



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:46 AM UTC

PDB ID : 9JKC / pdb_00009jkc
Title : Crystal structure of Aspergillus fumigatus polmycovirus 1 ploymerase
(residues 85-763) in its apo state
Authors : Jia, H.; Cao, S.; Gong, P.
Deposited on : 2024-09-15
Resolution : 3.40 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

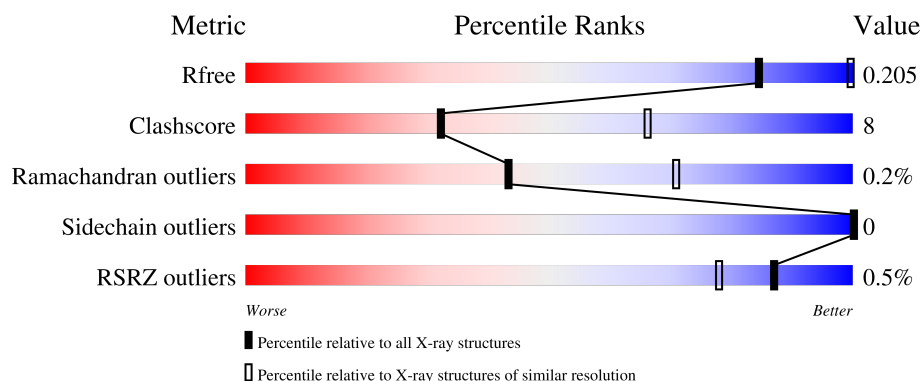
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	690	78% 18% •
1	B	690	78% 18% •
1	C	690	78% 17% 5%
1	D	690	76% 19% 5%
1	E	690	79% 16% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25293 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	661	Total	C	N	O	S	0	0	0
			5100	3214	920	945	21			
1	B	660	Total	C	N	O	S	0	1	0
			5100	3215	916	948	21			
1	C	656	Total	C	N	O	S	0	0	0
			5041	3186	908	926	21			
1	D	655	Total	C	N	O	S	0	0	0
			4988	3149	894	924	21			
1	E	660	Total	C	N	O	S	0	0	0
			5035	3175	908	931	21			

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	84	MET	-	initiating methionine	UNP A0A0H5BRR0
A	764	GLY	-	expression tag	UNP A0A0H5BRR0
A	765	SER	-	expression tag	UNP A0A0H5BRR0
A	766	SER	-	expression tag	UNP A0A0H5BRR0
A	767	SER	-	expression tag	UNP A0A0H5BRR0
A	768	HIS	-	expression tag	UNP A0A0H5BRR0
A	769	HIS	-	expression tag	UNP A0A0H5BRR0
A	770	HIS	-	expression tag	UNP A0A0H5BRR0
A	771	HIS	-	expression tag	UNP A0A0H5BRR0
A	772	HIS	-	expression tag	UNP A0A0H5BRR0
A	773	HIS	-	expression tag	UNP A0A0H5BRR0
B	84	MET	-	initiating methionine	UNP A0A0H5BRR0
B	764	GLY	-	expression tag	UNP A0A0H5BRR0
B	765	SER	-	expression tag	UNP A0A0H5BRR0
B	766	SER	-	expression tag	UNP A0A0H5BRR0
B	767	SER	-	expression tag	UNP A0A0H5BRR0
B	768	HIS	-	expression tag	UNP A0A0H5BRR0
B	769	HIS	-	expression tag	UNP A0A0H5BRR0
B	770	HIS	-	expression tag	UNP A0A0H5BRR0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	771	HIS	-	expression tag	UNP A0A0H5BRR0
B	772	HIS	-	expression tag	UNP A0A0H5BRR0
B	773	HIS	-	expression tag	UNP A0A0H5BRR0
C	84	MET	-	initiating methionine	UNP A0A0H5BRR0
C	764	GLY	-	expression tag	UNP A0A0H5BRR0
C	765	SER	-	expression tag	UNP A0A0H5BRR0
C	766	SER	-	expression tag	UNP A0A0H5BRR0
C	767	SER	-	expression tag	UNP A0A0H5BRR0
C	768	HIS	-	expression tag	UNP A0A0H5BRR0
C	769	HIS	-	expression tag	UNP A0A0H5BRR0
C	770	HIS	-	expression tag	UNP A0A0H5BRR0
C	771	HIS	-	expression tag	UNP A0A0H5BRR0
C	772	HIS	-	expression tag	UNP A0A0H5BRR0
C	773	HIS	-	expression tag	UNP A0A0H5BRR0
D	84	MET	-	initiating methionine	UNP A0A0H5BRR0
D	764	GLY	-	expression tag	UNP A0A0H5BRR0
D	765	SER	-	expression tag	UNP A0A0H5BRR0
D	766	SER	-	expression tag	UNP A0A0H5BRR0
D	767	SER	-	expression tag	UNP A0A0H5BRR0
D	768	HIS	-	expression tag	UNP A0A0H5BRR0
D	769	HIS	-	expression tag	UNP A0A0H5BRR0
D	770	HIS	-	expression tag	UNP A0A0H5BRR0
D	771	HIS	-	expression tag	UNP A0A0H5BRR0
D	772	HIS	-	expression tag	UNP A0A0H5BRR0
D	773	HIS	-	expression tag	UNP A0A0H5BRR0
E	84	MET	-	initiating methionine	UNP A0A0H5BRR0
E	764	GLY	-	expression tag	UNP A0A0H5BRR0
E	765	SER	-	expression tag	UNP A0A0H5BRR0
E	766	SER	-	expression tag	UNP A0A0H5BRR0
E	767	SER	-	expression tag	UNP A0A0H5BRR0
E	768	HIS	-	expression tag	UNP A0A0H5BRR0
E	769	HIS	-	expression tag	UNP A0A0H5BRR0
E	770	HIS	-	expression tag	UNP A0A0H5BRR0
E	771	HIS	-	expression tag	UNP A0A0H5BRR0
E	772	HIS	-	expression tag	UNP A0A0H5BRR0
E	773	HIS	-	expression tag	UNP A0A0H5BRR0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	10	Total 10	O 10	0	0
2	C	6	Total 6	O 6	0	0
2	D	6	Total 6	O 6	0	0
2	E	1	Total 1	O 1	0	0

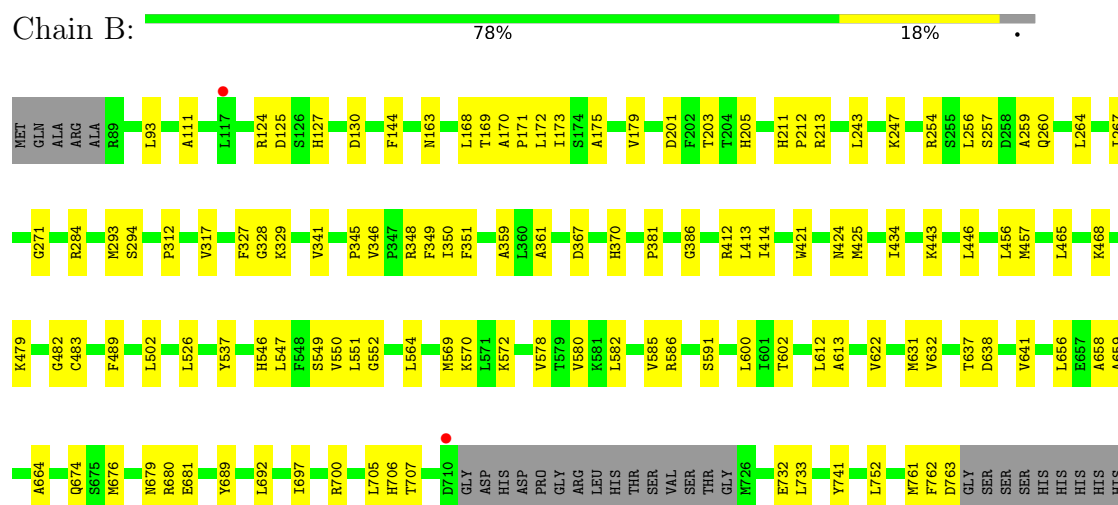
3 Residue-property plots [i](#)

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



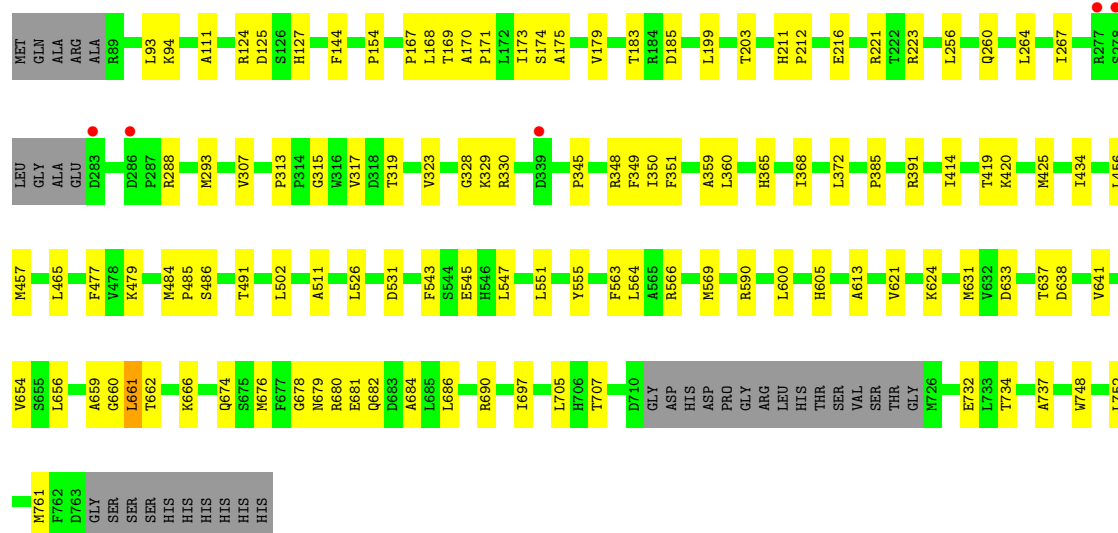
• Molecule 1: RNA dependent RNA polymerase



HIS

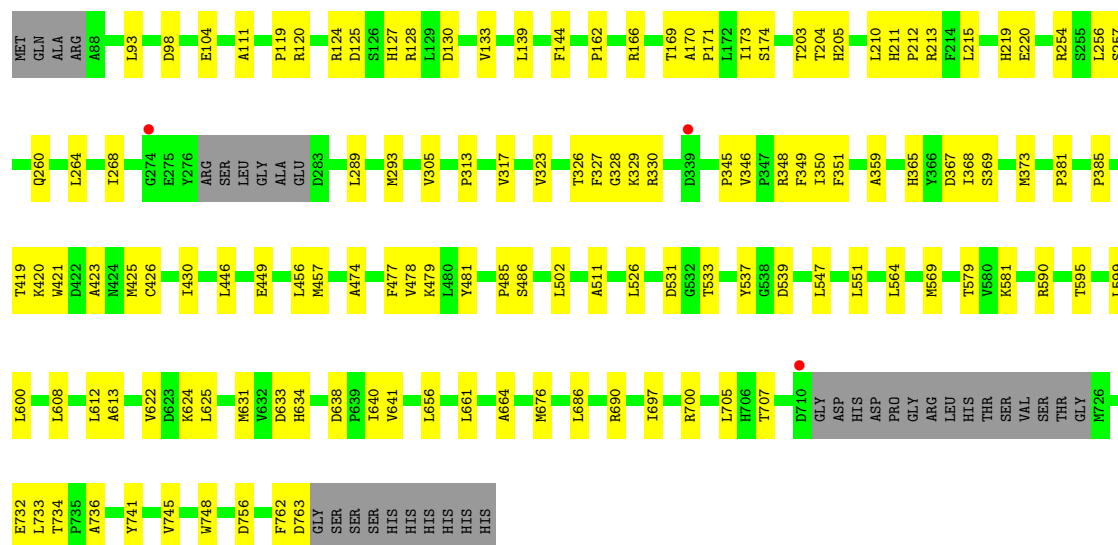
- Molecule 1: RNA dependent RNA polymerase

Chain C:  78% 17% 5%



- Molecule 1: RNA dependent RNA polymerase

Chain D:  76% 19% 5%



- Molecule 1: RNA dependent RNA polymerase

Chain E:  79% 16% 5%



P347	R348	F349	I350	F351	A359	L360	A361	D367	P377	P381	P385	R404	F405	S406	T407	P408	I414	M415	T419	K420	M425	I434	L437	L456	R459	F477	V478	K479	L480	Y481	P485	S486	F489	Y490	T491	N500	I501	L502	R510	A511				
Y537	F543	L551	G552	L553	A561	L564	M569	K570	L571	E577	R586	R590	T595	P596	H597	L608	L612	A613	M631	V632	D633	H634	D638	P639	I640	V641	Y642	L645	G660	L661	Q674	S675	M676	F677	G678	N679	R680	E681	Q682	D683	A684	I697		
D698	R699	A700	L702	T707	F708	R709	D710	GLY	ASP	HIS	ASP	PRO	GLY	ARG	LEU	HIS	THR	SER	VAL	SER	THR	GLY	W726	G731	E732	L733	T734	W739	A740	Y741	V745	W748	Y751	L752	P763	GLY	SER	SER	SER	HIS	HIS	HIS	HIS	HIS

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	257.96Å 182.92Å 118.68Å 90.00° 103.79° 90.00°	Depositor
Resolution (Å)	29.88 – 3.40 29.88 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.88-3.40) 99.2 (29.88-3.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.09 (at 3.39Å)	Xtriage
Refinement program	PHENIX 1.19	Depositor
R, R_{free}	0.158 , 0.206 0.158 , 0.205	Depositor DCC
R_{free} test set	3723 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	59.7	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25293	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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	0.48	0/5216	0.72	0/7083
1	B	0.48	0/5216	0.73	0/7083
1	C	0.46	0/5156	0.73	0/7005
1	D	0.46	0/5102	0.71	0/6942
1	E	0.42	0/5151	0.67	2/7005 (0.0%)
All	All	0.46	0/25841	0.71	2/35118 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	209	THR	CA-C-N	5.33	127.86	120.29
1	E	209	THR	C-N-CA	5.33	127.86	120.29

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5100	0	4975	86	0
1	B	5100	0	4975	81	0
1	C	5041	0	4920	85	0
1	D	4988	0	4816	83	0
1	E	5035	0	4869	75	0
2	A	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	0	1	0
2	C	6	0	0	0	0
2	D	6	0	0	0	0
2	E	1	0	0	0	0
All	All	25293	0	24555	400	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 8.

All (400) 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:676:MET:HE2	1:A:705:LEU:HD22	1.53	0.89
1:A:169:THR:HG22	1:A:613:ALA:HA	1.53	0.88
1:B:169:THR:HG22	1:B:613:ALA:HA	1.58	0.84
1:D:169:THR:HG22	1:D:613:ALA:HA	1.60	0.84
1:C:676:MET:HE2	1:C:705:LEU:HD22	1.61	0.82
1:B:676:MET:HE2	1:B:705:LEU:HD22	1.63	0.81
1:D:676:MET:HE2	1:D:705:LEU:HD22	1.64	0.80
1:E:169:THR:HG22	1:E:613:ALA:HA	1.63	0.80
1:C:169:THR:HG22	1:C:613:ALA:HA	1.65	0.79
1:D:317:VAL:HG11	1:D:456:LEU:HD22	1.69	0.74
1:A:213:ARG:HH21	1:A:346:VAL:HB	1.53	0.74
1:B:317:VAL:HG11	1:B:456:LEU:HD22	1.71	0.73
1:E:323:VAL:HG23	1:E:477:PHE:HE1	1.53	0.72
1:E:317:VAL:HG11	1:E:456:LEU:HD22	1.73	0.70
1:B:328:GLY:HA2	1:B:348:ARG:O	1.92	0.69
1:B:205:HIS:ND1	1:B:327:PHE:O	2.26	0.69
1:C:600:LEU:HD23	1:C:637:THR:HG23	1.75	0.69
1:B:600:LEU:HD23	1:B:637:THR:HG23	1.74	0.68
1:E:254:ARG:NH1	1:E:367:ASP:OD1	2.27	0.68
1:A:199:LEU:HD21	1:A:337:ILE:HG23	1.73	0.67
1:A:305:VAL:HG22	1:A:449:GLU:HG2	1.76	0.67
1:A:631:MET:HE1	1:A:697:ILE:HB	1.76	0.66
1:A:511:ALA:HB2	1:A:551:LEU:HD13	1.76	0.66
1:E:168:LEU:HD23	1:E:612:LEU:HD22	1.77	0.66
1:B:329:LYS:HE2	1:B:350:ILE:HD11	1.78	0.65
1:C:638:ASP:OD1	1:C:748:TRP:NE1	2.30	0.65
1:D:328:GLY:HA2	1:D:348:ARG:O	1.96	0.65
1:A:317:VAL:HG11	1:A:456:LEU:HD22	1.76	0.65
1:D:305:VAL:HG22	1:D:449:GLU:HG2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:590:ARG:NH2	1:D:633:ASP:OD1	2.29	0.65
1:E:293:MET:HE2	1:E:359:ALA:HB2	1.79	0.64
1:D:93:LEU:HD22	1:D:104:GLU:HB3	1.78	0.64
1:C:638:ASP:HB3	1:C:641:VAL:H	1.63	0.64
1:E:328:GLY:HA2	1:E:348:ARG:O	1.98	0.64
1:C:216:GLU:OE1	1:C:420:LYS:HD2	1.98	0.64
1:C:605:HIS:NE2	1:C:638:ASP:OD2	2.30	0.63
1:C:323:VAL:HG23	1:C:477:PHE:HE1	1.62	0.63
1:A:502:LEU:HD13	1:A:564:LEU:HD22	1.81	0.62
1:B:327:PHE:HB2	1:B:350:ILE:HB	1.81	0.62
1:C:631:MET:HE1	1:C:697:ILE:HB	1.81	0.61
1:E:631:MET:HE1	1:E:697:ILE:HB	1.83	0.61
1:E:349:PHE:CE2	1:E:351:PHE:HE2	2.18	0.61
1:E:674:GLN:HG3	1:E:680:ARG:HE	1.66	0.61
1:C:183:THR:HG22	1:C:185:ASP:H	1.65	0.60
1:C:385:PRO:HB3	1:C:590:ARG:NE	2.16	0.60
1:E:349:PHE:CD2	1:E:351:PHE:HE2	2.19	0.60
1:A:203:THR:O	1:A:330:ARG:HA	2.01	0.60
1:D:595:THR:HG21	1:D:600:LEU:HD22	1.82	0.60
1:C:328:GLY:HA2	1:C:348:ARG:O	2.00	0.60
1:C:93:LEU:HD23	1:D:119:PRO:HG2	1.82	0.60
1:A:600:LEU:HD23	1:A:637:THR:HG23	1.83	0.60
1:A:586:ARG:HG3	1:A:586:ARG:HH11	1.67	0.60
1:C:686:LEU:HD22	1:C:690:ARG:NH2	2.17	0.59
1:D:511:ALA:HB2	1:D:551:LEU:HD13	1.83	0.59
1:A:170:ALA:HB3	1:A:171:PRO:HD3	1.84	0.59
1:D:173:ILE:HG13	1:D:174:SER:N	2.17	0.59
1:A:600:LEU:HG	1:A:706:HIS:CE1	2.38	0.59
1:E:361:ALA:HB1	1:E:489:PHE:CD1	2.38	0.58
1:B:170:ALA:HB3	1:B:171:PRO:HD3	1.86	0.58
1:C:203:THR:CG2	1:C:345:PRO:HB2	2.33	0.58
1:E:674:GLN:NE2	1:E:678:GLY:O	2.37	0.58
1:C:486:SER:HA	1:C:491:THR:HG21	1.85	0.58
1:B:591:SER:HB2	1:B:602:THR:CG2	2.34	0.57
1:E:170:ALA:HB3	1:E:171:PRO:HD3	1.86	0.57
1:A:205:HIS:ND1	1:A:327:PHE:O	2.37	0.57
1:A:409:ASP:OD1	1:A:411:ALA:HB3	2.05	0.57
1:D:631:MET:HE1	1:D:697:ILE:HB	1.86	0.57
1:A:173:ILE:HG13	1:A:174:SER:N	2.19	0.57
1:C:221:ARG:NH1	1:C:223:ARG:HH21	2.02	0.57
1:E:596:PRO:HD3	1:E:751:TYR:CE2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:MET:HE2	1:B:359:ALA:HB2	1.87	0.56
1:C:679:ASN:HB3	1:C:681:GLU:HG3	1.86	0.56
1:E:213:ARG:HH21	1:E:346:VAL:HB	1.70	0.56
1:A:608:LEU:HD11	1:A:645:LEU:HD11	1.87	0.56
1:E:425:MET:HA	1:E:569:MET:HE1	1.86	0.56
1:A:119:PRO:HG2	1:B:93:LEU:HD23	1.88	0.56
1:C:167:PRO:HG2	1:C:168:LEU:HD22	1.88	0.56
1:C:564:LEU:HB3	1:C:569:MET:HB2	1.88	0.56
1:D:686:LEU:HD22	1:D:690:ARG:HH21	1.71	0.55
1:C:419:THR:HG22	1:C:420:LYS:HG2	1.88	0.55
1:E:608:LEU:HD11	1:E:645:LEU:HD11	1.89	0.55
1:A:674:GLN:HG3	1:A:680:ARG:NH1	2.22	0.55
1:D:624:LYS:HG2	1:D:656:LEU:HD11	1.88	0.55
1:C:349:PHE:CE2	1:C:351:PHE:HE2	2.25	0.54
1:B:256:LEU:HD21	1:B:457:MET:HE1	1.89	0.54
1:B:127:HIS:HA	1:B:130:ASP:OD1	2.07	0.54
1:A:175:ALA:O	1:A:179:VAL:HG23	2.07	0.54
1:A:328:GLY:HA2	1:A:348:ARG:O	2.08	0.54
1:A:486:SER:HA	1:A:491:THR:HG21	1.90	0.54
1:D:640:ILE:HG12	1:D:745:VAL:HG13	1.89	0.54
1:D:205:HIS:ND1	1:D:327:PHE:O	2.41	0.54
1:A:700:ARG:HG3	1:A:741:TYR:CE1	2.43	0.54
1:C:624:LYS:HD3	1:C:654:VAL:HG23	1.90	0.54
1:E:404:ARG:HB2	1:E:406:SER:O	2.08	0.54
1:D:264:LEU:O	1:D:268:ILE:HG12	2.08	0.53
1:A:128:ARG:NH1	1:A:473:PRO:O	2.40	0.53
1:B:349:PHE:CD2	1:B:351:PHE:HE2	2.26	0.53
1:D:257:SER:O	1:D:260:GLN:HG2	2.08	0.53
1:A:640:ILE:HG12	1:A:745:VAL:HG13	1.90	0.53
1:B:271:GLY:HA3	1:B:284:ARG:NH1	2.24	0.53
1:B:170:ALA:O	1:B:173:ILE:HG13	2.07	0.53
1:D:707:THR:HG21	1:D:733:LEU:HA	1.91	0.53
1:B:631:MET:HE1	1:B:697:ILE:HB	1.92	0.53
1:D:170:ALA:HB3	1:D:171:PRO:HD3	1.90	0.52
1:D:381:PRO:HA	1:D:537:TYR:CE2	2.44	0.52
1:B:468:LYS:HE3	1:B:483:CYS:H	1.74	0.52
1:E:638:ASP:HB3	1:E:641:VAL:HB	1.92	0.52
1:B:349:PHE:CE2	1:B:351:PHE:HE2	2.28	0.52
1:C:434:ILE:HD12	1:C:465:LEU:HD22	1.92	0.52
1:C:183:THR:HG22	1:C:185:ASP:N	2.24	0.52
1:A:351:PHE:CE1	1:A:485:PRO:HG2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:LEU:O	1:A:468:LYS:NZ	2.43	0.52
1:A:257:SER:O	1:A:260:GLN:HG2	2.10	0.51
1:B:425:MET:HA	1:B:569:MET:CE	2.40	0.51
1:C:434:ILE:HD12	1:C:465:LEU:CD2	2.40	0.51
1:D:599:LEU:O	1:D:600:LEU:HD12	2.11	0.51
1:E:700:ARG:HG3	1:E:741:TYR:CE1	2.46	0.51
1:E:707:THR:HG21	1:E:733:LEU:HA	1.91	0.51
1:D:502:LEU:HD13	1:D:564:LEU:HD22	1.91	0.51
1:E:201:ASP:HB3	1:E:345:PRO:HG2	1.91	0.51
1:A:213:ARG:NH2	1:A:346:VAL:HB	2.23	0.51
1:A:329:LYS:HD3	1:A:350:ILE:HD11	1.91	0.51
1:B:591:SER:HB2	1:B:602:THR:HG23	1.92	0.51
1:D:526:LEU:HD11	1:D:551:LEU:HD11	1.92	0.51
1:A:586:ARG:HG3	1:A:586:ARG:NH1	2.25	0.51
1:B:386:GLY:HA3	1:B:676:MET:HE1	1.93	0.50
1:D:590:ARG:HH22	1:D:633:ASP:CG	2.17	0.50
1:C:256:LEU:HD21	1:C:457:MET:HE1	1.93	0.50
1:D:581:LYS:HD3	1:D:756:ASP:OD2	2.12	0.50
1:E:510:ARG:HH21	1:E:553:LEU:HD22	1.76	0.50
1:C:621:VAL:HG13	1:C:656:LEU:CD2	2.41	0.50
1:D:638:ASP:HB3	1:D:641:VAL:H	1.76	0.50
1:E:486:SER:HA	1:E:491:THR:HG21	1.93	0.50
1:A:300:TYR:O	1:A:453:THR:HG23	2.11	0.50
1:B:700:ARG:HG3	1:B:741:TYR:CE1	2.47	0.50
1:C:329:LYS:HG2	1:C:350:ILE:HD11	1.94	0.50
1:C:368:ILE:O	1:C:372:LEU:HG	2.12	0.50
1:A:661:LEU:HD13	1:A:666:LYS:HE2	1.93	0.49
1:B:570:LYS:HD2	1:B:572:LYS:NZ	2.27	0.49
1:B:370:HIS:HB3	2:B:805:HOH:O	2.11	0.49
1:B:254:ARG:NH1	1:B:367:ASP:OD1	2.45	0.49
1:B:381:PRO:HA	1:B:537:TYR:CE2	2.47	0.49
1:A:414:ILE:HG13	1:A:543:PHE:CE2	2.47	0.49
1:D:323:VAL:HG23	1:D:477:PHE:HE1	1.77	0.49
1:C:329:LYS:HE3	1:C:348:ARG:CZ	2.43	0.49
1:D:425:MET:HA	1:D:569:MET:HE1	1.94	0.49
1:E:564:LEU:HB3	1:E:569:MET:HB2	1.94	0.49
1:C:216:GLU:CD	1:C:420:LYS:HD2	2.38	0.48
1:A:125:ASP:O	1:A:128:ARG:HG3	2.13	0.48
1:A:201:ASP:HB3	1:A:345:PRO:HG2	1.95	0.48
1:E:682:GLN:O	1:E:683:ASP:HB2	2.14	0.48
1:D:213:ARG:HH21	1:D:346:VAL:HB	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:HIS:NE2	1:D:423:ALA:O	2.47	0.48
1:E:385:PRO:HB3	1:E:590:ARG:CD	2.44	0.48
1:B:413:LEU:HD22	1:B:585:VAL:HG21	1.95	0.48
1:C:111:ALA:HB3	1:C:124:ARG:HD2	1.95	0.48
1:A:434:ILE:HD12	1:A:465:LEU:CD2	2.44	0.48
1:A:674:GLN:HE21	1:A:680:ARG:HG2	1.78	0.48
1:B:168:LEU:HD23	1:B:612:LEU:HD23	1.94	0.48
1:D:111:ALA:HB3	1:D:124:ARG:HD2	1.96	0.48
1:C:203:THR:O	1:C:330:ARG:HA	2.13	0.48
1:C:329:LYS:HE3	1:C:348:ARG:NH1	2.29	0.48
1:E:511:ALA:HB2	1:E:551:LEU:HD13	1.96	0.48
1:E:748:TRP:NE1	1:E:752:LEU:HD11	2.29	0.48
1:B:213:ARG:HH21	1:B:346:VAL:HB	1.79	0.48
1:B:361:ALA:HB1	1:B:489:PHE:CD1	2.49	0.47
1:B:425:MET:HA	1:B:569:MET:HE1	1.95	0.47
1:B:707:THR:HG21	1:B:733:LEU:HA	1.95	0.47
1:D:313:PRO:HG2	1:E:660:GLY:HA2	1.96	0.47
1:B:201:ASP:HB3	1:B:345:PRO:HG2	1.96	0.47
1:D:419:THR:HG22	1:D:420:LYS:HG2	1.96	0.47
1:E:590:ARG:HH22	1:E:633:ASP:CG	2.22	0.47
1:B:412:ARG:HG2	1:B:580:VAL:HG13	1.95	0.47
1:D:128:ARG:HB2	1:D:474:ALA:HB2	1.95	0.47
1:D:162:PRO:HB3	1:D:204:THR:HG21	1.95	0.47
1:A:465:LEU:HD12	1:A:465:LEU:HA	1.69	0.47
1:E:349:PHE:CD2	1:E:351:PHE:CE2	3.02	0.47
1:B:674:GLN:HE21	1:B:680:ARG:HG2	1.79	0.47
1:E:640:ILE:HG12	1:E:745:VAL:HG13	1.97	0.47
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.75	0.47
1:A:762:PHE:O	1:A:763:ASP:HB2	2.14	0.47
1:C:365:HIS:HB3	1:C:368:ILE:CG2	2.44	0.47
1:C:707:THR:HG21	1:C:732:GLU:O	2.14	0.47
1:D:98:ASP:HB3	1:D:133:VAL:HG13	1.97	0.47
1:D:256:LEU:HD21	1:D:457:MET:HE1	1.96	0.47
1:A:638:ASP:HB3	1:A:641:VAL:HB	1.97	0.47
1:B:674:GLN:HG3	1:B:680:ARG:HE	1.79	0.47
1:C:734:THR:HB	1:C:737:ALA:H	1.80	0.47
1:D:139:LEU:HD22	1:D:220:GLU:HG2	1.97	0.47
1:B:203:THR:HG22	1:B:345:PRO:HB2	1.97	0.47
1:B:502:LEU:HD13	1:B:564:LEU:HD22	1.96	0.47
1:B:526:LEU:HD11	1:B:551:LEU:HD11	1.97	0.47
1:D:329:LYS:HG2	1:D:350:ILE:CG1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:HIS:CG	1:B:212:PRO:HD3	2.50	0.47
1:B:692:LEU:HA	1:B:697:ILE:HD11	1.97	0.46
1:C:94:LYS:HA	1:D:120:ARG:HE	1.80	0.46
1:C:682:GLN:C	1:C:684:ALA:H	2.23	0.46
1:A:446:LEU:HD23	1:A:446:LEU:HA	1.65	0.46
1:D:700:ARG:HG3	1:D:741:TYR:CE1	2.50	0.46
1:C:170:ALA:HB3	1:C:171:PRO:HD3	1.97	0.46
1:A:465:LEU:HD11	1:A:484:MET:HE1	1.97	0.46
1:D:762:PHE:O	1:D:763:ASP:HB2	2.16	0.46
1:A:381:PRO:HA	1:A:537:TYR:CE2	2.50	0.46
1:E:707:THR:HG22	1:E:734:THR:H	1.81	0.46
1:A:577:GLU:OE1	1:A:584:ARG:HD3	2.16	0.46
1:A:600:LEU:CD2	1:A:637:THR:HG23	2.46	0.46
1:C:211:HIS:CG	1:C:212:PRO:HD3	2.51	0.46
1:C:293:MET:HE2	1:C:359:ALA:HB2	1.98	0.46
1:D:385:PRO:HB3	1:D:590:ARG:NE	2.31	0.46
1:C:351:PHE:CE1	1:C:485:PRO:HG2	2.51	0.46
1:A:264:LEU:HD23	1:A:264:LEU:HA	1.78	0.46
1:B:659:ALA:O	1:E:313:PRO:HD2	2.16	0.46
1:C:124:ARG:HG3	1:C:154:PRO:HG3	1.98	0.46
1:B:414:ILE:HG23	1:B:578:VAL:HG22	1.98	0.45
1:C:660:GLY:O	1:C:662:THR:N	2.47	0.45
1:D:661:LEU:HD23	1:D:661:LEU:HA	1.78	0.45
1:A:271:GLY:HA3	1:A:284:ARG:NH1	2.31	0.45
1:A:502:LEU:HD23	1:A:502:LEU:HA	1.76	0.45
1:E:502:LEU:HD13	1:E:564:LEU:HD22	1.97	0.45
1:A:172:LEU:HD23	1:A:648:ILE:HD11	1.97	0.45
1:A:364:LEU:HB3	1:A:365:HIS:CE1	2.52	0.45
1:D:203:THR:CG2	1:D:345:PRO:HB2	2.47	0.45
1:D:326:THR:HB	1:D:349:PHE:HE1	1.80	0.45
1:A:264:LEU:O	1:A:268:ILE:HG12	2.16	0.45
1:B:638:ASP:HB3	1:B:641:VAL:HB	1.97	0.45
1:D:125:ASP:O	1:D:128:ARG:HG3	2.16	0.45
1:D:351:PHE:CD1	1:D:485:PRO:HG2	2.51	0.45
1:D:564:LEU:HB3	1:D:569:MET:HB2	1.99	0.45
1:A:144:PHE:HD1	1:A:478:VAL:CG1	2.29	0.45
1:B:259:ALA:O	1:B:294:SER:OG	2.25	0.45
1:E:139:LEU:HD22	1:E:220:GLU:HG2	1.99	0.45
1:E:707:THR:HG21	1:E:732:GLU:O	2.16	0.45
1:D:479:LYS:HD2	1:D:481:TYR:OH	2.16	0.45
1:B:622:VAL:HG11	1:B:664:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:ILE:HG13	1:C:174:SER:H	1.81	0.45
1:E:404:ARG:HG3	1:E:408:PRO:HG3	1.99	0.45
1:B:570:LYS:HE3	1:B:572:LYS:HZ2	1.82	0.45
1:C:144:PHE:HA	1:C:479:LYS:O	2.17	0.45
1:C:307:VAL:HG22	1:C:313:PRO:HD3	1.99	0.45
1:D:211:HIS:CG	1:D:212:PRO:HD3	2.52	0.45
1:D:612:LEU:HD23	1:D:612:LEU:HA	1.74	0.45
1:C:526:LEU:HD22	1:C:547:LEU:HD22	1.98	0.45
1:E:323:VAL:CG2	1:E:477:PHE:HE1	2.25	0.45
1:A:385:PRO:HB3	1:A:590:ARG:NE	2.31	0.44
1:D:293:MET:HE2	1:D:359:ALA:HB2	1.98	0.44
1:E:415:MET:HE3	1:E:577:GLU:O	2.16	0.44
1:C:173:ILE:HG13	1:C:174:SER:N	2.32	0.44
1:B:570:LYS:CD	1:B:572:LYS:HZ2	2.30	0.44
1:C:661:LEU:HD13	1:C:666:LYS:HE2	1.98	0.44
1:A:203:THR:CG2	1:A:345:PRO:HB2	2.47	0.44
1:B:679:ASN:HB3	1:B:681:GLU:HG3	1.99	0.44
1:C:465:LEU:HG	1:C:484:MET:HE1	1.99	0.44
1:D:426:CYS:O	1:D:430:ILE:HG13	2.17	0.44
1:B:752:LEU:HD12	1:B:761:MET:HE2	1.99	0.44
1:C:175:ALA:O	1:C:179:VAL:HG23	2.18	0.44
1:E:586:ARG:NH1	1:E:586:ARG:HG3	2.33	0.44
1:B:689:TYR:CE2	1:E:312:PRO:HB3	2.52	0.44
1:E:204:THR:HG22	1:E:330:ARG:HG2	2.00	0.44
1:E:434:ILE:HA	1:E:437:LEU:HD12	1.99	0.44
1:E:586:ARG:HG3	1:E:586:ARG:HH11	1.83	0.44
1:C:199:LEU:HD23	1:C:199:LEU:HA	1.80	0.44
1:D:127:HIS:HA	1:D:130:ASP:OD1	2.17	0.44
1:C:288:ARG:HD3	1:C:288:ARG:H	1.82	0.44
1:C:317:VAL:HG11	1:C:456:LEU:HD22	1.99	0.44
1:E:661:LEU:HD23	1:E:661:LEU:HA	1.73	0.44
1:B:424:ASN:O	1:B:569:MET:HE2	2.18	0.44
1:C:590:ARG:HH22	1:C:633:ASP:CG	2.25	0.44
1:B:549:SER:O	1:B:552:GLY:N	2.35	0.43
1:D:369:SER:O	1:D:373:MET:HG3	2.18	0.43
1:A:329:LYS:CD	1:A:350:ILE:HD11	2.48	0.43
1:C:545:GLU:OE2	1:C:555:TYR:N	2.37	0.43
1:E:631:MET:HE3	1:E:702:LEU:HD11	2.00	0.43
1:A:199:LEU:HD23	1:A:199:LEU:HA	1.78	0.43
1:A:692:LEU:HA	1:A:697:ILE:HD11	1.99	0.43
1:C:425:MET:HA	1:C:569:MET:HE1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:661:LEU:HD23	1:C:661:LEU:HA	1.84	0.43
1:E:596:PRO:HG2	1:E:739:TRP:CD1	2.53	0.43
1:E:608:LEU:HG	1:E:634:HIS:CE1	2.53	0.43
1:A:387:ARG:NH1	1:A:709:ARG:NH1	2.66	0.43
1:B:111:ALA:HB3	1:B:124:ARG:HD2	2.00	0.43
1:C:563:PHE:O	1:C:566:ARG:HB2	2.18	0.43
1:C:674:GLN:HE21	1:C:680:ARG:HG2	1.83	0.43
1:D:595:THR:CG2	1:D:600:LEU:HD22	2.48	0.43
1:E:144:PHE:HA	1:E:479:LYS:O	2.18	0.43
1:E:595:THR:C	1:E:597:HIS:H	2.26	0.43
1:D:350:ILE:HD13	1:D:486:SER:HB2	2.00	0.43
1:D:533:THR:CG2	1:D:547:LEU:HG	2.48	0.43
1:D:707:THR:HG21	1:D:732:GLU:O	2.18	0.43
1:B:175:ALA:O	1:B:179:VAL:HG23	2.19	0.43
1:B:546:HIS:O	1:B:550:VAL:HG13	2.19	0.43
1:B:570:LYS:CD	1:B:572:LYS:NZ	2.81	0.43
1:B:172:LEU:HD23	1:B:172:LEU:HA	1.81	0.43
1:C:256:LEU:HD23	1:C:256:LEU:HA	1.68	0.43
1:D:365:HIS:HB3	1:D:368:ILE:HG22	2.01	0.43
1:E:414:ILE:HB	1:E:543:PHE:CE1	2.53	0.43
1:E:247:LYS:HE2	1:E:377:PRO:HD3	2.01	0.43
1:A:707:THR:HG21	1:A:732:GLU:O	2.19	0.42
1:C:621:VAL:HG13	1:C:656:LEU:HD21	2.00	0.42
1:D:256:LEU:HA	1:D:256:LEU:HD23	1.77	0.42
1:D:329:LYS:HG2	1:D:350:ILE:HG12	2.01	0.42
1:B:125:ASP:OD2	1:B:127:HIS:HB2	2.18	0.42
1:B:243:LEU:O	1:B:247:LYS:HG2	2.19	0.42
1:B:631:MET:CE	1:B:697:ILE:HB	2.49	0.42
1:C:360:LEU:HD11	1:C:457:MET:HB3	2.00	0.42
1:C:502:LEU:HD13	1:C:564:LEU:HD22	2.00	0.42
1:D:210:LEU:HD21	1:D:349:PHE:CE1	2.55	0.42
1:A:226:ASP:OD1	1:A:228:PRO:HD2	2.19	0.42
1:A:386:GLY:HA3	1:A:676:MET:HE1	2.01	0.42
1:B:762:PHE:O	1:B:763:ASP:HB2	2.19	0.42
1:D:144:PHE:HA	1:D:479:LYS:O	2.19	0.42
1:D:254:ARG:NH1	1:D:367:ASP:OD1	2.52	0.42
1:D:203:THR:O	1:D:330:ARG:HA	2.20	0.42
1:A:106:ARG:H	1:A:106:ARG:HG2	1.70	0.42
1:A:243:LEU:O	1:A:247:LYS:HG2	2.19	0.42
1:C:674:GLN:NE2	1:C:678:GLY:O	2.52	0.42
1:D:93:LEU:HD23	1:E:119:PRO:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:THR:HG22	1:D:345:PRO:HB2	2.01	0.42
1:A:421:TRP:CB	1:A:539:ASP:HB3	2.50	0.42
1:A:434:ILE:HD12	1:A:465:LEU:HD23	2.01	0.42
1:C:221:ARG:CZ	1:C:223:ARG:HH21	2.32	0.42
1:D:144:PHE:HD1	1:D:478:VAL:HG13	1.85	0.42
1:B:658:ALA:HB3	1:E:459:ARG:HH22	1.85	0.42
1:B:707:THR:HG21	1:B:732:GLU:O	2.19	0.42
1:C:414:ILE:HG13	1:C:543:PHE:CE2	2.54	0.42
1:D:579:THR:HB	1:D:581:LYS:H	1.84	0.42
1:D:622:VAL:HG11	1:D:664:ALA:HB1	2.02	0.42
1:A:628:ARG:NH1	1:A:656:LEU:HD12	2.34	0.42
1:B:168:LEU:HD23	1:B:612:LEU:CD2	2.50	0.42
1:C:368:ILE:HD12	1:C:368:ILE:HA	1.71	0.42
1:D:421:TRP:CB	1:D:539:ASP:HB3	2.50	0.42
1:E:157:PHE:HD2	1:E:327:PHE:HE2	1.68	0.42
1:E:385:PRO:HB3	1:E:590:ARG:NE	2.35	0.42
1:C:125:ASP:C	1:C:127:HIS:N	2.78	0.42
1:C:511:ALA:HB2	1:C:551:LEU:HD13	2.01	0.42
1:C:621:VAL:HG13	1:C:656:LEU:HD23	2.02	0.42
1:E:213:ARG:HG2	1:E:349:PHE:HD1	1.84	0.42
1:E:681:GLU:O	1:E:684:ALA:HB3	2.19	0.42
1:A:661:LEU:HD23	1:A:661:LEU:HA	1.71	0.41
1:B:600:LEU:HG	1:B:706:HIS:CE1	2.55	0.41
1:C:365:HIS:HB3	1:C:368:ILE:HG22	2.01	0.41
1:E:349:PHE:HD2	1:E:351:PHE:CE2	2.37	0.41
1:B:257:SER:O	1:B:260:GLN:HG2	2.20	0.41
1:B:443:LYS:HE2	1:B:443:LYS:HB2	1.91	0.41
1:E:419:THR:HG22	1:E:420:LYS:HG2	2.02	0.41
1:E:709:ARG:HB3	1:E:710:ASP:H	1.68	0.41
1:B:446:LEU:HA	1:B:446:LEU:HD23	1.70	0.41
1:E:608:LEU:HD23	1:E:608:LEU:HA	1.89	0.41
1:E:700:ARG:NH1	1:E:731:GLY:O	2.44	0.41
1:A:88:ALA:HB1	1:A:151:LEU:HD22	2.02	0.41
1:B:421:TRP:CD1	1:B:421:TRP:C	2.98	0.41
1:C:264:LEU:HD23	1:C:267:ILE:HD11	2.02	0.41
1:A:472:HIS:CG	1:A:473:PRO:HD2	2.55	0.41
1:C:349:PHE:O	1:C:350:ILE:HD13	2.20	0.41
1:E:642:TYR:CE2	1:E:699:ARG:HB2	2.55	0.41
1:A:689:TYR:CD1	1:B:312:PRO:HG3	2.56	0.41
1:B:144:PHE:HA	1:B:479:LYS:O	2.20	0.41
1:E:479:LYS:HD2	1:E:481:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:PHE:CZ	1:A:485:PRO:HG2	2.56	0.41
1:A:405:PHE:CE1	1:A:594:ARG:HB3	2.56	0.41
1:D:446:LEU:HD23	1:D:446:LEU:HA	1.78	0.41
1:D:608:LEU:HD13	1:D:634:HIS:CE1	2.56	0.41
1:E:385:PRO:HG2	1:E:676:MET:HE2	2.03	0.41
1:A:313:PRO:HD2	1:C:659:ALA:O	2.21	0.41
1:B:656:LEU:HA	1:B:656:LEU:HD23	1.68	0.41
1:C:349:PHE:CD2	1:C:351:PHE:HE2	2.39	0.41
1:A:320:THR:HG23	1:A:320:THR:O	2.20	0.41
1:A:458:TYR:CE2	1:A:462:ARG:HD2	2.56	0.41
1:A:634:HIS:CD2	1:A:641:VAL:HG11	2.56	0.41
1:B:264:LEU:HD23	1:B:267:ILE:HD11	2.03	0.41
1:B:586:ARG:NH1	1:B:591:SER:OG	2.53	0.41
1:C:125:ASP:C	1:C:127:HIS:H	2.29	0.41
1:C:752:LEU:HD12	1:C:761:MET:HE2	2.03	0.41
1:D:289:LEU:HD23	1:D:289:LEU:HA	1.86	0.41
1:D:600:LEU:HD13	1:D:736:ALA:HB1	2.03	0.41
1:E:124:ARG:HG3	1:E:154:PRO:HG3	2.03	0.41
1:E:240:PHE:CZ	1:E:500:ASN:HB3	2.56	0.41
1:E:351:PHE:CE1	1:E:485:PRO:HG2	2.56	0.41
1:B:434:ILE:HD12	1:B:465:LEU:CD2	2.51	0.41
1:B:547:LEU:HD23	1:B:547:LEU:HA	1.89	0.40
1:A:125:ASP:OD2	1:A:127:HIS:HB2	2.21	0.40
1:A:329:LYS:HE3	1:A:348:ARG:HB3	2.04	0.40
1:A:631:MET:HE3	1:A:702:LEU:HD11	2.04	0.40
1:B:632:VAL:HG21	1:B:692:LEU:HD21	2.04	0.40
1:D:638:ASP:OD1	1:D:748:TRP:NE1	2.54	0.40
1:E:561:ALA:HB2	1:E:571:LEU:HD23	2.02	0.40
1:A:223:ARG:H	1:A:223:ARG:HG3	1.64	0.40
1:C:315:GLY:O	1:C:319:THR:HG23	2.21	0.40
1:D:166:ARG:HA	1:D:166:ARG:HD3	1.92	0.40
1:D:625:LEU:HD23	1:D:656:LEU:HD13	2.02	0.40
1:E:157:PHE:HD2	1:E:327:PHE:CE2	2.39	0.40
1:E:381:PRO:HA	1:E:537:TYR:CE2	2.56	0.40
1:A:206:ASP:CG	1:A:209:THR:HG23	2.46	0.40
1:B:256:LEU:HD23	1:B:256:LEU:HA	1.75	0.40
1:C:391:ARG:H	1:C:391:ARG:HG2	1.74	0.40
1:C:682:GLN:C	1:C:684:ALA:N	2.79	0.40
1:D:212:PRO:HA	1:D:215:LEU:HD12	2.03	0.40
1:A:319:THR:O	1:A:320:THR:C	2.64	0.40
1:A:656:LEU:HD23	1:A:656:LEU:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:GLN:H	1:C:260:GLN:HG2	1.62	0.40
1:D:707:THR:HG22	1:D:734:THR:H	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	657/690 (95%)	613 (93%)	43 (6%)	1 (0%)	43	71
1	B	657/690 (95%)	614 (94%)	39 (6%)	4 (1%)	21	50
1	C	650/690 (94%)	612 (94%)	36 (6%)	2 (0%)	36	65
1	D	649/690 (94%)	614 (95%)	34 (5%)	1 (0%)	43	71
1	E	656/690 (95%)	619 (94%)	37 (6%)	0	100	100
All	All	3269/3450 (95%)	3072 (94%)	189 (6%)	8 (0%)	43	71

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	531	ASP
1	B	341	VAL
1	D	531	ASP
1	B	582	LEU
1	A	531	ASP
1	C	661	LEU
1	B	482	GLY
1	B	163	ASN

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	528/575 (92%)	528 (100%)	0	100	100
1	B	530/575 (92%)	530 (100%)	0	100	100
1	C	520/575 (90%)	520 (100%)	0	100	100
1	D	510/575 (89%)	510 (100%)	0	100	100
1	E	515/575 (90%)	515 (100%)	0	100	100
All	All	2603/2875 (90%)	2603 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	HIS
1	A	181	GLN
1	A	263	ASN
1	A	306	GLN
1	A	343	GLN
1	A	506	HIS
1	A	634	HIS
1	A	674	GLN
1	B	153	HIS
1	B	163	ASN
1	B	211	HIS
1	B	237	GLN
1	B	263	ASN
1	B	357	ASN
1	B	519	HIS
1	B	674	GLN
1	C	163	ASN
1	C	181	GLN
1	C	506	HIS
1	C	634	HIS
1	C	674	GLN

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Mol	Chain	Res	Type
1	D	113	ASN
1	D	163	ASN
1	D	263	ASN
1	D	357	ASN
1	D	618	HIS
1	D	634	HIS
1	D	674	GLN
1	E	163	ASN
1	E	181	GLN
1	E	237	GLN
1	E	263	ASN
1	E	357	ASN
1	E	618	HIS
1	E	706	HIS
1	E	750	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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

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	661/690 (95%)	-0.56	5 (0%) 82 71	22, 41, 72, 120	0
1	B	660/690 (95%)	-0.58	2 (0%) 90 84	18, 41, 75, 113	1 (0%)
1	C	656/690 (95%)	-0.50	5 (0%) 82 71	25, 44, 74, 113	0
1	D	655/690 (94%)	-0.54	3 (0%) 87 78	28, 44, 73, 111	0
1	E	660/690 (95%)	-0.38	2 (0%) 90 84	28, 54, 83, 122	0
All	All	3292/3450 (95%)	-0.51	17 (0%) 87 78	18, 45, 78, 122	1 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	278	SER	3.5
1	A	278	SER	3.4
1	C	283	ASP	3.3
1	E	283	ASP	3.1
1	D	710	ASP	2.7
1	C	286	ASP	2.6
1	A	279	LEU	2.4
1	A	710	ASP	2.4
1	B	117	LEU	2.3
1	A	339	ASP	2.3
1	E	341	VAL	2.3
1	D	274	GLY	2.2
1	A	272	SER	2.2
1	D	339	ASP	2.1
1	C	277	ARG	2.0
1	C	339	ASP	2.0
1	B	710	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.