



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2025 – 12:41 AM JST

PDB ID : 9IMX / pdb\_00009imx  
Title : Immune complex of HEV E2s and P1-5B nanobody  
Authors : Tingting, L.; Wenhui, X.; Ying, G.; Shaowei, L.  
Deposited on : 2024-07-04  
Resolution : 2.20 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](mailto: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>.

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

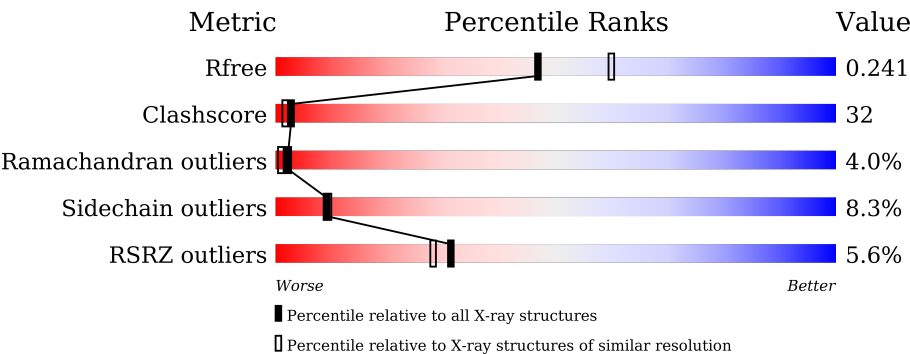
MolProbity : 4-5-2 with Phenix2.0rc1  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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  $\geq 3$ , 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	150	<div><div>6%</div><div>46%</div><div>45%</div><div>6%</div><div></div></div>
1	B	150	<div><div>2%</div><div>46%</div><div>44%</div><div>5%</div><div></div></div>
1	E	150	<div><div>4%</div><div>45%</div><div>46%</div><div>5%</div><div></div></div>
1	F	150	<div><div>3%</div><div>48%</div><div>42%</div><div>6%</div><div></div></div>
2	C	132	<div><div>3%</div><div>29%</div><div>36%</div><div>7%</div><div>27%</div></div>
2	D	132	<div><div>7%</div><div>30%</div><div>37%</div><div></div><div>28%</div></div>

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Mol	Chain	Length	Quality of chain
2	G	132	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>8%30%38%••27%</div></div>
2	H	132	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>5%35%30%5%•28%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7390 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 Secreted protein ORF2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	0	0	0
			1096	698	183	215			
1	B	144	Total	C	N	O	0	0	0
			1084	690	181	213			
1	E	146	Total	C	N	O	0	0	0
			1096	698	183	215			
1	F	144	Total	C	N	O	0	0	0
			1084	690	181	213			

- Molecule 2 is a protein called P1-5B nanobody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	96	Total	C	N	O	S	0	0	0
			732	463	120	145	4			
2	D	95	Total	C	N	O	S	0	0	0
			724	459	119	142	4			
2	G	96	Total	C	N	O	S	0	0	0
			732	463	120	145	4			
2	H	95	Total	C	N	O	S	0	0	0
			724	459	119	142	4			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total	O	0	0
			24	24		
3	B	22	Total	O	0	0
			22	22		
3	C	21	Total	O	0	0
			21	21		
3	D	12	Total	O	0	0
			12	12		

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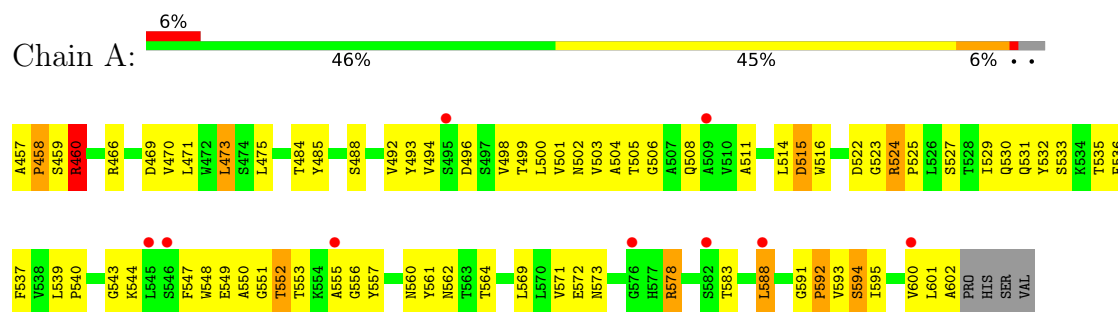
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	13	Total 13	O 13	0	0
3	F	15	Total 15	O 15	0	0
3	G	6	Total 6	O 6	0	0
3	H	5	Total 5	O 5	0	0

### 3 Residue-property plots

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

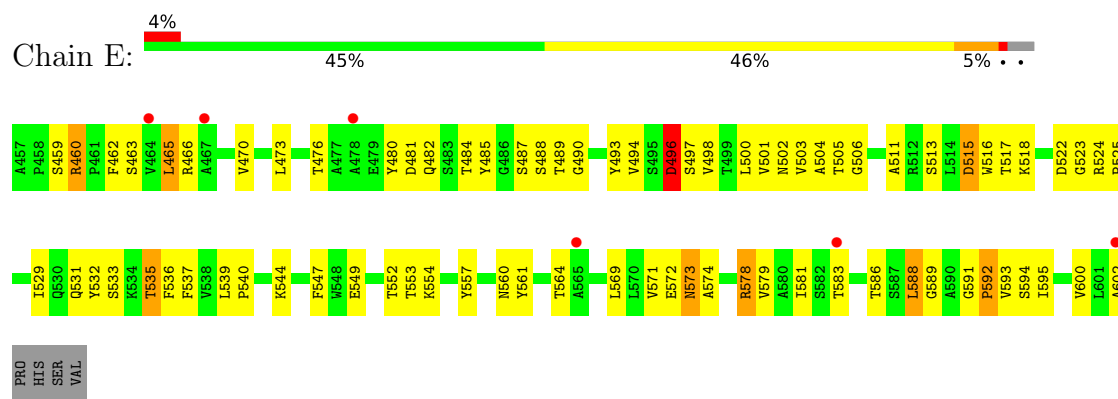
#### • Molecule 1: Secreted protein ORF2



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#### • Molecule 1: Secreted protein ORF2

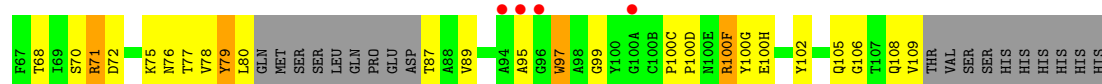
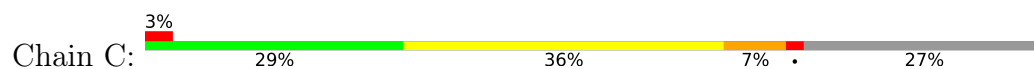


#### • Molecule 1: Secreted protein ORF2

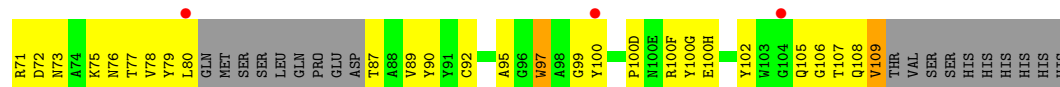




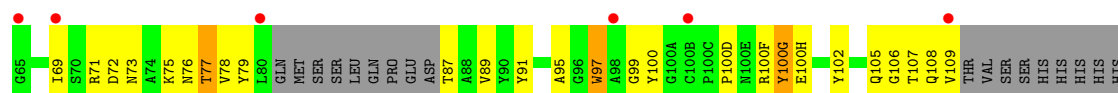
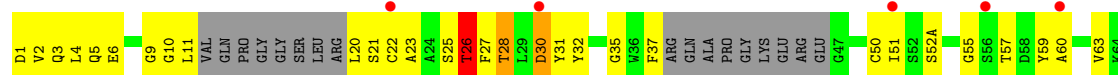
• Molecule 2: P1-5B nanobody



• Molecule 2: P1-5B nanobody

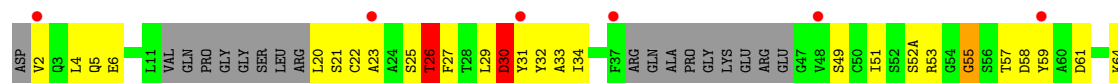


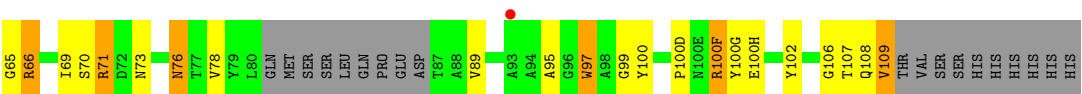
• Molecule 2: P1-5B nanobody



HIS

• Molecule 2: P1-5B nanobody







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.39Å 51.40Å 265.17Å 90.00° 92.74° 90.00°	Depositor
Resolution (Å)	66.22 – 2.20 66.22 – 2.20	Depositor EDS
% Data completeness (in resolution range)	85.3 (66.22-2.20) 100.0 (66.22-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.09 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0403	Depositor
R, $R_{free}$	0.217 , 0.245 0.213 , 0.241	Depositor DCC
$R_{free}$ test set	2124 reflections (2.58%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.9	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 73.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.044 for -k,-h,-l 0.042 for k,h,-l 0.059 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7390	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.73	0/1121	1.24	1/1538 (0.1%)
1	B	0.76	0/1108	1.25	3/1519 (0.2%)
1	E	0.67	0/1121	1.22	4/1538 (0.3%)
1	F	0.67	0/1108	1.21	2/1519 (0.1%)
2	C	0.71	0/749	1.09	0/1015
2	D	0.71	0/741	1.12	2/1004 (0.2%)
2	G	0.69	0/749	1.04	0/1015
2	H	0.60	0/741	1.03	1/1004 (0.1%)
All	All	0.70	0/7438	1.17	13/10152 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	E	0	2
1	F	0	1
2	C	0	4
2	H	0	3
All	All	0	14

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	528	THR	CA-CB-OG1	-7.43	98.45	109.60
1	E	487	SER	CA-C-N	6.34	129.10	120.54
1	E	487	SER	C-N-CA	6.34	129.10	120.54
2	H	30	ASP	CA-CB-CG	5.92	118.52	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	499	THR	CB-CA-C	5.88	119.95	109.38
1	B	531	GLN	CB-CG-CD	-5.87	102.62	112.60
2	D	37	PHE	CA-C-O	-5.71	111.10	120.80
1	E	496	ASP	CA-CB-CG	5.67	118.27	112.60
1	F	499	THR	CB-CA-C	5.48	119.83	109.37
2	D	30	ASP	CA-CB-CG	5.45	118.05	112.60
1	F	542	ARG	NE-CZ-NH1	-5.25	116.25	121.50
1	B	499	THR	CB-CA-C	5.23	118.79	109.38
1	E	573	ASN	N-CA-CB	5.05	116.00	110.35

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	460	ARG	Sidechain
1	A	524	ARG	Sidechain
1	A	578	ARG	Sidechain
1	B	542	ARG	Sidechain
2	C	100(F)	ARG	Sidechain
2	C	53	ARG	Sidechain
2	C	66	ARG	Sidechain
2	C	71	ARG	Sidechain
1	E	460	ARG	Sidechain
1	E	578	ARG	Sidechain
1	F	460	ARG	Sidechain
2	H	100(F)	ARG	Sidechain
2	H	66	ARG	Sidechain
2	H	97	TRP	Peptide

## 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	1096	0	1085	82	0
1	B	1084	0	1073	79	0
1	E	1096	0	1085	73	0
1	F	1084	0	1073	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	732	0	665	60	2
2	D	724	0	658	52	0
2	G	732	0	665	58	0
2	H	724	0	658	41	0
3	A	24	0	0	15	0
3	B	22	0	0	22	0
3	C	21	0	0	11	0
3	D	12	0	0	6	0
3	E	13	0	0	4	0
3	F	15	0	0	7	0
3	G	6	0	0	6	0
3	H	5	0	0	4	0
All	All	7390	0	6962	459	2

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 32.

All (459) 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)
2:C:77:THR:HB	3:C:201:HOH:O	1.49	1.13
1:A:504:ALA:HA	3:B:701:HOH:O	1.49	1.08
2:C:60:ALA:N	3:C:202:HOH:O	1.84	1.07
1:B:503:VAL:C	3:B:701:HOH:O	1.99	1.05
2:G:37:PHE:HD2	3:G:202:HOH:O	1.42	1.01
1:B:577:HIS:ND1	3:B:702:HOH:O	1.97	0.97
2:C:80:LEU:N	3:C:203:HOH:O	1.99	0.95
1:F:468:ASN:ND2	1:F:542:ARG:HH12	1.64	0.95
1:A:516:TRP:HE3	3:A:715:HOH:O	1.50	0.95
2:C:66:ARG:HG3	2:C:66:ARG:HH11	1.32	0.94
1:F:468:ASN:ND2	1:F:542:ARG:NH1	2.17	0.93
2:C:60:ALA:HB3	2:C:63:VAL:HB	1.52	0.92
1:A:588:LEU:HD22	1:A:592:PRO:HB3	1.52	0.92
1:A:492:VAL:O	3:A:702:HOH:O	1.87	0.91
1:A:530:GLN:O	3:A:701:HOH:O	1.87	0.91
1:E:493:TYR:CE1	1:E:592:PRO:HG3	2.06	0.91
1:A:457:ALA:O	1:A:459:SER:N	2.04	0.89
2:H:51:ILE:HG22	3:H:201:HOH:O	1.72	0.89
2:G:1:ASP:OD1	2:G:26:THR:OG1	1.90	0.89
1:F:503:VAL:O	3:F:702:HOH:O	1.90	0.88
1:B:524:ARG:NH2	2:G:105:GLN:OE1	2.07	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:61:ASP:OD1	3:D:201:HOH:O	1.92	0.87
2:H:34:ILE:O	3:H:201:HOH:O	1.91	0.86
1:F:549:GLU:N	3:F:703:HOH:O	2.05	0.86
1:B:531:GLN:NE2	3:B:703:HOH:O	2.04	0.86
1:E:549:GLU:HB2	1:E:588:LEU:HD11	1.57	0.85
1:F:468:ASN:HD21	1:F:542:ARG:NH1	1.73	0.84
1:F:468:ASN:HD21	1:F:542:ARG:HH12	1.26	0.84
1:A:505:THR:O	3:A:703:HOH:O	1.95	0.84
3:A:707:HOH:O	1:B:548:TRP:CB	2.26	0.84
1:A:493:TYR:CE1	1:A:592:PRO:HG3	2.13	0.83
1:B:592:PRO:HB2	1:B:595:ILE:HD11	1.62	0.81
1:A:504:ALA:CA	3:B:701:HOH:O	2.12	0.81
1:B:503:VAL:HG12	3:B:701:HOH:O	1.79	0.81
2:G:30:ASP:OD2	3:G:201:HOH:O	2.00	0.79
1:A:524:ARG:HH12	2:C:2:VAL:HG23	1.48	0.79
1:A:588:LEU:HD22	1:A:592:PRO:CB	2.14	0.78
1:B:503:VAL:O	3:B:701:HOH:O	1.92	0.78
1:B:512:ARG:HB3	3:B:705:HOH:O	1.83	0.78
2:C:25:SER:O	2:C:27:PHE:N	2.16	0.78
1:A:549:GLU:O	3:A:704:HOH:O	2.03	0.77
2:G:60:ALA:HB3	2:G:63:VAL:HB	1.65	0.77
1:B:572:GLU:O	3:B:702:HOH:O	2.03	0.76
2:H:25:SER:O	2:H:27:PHE:N	2.19	0.76
2:D:25:SER:O	2:D:27:PHE:N	2.19	0.76
1:F:515:ASP:O	1:F:519:VAL:HG23	1.87	0.75
2:C:71:ARG:HB2	2:C:78:VAL:HG22	1.68	0.75
1:A:548:TRP:CD1	3:A:704:HOH:O	2.39	0.74
1:E:544:LYS:NZ	1:E:560:ASN:O	2.17	0.74
2:G:25:SER:O	2:G:27:PHE:N	2.21	0.74
2:D:108:GLN:NE2	2:D:109:VAL:O	2.21	0.74
2:C:36:TRP:NE1	3:C:203:HOH:O	2.20	0.74
2:H:108:GLN:NE2	2:H:109:VAL:O	2.21	0.73
2:C:70:SER:CB	3:C:204:HOH:O	2.36	0.73
1:B:481:ASP:OD2	3:B:704:HOH:O	2.08	0.72
2:D:87:THR:N	2:D:90:TYR:HH	1.88	0.71
1:E:552:THR:CB	3:E:701:HOH:O	2.33	0.71
1:F:468:ASN:OD1	2:H:97:TRP:CD1	2.44	0.70
1:F:485:TYR:OH	1:F:572:GLU:OE2	2.10	0.70
1:E:561:TYR:CD1	1:F:561:TYR:CD1	2.79	0.70
1:A:460:ARG:HB3	2:C:31:TYR:CE2	2.26	0.70
1:B:531:GLN:OE1	3:B:703:HOH:O	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:493:TYR:CD1	1:E:592:PRO:HG3	2.27	0.69
1:F:519:VAL:CG1	1:F:526:LEU:HD11	2.22	0.69
1:F:519:VAL:HG12	1:F:526:LEU:HD11	1.73	0.69
3:A:707:HOH:O	1:B:548:TRP:HB2	1.89	0.69
1:A:503:VAL:HG21	1:B:470:VAL:HG21	1.75	0.68
1:B:477:ALA:H	1:B:594:SER:H	1.41	0.68
1:E:496:ASP:HA	1:E:578:ARG:HG2	1.73	0.68
1:A:496:ASP:HA	1:A:578:ARG:HG2	1.75	0.68
2:D:105:GLN:HG3	3:D:202:HOH:O	1.94	0.68
1:F:592:PRO:HB3	1:F:595:ILE:HD11	1.76	0.68
1:E:592:PRO:HB2	1:E:595:ILE:HD11	1.76	0.67
2:C:108:GLN:HG3	2:C:109:VAL:HG23	1.74	0.67
1:F:470:VAL:O	1:F:503:VAL:HG12	1.94	0.67
1:A:473:LEU:HD12	1:A:500:LEU:HD23	1.76	0.67
1:A:493:TYR:CD1	1:A:592:PRO:HG3	2.29	0.67
1:B:504:ALA:HA	3:B:701:HOH:O	1.95	0.67
1:B:513:SER:N	3:B:705:HOH:O	2.26	0.67
1:B:512:ARG:CB	3:B:705:HOH:O	2.39	0.67
2:G:108:GLN:HG3	2:G:109:VAL:HG23	1.77	0.66
1:B:515:ASP:OD2	1:B:518:LYS:HB2	1.95	0.66
1:E:549:GLU:CB	1:E:588:LEU:HD11	2.27	0.65
1:F:468:ASN:OD1	2:H:97:TRP:NE1	2.29	0.65
1:A:457:ALA:O	1:A:458:PRO:C	2.36	0.65
2:G:51:ILE:HG23	2:G:71:ARG:HH21	1.62	0.65
1:B:531:GLN:CD	3:B:703:HOH:O	2.34	0.65
2:D:59:TYR:CE1	2:D:100(D):PRO:HB3	2.32	0.64
2:H:69:ILE:HD13	3:H:201:HOH:O	1.97	0.64
2:D:3:GLN:HE22	2:G:2:VAL:HB	1.63	0.64
1:E:513:SER:O	1:E:513:SER:OG	2.14	0.64
1:F:588:LEU:O	3:F:704:HOH:O	2.14	0.64
1:A:550:ALA:HA	3:A:704:HOH:O	1.97	0.63
1:F:483:SER:OG	3:F:701:HOH:O	1.65	0.63
1:A:547:PHE:CZ	1:A:556:GLY:HA3	2.33	0.63
1:A:473:LEU:N	1:A:473:LEU:HD22	2.15	0.62
2:D:20:LEU:O	2:D:21:SER:OG	2.18	0.62
1:A:522:ASP:OD1	2:C:32:TYR:OH	2.18	0.61
1:A:553:THR:O	1:B:566:SER:OG	2.09	0.61
2:D:105:GLN:NE2	3:D:202:HOH:O	2.24	0.61
1:B:504:ALA:CA	3:B:701:HOH:O	2.49	0.61
1:A:466:ARG:NH1	2:C:28:THR:O	2.33	0.61
2:C:59:TYR:CE1	2:C:100(D):PRO:HB3	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:536:PHE:HD1	1:F:572:GLU:HA	1.66	0.60
1:B:472:TRP:HZ3	1:B:474:SER:HG	1.49	0.60
1:B:502:ASN:O	1:B:506:GLY:N	2.31	0.60
2:H:52(A):SER:HB3	2:H:99:GLY:HA2	1.85	0.59
1:B:504:ALA:N	3:B:701:HOH:O	2.22	0.59
1:E:523:GLY:HA3	2:G:26:THR:HG22	1.83	0.59
1:F:523:GLY:HA3	2:H:26:THR:HG22	1.83	0.59
1:F:529:ILE:HD12	1:F:531:GLN:HE21	1.68	0.59
1:A:470:VAL:HG11	1:B:470:VAL:HG11	1.84	0.59
1:A:592:PRO:HB2	1:A:595:ILE:HD11	1.85	0.59
1:A:502:ASN:O	1:A:506:GLY:N	2.29	0.59
2:C:3:GLN:HA	3:C:211:HOH:O	2.03	0.58
1:E:522:ASP:OD1	2:G:32:TYR:OH	2.19	0.58
1:E:591:GLY:O	1:E:593:VAL:N	2.36	0.58
2:G:10:GLY:N	2:G:109:VAL:O	2.37	0.58
1:E:554:LYS:CB	3:E:701:HOH:O	2.51	0.58
1:B:516:TRP:CZ2	1:B:571:VAL:HG11	2.39	0.58
1:B:524:ARG:NH2	2:G:5:GLN:HA	2.19	0.58
1:E:561:TYR:HB2	1:F:561:TYR:HB2	1.84	0.58
2:D:11:LEU:H	1:E:531:GLN:HG2	1.69	0.58
1:E:470:VAL:HG11	1:F:470:VAL:HG11	1.84	0.58
1:B:544:LYS:NZ	1:B:560:ASN:O	2.26	0.57
1:E:465:LEU:N	1:E:465:LEU:HD22	2.19	0.57
1:A:591:GLY:O	1:A:593:VAL:N	2.37	0.57
1:E:502:ASN:O	1:E:506:GLY:N	2.30	0.57
1:F:515:ASP:O	1:F:515:ASP:OD1	2.22	0.57
2:H:53:ARG:HE	2:H:100:TYR:HA	1.67	0.57
2:H:61:ASP:HA	2:H:64:LYS:HB2	1.87	0.57
1:F:474:SER:O	1:F:474:SER:OG	2.21	0.57
1:A:532:TYR:O	1:A:533:SER:HB3	2.05	0.57
1:B:530:GLN:N	2:G:9:GLY:O	2.38	0.57
2:C:60:ALA:CA	3:C:202:HOH:O	2.43	0.57
2:H:69:ILE:CD1	3:H:201:HOH:O	2.51	0.57
1:E:540:PRO:HB2	1:E:602:ALA:HB3	1.86	0.57
2:H:65:GLY:O	2:H:66:ARG:NH1	2.38	0.57
2:C:72:ASP:HB3	2:C:75:LYS:HB2	1.87	0.56
1:F:477:ALA:H	1:F:594:SER:H	1.53	0.56
1:A:543:GLY:N	3:A:707:HOH:O	2.37	0.56
2:G:108:GLN:OE1	2:G:109:VAL:HG23	2.05	0.56
1:A:539:LEU:HB2	1:A:569:LEU:HB2	1.88	0.56
2:H:20:LEU:O	2:H:21:SER:OG	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:ARG:NH1	2:C:2:VAL:HG23	2.18	0.56
1:A:540:PRO:HB2	1:A:602:ALA:HB3	1.87	0.56
1:E:524:ARG:HH12	2:G:2:VAL:HG23	1.71	0.56
1:E:552:THR:HB	3:E:701:HOH:O	2.01	0.56
1:F:591:GLY:N	1:F:592:PRO:HD3	2.21	0.56
1:B:591:GLY:O	1:B:593:VAL:N	2.38	0.56
1:A:561:TYR:CD1	1:B:561:TYR:CD1	2.94	0.55
2:C:1:ASP:OD1	3:C:205:HOH:O	2.18	0.55
2:D:3:GLN:NE2	2:G:2:VAL:HB	2.21	0.55
2:H:29:LEU:O	2:H:71:ARG:NH2	2.39	0.55
1:E:473:LEU:N	1:E:473:LEU:HD22	2.21	0.55
1:A:457:ALA:N	1:A:458:PRO:CD	2.69	0.55
1:A:516:TRP:CH2	1:A:571:VAL:HG11	2.42	0.55
1:A:555:ALA:CB	1:B:543:GLY:HA2	2.37	0.55
1:F:470:VAL:HG22	1:F:600:VAL:HG22	1.88	0.55
1:E:459:SER:C	2:G:31:TYR:OH	2.50	0.55
2:C:29:LEU:O	2:C:71:ARG:NH2	2.40	0.55
1:A:547:PHE:CE1	1:A:556:GLY:C	2.85	0.54
2:C:108:GLN:O	2:C:109:VAL:C	2.50	0.54
1:F:591:GLY:O	1:F:593:VAL:N	2.40	0.54
1:E:553:THR:HG22	1:F:542:ARG:HG2	1.89	0.54
2:C:20:LEU:O	2:C:21:SER:OG	2.19	0.54
1:E:476:THR:HB	1:E:497:SER:HB2	1.89	0.54
2:G:108:GLN:O	2:G:109:VAL:C	2.50	0.54
1:B:466:ARG:NH1	2:D:28:THR:O	2.41	0.54
1:F:470:VAL:HB	1:F:503:VAL:CG1	2.38	0.54
1:A:549:GLU:C	3:A:704:HOH:O	2.47	0.54
1:B:516:TRP:HB3	1:B:537:PHE:CE2	2.43	0.54
1:F:470:VAL:HB	1:F:503:VAL:HG11	1.90	0.53
1:F:514:LEU:HD23	1:F:516:TRP:CH2	2.42	0.53
1:A:492:VAL:C	3:A:702:HOH:O	2.44	0.53
1:B:523:GLY:HA3	2:D:26:THR:HG22	1.90	0.53
1:E:572:GLU:HG2	1:E:574:ALA:HB3	1.89	0.53
1:B:524:ARG:HH21	2:G:5:GLN:HA	1.73	0.53
2:C:97:TRP:CZ3	2:C:100(C):PRO:HG3	2.44	0.53
2:H:53:ARG:HG3	2:H:99:GLY:O	2.08	0.53
2:D:2:VAL:HG11	2:D:102:TYR:CG	2.42	0.53
2:D:29:LEU:O	2:D:71:ARG:NH2	2.42	0.53
1:E:504:ALA:HB2	1:F:503:VAL:HG23	1.91	0.53
1:B:530:GLN:O	2:G:10:GLY:HA3	2.08	0.53
1:B:532:TYR:O	1:B:533:SER:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:588:LEU:HD13	1:E:595:ILE:CD1	2.38	0.53
1:E:463:SER:O	1:E:465:LEU:HD22	2.09	0.53
1:E:532:TYR:O	1:E:533:SER:HB3	2.08	0.53
2:H:53:ARG:NH1	2:H:55:GLY:HA3	2.24	0.53
2:D:61:ASP:O	2:D:62:SER:HB2	2.10	0.52
1:E:554:LYS:HB3	3:E:701:HOH:O	2.07	0.52
1:A:529:ILE:HD12	1:A:531:GLN:NE2	2.24	0.52
1:A:562:ASN:HA	1:B:557:TYR:CE2	2.44	0.52
1:B:498:VAL:HG11	1:B:579:VAL:HG21	1.91	0.52
1:A:459:SER:C	2:C:31:TYR:OH	2.52	0.52
2:C:72:ASP:CB	2:C:75:LYS:HB2	2.40	0.52
1:F:561:TYR:HE2	1:F:584:TYR:CD1	2.28	0.52
1:E:470:VAL:HG22	1:E:600:VAL:HG22	1.91	0.52
1:B:536:PHE:HD1	1:B:572:GLU:HA	1.74	0.52
2:C:6:GLU:CD	2:C:106:GLY:H	2.18	0.52
1:E:516:TRP:CZ2	1:E:571:VAL:HG11	2.44	0.52
2:G:10:GLY:H	2:G:109:VAL:C	2.17	0.52
2:D:100(G):TYR:HD1	2:D:100(G):TYR:H	1.57	0.51
1:B:517:THR:HA	3:B:707:HOH:O	2.10	0.51
2:C:87:THR:HG23	2:C:109:VAL:HG21	1.92	0.51
1:E:489:THR:HG22	1:E:489:THR:O	2.11	0.51
1:F:532:TYR:O	1:F:533:SER:HB3	2.10	0.51
2:G:100(F):ARG:C	2:G:100(F):ARG:HD2	2.36	0.51
2:D:2:VAL:N	2:G:1:ASP:H2	2.08	0.51
1:A:470:VAL:HG22	1:A:600:VAL:HG22	1.92	0.51
1:A:523:GLY:HA3	2:C:26:THR:HG22	1.93	0.51
1:E:500:LEU:HD11	1:E:511:ALA:HB2	1.93	0.51
1:A:561:TYR:HB2	1:B:561:TYR:HB2	1.93	0.51
1:E:462:PHE:O	1:E:465:LEU:HD11	2.10	0.51
1:A:460:ARG:HB3	2:C:31:TYR:CZ	2.46	0.51
1:B:470:VAL:HG22	1:B:600:VAL:HG22	1.92	0.51
2:D:6:GLU:CD	2:D:106:GLY:H	2.18	0.51
1:E:522:ASP:OD2	2:G:102:TYR:OH	2.27	0.51
1:F:512:ARG:NE	1:F:576:GLY:HA2	2.26	0.51
2:G:52(A):SER:HB3	2:G:99:GLY:HA2	1.92	0.51
2:G:59:TYR:CE2	2:G:100(D):PRO:HB3	2.46	0.51
2:H:100(F):ARG:HD2	2:H:100(F):ARG:C	2.36	0.51
2:C:53:ARG:NH2	2:C:55:GLY:HA3	2.26	0.50
1:F:542:ARG:CD	1:F:602:ALA:HA	2.40	0.50
1:F:568:GLN:NE2	1:F:570:LEU:HD11	2.26	0.50
1:F:508:GLN:NE2	2:G:100:TYR:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:53:ARG:HH12	2:H:55:GLY:HA3	1.76	0.50
2:C:70:SER:O	2:C:78:VAL:HG13	2.11	0.50
1:B:472:TRP:HZ3	1:B:474:SER:OG	1.94	0.50
2:G:71:ARG:HD3	2:G:73:ASN:OD1	2.10	0.50
1:A:459:SER:C	2:C:31:TYR:HH	2.20	0.50
1:E:549:GLU:CA	1:E:588:LEU:HD11	2.42	0.50
1:B:529:ILE:HD11	1:B:570:LEU:HD22	1.92	0.50
1:F:552:THR:OG1	3:F:703:HOH:O	2.19	0.50
2:G:100(F):ARG:C	2:G:100(H):GLU:H	2.20	0.50
1:B:476:THR:HA	1:B:594:SER:HA	1.94	0.50
2:C:36:TRP:CD1	2:C:80:LEU:HD12	2.47	0.50
1:E:557:TYR:O	1:E:583:THR:HA	2.12	0.50
1:F:500:LEU:HD11	1:F:511:ALA:HB2	1.94	0.49
2:D:70:SER:O	2:D:78:VAL:HG13	2.11	0.49
1:E:481:ASP:HB2	1:E:494:VAL:HG23	1.94	0.49
1:A:535:THR:HB	1:A:573:ASN:HB3	1.94	0.49
2:H:70:SER:O	2:H:78:VAL:HG13	2.11	0.49
1:F:468:ASN:HD21	1:F:542:ARG:CZ	2.24	0.49
2:D:100(F):ARG:C	2:D:100(H):GLU:H	2.20	0.49
1:A:553:THR:HG22	1:B:542:ARG:HG2	1.94	0.49
1:E:481:ASP:HB2	1:E:494:VAL:CG2	2.43	0.49
1:F:533:SER:O	1:F:533:SER:OG	2.29	0.49
1:A:516:TRP:CZ2	1:A:571:VAL:HG11	2.48	0.49
1:A:504:ALA:N	3:B:701:HOH:O	2.38	0.49
1:F:542:ARG:HD2	1:F:602:ALA:HA	1.94	0.49
1:F:529:ILE:CD1	1:F:531:GLN:HE21	2.25	0.48
2:G:22:CYS:N	2:G:78:VAL:O	2.46	0.48
2:H:100(F):ARG:C	2:H:100(H):GLU:H	2.21	0.48
2:H:6:GLU:CD	2:H:106:GLY:H	2.20	0.48
2:H:59:TYR:CE1	2:H:100(D):PRO:HB3	2.49	0.48
2:C:70:SER:OG	2:C:79:TYR:HD1	1.96	0.48
1:F:535:THR:HB	3:F:709:HOH:O	2.12	0.48
1:B:476:THR:HB	1:B:497:SER:HB2	1.96	0.48
2:C:66:ARG:HG3	2:C:66:ARG:NH1	2.08	0.48
1:E:503:VAL:HG12	1:F:503:VAL:HG22	1.96	0.48
2:D:22:CYS:N	2:D:78:VAL:O	2.46	0.48
1:E:539:LEU:HB2	1:E:569:LEU:HB2	1.96	0.48
1:F:473:LEU:N	1:F:473:LEU:HD22	2.28	0.48
2:G:3:GLN:HB2	2:G:25:SER:OG	2.14	0.48
1:A:460:ARG:HB3	2:C:31:TYR:HE2	1.76	0.48
2:C:100(F):ARG:HD2	2:C:100(F):ARG:C	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:460:ARG:HD2	1:E:505:THR:OG1	2.13	0.47
1:A:475:LEU:HG	1:A:498:VAL:HG13	1.96	0.47
2:C:23:ALA:HA	2:C:76:ASN:O	2.14	0.47
2:D:2:VAL:HG11	2:D:102:TYR:CD2	2.48	0.47
2:H:22:CYS:N	2:H:78:VAL:O	2.47	0.47
2:D:37:PHE:HD1	2:D:47:GLY:HA2	1.80	0.47
1:E:460:ARG:NH1	1:E:505:THR:OG1	2.43	0.47
2:G:91:TYR:C	3:G:202:HOH:O	2.57	0.47
1:A:562:ASN:HA	1:B:557:TYR:CD2	2.49	0.47
1:B:484:THR:HG22	1:B:485:TYR:CD1	2.49	0.47
2:C:22:CYS:N	2:C:78:VAL:O	2.47	0.47
1:F:463:SER:HA	1:F:519:VAL:HG22	1.96	0.47
1:B:512:ARG:CA	3:B:705:HOH:O	2.63	0.47
2:H:5:GLN:HB2	2:H:23:ALA:HB3	1.97	0.47
2:H:71:ARG:HB2	2:H:78:VAL:HG22	1.96	0.47
1:A:588:LEU:CD2	1:A:592:PRO:HB3	2.34	0.47
2:D:100(G):TYR:CD1	2:D:100(G):TYR:N	2.82	0.47
1:F:588:LEU:C	1:F:592:PRO:HG3	2.39	0.47
1:A:547:PHE:CE1	1:A:556:GLY:HA3	2.50	0.47
1:A:600:VAL:HG11	1:B:548:TRP:CH2	2.48	0.47
1:B:501:VAL:HG22	1:B:508:GLN:HB3	1.96	0.47
2:C:52(A):SER:HB3	2:C:99:GLY:HA2	1.95	0.47
1:E:466:ARG:NH1	2:G:28:THR:O	2.47	0.47
1:F:476:THR:HA	1:F:594:SER:HA	1.97	0.47
1:F:536:PHE:CD1	1:F:572:GLU:HA	2.48	0.47
1:A:536:PHE:HD1	1:A:572:GLU:HA	1.79	0.47
1:A:500:LEU:HD11	1:A:511:ALA:HB2	1.97	0.47
2:C:100(F):ARG:C	2:C:100(H):GLU:H	2.23	0.47
1:E:588:LEU:HD22	1:E:592:PRO:HB3	1.96	0.47
2:G:59:TYR:HE2	2:G:100(D):PRO:HB3	1.79	0.47
1:E:515:ASP:OD1	1:E:515:ASP:O	2.32	0.46
2:C:31:TYR:CD1	2:C:31:TYR:N	2.82	0.46
2:D:105:GLN:CG	3:D:202:HOH:O	2.60	0.46
1:E:529:ILE:HG12	1:E:536:PHE:HB2	1.97	0.46
2:G:6:GLU:CD	2:G:106:GLY:H	2.22	0.46
2:H:2:VAL:HG11	2:H:102:TYR:CG	2.50	0.46
1:A:557:TYR:O	1:A:583:THR:HA	2.14	0.46
1:A:588:LEU:HD22	1:A:595:ILE:HD11	1.97	0.46
2:C:79:TYR:C	3:C:203:HOH:O	2.47	0.46
2:H:89:VAL:HG22	2:H:108:GLN:HB2	1.96	0.46
1:F:466:ARG:CD	2:H:32:TYR:HE1	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:23:ALA:HA	2:G:76:ASN:O	2.16	0.46
2:H:23:ALA:HA	2:H:76:ASN:O	2.16	0.46
1:A:484:THR:HG22	1:A:485:TYR:CD1	2.51	0.46
1:A:593:VAL:O	1:A:594:SER:O	2.33	0.46
1:F:549:GLU:CB	3:F:703:HOH:O	2.63	0.46
1:A:540:PRO:CB	1:A:602:ALA:HB3	2.46	0.46
2:D:72:ASP:HB2	2:D:79:TYR:OH	2.16	0.45
2:D:92:CYS:O	2:D:92:CYS:SG	2.75	0.45
2:D:21:SER:HB3	2:D:77:THR:HG22	1.98	0.45
2:D:87:THR:N	2:D:90:TYR:OH	2.49	0.45
1:B:546:SER:CB	1:B:598:VAL:HG12	2.46	0.45
2:D:72:ASP:HB3	2:D:75:LYS:HG3	1.98	0.45
1:E:498:VAL:HG11	1:E:579:VAL:HG21	1.98	0.45
2:C:3:GLN:HB2	2:C:25:SER:OG	2.15	0.45
1:E:553:THR:HG22	1:F:542:ARG:CG	2.47	0.45
2:H:49:SER:OG	2:H:58:ASP:OD1	2.32	0.45
2:H:30:ASP:HA	2:H:73:ASN:OD1	2.16	0.45
2:D:25:SER:CB	2:G:1:ASP:HB2	2.47	0.45
1:B:515:ASP:O	1:B:519:VAL:HG23	2.17	0.45
1:E:516:TRP:HB3	1:E:537:PHE:CE2	2.52	0.45
2:D:30:ASP:HA	2:D:73:ASN:OD1	2.17	0.45
1:F:593:VAL:O	1:F:594:SER:O	2.35	0.45
2:G:89:VAL:HA	2:G:108:GLN:HA	1.98	0.45
1:A:544:LYS:NZ	1:A:560:ASN:O	2.24	0.44
1:F:480:TYR:HB2	1:F:590:ALA:HA	1.99	0.44
1:B:512:ARG:C	3:B:705:HOH:O	2.60	0.44
1:F:544:LYS:NZ	1:F:560:ASN:O	2.26	0.44
1:F:552:THR:OG1	1:F:553:THR:N	2.49	0.44
1:F:591:GLY:N	1:F:592:PRO:CD	2.80	0.44
2:G:51:ILE:HB	2:G:69:ILE:HD13	1.99	0.44
1:A:588:LEU:HD13	1:A:595:ILE:HD12	1.99	0.44
1:A:548:TRP:NE1	3:A:704:HOH:O	2.45	0.44
1:B:530:GLN:H	2:G:10:GLY:CA	2.31	0.44
1:E:524:ARG:NH1	2:G:2:VAL:HG23	2.32	0.44
1:E:588:LEU:HB3	1:E:592:PRO:HB3	2.00	0.44
1:F:514:LEU:O	1:F:516:TRP:CD1	2.71	0.44
2:D:2:VAL:HG23	2:G:3:GLN:NE2	2.33	0.44
2:H:100(F):ARG:HG3	2:H:100(G):TYR:CD1	2.52	0.44
1:B:515:ASP:O	1:B:515:ASP:CG	2.61	0.44
1:B:516:TRP:CD1	3:B:702:HOH:O	2.70	0.44
1:B:533:SER:O	1:B:533:SER:OG	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:466:ARG:NH1	3:G:201:HOH:O	2.36	0.44
1:B:568:GLN:HE21	1:B:568:GLN:HB2	1.65	0.43
2:D:30:ASP:O	2:D:71:ARG:NH1	2.51	0.43
2:G:87:THR:HG23	2:G:109:VAL:HG21	2.00	0.43
1:B:500:LEU:HD11	1:B:511:ALA:HB2	2.00	0.43
1:A:522:ASP:OD2	2:C:102:TYR:OH	2.35	0.43
1:A:555:ALA:HB2	1:B:566:SER:HA	2.01	0.43
2:D:23:ALA:HA	2:D:76:ASN:O	2.18	0.43
1:F:547:PHE:CD2	1:F:581:ILE:HD12	2.52	0.43
2:H:57:THR:HG21	2:H:59:TYR:CZ	2.54	0.43
1:B:460:ARG:HD2	2:D:31:TYR:CE2	2.54	0.43
2:H:33:ALA:N	2:H:95:ALA:O	2.50	0.43
1:B:588:LEU:O	1:B:592:PRO:HD3	2.18	0.43
1:E:535:THR:HB	1:E:573:ASN:HB3	2.00	0.43
1:E:553:THR:O	1:F:566:SER:HB3	2.18	0.43
1:F:560:ASN:HB3	1:F:563:THR:OG1	2.19	0.43
1:E:547:PHE:CD2	1:E:581:ILE:HD12	2.53	0.43
1:F:460:ARG:HD2	2:H:31:TYR:CE2	2.54	0.43
2:G:5:GLN:HB2	2:G:23:ALA:HB3	2.00	0.43
2:G:37:PHE:CD2	3:G:202:HOH:O	2.33	0.43
1:B:561:TYR:HE2	1:B:584:TYR:CD1	2.36	0.43
1:F:531:GLN:O	1:F:534:LYS:N	2.48	0.43
1:F:542:ARG:HG3	1:F:602:ALA:HB2	2.00	0.43
2:G:21:SER:HB3	2:G:77:THR:HG22	2.01	0.43
2:G:100(G):TYR:CD1	2:G:100(G):TYR:N	2.86	0.43
2:H:30:ASP:O	2:H:71:ARG:NH1	2.52	0.43
1:E:561:TYR:CD1	1:F:561:TYR:HD1	2.35	0.43
2:H:89:VAL:HA	2:H:108:GLN:HA	2.01	0.43
1:B:531:GLN:HE21	1:B:531:GLN:HB3	1.42	0.43
1:B:591:GLY:N	1:B:592:PRO:CD	2.82	0.43
2:C:89:VAL:HG22	2:C:108:GLN:OE1	2.18	0.43
2:D:105:GLN:HA	3:D:206:HOH:O	2.19	0.43
1:B:531:GLN:O	1:B:534:LYS:N	2.48	0.43
1:B:557:TYR:O	1:B:583:THR:HA	2.19	0.43
2:D:37:PHE:CD1	2:D:47:GLY:HA2	2.53	0.43
2:G:95:ALA:HB1	2:G:97:TRP:CD1	2.54	0.43
2:D:48:VAL:CG2	3:D:203:HOH:O	2.67	0.42
1:F:459:SER:OG	1:F:460:ARG:N	2.50	0.42
2:D:100(F):ARG:C	2:D:100(F):ARG:HD2	2.44	0.42
1:E:500:LEU:HD12	1:E:500:LEU:N	2.34	0.42
1:E:511:ALA:O	1:E:516:TRP:NE1	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:586:THR:HB	1:E:589:GLY:HA2	2.01	0.42
2:H:6:GLU:HB2	2:H:107:THR:HG23	2.00	0.42
1:A:460:ARG:HB3	2:C:31:TYR:OH	2.19	0.42
1:F:475:LEU:HD13	1:F:595:ILE:HG22	2.01	0.42
2:D:2:VAL:HG21	2:D:102:TYR:CZ	2.53	0.42
1:E:536:PHE:HD1	1:E:572:GLU:HA	1.85	0.42
1:A:515:ASP:O	1:A:515:ASP:OD1	2.38	0.42
2:C:36:TRP:CG	2:C:80:LEU:HD12	2.54	0.42
2:C:60:ALA:O	2:C:64:LYS:HB2	2.20	0.42
1:E:484:THR:HG22	1:E:485:TYR:CD1	2.55	0.42
1:F:498:VAL:HG11	1:F:579:VAL:HG21	2.02	0.42
1:F:539:LEU:HB2	1:F:569:LEU:HB2	2.01	0.42
1:F:460:ARG:HH12	1:F:469:ASP:CG	2.27	0.42
2:G:20:LEU:O	2:G:21:SER:OG	2.31	0.42
2:G:108:GLN:CG	2:G:109:VAL:HG23	2.49	0.42
1:B:546:SER:HB3	1:B:598:VAL:HG12	2.02	0.42
2:C:30:ASP:O	2:C:71:ARG:NH1	2.51	0.42
2:C:70:SER:OG	3:C:204:HOH:O	2.06	0.42
1:B:468:ASN:OD1	1:B:542:ARG:NH1	2.53	0.41
2:G:100(G):TYR:H	2:G:100(G):TYR:HD1	1.66	0.41
1:A:530:GLN:OE1	3:A:705:HOH:O	2.21	0.41
2:C:22:CYS:HB2	2:C:36:TRP:CZ2	2.55	0.41
2:D:33:ALA:N	2:D:95:ALA:O	2.53	0.41
1:F:557:TYR:O	1:F:583:THR:HA	2.20	0.41
1:A:500:LEU:HD12	1:A:500:LEU:N	2.35	0.41
1:B:514:LEU:O	1:B:516:TRP:CD1	2.74	0.41
1:B:586:THR:HB	1:B:589:GLY:HA2	2.02	0.41
2:D:53:ARG:HG3	2:D:99:GLY:O	2.20	0.41
1:E:466:ARG:HD3	2:G:32:TYR:HE1	1.86	0.41
2:G:30:ASP:O	2:G:71:ARG:NH1	2.52	0.41
2:C:3:GLN:CA	3:C:211:HOH:O	2.63	0.41
2:D:23:ALA:N	2:D:77:THR:HG23	2.35	0.41
2:G:35:GLY:HA2	2:G:50:CYS:HA	2.02	0.41
2:C:33:ALA:N	2:C:95:ALA:O	2.51	0.41
2:C:72:ASP:OD2	2:C:75:LYS:HD2	2.21	0.41
2:D:52(A):SER:HB3	2:D:99:GLY:HA2	2.02	0.41
1:E:531:GLN:HB2	1:E:536:PHE:HE2	1.86	0.41
2:G:72:ASP:CG	2:G:75:LYS:HD2	2.46	0.41
1:A:514:LEU:O	1:A:516:TRP:CD1	2.73	0.41
1:A:457:ALA:O	1:A:459:SER:OG	2.22	0.41
1:E:466:ARG:NH2	3:G:201:HOH:O	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:475:LEU:HB2	1:F:595:ILE:HB	2.03	0.41
2:C:72:ASP:CG	2:C:75:LYS:HD2	2.46	0.41
1:E:480:TYR:CE2	1:E:482:GLN:HG2	2.56	0.41
1:A:469:ASP:O	1:A:600:VAL:HA	2.20	0.41
1:A:537:PHE:HB2	1:A:571:VAL:HB	2.03	0.41
1:B:472:TRP:CZ3	1:B:474:SER:OG	2.71	0.41
2:D:6:GLU:HB2	2:D:107:THR:HG23	2.03	0.41
2:D:100(F):ARG:HG3	2:D:100(G):TYR:CD1	2.55	0.41
1:E:503:VAL:HG21	1:F:470:VAL:HG21	2.03	0.41
1:E:515:ASP:HB2	1:E:518:LYS:HD3	2.01	0.41
1:F:519:VAL:HG11	1:F:526:LEU:HD11	1.97	0.41
3:A:707:HOH:O	1:B:548:TRP:HB3	2.05	0.41
2:C:66:ARG:HH11	2:C:66:ARG:CG	2.13	0.41
2:D:89:VAL:HG22	2:D:108:GLN:HB2	2.03	0.41
1:E:588:LEU:HD13	1:E:595:ILE:HD12	2.03	0.41
1:B:468:ASN:ND2	2:D:97:TRP:CD1	2.89	0.40
1:F:460:ARG:HB2	2:H:31:TYR:CE2	2.56	0.40
1:A:551:GLY:O	1:A:552:THR:O	2.38	0.40
2:C:37:PHE:CD1	2:C:47:GLY:HA2	2.57	0.40
1:F:586:THR:HB	1:F:589:GLY:HA2	2.02	0.40
2:G:51:ILE:HG23	2:G:51:ILE:O	2.20	0.40
1:A:508:GLN:NE2	2:D:100:TYR:O	2.54	0.40
1:E:557:TYR:CD2	1:F:561:TYR:O	2.75	0.40
2:D:5:GLN:HB2	2:D:23:ALA:HB3	2.04	0.40
1:A:471:LEU:HD12	1:A:601:LEU:HD21	2.04	0.40
2:C:53:ARG:HG3	2:C:99:GLY:O	2.21	0.40
1:F:522:ASP:OD1	2:H:32:TYR:OH	2.38	0.40
2:G:6:GLU:HB2	2:G:107:THR:HG23	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:75:LYS:NZ	2:C:77:THR:OG1[2_655]	1.98	0.22
2:C:75:LYS:O	2:C:75:LYS:NZ[2_655]	2.11	0.09



## 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	144/150 (96%)	124 (86%)	14 (10%)	6 (4%)	2	1
1	B	142/150 (95%)	122 (86%)	16 (11%)	4 (3%)	4	2
1	E	144/150 (96%)	126 (88%)	13 (9%)	5 (4%)	3	1
1	F	142/150 (95%)	126 (89%)	12 (8%)	4 (3%)	4	2
2	C	88/132 (67%)	70 (80%)	12 (14%)	6 (7%)	1	0
2	D	87/132 (66%)	71 (82%)	11 (13%)	5 (6%)	1	0
2	G	88/132 (67%)	71 (81%)	12 (14%)	5 (6%)	1	0
2	H	87/132 (66%)	71 (82%)	14 (16%)	2 (2%)	5	3
All	All	922/1128 (82%)	781 (85%)	104 (11%)	37 (4%)	2	1

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	26	THR
2	D	26	THR
2	D	97	TRP
2	G	26	THR
2	H	26	THR
1	A	458	PRO
1	A	552	THR
1	A	592	PRO
1	A	594	SER
1	B	525	PRO
2	C	55	GLY
2	D	62	SER
1	F	525	PRO
1	F	592	PRO
1	F	594	SER
2	G	55	GLY
2	H	55	GLY

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Mol	Chain	Res	Type
1	B	594	SER
1	E	515	ASP
1	E	592	PRO
1	E	594	SER
2	G	97	TRP
1	B	592	PRO
2	C	57	THR
2	C	100(G)	TYR
2	D	55	GLY
1	E	525	PRO
2	G	57	THR
1	A	515	ASP
1	A	525	PRO
2	C	97	TRP
2	D	57	THR
2	G	100(G)	TYR
1	F	490	GLY
1	B	490	GLY
2	C	9	GLY
1	E	490	GLY

### 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	118/122 (97%)	110 (93%)	8 (7%)	13	15
1	B	117/122 (96%)	106 (91%)	11 (9%)	7	7
1	E	118/122 (97%)	110 (93%)	8 (7%)	13	15
1	F	117/122 (96%)	110 (94%)	7 (6%)	16	19
2	C	73/105 (70%)	62 (85%)	11 (15%)	2	2
2	D	72/105 (69%)	67 (93%)	5 (7%)	13	14
2	G	73/105 (70%)	66 (90%)	7 (10%)	7	6
2	H	72/105 (69%)	66 (92%)	6 (8%)	9	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	760/908 (84%)	697 (92%)	63 (8%)	<b>9</b> <b>9</b>

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	460	ARG
1	A	473	LEU
1	A	488	SER
1	A	494	VAL
1	A	501	VAL
1	A	527	SER
1	A	564	THR
1	A	588	LEU
1	B	493	TYR
1	B	494	VAL
1	B	501	VAL
1	B	508	GLN
1	B	517	THR
1	B	526	LEU
1	B	533	SER
1	B	538	VAL
1	B	564	THR
1	B	568	GLN
1	B	594	SER
2	C	4	LEU
2	C	21	SER
2	C	26	THR
2	C	28	THR
2	C	30	ASP
2	C	56	SER
2	C	58	ASP
2	C	66	ARG
2	C	68	THR
2	C	79	TYR
2	C	105	GLN
2	D	26	THR
2	D	30	ASP
2	D	62	SER
2	D	80	LEU
2	D	109	VAL
1	E	465	LEU
1	E	488	SER

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Mol	Chain	Res	Type
1	E	496	ASP
1	E	501	VAL
1	E	517	THR
1	E	535	THR
1	E	564	THR
1	E	588	LEU
1	F	474	SER
1	F	483	SER
1	F	503	VAL
1	F	517	THR
1	F	563	THR
1	F	564	THR
1	F	586	THR
2	G	4	LEU
2	G	11	LEU
2	G	26	THR
2	G	28	THR
2	G	30	ASP
2	G	77	THR
2	G	79	TYR
2	H	4	LEU
2	H	26	THR
2	H	30	ASP
2	H	71	ARG
2	H	76	ASN
2	H	109	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	468	ASN
1	A	531	GLN
1	A	568	GLN
1	B	502	ASN
1	B	568	GLN
1	E	531	GLN
1	F	468	ASN
1	F	482	GLN
1	F	531	GLN
2	G	76	ASN
2	H	76	ASN

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	146/150 (97%)	0.60	9 (6%) 28 25	21, 31, 37, 40	0
1	B	144/150 (96%)	0.46	3 (2%) 63 59	24, 31, 36, 38	0
1	E	146/150 (97%)	0.60	6 (4%) 42 38	26, 35, 40, 44	0
1	F	144/150 (96%)	0.60	5 (3%) 47 44	26, 34, 42, 45	0
2	C	96/132 (72%)	0.61	4 (4%) 41 37	25, 32, 38, 42	0
2	D	95/132 (71%)	0.69	9 (9%) 15 13	24, 33, 39, 45	0
2	G	96/132 (72%)	0.85	11 (11%) 11 9	30, 36, 42, 43	0
2	H	95/132 (71%)	0.85	7 (7%) 22 20	31, 38, 46, 50	0
All	All	962/1128 (85%)	0.64	54 (5%) 31 28	21, 33, 41, 50	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	467	ALA	4.7
1	E	602	ALA	4.5
2	H	31	TYR	4.1
2	H	23	ALA	4.0
2	C	94	ALA	3.6
2	G	69	ILE	3.3
2	C	95	ALA	3.1
2	H	37	PHE	3.0
1	A	582	SER	3.0
1	F	514	LEU	3.0
1	F	462	PHE	3.0
2	D	51	ILE	2.9
2	G	109	VAL	2.9
2	G	51	ILE	2.9
1	E	464	VAL	2.8
2	G	60	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	96	GLY	2.8
1	B	602	ALA	2.7
2	G	22	CYS	2.6
2	D	104	GLY	2.5
1	A	545	LEU	2.5
2	G	30	ASP	2.5
1	A	509	ALA	2.5
2	G	80	LEU	2.5
1	B	557	TYR	2.4
2	D	32	TYR	2.4
2	G	65	GLY	2.4
1	F	550	ALA	2.4
2	G	98	ALA	2.4
2	D	7	SER	2.3
2	D	100	TYR	2.3
2	H	93	ALA	2.3
2	H	2	VAL	2.3
1	A	600	VAL	2.3
1	E	478	ALA	2.2
1	A	546	SER	2.2
2	G	56	SER	2.2
1	F	535	THR	2.2
2	H	48	VAL	2.2
1	A	576	GLY	2.2
1	A	588	LEU	2.2
1	E	583	THR	2.2
1	B	598	VAL	2.2
1	A	495	SER	2.1
2	D	80	LEU	2.1
1	A	555	ALA	2.1
2	H	59	TYR	2.1
2	C	100(A)	GLY	2.1
1	F	521	LEU	2.1
2	D	20	LEU	2.1
2	D	57	THR	2.1
2	G	100(B)	CYS	2.0
1	E	565	ALA	2.0
2	D	56	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates [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.