WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Apr 27, 2024 – 04:06 pm BST

PDB ID	:	2J7O
Title	:	STRUCTURE OF THE RNAI POLYMERASE FROM NEUROSPORA CRASSA
Authors	:	Salgado, P.S.; Koivunen, M.R.L.; Makeyev, E.V.; Bamford, D.H.; Stuart, D.I.; Grimes, J.M.
Deposited on	:	2006-10-13
Resolution	:	3.50 Å(reported)

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.50 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.
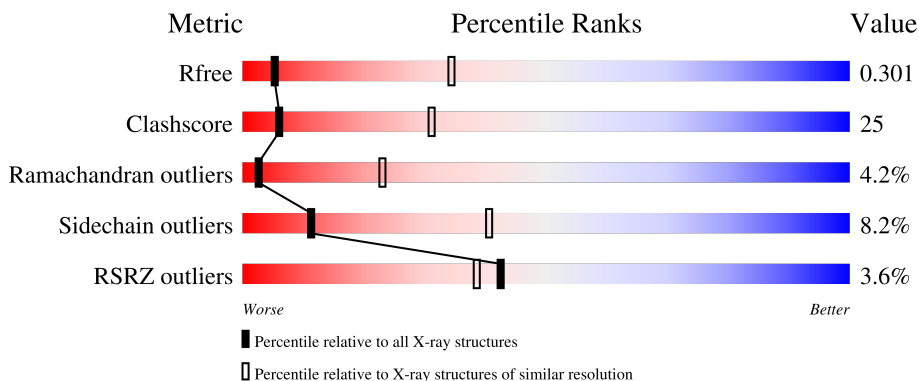
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 <=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	1022	3% 61% 23% 6% · 9%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 7521 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 RNA DEPENDENT RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	935	Total 7520	C 4814	N 1304	O 1368	S 34	0	0	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	559	ALA	GLY	conflict	UNP Q9Y7G6

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mg 1	0	0

3 Residue-property plots ⓘ

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

• Molecule 1: RNA DEPENDENT RNA POLYMERASE
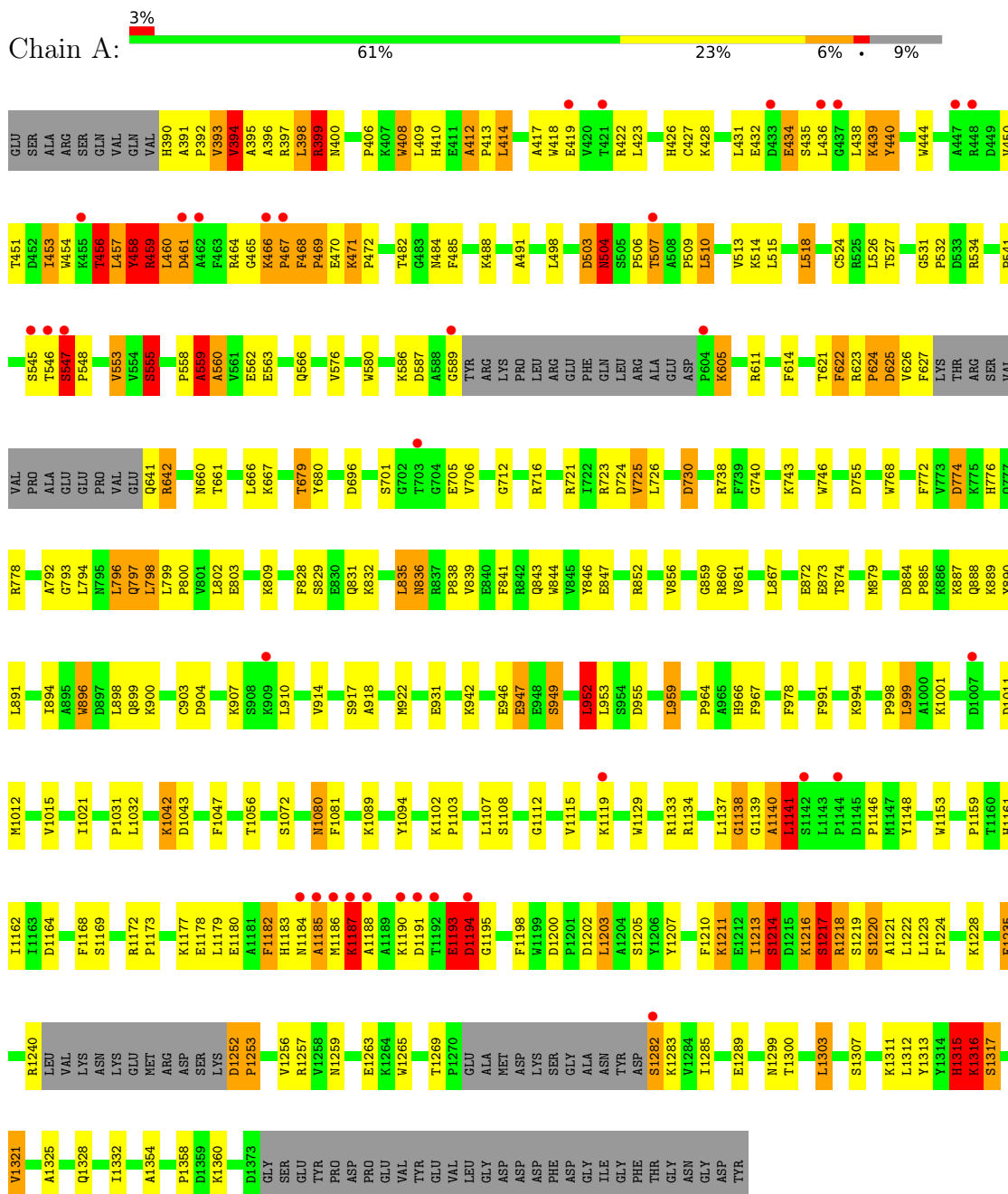
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	114.60Å 125.02Å 102.20Å 90.00° 108.75° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50 19.95 – 3.50	Depositor EDS
% Data completeness (in resolution range)	91.4 (20.00-3.50) 91.4 (19.95-3.50)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 3.52Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.353 , 0.360 0.301 , 0.301	Depositor DCC
R_{free} test set	773 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	103.5	Xtriage
Anisotropy	0.584	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 53.1	EDS
L-test for twinning[2]	$< |L| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	7521	wwPDB-VP
Average B, all atoms (Å^2)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	1.00	14/7711 (0.2%)	0.80	16/10433 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	18

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	434	GLU	CD-OE2	49.94	1.80	1.25
1	A	1042	LYS	C-N	27.46	1.97	1.34
1	A	434	GLU	CD-OE1	25.46	1.53	1.25
1	A	1080	ASN	C-N	18.42	1.76	1.34
1	A	432	GLU	CD-OE1	16.69	1.44	1.25
1	A	436	LEU	C-N	16.09	1.62	1.33
1	A	679	THR	C-N	15.74	1.70	1.34
1	A	888	GLN	C-N	12.20	1.62	1.34
1	A	434	GLU	C-O	10.17	1.42	1.23
1	A	434	GLU	CG-CD	7.69	1.63	1.51
1	A	1257	ARG	CZ-NH1	7.61	1.43	1.33
1	A	436	LEU	C-O	6.47	1.35	1.23
1	A	435	SER	CA-CB	-6.22	1.43	1.52
1	A	435	SER	CB-OG	-5.36	1.35	1.42

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	836	ASN	O-C-N	-14.80	99.02	122.70
1	A	434	GLU	OE1-CD-OE2	13.00	138.90	123.30
1	A	679	THR	O-C-N	12.84	143.24	122.70
1	A	679	THR	CA-C-N	-9.90	95.43	117.20
1	A	836	ASN	CA-C-N	9.28	137.62	117.20
1	A	836	ASN	C-N-CA	8.56	143.09	121.70
1	A	679	THR	C-N-CA	-7.67	102.54	121.70
1	A	436	LEU	O-C-N	7.02	135.14	123.20
1	A	952	LEU	CA-CB-CG	6.90	131.17	115.30
1	A	1316	LYS	N-CA-C	-6.57	93.25	111.00
1	A	1283	LYS	N-CA-C	-6.53	93.37	111.00
1	A	432	GLU	OE1-CD-OE2	6.29	130.85	123.30
1	A	436	LEU	CA-C-N	-6.07	104.06	116.20
1	A	798	LEU	CA-CB-CG	5.55	128.07	115.30
1	A	560	ALA	N-CA-C	5.21	125.08	111.00
1	A	459	ARG	N-CA-C	5.09	124.76	111.00

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1138	GLY	Peptide
1	A	1139	GLY	Peptide
1	A	1161	HIS	Mainchain
1	A	1213	ILE	Peptide
1	A	1217	SER	Peptide
1	A	1220	SER	Peptide
1	A	1252	ASP	Peptide
1	A	1282	SER	Peptide
1	A	1315	HIS	Peptide
1	A	456	THR	Peptide
1	A	504	ASN	Peptide
1	A	506	PRO	Peptide
1	A	545	SER	Peptide
1	A	547	SER	Peptide
1	A	555	SER	Peptide
1	A	559	ALA	Peptide
1	A	624	PRO	Peptide
1	A	836	ASN	Mainchain

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	7520	0	7464	372	0
2	A	1	0	0	0	0
All	All	7521	0	7464	372	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 25.

All (372) 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:679:THR:C	1:A:680:TYR:N	1.70	1.43
1:A:641:GLN:CB	1:A:642:ARG:HB2	1.50	1.41
1:A:1080:ASN:C	1:A:1081:PHE:N	1.76	1.38
1:A:1184:ASN:N	1:A:1185:ALA:HB3	1.49	1.27
1:A:1193:GLU:HA	1:A:1194:ASP:O	1.37	1.25
1:A:399:ARG:CB	1:A:400:ASN:HB3	1.69	1.22
1:A:434:GLU:OE2	1:A:434:GLU:CD	1.80	1.19
1:A:1042:LYS:C	1:A:1043:ASP:N	1.97	1.18
1:A:503:ASP:O	1:A:504:ASN:HB2	1.38	1.18
1:A:439:LYS:HG3	1:A:440:TYR:H	1.06	1.17
1:A:1315:HIS:HB2	1:A:1316:LYS:CB	1.72	1.17
1:A:438:LEU:HA	1:A:439:LYS:CB	1.71	1.17
1:A:465:GLY:HA2	1:A:466:LYS:HB2	1.29	1.15
1:A:1210:PHE:O	1:A:1214:SER:HB2	1.47	1.14
1:A:641:GLN:HB2	1:A:642:ARG:CB	1.77	1.13
1:A:667:LYS:HE2	1:A:1119:LYS:O	1.45	1.13
1:A:393:VAL:HG23	1:A:394:VAL:HG23	1.14	1.12
1:A:438:LEU:HA	1:A:439:LYS:HB3	1.18	1.12
1:A:1186:MET:H	1:A:1187:LYS:HB3	1.01	1.12
1:A:399:ARG:HD2	1:A:507:THR:HG22	1.23	1.10
1:A:1315:HIS:CB	1:A:1316:LYS:HB2	1.81	1.07
1:A:723:ARG:HH11	1:A:723:ARG:HG2	1.00	1.07
1:A:1194:ASP:HB2	1:A:1195:GLY:HA2	1.35	1.06
1:A:828:PHE:CD1	1:A:1178:GLU:HG2	1.89	1.05
1:A:1184:ASN:H	1:A:1185:ALA:CB	1.68	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ALA:HB1	1:A:413:PRO:HA	1.37	1.04
1:A:438:LEU:CA	1:A:439:LYS:HB3	1.86	1.04
1:A:457:LEU:HB3	1:A:458:TYR:CB	1.90	1.01
1:A:896:TRP:CZ2	1:A:1186:MET:HE3	1.95	1.01
1:A:399:ARG:HB3	1:A:400:ASN:CB	1.91	1.00
1:A:412:ALA:HB1	1:A:413:PRO:CA	1.90	1.00
1:A:439:LYS:HG3	1:A:440:TYR:N	1.65	1.00
1:A:835:LEU:HD13	1:A:841:PHE:CE1	1.96	1.00
1:A:896:TRP:HH2	1:A:1183:HIS:HD1	1.01	0.99
1:A:412:ALA:CB	1:A:413:PRO:HA	1.92	0.98
1:A:399:ARG:HE	1:A:399:ARG:HA	1.29	0.97
1:A:1220:SER:N	1:A:1221:ALA:HB3	1.80	0.97
1:A:399:ARG:HB3	1:A:400:ASN:HB3	0.96	0.96
1:A:624:PRO:HA	1:A:625:ASP:HB2	1.45	0.96
1:A:723:ARG:HG2	1:A:723:ARG:NH1	1.77	0.95
1:A:1217:SER:CB	1:A:1221:ALA:HB2	1.97	0.95
1:A:1193:GLU:CA	1:A:1194:ASP:O	2.14	0.94
1:A:1186:MET:N	1:A:1187:LYS:HB3	1.83	0.94
1:A:457:LEU:HB3	1:A:458:TYR:HB3	1.48	0.94
1:A:838:PRO:HA	1:A:879:MET:HE1	1.50	0.94
1:A:705:GLU:OE2	1:A:1001:LYS:NZ	2.00	0.93
1:A:1217:SER:OG	1:A:1221:ALA:HB2	1.70	0.92
1:A:395:ALA:HB1	1:A:396:ALA:HA	1.52	0.91
1:A:399:ARG:CB	1:A:400:ASN:CB	2.48	0.90
1:A:456:THR:HG22	1:A:457:LEU:HA	1.53	0.90
1:A:439:LYS:CG	1:A:440:TYR:N	2.33	0.90
1:A:1194:ASP:CB	1:A:1195:GLY:HA2	1.98	0.90
1:A:828:PHE:CE1	1:A:1178:GLU:HG2	2.06	0.90
1:A:828:PHE:CG	1:A:1178:GLU:HG2	2.07	0.88
1:A:1210:PHE:O	1:A:1214:SER:CB	2.20	0.88
1:A:466:LYS:H	1:A:467:PRO:HA	1.39	0.88
1:A:1194:ASP:HB2	1:A:1195:GLY:CA	2.04	0.88
1:A:393:VAL:H	1:A:394:VAL:C	1.77	0.87
1:A:641:GLN:CB	1:A:642:ARG:CB	2.45	0.87
1:A:679:THR:CA	1:A:680:TYR:N	2.37	0.86
1:A:559:ALA:CB	1:A:562:GLU:OE1	2.23	0.86
1:A:1140:ALA:O	1:A:1141:LEU:O	1.94	0.86
1:A:828:PHE:CD2	1:A:1178:GLU:HG3	2.10	0.85
1:A:468:PHE:HA	1:A:469:PRO:O	1.76	0.85
1:A:879:MET:HE3	1:A:885:PRO:HG3	1.60	0.84
1:A:679:THR:C	1:A:680:TYR:CA	2.46	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:TRP:O	1:A:458:TYR:HB3	1.77	0.84
1:A:1217:SER:HB3	1:A:1221:ALA:HB2	1.59	0.83
1:A:417:ALA:HB1	1:A:576:VAL:HG13	1.60	0.83
1:A:922:MET:HE1	1:A:1011:ASP:HB3	1.61	0.83
1:A:559:ALA:HB1	1:A:562:GLU:OE1	1.78	0.82
1:A:828:PHE:CG	1:A:1178:GLU:CG	2.62	0.82
1:A:457:LEU:HB3	1:A:458:TYR:HB2	1.60	0.81
1:A:1159:PRO:HB3	1:A:1164:ASP:HB3	1.61	0.81
1:A:1186:MET:H	1:A:1187:LYS:CB	1.90	0.81
1:A:641:GLN:HB2	1:A:642:ARG:HB2	0.85	0.81
1:A:423:LEU:HD11	1:A:458:TYR:CE1	2.16	0.80
1:A:831:GLN:CG	1:A:844:TRP:CZ2	2.66	0.79
1:A:412:ALA:CB	1:A:413:PRO:CA	2.55	0.79
1:A:1315:HIS:HB2	1:A:1316:LYS:HB2	0.85	0.79
1:A:453:ILE:O	1:A:454:TRP:HD1	1.66	0.79
1:A:828:PHE:CD2	1:A:1178:GLU:CG	2.67	0.78
1:A:896:TRP:CE2	1:A:1186:MET:HE3	2.18	0.78
1:A:450:VAL:HG11	1:A:472:PRO:HD2	1.64	0.78
1:A:896:TRP:CZ2	1:A:1186:MET:CE	2.67	0.78
1:A:457:LEU:HD12	1:A:457:LEU:O	1.84	0.77
1:A:1112:GLY:O	1:A:1115:VAL:HG22	1.84	0.77
1:A:393:VAL:HG23	1:A:394:VAL:CG2	2.07	0.77
1:A:399:ARG:HB2	1:A:400:ASN:O	1.86	0.76
1:A:829:SER:HA	1:A:832:LYS:HE3	1.68	0.76
1:A:896:TRP:CE2	1:A:1186:MET:CE	2.68	0.75
1:A:576:VAL:O	1:A:576:VAL:HG12	1.87	0.75
1:A:796:LEU:HA	1:A:799:LEU:HD12	1.67	0.75
1:A:423:LEU:HD21	1:A:458:TYR:HD1	1.52	0.75
1:A:438:LEU:HA	1:A:439:LYS:HB2	1.66	0.75
1:A:831:GLN:HG3	1:A:844:TRP:CZ2	2.21	0.74
1:A:896:TRP:CH2	1:A:1183:HIS:ND1	2.55	0.74
1:A:399:ARG:HD2	1:A:507:THR:CG2	2.13	0.74
1:A:1214:SER:HA	1:A:1217:SER:OG	1.89	0.73
1:A:465:GLY:CA	1:A:466:LYS:HB2	2.16	0.72
1:A:408:TRP:HZ3	1:A:431:LEU:O	1.71	0.72
1:A:835:LEU:CD1	1:A:841:PHE:CE1	2.71	0.72
1:A:470:GLU:O	1:A:471:LYS:HB3	1.89	0.72
1:A:466:LYS:N	1:A:467:PRO:HA	2.06	0.71
1:A:831:GLN:HG2	1:A:844:TRP:CZ2	2.25	0.71
1:A:896:TRP:HH2	1:A:1183:HIS:ND1	1.81	0.71
1:A:503:ASP:O	1:A:504:ASN:CB	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:LEU:N	1:A:459:ARG:HB2	2.06	0.71
1:A:457:LEU:H	1:A:459:ARG:HB2	1.55	0.70
1:A:641:GLN:CA	1:A:642:ARG:HB2	2.20	0.70
1:A:903:CYS:SG	1:A:1179:LEU:HD21	2.31	0.70
1:A:879:MET:CE	1:A:885:PRO:HD3	2.22	0.70
1:A:1184:ASN:CA	1:A:1185:ALA:HB3	2.22	0.69
1:A:408:TRP:CZ3	1:A:431:LEU:O	2.45	0.69
1:A:498:LEU:HD22	1:A:513:VAL:HG22	1.75	0.69
1:A:667:LYS:CE	1:A:1119:LYS:O	2.35	0.69
1:A:1219:SER:C	1:A:1221:ALA:HB3	2.13	0.69
1:A:1253:PRO:HD2	1:A:1256:VAL:HB	1.73	0.69
1:A:399:ARG:HB2	1:A:400:ASN:CB	2.23	0.69
1:A:397:ARG:O	1:A:398:LEU:HB2	1.93	0.68
1:A:723:ARG:HH11	1:A:723:ARG:CG	1.87	0.68
1:A:395:ALA:HB1	1:A:396:ALA:CA	2.23	0.68
1:A:393:VAL:CG2	1:A:394:VAL:HG23	2.08	0.68
1:A:438:LEU:CA	1:A:439:LYS:CB	2.52	0.67
1:A:412:ALA:HB1	1:A:413:PRO:C	2.14	0.67
1:A:879:MET:HE3	1:A:885:PRO:CG	2.23	0.67
1:A:391:ALA:HB3	1:A:392:PRO:HA	1.76	0.66
1:A:831:GLN:HG2	1:A:844:TRP:CE2	2.31	0.66
1:A:453:ILE:O	1:A:454:TRP:CD1	2.48	0.66
1:A:560:ALA:HB1	1:A:563:GLU:HB3	1.78	0.65
1:A:456:THR:O	1:A:459:ARG:HD2	1.95	0.65
1:A:1217:SER:OG	1:A:1221:ALA:CB	2.44	0.65
1:A:459:ARG:O	1:A:461:ASP:N	2.23	0.64
1:A:942:LYS:HG3	1:A:949:SER:OG	1.97	0.64
1:A:605:LYS:HD2	1:A:605:LYS:H	1.63	0.64
1:A:796:LEU:HD12	1:A:797:GLN:N	2.12	0.63
1:A:418:TRP:CD1	1:A:518:LEU:HD13	2.32	0.63
1:A:1216:LYS:HE3	1:A:1216:LYS:HA	1.81	0.63
1:A:1180:GLU:OE1	1:A:1180:GLU:HA	1.99	0.63
1:A:624:PRO:CA	1:A:625:ASP:HB2	2.27	0.62
1:A:423:LEU:HD11	1:A:458:TYR:HE1	1.63	0.62
1:A:1220:SER:N	1:A:1221:ALA:CB	2.58	0.62
1:A:412:ALA:HB3	1:A:413:PRO:HA	1.82	0.62
1:A:626:VAL:N	1:A:627:PHE:HA	2.15	0.62
1:A:723:ARG:NH1	1:A:723:ARG:CG	2.53	0.62
1:A:390:HIS:CE1	1:A:566:GLN:HE22	2.18	0.61
1:A:922:MET:HE2	1:A:1012:MET:C	2.20	0.61
1:A:460:LEU:O	1:A:461:ASP:CB	2.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1202:ASP:O	1:A:1205:SER:HB2	1.99	0.61
1:A:828:PHE:CZ	1:A:1178:GLU:HG2	2.36	0.61
1:A:457:LEU:O	1:A:460:LEU:HB2	2.01	0.61
1:A:879:MET:HE3	1:A:885:PRO:CD	2.31	0.61
1:A:408:TRP:CH2	1:A:438:LEU:HD13	2.36	0.60
1:A:1186:MET:HB2	1:A:1187:LYS:HB2	1.82	0.60
1:A:1300:THR:HA	1:A:1303:LEU:HD23	1.82	0.60
1:A:723:ARG:NH1	1:A:724:ASP:OD1	2.33	0.60
1:A:797:GLN:O	1:A:797:GLN:HG3	1.97	0.60
1:A:509:PRO:O	1:A:510:LEU:HB3	2.01	0.60
1:A:399:ARG:HA	1:A:399:ARG:NE	2.10	0.60
1:A:1184:ASN:N	1:A:1185:ALA:CB	2.41	0.60
1:A:1207:TYR:CD2	1:A:1311:LYS:HG3	2.36	0.60
1:A:1184:ASN:CA	1:A:1185:ALA:CB	2.79	0.60
1:A:393:VAL:N	1:A:394:VAL:O	2.25	0.60
1:A:453:ILE:O	1:A:453:ILE:HG22	2.02	0.59
1:A:884:ASP:HB3	1:A:887:LYS:HB2	1.84	0.59
1:A:922:MET:CE	1:A:1012:MET:C	2.71	0.59
1:A:491:ALA:HB1	1:A:532:PRO:HB3	1.84	0.59
1:A:395:ALA:CB	1:A:396:ALA:HA	2.31	0.58
1:A:879:MET:HE2	1:A:885:PRO:HD3	1.84	0.58
1:A:393:VAL:N	1:A:394:VAL:C	2.54	0.58
1:A:1285:ILE:O	1:A:1289:GLU:HB2	2.03	0.58
1:A:828:PHE:CE2	1:A:1178:GLU:CG	2.87	0.58
1:A:861:VAL:HG13	1:A:873:GLU:HG2	1.86	0.58
1:A:879:MET:CE	1:A:885:PRO:CD	2.81	0.58
1:A:1235:GLU:HG2	1:A:1313:TYR:CZ	2.39	0.57
1:A:423:LEU:HD21	1:A:458:TYR:CD1	2.35	0.57
1:A:408:TRP:CD1	1:A:408:TRP:C	2.78	0.57
1:A:838:PRO:HA	1:A:879:MET:CE	2.31	0.57
1:A:922:MET:HE1	1:A:1011:ASP:CB	2.34	0.57
1:A:456:THR:O	1:A:459:ARG:NH1	2.38	0.56
1:A:547:SER:HB2	1:A:548:PRO:CA	2.35	0.56
1:A:622:PHE:HA	1:A:642:ARG:O	2.05	0.56
1:A:456:THR:HG22	1:A:457:LEU:CA	2.33	0.56
1:A:1186:MET:N	1:A:1187:LYS:CB	2.60	0.56
1:A:1315:HIS:HB2	1:A:1316:LYS:CA	2.36	0.56
1:A:1159:PRO:HB3	1:A:1164:ASP:CB	2.32	0.56
1:A:1259:ASN:O	1:A:1263:GLU:HG3	2.05	0.56
1:A:555:SER:O	1:A:555:SER:OG	2.21	0.56
1:A:454:TRP:O	1:A:458:TYR:CB	2.52	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:PRO:O	1:A:510:LEU:CB	2.53	0.55
1:A:899:GLN:HA	1:A:899:GLN:OE1	2.07	0.55
1:A:1193:GLU:N	1:A:1194:ASP:O	2.40	0.55
1:A:1217:SER:OG	1:A:1221:ALA:N	2.40	0.55
1:A:399:ARG:CB	1:A:400:ASN:CA	2.85	0.54
1:A:828:PHE:CD2	1:A:1178:GLU:HG2	2.36	0.54
1:A:624:PRO:HA	1:A:625:ASP:CB	2.27	0.54
1:A:466:LYS:HB3	1:A:467:PRO:O	2.08	0.54
1:A:1213:ILE:O	1:A:1216:LYS:HB3	2.08	0.53
1:A:580:TRP:HB3	1:A:614:PHE:HB3	1.90	0.53
1:A:438:LEU:CB	1:A:439:LYS:HB3	2.38	0.53
1:A:1210:PHE:O	1:A:1213:ILE:HG22	2.08	0.53
1:A:586:LYS:HG2	1:A:587:ASP:N	2.24	0.53
1:A:942:LYS:CG	1:A:949:SER:OG	2.56	0.53
1:A:417:ALA:CB	1:A:576:VAL:HG13	2.36	0.53
1:A:391:ALA:HB1	1:A:393:VAL:HG22	1.91	0.53
1:A:397:ARG:O	1:A:398:LEU:CB	2.56	0.53
1:A:1315:HIS:H	1:A:1315:HIS:CD2	2.26	0.52
1:A:1146:PRO:HB3	1:A:1148:TYR:CE2	2.44	0.52
1:A:451:THR:OG1	1:A:471:LYS:HE3	2.09	0.52
1:A:666:LEU:HD23	1:A:1072:SER:OG	2.10	0.52
1:A:1203:LEU:O	1:A:1307:SER:HB2	2.10	0.52
1:A:391:ALA:HB3	1:A:392:PRO:CA	2.40	0.51
1:A:843:GLN:NE2	1:A:1360:LYS:HA	2.25	0.51
1:A:890:TYR:CE2	1:A:894:ILE:HD11	2.45	0.51
1:A:605:LYS:HD2	1:A:605:LYS:N	2.25	0.51
1:A:458:TYR:CZ	1:A:465:GLY:O	2.64	0.51
1:A:465:GLY:HA2	1:A:466:LYS:CB	2.15	0.51
1:A:797:GLN:NE2	1:A:964:PRO:HB2	2.24	0.51
1:A:774:ASP:OD1	1:A:776:HIS:N	2.43	0.51
1:A:828:PHE:CE2	1:A:1178:GLU:HG3	2.45	0.51
1:A:859:GLY:O	1:A:860:ARG:HB3	2.11	0.51
1:A:1129:TRP:CZ2	1:A:1133:ARG:HD3	2.46	0.51
1:A:1194:ASP:OD2	1:A:1194:ASP:N	2.43	0.51
1:A:399:ARG:CD	1:A:507:THR:HG22	2.16	0.50
1:A:1219:SER:CA	1:A:1221:ALA:HB3	2.41	0.50
1:A:534:ARG:HD2	1:A:642:ARG:HD2	1.92	0.50
1:A:558:PRO:O	1:A:559:ALA:C	2.50	0.50
1:A:1186:MET:CA	1:A:1187:LYS:CB	2.90	0.50
1:A:427:CYS:O	1:A:428:LYS:HB2	2.10	0.50
1:A:967:PHE:CD2	1:A:1031:PRO:HG3	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1328:GLN:O	1:A:1332:ILE:HG13	2.12	0.50
1:A:439:LYS:O	1:A:440:TYR:HB2	2.11	0.50
1:A:1312:LEU:O	1:A:1315:HIS:CD2	2.64	0.50
1:A:917:SER:HA	1:A:1015:VAL:O	2.12	0.50
1:A:904:ASP:HA	1:A:907:LYS:HE2	1.93	0.50
1:A:400:ASN:C	1:A:400:ASN:OD1	2.50	0.49
1:A:1300:THR:HA	1:A:1303:LEU:CD2	2.42	0.49
1:A:803:GLU:O	1:A:809:LYS:HE2	2.12	0.49
1:A:991:PHE:CD2	1:A:999:LEU:HB3	2.48	0.49
1:A:576:VAL:O	1:A:576:VAL:CG1	2.58	0.48
1:A:450:VAL:HG12	1:A:471:LYS:HE2	1.94	0.48
1:A:679:THR:C	1:A:680:TYR:HA	2.31	0.48
1:A:457:LEU:CB	1:A:458:TYR:CB	2.78	0.48
1:A:498:LEU:O	1:A:541:PRO:HD3	2.13	0.48
1:A:524:CYS:SG	1:A:527:THR:HG23	2.53	0.48
1:A:872:GLU:HG3	1:A:898:LEU:HD11	1.95	0.48
1:A:1211:LYS:O	1:A:1214:SER:HB3	2.14	0.48
1:A:1317:SER:O	1:A:1321:VAL:HG12	2.13	0.48
1:A:1220:SER:H	1:A:1221:ALA:HB3	1.74	0.48
1:A:458:TYR:CE2	1:A:465:GLY:O	2.67	0.48
1:A:468:PHE:CA	1:A:469:PRO:O	2.56	0.47
1:A:705:GLU:HG2	1:A:998:PRO:HD2	1.95	0.47
1:A:1200:ASP:OD1	1:A:1202:ASP:HB2	2.15	0.47
1:A:458:TYR:N	1:A:459:ARG:C	2.68	0.47
1:A:406:PRO:HG3	1:A:431:LEU:HB3	1.97	0.47
1:A:900:LYS:HB2	1:A:900:LYS:HE3	1.58	0.47
1:A:464:ARG:HA	1:A:465:GLY:O	2.15	0.47
1:A:466:LYS:N	1:A:467:PRO:CA	2.77	0.47
1:A:721:ARG:O	1:A:725:VAL:HG13	2.15	0.47
1:A:796:LEU:HB3	1:A:910:LEU:HB2	1.96	0.47
1:A:828:PHE:CE2	1:A:1178:GLU:HG2	2.50	0.47
1:A:1224:PHE:CE2	1:A:1228:LYS:HE3	2.50	0.47
1:A:444:TRP:CE2	1:A:453:ILE:HG23	2.50	0.47
1:A:395:ALA:HA	1:A:397:ARG:O	2.15	0.46
1:A:399:ARG:HB2	1:A:400:ASN:CA	2.45	0.46
1:A:434:GLU:OE2	1:A:434:GLU:N	2.49	0.46
1:A:774:ASP:OD1	1:A:774:ASP:C	2.53	0.46
1:A:1169:SER:O	1:A:1173:PRO:HG2	2.15	0.46
1:A:1217:SER:OG	1:A:1221:ALA:CA	2.64	0.46
1:A:456:THR:O	1:A:459:ARG:HB2	2.16	0.46
1:A:456:THR:O	1:A:459:ARG:CD	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:TYR:H	1:A:459:ARG:C	2.19	0.46
1:A:457:LEU:HA	1:A:457:LEU:HD13	1.80	0.46
1:A:860:ARG:HA	1:A:1354:ALA:HB2	1.98	0.46
1:A:1186:MET:CB	1:A:1187:LYS:HB2	2.45	0.46
1:A:847:GLU:OE2	1:A:1360:LYS:NZ	2.42	0.46
1:A:456:THR:C	1:A:459:ARG:HB2	2.36	0.46
1:A:484:ASN:O	1:A:485:PHE:HB2	2.16	0.45
1:A:889:LYS:HG2	1:A:1198:PHE:CZ	2.50	0.45
1:A:966:HIS:ND1	1:A:1089:LYS:CE	2.79	0.45
1:A:1190:LYS:HG3	1:A:1191:ASP:H	1.81	0.45
1:A:712:GLY:O	1:A:746:TRP:HA	2.15	0.45
1:A:589:GLY:H	1:A:611:ARG:HH21	1.63	0.45
1:A:456:THR:O	1:A:459:ARG:CZ	2.64	0.45
1:A:738:ARG:HD3	1:A:743:LYS:HG2	1.99	0.45
1:A:1182:PHE:N	1:A:1182:PHE:CD2	2.83	0.45
1:A:622:PHE:CD1	1:A:622:PHE:N	2.84	0.45
1:A:1185:ALA:H	1:A:1188:ALA:HB2	1.81	0.45
1:A:723:ARG:HD3	1:A:730:ASP:C	2.37	0.45
1:A:952:LEU:HG	1:A:978:PHE:CD1	2.52	0.45
1:A:1140:ALA:O	1:A:1141:LEU:C	2.54	0.45
1:A:1193:GLU:CA	1:A:1194:ASP:C	2.84	0.45
1:A:467:PRO:HB2	1:A:468:PHE:H	1.53	0.45
1:A:666:LEU:CD2	1:A:1072:SER:HA	2.47	0.45
1:A:406:PRO:O	1:A:410:HIS:CD2	2.71	0.44
1:A:466:LYS:H	1:A:467:PRO:CA	2.18	0.44
1:A:1193:GLU:H	1:A:1194:ASP:C	2.20	0.44
1:A:414:LEU:HD13	1:A:485:PHE:CZ	2.53	0.44
1:A:547:SER:CB	1:A:548:PRO:CA	2.96	0.44
1:A:1182:PHE:HA	1:A:1185:ALA:CB	2.47	0.44
1:A:457:LEU:HD12	1:A:457:LEU:C	2.35	0.44
1:A:396:ALA:HB1	1:A:399:ARG:CZ	2.48	0.44
1:A:835:LEU:HD13	1:A:841:PHE:CD1	2.49	0.44
1:A:879:MET:HE3	1:A:885:PRO:HD3	1.93	0.44
1:A:1153:TRP:CE3	1:A:1168:PHE:CD1	3.05	0.44
1:A:1177:LYS:HB2	1:A:1177:LYS:HE2	1.67	0.44
1:A:959:LEU:HD22	1:A:1021:ILE:HG22	2.00	0.44
1:A:399:ARG:HB2	1:A:400:ASN:C	2.38	0.43
1:A:1102:LYS:N	1:A:1103:PRO:HD2	2.32	0.43
1:A:867:LEU:HD22	1:A:874:THR:HG23	1.99	0.43
1:A:1184:ASN:H	1:A:1185:ALA:HB3	0.71	0.43
1:A:464:ARG:HA	1:A:465:GLY:C	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:896:TRP:CE2	1:A:1186:MET:HE1	2.53	0.43
1:A:391:ALA:CB	1:A:393:VAL:HG22	2.47	0.43
1:A:444:TRP:CD1	1:A:453:ILE:HG23	2.54	0.43
1:A:456:THR:HG22	1:A:457:LEU:HD13	2.01	0.43
1:A:454:TRP:HA	1:A:457:LEU:HD23	2.01	0.43
1:A:792:ALA:HB2	1:A:918:ALA:HA	2.01	0.43
1:A:1080:ASN:CA	1:A:1081:PHE:N	2.75	0.43
1:A:1194:ASP:CB	1:A:1195:GLY:CA	2.76	0.43
1:A:1094:TYR:CE2	1:A:1146:PRO:HA	2.53	0.43
1:A:1141:LEU:HD13	1:A:1141:LEU:HA	1.89	0.43
1:A:1220:SER:H	1:A:1221:ALA:CB	2.29	0.43
1:A:1222:LEU:HD12	1:A:1222:LEU:HA	1.86	0.43
1:A:641:GLN:HB3	1:A:642:ARG:HB2	1.75	0.43
1:A:408:TRP:CH2	1:A:431:LEU:HD23	2.54	0.42
1:A:444:TRP:CD2	1:A:453:ILE:HG23	2.54	0.42
1:A:624:PRO:CA	1:A:625:ASP:CB	2.92	0.42
1:A:931:GLU:OE2	1:A:994:LYS:NZ	2.51	0.42
1:A:740:GLY:HA3	1:A:772:PHE:CE2	2.54	0.42
1:A:846:TYR:CD1	1:A:1358:PRO:HD2	2.54	0.42
1:A:1190:LYS:HG3	1:A:1191:ASP:N	2.34	0.42
1:A:419:GLU:OE1	1:A:422:ARG:HD3	2.20	0.42
1:A:966:HIS:HB3	1:A:1108:SER:OG	2.20	0.42
1:A:1299:ASN:O	1:A:1303:LEU:HD22	2.19	0.42
1:A:467:PRO:HG2	1:A:468:PHE:HD2	1.85	0.42
1:A:547:SER:CB	1:A:548:PRO:HA	2.50	0.42
1:A:559:ALA:HB2	1:A:562:GLU:OE1	2.13	0.42
1:A:772:PHE:O	1:A:778:ARG:CD	2.67	0.42
1:A:454:TRP:O	1:A:458:TYR:CG	2.72	0.42
1:A:852:ARG:O	1:A:856:VAL:HG23	2.19	0.42
1:A:426:HIS:HB3	1:A:469:PRO:HD3	2.02	0.42
1:A:457:LEU:CB	1:A:458:TYR:HB3	2.33	0.42
1:A:696:ASP:HB3	1:A:706:VAL:HG13	2.02	0.42
1:A:793:GLY:HA2	1:A:914:VAL:H	1.84	0.42
1:A:531:GLY:HA2	1:A:532:PRO:HD3	1.86	0.41
1:A:444:TRP:HZ2	1:A:456:THR:HG21	1.84	0.41
1:A:457:LEU:CB	1:A:458:TYR:HB2	2.40	0.41
1:A:470:GLU:O	1:A:471:LYS:CB	2.64	0.41
1:A:799:LEU:HB2	1:A:800:PRO:HD3	2.03	0.41
1:A:1182:PHE:HA	1:A:1185:ALA:HB1	2.01	0.41
1:A:464:ARG:HA	1:A:464:ARG:HD2	1.70	0.41
1:A:828:PHE:CD1	1:A:1178:GLU:CG	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:828:PHE:CZ	1:A:1178:GLU:CG	3.03	0.41
1:A:1207:TYR:CE2	1:A:1311:LYS:HG3	2.55	0.41
1:A:1183:HIS:HA	1:A:1186:MET:HG3	2.03	0.41
1:A:1252:ASP:O	1:A:1252:ASP:CG	2.58	0.41
1:A:485:PHE:HB3	1:A:532:PRO:HB2	2.02	0.41
1:A:860:ARG:HA	1:A:1354:ALA:CB	2.50	0.41
1:A:660:ASN:OD1	1:A:768:TRP:HB2	2.21	0.41
1:A:861:VAL:CG1	1:A:873:GLU:HG2	2.49	0.41
1:A:946:GLU:HB3	1:A:947:GLU:H	1.78	0.41
1:A:884:ASP:HA	1:A:885:PRO:HD2	1.92	0.41
1:A:661:THR:HA	1:A:1047:PHE:HB3	2.03	0.40
1:A:1089:LYS:HB2	1:A:1107:LEU:HB3	2.03	0.40
1:A:1146:PRO:CB	1:A:1148:TYR:CE2	3.04	0.40
1:A:394:VAL:HA	1:A:395:ALA:HA	1.76	0.40
1:A:423:LEU:HD11	1:A:458:TYR:CD1	2.53	0.40
1:A:1265:TRP:CZ2	1:A:1325:ALA:HB2	2.56	0.40
1:A:794:LEU:HD11	1:A:802:LEU:HD11	2.03	0.40
1:A:460:LEU:O	1:A:461:ASP:HB3	2.19	0.40
1:A:514:LYS:HB3	1:A:514:LYS:HE3	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	921/1022 (90%)	829 (90%)	53 (6%)	39 (4%)	3	23

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	399	ARG
1	A	412	ALA

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Mol	Chain	Res	Type
1	A	439	LYS
1	A	440	TYR
1	A	459	ARG
1	A	460	LEU
1	A	466	LYS
1	A	467	PRO
1	A	504	ASN
1	A	510	LEU
1	A	547	SER
1	A	553	VAL
1	A	621	THR
1	A	625	ASP
1	A	642	ARG
1	A	1140	ALA
1	A	1141	LEU
1	A	1193	GLU
1	A	1194	ASP
1	A	394	VAL
1	A	398	LEU
1	A	461	ASP
1	A	503	ASP
1	A	1138	GLY
1	A	1162	ILE
1	A	1185	ALA
1	A	1187	LYS
1	A	1214	SER
1	A	1316	LYS
1	A	559	ALA
1	A	1218	ARG
1	A	1315	HIS
1	A	458	TYR
1	A	469	PRO
1	A	471	LYS
1	A	488	LYS
1	A	468	PHE
1	A	453	ILE
1	A	1253	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	815/891 (92%)	748 (92%)	67 (8%)	11	40

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	393	VAL
1	A	394	VAL
1	A	399	ARG
1	A	408	TRP
1	A	409	LEU
1	A	414	LEU
1	A	456	THR
1	A	457	LEU
1	A	458	TYR
1	A	482	THR
1	A	504	ASN
1	A	507	THR
1	A	515	LEU
1	A	518	LEU
1	A	526	LEU
1	A	546	THR
1	A	547	SER
1	A	553	VAL
1	A	555	SER
1	A	605	LYS
1	A	622	PHE
1	A	623	ARG
1	A	701	SER
1	A	716	ARG
1	A	725	VAL
1	A	726	LEU
1	A	730	ASP
1	A	755	ASP
1	A	774	ASP
1	A	796	LEU
1	A	797	GLN
1	A	798	LEU
1	A	835	LEU
1	A	839	VAL

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Mol	Chain	Res	Type
1	A	891	LEU
1	A	896	TRP
1	A	947	GLU
1	A	949	SER
1	A	952	LEU
1	A	953	LEU
1	A	955	ASP
1	A	959	LEU
1	A	999	LEU
1	A	1032	LEU
1	A	1056	THR
1	A	1134	ARG
1	A	1137	LEU
1	A	1141	LEU
1	A	1172	ARG
1	A	1182	PHE
1	A	1187	LYS
1	A	1193	GLU
1	A	1194	ASP
1	A	1203	LEU
1	A	1211	LYS
1	A	1214	SER
1	A	1216	LYS
1	A	1217	SER
1	A	1218	ARG
1	A	1223	LEU
1	A	1235	GLU
1	A	1240	ARG
1	A	1269	THR
1	A	1282	SER
1	A	1303	LEU
1	A	1317	SER
1	A	1321	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	390	HIS
1	A	557	GLN
1	A	566	GLN
1	A	579	GLN
1	A	665	HIS

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Mol	Chain	Res	Type
1	A	843	GLN
1	A	871	GLN
1	A	1120	GLN
1	A	1315	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	7

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	908:SER	C	909:LYS	N	3.26
1	A	1189:ALA	C	1190:LYS	N	2.78
1	A	1042:LYS	C	1043:ASP	N	1.97
1	A	1080:ASN	C	1081:PHE	N	1.76
1	A	679:THR	C	680:TYR	N	1.70
1	A	436:LEU	C	437:GLY	N	1.62
1	A	888:GLN	C	889:LYS	N	1.62

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	935/1022 (91%)	-0.04	34 (3%)	42	38	44, 119, 150, 150	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	909	LYS	5.1
1	A	1142	SER	4.5
1	A	437	GLY	4.3
1	A	1191	ASP	3.7
1	A	461	ASP	3.4
1	A	1190	LYS	3.3
1	A	455	LYS	3.2
1	A	462	ALA	3.0
1	A	1187	LYS	3.0
1	A	1194	ASP	3.0
1	A	448	ARG	3.0
1	A	1186	MET	3.0
1	A	703	THR	2.9
1	A	507	THR	2.8
1	A	546	THR	2.8
1	A	604	PRO	2.7
1	A	433	ASP	2.6
1	A	436	LEU	2.6
1	A	1119	LYS	2.5
1	A	1185	ALA	2.5
1	A	1007	ASP	2.5
1	A	1192	THR	2.5
1	A	589	GLY	2.4
1	A	547	SER	2.4
1	A	1188	ALA	2.4
1	A	466	LYS	2.3
1	A	545	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1282	SER	2.2
1	A	1184	ASN	2.2
1	A	1144	PRO	2.1
1	A	447	ALA	2.1
1	A	421	THR	2.1
1	A	467	PRO	2.1
1	A	419	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 monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	A	2373	1/1	0.13	0.34	150,150,150,150	0

6.5 Other polymers ⓘ

There are no such residues in this entry.