



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2024 – 07:49 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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

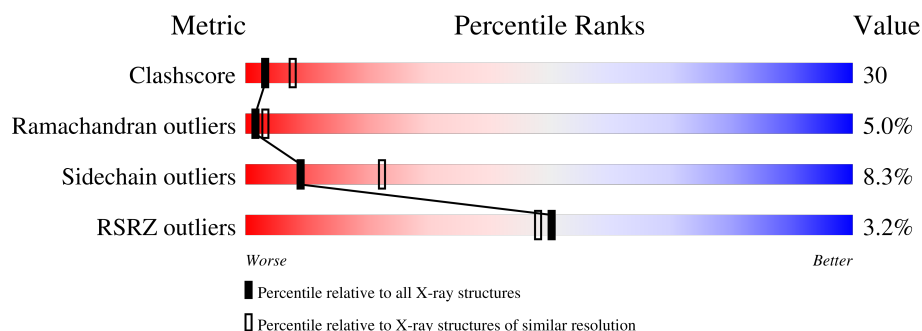
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	1054	

2 Entry composition

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

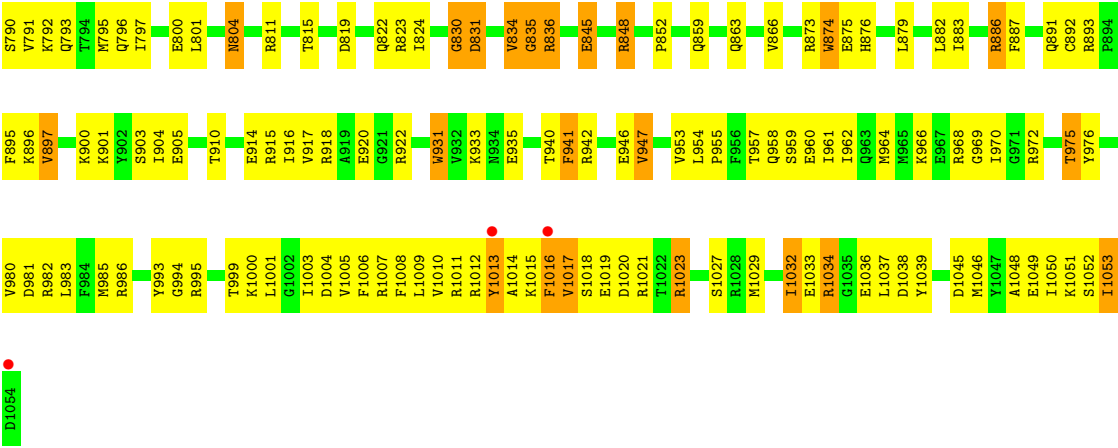
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1011	Total	C	N	O	S	0	0	0
			8151	5196	1437	1493	25			

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		



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 41.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (41.00-2.70) 99.2 (41.00-2.70)	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 0.229 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	54.0	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 82.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

All (498) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B: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:HB3	1:B:610:ARG:HH11	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:101:ARG:HA	1:B:157:LYS:O	1.86	0.74
1:B:374:TYR:O	1:B:375:LEU:HB2	1.87	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:466:ALA:HB1	1:B:472:GLU:HB3	1.71	0.72
1:B:572:GLY:O	1:B:573:ARG:HG3	1.90	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:143:LYS:O	1:B:147:GLU:HG3	1.90	0.71
1:B:288:ALA:O	1:B:324:ILE:HD11	1.91	0.71
1:B:486:ARG:O	1:B:490: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:358:ILE:HB	1:B:419:GLY:HA2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:610:ARG:HB3	1:B:610:ARG:NH1	2.08	0.69
1:B:662:THR:HG23	1:B:665:ALA:H	1.57	0.69
1:B:694:ILE:HD12	1:B:1050:ILE:HD11	1.75	0.69
1:B:1034:ARG:HB3	1:B:1036:GLU:HG3	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:559:LEU:HD12	1:B:692:ARG:NH1	2.08	0.68
1:B:704:GLU:HG3	1:B:705:ARG:N	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:304:VAL:HG23	1:B:323:LEU:HD11	1.75	0.67
1:B:361:ILE:HD12	1:B:361:ILE:H	1.58	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:N	1:B:804:ASN:HD22	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:283:ARG:HB2	1:B:287:GLU:OE2	1.98	0.64
1:B:367:GLN:HG3	1:B:368:MET:N	2.12	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:321:ASP:HA	1:B:342:ARG:NH2	2.13	0.63
1:B:427:ARG:O	1:B:431:GLN:HG3	1.98	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:222:VAL:HG12	1:B:224:THR:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:774:TYR:CE1	1:B:886:ARG:HG3	2.33	0.63
1:B:793:GLN:O	1:B:797:ILE:HG12	1.98	0.63
1:B:1017:VAL:HG12	1:B:1017:VAL:O	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:N	1:B:739:ILE:HD12	2.15	0.60
1:B:171:ARG:O	1:B:172:GLU:HB2	2.00	0.60
1:B:499:GLN:HG2	1:B:500:GLU:OE2	2.01	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:261:ASP:OD2	1:B:267:LEU:HG	2.01	0.60
1:B:901:LYS:HB3	1:B:914:GLU:HG2	1.83	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:248:ARG:HG2	1:B:526:LYS:HB3	1.84	0.59
1:B:662:THR:CG2	1:B:665:ALA:H	2.15	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:975:THR:HG21	2:B:2155:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1006:PHE:O	1:B:1010:VAL:HG12	2.03	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
1:B:140:ARG:O	1:B:142:PRO:HD3	2.03	0.59
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:340:PRO:HG3	1:B:438:ARG:NH1	2.18	0.59
1:B:335:ARG:HD3	1:B:336:GLY:H	1.68	0.58
1:B:706:PHE:O	1:B:707:ASN:C	2.41	0.58
1:B:560:ILE:HD12	1:B:561:THR:H	1.67	0.58
1:B:734:ARG:HG3	1:B:734:ARG:HH11	1.69	0.58
1:B:1003:ILE:O	1:B:1007:ARG:HG3	2.03	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:4:ALA:HA	1:B:11:ALA:O	2.03	0.58
1:B:305:THR:O	1:B:306:ALA:HB3	2.04	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: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: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: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:HD13	1:B:465:ARG:HG3	1.85	0.57
1:B:426:LEU:O	1:B:430:ILE:HG13	2.04	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:99:GLY:HA2	1:B:157:LYS:NZ	2.19	0.56
1:B:761:VAL:CG2	1:B:903:SER:HB2	2.35	0.56
1:B:409:PRO:HG2	1:B:416:VAL:HB	1.87	0.56
1:B:417:ARG:NH2	1:B:455:ASP:OD2	2.35	0.56
1:B:564:GLY:HA3	1:B:569:LEU:H	1.71	0.56
1:B:972:ARG:NH2	1:B:1029:MET:HB2	2.20	0.56
1:B:1010:VAL:O	1:B:1010:VAL:HG22	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:MET:HA	1:B:66:LYS:HD2	1.86	0.56
1:B:295:LEU:O	1:B:298:LYS:O	2.23	0.56
1:B:791:VAL:HG21	1:B:980:VAL:CG1	2.36	0.56
1:B:142:PRO:HG2	1:B:145:GLU:OE1	2.04	0.56
1:B:477:ASP:HA	1:B:479:VAL:CG1	2.36	0.56
1:B:222:VAL:HG12	1:B:223:SER:N	2.20	0.56
1:B:364:LEU:O	1:B:397:ARG:NH1	2.38	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:563:ARG:HA	1:B:563:ARG:HE	1.72	0.55
1:B:697:VAL:O	1:B:700:GLN:HB3	2.05	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:249:ILE:N	1:B:249:ILE:HD12	2.21	0.55
1:B:378:ASN:HD21	1:B:380:ASP:HB2	1.72	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:HG2	1:B:612:ARG:HH11	1.71	0.54
1:B:900:LYS:HB2	1:B:917:VAL:HG21	1.89	0.54
1:B:361:ILE:HD13	1:B:401:LYS:HG2	1.89	0.54
1:B:703:TRP:O	1:B:707:ASN:HA	2.08	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:191:SER:HB2	1:B:232:LYS:CE	2.39	0.53
1:B:972:ARG:HH22	1:B:1029:MET:CB	2.20	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:100:LYS:O	1:B:177:ASP:HB2	2.09	0.52
1:B:265:SER:C	1:B:267:LEU:H	2.12	0.52
1:B:717:GLN:HG3	1:B:982:ARG:NE	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:VAL:HG11	1:B:225:ALA:HB2	1.90	0.52
1:B:623:ALA:O	1:B:624:GLU:HB2	2.08	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:901:LYS:HA	1:B:914:GLU:HA	1.91	0.52
1:B:163:THR:HB	1:B:187:ILE:HD13	1.91	0.52
1:B:335:ARG:HH11	1:B:335:ARG:HG2	1.74	0.52
1:B:370:LYS:O	1:B:373:ALA:HB3	2.10	0.52
1:B:559:LEU:HD11	1:B:567:GLY:O	2.09	0.52
1:B:608:ASN:HD21	1:B:610:ARG:HB2	1.72	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:252:ARG:NH2	1:B:256:ASP:OD2	2.42	0.52
1:B:790:SER:HB2	1:B:958:GLN:HE22	1.74	0.52
1:B:700:GLN:HA	1:B:703:TRP:CE3	2.44	0.52
1:B:660:GLU:OE2	1:B:662:THR:HG21	2.10	0.52
1:B:756:LEU:O	1:B:940:THR:HA	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:OD1	1:B:195:ASP:N	2.42	0.51
1:B:470:ASP:C	1:B:471:ILE:O	2.46	0.51
1:B:750:ASP:O	1:B:947:VAL:HG21	2.10	0.51
1:B:387:PRO:HA	1:B:391:ARG:O	2.10	0.51
1:B:709:ARG:HG3	1:B:710:ASN:H	1.75	0.51
1:B:389:VAL:HG23	1:B:390:GLU:N	2.26	0.51
1:B:715:ARG:NH1	1:B:1049:GLU:OE2	2.43	0.51
1:B:142:PRO:HB2	1:B:145:GLU:CB	2.40	0.51
1:B:265:SER:O	1:B:267:LEU:N	2.44	0.51
1:B:337:LEU:N	1:B:337:LEU:HD12	2.26	0.51
1:B:761:VAL:HG21	1:B:903:SER:HB2	1.92	0.51
1:B:36:LEU:HD22	1:B:40:ASP:OD2	2.11	0.51
1:B:1016:PHE:HB3	1:B:1021:ARG:HH11	1.75	0.51
1:B:693:TRP:O	1:B:697:VAL:HG23	2.10	0.51
1:B:1019:GLU:O	1:B:1023:ARG:HB2	2.11	0.51
1:B:835:GLY:O	1:B:891:GLN:OE1	2.28	0.50
1:B:791:VAL:HG21	1:B:980:VAL:HG13	1.93	0.50
1:B:1032:ILE:HG23	1:B:1033:GLU:N	2.26	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:93:LEU:HA	1:B:158:ILE:HD11	1.94	0.50
1:B:108:THR:HG22	1:B:110:LEU:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:848:ARG:HB2	1:B:887:PHE:CD1	2.46	0.50
1:B:957:THR:HG22	1:B:994:GLY:O	2.12	0.50
1:B:378:ASN:HD22	1:B:381:GLU:H	1.58	0.50
1:B:574:PHE:HE2	1:B:693:TRP:HH2	1.58	0.50
1:B:133:LEU:HD13	1:B:133:LEU:O	2.12	0.50
1:B:207:LEU:N	1:B:207:LEU:HD22	2.27	0.49
1:B:49:PHE:HZ	1:B:93:LEU:HD23	1.77	0.49
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:234:GLU:OE2	1:B:237:ARG:NE	2.35	0.49
1:B:335:ARG:CD	1:B:336:GLY:H	2.24	0.49
1:B:701:LYS:HA	1:B:704:GLU:HG2	1.94	0.49
1:B:130:THR:CG2	1:B:131:GLU:H	2.15	0.49
1:B:307:THR:HG22	1:B:308:LYS:N	2.27	0.49
1:B:372:LEU:O	1:B:374:TYR:O	2.30	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:361:ILE:HD12	1:B:361:ILE:N	2.27	0.48
1:B:764:ARG:HH11	1:B:764:ARG:HG2	1.78	0.48
1:B:901:LYS:HG3	1:B:901:LYS:O	2.13	0.48
1:B:901:LYS:CB	1:B:914:GLU:HG2	2.43	0.48
1:B:766:GLU:O	1:B:896:LYS:HA	2.13	0.48
1:B:222:VAL:CG1	1:B:223:SER:N	2.76	0.48
1:B:383:GLU:C	1:B:385:LEU:H	2.17	0.48
1:B:714:GLY:N	1:B:717:GLN:OE1	2.46	0.48
1:B:530:LYS:HB3	1:B:537:VAL:CG1	2.43	0.48
1:B:749:HIS:CD2	1:B:750:ASP:H	2.32	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:120:ARG:HG2	1:B:120:ARG:HH11	1.79	0.47
1:B:123:ALA:HB1	1:B:128:VAL:HG13	1.95	0.47
1:B:168:LYS:HG3	1:B:169:HIS:N	2.30	0.47
1:B:471:ILE:HG22	1:B:472:GLU:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:95:LEU:O	1:B:100:LYS:HB2	2.15	0.47
1:B:141:ILE:HG22	1:B:143:LYS:N	2.28	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:49:PHE:O	1:B:53:CYS:HB2	2.14	0.47
1:B:141:ILE:CG2	1:B:146:LYS:HD3	2.44	0.47
1:B:366:PRO:HG3	1:B:393:ILE:CD1	2.44	0.47
1:B:1032:ILE:CG2	1:B:1033:GLU:N	2.77	0.47
1:B:133:LEU:HD13	1:B:133:LEU:C	2.35	0.47
1:B:142:PRO:HB2	1:B:145:GLU:HB3	1.96	0.47
1:B:463:ILE:CD1	1:B:474:LYS:HG3	2.45	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: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:1051:LYS:C	1:B:1053:ILE:H	2.18	0.46
1:B:168:LYS:HG3	1:B:169:HIS:H	1.81	0.46
1:B:274:LEU:HD13	1:B:481:PHE:HD1	1.81	0.46
1:B:389:VAL:CG2	1:B:390:GLU:N	2.78	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:480:ASP:OD1	1:B:482:GLU:HG2	2.15	0.46
1:B:702:LEU:HD21	1:B:1005:VAL:HG13	1.97	0.46
1:B:709:ARG:C	1:B:711:LEU:H	2.19	0.46
1:B:123:ALA:C	1:B:125:LYS:H	2.19	0.46
1:B:134:ILE:HD13	1:B:134:ILE:C	2.36	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: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:280:ILE:N	1:B:280:ILE:HD12	2.30	0.46
1:B:360:ASP:C	1:B:362:ASP:N	2.70	0.46
1:B:563:ARG:O	1:B:564:GLY:O	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:708:ASN:HD22	1:B:709:ARG:N	2.14	0.45
1:B:768:ARG:HB2	1:B:895:PHE:CE1	2.51	0.45
1:B:897:VAL:HG22	1:B:916:ILE:CG2	2.44	0.45
1:B:57:PRO:HG2	1:B:62:LYS:HE3	1.98	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:183:ASP:CB	1:B:186:ALA:HB3	2.45	0.45
1:B:58:ARG:H	1:B:61:GLN:HE21	1.64	0.45
1:B:266:THR:HG22	1:B:266:THR:O	2.16	0.45
1:B:373:ALA:C	1:B:374:TYR:O	2.49	0.45
1:B:759:LYS:NZ	1:B:905:GLU:HG2	2.32	0.45
1:B:299:PHE:HB2	1:B:301:ILE:HG12	1.99	0.45
1:B:791:VAL:HG11	1:B:962:ILE:HD11	1.98	0.45
1:B:274:LEU:HD12	1:B:274:LEU:HA	1.80	0.45
1:B:67:ARG:O	1:B:72:GLU:HB2	2.17	0.45
1:B:905:GLU:OE1	1:B:910:THR:HG22	2.16	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:233:ALA:HB1	1:B:244:ILE:HD11	1.99	0.45
1:B:459:LEU:O	1:B:463:ILE:HG12	2.17	0.45
1:B:191:SER:HB2	1:B:232:LYS:HE2	1.99	0.45
1:B:380:ASP:O	1:B:384:ARG:CB	2.65	0.44
1:B:715:ARG:HH21	1:B:1021:ARG:HG2	1.82	0.44
1:B:80:THR:O	1:B:440:PHE:HB2	2.18	0.44
1:B:355:ARG:HG3	1:B:422:ILE:HG12	1.98	0.44
1:B:701:LYS:C	1:B:704:GLU:HG2	2.37	0.44
1:B:955:PRO:HD2	1:B:995:ARG:HD2	1.99	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:HG3	1:B:492:ARG:HH11	1.82	0.44
1:B:1013:TYR:CZ	1:B:1015:LYS:HD3	2.53	0.44
1:B:71:LYS:HD2	1:B:71:LYS:O	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:NH1	1:B:873:ARG:HG3	2.33	0.44
1:B:106:PHE:CE2	1:B:115:ALA:HB2	2.53	0.44
1:B:559:LEU:HD12	1:B:692:ARG:HH11	1.82	0.44
1:B:119:ILE:HD12	1:B:160:ILE:HD11	1.99	0.44
1:B:557:VAL:HA	1:B:581:ILE:HG13	2.00	0.44
1:B:895:PHE:HD1	1:B:895:PHE:H	1.66	0.44
1:B:265:SER:C	1:B:267:LEU:N	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:ILE:HD13	1:B:541:PRO:N	2.33	0.44
1:B:564:GLY:O	1:B:566:HIS:N	2.51	0.44
1:B:700:GLN:OE1	1:B:701:LYS:NZ	2.51	0.44
1:B:226:THR:OG1	1:B:228:LYS:HG3	2.18	0.44
1:B:267:LEU:HD13	1:B:267:LEU:HA	1.83	0.44
1:B:608:ASN:ND2	1:B:610:ARG:H	2.16	0.44
1:B:386:LEU:HB3	1:B:389:VAL:CG2	2.47	0.43
1:B:900:LYS:HB2	1:B:917:VAL:CG2	2.47	0.43
1:B:900:LYS:HD2	1:B:917:VAL:HG21	2.00	0.43
1:B:1019:GLU:O	1:B:1019:GLU:HG2	2.17	0.43
1:B:780:LEU:HD21	1:B:795:MET:SD	2.58	0.43
1:B:37:PHE:HB3	1:B:38:PRO:HD2	2.00	0.43
1:B:756:LEU:O	1:B:756:LEU:HD12	2.18	0.43
1:B:298:LYS:NZ	2:B:2040:HOH:O	2.51	0.43
1:B:339:LEU:HB2	1:B:343:ILE:HG13	2.00	0.43
1:B:702:LEU:HD11	1:B:1009:LEU:HD21	2.01	0.43
1:B:738:ALA:N	1:B:747:LEU:O	2.51	0.43
1:B:773:PRO:HD2	1:B:815:THR:HB	1.99	0.43
1:B:904:ILE:O	1:B:910:THR:HA	2.18	0.43
1:B:175:HIS:HD2	2:B:2016:HOH:O	2.00	0.43
1:B:226:THR:C	1:B:228:LYS:N	2.72	0.43
1:B:400:LEU:O	1:B:404:MET:HG3	2.19	0.43
1:B:1037:LEU:HD13	1:B:1038:ASP:O	2.19	0.43
1:B:365:SER:OG	1:B:367:GLN:HG2	2.18	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:170:TYR:HA	1:B:173:LEU:HD12	2.00	0.43
1:B:682:LYS:CB	1:B:1032:ILE:HD11	2.48	0.43
1:B:104:VAL:O	1:B:160:ILE:HA	2.19	0.43
1:B:800:GLU:OE1	1:B:876:HIS:HE1	2.02	0.43
1:B:303:ILE:HA	1:B:324:ILE:O	2.19	0.43
1:B:715:ARG:O	1:B:715:ARG:HG3	2.18	0.43
1:B:873:ARG:HG3	1:B:873:ARG:HH11	1.83	0.43
1:B:873:ARG:HB2	1:B:875:GLU:OE1	2.19	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:703:TRP:NE1	1:B:711:LEU:O	2.52	0.42
1:B:705:ARG:O	1:B:706:PHE:C	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:931:TRP:HZ3	1:B:933:LYS:HG2	1.83	0.42
1:B:49:PHE:CE2	1:B:94:PHE:HB2	2.54	0.42
1:B:77:THR:OG1	1:B:224:THR:HG21	2.19	0.42
1:B:266:THR:C	1:B:267:LEU:HD22	2.40	0.42
1:B:717:GLN:HG2	1:B:983:LEU:CD2	2.49	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: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: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:1015:LYS:HZ2	1:B:1016:PHE:HD2	1.66	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:107:PRO:CD	1:B:183:ASP:HB3	2.49	0.42
1:B:470:ASP:O	1:B:473:PHE:CD1	2.73	0.42
1:B:508:LEU:HD12	1:B:548:MET:O	2.19	0.42
1:B:957:THR:OG1	1:B:960:GLU:HG2	2.20	0.42
1:B:307:THR:CG2	1:B:308:LYS:N	2.82	0.42
1:B:76:ALA:O	1:B:224:THR:HB	2.20	0.42
1:B:148:ASN:HA	1:B:151:GLN:NE2	2.19	0.42
1:B:296:LYS:C	1:B:298:LYS:H	2.21	0.42
1:B:426:LEU:HD21	1:B:466:ALA:CB	2.50	0.42
1:B:274:LEU:HD13	1:B:481:PHE:CD1	2.55	0.42
1:B:305:THR:HG23	2:B:2041:HOH:O	2.19	0.42
1:B:504:ILE:N	1:B:504:ILE:HD12	2.35	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:142:PRO:O	1:B:144:ARG:N	2.45	0.42
1:B:532:LEU:HD12	1:B:619:LEU:HD11	2.02	0.42
1:B:285:GLY:O	1:B:289:GLU:HG3	2.19	0.41
1:B:468:LEU:CD2	1:B:866:VAL:HG11	2.50	0.41
1:B:123:ALA:CB	1:B:128:VAL:HG13	2.49	0.41
1:B:611:SER:HA	1:B:614:GLU:OE2	2.20	0.41
1:B:819:ASP:HA	1:B:822:GLN:HB2	2.01	0.41
1:B:859:GLN:O	1:B:863:GLN:HG2	2.20	0.41
1:B:874:TRP:NE1	1:B:875:GLU:HG3	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:LYS:C	1:B:298:LYS:N	2.73	0.41
1:B:304:VAL:O	1:B:307:THR:HB	2.20	0.41
1:B:532:LEU:C	1:B:534:GLY:N	2.73	0.41
1:B:628:VAL:HG11	1:B:640:ALA:CB	2.51	0.41
1:B:705:ARG:C	1:B:707:ASN:N	2.73	0.41
1:B:196:LYS:O	1:B:200:LEU:HG	2.21	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: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:141:ILE:HG23	1:B:146:LYS:HD3	2.02	0.41
1:B:301:ILE:HG23	1:B:322:HIS:HB2	2.03	0.41
1:B:305:THR:HG21	1:B:326:THR:CB	2.30	0.41
1:B:385:LEU:O	1:B:386:LEU:C	2.58	0.41
1:B:472:GLU:CA	1:B:472:GLU:OE1	2.69	0.41
1:B:570:VAL:O	1:B:571:ASN:CB	2.68	0.41
1:B:702:LEU:HD21	1:B:1009:LEU:HD21	2.02	0.41
1:B:715:ARG:NH2	1:B:1021:ARG:HD3	2.36	0.41
1:B:757:THR:O	1:B:904:ILE:HA	2.21	0.41
1:B:969:GLY:C	1:B:970:ILE:HD12	2.40	0.41
1:B:1015:LYS:HZ3	1:B:1021:ARG:HH12	1.68	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: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:709:ARG:CG	1:B:710:ASN:H	2.34	0.41
1:B:436:THR:HG23	1:B:447:GLY:CA	2.31	0.40
1:B:107:PRO:CG	1:B:183:ASP:HB3	2.51	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:259:VAL:O	1:B:452:LEU:HA	2.22	0.40
1:B:373:ALA:HB1	1:B:382:ILE:HD12	2.01	0.40
1:B:513:SER:HA	1:B:514:PRO:HD3	1.94	0.40
1:B:690:GLU:HB2	1:B:1046:MET:SD	2.61	0.40
1:B:335:ARG:HG2	1:B:335:ARG:NH1	2.35	0.40
1:B:638:LYS:HG2	1:B:684:GLN:OE1	2.21	0.40
1:B:702:LEU:HD21	1:B:1009:LEU:CD2	2.52	0.40
1:B:764:ARG:HG2	1:B:764:ARG:NH1	2.35	0.40
1:B:217:ARG:HH11	1:B:217:ARG:HG2	1.87	0.40
1:B:295:LEU:HB3	1:B:301:ILE:CD1	2.51	0.40
1:B:426:LEU:HD22	1:B:466:ALA:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:ASN:HB2	1:B:573:ARG:HH21	1.86	0.40
1:B:1:ALA:HB1	1:B:14:ALA:N	2.36	0.40
1:B:37:PHE:N	1:B:37:PHE:CD1	2.90	0.40
1:B:484:LEU:O	1:B:488:LEU:HG	2.21	0.40
1:B:527:PRO:HB3	1:B:540:ILE:HB	2.02	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	B	999/1054 (95%)	859 (86%)	90 (9%)	50 (5%)	1 3

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

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Mol	Chain	Res	Type
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
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%)	9	22

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
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

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Mol	Chain	Res	Type
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
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

Sometimes 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

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Mol	Chain	Res	Type
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
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 molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	21:ALA	C	33:SER	N	21.87
1	B	6:ALA	C	8:ALA	N	15.79
1	B	12:ALA	C	14:ALA	N	13.81

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%)	0.05	32 (3%)	50 48	19, 51, 90, 113	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	472	GLU	4.8
1	B	358	ILE	4.1
1	B	3	ALA	3.9
1	B	15	ALA	3.7
1	B	1	ALA	3.6
1	B	14	ALA	3.2
1	B	1013	TYR	3.2
1	B	34	LEU	3.1
1	B	224	THR	3.1
1	B	223	SER	3.1
1	B	399	ILE	2.8
1	B	142	PRO	2.7
1	B	127	GLY	2.7
1	B	169	HIS	2.7
1	B	756	LEU	2.7
1	B	129	GLY	2.7
1	B	1054	ASP	2.7
1	B	392	HIS	2.7
1	B	306	ALA	2.6
1	B	410	GLN	2.6
1	B	1016	PHE	2.5
1	B	128	VAL	2.4
1	B	388	ALA	2.4
1	B	171	ARG	2.3
1	B	2	ALA	2.3
1	B	190	ALA	2.3
1	B	18	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	406	LYS	2.2
1	B	4	ALA	2.2
1	B	6	ALA	2.1
1	B	188	LEU	2.0
1	B	126	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.