
1:B:248:ARG:HG2	1:B:526:LYS:HB3	1.84	0.59
1:B:1046:MET:O	1:B:1050:ILE:HG12	2.01	0.59
1:B:9:ALA:HA	1:B:17:ALA:O	2.03	0.59
1:B:1006:PHE:O	1:B:1010:VAL:HG12	2.03	0.59
1:B:975:THR:HG21	2:B:2155:HOH:O	2.01	0.59
1:B:183:ASP:OD2	1:B:186:ALA:HB3	2.03	0.59
1:B:964:MET:O	1:B:968:ARG:HG2	2.03	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:141:ILE:HG22	1:B:143:LYS:H	1.68	0.59
1:B:380:ASP:O	1:B:384:ARG:HB2	2.01	0.59
1:B:140:ARG:O	1:B:142:PRO:HD3	2.03	0.59
1:B:340:PRO:HG3	1:B:438:ARG:NH1	2.18	0.59
1:B:706:PHE:O	1:B:707:ASN:C	2.41	0.58
1:B:335:ARG:HD3	1:B:336:GLY:H	1.68	0.58
1:B:560:ILE:HD12	1:B:561:THR:H	1.67	0.58
1:B:1003:ILE:O	1:B:1007:ARG:HG3	2.03	0.58
1:B:734:ARG:HH11	1:B:734:ARG:HG3	1.69	0.58
1:B:515:THR:HG21	1:B:804:ASN:ND2	2.18	0.58
1:B:335:ARG:NH2	1:B:338:ASP:N	2.51	0.58
1:B:305:THR:O	1:B:306:ALA:HB3	2.04	0.58
1:B:4:ALA:HA	1:B:11:ALA:O	2.03	0.58
1:B:468:LEU:HD23	1:B:866:VAL:HG11	1.84	0.58
1:B:783:ALA:O	1:B:787:LEU:O	2.21	0.58
1:B:687:ARG:HG2	1:B:1029:MET:SD	2.44	0.58
1:B:736:LYS:HD2	1:B:749:HIS:C	2.24	0.57
1:B:745:LEU:HD11	1:B:904:ILE:HD13	1.86	0.57
1:B:917:VAL:HG13	1:B:935:GLU:HG2	1.85	0.57
1:B:125:LYS:O	1:B:126:ALA:HB2	2.05	0.57
1:B:1023:ARG:NH2	1:B:1027:SER:HB2	2.19	0.57
1:B:8:ALA:O	1:B:9:ALA:HB3	2.04	0.57
1:B:106:PHE:O	1:B:162:THR:HA	2.05	0.57
1:B:1015:LYS:NZ	1:B:1021:ARG:HH12	2.03	0.57
1:B:121:LYS:O	1:B:124:GLU:HB2	2.04	0.57
1:B:563:ARG:HA	1:B:563:ARG:NE	2.19	0.57
1:B:208:LYS:CG	1:B:209:THR:H	2.08	0.57
1:B:426:LEU:O	1:B:430:ILE:HG13	2.04	0.57
1:B:426:LEU:HD13	1:B:465:ARG:HG3	1.85	0.57
1:B:657:GLU:OE2	1:B:659:HIS:HE1	1.87	0.57
1:B:784:ASN:HD22	1:B:959:SER:N	2.03	0.57
1:B:761:VAL:CG2	1:B:903:SER:HB2	2.35	0.56
1:B:99:GLY:HA2	1:B:157:LYS:NZ	2.19	0.56
1:B:409:PRO:HG2	1:B:416:VAL:HB	1.87	0.56
1:B:1010:VAL:O	1:B:1010:VAL:HG22	2.06	0.56
1:B:972:ARG:NH2	1:B:1029:MET:HB2	2.20	0.56
1:B:564:GLY:HA3	1:B:569:LEU:H	1.71	0.56
1:B:417:ARG:NH2	1:B:455:ASP:OD2	2.35	0.56
1:B:791:VAL:HG21	1:B:980:VAL:CG1	2.36	0.56
1:B:295:LEU:O	1:B:298:LYS:O	2.23	0.56
1:B:63:MET:HA	1:B:66:LYS:HD2	1.86	0.56
1:B:142:PRO:HG2	1:B:145:GLU:OE1	2.04	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:477:ASP:HA	1:B:479:VAL:CG1	2.36	0.56
1:B:364:LEU:O	1:B:397:ARG:NH1	2.38	0.56
1:B:222:VAL:HG12	1:B:223:SER:N	2.20	0.56
1:B:1001:LEU:O	1:B:1005:VAL:HG23	2.06	0.55
1:B:185:ASP:OD1	1:B:228:LYS:HD2	2.07	0.55
1:B:483:LYS:NZ	2:B:2070:HOH:O	2.38	0.55
1:B:263:SER:O	1:B:265:SER:N	2.34	0.55
1:B:634:THR:HB	1:B:684:GLN:HB2	1.89	0.55
1:B:697:VAL:O	1:B:700:GLN:HB3	2.05	0.55
1:B:563:ARG:HE	1:B:563:ARG:HA	1.72	0.55
1:B:100:LYS:O	1:B:177:ASP:OD2	2.25	0.55
1:B:183:ASP:OD2	1:B:187:ILE:HG12	2.07	0.55
1:B:378:ASN:HD21	1:B:380:ASP:HB2	1.72	0.55
1:B:249:ILE:N	1:B:249:ILE:HD12	2.21	0.55
1:B:361:ILE:CG2	1:B:397:ARG:HG3	2.38	0.55
1:B:776:THR:O	1:B:780:LEU:HG	2.07	0.55
1:B:361:ILE:HG22	1:B:397:ARG:HG3	1.89	0.54
1:B:761:VAL:HB	1:B:901:LYS:HG3	1.89	0.54
1:B:612:ARG:HH11	1:B:612:ARG:HG2	1.71	0.54
1:B:900:LYS:HB2	1:B:917:VAL:HG21	1.89	0.54
1:B:703:TRP:O	1:B:707:ASN:HA	2.08	0.54
1:B:361:ILE:HD13	1:B:401:LYS:HG2	1.89	0.54
1:B:514:PRO:HB3	1:B:518:ARG:HH12	1.72	0.54
1:B:233:ALA:CB	1:B:244:ILE:HD11	2.38	0.53
1:B:698:LEU:HB2	1:B:713:ALA:HB3	1.91	0.53
1:B:541:PRO:HA	1:B:546:VAL:HA	1.91	0.53
1:B:570:VAL:O	1:B:571:ASN:HB2	2.08	0.53
1:B:845:GLU:OE1	1:B:848:ARG:NH1	2.40	0.53
1:B:972:ARG:HH22	1:B:1029:MET:CB	2.20	0.53
1:B:191:SER:HB2	1:B:232:LYS:CE	2.39	0.53
1:B:917:VAL:CG1	1:B:935:GLU:HG2	2.39	0.53
1:B:305:THR:O	1:B:306:ALA:CB	2.57	0.53
1:B:784:ASN:ND2	1:B:959:SER:N	2.56	0.53
1:B:58:ARG:HH22	1:B:499:GLN:HA	1.73	0.53
1:B:265:SER:C	1:B:267:LEU:H	2.12	0.52
1:B:100:LYS:O	1:B:177:ASP:HB2	2.09	0.52
1:B:717:GLN:HG3	1:B:982:ARG:NE	2.23	0.52
1:B:184:VAL:HG11	1:B:225:ALA:HB2	1.90	0.52
1:B:942:ARG:HG3	1:B:942:ARG:O	2.09	0.52
1:B:1037:LEU:HD22	1:B:1038:ASP:N	2.24	0.52
1:B:623:ALA:O	1:B:624:GLU:HB2	2.08	0.52
1:B:901:LYS:HA	1:B:914:GLU:HA	1.91	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:608:ASN:HD21	1:B:610:ARG:HB2	1.72	0.52
1:B:370:LYS:O	1:B:373:ALA:HB3	2.10	0.52
1:B:335:ARG:HH11	1:B:335:ARG:HG2	1.74	0.52
1:B:163:THR:HB	1:B:187:ILE:HD13	1.91	0.52
1:B:559:LEU:HD11	1:B:567:GLY:O	2.09	0.52
1:B:719:LEU:HD11	1:B:1019:GLU:HB2	1.92	0.52
1:B:321:ASP:HA	1:B:342:ARG:HH22	1.74	0.52
1:B:790:SER:HB2	1:B:958:GLN:HE22	1.74	0.52
1:B:252:ARG:NH2	1:B:256:ASP:OD2	2.42	0.52
1:B:700:GLN:HA	1:B:703:TRP:CE3	2.44	0.52
1:B:756:LEU:O	1:B:940:THR:HA	2.10	0.52
1:B:660:GLU:OE2	1:B:662:THR:HG21	2.10	0.52
1:B:941:PHE:CD1	1:B:941:PHE:N	2.78	0.52
1:B:226:THR:C	1:B:228:LYS:H	2.12	0.51
1:B:195:ASP:N	1:B:195:ASP:OD1	2.42	0.51
1:B:750:ASP:O	1:B:947:VAL:HG21	2.10	0.51
1:B:470:ASP:C	1:B:471:ILE:O	2.46	0.51
1:B:709:ARG:HG3	1:B:710:ASN:H	1.75	0.51
1:B:387:PRO:HA	1:B:391:ARG:O	2.10	0.51
1:B:715:ARG:NH1	1:B:1049:GLU:OE2	2.43	0.51
1:B:389:VAL:HG23	1:B:390:GLU:N	2.26	0.51
1:B:142:PRO:HB2	1:B:145:GLU:CB	2.40	0.51
1:B:761:VAL:HG21	1:B:903:SER:HB2	1.92	0.51
1:B:265:SER:O	1:B:267:LEU:N	2.44	0.51
1:B:337:LEU:HD12	1:B:337:LEU:N	2.26	0.51
1:B:1016:PHE:HB3	1:B:1021:ARG:HH11	1.75	0.51
1:B:36:LEU:HD22	1:B:40:ASP:OD2	2.11	0.51
1:B:1019:GLU:O	1:B:1023:ARG:HB2	2.11	0.51
1:B:693:TRP:O	1:B:697:VAL:HG23	2.10	0.51
1:B:835:GLY:O	1:B:891:GLN:OE1	2.28	0.50
1:B:1032:ILE:HG23	1:B:1033:GLU:N	2.26	0.50
1:B:791:VAL:HG21	1:B:980:VAL:HG13	1.93	0.50
1:B:931:TRP:CZ3	1:B:933:LYS:HG2	2.47	0.50
1:B:192:LYS:O	1:B:196:LYS:HG3	2.12	0.50
1:B:108:THR:HG22	1:B:110:LEU:N	2.27	0.50
1:B:957:THR:HG22	1:B:994:GLY:O	2.12	0.50
1:B:848:ARG:HB2	1:B:887:PHE:CD1	2.46	0.50
1:B:93:LEU:HA	1:B:158:ILE:HD11	1.94	0.50
1:B:574:PHE:HE2	1:B:693:TRP:HH2	1.58	0.50
1:B:378:ASN:HD22	1:B:381:GLU:H	1.58	0.50
1:B:133:LEU:O	1:B:133:LEU:HD13	2.12	0.50
1:B:207:LEU:N	1:B:207:LEU:HD22	2.27	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:101:ARG:NH2	1:B:154:ARG:HA	2.27	0.49
1:B:184:VAL:CG1	1:B:225:ALA:HB2	2.42	0.49
1:B:49:PHE:HZ	1:B:93:LEU:HD23	1.77	0.49
1:B:701:LYS:HA	1:B:704:GLU:HG2	1.94	0.49
1:B:335:ARG:CD	1:B:336:GLY:H	2.24	0.49
1:B:234:GLU:OE2	1:B:237:ARG:NE	2.35	0.49
1:B:130:THR:CG2	1:B:131:GLU:H	2.15	0.49
1:B:372:LEU:O	1:B:374:TYR:O	2.30	0.49
1:B:307:THR:HG22	1:B:308:LYS:N	2.27	0.49
1:B:560:ILE:O	1:B:567:GLY:HA3	2.12	0.49
1:B:714:GLY:HA3	1:B:982:ARG:NH2	2.28	0.49
1:B:267:LEU:O	1:B:271:LEU:HG	2.11	0.49
1:B:379:VAL:HG21	1:B:863:GLN:HG3	1.95	0.49
1:B:741:ARG:O	1:B:742:ASP:HB2	2.13	0.49
1:B:377:ARG:HB2	1:B:382:ILE:HD11	1.95	0.48
1:B:754:PHE:CD1	1:B:754:PHE:N	2.81	0.48
1:B:901:LYS:O	1:B:901:LYS:HG3	2.13	0.48
1:B:901:LYS:CB	1:B:914:GLU:HG2	2.43	0.48
1:B:361:ILE:N	1:B:361:ILE:HD12	2.27	0.48
1:B:764:ARG:HG2	1:B:764:ARG:HH11	1.78	0.48
1:B:766:GLU:O	1:B:896:LYS:HA	2.13	0.48
1:B:383:GLU:C	1:B:385:LEU:H	2.17	0.48
1:B:222:VAL:CG1	1:B:223:SER:N	2.76	0.48
1:B:714:GLY:N	1:B:717:GLN:OE1	2.46	0.48
1:B:749:HIS:CD2	1:B:750:ASP:H	2.32	0.48
1:B:530:LYS:HB3	1:B:537:VAL:CG1	2.43	0.48
1:B:957:THR:H	1:B:960:GLU:HG2	1.79	0.48
1:B:66:LYS:HD3	1:B:622:ASP:HA	1.96	0.48
1:B:463:ILE:HD12	1:B:474:LYS:HG3	1.95	0.47
1:B:662:THR:HG22	1:B:665:ALA:CB	2.44	0.47
1:B:985:MET:SD	1:B:986:ARG:NH1	2.87	0.47
1:B:123:ALA:HB1	1:B:128:VAL:HG13	1.95	0.47
1:B:471:ILE:HG22	1:B:472:GLU:H	1.79	0.47
1:B:120:ARG:HG2	1:B:120:ARG:HH11	1.79	0.47
1:B:168:LYS:HG3	1:B:169:HIS:N	2.30	0.47
1:B:335:ARG:HD3	1:B:335:ARG:N	2.29	0.47
1:B:662:THR:HG22	1:B:665:ALA:HB2	1.97	0.47
1:B:163:THR:HB	1:B:187:ILE:HD11	1.96	0.47
1:B:511:VAL:HB	1:B:516:LYS:HD3	1.96	0.47
1:B:736:LYS:O	1:B:736:LYS:HG3	2.15	0.47
1:B:756:LEU:HA	1:B:905:GLU:O	2.15	0.47
1:B:141:ILE:HG22	1:B:143:LYS:N	2.28	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:95:LEU:O	1:B:100:LYS:HB2	2.15	0.47
1:B:141:ILE:CG2	1:B:146:LYS:HD3	2.44	0.47
1:B:1032:ILE:CG2	1:B:1033:GLU:N	2.77	0.47
1:B:49:PHE:O	1:B:53:CYS:HB2	2.14	0.47
1:B:366:PRO:HG3	1:B:393:ILE:CD1	2.44	0.47
1:B:463:ILE:CD1	1:B:474:LYS:HG3	2.45	0.47
1:B:142:PRO:HB2	1:B:145:GLU:HB3	1.96	0.47
1:B:133:LEU:C	1:B:133:LEU:HD13	2.35	0.47
1:B:183:ASP:HB2	1:B:186:ALA:CB	2.43	0.47
1:B:415:VAL:HB	1:B:422:ILE:HB	1.97	0.47
1:B:1018:SER:C	1:B:1020:ASP:H	2.17	0.47
1:B:184:VAL:HG21	1:B:224:THR:O	2.14	0.47
1:B:426:LEU:HD21	1:B:466:ALA:HB2	1.96	0.46
1:B:792:LYS:HG3	1:B:981:ASP:CG	2.35	0.46
1:B:1051:LYS:C	1:B:1053:ILE:H	2.18	0.46
1:B:477:ASP:HA	1:B:479:VAL:HG13	1.96	0.46
1:B:1018:SER:C	1:B:1020:ASP:N	2.66	0.46
1:B:168:LYS:HG3	1:B:169:HIS:H	1.81	0.46
1:B:389:VAL:CG2	1:B:390:GLU:N	2.78	0.46
1:B:274:LEU:HD13	1:B:481:PHE:HD1	1.81	0.46
1:B:168:LYS:CE	1:B:169:HIS:HB2	2.46	0.46
1:B:699:SER:OG	1:B:712:SER:HA	2.15	0.46
1:B:709:ARG:C	1:B:711:LEU:H	2.19	0.46
1:B:702:LEU:HD21	1:B:1005:VAL:HG13	1.97	0.46
1:B:480:ASP:OD1	1:B:482:GLU:HG2	2.15	0.46
1:B:123:ALA:C	1:B:125:LYS:H	2.19	0.46
1:B:694:ILE:CD1	1:B:1050:ILE:HD11	2.42	0.46
1:B:717:GLN:HB2	1:B:982:ARG:HE	1.81	0.46
1:B:134:ILE:C	1:B:134:ILE:HD13	2.36	0.46
1:B:168:LYS:HE3	1:B:169:HIS:HB2	1.97	0.46
1:B:227:ALA:O	1:B:229:LYS:N	2.48	0.46
1:B:360:ASP:C	1:B:362:ASP:N	2.70	0.46
1:B:280:ILE:HD12	1:B:280:ILE:N	2.30	0.46
1:B:897:VAL:HG22	1:B:916:ILE:CG2	2.44	0.45
1:B:708:ASN:HD22	1:B:709:ARG:N	2.14	0.45
1:B:563:ARG:O	1:B:564:GLY:O	2.34	0.45
1:B:768:ARG:HB2	1:B:895:PHE:CE1	2.51	0.45
1:B:559:LEU:CD1	1:B:567:GLY:HA3	2.46	0.45
1:B:819:ASP:O	1:B:823:ARG:HG3	2.16	0.45
1:B:57:PRO:HG2	1:B:62:LYS:HE3	1.98	0.45
1:B:183:ASP:CB	1:B:186:ALA:HB3	2.45	0.45
1:B:759:LYS:NZ	1:B:905:GLU:HG2	2.32	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:373:ALA:C	1:B:374:TYR:O	2.49	0.45
1:B:58:ARG:H	1:B:61:GLN:HE21	1.64	0.45
1:B:266:THR:O	1:B:266:THR:HG22	2.16	0.45
1:B:791:VAL:HG11	1:B:962:ILE:HD11	1.98	0.45
1:B:299:PHE:HB2	1:B:301:ILE:HG12	1.99	0.45
1:B:274:LEU:HD12	1:B:274:LEU:HA	1.80	0.45
1:B:905:GLU:OE1	1:B:910:THR:HG22	2.16	0.45
1:B:67:ARG:O	1:B:72:GLU:HB2	2.17	0.45
1:B:470:ASP:O	1:B:471:ILE:O	2.35	0.45
1:B:671:GLU:HA	1:B:671:GLU:OE1	2.17	0.45
1:B:459:LEU:O	1:B:463:ILE:HG12	2.17	0.45
1:B:233:ALA:HB1	1:B:244:ILE:HD11	1.99	0.45
1:B:191:SER:HB2	1:B:232:LYS:HE2	1.99	0.45
1:B:715:ARG:HH21	1:B:1021:ARG:HG2	1.82	0.44
1:B:380:ASP:O	1:B:384:ARG:CB	2.65	0.44
1:B:701:LYS:C	1:B:704:GLU:HG2	2.37	0.44
1:B:355:ARG:HG3	1:B:422:ILE:HG12	1.98	0.44
1:B:955:PRO:HD2	1:B:995:ARG:HD2	1.99	0.44
1:B:80:THR:O	1:B:440:PHE:HB2	2.18	0.44
1:B:1013:TYR:CZ	1:B:1015:LYS:HD3	2.53	0.44
1:B:40:ASP:O	1:B:43:LEU:HB3	2.17	0.44
1:B:75:ALA:HA	1:B:222:VAL:HB	1.99	0.44
1:B:492:ARG:HH11	1:B:492:ARG:HG3	1.82	0.44
1:B:71:LYS:O	1:B:71:LYS:HD2	2.17	0.44
1:B:879:LEU:O	1:B:883:ILE:HG13	2.18	0.44
1:B:759:LYS:HE2	1:B:903:SER:HB3	1.99	0.44
1:B:873:ARG:HG3	1:B:873:ARG:NH1	2.33	0.44
1:B:559:LEU:HD12	1:B:692:ARG:HH11	1.82	0.44
1:B:106:PHE:CE2	1:B:115:ALA:HB2	2.53	0.44
1:B:895:PHE:H	1:B:895:PHE:HD1	1.66	0.44
1:B:557:VAL:HA	1:B:581:ILE:HG13	2.00	0.44
1:B:119:ILE:HD12	1:B:160:ILE:HD11	1.99	0.44
1:B:700:GLN:OE1	1:B:701:LYS:NZ	2.51	0.44
1:B:540:ILE:HD13	1:B:541:PRO:N	2.33	0.44
1:B:265:SER:C	1:B:267:LEU:N	2.70	0.44
1:B:564:GLY:O	1:B:566:HIS:N	2.51	0.44
1:B:608:ASN:ND2	1:B:610:ARG:H	2.16	0.44
1:B:267:LEU:HA	1:B:267:LEU:HD13	1.83	0.44
1:B:226:THR:OG1	1:B:228:LYS:HG3	2.18	0.44
1:B:1019:GLU:O	1:B:1019:GLU:HG2	2.17	0.43
1:B:386:LEU:HB3	1:B:389:VAL:CG2	2.47	0.43
1:B:900:LYS:HD2	1:B:917:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:900:LYS:HB2	1:B:917:VAL:CG2	2.47	0.43
1:B:780:LEU:HD21	1:B:795:MET:SD	2.58	0.43
1:B:756:LEU:O	1:B:756:LEU:HD12	2.18	0.43
1:B:37:PHE:HB3	1:B:38:PRO:HD2	2.00	0.43
1:B:738:ALA:N	1:B:747:LEU:O	2.51	0.43
1:B:904:ILE:O	1:B:910:THR:HA	2.18	0.43
1:B:298:LYS:NZ	2:B:2040:HOH:O	2.51	0.43
1:B:702:LEU:HD11	1:B:1009:LEU:HD21	2.01	0.43
1:B:773:PRO:HD2	1:B:815:THR:HB	1.99	0.43
1:B:339:LEU:HB2	1:B:343:ILE:HG13	2.00	0.43
1:B:226:THR:C	1:B:228:LYS:N	2.72	0.43
1:B:1037:LEU:HD13	1:B:1038:ASP:O	2.19	0.43
1:B:175:HIS:HD2	2:B:2016:HOH:O	2.00	0.43
1:B:400:LEU:O	1:B:404:MET:HG3	2.19	0.43
1:B:560:ILE:CD1	1:B:561:THR:H	2.31	0.43
1:B:682:LYS:HB2	1:B:1032:ILE:HD11	2.01	0.43
1:B:365:SER:OG	1:B:367:GLN:HG2	2.18	0.43
1:B:682:LYS:CB	1:B:1032:ILE:HD11	2.48	0.43
1:B:170:TYR:HA	1:B:173:LEU:HD12	2.00	0.43
1:B:800:GLU:OE1	1:B:876:HIS:HE1	2.02	0.43
1:B:104:VAL:O	1:B:160:ILE:HA	2.19	0.43
1:B:715:ARG:O	1:B:715:ARG:HG3	2.18	0.43
1:B:303:ILE:HA	1:B:324:ILE:O	2.19	0.43
1:B:873:ARG:HB2	1:B:875:GLU:OE1	2.19	0.43
1:B:873:ARG:HG3	1:B:873:ARG:HH11	1.83	0.43
1:B:892:CYS:SG	1:B:922:ARG:HB3	2.59	0.43
1:B:915:ARG:O	1:B:917:VAL:HG23	2.19	0.43
1:B:224:THR:OG1	1:B:246:SER:HB3	2.19	0.42
1:B:8:ALA:O	1:B:9:ALA:CB	2.67	0.42
1:B:1045:ASP:O	1:B:1048:ALA:HB3	2.19	0.42
1:B:705:ARG:O	1:B:706:PHE:C	2.56	0.42
1:B:703:TRP:NE1	1:B:711:LEU:O	2.52	0.42
1:B:931:TRP:HZ3	1:B:933:LYS:HG2	1.83	0.42
1:B:77:THR:OG1	1:B:224:THR:HG21	2.19	0.42
1:B:717:GLN:HG2	1:B:983:LEU:CD2	2.49	0.42
1:B:266:THR:C	1:B:267:LEU:HD22	2.40	0.42
1:B:791:VAL:CG2	1:B:792:LYS:N	2.82	0.42
1:B:976:TYR:O	1:B:980:VAL:HG12	2.19	0.42
1:B:49:PHE:CE2	1:B:94:PHE:HB2	2.54	0.42
1:B:985:MET:HG3	1:B:986:ARG:HD2	2.02	0.42
1:B:305:THR:CG2	1:B:326:THR:HB	2.30	0.42
1:B:1015:LYS:HZ2	1:B:1016:PHE:HD2	1.66	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:416:VAL:HG22	1:B:421:VAL:HG22	2.02	0.42
1:B:685:VAL:O	1:B:689:ILE:HG12	2.20	0.42
1:B:1008:PHE:CE1	1:B:1012:ARG:HD2	2.55	0.42
1:B:470:ASP:O	1:B:473:PHE:CD1	2.73	0.42
1:B:107:PRO:CD	1:B:183:ASP:HB3	2.49	0.42
1:B:957:THR:OG1	1:B:960:GLU:HG2	2.20	0.42
1:B:53:CYS:SG	1:B:122:TYR:HB3	2.59	0.42
1:B:103:TYR:HB2	1:B:176:PHE:CD1	2.54	0.42
1:B:508:LEU:HD12	1:B:548:MET:O	2.19	0.42
1:B:307:THR:CG2	1:B:308:LYS:N	2.82	0.42
1:B:148:ASN:HA	1:B:151:GLN:NE2	2.19	0.42
1:B:426:LEU:HD21	1:B:466:ALA:CB	2.50	0.42
1:B:76:ALA:O	1:B:224:THR:HB	2.20	0.42
1:B:296:LYS:C	1:B:298:LYS:H	2.21	0.42
1:B:305:THR:HG23	2:B:2041:HOH:O	2.19	0.42
1:B:736:LYS:HD2	1:B:749:HIS:O	2.19	0.42
1:B:946:GLU:O	1:B:947:VAL:O	2.38	0.42
1:B:1000:LYS:O	1:B:1003:ILE:HG23	2.19	0.42
1:B:274:LEU:HD13	1:B:481:PHE:CD1	2.55	0.42
1:B:504:ILE:HD12	1:B:504:ILE:N	2.35	0.42
1:B:532:LEU:HD12	1:B:619:LEU:HD11	2.02	0.42
1:B:142:PRO:O	1:B:144:ARG:N	2.45	0.42
1:B:468:LEU:CD2	1:B:866:VAL:HG11	2.50	0.41
1:B:285:GLY:O	1:B:289:GLU:HG3	2.19	0.41
1:B:611:SER:HA	1:B:614:GLU:OE2	2.20	0.41
1:B:123:ALA:CB	1:B:128:VAL:HG13	2.49	0.41
1:B:874:TRP:NE1	1:B:875:GLU:HG3	2.35	0.41
1:B:859:GLN:O	1:B:863:GLN:HG2	2.20	0.41
1:B:819:ASP:HA	1:B:822:GLN:HB2	2.01	0.41
1:B:848:ARG:HB2	1:B:887:PHE:CG	2.55	0.41
1:B:141:ILE:CG2	1:B:143:LYS:H	2.31	0.41
1:B:296:LYS:C	1:B:298:LYS:N	2.73	0.41
1:B:532:LEU:C	1:B:534:GLY:N	2.73	0.41
1:B:705:ARG:C	1:B:707:ASN:N	2.73	0.41
1:B:304:VAL:O	1:B:307:THR:HB	2.20	0.41
1:B:628:VAL:HG11	1:B:640:ALA:CB	2.51	0.41
1:B:693:TRP:O	1:B:694:ILE:C	2.59	0.41
1:B:708:ASN:ND2	1:B:709:ARG:N	2.68	0.41
1:B:196:LYS:O	1:B:200:LEU:HG	2.21	0.41
1:B:436:THR:CG2	1:B:447:GLY:HA3	2.31	0.41
1:B:953:VAL:HG12	1:B:954:LEU:N	2.35	0.41
1:B:305:THR:HG21	1:B:326:THR:CB	2.30	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:757:THR:O	1:B:904:ILE:HA	2.21	0.41
1:B:570:VAL:O	1:B:571:ASN:CB	2.68	0.41
1:B:472:GLU:OE1	1:B:472:GLU:CA	2.69	0.41
1:B:715:ARG:NH2	1:B:1021:ARG:HD3	2.36	0.41
1:B:1015:LYS:HZ3	1:B:1021:ARG:HH12	1.68	0.41
1:B:141:ILE:HG23	1:B:146:LYS:HD3	2.02	0.41
1:B:385:LEU:O	1:B:386:LEU:C	2.58	0.41
1:B:301:ILE:HG23	1:B:322:HIS:HB2	2.03	0.41
1:B:702:LEU:HD21	1:B:1009:LEU:HD21	2.02	0.41
1:B:969:GLY:C	1:B:970:ILE:HD12	2.40	0.41
1:B:709:ARG:CG	1:B:710:ASN:H	2.34	0.41
1:B:335:ARG:NE	1:B:336:GLY:H	2.18	0.41
1:B:386:LEU:O	1:B:390:GLU:O	2.39	0.41
1:B:58:ARG:H	1:B:61:GLN:NE2	2.17	0.41
1:B:120:ARG:HD2	1:B:120:ARG:HA	1.89	0.41
1:B:436:THR:HG23	1:B:447:GLY:CA	2.31	0.40
1:B:108:THR:O	1:B:112:VAL:HG23	2.20	0.40
1:B:108:THR:CG2	1:B:110:LEU:H	2.34	0.40
1:B:373:ALA:HB1	1:B:382:ILE:HD12	2.01	0.40
1:B:690:GLU:HB2	1:B:1046:MET:SD	2.61	0.40
1:B:107:PRO:CG	1:B:183:ASP:HB3	2.51	0.40
1:B:513:SER:HA	1:B:514:PRO:HD3	1.94	0.40
1:B:259:VAL:O	1:B:452:LEU:HA	2.22	0.40
1:B:335:ARG:HG2	1:B:335:ARG:NH1	2.35	0.40
1:B:702:LEU:HD21	1:B:1009:LEU:CD2	2.52	0.40
1:B:638:LYS:HG2	1:B:684:GLN:OE1	2.21	0.40
1:B:764:ARG:HG2	1:B:764:ARG:NH1	2.35	0.40
1:B:571:ASN:HB2	1:B:573:ARG:HH21	1.86	0.40
1:B:426:LEU:HD22	1:B:466:ALA:HA	2.03	0.40
1:B:295:LEU:HB3	1:B:301:ILE:CD1	2.51	0.40
1:B:217:ARG:HH11	1:B:217:ARG:HG2	1.87	0.40
1:B:527:PRO:HB3	1:B:540:ILE:HB	2.02	0.40
1:B:37:PHE:N	1:B:37:PHE:CD1	2.90	0.40
1:B:1:ALA:HB1	1:B:14:ALA:N	2.36	0.40
1:B:484:LEU:O	1:B:488:LEU:HG	2.21	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	B	999/1054 (95%)	859 (86%)	90 (9%)	50 (5%)	3 6

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	126	ALA
1	B	224	THR
1	B	226	THR
1	B	309	LYS
1	B	418	GLU
1	B	470	ASP
1	B	471	ILE
1	B	533	ASP
1	B	716	ALA
1	B	835	GLY
1	B	1053	ILE
1	B	16	ALA
1	B	191	SER
1	B	264	ILE
1	B	266	THR
1	B	299	PHE
1	B	306	ALA
1	B	406	LYS
1	B	564	GLY
1	B	571	ASN
1	B	707	ASN
1	B	830	GLY
1	B	831	ASP
1	B	56	GLU
1	B	124	GLU
1	B	228	LYS
1	B	261	ASP
1	B	384	ARG
1	B	709	ARG

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Mol	Chain	Res	Type
1	B	761	VAL
1	B	947	VAL
1	B	1017	VAL
1	B	9	ALA
1	B	153	LEU
1	B	308	LYS
1	B	391	ARG
1	B	498	ARG
1	B	563	ARG
1	B	574	PHE
1	B	726	ASP
1	B	751	GLU
1	B	565	PHE
1	B	570	VAL
1	B	101	ARG
1	B	245	GLY
1	B	836	ARG
1	B	393	ILE
1	B	55	GLY
1	B	184	VAL
1	B	834	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	B	868/895 (97%)	796 (92%)	72 (8%)	16	35

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	36	LEU
1	B	47	VAL
1	B	58	ARG
1	B	71	LYS
1	B	95	LEU
1	B	98	LYS
1	B	110	LEU

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Mol	Chain	Res	Type
1	B	134	ILE
1	B	138	HIS
1	B	153	LEU
1	B	157	LYS
1	B	163	THR
1	B	168	LYS
1	B	195	ASP
1	B	197	LEU
1	B	198	LEU
1	B	199	HIS
1	B	252	ARG
1	B	301	ILE
1	B	320	ILE
1	B	324	ILE
1	B	326	THR
1	B	335	ARG
1	B	372	LEU
1	B	394	ASP
1	B	397	ARG
1	B	400	LEU
1	B	426	LEU
1	B	436	THR
1	B	438	ARG
1	B	452	LEU
1	B	479	VAL
1	B	484	LEU
1	B	499	GLN
1	B	540	ILE
1	B	550	THR
1	B	559	LEU
1	B	612	ARG
1	B	648	SER
1	B	663	ARG
1	B	667	LEU
1	B	671	GLU
1	B	687	ARG
1	B	690	GLU
1	B	705	ARG
1	B	745	LEU
1	B	747	LEU
1	B	754	PHE
1	B	759	LYS

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Mol	Chain	Res	Type
1	B	782	ASP
1	B	796	GLN
1	B	801	LEU
1	B	804	ASN
1	B	845	GLU
1	B	848	ARG
1	B	874	TRP
1	B	882	LEU
1	B	886	ARG
1	B	897	VAL
1	B	920	GLU
1	B	931	TRP
1	B	941	PHE
1	B	966	LYS
1	B	975	THR
1	B	993	TYR
1	B	1004	ASP
1	B	1013	TYR
1	B	1016	PHE
1	B	1023	ARG
1	B	1032	ILE
1	B	1034	ARG
1	B	1039	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	61	GLN
1	B	114	GLN
1	B	151	GLN
1	B	155	ASN
1	B	169	HIS
1	B	238	GLN
1	B	241	ASN
1	B	260	ASN
1	B	367	GLN
1	B	378	ASN
1	B	499	GLN
1	B	608	ASN
1	B	621	HIS
1	B	659	HIS
1	B	708	ASN

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Mol	Chain	Res	Type
1	B	749	HIS
1	B	784	ASN
1	B	796	GLN
1	B	799	GLN
1	B	804	ASN
1	B	859	GLN
1	B	876	HIS
1	B	958	GLN
1	B	963	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 ⓘ

There are no ligands in this entry.

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	B	1011/1054 (95%)	0.01	34 (3%)	43 48	19, 51, 90, 113	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	306	ALA	6.1
1	B	1013	TYR	4.2
1	B	756	LEU	4.1
1	B	305	THR	3.3
1	B	358	ILE	3.3
1	B	1054	ASP	3.2
1	B	130	THR	3.1
1	B	169	HIS	3.1
1	B	563	ARG	3.0
1	B	472	GLU	3.0
1	B	224	THR	2.9
1	B	388	ALA	2.9
1	B	399	ILE	2.8
1	B	15	ALA	2.8
1	B	141	ILE	2.7
1	B	3	ALA	2.7
1	B	301	ILE	2.6
1	B	1012	ARG	2.6
1	B	704	GLU	2.6
1	B	402	LYS	2.5
1	B	120	ARG	2.4
1	B	406	LYS	2.4
1	B	571	ASN	2.4
1	B	1053	ILE	2.3
1	B	573	ARG	2.3
1	B	309	LYS	2.2
1	B	758	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	743	PHE	2.2
1	B	572	GLY	2.2
1	B	337	LEU	2.2
1	B	144	ARG	2.2
1	B	574	PHE	2.1
1	B	1015	LYS	2.1
1	B	1016	PHE	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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.