



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:35 PM UTC

PDB ID : 5J7O / pdb_00005j7o
Title : Faustovirus major capsid protein
Authors : Klose, T.; Rossmann, M.G.
Deposited on : 2016-04-06
Resolution : 2.37 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

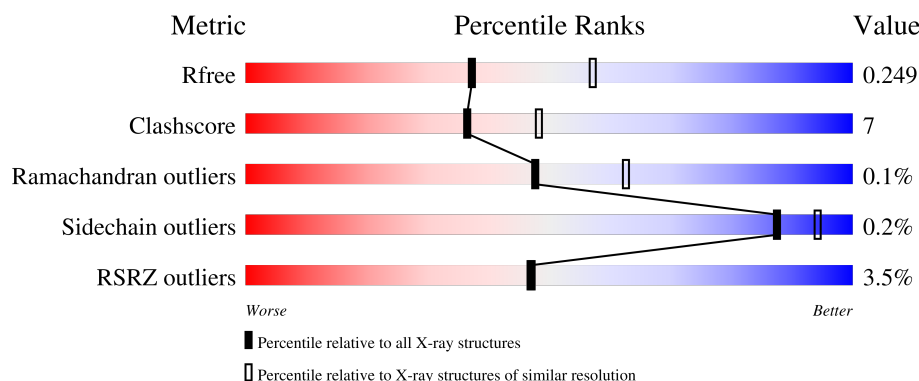
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	645	2% 83% 11% 5%
1	B	645	2% 85% 11% .
1	C	645	3% 84% 11% .
1	D	645	3% 82% 12% 5%
1	E	645	4% 81% 14% 5%

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Mol	Chain	Length	Quality of chain
1	F	645	5% 82% 14%
2	G	21	90% 10%
2	H	21	95% 5%
2	I	21	95% 5%
2	J	21	81% 19%
2	K	21	90% 10%
2	L	21	81% 10% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30884 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 major capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	611	Total	C	N	O	S	0	0	0
			4799	3067	805	913	14			
1	B	616	Total	C	N	O	S	0	0	0
			4837	3092	812	919	14			
1	C	616	Total	C	N	O	S	0	0	0
			4842	3098	812	918	14			
1	D	610	Total	C	N	O	S	0	0	0
			4793	3064	804	911	14			
1	E	614	Total	C	N	O	S	0	0	0
			4823	3083	810	916	14			
1	F	622	Total	C	N	O	S	0	0	0
			4878	3118	818	928	14			

- Molecule 2 is a protein called unknown.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	21	Total	C	N	O	0	0	0
			105	63	21	21			
2	H	21	Total	C	N	O	0	0	0
			105	63	21	21			
2	I	21	Total	C	N	O	0	0	0
			105	63	21	21			
2	J	21	Total	C	N	O	0	0	0
			105	63	21	21			
2	K	21	Total	C	N	O	0	0	0
			105	63	21	21			
2	L	19	Total	C	N	O	0	0	0
			95	57	19	19			

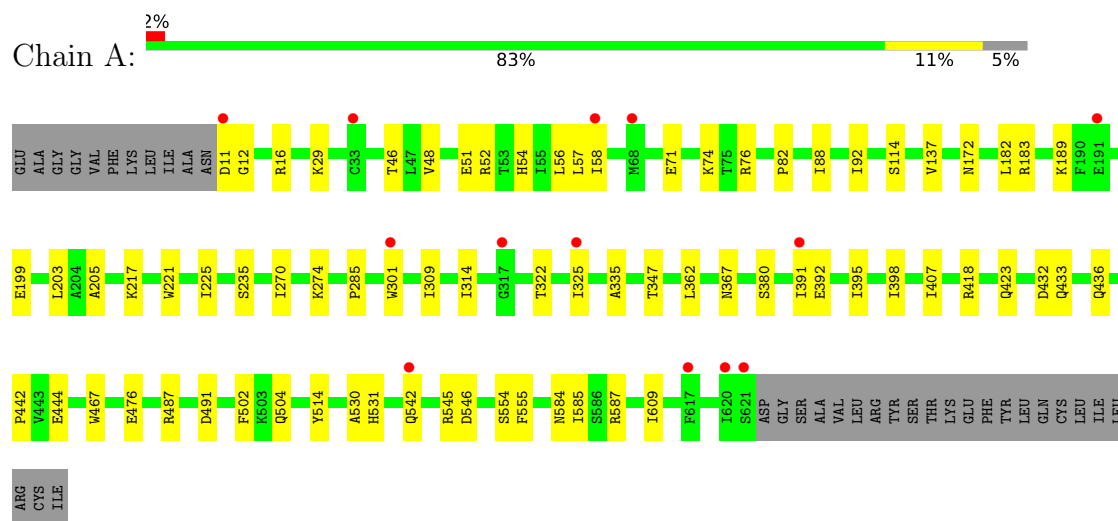
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	221	Total 221	O 221	0	0
3	B	220	Total 220	O 220	0	0
3	C	227	Total 227	O 227	0	0
3	D	198	Total 198	O 198	0	0
3	E	194	Total 194	O 194	0	0
3	F	206	Total 206	O 206	0	0
3	G	6	Total 6	O 6	0	0
3	H	2	Total 2	O 2	0	0
3	I	8	Total 8	O 8	0	0
3	J	3	Total 3	O 3	0	0
3	K	3	Total 3	O 3	0	0
3	L	4	Total 4	O 4	0	0

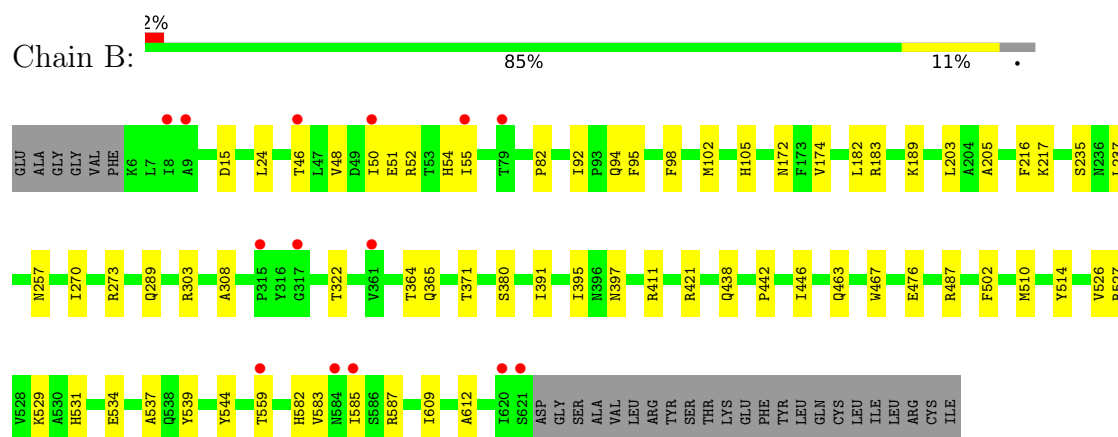
3 Residue-property plots [i](#)

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.

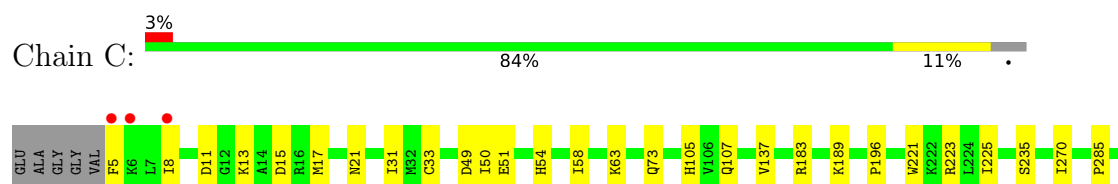
- Molecule 1: major capsid protein

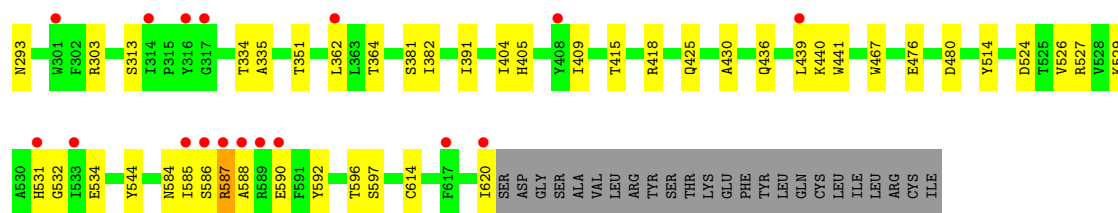


- Molecule 1: major capsid protein

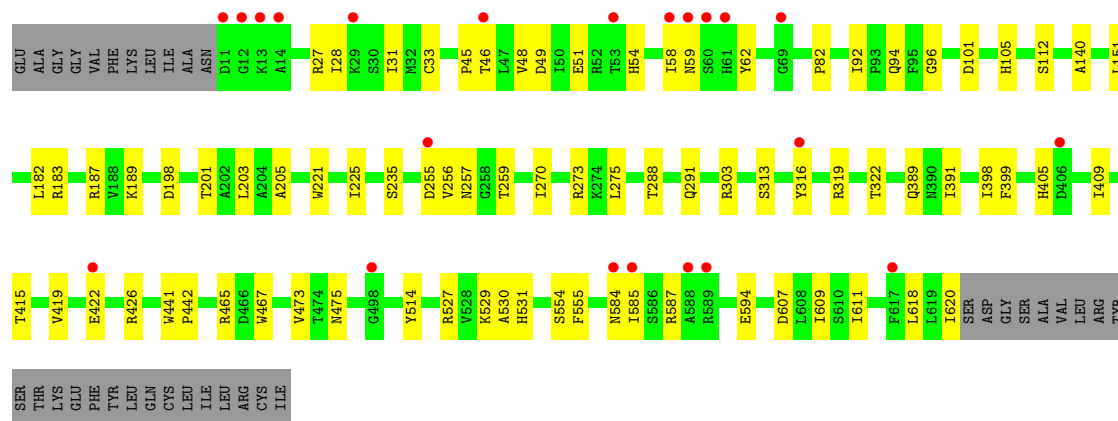
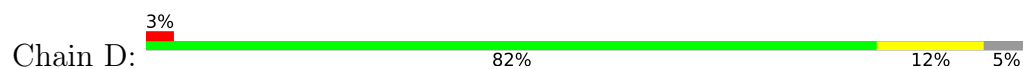


- Molecule 1: major capsid protein

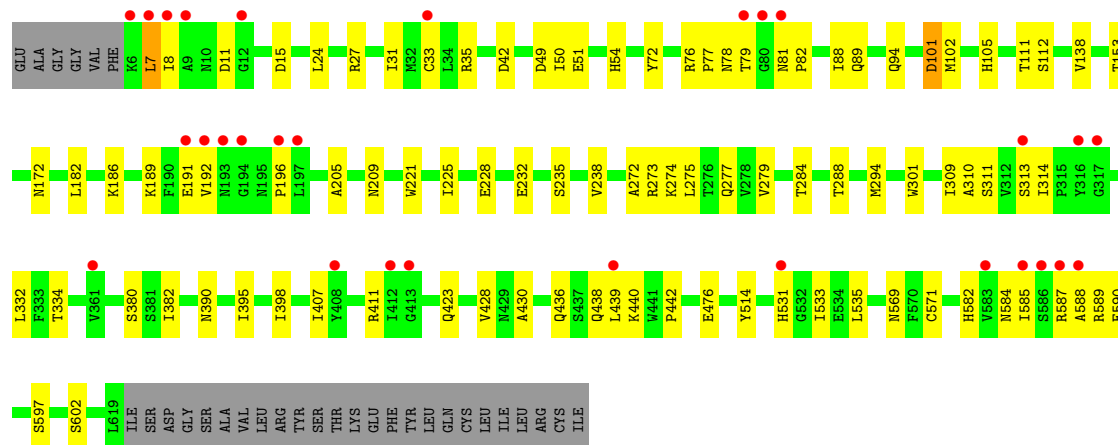
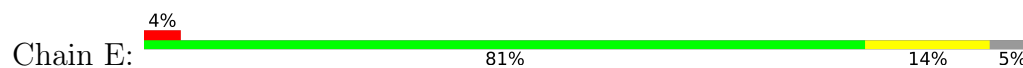




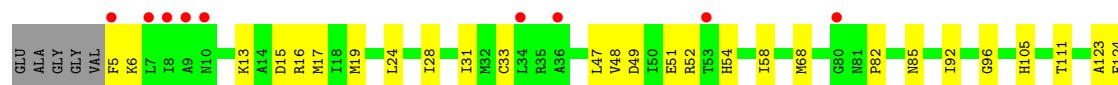
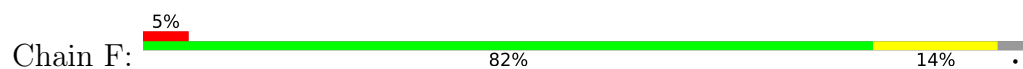
• Molecule 1: major capsid protein

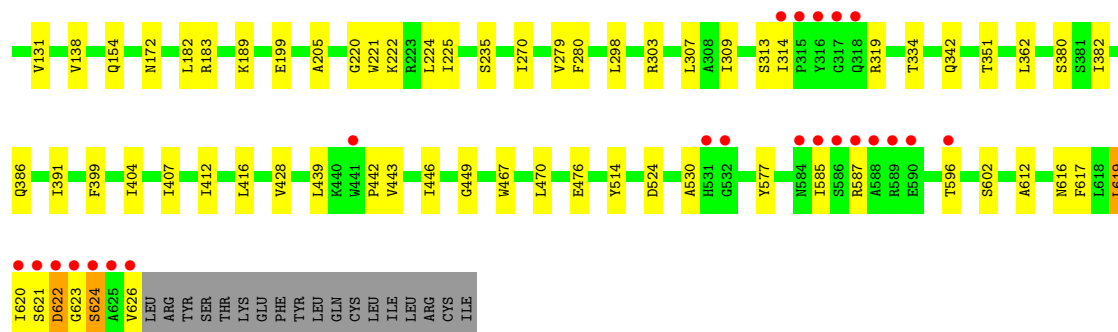


• Molecule 1: major capsid protein



• Molecule 1: major capsid protein





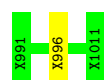
• Molecule 2: unknown

Chain G: 90% 10%



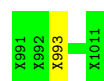
• Molecule 2: unknown

Chain H: 95% 5%



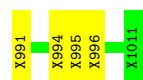
• Molecule 2: unknown

Chain I: 95% 5%



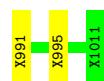
• Molecule 2: unknown

Chain J: 81% 19%



• Molecule 2: unknown

Chain K: 90% 10%



• Molecule 2: unknown

Chain L: 81% 10% 10%

X991	X1006	X1009	UNK	UNK
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.33Å 390.65Å 79.49Å 90.00° 112.91° 90.00°	Depositor
Resolution (Å)	70.07 – 2.37 70.07 – 2.37	Depositor EDS
% Data completeness (in resolution range)	89.8 (70.07-2.37) 89.8 (70.07-2.37)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.37Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.203 , 0.247 0.205 , 0.249	Depositor DCC
R_{free} test set	7642 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.038 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	30884	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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	0.13	0/4915	0.32	0/6716
1	B	0.10	0/4953	0.31	0/6767
1	C	0.11	0/4959	0.32	0/6775
1	D	0.09	0/4909	0.30	0/6708
1	E	0.20	0/4939	0.35	0/6748
1	F	0.19	0/4995	0.33	0/6824
All	All	0.14	0/29670	0.32	0/40538

There are no bond length outliers.

There are no bond angle outliers.

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	4799	0	4720	72	0
1	B	4837	0	4766	61	0
1	C	4842	0	4770	87	0
1	D	4793	0	4715	84	0
1	E	4823	0	4750	112	0
1	F	4878	0	4801	79	0
2	G	105	0	24	2	0
2	H	105	0	24	1	0
2	I	105	0	25	1	0
2	J	105	0	24	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	105	0	25	2	0
2	L	95	0	21	2	0
3	A	221	0	0	3	0
3	B	220	0	0	4	0
3	C	227	0	0	10	0
3	D	198	0	0	0	0
3	E	194	0	0	1	0
3	F	206	0	0	5	0
3	G	6	0	0	1	0
3	H	2	0	0	0	0
3	I	8	0	0	2	0
3	J	3	0	0	1	0
3	K	3	0	0	0	0
3	L	4	0	0	1	0
All	All	30884	0	28665	419	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 7.

All (419) 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:C:585:ILE:HG12	1:C:588:ALA:CB	1.20	1.58
1:D:584:ASN:CG	1:E:8:ILE:HD11	1.35	1.46
1:C:585:ILE:CG1	1:C:588:ALA:HB3	1.53	1.39
1:E:531:HIS:NE2	1:E:587:ARG:C	1.90	1.27
1:C:584:ASN:C	1:C:586:SER:HB3	1.60	1.27
1:E:531:HIS:NE2	1:E:588:ALA:N	1.66	1.26
1:D:584:ASN:CG	1:E:8:ILE:CD1	2.08	1.24
1:C:585:ILE:CG1	1:C:588:ALA:CB	2.12	1.21
1:E:112:SER:OG	1:E:288:THR:HG22	1.38	1.20
1:C:585:ILE:N	1:C:586:SER:HB3	1.57	1.20
1:E:531:HIS:HD2	1:F:6:LYS:NZ	1.44	1.14
1:A:88:ILE:HD12	1:A:325:ILE:HD11	1.19	1.11
1:A:88:ILE:HD13	1:A:391:ILE:CD1	1.80	1.10
1:F:351:THR:HG23	1:F:362:LEU:HD23	1.27	1.10
1:C:585:ILE:CA	1:C:586:SER:HB3	1.81	1.09
1:F:351:THR:CG2	1:F:362:LEU:HD23	1.82	1.08
1:E:531:HIS:CD2	1:F:6:LYS:NZ	2.24	1.06
1:C:585:ILE:HG12	1:C:588:ALA:HB1	1.34	1.05
1:C:584:ASN:C	1:C:586:SER:CB	2.28	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:584:ASN:OD1	1:E:8:ILE:HD11	1.58	1.04
3:B:913:HOH:O	1:C:8:ILE:HD11	1.58	1.03
1:E:79:THR:CG2	1:E:89:GLN:H	1.76	0.99
1:A:542:GLN:HG3	1:A:546:ASP:OD2	1.62	0.99
1:D:584:ASN:CB	1:E:8:ILE:HD11	1.94	0.96
1:C:351:THR:OG1	1:C:362:LEU:HD22	1.63	0.96
1:E:531:HIS:CD2	1:F:6:LYS:HZ3	1.83	0.95
1:B:55:ILE:HG13	1:C:63:LYS:HE2	1.47	0.94
1:B:55:ILE:CD1	1:C:63:LYS:HB2	1.98	0.93
1:E:531:HIS:HD2	1:F:6:LYS:HZ3	1.09	0.92
1:A:88:ILE:CD1	1:A:325:ILE:HD11	1.98	0.92
1:A:88:ILE:HD13	1:A:391:ILE:HD13	1.50	0.91
1:F:351:THR:CG2	1:F:362:LEU:CD2	2.49	0.90
1:C:436:GLN:HB3	1:C:439:LEU:HD13	1.54	0.90
1:C:585:ILE:N	1:C:586:SER:CB	2.33	0.90
1:E:79:THR:HG21	1:E:89:GLN:N	1.87	0.89
1:E:7:LEU:HD13	1:E:8:ILE:N	1.88	0.88
1:C:584:ASN:O	1:C:586:SER:HB3	1.73	0.86
1:C:585:ILE:HA	1:C:586:SER:HB3	1.58	0.85
1:A:58:ILE:HD12	1:B:308:ALA:HB3	1.57	0.85
1:A:88:ILE:HD12	1:A:325:ILE:CD1	2.04	0.83
1:D:255:ASP:OD2	1:F:123:ALA:HB3	1.77	0.83
3:B:913:HOH:O	1:C:8:ILE:CD1	2.20	0.82
1:E:79:THR:HG21	1:E:89:GLN:H	1.41	0.82
1:E:79:THR:CG2	1:E:89:GLN:N	2.42	0.81
1:A:58:ILE:CD1	1:B:308:ALA:HB3	2.09	0.81
1:C:585:ILE:CB	1:C:588:ALA:HB3	2.12	0.79
1:D:273:ARG:HE	1:E:284:THR:HG22	1.48	0.79
1:D:584:ASN:ND2	1:E:8:ILE:CD1	2.46	0.79
1:A:88:ILE:CD1	1:A:325:ILE:CD1	2.61	0.77
1:D:584:ASN:CB	1:E:8:ILE:CD1	2.58	0.77
1:E:79:THR:HG23	1:E:89:GLN:H	1.49	0.76
1:D:584:ASN:ND2	1:E:8:ILE:HG13	2.01	0.76
1:D:46:THR:HG23	1:E:411:ARG:HE	1.49	0.75
1:E:35:ARG:NH1	1:E:42:ASP:O	2.19	0.75
1:F:313:SER:HA	1:F:621:SER:HB3	1.68	0.74
1:E:27:ARG:NH2	1:E:49:ASP:O	2.20	0.74
1:C:585:ILE:HG12	1:C:588:ALA:HB3	0.75	0.74
1:A:74:LYS:HD2	1:A:392:GLU:OE1	1.87	0.74
1:E:531:HIS:HD2	1:F:6:LYS:HZ1	1.35	0.74
1:D:465:ARG:NH1	1:D:473:VAL:HG11	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:THR:HG22	1:D:48:VAL:H	1.52	0.73
1:C:293:ASN:OD1	3:C:701:HOH:O	2.06	0.73
1:C:584:ASN:CG	1:C:586:SER:HB2	2.14	0.72
1:D:255:ASP:OD1	1:D:256:VAL:N	2.23	0.72
1:C:13:LYS:HG2	1:C:17:MET:HE2	1.72	0.71
1:D:27:ARG:NH2	1:D:49:ASP:O	2.21	0.71
1:B:55:ILE:HD12	1:C:63:LYS:HB2	1.73	0.70
2:L:1006:UNK:N	3:L:1101:HOH:O	2.24	0.69
1:A:82:PRO:HB3	1:A:391:ILE:CD1	2.23	0.69
1:A:88:ILE:HG21	1:A:391:ILE:HD12	1.75	0.69
1:C:584:ASN:O	1:C:586:SER:CB	2.37	0.67
1:E:7:LEU:HD13	1:E:7:LEU:C	2.20	0.67
1:E:411:ARG:O	1:E:411:ARG:NH1	2.29	0.66
1:D:527:ARG:HB3	1:D:594:GLU:HB2	1.77	0.66
1:C:531:HIS:CE1	1:C:587:ARG:O	2.50	0.65
1:A:46:THR:HG22	1:A:48:VAL:H	1.61	0.64
1:A:542:GLN:HG3	1:A:545:ARG:HH21	1.62	0.64
1:A:542:GLN:CG	1:A:546:ASP:OD2	2.43	0.64
1:F:33:CYS:SG	2:L:991:UNK:N	2.70	0.64
1:A:76:ARG:NH2	3:A:709:HOH:O	2.29	0.64
1:E:531:HIS:NE2	1:E:587:ARG:CA	2.61	0.64
1:E:192:VAL:HG21	1:E:314:ILE:HD13	1.80	0.63
1:F:313:SER:HA	1:F:621:SER:CB	2.28	0.63
1:A:16:ARG:NH2	3:A:711:HOH:O	2.32	0.63
1:B:55:ILE:HD11	1:C:63:LYS:HB2	1.80	0.63
1:C:529:LYS:HE2	1:C:532:GLY:HA2	1.80	0.63
1:A:530:ALA:HB1	1:A:587:ARG:HB3	1.81	0.63
1:C:107:GLN:NE2	3:C:701:HOH:O	2.30	0.63
1:D:584:ASN:ND2	1:E:8:ILE:CG1	2.62	0.62
1:D:187:ARG:HG2	1:D:201:THR:HG22	1.82	0.62
1:B:55:ILE:HG13	1:C:63:LYS:CE	2.26	0.62
1:D:584:ASN:HD21	1:E:8:ILE:HG13	1.65	0.61
1:A:274:LYS:NZ	1:C:480:ASP:OD1	2.32	0.61
1:C:313:SER:HB2	1:C:620:ILE:HG23	1.82	0.61
1:A:88:ILE:CD1	1:A:391:ILE:HD13	2.26	0.61
1:C:586:SER:C	1:C:588:ALA:H	2.09	0.61
1:E:79:THR:HG21	1:E:88:ILE:HA	1.82	0.61
1:E:72:TYR:OH	1:E:101:ASP:OD2	2.12	0.61
2:I:993:UNK:O	3:I:1101:HOH:O	2.16	0.60
1:D:531:HIS:HB2	1:D:587:ARG:HA	1.82	0.60
1:C:585:ILE:HG22	1:C:585:ILE:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:584:ASN:HB2	1:E:8:ILE:HD11	1.80	0.60
1:E:182:LEU:HD22	1:E:205:ALA:HB1	1.84	0.60
1:C:105:HIS:ND1	3:C:716:HOH:O	2.32	0.59
1:A:52:ARG:NH2	2:G:996:UNK:O	2.36	0.59
1:B:371:THR:HB	1:B:510:MET:HE3	1.83	0.59
1:F:13:LYS:HG2	1:F:16:ARG:HH21	1.66	0.58
1:A:92:ILE:HG23	1:A:395:ILE:HD13	1.85	0.58
1:F:442:PRO:HD3	1:F:585:ILE:HD11	1.85	0.58
1:B:46:THR:HG22	1:B:48:VAL:H	1.68	0.58
1:E:440:LYS:HA	1:E:585:ILE:HG13	1.86	0.57
1:B:364:THR:HG22	1:B:365:GLN:HG3	1.85	0.57
1:B:527:ARG:NH1	1:B:534:GLU:OE2	2.36	0.57
1:D:584:ASN:CG	1:E:8:ILE:CG1	2.76	0.57
1:A:442:PRO:HD3	1:A:585:ILE:HD11	1.85	0.57
1:F:82:PRO:HG3	1:F:391:ILE:HG22	1.86	0.57
1:F:623:GLY:O	1:F:624:SER:OG	2.11	0.56
1:B:529:LYS:NZ	3:B:718:HOH:O	2.37	0.56
1:D:584:ASN:HB2	1:E:8:ILE:CD1	2.35	0.56
1:F:351:THR:HG22	1:F:362:LEU:HG	1.86	0.56
1:A:82:PRO:HB3	1:A:391:ILE:HD13	1.88	0.56
1:E:531:HIS:NE2	1:E:587:ARG:HB3	2.20	0.56
1:C:293:ASN:ND2	3:C:729:HOH:O	2.38	0.56
1:D:33:CYS:SG	2:J:991:UNK:N	2.79	0.56
1:D:398:ILE:HG21	1:F:58:ILE:HD11	1.86	0.56
1:B:182:LEU:HD22	1:B:205:ALA:HB1	1.88	0.56
1:A:88:ILE:HD13	1:A:391:ILE:HD12	1.80	0.56
1:C:405:HIS:CE1	1:C:409:ILE:HD11	2.40	0.56
1:A:221:TRP:O	1:A:225:ILE:HG13	2.06	0.55
1:B:24:LEU:HD11	1:B:50:ILE:HG23	1.87	0.55
1:E:102:MET:HG2	1:E:395:ILE:HG12	1.87	0.55
1:E:423:GLN:HB2	1:E:438:GLN:HB2	1.87	0.55
1:A:407:ILE:HD13	1:C:50:ILE:HD11	1.88	0.55
1:D:27:ARG:HH11	2:J:995:UNK:HA	1.72	0.55
1:D:465:ARG:NH2	1:D:475:ASN:OD1	2.31	0.55
1:E:76:ARG:NH1	1:E:390:ASN:OD1	2.39	0.55
1:C:351:THR:HG1	1:C:362:LEU:HD22	1.66	0.55
1:D:530:ALA:HB1	1:D:587:ARG:HB3	1.89	0.55
1:F:24:LEU:O	1:F:28:ILE:HG12	2.07	0.55
1:E:94:GLN:OE1	1:E:311:SER:OG	2.18	0.55
1:E:334:THR:HG23	1:E:382:ILE:HG23	1.88	0.54
1:D:58:ILE:HD11	1:E:398:ILE:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:428:VAL:CG2	1:F:602:SER:HA	2.38	0.54
1:A:11:ASP:HB3	1:A:12:GLY:HA2	1.89	0.54
1:B:531:HIS:HB2	1:B:587:ARG:HA	1.88	0.54
1:E:428:VAL:HG13	1:E:602:SER:HA	1.89	0.54
1:A:71:GLU:OE1	1:C:5:PHE:HB2	2.07	0.54
1:C:425:GLN:NE2	3:C:731:HOH:O	2.39	0.54
1:D:442:PRO:HD3	1:D:585:ILE:HD11	1.90	0.54
1:E:78:ASN:ND2	3:E:716:HOH:O	2.41	0.53
1:E:7:LEU:C	1:E:7:LEU:CD1	2.82	0.53
1:C:223:ARG:NH1	3:C:715:HOH:O	2.30	0.53
1:B:237:LEU:HD23	1:B:273:ARG:HG2	1.90	0.53
1:C:334:THR:HG21	1:C:381:SER:HA	1.90	0.53
1:E:533:ILE:HG22	1:F:5:PHE:CZ	2.44	0.53
1:D:584:ASN:CG	1:E:8:ILE:HD12	2.25	0.53
1:B:82:PRO:HG3	1:B:391:ILE:HG22	1.90	0.53
1:A:487:ARG:HB3	1:A:502:PHE:CE1	2.44	0.53
1:E:584:ASN:OD1	1:E:585:ILE:N	2.41	0.53
1:B:51:GLU:HA	1:B:54:HIS:O	2.09	0.52
1:A:74:LYS:HD2	1:A:392:GLU:CD	2.34	0.52
1:D:514:TYR:CE2	1:F:235:SER:HB3	2.44	0.52
1:A:58:ILE:HD11	1:B:308:ALA:HB3	1.90	0.52
1:E:272:ALA:HB2	1:F:280:PHE:HB3	1.92	0.52
1:C:33:CYS:SG	3:I:1106:HOH:O	2.58	0.51
1:D:235:SER:HB3	1:E:514:TYR:CE2	2.44	0.51
1:E:31:ILE:O	1:E:35:ARG:HG3	2.10	0.51
1:F:412:ILE:CG2	1:F:620:ILE:HD12	2.41	0.51
1:B:105:HIS:O	1:B:391:ILE:HA	2.10	0.51
1:A:51:GLU:HA	1:A:54:HIS:O	2.10	0.51
1:C:362:LEU:HD23	1:C:364:THR:HG23	1.93	0.51
1:D:45:PRO:HD2	1:E:407:ILE:HG12	1.92	0.51
1:E:588:ALA:C	1:E:590:GLU:H	2.17	0.51
1:F:351:THR:HG22	1:F:362:LEU:CG	2.40	0.51
1:D:255:ASP:OD1	1:D:256:VAL:HG22	2.11	0.51
1:B:24:LEU:HD21	1:C:404:ILE:HD11	1.92	0.51
1:E:51:GLU:HA	1:E:54:HIS:O	2.11	0.51
1:B:257:ASN:ND2	3:B:717:HOH:O	2.36	0.51
1:D:183:ARG:HB2	1:D:467:TRP:CZ2	2.46	0.51
1:C:362:LEU:HD23	1:C:362:LEU:O	2.11	0.50
1:B:235:SER:HB3	1:C:514:TYR:CE2	2.47	0.50
1:D:82:PRO:HG3	1:D:391:ILE:HG22	1.93	0.50
1:D:62:TYR:OH	1:F:17:MET:O	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:ILE:CG1	1:C:63:LYS:HE2	2.32	0.50
1:E:79:THR:HG23	1:E:89:GLN:N	2.18	0.50
1:E:442:PRO:HB3	1:E:582:HIS:CD2	2.46	0.50
1:F:439:LEU:HD13	1:F:443:VAL:HG21	1.93	0.50
1:D:313:SER:HB2	1:D:620:ILE:HG23	1.93	0.50
1:E:11:ASP:HB3	1:E:15:ASP:OD2	2.12	0.50
1:E:588:ALA:HB3	1:E:590:GLU:HB2	1.94	0.50
1:B:487:ARG:HB3	1:B:502:PHE:CE1	2.47	0.49
1:E:235:SER:HB3	1:F:514:TYR:CE2	2.47	0.49
1:E:27:ARG:HH11	2:K:995:UNK:HA	1.77	0.49
1:E:189:LYS:HD2	1:E:196:PRO:HG3	1.94	0.49
1:F:621:SER:CB	3:F:771:HOH:O	2.60	0.49
1:B:55:ILE:HD11	1:C:63:LYS:HD3	1.95	0.49
1:F:51:GLU:HA	1:F:54:HIS:O	2.12	0.49
1:F:449:GLY:HA3	1:F:470:LEU:HD13	1.94	0.49
1:E:531:HIS:NE2	1:E:587:ARG:CB	2.75	0.49
1:F:621:SER:HB3	3:F:771:HOH:O	2.12	0.49
1:A:301:TRP:H	1:A:301:TRP:CD1	2.30	0.49
1:D:415:THR:HG22	1:D:618:LEU:HB3	1.95	0.49
1:E:531:HIS:CD2	1:F:6:LYS:HZ1	2.17	0.49
1:D:422:GLU:HG3	1:D:611:ILE:HG12	1.95	0.49
1:F:131:VAL:HG22	1:F:138:VAL:HB	1.95	0.49
1:B:94:GLN:CD	1:D:316:TYR:H	2.21	0.49
1:B:92:ILE:HG23	1:B:395:ILE:HD13	1.96	0.48
1:C:221:TRP:O	1:C:225:ILE:HG13	2.14	0.48
1:C:415:THR:HG22	1:C:620:ILE:HD11	1.95	0.48
1:D:255:ASP:N	1:D:259:THR:O	2.43	0.48
1:E:531:HIS:O	1:E:533:ILE:HG12	2.12	0.48
1:F:13:LYS:HG2	1:F:16:ARG:NH2	2.29	0.48
1:A:270:ILE:HG12	1:C:476:GLU:HG2	1.95	0.48
1:D:189:LYS:HG3	1:D:322:THR:HB	1.96	0.48
1:D:46:THR:HA	1:E:411:ARG:HG3	1.96	0.48
1:C:183:ARG:HB2	1:C:467:TRP:CZ2	2.48	0.48
1:E:535:LEU:HD23	1:F:5:PHE:HE2	1.78	0.48
1:F:85:ASN:OD1	3:F:701:HOH:O	2.20	0.48
1:A:51:GLU:HG2	1:A:56:LEU:HD23	1.96	0.47
1:E:24:LEU:HD21	1:F:404:ILE:HD11	1.95	0.47
1:A:584:ASN:ND2	1:B:15:ASP:OD2	2.35	0.47
1:E:79:THR:HG21	1:E:88:ILE:CA	2.44	0.47
1:E:228:GLU:OE1	1:E:284:THR:HG23	2.14	0.47
1:F:31:ILE:HD13	1:F:49:ASP:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1006:UNK:O	3:G:1101:HOH:O	2.19	0.47
1:C:189:LYS:HD2	1:C:196:PRO:HB3	1.94	0.47
1:C:334:THR:HG23	1:C:382:ILE:HG23	1.97	0.47
1:D:28:ILE:HG23	1:D:45:PRO:HG2	1.97	0.47
1:D:182:LEU:HD22	1:D:205:ALA:HB1	1.97	0.47
1:F:19:MET:O	1:F:54:HIS:NE2	2.47	0.47
1:A:82:PRO:HB3	1:A:391:ILE:HD11	1.95	0.47
1:A:398:ILE:HG21	1:C:58:ILE:HD11	1.97	0.47
1:D:112:SER:HB3	1:D:288:THR:HG22	1.97	0.47
1:D:465:ARG:HH12	1:D:473:VAL:HG11	1.79	0.47
1:E:310:ALA:O	1:E:313:SER:OG	2.24	0.47
1:F:412:ILE:HG23	1:F:620:ILE:HD12	1.96	0.47
1:B:172:ASN:ND2	1:B:380:SER:HB3	2.30	0.47
1:D:527:ARG:N	1:D:594:GLU:O	2.40	0.47
1:D:554:SER:OG	1:D:555:PHE:N	2.47	0.47
1:E:33:CYS:SG	2:K:991:UNK:N	2.87	0.47
1:B:55:ILE:CG1	1:C:63:LYS:HB2	2.44	0.46
1:D:255:ASP:C	1:D:257:ASN:N	2.72	0.46
1:B:442:PRO:HD3	1:B:585:ILE:HD11	1.96	0.46
1:D:105:HIS:O	1:D:391:ILE:HA	2.14	0.46
1:E:436:GLN:HB3	1:E:439:LEU:HG	1.97	0.46
1:A:423:GLN:HE22	1:A:436:GLN:HA	1.80	0.46
1:E:79:THR:HG23	1:E:89:GLN:HB3	1.98	0.46
1:E:111:THR:HG21	1:E:332:LEU:HD21	1.95	0.46
1:E:582:HIS:NE2	1:F:15:ASP:OD1	2.34	0.46
1:F:48:VAL:O	1:F:52:ARG:HG3	2.15	0.46
1:E:7:LEU:HD13	1:E:8:ILE:C	2.41	0.46
1:F:351:THR:HG21	1:F:362:LEU:CD2	2.42	0.46
1:F:530:ALA:HB1	1:F:587:ARG:HB3	1.97	0.46
1:E:535:LEU:HD23	1:F:5:PHE:CE2	2.51	0.46
1:C:430:ALA:O	1:C:597:SER:N	2.47	0.46
1:D:465:ARG:HH11	1:D:473:VAL:HG11	1.75	0.46
1:E:172:ASN:ND2	1:E:380:SER:HB3	2.31	0.46
1:C:586:SER:C	1:C:588:ALA:N	2.73	0.46
1:F:446:ILE:HG12	1:F:612:ALA:HB2	1.98	0.46
1:C:105:HIS:O	1:C:391:ILE:HA	2.15	0.46
1:E:238:VAL:HG11	1:E:274:LYS:HE2	1.97	0.45
1:B:52:ARG:NH2	2:H:996:UNK:O	2.49	0.45
1:C:590:GLU:HB3	1:C:592:TYR:HE1	1.81	0.45
1:E:138:VAL:HG22	1:E:153:THR:HG23	1.97	0.45
1:A:29:LYS:HB3	1:A:29:LYS:HE2	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:THR:HG22	1:B:48:VAL:N	2.30	0.45
1:C:524:ASP:HB2	1:C:596:THR:HG22	1.97	0.45
1:E:189:LYS:HG2	1:E:191:GLU:HG3	1.98	0.45
1:D:584:ASN:ND2	1:E:15:ASP:OD2	2.43	0.45
1:A:58:ILE:HG23	1:A:58:ILE:O	2.17	0.45
1:C:11:ASP:HB3	1:C:15:ASP:OD2	2.17	0.45
1:A:487:ARG:HD3	1:A:504:GLN:HG2	1.98	0.45
1:C:584:ASN:ND2	1:C:586:SER:HB2	2.31	0.45
1:D:584:ASN:CB	1:E:8:ILE:HD12	2.44	0.45
1:A:217:LYS:HA	1:B:559:THR:HG23	1.98	0.45
1:A:347:THR:OG1	1:A:367:ASN:HB2	2.17	0.45
1:E:50:ILE:HD11	1:F:407:ILE:HD13	1.98	0.45
1:A:235:SER:HB3	1:B:514:TYR:CE2	2.52	0.45
1:D:405:HIS:O	1:D:409:ILE:HG12	2.17	0.45
1:E:112:SER:HG	1:E:288:THR:HG22	1.69	0.45
1:F:182:LEU:HD22	1:F:205:ALA:HB1	1.98	0.45
1:F:298:LEU:O	1:F:303:ARG:NH1	2.49	0.45
1:D:465:ARG:HH12	1:D:473:VAL:CG1	2.30	0.45
1:E:232:GLU:CD	1:E:275:LEU:HD13	2.42	0.45
1:F:351:THR:CG2	1:F:362:LEU:CG	2.95	0.45
1:E:588:ALA:C	1:E:590:GLU:N	2.75	0.44
1:D:426:ARG:NE	1:D:607:ASP:OD1	2.50	0.44
1:D:527:ARG:CZ	1:D:529:LYS:HD2	2.47	0.44
1:F:616:ASN:OD1	1:F:617:PHE:N	2.40	0.44
1:B:95:PHE:HB3	1:B:397:ASN:OD1	2.17	0.44
1:B:102:MET:O	1:B:303:ARG:NH2	2.50	0.44
1:B:183:ARG:HB2	1:B:467:TRP:CZ2	2.52	0.44
1:E:112:SER:OG	1:E:288:THR:CG2	2.33	0.44
1:A:182:LEU:HD22	1:A:205:ALA:HB1	1.99	0.44
1:B:442:PRO:HB3	1:B:582:HIS:CD2	2.53	0.44
1:D:198:ASP:HB2	1:D:419:VAL:HG12	1.98	0.44
1:E:430:ALA:O	1:E:597:SER:N	2.50	0.44
1:A:58:ILE:CD1	1:B:98:PHE:CD2	3.01	0.44
1:B:95:PHE:O	1:D:94:GLN:NE2	2.51	0.44
1:C:531:HIS:ND1	1:C:587:ARG:O	2.50	0.44
1:C:587:ARG:NH2	3:C:750:HOH:O	2.50	0.44
1:D:51:GLU:HA	1:D:54:HIS:O	2.17	0.44
1:E:79:THR:CG2	1:E:89:GLN:HB3	2.48	0.44
1:F:313:SER:HB3	1:F:620:ILE:HG23	1.99	0.44
1:A:491:ASP:OD2	3:A:702:HOH:O	2.21	0.44
1:D:255:ASP:C	1:D:257:ASN:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:416:LEU:HD12	1:F:617:PHE:CE2	2.52	0.44
1:B:203:LEU:HD22	1:B:609:ILE:HD13	2.00	0.44
1:E:569:ASN:ND2	1:E:571:CYS:O	2.51	0.44
1:A:88:ILE:HD11	1:A:325:ILE:CD1	2.46	0.43
1:E:77:PRO:HB2	1:E:79:THR:OG1	2.18	0.43
1:F:428:VAL:HG22	1:F:428:VAL:O	2.18	0.43
1:A:189:LYS:HG3	1:A:322:THR:HB	1.99	0.43
1:A:285:PRO:HB3	1:A:335:ALA:HB3	2.01	0.43
1:D:415:THR:CG2	1:D:618:LEU:HB3	2.47	0.43
1:E:81:ASN:HA	1:E:82:PRO:HD3	1.89	0.43
1:F:220:GLY:O	1:F:224:LEU:HG	2.19	0.43
1:D:92:ILE:HB	1:D:319:ARG:HG3	1.99	0.43
1:C:303:ARG:NH2	3:C:738:HOH:O	2.44	0.43
1:C:285:PRO:HB3	1:C:335:ALA:HB3	2.01	0.43
1:C:587:ARG:NH1	1:C:587:ARG:HB2	2.34	0.43
1:A:58:ILE:HD13	1:B:98:PHE:CD2	2.53	0.43
1:B:487:ARG:HD3	1:B:502:PHE:CZ	2.54	0.43
1:C:440:LYS:HA	1:C:585:ILE:HG21	2.01	0.43
1:D:140:ALA:HB2	1:D:151:LEU:HD12	2.01	0.43
1:D:270:ILE:HG12	1:F:476:GLU:HG2	1.99	0.43
1:D:275:LEU:HB2	1:E:277:GLN:HB2	2.01	0.43
1:E:105:HIS:HA	1:E:294:MET:O	2.18	0.43
1:E:221:TRP:O	1:E:225:ILE:HG12	2.19	0.43
1:F:96:GLY:HA2	1:F:399:PHE:CE2	2.54	0.43
1:D:46:THR:HG23	1:E:411:ARG:HH21	1.84	0.42
1:E:531:HIS:CD2	1:E:587:ARG:C	2.88	0.42
2:J:991:UNK:N	3:J:1102:HOH:O	2.36	0.42
1:D:46:THR:HG22	1:D:48:VAL:N	2.26	0.42
1:D:203:LEU:HD22	1:D:609:ILE:HD13	2.00	0.42
1:E:209:ASN:OD1	1:E:221:TRP:NE1	2.39	0.42
1:A:542:GLN:HG3	1:A:545:ARG:NH2	2.32	0.42
1:B:55:ILE:CG1	1:C:63:LYS:CE	2.96	0.42
1:D:46:THR:HG23	1:E:411:ARG:NE	2.25	0.42
1:C:73:GLN:NE2	3:C:727:HOH:O	2.38	0.42
1:C:584:ASN:C	1:C:586:SER:HB2	2.35	0.42
1:A:189:LYS:HB3	1:A:199:GLU:HB3	2.02	0.42
1:B:55:ILE:HG13	1:C:63:LYS:CB	2.49	0.42
1:D:101:ASP:HB3	1:D:303:ARG:HG3	2.01	0.42
1:D:419:VAL:HG21	1:D:441:TRP:CZ3	2.54	0.42
1:D:584:ASN:ND2	1:E:8:ILE:HD12	2.32	0.42
1:E:476:GLU:HG2	1:F:270:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ARG:HB2	1:A:467:TRP:CZ2	2.53	0.42
1:C:137:VAL:HG13	1:C:137:VAL:O	2.19	0.42
1:B:174:VAL:HG23	1:B:289:GLN:HG2	2.01	0.42
1:B:189:LYS:HB2	1:B:322:THR:HB	2.00	0.42
1:B:216:PHE:CD1	1:B:217:LYS:HG2	2.55	0.42
1:E:273:ARG:HG3	1:F:279:VAL:HG23	2.02	0.42
1:A:82:PRO:HG3	1:A:391:ILE:HG12	2.01	0.42
1:A:88:ILE:HD13	1:A:391:ILE:HD11	1.90	0.42
1:E:186:LYS:HB3	1:E:186:LYS:HE2	1.76	0.42
1:F:154:GLN:HA	1:F:342:GLN:O	2.20	0.42
1:A:203:LEU:HD22	1:A:609:ILE:HD13	2.02	0.42
1:B:421:ARG:HD2	1:B:438:GLN:O	2.19	0.42
1:C:584:ASN:O	1:C:586:SER:OG	2.38	0.42
1:F:105:HIS:O	1:F:391:ILE:HA	2.19	0.42
1:F:309:ILE:HG21	1:F:314:ILE:HD12	2.02	0.42
1:A:114:SER:O	1:A:380:SER:OG	2.37	0.41
1:A:432:ASP:OD1	1:A:433:GLN:N	2.53	0.41
1:B:476:GLU:HG2	1:C:270:ILE:HG12	2.02	0.41
1:D:221:TRP:O	1:D:225:ILE:HG12	2.19	0.41
1:D:273:ARG:HG3	1:E:279:VAL:HG23	2.02	0.41
1:A:57:LEU:HD23	1:A:57:LEU:HA	1.91	0.41
1:A:172:ASN:ND2	1:A:380:SER:O	2.52	0.41
1:F:189:LYS:HG2	1:F:199:GLU:HB3	2.02	0.41
1:B:526:VAL:HB	1:B:544:TYR:CE2	2.55	0.41
1:B:537:ALA:HB3	1:B:539:TYR:CZ	2.56	0.41
1:D:31:ILE:HG23	1:D:45:PRO:HG3	2.03	0.41
1:E:587:ARG:HA	1:E:588:ALA:HA	1.53	0.41
1:F:619:LEU:N	1:F:619:LEU:HD22	2.35	0.41
1:F:626:VAL:HA	3:F:745:HOH:O	2.20	0.41
1:A:514:TYR:CE2	1:C:235:SER:HB3	2.55	0.41
1:C:440:LYS:HE2	1:C:441:TRP:CE2	2.56	0.41
1:C:440:LYS:HE3	1:C:440:LYS:HB2	1.93	0.41
1:A:46:THR:HA	1:B:411:ARG:HD2	2.01	0.41
1:A:137:VAL:O	1:A:137:VAL:HG13	2.21	0.41
1:A:554:SER:OG	1:A:555:PHE:N	2.53	0.41
1:B:446:ILE:HG12	1:B:612:ALA:HB2	2.01	0.41
1:C:21:ASN:ND2	3:C:713:HOH:O	2.29	0.41
1:E:79:THR:HG21	1:E:88:ILE:C	2.42	0.41
1:F:172:ASN:ND2	1:F:380:SER:HB3	2.36	0.41
1:F:524:ASP:HB2	1:F:596:THR:HG23	2.02	0.41
1:B:463:GLN:HE21	1:B:463:GLN:HB3	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:ARG:O	1:D:31:ILE:HG22	2.20	0.41
1:D:96:GLY:HA2	1:D:399:PHE:CE2	2.55	0.41
1:F:92:ILE:HB	1:F:319:ARG:HG3	2.02	0.41
1:C:418:ARG:HA	1:C:614:CYS:O	2.20	0.41
1:D:255:ASP:OD1	1:F:124:PHE:O	2.39	0.41
1:E:301:TRP:CZ2	1:E:309:ILE:HD11	2.56	0.41
1:F:334:THR:HG23	1:F:382:ILE:HG23	2.03	0.41
1:A:531:HIS:HB2	1:A:587:ARG:HA	2.02	0.41
1:B:442:PRO:HA	1:B:583:VAL:O	2.20	0.41
1:F:183:ARG:HB2	1:F:467:TRP:CZ2	2.56	0.41
1:C:51:GLU:HA	1:C:54:HIS:O	2.21	0.41
1:C:526:VAL:HB	1:C:544:TYR:CE2	2.55	0.41
1:E:585:ILE:HG22	1:E:589:ARG:HA	2.03	0.41
1:F:307:LEU:HD21	1:F:577:TYR:CE1	2.55	0.41
2:J:994:UNK:O	2:J:996:UNK:N	2.54	0.41
1:A:217:LYS:HA	1:B:559:THR:CG2	2.51	0.41
1:C:31:ILE:HD13	1:C:49:ASP:HB3	2.02	0.41
1:F:621:SER:O	1:F:622:ASP:HB3	2.21	0.41
1:A:309:ILE:HG21	1:A:314:ILE:HD12	2.03	0.40
1:C:527:ARG:NH2	1:C:534:GLU:OE2	2.48	0.40
1:D:51:GLU:OE2	1:D:59:ASN:ND2	2.54	0.40
1:D:291:GLN:NE2	1:D:389:GLN:OE1	2.45	0.40
1:F:222:LYS:NZ	3:F:737:HOH:O	2.54	0.40
1:F:621:SER:O	1:F:622:ASP:CB	2.69	0.40
1:A:418:ARG:NH2	1:A:444:GLU:OE2	2.36	0.40
1:F:47:LEU:O	1:F:51:GLU:HG3	2.21	0.40
1:A:476:GLU:HG2	1:B:270:ILE:HG12	2.03	0.40
1:D:527:ARG:NH1	1:D:529:LYS:HD2	2.37	0.40
1:B:55:ILE:HG13	1:C:63:LYS:HB2	2.04	0.40
1:F:111:THR:HG21	1:F:386:GLN:HB2	2.04	0.40
1:F:221:TRP:O	1:F:225:ILE:HG12	2.22	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	609/645 (94%)	591 (97%)	18 (3%)	0	100	100
1	B	614/645 (95%)	601 (98%)	13 (2%)	0	100	100
1	C	614/645 (95%)	594 (97%)	19 (3%)	1 (0%)	43	56
1	D	608/645 (94%)	596 (98%)	12 (2%)	0	100	100
1	E	612/645 (95%)	595 (97%)	17 (3%)	0	100	100
1	F	620/645 (96%)	599 (97%)	19 (3%)	2 (0%)	36	48
All	All	3677/3870 (95%)	3576 (97%)	98 (3%)	3 (0%)	48	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	622	ASP
1	F	624	SER
1	C	587	ARG

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	526/554 (95%)	525 (100%)	1 (0%)	87	94
1	B	530/554 (96%)	530 (100%)	0	100	100
1	C	530/554 (96%)	530 (100%)	0	100	100
1	D	525/554 (95%)	525 (100%)	0	100	100
1	E	528/554 (95%)	526 (100%)	2 (0%)	84	91
1	F	534/554 (96%)	532 (100%)	2 (0%)	84	91
All	All	3173/3324 (96%)	3168 (100%)	5 (0%)	87	94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	362	LEU
1	E	7	LEU
1	E	101	ASP
1	F	68	MET
1	F	619	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	89	GLN
1	A	164	GLN
1	A	483	GLN
1	A	556	ASN
1	B	107	GLN
1	B	367	ASN
1	C	21	ASN
1	C	78	ASN
1	C	291	GLN
1	C	293	ASN
1	C	327	GLN
1	C	390	ASN
1	C	504	GLN
1	C	556	ASN
1	D	61	HIS
1	D	164	GLN
1	D	193	ASN
1	D	454	ASN
1	D	504	GLN
1	D	511	GLN
1	E	21	ASN
1	E	59	ASN
1	E	73	GLN
1	E	107	GLN
1	E	277	GLN
1	E	293	ASN
1	E	436	GLN
1	E	438	GLN
1	E	511	GLN
1	E	531	HIS
1	E	556	ASN
1	F	73	GLN
1	F	107	GLN

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Mol	Chain	Res	Type
1	F	367	ASN
1	F	511	GLN
1	F	531	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	611/645 (94%)	0.25	13 (2%) 63 62	29, 42, 61, 90	0
1	B	616/645 (95%)	0.31	14 (2%) 61 60	27, 41, 65, 92	0
1	C	616/645 (95%)	0.26	20 (3%) 50 50	26, 41, 67, 138	0
1	D	610/645 (94%)	0.32	22 (3%) 46 46	29, 43, 70, 108	0
1	E	614/645 (95%)	0.41	29 (4%) 36 36	32, 45, 75, 145	0
1	F	622/645 (96%)	0.41	32 (5%) 33 33	26, 44, 71, 122	0
2	G	0/21	-	-	-	-
2	H	0/21	-	-	-	-
2	I	0/21	-	-	-	-
2	J	0/21	-	-	-	-
2	K	0/21	-	-	-	-
2	L	0/21	-	-	-	-
All	All	3689/3996 (92%)	0.33	130 (3%) 47 47	26, 43, 68, 145	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	5	PHE	7.1
1	F	588	ALA	6.2
1	D	255	ASP	5.0
1	A	617	PHE	4.6
1	A	542	GLN	4.5
1	F	586	SER	4.4
1	E	585	ILE	4.3
1	F	317	GLY	4.3
1	E	9	ALA	4.3
1	C	620	ILE	4.2
1	C	439	LEU	4.1
1	D	12	GLY	4.0
1	C	588	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	55	ILE	3.8
1	C	587	ARG	3.6
1	A	68	MET	3.6
1	F	585	ILE	3.5
1	E	531	HIS	3.5
1	C	586	SER	3.5
1	D	11	ASP	3.5
1	B	50	ILE	3.4
1	C	590	GLU	3.4
1	E	6	LYS	3.4
1	D	14	ALA	3.3
1	A	391	ILE	3.3
1	E	193	ASN	3.3
1	F	584	ASN	3.2
1	F	587	ARG	3.2
1	C	585	ILE	3.2
1	E	586	SER	3.2
1	C	589	ARG	3.2
1	D	422	GLU	3.2
1	E	316	TYR	3.2
1	E	317	GLY	3.2
1	F	315	PRO	3.2
1	C	617	PHE	3.1
1	A	33	CYS	3.1
1	A	58	ILE	3.0
1	F	9	ALA	3.0
1	E	79	THR	3.0
1	F	622	ASP	3.0
1	B	9	ALA	3.0
1	E	408	TYR	3.0
1	F	624	SER	3.0
1	D	61	HIS	2.9
1	E	587	ARG	2.9
1	E	412	ILE	2.8
1	F	532	GLY	2.8
1	B	8	ILE	2.7
1	D	46	THR	2.7
1	F	531	HIS	2.7
1	F	318	GLN	2.7
1	F	626	VAL	2.7
1	C	314	ILE	2.7
1	E	313	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	361	VAL	2.7
1	D	316	TYR	2.6
1	E	194	GLY	2.6
1	D	588	ALA	2.6
1	F	7	LEU	2.6
1	B	79	THR	2.5
1	E	80	GLY	2.5
1	A	325	ILE	2.5
1	F	621	SER	2.5
1	F	316	TYR	2.5
1	D	29	LYS	2.5
1	C	531	HIS	2.5
1	C	5	PHE	2.5
1	E	361	VAL	2.5
1	E	7	LEU	2.5
1	A	621	SER	2.4
1	B	620	ILE	2.4
1	C	301	TRP	2.4
1	E	588	ALA	2.4
1	B	559	THR	2.4
1	B	621	SER	2.4
1	D	585	ILE	2.4
1	B	584	ASN	2.4
1	C	317	GLY	2.4
1	B	317	GLY	2.4
1	F	620	ILE	2.4
1	E	439	LEU	2.4
1	A	11	ASP	2.3
1	C	408	TYR	2.3
1	A	317	GLY	2.3
1	F	80	GLY	2.3
1	F	625	ALA	2.3
1	E	8	ILE	2.3
1	C	362	LEU	2.3
1	D	59	ASN	2.3
1	E	33	CYS	2.3
1	F	441	TRP	2.3
1	D	406	ASP	2.2
1	D	589	ARG	2.2
1	F	596	THR	2.2
1	F	8	ILE	2.2
1	E	197	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	6	LYS	2.2
1	D	53	THR	2.2
1	A	620	ILE	2.2
1	C	8	ILE	2.2
1	E	192	VAL	2.2
1	B	315	PRO	2.2
1	F	36	ALA	2.2
1	F	34	LEU	2.1
1	E	81	ASN	2.1
1	F	10	ASN	2.1
1	A	191	GLU	2.1
1	F	590	GLU	2.1
1	D	60	SER	2.1
1	F	53	THR	2.1
1	F	589	ARG	2.1
1	D	58	ILE	2.1
1	D	617	PHE	2.1
1	E	196	PRO	2.1
1	E	12	GLY	2.1
1	F	623	GLY	2.1
1	E	583	VAL	2.1
1	D	498	GLY	2.1
1	E	413	GLY	2.1
1	B	46	THR	2.1
1	D	13	LYS	2.1
1	D	69	GLY	2.1
1	A	301	TRP	2.1
1	D	584	ASN	2.0
1	B	585	ILE	2.0
1	C	533	ILE	2.0
1	C	316	TYR	2.0
1	E	191	GLU	2.0
1	F	314	ILE	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.