



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:27 AM UTC

PDB ID : 7W82 / pdb_00007w82
Title : Crystal structure of maize RDR2
Authors : Du, X.; Yang, Z.; Du, J.
Deposited on : 2021-12-07
Resolution : 3.10 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

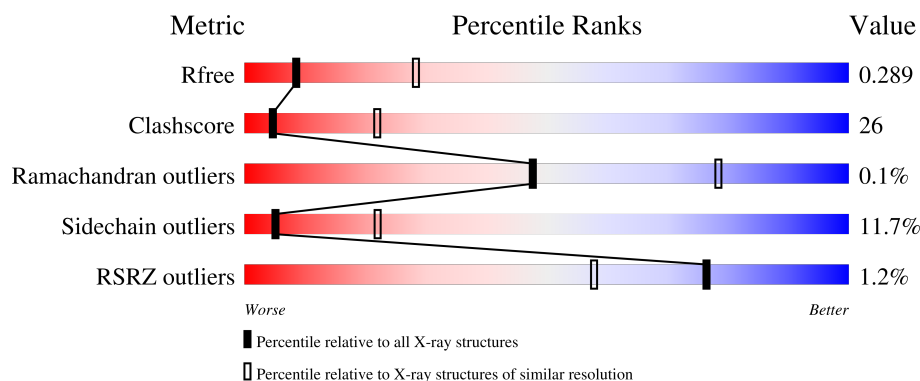
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	A	1024	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7492 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	944	Total	C	N	O	S	0	0	0
			7492	4758	1303	1384	47			

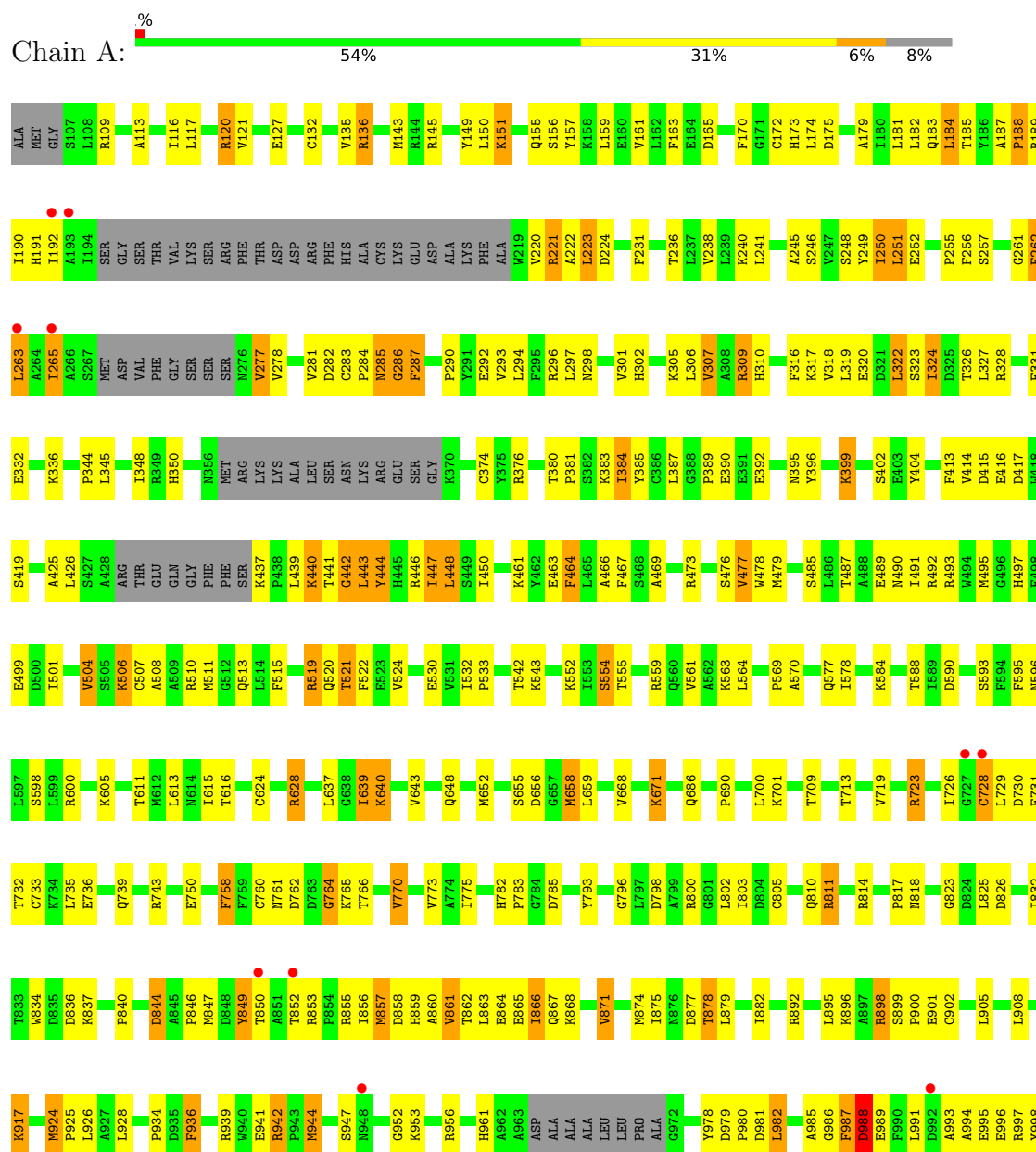
There are 8 discrepancies between the modelled and reference sequences:

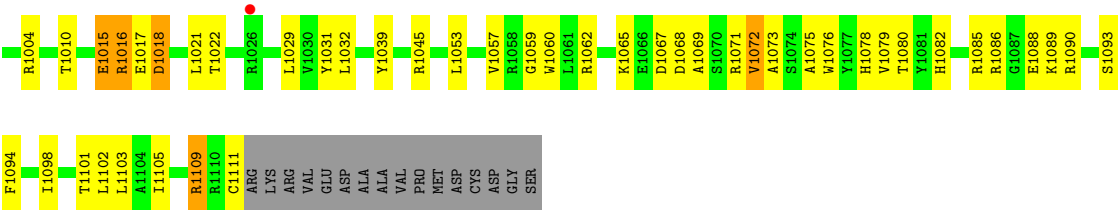
Chain	Residue	Modelled	Actual	Comment	Reference
A	104	ALA	-	expression tag	UNP Q19VG2
A	105	MET	-	expression tag	UNP Q19VG2
A	106	GLY	-	expression tag	UNP Q19VG2
A	841	ALA	GLU	engineered mutation	UNP Q19VG2
A	842	ALA	LYS	engineered mutation	UNP Q19VG2
A	962	ALA	GLU	engineered mutation	UNP Q19VG2
A	963	ALA	GLU	engineered mutation	UNP Q19VG2
A	966	ALA	GLU	engineered mutation	UNP Q19VG2

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	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	149.04Å 149.04Å 345.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.02 – 3.10 43.02 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.02-3.10) 99.6 (43.02-3.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.230 , 0.270 0.258 , 0.289	Depositor DCC
R_{free} test set	1357 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	83.8	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 61.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k +1/3*l 0.000 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/ 3*k+1/3*l 0.016 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+ 1/3*l,-4/3*h+4/3*k+1/3*l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7492	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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	A	0.77	3/7657 (0.0%)	0.96	16/10352 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	979	ASP	CA-C	-6.01	1.45	1.52
1	A	847	MET	CA-C	-5.62	1.45	1.52
1	A	188	PRO	N-CD	5.07	1.54	1.47

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	860	ALA	N-CA-C	-9.82	97.86	110.53
1	A	892	ARG	N-CA-C	8.00	119.78	111.14
1	A	985	ALA	N-CA-C	7.80	119.78	111.28
1	A	263	LEU	N-CA-C	7.60	120.33	110.53
1	A	785	ASP	N-CA-C	-7.21	103.95	112.89
1	A	861	VAL	N-CA-C	7.12	119.07	108.54
1	A	936	PHE	N-CA-C	6.81	118.78	111.36
1	A	286	GLY	N-CA-C	6.74	120.82	112.73
1	A	184	LEU	N-CA-C	5.64	117.71	108.52
1	A	944	MET	N-CA-C	5.63	118.25	109.52
1	A	442	GLY	CA-C-N	-5.52	112.89	120.28
1	A	442	GLY	C-N-CA	-5.52	112.89	120.28
1	A	262	GLU	N-CA-C	5.31	116.91	108.79
1	A	978	TYR	N-CA-C	-5.29	102.45	110.28
1	A	764	GLY	N-CA-C	-5.07	109.05	115.08
1	A	934	PRO	N-CA-C	5.01	118.24	111.22

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	7492	0	7444	385	0
All	All	7492	0	7444	385	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 26.

All (385) 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:448:LEU:HD21	1:A:868:LYS:HD3	1.19	1.17
1:A:189:ARG:CG	1:A:221:ARG:HH12	1.61	1.14
1:A:818:ASN:HA	1:A:823:GLY:HA3	1.24	1.12
1:A:444:TYR:CD2	1:A:875:ILE:HD11	1.90	1.07
1:A:189:ARG:HG3	1:A:221:ARG:NH1	1.70	1.06
1:A:189:ARG:HB3	1:A:221:ARG:HH22	1.15	1.05
1:A:189:ARG:HG3	1:A:221:ARG:HH12	0.91	1.05
1:A:223:LEU:H	1:A:223:LEU:HD12	1.24	0.99
1:A:425:ALA:O	1:A:443:LEU:HD12	1.62	0.99
1:A:758:PHE:O	1:A:770:VAL:HG23	1.63	0.98
1:A:489:GLU:HG2	1:A:493:ARG:HH21	1.25	0.98
1:A:760:CYS:SG	1:A:761:ASN:N	2.32	0.95
1:A:187:ALA:HB3	1:A:416:GLU:OE1	1.67	0.95
1:A:121:VAL:HG21	1:A:309:ARG:HH22	1.31	0.94
1:A:760:CYS:HB3	1:A:770:VAL:HG21	1.47	0.94
1:A:448:LEU:HD21	1:A:868:LYS:CD	1.98	0.94
1:A:189:ARG:HB3	1:A:221:ARG:NH2	1.84	0.92
1:A:818:ASN:CA	1:A:823:GLY:HA3	2.00	0.91
1:A:309:ARG:HH11	1:A:309:ARG:HG2	1.36	0.90
1:A:444:TYR:HD2	1:A:875:ILE:HD11	1.37	0.90
1:A:1069:ALA:HA	1:A:1072:VAL:CG2	2.02	0.90
1:A:817:PRO:O	1:A:823:GLY:HA2	1.72	0.89
1:A:121:VAL:CG2	1:A:309:ARG:HH22	1.86	0.88
1:A:1086:ARG:HB2	1:A:1089:LYS:HE2	1.57	0.87
1:A:1004:ARG:HH11	1:A:1004:ARG:HG3	1.40	0.86
1:A:878:THR:O	1:A:882:ILE:HG13	1.76	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:862:THR:HG23	1:A:865:GLU:OE2	1.76	0.86
1:A:192:ILE:HG12	1:A:222:ALA:HB2	1.57	0.86
1:A:174:LEU:HD12	1:A:240:LYS:HD2	1.54	0.86
1:A:1065:LYS:HD3	1:A:1067:ASP:OD2	1.75	0.86
1:A:444:TYR:CE2	1:A:875:ILE:HD11	2.12	0.85
1:A:1069:ALA:C	1:A:1072:VAL:HG23	2.02	0.84
1:A:324:ILE:HD12	1:A:324:ILE:O	1.77	0.84
1:A:1069:ALA:HA	1:A:1072:VAL:HG23	1.58	0.84
1:A:1069:ALA:O	1:A:1072:VAL:HG23	1.77	0.83
1:A:862:THR:O	1:A:866:ILE:HD13	1.79	0.82
1:A:293:VAL:HG22	1:A:327:LEU:HD23	1.60	0.82
1:A:277:VAL:HG11	1:A:384:ILE:HD12	1.62	0.81
1:A:310:HIS:HD2	1:A:344:PRO:HD2	1.46	0.81
1:A:552:LYS:HG3	1:A:598:SER:HB2	1.64	0.80
1:A:1069:ALA:CA	1:A:1072:VAL:HG23	2.12	0.80
1:A:817:PRO:O	1:A:823:GLY:CA	2.30	0.80
1:A:1065:LYS:CB	1:A:1068:ASP:HB2	2.12	0.80
1:A:1065:LYS:HB3	1:A:1068:ASP:HB2	1.63	0.79
1:A:817:PRO:C	1:A:823:GLY:HA2	2.07	0.79
1:A:192:ILE:HD11	1:A:222:ALA:HB3	1.65	0.79
1:A:489:GLU:HG3	1:A:493:ARG:HE	1.48	0.78
1:A:121:VAL:HG21	1:A:309:ARG:NH2	1.98	0.78
1:A:504:VAL:HG23	1:A:866:ILE:HD12	1.64	0.78
1:A:998:TYR:CE2	1:A:1089:LYS:HD2	2.19	0.77
1:A:282:ASP:OD2	1:A:283:CYS:N	2.18	0.77
1:A:656:ASP:OD2	1:A:961:HIS:CE1	2.37	0.77
1:A:135:VAL:HG22	1:A:150:LEU:HD13	1.67	0.77
1:A:113:ALA:HB2	1:A:241:LEU:HD23	1.69	0.74
1:A:121:VAL:CG1	1:A:309:ARG:HH12	1.99	0.74
1:A:223:LEU:HD12	1:A:223:LEU:N	2.02	0.74
1:A:817:PRO:C	1:A:823:GLY:CA	2.60	0.74
1:A:733:CYS:HB2	1:A:810:GLN:OE1	1.87	0.74
1:A:628:ARG:NH1	1:A:713:THR:O	2.21	0.73
1:A:309:ARG:HG2	1:A:309:ARG:NH1	2.03	0.73
1:A:1004:ARG:HG3	1:A:1004:ARG:NH1	2.01	0.73
1:A:600:ARG:NH2	1:A:731:GLU:OE2	2.22	0.72
1:A:192:ILE:HG12	1:A:222:ALA:CB	2.20	0.72
1:A:174:LEU:HD13	1:A:175:ASP:OD2	1.89	0.72
1:A:761:ASN:ND2	1:A:793:TYR:CZ	2.58	0.71
1:A:1065:LYS:O	1:A:1068:ASP:N	2.24	0.71
1:A:987:PHE:O	1:A:988:ASP:HB2	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ARG:NH2	1:A:252:GLU:OE1	2.22	0.70
1:A:413:PHE:HB2	1:A:874:MET:HE1	1.72	0.70
1:A:690:PRO:HG3	1:A:700:LEU:HD12	1.72	0.70
1:A:121:VAL:HG13	1:A:309:ARG:HH12	1.56	0.70
1:A:192:ILE:N	1:A:220:VAL:O	2.21	0.70
1:A:336:LYS:HE2	1:A:1010:THR:HG21	1.72	0.70
1:A:344:PRO:O	1:A:348:ILE:HD12	1.92	0.70
1:A:319:LEU:O	1:A:322:LEU:CB	2.39	0.69
1:A:506:LYS:HD3	1:A:917:LYS:HE3	1.74	0.69
1:A:760:CYS:HB3	1:A:770:VAL:CG2	2.20	0.69
1:A:285:ASN:HD22	1:A:285:ASN:N	1.91	0.69
1:A:323:SER:O	1:A:326:THR:HG22	1.92	0.69
1:A:1069:ALA:HA	1:A:1072:VAL:HG21	1.74	0.67
1:A:189:ARG:CB	1:A:221:ARG:HH22	2.02	0.67
1:A:1015:GLU:HG2	1:A:1016:ARG:HG3	1.75	0.67
1:A:469:ALA:O	1:A:473:ARG:NH1	2.27	0.67
1:A:1069:ALA:O	1:A:1072:VAL:N	2.27	0.67
1:A:1079:VAL:O	1:A:1089:LYS:NZ	2.25	0.66
1:A:293:VAL:HG22	1:A:327:LEU:CD2	2.25	0.66
1:A:997:ARG:HG3	1:A:1060:TRP:CE3	2.31	0.66
1:A:323:SER:OG	1:A:326:THR:HG22	1.95	0.66
1:A:165:ASP:OD2	1:A:189:ARG:NH1	2.29	0.65
1:A:183:GLN:C	1:A:184:LEU:HD12	2.20	0.65
1:A:444:TYR:CE2	1:A:875:ILE:CD1	2.79	0.65
1:A:1098:ILE:HG22	1:A:1101:THR:HB	1.78	0.65
1:A:446:ARG:O	1:A:450:ILE:HG12	1.97	0.65
1:A:157:TYR:CD1	1:A:192:ILE:HD12	2.32	0.65
1:A:426:LEU:HA	1:A:441:THR:CG2	2.27	0.65
1:A:1086:ARG:HB2	1:A:1089:LYS:CE	2.25	0.65
1:A:426:LEU:HA	1:A:441:THR:HG21	1.79	0.65
1:A:761:ASN:ND2	1:A:793:TYR:CE2	2.65	0.65
1:A:1021:LEU:HD11	1:A:1093:SER:OG	1.97	0.64
1:A:307:VAL:HG21	1:A:310:HIS:ND1	2.12	0.64
1:A:510:ARG:HD2	1:A:605:LYS:HB3	1.80	0.64
1:A:344:PRO:C	1:A:348:ILE:HD12	2.22	0.64
1:A:732:THR:HG22	1:A:800:ARG:HH11	1.62	0.64
1:A:941:GLU:HG2	1:A:942:ARG:HG2	1.78	0.64
1:A:648:GLN:O	1:A:652:MET:HG3	1.97	0.64
1:A:174:LEU:CD1	1:A:240:LYS:HD2	2.27	0.64
1:A:192:ILE:CD1	1:A:222:ALA:HB3	2.28	0.64
1:A:489:GLU:CG	1:A:493:ARG:HE	2.10	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:GLU:HG2	1:A:493:ARG:NH2	2.06	0.63
1:A:324:ILE:HD12	1:A:324:ILE:C	2.22	0.63
1:A:189:ARG:HH21	1:A:417:ASP:CG	2.07	0.62
1:A:302:HIS:HD1	1:A:385:TYR:HA	1.65	0.62
1:A:1102:LEU:O	1:A:1105:ILE:HG12	1.98	0.62
1:A:743:ARG:HG2	1:A:803:ILE:HG13	1.80	0.62
1:A:1086:ARG:HD2	1:A:1089:LYS:HE3	1.82	0.61
1:A:628:ARG:NH2	1:A:936:PHE:HB2	2.16	0.61
1:A:862:THR:CG2	1:A:865:GLU:OE2	2.47	0.61
1:A:861:VAL:HG12	1:A:866:ILE:CD1	2.30	0.61
1:A:862:THR:OG1	1:A:865:GLU:N	2.21	0.61
1:A:993:ALA:O	1:A:996:GLU:HB2	2.00	0.61
1:A:121:VAL:CG2	1:A:309:ARG:NH2	2.58	0.61
1:A:285:ASN:ND2	1:A:286:GLY:H	1.99	0.61
1:A:448:LEU:HD22	1:A:871:VAL:HG21	1.83	0.61
1:A:310:HIS:CD2	1:A:344:PRO:HD2	2.33	0.60
1:A:563:LYS:HB2	1:A:569:PRO:HG3	1.82	0.60
1:A:189:ARG:CB	1:A:221:ARG:HH12	2.14	0.60
1:A:997:ARG:HG3	1:A:1060:TRP:CZ3	2.36	0.60
1:A:659:LEU:HD21	1:A:701:LYS:HG2	1.82	0.60
1:A:861:VAL:CG1	1:A:866:ILE:HD11	2.32	0.59
1:A:1086:ARG:CB	1:A:1089:LYS:HE2	2.31	0.59
1:A:285:ASN:HD22	1:A:285:ASN:H	1.50	0.59
1:A:319:LEU:O	1:A:322:LEU:HB2	2.02	0.59
1:A:425:ALA:HB1	1:A:443:LEU:CD1	2.33	0.58
1:A:590:ASP:OD2	1:A:800:ARG:NH2	2.36	0.58
1:A:319:LEU:HA	1:A:322:LEU:HB2	1.84	0.58
1:A:157:TYR:HE1	1:A:192:ILE:HG23	1.66	0.58
1:A:425:ALA:O	1:A:443:LEU:CD1	2.45	0.58
1:A:489:GLU:HG3	1:A:493:ARG:NE	2.17	0.58
1:A:1075:ALA:O	1:A:1079:VAL:HG13	2.04	0.57
1:A:192:ILE:CG1	1:A:222:ALA:CB	2.81	0.57
1:A:709:THR:O	1:A:713:THR:OG1	2.23	0.57
1:A:287:PHE:N	1:A:287:PHE:CD1	2.72	0.57
1:A:1069:ALA:O	1:A:1072:VAL:CG2	2.51	0.57
1:A:296:ARG:HE	1:A:389:PRO:HD2	1.69	0.57
1:A:743:ARG:NH2	1:A:798:ASP:O	2.38	0.56
1:A:307:VAL:HG21	1:A:310:HIS:CE1	2.41	0.56
1:A:223:LEU:H	1:A:223:LEU:CD1	2.06	0.56
1:A:817:PRO:C	1:A:823:GLY:HA3	2.28	0.56
1:A:658:MET:HE2	1:A:700:LEU:HD22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:LEU:HD13	1:A:175:ASP:CG	2.31	0.56
1:A:1073:ALA:O	1:A:1076:TRP:HB2	2.05	0.56
1:A:497:HIS:ND1	1:A:499:GLU:OE2	2.39	0.56
1:A:249:TYR:CD1	1:A:250:ILE:CD1	2.89	0.55
1:A:1101:THR:O	1:A:1105:ILE:HG23	2.06	0.55
1:A:762:ASP:OD1	1:A:764:GLY:N	2.37	0.55
1:A:988:ASP:HA	1:A:991:LEU:HD13	1.89	0.55
1:A:818:ASN:N	1:A:823:GLY:HA3	2.22	0.54
1:A:293:VAL:CG2	1:A:327:LEU:CD2	2.85	0.54
1:A:1065:LYS:CB	1:A:1068:ASP:CB	2.85	0.54
1:A:1065:LYS:HB2	1:A:1068:ASP:HB2	1.89	0.54
1:A:163:PHE:CD2	1:A:255:PRO:HD3	2.43	0.54
1:A:994:ALA:HB3	1:A:1079:VAL:HG11	1.90	0.54
1:A:861:VAL:CG1	1:A:866:ILE:CD1	2.85	0.54
1:A:157:TYR:CE1	1:A:192:ILE:HG23	2.42	0.54
1:A:506:LYS:O	1:A:510:ARG:HG2	2.07	0.54
1:A:991:LEU:HD22	1:A:1085:ARG:NH1	2.23	0.54
1:A:132:CYS:SG	1:A:150:LEU:HD11	2.48	0.54
1:A:189:ARG:N	1:A:189:ARG:CD	2.71	0.54
1:A:521:THR:OG1	1:A:613:LEU:O	2.22	0.54
1:A:182:LEU:HB3	1:A:184:LEU:HD11	1.90	0.53
1:A:464:PHE:C	1:A:464:PHE:CD2	2.86	0.53
1:A:655:SER:O	1:A:658:MET:HG3	2.09	0.53
1:A:686:GLN:HG3	1:A:1103:LEU:HD22	1.90	0.53
1:A:159:LEU:HD21	1:A:231:PHE:CZ	2.43	0.53
1:A:189:ARG:NH2	1:A:417:ASP:CG	2.66	0.53
1:A:223:LEU:O	1:A:224:ASP:C	2.51	0.53
1:A:444:TYR:C	1:A:444:TYR:CD1	2.86	0.53
1:A:773:VAL:HG12	1:A:834:TRP:HB3	1.89	0.53
1:A:510:ARG:HH22	1:A:917:LYS:HZ1	1.56	0.53
1:A:554:SER:HB3	1:A:596:ASN:HA	1.90	0.53
1:A:882:ILE:HD13	1:A:908:LEU:HB3	1.90	0.53
1:A:1076:TRP:O	1:A:1079:VAL:HG22	2.09	0.53
1:A:448:LEU:CD2	1:A:868:LYS:HD3	2.13	0.53
1:A:425:ALA:O	1:A:441:THR:HG21	2.09	0.52
1:A:861:VAL:HG12	1:A:866:ILE:HD11	1.92	0.52
1:A:294:LEU:HA	1:A:297:LEU:HD12	1.92	0.52
1:A:120:ARG:HD3	1:A:181:LEU:HD21	1.92	0.52
1:A:157:TYR:CE1	1:A:192:ILE:HD12	2.44	0.52
1:A:998:TYR:HA	1:A:1094:PHE:CE1	2.44	0.52
1:A:413:PHE:CG	1:A:447:ILE:CG2	2.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:ASP:OD2	1:A:961:HIS:NE2	2.41	0.52
1:A:290:PRO:HG2	1:A:293:VAL:HG23	1.92	0.52
1:A:866:ILE:CD1	1:A:866:ILE:N	2.73	0.52
1:A:1032:LEU:HD13	1:A:1039:TYR:HD1	1.74	0.52
1:A:121:VAL:HG11	1:A:309:ARG:HH12	1.75	0.52
1:A:307:VAL:CG2	1:A:310:HIS:ND1	2.73	0.52
1:A:504:VAL:O	1:A:507:CYS:HB3	2.10	0.51
1:A:862:THR:OG1	1:A:865:GLU:OE2	2.28	0.51
1:A:1059:GLY:O	1:A:1060:TRP:C	2.49	0.51
1:A:292:GLU:HG3	1:A:389:PRO:HG2	1.91	0.51
1:A:319:LEU:C	1:A:322:LEU:HB2	2.35	0.51
1:A:319:LEU:CA	1:A:322:LEU:HB2	2.40	0.51
1:A:161:VAL:HG22	1:A:188:PRO:HB3	1.92	0.51
1:A:172:CYS:HG	1:A:179:ALA:C	2.19	0.51
1:A:997:ARG:CG	1:A:1060:TRP:CE3	2.93	0.51
1:A:444:TYR:HE2	1:A:875:ILE:CD1	2.23	0.51
1:A:116:ILE:HB	1:A:238:VAL:HB	1.93	0.51
1:A:283:CYS:SG	1:A:284:PRO:HD2	2.51	0.51
1:A:732:THR:CG2	1:A:800:ARG:HH11	2.24	0.51
1:A:464:PHE:HA	1:A:479:MET:HG2	1.92	0.50
1:A:489:GLU:HA	1:A:492:ARG:HG3	1.92	0.50
1:A:899:SER:O	1:A:902:CYS:N	2.43	0.50
1:A:467:PHE:CZ	1:A:508:ALA:HB1	2.46	0.50
1:A:844:ASP:OD1	1:A:898:ARG:NH1	2.45	0.50
1:A:191:HIS:C	1:A:192:ILE:HD13	2.36	0.50
1:A:285:ASN:ND2	1:A:286:GLY:N	2.60	0.50
1:A:318:VAL:O	1:A:322:LEU:HB2	2.12	0.49
1:A:413:PHE:CD1	1:A:447:ILE:HG23	2.47	0.49
1:A:668:VAL:HA	1:A:671:LYS:HE3	1.95	0.49
1:A:521:THR:HG21	1:A:561:VAL:HG13	1.95	0.49
1:A:995:GLU:OE2	1:A:1079:VAL:HB	2.13	0.49
1:A:310:HIS:HD2	1:A:344:PRO:CD	2.20	0.49
1:A:376:ARG:HB2	1:A:387:LEU:HB2	1.94	0.49
1:A:584:LYS:HE3	1:A:605:LYS:HE3	1.95	0.49
1:A:939:ARG:HB3	1:A:942:ARG:HG3	1.95	0.49
1:A:293:VAL:CG2	1:A:327:LEU:HD23	2.38	0.49
1:A:425:ALA:HB1	1:A:443:LEU:HD13	1.94	0.49
1:A:796:GLY:O	1:A:800:ARG:HG3	2.13	0.49
1:A:322:LEU:HB3	1:A:327:LEU:HD13	1.94	0.48
1:A:542:THR:HG21	1:A:849:TYR:CD2	2.48	0.48
1:A:1109:ARG:O	1:A:1111:CYS:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ASN:O	1:A:302:HIS:HD2	1.96	0.48
1:A:302:HIS:HE1	1:A:384:ILE:HG23	1.79	0.48
1:A:417:ASP:OD1	1:A:419:SER:OG	2.24	0.48
1:A:998:TYR:HD1	1:A:1094:PHE:CD1	2.32	0.48
1:A:189:ARG:CG	1:A:221:ARG:NH1	2.45	0.47
1:A:374:CYS:O	1:A:389:PRO:HA	2.14	0.47
1:A:590:ASP:HB3	1:A:593:SER:HB2	1.95	0.47
1:A:765:LYS:C	1:A:766:THR:CG2	2.87	0.47
1:A:1109:ARG:C	1:A:1109:ARG:HD3	2.40	0.47
1:A:191:HIS:HA	1:A:221:ARG:HA	1.96	0.47
1:A:640:LYS:O	1:A:643:VAL:HG22	2.14	0.47
1:A:1015:GLU:HG2	1:A:1016:ARG:CG	2.43	0.47
1:A:189:ARG:HB3	1:A:221:ARG:CZ	2.42	0.47
1:A:861:VAL:HG11	1:A:866:ILE:HD11	1.96	0.47
1:A:905:LEU:HD22	1:A:924:MET:HE1	1.97	0.47
1:A:287:PHE:HE2	1:A:317:LYS:HB2	1.78	0.47
1:A:307:VAL:HG23	1:A:310:HIS:CG	2.50	0.47
1:A:732:THR:O	1:A:733:CYS:HB3	2.14	0.47
1:A:862:THR:HG1	1:A:865:GLU:HB2	1.78	0.47
1:A:302:HIS:ND1	1:A:385:TYR:HA	2.30	0.47
1:A:173:HIS:H	1:A:261:GLY:HA2	1.79	0.47
1:A:530:GLU:HB2	1:A:595:PHE:CG	2.49	0.47
1:A:284:PRO:HD3	1:A:316:PHE:CD2	2.49	0.47
1:A:980:PRO:O	1:A:981:ASP:C	2.58	0.46
1:A:172:CYS:N	1:A:179:ALA:O	2.46	0.46
1:A:732:THR:HG22	1:A:800:ARG:NH1	2.30	0.46
1:A:181:LEU:HD11	1:A:236:THR:HG22	1.97	0.46
1:A:322:LEU:HG	1:A:327:LEU:CD1	2.45	0.46
1:A:495:MET:HE1	1:A:511:MET:O	2.15	0.46
1:A:765:LYS:O	1:A:766:THR:HG22	2.15	0.46
1:A:877:ASP:OD1	1:A:878:THR:N	2.49	0.46
1:A:1018:ASP:O	1:A:1022:THR:OG1	2.31	0.46
1:A:136:ARG:HE	1:A:149:TYR:HB2	1.81	0.46
1:A:782:HIS:ND1	1:A:783:PRO:O	2.48	0.46
1:A:223:LEU:CD2	1:A:446:ARG:HB2	2.45	0.46
1:A:578:ILE:HG22	1:A:615:ILE:HD13	1.98	0.46
1:A:584:LYS:NZ	1:A:826:ASP:OD1	2.45	0.46
1:A:143:MET:HG3	1:A:145:ARG:HH21	1.81	0.46
1:A:287:PHE:N	1:A:287:PHE:HD1	2.14	0.46
1:A:381:PRO:HD3	1:A:414:VAL:O	2.16	0.46
1:A:501:ILE:C	1:A:501:ILE:HD12	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:SER:O	1:A:252:GLU:HG3	2.16	0.45
1:A:285:ASN:N	1:A:285:ASN:ND2	2.60	0.45
1:A:172:CYS:SG	1:A:179:ALA:HB3	2.57	0.45
1:A:307:VAL:HG23	1:A:310:HIS:HB2	1.97	0.45
1:A:323:SER:O	1:A:327:LEU:N	2.45	0.45
1:A:1072:VAL:O	1:A:1075:ALA:HB3	2.17	0.45
1:A:241:LEU:HD13	1:A:245:ALA:HB1	1.99	0.45
1:A:510:ARG:CD	1:A:605:LYS:HB3	2.45	0.45
1:A:249:TYR:CD1	1:A:250:ILE:HD12	2.52	0.45
1:A:284:PRO:HD3	1:A:316:PHE:CE2	2.51	0.45
1:A:309:ARG:NH1	1:A:309:ARG:CG	2.73	0.45
1:A:441:THR:HG23	1:A:443:LEU:N	2.31	0.45
1:A:1109:ARG:NH1	1:A:1111:CYS:O	2.50	0.45
1:A:487:THR:O	1:A:490:ASN:HB2	2.17	0.45
1:A:504:VAL:HG21	1:A:865:GLU:HB3	1.97	0.45
1:A:723:ARG:HH22	1:A:750:GLU:CD	2.25	0.45
1:A:165:ASP:CG	1:A:189:ARG:HH12	2.25	0.44
1:A:184:LEU:N	1:A:184:LEU:CD1	2.80	0.44
1:A:588:THR:HG21	1:A:728:CYS:HB3	1.98	0.44
1:A:127:GLU:HA	1:A:265:ILE:O	2.17	0.44
1:A:817:PRO:O	1:A:823:GLY:HA3	2.17	0.44
1:A:1029:LEU:HD23	1:A:1031:TYR:HE1	1.83	0.44
1:A:1004:ARG:NH1	1:A:1004:ARG:CG	2.73	0.44
1:A:350:HIS:ND1	1:A:350:HIS:C	2.76	0.44
1:A:501:ILE:HD12	1:A:501:ILE:O	2.18	0.44
1:A:624:CYS:HB3	1:A:719:VAL:O	2.17	0.44
1:A:319:LEU:O	1:A:322:LEU:HB3	2.16	0.44
1:A:395:ASN:O	1:A:399:LYS:HB2	2.18	0.44
1:A:510:ARG:HA	1:A:513:GLN:HG3	2.00	0.44
1:A:223:LEU:HD21	1:A:446:ARG:HB2	1.99	0.44
1:A:555:THR:O	1:A:559:ARG:HG3	2.17	0.44
1:A:1069:ALA:O	1:A:1072:VAL:CB	2.66	0.44
1:A:1079:VAL:C	1:A:1089:LYS:HZ1	2.17	0.44
1:A:1080:THR:O	1:A:1086:ARG:HD3	2.18	0.44
1:A:192:ILE:CG1	1:A:222:ALA:HB2	2.35	0.44
1:A:404:TYR:HE1	1:A:485:SER:HB2	1.82	0.44
1:A:735:LEU:O	1:A:811:ARG:HG3	2.18	0.44
1:A:899:SER:O	1:A:900:PRO:C	2.60	0.44
1:A:223:LEU:HD11	1:A:442:GLY:HA3	1.99	0.43
1:A:530:GLU:HG2	1:A:532:ILE:HG23	1.99	0.43
1:A:590:ASP:CG	1:A:800:ARG:NH2	2.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:GLN:OE1	1:A:520:GLN:N	2.49	0.43
1:A:380:THR:HG23	1:A:416:GLU:HA	1.99	0.43
1:A:867:GLN:O	1:A:871:VAL:HG23	2.19	0.43
1:A:590:ASP:CG	1:A:800:ARG:HH22	2.26	0.43
1:A:729:LEU:HD12	1:A:730:ASP:H	1.83	0.43
1:A:1073:ALA:O	1:A:1076:TRP:N	2.52	0.43
1:A:190:ILE:O	1:A:221:ARG:HA	2.19	0.43
1:A:380:THR:HB	1:A:383:LYS:HB2	2.01	0.43
1:A:415:ASP:OD1	1:A:416:GLU:N	2.40	0.43
1:A:476:SER:OG	1:A:477:VAL:N	2.52	0.43
1:A:559:ARG:NH2	1:A:570:ALA:O	2.51	0.43
1:A:871:VAL:O	1:A:874:MET:HB2	2.18	0.43
1:A:255:PRO:O	1:A:256:PHE:C	2.62	0.43
1:A:448:LEU:HD21	1:A:868:LYS:CE	2.49	0.43
1:A:905:LEU:HD23	1:A:905:LEU:HA	1.79	0.43
1:A:181:LEU:HD13	1:A:238:VAL:HG22	2.00	0.42
1:A:331:PHE:O	1:A:332:GLU:C	2.62	0.42
1:A:775:ILE:HG12	1:A:832:ILE:HG23	2.00	0.42
1:A:836:ASP:OD2	1:A:837:LYS:NZ	2.52	0.42
1:A:390:GLU:OE2	1:A:1045:ARG:NH1	2.52	0.42
1:A:917:LYS:O	1:A:917:LYS:HG3	2.19	0.42
1:A:986:GLY:C	1:A:1071:ARG:HD2	2.43	0.42
1:A:249:TYR:HD1	1:A:250:ILE:CD1	2.33	0.42
1:A:532:ILE:HB	1:A:533:PRO:HD2	2.00	0.42
1:A:307:VAL:CG2	1:A:310:HIS:CG	3.02	0.42
1:A:637:LEU:HD23	1:A:840:PRO:HG2	2.01	0.42
1:A:376:ARG:NE	1:A:392:GLU:OE2	2.49	0.42
1:A:519:ARG:HE	1:A:519:ARG:HB2	1.57	0.42
1:A:736:GLU:H	1:A:739:GLN:NE2	2.18	0.42
1:A:441:THR:HG23	1:A:444:TYR:H	1.85	0.42
1:A:542:THR:HG21	1:A:849:TYR:CE2	2.54	0.42
1:A:994:ALA:CB	1:A:1079:VAL:HG11	2.50	0.42
1:A:1017:GLU:HG2	1:A:1021:LEU:CD1	2.50	0.42
1:A:150:LEU:HD12	1:A:151:LYS:H	1.84	0.42
1:A:521:THR:HB	1:A:522:PHE:H	1.66	0.42
1:A:1057:VAL:O	1:A:1060:TRP:N	2.53	0.41
1:A:310:HIS:CD2	1:A:344:PRO:CD	3.01	0.41
1:A:466:ALA:O	1:A:478:TRP:HB2	2.21	0.41
1:A:863:LEU:HD23	1:A:863:LEU:HA	1.71	0.41
1:A:221:ARG:HH11	1:A:415:ASP:CG	2.28	0.41
1:A:248:SER:HA	1:A:251:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:HIS:HE1	1:A:384:ILE:CG2	2.33	0.41
1:A:322:LEU:HD13	1:A:322:LEU:HA	1.88	0.41
1:A:524:VAL:O	1:A:611:THR:HB	2.20	0.41
1:A:189:ARG:HD2	1:A:416:GLU:HG3	2.02	0.41
1:A:1053:LEU:O	1:A:1057:VAL:HG23	2.21	0.41
1:A:1078:HIS:CD2	1:A:1082:HIS:HB2	2.56	0.41
1:A:155:GLN:OE1	1:A:156:SER:N	2.52	0.41
1:A:183:GLN:C	1:A:184:LEU:CD1	2.92	0.41
1:A:577:GLN:O	1:A:616:THR:N	2.48	0.41
1:A:925:PRO:HG2	1:A:928:LEU:HB2	2.02	0.41
1:A:947:SER:O	1:A:956:ARG:NH2	2.50	0.41
1:A:982:LEU:HD12	1:A:982:LEU:HA	1.72	0.41
1:A:639:ILE:HD13	1:A:639:ILE:HA	1.76	0.41
1:A:765:LYS:C	1:A:766:THR:HG23	2.44	0.41
1:A:298:ASN:O	1:A:301:VAL:N	2.54	0.41
1:A:487:THR:O	1:A:491:ILE:HD12	2.21	0.41
1:A:1065:LYS:C	1:A:1068:ASP:H	2.29	0.41
1:A:181:LEU:HD11	1:A:236:THR:CG2	2.51	0.41
1:A:466:ALA:HB3	1:A:515:PHE:CE2	2.56	0.41
1:A:857:MET:HE2	1:A:861:VAL:HG22	2.03	0.41
1:A:952:GLY:O	1:A:956:ARG:HG3	2.21	0.41
1:A:170:PHE:HB2	1:A:181:LEU:HB3	2.03	0.40
1:A:440:LYS:HD3	1:A:440:LYS:HA	1.53	0.40
1:A:543:LYS:HB3	1:A:543:LYS:HE2	1.89	0.40
1:A:1059:GLY:O	1:A:1062:ARG:N	2.48	0.40
1:A:564:LEU:HD12	1:A:564:LEU:HA	1.90	0.40
1:A:726:ILE:O	1:A:805:CYS:HB2	2.21	0.40
1:A:733:CYS:O	1:A:733:CYS:SG	2.78	0.40
1:A:814:ARG:NH1	1:A:846:PRO:HB2	2.36	0.40
1:A:250:ILE:CD1	1:A:250:ILE:N	2.84	0.40
1:A:396:TYR:HA	1:A:520:GLN:HE21	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	932/1024 (91%)	889 (95%)	42 (4%)	1 (0%)	48 78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	988	ASP

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	812/875 (93%)	717 (88%)	95 (12%)	5 22

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	LEU
1	A	120	ARG
1	A	136	ARG
1	A	151	LYS
1	A	185	THR
1	A	221	ARG
1	A	223	LEU
1	A	246	SER
1	A	250	ILE
1	A	251	LEU
1	A	257	SER
1	A	262	GLU
1	A	263	LEU
1	A	265	ILE
1	A	277	VAL
1	A	278	VAL
1	A	281	VAL
1	A	285	ASN

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Mol	Chain	Res	Type
1	A	287	PHE
1	A	305	LYS
1	A	306	LEU
1	A	307	VAL
1	A	309	ARG
1	A	320	GLU
1	A	322	LEU
1	A	324	ILE
1	A	328	ARG
1	A	345	LEU
1	A	384	ILE
1	A	399	LYS
1	A	402	SER
1	A	437	LYS
1	A	439	LEU
1	A	440	LYS
1	A	443	LEU
1	A	444	TYR
1	A	447	ILE
1	A	448	LEU
1	A	461	LYS
1	A	463	GLU
1	A	464	PHE
1	A	477	VAL
1	A	504	VAL
1	A	506	LYS
1	A	519	ARG
1	A	521	THR
1	A	554	SER
1	A	628	ARG
1	A	639	ILE
1	A	640	LYS
1	A	658	MET
1	A	671	LYS
1	A	723	ARG
1	A	728	CYS
1	A	758	PHE
1	A	770	VAL
1	A	802	LEU
1	A	811	ARG
1	A	825	LEU
1	A	844	ASP

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Mol	Chain	Res	Type
1	A	849	TYR
1	A	850	THR
1	A	852	THR
1	A	853	ARG
1	A	855	ARG
1	A	856	ILE
1	A	857	MET
1	A	858	ASP
1	A	859	HIS
1	A	864	GLU
1	A	866	ILE
1	A	871	VAL
1	A	878	THR
1	A	879	LEU
1	A	895	LEU
1	A	896	LYS
1	A	898	ARG
1	A	901	GLU
1	A	917	LYS
1	A	924	MET
1	A	926	LEU
1	A	942	ARG
1	A	944	MET
1	A	953	LYS
1	A	982	LEU
1	A	987	PHE
1	A	988	ASP
1	A	989	GLU
1	A	1015	GLU
1	A	1016	ARG
1	A	1018	ASP
1	A	1072	VAL
1	A	1088	GLU
1	A	1090	ARG
1	A	1109	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	GLN
1	A	285	ASN
1	A	302	HIS

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Mol	Chain	Res	Type
1	A	560	GLN
1	A	577	GLN
1	A	1054	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	944/1024 (92%)	0.18	11 (1%) 76 58	24, 80, 127, 181	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	728	CYS	4.0
1	A	263	LEU	3.0
1	A	850	THR	3.0
1	A	265	ILE	2.9
1	A	727	GLY	2.7
1	A	852	THR	2.6
1	A	1026	ARG	2.4
1	A	193	ALA	2.3
1	A	192	ILE	2.3
1	A	948	ASN	2.3
1	A	992	ASP	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 oligosaccharides 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.