



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:53 AM UTC

PDB ID : 9UZA / pdb_00009uza
Title : Crystal structure of Crimean-Congo hemorrhagic fever virus cap-snatching endonuclease
Authors : Deng, Z.; Kuang, W.; Tian, Z.
Deposited on : 2025-05-16
Resolution : 3.05 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

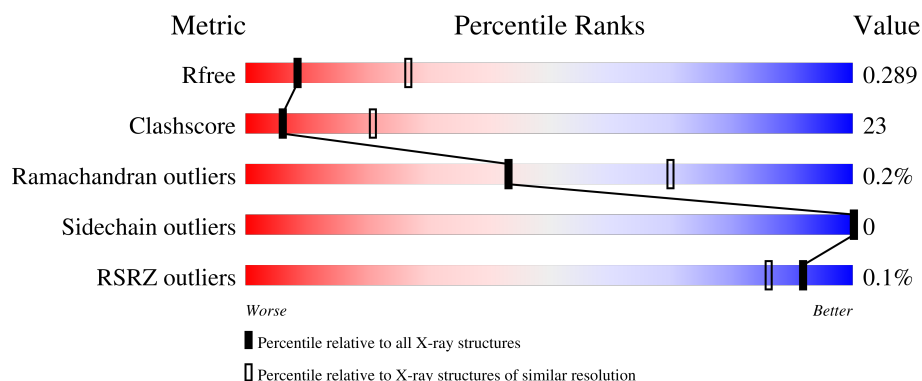
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	319	49% 31% 20%
1	B	319	49% 31% 20%
2	C	228	53% 38% 8%
2	H	228	56% 35% 8%
3	D	219	58% 41% .

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Mol	Chain	Length	Quality of chain
3	L	219	63% 35% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10709 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-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			2083	1328	356	386	13			
1	B	255	Total	C	N	O	S	0	0	0
			2083	1328	356	386	13			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	580	GLY	-	expression tag	UNP D5MEH7
A	581	PRO	-	expression tag	UNP D5MEH7
A	582	LEU	-	expression tag	UNP D5MEH7
A	583	GLY	-	expression tag	UNP D5MEH7
A	584	SER	-	expression tag	UNP D5MEH7
B	580	GLY	-	expression tag	UNP D5MEH7
B	581	PRO	-	expression tag	UNP D5MEH7
B	582	LEU	-	expression tag	UNP D5MEH7
B	583	GLY	-	expression tag	UNP D5MEH7
B	584	SER	-	expression tag	UNP D5MEH7

- Molecule 2 is a protein called mAb G5 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	210	Total	C	N	O	S	0	0	0
			1600	1021	260	314	5			
2	C	210	Total	C	N	O	S	0	0	0
			1599	1020	260	314	5			

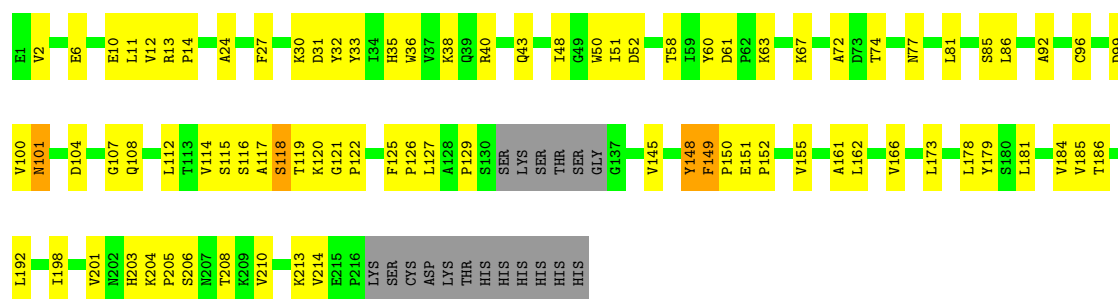
- Molecule 3 is a protein called mAb G5 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	216	Total	C	N	O	S	0	0	0
			1672	1051	285	331	5			

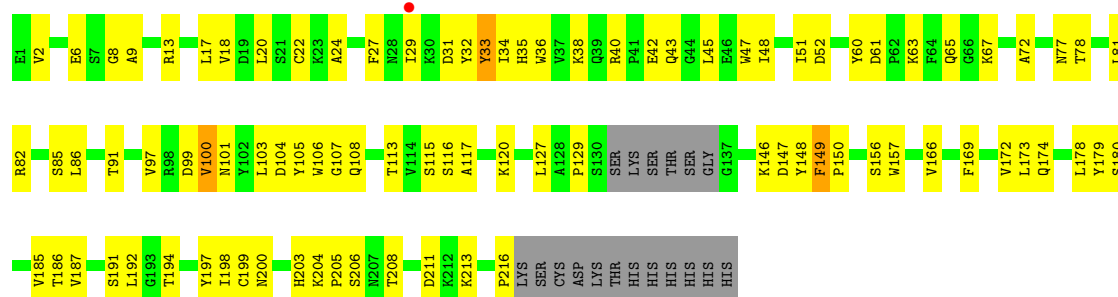
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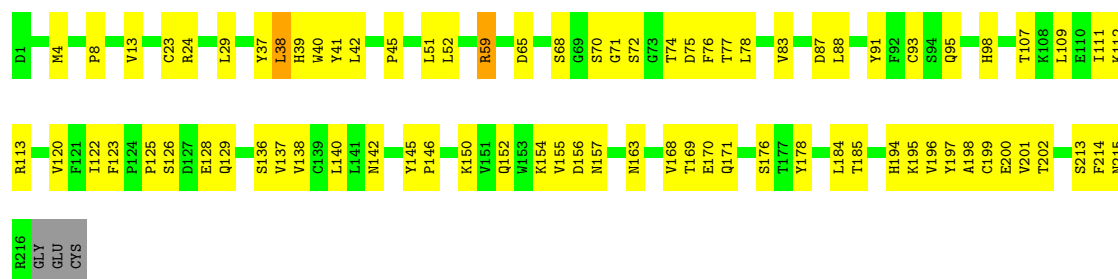
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	216	Total	C	N	O	S	0	0	0
			1672	1051	285	331	5			



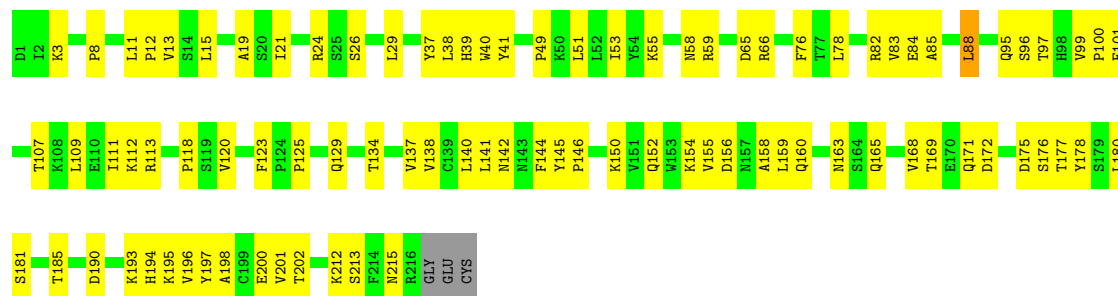
• Molecule 2: mAb G5 Fab heavy chain



• Molecule 3: mAb G5 Fab light chain



• Molecule 3: mAb G5 Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.77Å 99.78Å 180.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.11 – 3.05 29.11 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.11-3.05) 99.5 (29.11-3.05)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.07Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.226 , 0.295 0.223 , 0.289	Depositor DCC
R_{free} test set	1786 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	120.7	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 93.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.005 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10709	wwPDB-VP
Average B, all atoms (Å ²)	137.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.48% 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

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.55	0/2132	0.84	0/2881
1	B	0.54	0/2132	0.81	0/2881
2	C	0.64	0/1639	1.01	2/2242 (0.1%)
2	H	0.63	0/1640	0.97	3/2244 (0.1%)
3	D	0.59	0/1710	0.88	1/2317 (0.0%)
3	L	0.58	1/1710 (0.1%)	0.93	1/2317 (0.0%)
All	All	0.59	1/10963 (0.0%)	0.90	7/14882 (0.0%)

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
2	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	38	LEU	CG-CD1	-5.37	1.34	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	148	TYR	CA-C-N	-5.56	108.24	121.80
2	H	148	TYR	C-N-CA	-5.56	108.24	121.80
2	H	101	ASN	N-CA-C	-5.34	105.40	113.51
3	D	88	LEU	CA-CB-CG	-5.22	98.01	116.30
3	L	59	ARG	CA-CB-CG	-5.21	103.69	114.10
2	C	100	VAL	CA-C-N	5.01	131.10	121.54
2	C	100	VAL	C-N-CA	5.01	131.10	121.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	33	TYR	Sidechain

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	2083	0	2048	96	0
1	B	2083	0	2048	100	0
2	C	1599	0	1563	74	0
2	H	1600	0	1565	85	0
3	D	1672	0	1640	91	0
3	L	1672	0	1640	69	0
All	All	10709	0	10504	478	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 23.

All (478) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:753:MET:HE2	1:B:858:SER:HB3	1.32	1.10
2:H:120:LYS:HG3	2:H:148:TYR:HA	1.41	1.00
1:B:738:LEU:HB2	2:C:101:ASN:HD21	1.26	1.00
3:D:12:PRO:HB2	3:D:112:LYS:HE3	1.46	0.98
2:H:35:HIS:NE2	2:H:99:ASP:OD2	1.98	0.96
1:B:844:LYS:HE2	1:B:848:LYS:HE3	1.48	0.95
1:B:733:ARG:NH1	1:B:735:MET:O	2.00	0.95
3:L:59:ARG:NH1	3:L:65:ASP:HA	1.83	0.94
1:B:740:GLU:OE2	3:D:37:TYR:OH	1.87	0.92
3:L:152:GLN:NE2	3:L:200:GLU:OE1	2.03	0.91
2:H:13:ARG:HH21	2:H:117:ALA:HB2	1.40	0.87
2:C:100:VAL:O	2:C:101:ASN:ND2	2.08	0.86
1:A:665:LEU:HD11	1:A:695:SER:HB3	1.57	0.85
1:A:759:LEU:HD12	1:A:797:TYR:HE2	1.41	0.85
1:B:637:LYS:HA	1:B:887:VAL:HG11	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:ILE:HD11	1:A:890:LEU:HD13	1.58	0.84
3:L:59:ARG:HH12	3:L:65:ASP:HA	1.39	0.84
1:A:800:ARG:HG2	1:A:832:ILE:HG21	1.58	0.83
1:A:733:ARG:NH1	1:A:735:MET:O	2.12	0.83
1:B:753:MET:CE	1:B:858:SER:HB3	2.09	0.81
1:B:836:ILE:HG23	1:B:861:ALA:HB3	1.62	0.80
1:A:586:PRO:HG2	1:A:589:ILE:HD12	1.64	0.79
1:B:800:ARG:HG2	1:B:832:ILE:HG21	1.63	0.79
1:A:738:LEU:H	2:H:101:ASN:HD21	1.31	0.79
1:B:585:GLU:N	1:B:897:ASN:OD1	2.16	0.79
1:A:637:LYS:HA	1:A:887:VAL:HG11	1.66	0.77
3:L:156:ASP:OD2	3:L:194:HIS:HB3	1.84	0.77
1:A:839:ASP:HB3	1:A:843:TRP:CD1	2.20	0.76
3:L:24:ARG:HG2	3:L:75:ASP:OD1	1.86	0.76
3:L:71:GLY:HA3	3:L:76:PHE:HA	1.67	0.76
1:A:839:ASP:HB3	1:A:843:TRP:HD1	1.49	0.76
3:D:171:GLN:HG3	3:D:178:TYR:CE1	2.19	0.76
3:D:125:PRO:HD3	3:D:137:VAL:HG22	1.68	0.76
1:A:759:LEU:HD12	1:A:797:TYR:CE2	2.21	0.75
1:B:733:ARG:NH2	2:C:99:ASP:OD2	2.20	0.75
3:L:150:LYS:NZ	3:L:152:GLN:OE1	2.20	0.74
1:A:685:PRO:O	3:D:24:ARG:NH1	2.21	0.73
3:D:150:LYS:HB3	3:D:202:THR:HB	1.70	0.73
1:B:839:ASP:HB3	1:B:843:TRP:CD1	2.23	0.73
1:B:800:ARG:NH1	1:B:864:ASP:OD1	2.22	0.73
1:B:665:LEU:HD11	1:B:695:SER:HB3	1.71	0.73
3:L:59:ARG:HH12	3:L:65:ASP:CA	2.02	0.73
1:A:673:LYS:HD2	1:A:853:LEU:O	1.88	0.72
1:A:753:MET:CE	1:A:858:SER:HB3	2.19	0.72
2:C:13:ARG:HG2	2:C:116:SER:HA	1.73	0.71
3:L:152:GLN:HB3	3:L:200:GLU:HB3	1.73	0.71
3:L:38:LEU:HD23	3:L:39:HIS:N	2.07	0.70
1:B:661:SER:HA	1:B:691:THR:HG22	1.74	0.69
2:H:129:PRO:HG2	2:H:192:LEU:HD21	1.75	0.69
3:D:171:GLN:HG3	3:D:178:TYR:CZ	2.27	0.69
2:H:67:LYS:NZ	2:H:85:SER:O	2.25	0.69
1:B:696:LEU:HD13	1:B:746:VAL:HG11	1.75	0.69
2:C:146:LYS:NZ	2:C:174:GLN:OE1	2.25	0.69
3:D:113:ARG:HG2	3:D:113:ARG:HH11	1.56	0.69
3:L:59:ARG:CZ	3:L:65:ASP:HA	2.23	0.69
3:D:152:GLN:NE2	3:D:200:GLU:OE1	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:759:LEU:HD12	1:B:797:TYR:HE2	1.58	0.69
1:A:800:ARG:NH1	1:A:864:ASP:OD1	2.27	0.68
3:D:8:PRO:O	3:D:107:THR:HG23	1.94	0.68
2:C:149:PHE:HB3	2:C:150:PRO:HD3	1.77	0.67
3:D:37:TYR:CE1	3:D:55:LYS:HE2	2.29	0.67
2:C:127:LEU:HB3	3:D:123:PHE:CD1	2.29	0.67
2:C:150:PRO:HG2	2:C:205:PRO:HB2	1.76	0.67
2:H:118:SER:CB	2:H:149:PHE:HD2	2.08	0.67
2:H:24:ALA:O	2:H:77:ASN:ND2	2.28	0.67
2:H:127:LEU:HB3	3:L:123:PHE:CD2	2.29	0.67
1:A:832:ILE:HG23	1:A:863:ALA:HB3	1.75	0.66
1:B:637:LYS:HD3	1:B:891:PHE:CE2	2.30	0.66
2:C:150:PRO:HB2	2:C:205:PRO:HG2	1.77	0.66
1:A:637:LYS:HD3	1:A:891:PHE:CE2	2.31	0.66
2:H:10:GLU:OE2	2:H:204:LYS:HE2	1.95	0.65
2:H:125:PHE:CE2	3:L:129:GLN:HG3	2.31	0.65
3:L:125:PRO:HD3	3:L:137:VAL:HG22	1.78	0.65
3:D:38:LEU:HD23	3:D:39:HIS:N	2.12	0.65
2:H:13:ARG:NH2	2:H:117:ALA:HB2	2.09	0.65
1:B:736:PHE:HB3	2:C:101:ASN:OD1	1.96	0.65
2:H:149:PHE:HB3	2:H:150:PRO:HD3	1.79	0.65
1:A:753:MET:HE2	1:A:858:SER:HB3	1.80	0.64
1:A:797:TYR:HE1	1:A:872:ARG:O	1.79	0.64
3:L:13:VAL:HG21	3:L:83:VAL:HG21	1.80	0.64
1:B:802:ILE:HG13	1:B:836:ILE:CG2	2.28	0.64
1:B:758:ARG:HG2	1:B:759:LEU:HD22	1.79	0.64
1:A:758:ARG:HG2	1:A:759:LEU:HD22	1.79	0.64
1:B:759:LEU:HD12	1:B:797:TYR:CE2	2.32	0.64
1:B:832:ILE:HG23	1:B:863:ALA:HB3	1.80	0.64
3:D:29:LEU:HD12	3:D:38:LEU:HD12	1.80	0.64
2:H:30:LYS:HG3	2:H:74:THR:HG21	1.79	0.64
2:C:108:GLN:N	2:C:108:GLN:OE1	2.30	0.63
1:A:696:LEU:HB2	1:A:822:LEU:HB3	1.79	0.63
3:D:53:ILE:HD13	3:D:59:ARG:HA	1.80	0.63
2:H:10:GLU:HG2	2:H:152:PRO:HG3	1.80	0.63
2:H:120:LYS:HD3	2:H:121:GLY:N	2.14	0.63
1:A:637:LYS:HD3	1:A:891:PHE:HE2	1.64	0.63
1:B:682:GLN:HA	1:B:688:ARG:HH21	1.63	0.63
3:L:59:ARG:HH12	3:L:65:ASP:C	2.07	0.63
1:B:829:GLN:NE2	1:B:835:LYS:HD3	2.14	0.63
1:B:738:LEU:HB2	2:C:101:ASN:ND2	2.07	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:PRO:HD2	2:H:101:ASN:ND2	2.15	0.62
3:D:15:LEU:HD22	3:D:84:GLU:HA	1.81	0.62
1:A:733:ARG:NH2	2:H:99:ASP:OD1	2.33	0.62
1:A:659:LYS:HE2	1:A:693:ASP:HA	1.81	0.61
2:H:155:VAL:HG22	2:H:201:VAL:HG12	1.82	0.61
3:L:8:PRO:O	3:L:107:THR:HG23	2.00	0.61
1:A:646:ALA:HB2	1:A:694:PHE:HZ	1.66	0.61
3:D:120:VAL:HG21	3:D:201:VAL:HG21	1.83	0.61
1:A:733:ARG:HD3	1:A:736:PHE:CE2	2.35	0.61
1:A:672:ASP:N	1:A:672:ASP:OD1	2.34	0.60
1:A:759:LEU:O	1:A:797:TYR:HD2	1.84	0.60
3:L:29:LEU:HD12	3:L:38:LEU:HD12	1.82	0.60
1:A:821:LEU:HB3	1:A:857:CYS:SG	2.42	0.60
2:H:35:HIS:CE1	2:H:50:TRP:HB3	2.37	0.60
2:H:198:ILE:HD13	2:H:213:LYS:HG3	1.83	0.59
2:C:206:SER:OG	2:C:208:THR:OG1	2.15	0.59
2:H:13:ARG:HH21	2:H:117:ALA:CB	2.11	0.59
3:D:141:LEU:HB3	3:D:144:PHE:HE2	1.67	0.59
1:B:738:LEU:CB	2:C:101:ASN:HD21	2.09	0.59
1:A:685:PRO:HB2	3:D:24:ARG:NH1	2.17	0.59
1:A:646:ALA:HB2	1:A:694:PHE:CZ	2.37	0.59
1:B:646:ALA:HB2	1:B:694:PHE:CZ	2.38	0.59
1:B:829:GLN:OE1	1:B:835:LYS:HB2	2.03	0.59
3:D:120:VAL:HG12	3:D:212:LYS:HG3	1.84	0.59
1:A:832:ILE:HD11	1:A:865:CYS:SG	2.43	0.58
2:H:184:VAL:HG21	3:L:140:LEU:HD22	1.85	0.58
1:A:585:GLU:N	1:A:897:ASN:OD1	2.37	0.58
1:A:753:MET:HE3	1:A:858:SER:HB3	1.84	0.58
1:B:678:LEU:HD22	1:B:688:ARG:NH1	2.18	0.58
1:B:733:ARG:HD3	1:B:736:PHE:CZ	2.39	0.58
2:C:173:LEU:HD13	2:C:179:TYR:CE1	2.39	0.58
1:B:802:ILE:HG13	1:B:836:ILE:HG21	1.86	0.57
1:B:811:SER:H	1:B:814:ASP:HB2	1.69	0.57
1:B:797:TYR:HE1	1:B:872:ARG:O	1.88	0.57
1:A:678:LEU:HD22	1:A:688:ARG:NH1	2.20	0.57
2:H:206:SER:OG	2:H:208:THR:OG1	2.08	0.57
3:D:41:TYR:CE1	3:D:51:LEU:HD13	2.40	0.57
2:H:14:PRO:HD3	2:H:115:SER:O	2.05	0.57
2:H:127:LEU:HD21	3:L:138:VAL:HG21	1.86	0.57
3:L:197:TYR:HB2	3:L:214:PHE:CE1	2.40	0.57
1:A:800:ARG:HG2	1:A:832:ILE:HD13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:821:LEU:O	1:B:858:SER:N	2.34	0.56
3:D:152:GLN:HB3	3:D:200:GLU:HB3	1.86	0.56
1:B:673:LYS:HD2	1:B:853:LEU:O	2.05	0.56
1:B:859:PHE:CZ	1:B:861:ALA:HB2	2.39	0.56
1:B:730:VAL:HG12	1:B:731:THR:H	1.69	0.56
1:A:694:PHE:HB2	1:A:824:VAL:HB	1.86	0.56
2:H:186:THR:HG21	3:L:142:ASN:ND2	2.21	0.56
2:C:67:LYS:NZ	2:C:85:SER:O	2.39	0.56
2:C:9:ALA:HB3	2:C:18:VAL:HG23	1.87	0.56
1:A:685:PRO:HB2	3:D:24:ARG:CZ	2.36	0.56
3:L:155:VAL:HG13	3:L:197:TYR:CE1	2.41	0.56
3:D:13:VAL:HG23	3:D:83:VAL:HG11	1.87	0.55
2:H:108:GLN:N	2:H:108:GLN:OE1	2.40	0.55
2:C:120:LYS:HG3	2:C:148:TYR:HA	1.88	0.55
1:A:685:PRO:C	3:D:24:ARG:HH11	2.14	0.55
2:H:108:GLN:H	2:H:108:GLN:CD	2.13	0.55
3:D:37:TYR:O	3:D:95:GLN:HA	2.07	0.55
3:L:4:MET:HE3	3:L:23:CYS:SG	2.47	0.55
1:B:692:PRO:HG2	1:B:695:SER:OG	2.07	0.55
3:L:163:ASN:O	3:L:185:THR:HG22	2.07	0.55
1:B:659:LYS:HE2	1:B:693:ASP:HA	1.88	0.55
1:B:690:LEU:HD13	1:B:842:LYS:HD2	1.88	0.55
2:C:129:PRO:HG3	2:C:192:LEU:HD11	1.88	0.55
2:C:186:THR:HG21	3:D:142:ASN:OD1	2.06	0.55
2:C:35:HIS:CD2	2:C:99:ASP:HB2	2.42	0.54
2:C:91:THR:HG23	2:C:113:THR:HA	1.89	0.54
3:D:38:LEU:HD13	3:D:76:PHE:CG	2.43	0.54
2:H:12:VAL:HG21	2:H:86:LEU:HD13	1.89	0.54
2:H:120:LYS:HG2	2:H:178:LEU:HD22	1.90	0.54
2:H:151:GLU:O	2:H:151:GLU:HG2	2.07	0.54
1:B:696:LEU:HB2	1:B:822:LEU:HB3	1.89	0.54
3:D:190:ASP:OD1	3:D:193:LYS:HD3	2.08	0.54
3:L:171:GLN:HG3	3:L:178:TYR:CE1	2.42	0.54
2:H:35:HIS:O	2:H:96:CYS:HA	2.08	0.54
3:L:120:VAL:HG21	3:L:201:VAL:HG21	1.90	0.54
2:H:100:VAL:O	2:H:101:ASN:HB2	2.08	0.54
1:B:646:ALA:HB2	1:B:694:PHE:HZ	1.72	0.54
3:D:38:LEU:HD23	3:D:38:LEU:C	2.33	0.54
3:L:45:PRO:HG3	3:L:170:GLU:HG2	1.90	0.53
3:D:163:ASN:O	3:D:185:THR:HG22	2.09	0.53
1:B:849:LEU:HD12	1:B:849:LEU:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:759:LEU:O	1:B:797:TYR:HD2	1.92	0.53
1:A:598:MET:HG3	1:A:617:PHE:CE1	2.43	0.53
2:C:166:VAL:HG22	2:C:185:VAL:HB	1.89	0.53
1:A:616:LEU:HD13	1:A:636:LEU:HA	1.91	0.53
1:B:832:ILE:HD11	1:B:865:CYS:SG	2.49	0.53
1:A:692:PRO:HG2	1:A:695:SER:OG	2.09	0.53
1:A:702:PHE:HB2	3:L:72:SER:OG	2.08	0.53
2:C:33:TYR:HD1	2:C:52:ASP:HA	1.74	0.53
2:C:129:PRO:HD2	2:C:216:PRO:HA	1.90	0.53
1:B:694:PHE:HB2	1:B:824:VAL:HB	1.90	0.52
3:D:123:PHE:HB2	3:D:138:VAL:HB	1.92	0.52
3:D:13:VAL:HG21	3:D:83:VAL:HG21	1.90	0.52
2:H:11:LEU:HD22	2:H:150:PRO:HG3	1.92	0.52
2:H:120:LYS:HD3	2:H:121:GLY:H	1.74	0.52
3:D:141:LEU:HB3	3:D:144:PHE:CE2	2.45	0.52
3:D:155:VAL:CG2	3:D:160:GLN:HE22	2.23	0.52
3:L:40:TRP:CZ3	3:L:93:CYS:HB3	2.45	0.52
3:L:154:LYS:HE3	3:L:157:ASN:HA	1.90	0.52
2:C:127:LEU:HD22	3:D:123:PHE:HB3	1.92	0.52
2:H:13:ARG:HA	2:H:115:SER:O	2.10	0.52
2:H:118:SER:CB	2:H:149:PHE:CD2	2.92	0.52
3:D:11:LEU:HD21	3:D:19:ALA:HB1	1.91	0.52
1:B:649:TYR:CE2	1:B:756:PHE:HE1	2.29	0.51
1:B:630:TRP:HE3	1:B:894:LEU:HB3	1.75	0.51
1:B:637:LYS:HB2	1:B:891:PHE:HE2	1.75	0.51
2:H:120:LYS:HG3	2:H:148:TYR:CA	2.28	0.51
1:B:678:LEU:CD2	1:B:688:ARG:NH1	2.73	0.51
2:C:17:LEU:HD11	2:C:82:ARG:HD3	1.92	0.51
1:A:802:ILE:HG13	1:A:836:ILE:HG21	1.92	0.51
2:H:119:THR:HG23	2:H:205:PRO:O	2.10	0.51
1:B:859:PHE:HZ	1:B:861:ALA:HB2	1.76	0.51
3:L:145:TYR:CD1	3:L:146:PRO:HA	2.47	0.51
1:B:802:ILE:HG13	1:B:836:ILE:HG22	1.93	0.51
2:C:198:ILE:HD13	2:C:213:LYS:HG3	1.92	0.51
3:D:118:PRO:HB3	3:D:144:PHE:CD2	2.46	0.50
2:H:104:ASP:HA	3:L:51:LEU:HD22	1.92	0.50
1:B:630:TRP:CE3	1:B:894:LEU:HB3	2.47	0.50
3:D:156:ASP:OD2	3:D:194:HIS:HB3	2.11	0.50
2:H:30:LYS:HE3	2:H:74:THR:OG1	2.11	0.50
1:A:737:PRO:HG3	2:H:33:TYR:CD2	2.47	0.50
2:H:201:VAL:HG22	2:H:210:VAL:HB	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:51:ILE:HD13	2:H:72:ALA:HB2	1.93	0.50
1:B:680:ARG:HG3	1:B:849:LEU:HD11	1.94	0.50
3:D:38:LEU:CD1	3:D:76:PHE:CD2	2.94	0.50
3:D:88:LEU:HD21	3:D:111:ILE:HG12	1.94	0.49
1:A:844:LYS:HE2	1:A:848:LYS:HE3	1.94	0.49
2:H:173:LEU:HD13	2:H:179:TYR:CZ	2.46	0.49
3:L:59:ARG:NH2	3:L:65:ASP:HA	2.27	0.49
1:A:825:GLU:HB3	1:A:835:LYS:HE3	1.93	0.49
1:B:809:ARG:CD	1:B:809:ARG:H	2.25	0.49
2:C:29:ILE:HG22	2:C:34:ILE:HD11	1.94	0.49
3:D:198:ALA:HB2	3:D:213:SER:HB3	1.93	0.49
1:B:735:MET:HE3	1:B:735:MET:HA	1.94	0.49
1:B:651:TRP:CE2	1:B:696:LEU:HD11	2.48	0.49
1:B:672:ASP:OD1	1:B:672:ASP:N	2.43	0.49
3:D:125:PRO:CD	3:D:137:VAL:HG22	2.42	0.49
1:A:737:PRO:HD2	2:H:101:ASN:CG	2.37	0.49
2:H:125:PHE:CD2	3:L:129:GLN:HG3	2.48	0.49
1:B:733:ARG:HD3	1:B:736:PHE:CE2	2.47	0.49
2:C:6:GLU:OE2	2:C:107:GLY:HA3	2.13	0.49
1:A:690:LEU:HD22	1:A:842:LYS:HD2	1.95	0.49
1:A:733:ARG:HD3	1:A:736:PHE:CZ	2.48	0.48
1:A:661:SER:HA	1:A:691:THR:HG22	1.95	0.48
1:B:637:LYS:CA	1:B:887:VAL:HG11	2.38	0.48
2:H:166:VAL:HG22	2:H:185:VAL:HB	1.95	0.48
1:B:630:TRP:CH2	1:B:891:PHE:HD1	2.31	0.48
2:C:35:HIS:NE2	2:C:99:ASP:OD2	2.46	0.48
1:A:602:PHE:HA	1:A:605:LEU:HD12	1.95	0.48
1:A:736:PHE:HB3	2:H:101:ASN:OD1	2.14	0.48
3:D:145:TYR:CD1	3:D:146:PRO:HA	2.49	0.48
1:A:832:ILE:O	1:A:836:ILE:HD12	2.13	0.48
2:C:200:ASN:HD22	2:C:211:ASP:CG	2.22	0.48
3:D:196:VAL:HG22	3:D:215:ASN:OD1	2.13	0.48
2:C:156:SER:OG	2:C:200:ASN:HB2	2.14	0.48
2:C:150:PRO:HB2	2:C:203:HIS:HE2	1.79	0.47
2:C:18:VAL:HG12	2:C:86:LEU:HD11	1.95	0.47
3:D:21:ILE:HG22	3:D:40:TRP:CH2	2.50	0.47
3:D:120:VAL:HA	3:D:140:LEU:O	2.15	0.47
1:A:849:LEU:O	1:A:849:LEU:HD12	2.15	0.47
2:H:12:VAL:HG22	2:H:112:LEU:HD11	1.97	0.47
3:L:42:LEU:HD13	3:L:91:TYR:CE1	2.50	0.47
2:H:38:LYS:HB2	2:H:48:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2:VAL:HG13	2:C:27:PHE:CE1	2.50	0.47
3:D:15:LEU:HD23	3:D:83:VAL:HG12	1.97	0.47
3:D:129:GLN:HG2	3:D:134:THR:HG23	1.97	0.47
3:D:181:SER:O	3:D:181:SER:OG	2.33	0.47
3:L:23:CYS:HB2	3:L:40:TRP:CH2	2.50	0.47
3:L:52:LEU:HA	3:L:52:LEU:HD23	1.73	0.47
1:B:649:TYR:CE2	1:B:756:PHE:CE1	3.02	0.47
1:B:696:LEU:HD22	1:B:744:ASN:ND2	2.30	0.47
2:C:40:ARG:HB2	2:C:43:GLN:HB2	1.97	0.47
1:A:590:ILE:HD13	1:A:893:LYS:HB3	1.97	0.47
1:B:868:THR:HB	1:B:873:TRP:NE1	2.30	0.47
2:C:117:ALA:HB3	2:C:149:PHE:CE2	2.50	0.47
1:B:760:MET:HE2	1:B:798:GLY:HA2	1.97	0.46
3:D:168:VAL:HG22	3:D:180:LEU:HD12	1.97	0.46
1:B:808:MET:HB2	1:B:851:GLU:HG3	1.97	0.46
3:D:15:LEU:HD21	3:D:84:GLU:C	2.40	0.46
1:A:809:ARG:H	1:A:809:ARG:CD	2.28	0.46
3:L:38:LEU:HD23	3:L:38:LEU:C	2.39	0.46
3:D:38:LEU:HD13	3:D:76:PHE:CD2	2.50	0.46
1:A:850:LEU:HD23	1:A:850:LEU:HA	1.48	0.46
1:A:586:PRO:CG	1:A:589:ILE:HD12	2.40	0.46
2:H:61:ASP:OD1	2:H:63:LYS:HG2	2.16	0.46
1:B:873:TRP:HB2	1:B:880:VAL:HG21	1.97	0.46
1:A:665:LEU:HD11	1:A:695:SER:CB	2.38	0.46
2:H:122:PRO:HB3	2:H:148:TYR:CD2	2.51	0.46
1:B:696:LEU:O	1:B:821:LEU:HD12	2.15	0.46
2:C:86:LEU:HD23	2:C:86:LEU:HA	1.57	0.46
3:L:111:ILE:HB	3:L:176:SER:HB3	1.96	0.46
3:L:150:LYS:HB3	3:L:202:THR:HB	1.98	0.46
1:B:809:ARG:O	1:B:810:PHE:HD1	1.99	0.46
2:C:115:SER:OG	2:C:116:SER:N	2.49	0.46
2:H:2:VAL:HG13	2:H:27:PHE:CE1	2.51	0.46
3:D:111:ILE:HB	3:D:176:SER:HB3	1.98	0.46
3:D:113:ARG:NE	3:D:177:THR:HG22	2.30	0.46
1:A:682:GLN:HA	1:A:688:ARG:HH21	1.80	0.45
1:A:759:LEU:O	1:A:797:TYR:CD2	2.66	0.45
3:L:38:LEU:HD21	3:L:93:CYS:HB2	1.97	0.45
3:L:128:GLU:OE1	3:L:128:GLU:N	2.46	0.45
1:A:698:GLN:HG2	1:A:748:SER:HA	1.98	0.45
3:L:70:SER:O	3:L:77:THR:N	2.36	0.45
2:H:198:ILE:CD1	2:H:213:LYS:HG3	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:112:LYS:HA	3:L:145:TYR:OH	2.15	0.45
3:D:11:LEU:O	3:D:109:LEU:HD12	2.16	0.45
3:D:96:SER:HA	3:D:101:PHE:CD1	2.52	0.45
1:A:634:LEU:HA	1:A:891:PHE:HZ	1.82	0.45
1:A:696:LEU:HD22	1:A:744:ASN:HD22	1.82	0.45
2:C:51:ILE:HD13	2:C:72:ALA:HB2	1.99	0.45
1:A:654:ILE:HG21	1:A:659:LYS:HA	1.99	0.45
1:A:758:ARG:HG3	1:A:763:GLY:HA2	1.97	0.45
3:D:113:ARG:HE	3:D:177:THR:CG2	2.30	0.45
2:H:86:LEU:HD23	2:H:86:LEU:HA	1.79	0.45
2:H:126:PRO:HB3	2:H:214:VAL:HG22	1.99	0.45
1:B:839:ASP:HB3	1:B:843:TRP:NE1	2.31	0.45
3:D:15:LEU:CD2	3:D:84:GLU:C	2.90	0.45
3:D:15:LEU:HD11	3:D:85:ALA:HB2	1.99	0.45
1:A:594:ILE:CD1	1:A:890:LEU:HD13	2.38	0.45
2:H:43:GLN:H	2:H:43:GLN:HG2	1.50	0.45
3:D:65:ASP:OD1	3:D:65:ASP:N	2.49	0.45
1:A:732:GLU:O	1:A:734:LYS:HG3	2.17	0.44
3:D:113:ARG:HB3	3:D:145:TYR:CD2	2.52	0.44
1:B:802:ILE:HD12	1:B:840:HIS:ND1	2.31	0.44
1:B:821:LEU:HD12	1:B:821:LEU:HA	1.86	0.44
2:H:36:TRP:CE2	2:H:81:LEU:HB2	2.51	0.44
1:B:636:LEU:CD2	1:B:887:VAL:HG22	2.47	0.44
1:B:659:LYS:HE2	1:B:693:ASP:O	2.18	0.44
3:D:53:ILE:HA	3:D:58:ASN:O	2.18	0.44
3:D:152:GLN:HG2	3:D:154:LYS:HG3	2.00	0.44
2:H:184:VAL:HG21	3:L:140:LEU:CD2	2.48	0.44
3:L:122:ILE:HD12	3:L:199:CYS:HB2	2.00	0.44
3:L:171:GLN:HG3	3:L:178:TYR:CZ	2.53	0.44
1:B:663:THR:HG23	1:B:674:PHE:HE1	1.81	0.44
1:B:696:LEU:HD22	1:B:744:ASN:HD22	1.81	0.44
2:H:122:PRO:HB2	2:H:145:VAL:HG13	1.98	0.44
3:D:195:LYS:O	3:D:215:ASN:HA	2.18	0.44
1:A:696:LEU:HD13	1:A:746:VAL:HG11	1.98	0.44
2:C:38:LYS:HE2	2:C:40:ARG:NE	2.32	0.44
1:A:678:LEU:CD2	1:A:688:ARG:NH1	2.81	0.44
1:B:808:MET:CG	1:B:809:ARG:HH11	2.30	0.44
1:B:815:GLN:HG2	1:B:820:GLN:OE1	2.18	0.44
2:C:157:TRP:CH2	2:C:199:CYS:HB3	2.52	0.44
3:D:198:ALA:CB	3:D:213:SER:HB3	2.48	0.44
2:H:40:ARG:HG2	2:H:92:ALA:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:129:GLN:HE22	3:L:136:SER:CB	2.31	0.43
2:C:13:ARG:HA	2:C:115:SER:O	2.18	0.43
2:C:31:ASP:O	2:C:32:TYR:CG	2.71	0.43
2:C:32:TYR:HB3	2:C:99:ASP:O	2.18	0.43
2:C:129:PRO:CG	2:C:192:LEU:HD11	2.47	0.43
1:A:630:TRP:CH2	1:A:891:PHE:HD1	2.36	0.43
2:H:30:LYS:CG	2:H:74:THR:HG21	2.47	0.43
2:H:31:ASP:O	2:H:32:TYR:CG	2.71	0.43
2:C:61:ASP:OD1	2:C:63:LYS:HG2	2.18	0.43
2:H:186:THR:HG21	3:L:142:ASN:HD21	1.83	0.43
1:B:665:LEU:HD11	1:B:695:SER:CB	2.44	0.43
1:B:811:SER:N	1:B:814:ASP:HB2	2.32	0.43
3:D:113:ARG:HG2	3:D:113:ARG:NH1	2.29	0.43
3:D:15:LEU:HD22	3:D:84:GLU:CA	2.48	0.43
1:A:842:LYS:HE3	1:A:842:LYS:HB3	1.87	0.43
3:L:41:TYR:CD1	3:L:51:LEU:HA	2.54	0.43
1:B:601:LEU:HD22	1:B:886:SER:OG	2.17	0.43
3:D:3:LYS:H	3:D:26:SER:CB	2.31	0.43
1:A:687:PHE:CG	1:A:846:ILE:HD11	2.53	0.43
1:A:800:ARG:NH2	1:A:872:ARG:O	2.37	0.43
2:C:147:ASP:HB3	2:C:178:LEU:HD13	2.01	0.43
3:D:172:ASP:HB3	3:D:175:ASP:OD1	2.17	0.43
2:C:150:PRO:HD2	2:C:203:HIS:CE1	2.54	0.43
1:A:821:LEU:HG	1:A:823:LEU:HD21	2.00	0.43
1:A:836:ILE:HD12	1:A:836:ILE:H	1.83	0.43
3:L:24:ARG:HA	3:L:74:THR:O	2.18	0.43
1:B:585:GLU:HB3	1:B:897:ASN:HD21	1.83	0.43
3:D:3:LYS:H	3:D:26:SER:HB3	1.84	0.43
3:D:40:TRP:CE2	3:D:78:LEU:HB2	2.54	0.43
2:H:116:SER:O	2:H:117:ALA:HB3	2.19	0.43
2:C:45:LEU:HD23	2:C:45:LEU:HA	1.93	0.43
2:H:151:GLU:N	2:H:152:PRO:HD2	2.34	0.42
2:C:97:VAL:HG11	2:C:103:LEU:HB3	2.01	0.42
1:A:756:PHE:O	1:A:760:MET:HG3	2.19	0.42
1:B:627:SER:O	1:B:631:LYS:HG3	2.18	0.42
1:B:687:PHE:CG	1:B:846:ILE:HD11	2.54	0.42
1:B:689:ASP:O	1:B:691:THR:HG23	2.19	0.42
2:C:24:ALA:O	2:C:77:ASN:ND2	2.51	0.42
2:C:47:TRP:CZ3	3:D:100:PRO:HA	2.54	0.42
3:D:141:LEU:HD11	3:D:201:VAL:HG22	2.01	0.42
3:L:168:VAL:HG12	3:L:169:THR:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:678:LEU:CD2	1:B:688:ARG:HH11	2.32	0.42
1:B:796:ASP:CG	1:B:797:TYR:H	2.27	0.42
1:B:873:TRP:CB	1:B:880:VAL:HG21	2.49	0.42
3:D:155:VAL:HG23	3:D:160:GLN:HE22	1.83	0.42
1:A:609:CYS:HB2	1:A:653:TYR:CD2	2.54	0.42
2:H:12:VAL:HG21	2:H:86:LEU:CD1	2.50	0.42
2:H:32:TYR:CE1	2:H:100:VAL:HG12	2.55	0.42
3:L:195:LYS:O	3:L:215:ASN:HA	2.19	0.42
1:B:652:GLN:HG2	1:B:744:ASN:OD1	2.19	0.42
1:B:820:GLN:HG2	1:B:856:LYS:HB3	2.02	0.42
2:C:42:GLU:OE1	2:C:42:GLU:N	2.52	0.42
2:C:172:VAL:HG22	2:C:180:SER:O	2.18	0.42
1:A:732:GLU:HA	3:L:98:HIS:HA	2.01	0.42
1:B:654:ILE:HG22	1:B:659:LYS:HG3	2.02	0.42
3:D:141:LEU:HD22	3:D:180:LEU:HD22	2.02	0.42
3:L:59:ARG:HH22	3:L:65:ASP:CB	2.32	0.42
3:L:196:VAL:HG22	3:L:215:ASN:OD1	2.19	0.42
3:D:163:ASN:OD1	3:D:163:ASN:N	2.51	0.42
2:H:38:LYS:HE2	2:H:40:ARG:NE	2.35	0.42
2:H:120:LYS:CG	2:H:148:TYR:HA	2.31	0.42
3:D:152:GLN:HG3	3:D:159:LEU:HD13	2.02	0.42
1:A:735:MET:HE3	1:A:735:MET:HA	2.01	0.42
3:D:154:LYS:HE3	3:D:154:LYS:HB3	1.92	0.42
1:A:616:LEU:O	1:A:620:ILE:HG13	2.19	0.42
1:A:868:THR:HB	1:A:873:TRP:NE1	2.34	0.42
2:H:33:TYR:CE1	2:H:52:ASP:HB2	2.55	0.42
2:H:40:ARG:HG2	2:H:92:ALA:CB	2.49	0.42
2:C:169:PHE:CE1	3:D:169:THR:HG23	2.55	0.42
1:A:696:LEU:HD22	1:A:744:ASN:ND2	2.35	0.42
3:L:13:VAL:HG23	3:L:83:VAL:HG11	2.01	0.42
1:B:649:TYR:CD1	1:B:649:TYR:N	2.87	0.42
2:C:191:SER:O	2:C:194:THR:HB	2.20	0.42
3:D:13:VAL:HG22	3:D:109:LEU:HD11	2.02	0.42
1:A:598:MET:HE3	1:A:890:LEU:HD22	2.01	0.41
3:L:198:ALA:HB2	3:L:213:SER:HB3	2.00	0.41
1:A:829:GLN:H	1:A:829:GLN:HG2	1.66	0.41
3:L:87:ASP:O	3:L:109:LEU:HD23	2.20	0.41
3:L:88:LEU:HD21	3:L:111:ILE:HG12	2.01	0.41
2:C:104:ASP:OD1	2:C:105:TYR:N	2.51	0.41
2:H:148:TYR:CE1	2:H:179:TYR:HB2	2.56	0.41
3:L:13:VAL:HG22	3:L:109:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:31:ASP:C	2:C:32:TYR:CD2	2.98	0.41
2:C:22:CYS:C	2:C:78:THR:HG23	2.45	0.41
1:B:678:LEU:O	1:B:688:ARG:NH2	2.54	0.41
1:B:806:ASN:HB3	1:B:847:LEU:HD22	2.02	0.41
2:C:8:GLY:HA3	2:C:20:LEU:HD23	2.03	0.41
2:C:47:TRP:HZ3	3:D:99:VAL:HG13	1.85	0.41
2:C:60:TYR:HB2	2:C:65:GLN:HG3	2.03	0.41
3:L:37:TYR:O	3:L:95:GLN:HA	2.21	0.41
1:B:870:PRO:O	1:B:877:GLU:HG3	2.21	0.41
2:C:174:GLN:HA	3:D:165:GLN:OE1	2.20	0.41
3:D:120:VAL:CG2	3:D:201:VAL:HG21	2.49	0.41
1:A:590:ILE:O	1:A:594:ILE:HG12	2.20	0.41
1:A:811:SER:H	1:A:814:ASP:HB2	1.85	0.41
2:H:203:HIS:NE2	2:H:205:PRO:HG2	2.36	0.41
3:L:41:TYR:CE1	3:L:51:LEU:HD13	2.56	0.41
2:C:106:TRP:CZ3	3:D:49:PRO:HG2	2.56	0.41
2:C:150:PRO:CB	2:C:205:PRO:HG2	2.49	0.41
1:A:862:CYS:HB2	1:A:874:TRP:CE2	2.56	0.41
2:H:161:ALA:HB1	3:D:158:ALA:HB1	2.03	0.41
3:L:120:VAL:CG2	3:L:201:VAL:HG21	2.51	0.41
1:B:634:LEU:HA	1:B:891:PHE:HZ	1.85	0.41
1:B:749:ILE:HG12	1:B:822:LEU:HB2	2.01	0.41
3:D:88:LEU:HD13	3:D:171:GLN:HB3	2.03	0.41
2:H:162:LEU:HD21	2:H:185:VAL:HG21	2.02	0.41
1:A:587:ILE:HD13	1:A:629:ALA:HB2	2.03	0.40
2:H:58:THR:HB	2:H:60:TYR:CE1	2.56	0.40
2:C:36:TRP:CE2	2:C:81:LEU:HB2	2.55	0.40
2:C:187:VAL:HG11	2:C:197:TYR:CE1	2.56	0.40
2:C:204:LYS:HB3	2:C:205:PRO:HD3	2.03	0.40
3:D:37:TYR:HB2	3:D:97:THR:OG1	2.21	0.40
3:D:66:ARG:HD2	3:D:82:ARG:O	2.21	0.40
3:D:180:LEU:HD23	3:D:180:LEU:C	2.47	0.40
2:H:86:LEU:HB3	2:H:114:VAL:HG11	2.02	0.40
3:L:68:SER:O	3:L:78:LEU:HD12	2.21	0.40
3:L:113:ARG:HD2	3:L:176:SER:O	2.21	0.40
2:C:150:PRO:HB2	2:C:203:HIS:NE2	2.36	0.40
2:H:173:LEU:HD13	2:H:179:TYR:CE1	2.56	0.40
1:B:813:GLU:O	1:B:817:GLU:N	2.54	0.40
2:C:38:LYS:HB2	2:C:48:ILE:HD11	2.04	0.40
2:C:149:PHE:O	2:C:150:PRO:C	2.64	0.40
1:A:626:HIS:CE1	1:A:897:ASN:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:PRO:HD2	1:A:658:ILE:HG12	2.03	0.40
1:A:800:ARG:HD2	1:A:863:ALA:O	2.21	0.40
1:A:802:ILE:HG13	1:A:836:ILE:CG2	2.52	0.40
2:H:118:SER:CB	2:H:149:PHE:HB3	2.51	0.40
2:H:125:PHE:HB3	3:L:126:SER:OG	2.22	0.40
3:L:163:ASN:ND2	3:L:184:LEU:HD11	2.36	0.40
1:B:821:LEU:HG	1:B:823:LEU:HD21	2.04	0.40
2:C:149:PHE:CB	2:C:150:PRO:HD3	2.49	0.40
1:A:821:LEU:HA	1:A:821:LEU:HD12	1.77	0.40
2:H:6:GLU:OE2	2:H:107:GLY:HA3	2.21	0.40
2:H:181:LEU:C	2:H:181:LEU:HD12	2.46	0.40
3:D:155:VAL:HG22	3:D:197:TYR:CD1	2.56	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	249/319 (78%)	246 (99%)	3 (1%)	0	100	100
1	B	249/319 (78%)	245 (98%)	4 (2%)	0	100	100
2	C	206/228 (90%)	197 (96%)	8 (4%)	1 (0%)	24	52
2	H	206/228 (90%)	193 (94%)	11 (5%)	2 (1%)	12	37
3	D	214/219 (98%)	206 (96%)	8 (4%)	0	100	100
3	L	214/219 (98%)	206 (96%)	8 (4%)	0	100	100
All	All	1338/1532 (87%)	1293 (97%)	42 (3%)	3 (0%)	43	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	118	SER

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Mol	Chain	Res	Type
2	H	149	PHE
2	C	149	PHE

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	234/291 (80%)	234 (100%)	0	100	100
1	B	234/291 (80%)	234 (100%)	0	100	100
2	C	180/199 (90%)	180 (100%)	0	100	100
2	H	180/199 (90%)	180 (100%)	0	100	100
3	D	194/196 (99%)	194 (100%)	0	100	100
3	L	194/196 (99%)	194 (100%)	0	100	100
All	All	1216/1372 (89%)	1216 (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 (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	626	HIS
1	A	747	HIS
1	A	761	HIS
1	A	897	ASN
2	H	101	ASN
1	B	897	ASN
2	C	39	GLN
3	D	43	GLN
3	D	142	ASN
3	D	160	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 [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	255/319 (79%)	-0.71	0	100	100	114, 144, 188, 196	0
1	B	255/319 (79%)	-0.83	0	100	100	111, 142, 177, 195	0
2	C	210/228 (92%)	-0.73	1 (0%)	87	72	94, 122, 142, 151	0
2	H	210/228 (92%)	-0.80	0	100	100	103, 130, 158, 167	0
3	D	216/219 (98%)	-0.81	0	100	100	104, 125, 162, 171	0
3	L	216/219 (98%)	-0.75	0	100	100	110, 134, 176, 186	0
All	All	1362/1532 (88%)	-0.77	1 (0%)	92	86	94, 133, 174, 196	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	29	ILE	2.7

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.