



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:32 PM GMT

PDB ID : 1U0N  
Title : The ternary von Willebrand Factor A1-glycoprotein Ibalphabotrocetin complex  
Authors : Fukuda, K.; Liddington, R.C.  
Deposited on : 2004-07-13  
Resolution : 2.95 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

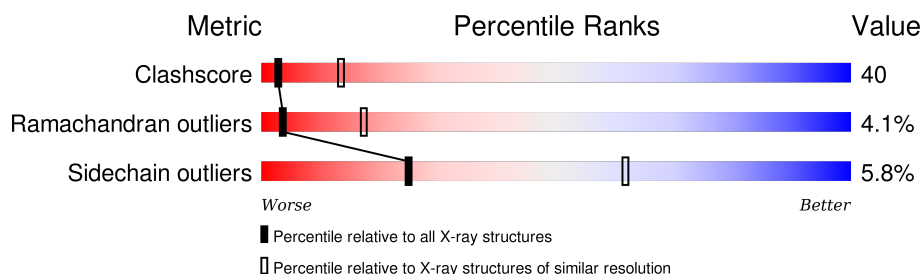
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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))
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	208	
2	B	133	
3	C	125	
4	D	265	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5864 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 Von Willebrand factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	1
			1664	1062	293	303	6			

- Molecule 2 is a protein called Botrocetin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	0	0
			1066	679	175	204	8			

- Molecule 3 is a protein called Botrocetin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	125	Total	C	N	O	S	0	0	0
			1060	682	166	202	10			

- Molecule 4 is a protein called Platelet glycoprotein Ib.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	265	Total	C	N	O	S	0	0	0
			2074	1334	344	387	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	21	GLN	ASN	ENGINEERED	UNP P07359
D	159	GLN	ASN	ENGINEERED	UNP P07359

### 3 Residue-property plots

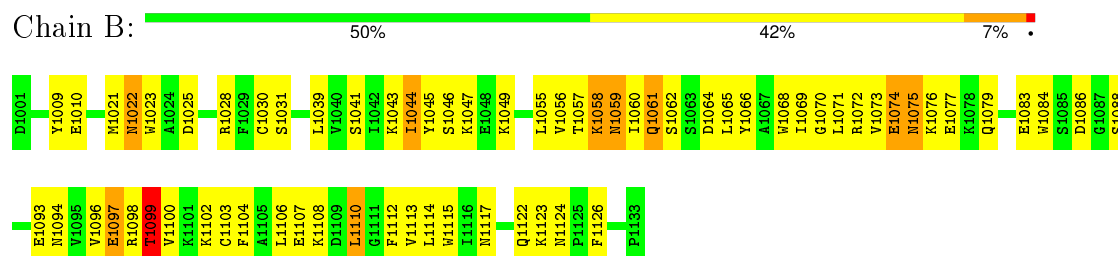
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

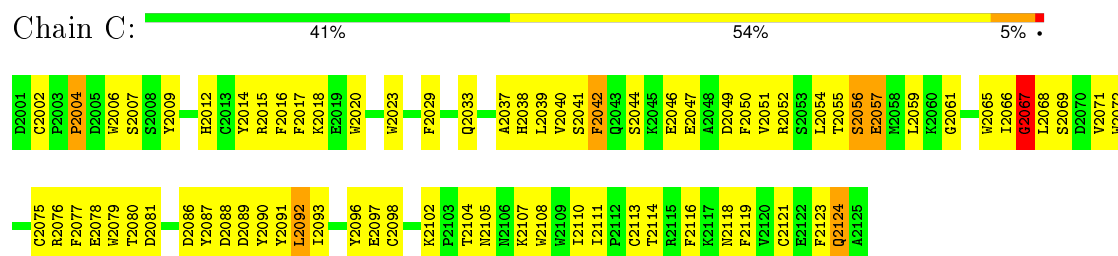
#### • Molecule 1: Von Willebrand factor



#### • Molecule 2: Botrocetin



#### • Molecule 3: Botrocetin



#### • Molecule 4: Platelet glycoprotein Ib



H1	P2	I3	C4	E5	V6	S7	K8	V9	H12	L13	E14	V15	M16	C17	D18	K19	R20	Q21	L22	L25	P26	L29	P30	T34	I35	L38	S39	L42	L43	Y44	S47	L48	A49	T50	L51	P52	T55	B56	L57	T58	Q59	L60	B61	L62	D63	B64	G65	B66	L67	T68			
K69	L70	Q71	V72	D73	G74	T75	V78	L79	G80	T81	L82	B83	L84	S85	H86	L89	L92	P93	L94	L95	T98	L99	P100	A101	L102	T103	V104	L105	D106	V107	R111	L115	P116	L117	G118	A119	P120	B121	G122	T123	G124	E125	L126	Q127	E128	L129	Y130	L131	K132	E135	L136	K137	
T138	L139	P140	L143	L144	T145	P146	L150	E151	K152	L153	S154	L155	A156	N157	N158	Q159	L160	T161	P164	A165	G166	L167	L168	E172	N173	L174	D175	T176	L177	L178	L179	Q180	E181	N182	S183	F192	G193	S194	H195	L196	L197	P198	F199	A200	F201	L202	E203	V207	L208	C209	N210	C211	E212
I213	F216	R217	L220	Q221	D222	N223	N226	V227	W230	K231	Q232	G233	V234	D235	V236	K237	A238	N239	V243	A244	S245	V246	Q247	C248	D249	N250	S251	D252	K253	F254	P255	V256	Y259	P260	Q261	K262	F265																

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.31Å 108.31Å 221.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.95	Depositor
% Data completeness (in resolution range)	94.5 (6.00-2.95)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.213 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5864	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

## 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	0.41	0/1696	0.68	0/2290
2	B	0.41	0/1094	0.66	0/1476
3	C	0.38	0/1098	0.56	1/1490 (0.1%)
4	D	0.36	0/2121	0.67	0/2895
All	All	0.39	0/6009	0.65	1/8151 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2067	GLY	N-CA-C	5.29	126.32	113.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1664	0	1708	152	0
2	B	1066	0	1009	82	0
3	C	1060	0	937	96	0
4	D	2074	0	2112	191	0
All	All	5864	0	5766	461	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 40.

All (461) 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)
4:D:75:THR:HA	4:D:98:THR:HG23	1.43	1.01
4:D:47:SER:HA	4:D:71:GLN:HB2	1.39	1.00
2:B:1074:GLU:HB2	3:C:2078:GLU:HG2	1.42	1.00
4:D:232:GLN:NE2	4:D:233:GLY:H	1.59	0.99
4:D:232:GLN:HE21	4:D:233:GLY:N	1.60	0.99
4:D:84:LEU:HB2	4:D:107:VAL:HG12	1.49	0.94
1:A:632:ARG:HH11	3:C:2114:THR:HG21	1.33	0.93
4:D:227:VAL:HG21	4:D:243:VAL:HG23	1.52	0.91
4:D:6:VAL:HG22	4:D:15:VAL:HG22	1.54	0.90
4:D:35:ILE:HG22	4:D:59:GLN:HB3	1.55	0.89
4:D:232:GLN:HE21	4:D:233:GLY:H	0.92	0.89
1:A:628:GLN:HE21	3:C:2092:LEU:HD21	1.37	0.89
2:B:1022:ASN:HD22	2:B:1022:ASN:H	1.19	0.88
4:D:227:VAL:HG11	4:D:243:VAL:HA	1.57	0.86
2:B:1009:TYR:OH	2:B:1047:LYS:HB3	1.75	0.86
4:D:154:SER:HA	4:D:178:LEU:HB2	1.57	0.86
3:C:2059:LEU:HD12	3:C:2059:LEU:H	1.40	0.86
2:B:1075:ASN:N	2:B:1075:ASN:HD22	1.71	0.85
4:D:12:HIS:HA	4:D:34:THR:HG21	1.60	0.83
1:A:552:ARG:HG3	1:A:611:ARG:NH2	1.96	0.80
4:D:209:CYS:HA	4:D:213:ILE:HG21	1.64	0.80
2:B:1022:ASN:ND2	2:B:1022:ASN:H	1.80	0.80
1:A:546:ILE:HD11	1:A:577:LEU:HD13	1.64	0.80
3:C:2061:GLY:HA2	3:C:2102:LYS:HE3	1.63	0.79
4:D:104:VAL:HG12	4:D:128:GLU:HB2	1.64	0.79
4:D:80:GLY:HA2	4:D:102:LEU:HA	1.65	0.79
4:D:58:THR:HA	4:D:79:LEU:HA	1.65	0.78
3:C:2012:HIS:CE1	3:C:2124:GLN:HB3	2.20	0.77
4:D:233:GLY:O	4:D:234:VAL:HG12	1.85	0.77
1:A:663:ARG:NH1	1:A:667:LYS:HD2	2.00	0.76
1:A:663:ARG:HH11	1:A:667:LYS:HD2	1.52	0.75
1:A:549:LYS:HB2	4:D:9:VAL:HG21	1.67	0.75
4:D:103:THR:HA	4:D:126:LEU:HA	1.69	0.75
1:A:660:LYS:O	1:A:664:LEU:HD13	1.86	0.74
2:B:1099:THR:HG21	3:C:2110:ILE:H	1.51	0.74
1:A:546:ILE:HG23	1:A:574:PRO:HG3	1.69	0.73
4:D:253:LYS:HG2	4:D:254:PHE:CE2	2.24	0.73
1:A:552:ARG:HG3	1:A:611:ARG:HH21	1.51	0.73
4:D:196:LEU:O	4:D:198:PRO:HD3	1.89	0.72
3:C:2012:HIS:ND1	3:C:2124:GLN:HB3	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:703:PRO:HB2	1:A:705:THR:N	2.04	0.71
1:A:663:ARG:HH22	3:C:2089:ASP:HA	1.55	0.71
2:B:1075:ASN:HD21	3:C:2076:ARG:H	1.38	0.70
1:A:666:GLU:HA	1:A:672:ASN:O	1.92	0.70
1:A:648:VAL:HB	1:A:672:ASN:HD21	1.57	0.69
1:A:664:LEU:HD21	3:C:2091:TYR:HB2	1.74	0.69
2:B:1044:ILE:HG13	3:C:2090:TYR:CE2	2.28	0.69
4:D:145:THR:HB	4:D:146:PRO:HD3	1.75	0.69
4:D:95:LEU:HD13	4:D:99:LEU:HD12	1.73	0.68
4:D:58:THR:HG22	4:D:78:VAL:O	1.93	0.68
4:D:39:SER:HB3	4:D:63:ASP:OD1	1.92	0.68
4:D:227:VAL:CG1	4:D:243:VAL:HA	2.23	0.68
1:A:616:ARG:HH21	1:A:645:LYS:HB2	1.58	0.68
4:D:8:LYS:HG2	4:D:13:LEU:CD1	2.24	0.68
4:D:44:TYR:HA	4:D:66:GLU:O	1.94	0.67
1:A:703:PRO:HG2	1:A:704:PRO:HA	1.77	0.67
4:D:60:LEU:HD23	4:D:82:LEU:CD1	2.25	0.67
4:D:111:ARG:HG2	4:D:135:GLU:OE2	1.94	0.66
3:C:2091:TYR:CE2	3:C:2092:LEU:HD12	2.29	0.66
3:C:2105:ASN:OD1	3:C:2107:LYS:HB2	1.95	0.66
4:D:247:GLN:HA	4:D:256:VAL:HG23	1.76	0.66
1:A:546:ILE:HD11	1:A:577:LEU:CD1	2.27	0.66
2:B:1075:ASN:H	2:B:1075:ASN:HD22	1.44	0.64
2:B:1075:ASN:N	2:B:1075:ASN:ND2	2.43	0.64
1:A:663:ARG:CZ	1:A:667:LYS:HZ3	2.10	0.64
3:C:2049:ASP:O	3:C:2052:ARG:HB3	1.97	0.64
1:A:629:ARG:HH11	1:A:629:ARG:HG3	1.63	0.64
3:C:2059:LEU:HD12	3:C:2059:LEU:N	2.11	0.64
4:D:81:THR:HA	4:D:104:VAL:HG23	1.80	0.64
1:A:663:ARG:HD2	1:A:664:LEU:HD12	1.78	0.63
1:A:554:ALA:HA	1:A:566:ILE:HG22	1.80	0.63
4:D:175:ASP:HA	4:D:198:PRO:HD2	1.80	0.63
4:D:217:ARG:O	4:D:221:GLN:HG3	1.99	0.63
4:D:223:ASN:HB3	4:D:226:ASN:HD22	1.63	0.63
4:D:49:ALA:O	4:D:52:MET:HG3	1.99	0.62
1:A:628:GLN:HE21	3:C:2092:LEU:CD2	2.10	0.62
1:A:580:ILE:HG23	4:D:235:ASP:OD2	1.99	0.62
1:A:499:ILE:HD11	1:A:574:PRO:HD3	1.82	0.62
1:A:703:PRO:HB2	1:A:704:PRO:C	2.20	0.62
3:C:2023:TRP:CE2	3:C:2069:SER:HB3	2.33	0.62
4:D:116:PRO:O	4:D:119:ALA:HB2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1047:LYS:O	2:B:1047:LYS:HD3	2.00	0.62
2:B:1044:ILE:HG13	3:C:2090:TYR:HE2	1.64	0.61
2:B:1096:VAL:O	2:B:1099:THR:HB	2.00	0.61
1:A:664:LEU:HD21	3:C:2091:TYR:CB	2.31	0.61
4:D:64:ARG:HA	4:D:86:HIS:O	2.00	0.61
1:A:648:VAL:HB	1:A:672:ASN:ND2	2.15	0.61
4:D:253:LYS:HE3	4:D:254:PHE:CE1	2.36	0.61
4:D:248:CYS:O	4:D:249:ASP:HB2	2.01	0.61
2:B:1084:TRP:HE3	3:C:2067:GLY:HA3	1.66	0.61
3:C:2059:LEU:CD1	3:C:2059:LEU:H	2.13	0.61
1:A:636:ARG:HG2	2:B:1114:LEU:CD1	2.31	0.61
1:A:629:ARG:NH1	1:A:629:ARG:HG3	2.16	0.61
1:A:701:ALA:C	1:A:703:PRO:HD2	2.21	0.60
2:B:1060:ILE:O	2:B:1061:GLN:C	2.39	0.60
1:A:628:GLN:NE2	3:C:2092:LEU:HD21	2.13	0.60
1:A:621:LEU:HD23	1:A:651:VAL:HB	1.84	0.60
2:B:1099:THR:HG23	3:C:2110:ILE:HB	1.84	0.60
2:B:1021:MET:HA	2:B:1123:LYS:NZ	2.17	0.60
4:D:84:LEU:HB2	4:D:107:VAL:CG1	2.27	0.60
4:D:120:LEU:HB3	4:D:123:LEU:HD12	1.84	0.60
1:A:529:GLU:HB3	1:A:680:VAL:HG11	1.84	0.60
1:A:499:ILE:HA	1:A:573:ARG:NH2	2.16	0.60
2:B:1061:GLN:O	2:B:1062:SER:OG	2.20	0.60
1:A:576:GLU:OE2	1:A:576:GLU:HA	2.01	0.59
3:C:2037:ALA:HB2	3:C:2123:PHE:HB3	1.84	0.59
4:D:209:CYS:HB3	4:D:259:TYR:CD1	2.37	0.59
1:A:513:LEU:HD12	1:A:514:ASP:N	2.17	0.59
4:D:259:TYR:CE2	4:D:261:GLY:HA2	2.37	0.59
1:A:511:ARG:NH1	1:A:696:ASP:HA	2.17	0.59
1:A:702:PRO:N	1:A:703:PRO:HD2	2.17	0.59
2:B:1009:TYR:HH	2:B:1047:LYS:HB3	1.64	0.59
1:A:549:LYS:CB	4:D:9:VAL:HG21	2.32	0.59
4:D:4:CYS:HB3	4:D:16:ASN:O	2.02	0.59
4:D:230:TRP:HH2	4:D:237:LYS:HD3	1.67	0.59
4:D:55:THR:O	4:D:56:ARG:HB2	2.03	0.58
4:D:25:LEU:HD11	4:D:29:LEU:CD1	2.33	0.58
1:A:499:ILE:HD11	1:A:574:PRO:CD	2.34	0.58
4:D:161:THR:HA	4:D:183:SER:O	2.04	0.58
2:B:1065:LEU:HA	2:B:1108:LYS:HB2	1.83	0.58
4:D:213:ILE:O	4:D:213:ILE:HG12	2.04	0.57
4:D:253:LYS:HE3	4:D:254:PHE:CD1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:155:LEU:HB2	4:D:179:LEU:HD23	1.84	0.57
1:A:677:LEU:HD12	1:A:677:LEU:N	2.20	0.57
1:A:573:ARG:HB2	1:A:573:ARG:HH11	1.69	0.57
1:A:608:LYS:HD2	4:D:128:GLU:OE2	2.03	0.57
2:B:1096:VAL:HG23	3:C:2108:TRP:O	2.05	0.57
4:D:193:GLY:HA3	4:D:195:HIS:CE1	2.39	0.57
3:C:2056:SER:O	3:C:2057:GLU:HB2	2.03	0.57
4:D:47:SER:OG	4:D:71:GLN:HG3	2.05	0.57
2:B:1099:THR:CG2	3:C:2110:ILE:HB	2.34	0.57
1:A:636:ARG:HG2	2:B:1114:LEU:HD13	1.87	0.57
4:D:52:MET:SD	4:D:75:THR:N	2.75	0.57
1:A:663:ARG:HH22	3:C:2089:ASP:CA	2.18	0.56
4:D:249:ASP:O	4:D:250:ASN:O	2.23	0.56
3:C:2065:TRP:HB2	3:C:2119:PHE:HB3	1.86	0.56
1:A:522:SER:HB3	1:A:592:ALA:HB2	1.88	0.55
1:A:499:ILE:C	1:A:499:ILE:HD13	2.26	0.55
4:D:144:LEU:HD11	4:D:153:LEU:HD22	1.89	0.55
4:D:14:GLU:HG3	4:D:35:ILE:CG1	2.35	0.55
4:D:34:THR:HA	4:D:56:ARG:O	2.05	0.55
4:D:6:VAL:HG21	4:D:30:PRO:HG2	1.88	0.55
2:B:1084:TRP:CG	3:C:2041:SER:HB2	2.42	0.55
2:B:1086:ASP:HA	3:C:2038:HIS:CD2	2.42	0.55
2:B:1041:SER:HA	3:C:2079:TRP:CZ3	2.42	0.55
1:A:664:LEU:O	1:A:668:GLN:HG2	2.07	0.54
2:B:1100:VAL:HG12	2:B:1102:LYS:HG3	1.88	0.54
2:B:1023:TRP:CZ3	2:B:1072:ARG:HD2	2.43	0.54
4:D:253:LYS:HG2	4:D:254:PHE:CD2	2.42	0.54
2:B:1075:ASN:ND2	2:B:1075:ASN:H	2.04	0.54
4:D:25:LEU:HD11	4:D:29:LEU:HD12	1.90	0.54
2:B:1093:GLU:HA	3:C:2108:TRP:CH2	2.43	0.54
4:D:207:TRP:HB2	4:D:248:CYS:HA	1.90	0.54
3:C:2006:TRP:CD2	3:C:2015:ARG:HB2	2.43	0.54
1:A:543:ARG:HG3	1:A:543:ARG:HH11	1.73	0.54
3:C:2097:GLU:C	3:C:2113:CYS:SG	2.87	0.54
4:D:209:CYS:SG	4:D:213:ILE:HD13	2.47	0.53
1:A:663:ARG:CD	1:A:664:LEU:HD12	2.37	0.53
4:D:67:LEU:HD23	4:D:89:LEU:HD21	1.91	0.53
4:D:34:THR:OG1	4:D:35:ILE:HD13	2.08	0.53
4:D:201:PHE:CZ	4:D:239:MET:HE2	2.43	0.53
4:D:135:GLU:HA	4:D:159:GLN:NE2	2.23	0.53
4:D:49:ALA:C	4:D:51:LEU:H	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:VAL:HG13	1:A:578:ARG:HG2	1.90	0.53
1:A:501:GLU:OE2	1:A:573:ARG:HD3	2.08	0.53
1:A:703:PRO:HG2	1:A:704:PRO:C	2.29	0.53
3:C:2097:GLU:HB3	3:C:2111:ILE:O	2.08	0.53
4:D:92:LEU:HD12	4:D:93:PRO:HD2	1.91	0.53
4:D:128:GLU:HG2	4:D:152:LYS:CG	2.39	0.53
1:A:647:ILE:HD12	1:A:647:ILE:H	1.74	0.53
4:D:202:LEU:HB2	4:D:246:VAL:HG22	1.90	0.53
1:A:628:GLN:HE22	3:C:2096:TYR:HE2	1.56	0.53
4:D:137:LYS:O	4:D:160:LEU:HA	2.09	0.53
4:D:164:PRO:O	4:D:167:LEU:N	2.42	0.53
1:A:581:ALA:O	1:A:584:VAL:HG23	2.09	0.52
4:D:220:LEU:HD11	4:D:246:VAL:HG11	1.90	0.52
1:A:636:ARG:NH2	2:B:1107:GLU:OE1	2.34	0.52
1:A:703:PRO:HG2	1:A:704:PRO:CA	2.38	0.52
1:A:682:GLU:OE1	1:A:685:GLN:NE2	2.43	0.52
1:A:622:MET:CE	1:A:658:ASN:HB3	2.39	0.52
2:B:1044:ILE:HG22	2:B:1045:TYR:CG	2.44	0.52
3:C:2015:ARG:HG2	3:C:2015:ARG:HH11	1.74	0.52
4:D:140:PRO:HG2	4:D:143:LEU:HB2	1.91	0.52
1:A:664:LEU:HD21	3:C:2091:TYR:CG	2.45	0.52
4:D:102:LEU:HD23	4:D:123:LEU:HD22	1.92	0.52
3:C:2042:PHE:HE2	3:C:2051:VAL:HG21	1.75	0.52
1:A:556:VAL:HA	1:A:563:HIS:O	2.09	0.52
4:D:125:GLU:O	4:D:127:GLN:HG3	2.10	0.51
4:D:202:LEU:HD13	4:D:216:PHE:CZ	2.45	0.51
2:B:1069:ILE:HG12	2:B:1104:PHE:O	2.09	0.51
1:A:505:HIS:HE1	1:A:542:GLU:OE1	1.94	0.51
4:D:49:ALA:HB2	4:D:73:ASP:O	2.10	0.51
1:A:628:GLN:NE2	3:C:2096:TYR:CE2	2.77	0.51
4:D:197:LEU:HD23	4:D:200:ALA:HB2	1.91	0.51
4:D:210:ASN:O	4:D:259:TYR:CE2	2.64	0.51
2:B:1075:ASN:ND2	3:C:2076:ARG:H	2.05	0.51
2:B:1030:CYS:SG	2:B:1039:LEU:HD23	2.50	0.51
2:B:1022:ASN:HD21	2:B:1025:ASP:CG	2.12	0.51
4:D:180:GLN:HG3	4:D:203:HIS:CE1	2.46	0.51
1:A:599:LYS:HE2	4:D:199:PHE:CE1	2.46	0.51
1:A:638:VAL:HG11	1:A:668:GLN:HG3	1.93	0.51
4:D:120:LEU:CB	4:D:123:LEU:HD12	2.41	0.51
2:B:1021:MET:HA	2:B:1123:LYS:HZ2	1.76	0.51
4:D:1:HIS:ND1	4:D:2:PRO:HD2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:LEU:O	1:A:536:PHE:HB3	2.11	0.50
4:D:47:SER:HB2	4:D:50:THR:HG23	1.92	0.50
1:A:628:GLN:NE2	3:C:2096:TYR:HE2	2.09	0.50
4:D:102:LEU:HD21	4:D:105:LEU:HD13	1.93	0.50
3:C:2116:PHE:HB2	4:D:221:GLN:HB3	1.92	0.50
3:C:2076:ARG:NH1	3:C:2076:ARG:HG3	2.27	0.50
1:A:557:GLU:OE2	1:A:559:HIS:ND1	2.44	0.50
1:A:665:ILE:CG2	1:A:672:ASN:HD22	2.24	0.50
2:B:1079:GLN:HB2	3:C:2071:VAL:HB	1.92	0.50
4:D:178:LEU:HD23	4:D:201:PHE:CD1	2.46	0.50
2:B:1073:VAL:HG13	3:C:2075:CYS:HB3	1.94	0.50
3:C:2086:ASP:C	3:C:2086:ASP:OD2	2.50	0.50
3:C:2009:TYR:HB3	3:C:2014:TYR:CE1	2.46	0.50
4:D:247:GLN:OE1	4:D:253:LYS:N	2.44	0.50
3:C:2046:GLU:H	3:C:2046:GLU:CD	2.15	0.50
4:D:132:LYS:HE3	4:D:157:ASN:OD1	2.12	0.50
4:D:233:GLY:O	4:D:235:ASP:N	2.39	0.50
2:B:1108:LYS:HA	2:B:1112:PHE:CZ	2.47	0.49
1:A:527:GLU:HA	1:A:586:TYR:CD1	2.47	0.49
2:B:1075:ASN:HD21	3:C:2076:ARG:N	2.05	0.49
1:A:593:SER:HB2	1:A:630:MET:HE1	1.93	0.49
4:D:35:ILE:HD13	4:D:35:ILE:H	1.76	0.49
3:C:2009:TYR:HB2	3:C:2050:PHE:CD2	2.48	0.49
4:D:197:LEU:O	4:D:226:ASN:HB3	2.12	0.49
1:A:609:ILE:HG22	1:A:609:ILE:O	2.11	0.49
1:A:501:GLU:OE1	1:A:573:ARG:HG2	2.12	0.49
2:B:1049:LYS:HD2	2:B:1113:VAL:HG13	1.93	0.49
1:A:622:MET:HE1	1:A:658:ASN:HB3	1.94	0.49
1:A:565:TYR:CD2	4:D:236:VAL:HG22	2.48	0.49
3:C:2076:ARG:HH11	3:C:2076:ARG:HG3	1.77	0.49
1:A:571:ARG:NH1	4:D:14:GLU:CD	2.66	0.49
4:D:6:VAL:HG22	4:D:15:VAL:CG2	2.36	0.49
1:A:616:ARG:HH11	1:A:616:ARG:HG3	1.76	0.49
2:B:1108:LYS:HA	2:B:1112:PHE:CE1	2.48	0.48
1:A:676:VAL:C	1:A:677:LEU:HD12	2.33	0.48
3:C:2065:TRP:HA	3:C:2065:TRP:CE3	2.47	0.48
2:B:1098:ARG:HG3	2:B:1098:ARG:O	2.13	0.48
1:A:632:ARG:HH11	3:C:2114:THR:CG2	2.15	0.48
4:D:208:LEU:HG	4:D:210:ASN:ND2	2.28	0.48
4:D:121:ARG:HA	4:D:146:PRO:HG2	1.96	0.48
4:D:95:LEU:HD12	4:D:105:LEU:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:TYR:CE2	4:D:236:VAL:HG22	2.48	0.48
1:A:579:ARG:HG2	1:A:579:ARG:HH11	1.77	0.48
4:D:172:GLU:C	4:D:173:ASN:OD1	2.52	0.48
1:A:530:PHE:O	1:A:534:LYS:HG3	2.13	0.48
3:C:2018:LYS:O	3:C:2018:LYS:HG3	2.12	0.48
2:B:1126:PHE:N	2:B:1126:PHE:CD1	2.79	0.48
1:A:604:GLN:HE21	4:D:239:MET:CE	2.26	0.48
2:B:1039:LEU:HB2	2:B:1070:GLY:HA2	1.95	0.48
3:C:2029:PHE:O	3:C:2033:GLN:HG2	2.14	0.48
2:B:1084:TRP:HD1	2:B:1088:SER:O	1.96	0.48
4:D:35:ILE:HD13	4:D:35:ILE:N	2.28	0.48
1:A:663:ARG:CZ	1:A:667:LYS:NZ	2.77	0.48
3:C:2016:PHE:HE1	3:C:2118:ASN:HB3	1.78	0.48
4:D:94:LEU:HD22	4:D:94:LEU:N	2.28	0.48
2:B:1060:ILE:HD11	2:B:1064:ASP:HB2	1.96	0.48
4:D:14:GLU:CB	4:D:35:ILE:HD11	2.44	0.48
1:A:616:ARG:NH2	1:A:645:LYS:HB2	2.26	0.48
1:A:512:LEU:HB2	1:A:699:PRO:HG2	1.96	0.47
1:A:535:ALA:O	1:A:539:ASP:HB2	2.14	0.47
2:B:1107:GLU:O	2:B:1112:PHE:HA	2.13	0.47
4:D:17:CYS:O	4:D:20:ARG:HB2	2.14	0.47
4:D:38:LEU:HB2	4:D:62:LEU:HD23	1.96	0.47
1:A:616:ARG:HG3	1:A:616:ARG:NH1	2.29	0.47
1:A:657:ALA:O	1:A:659:LEU:HD22	2.13	0.47
1:A:522:SER:C	1:A:524:ARG:H	2.17	0.47
3:C:2061:GLY:CA	3:C:2102:LYS:HE3	2.40	0.47
1:A:687:ARG:NH1	1:A:688:ASP:OD1	2.46	0.47
4:D:202:LEU:HD13	4:D:216:PHE:HZ	1.80	0.47
2:B:1110:LEU:HD12	2:B:1110:LEU:HA	1.67	0.47
1:A:523:SER:N	1:A:588:GLY:HA2	2.29	0.47
1:A:634:PHE:CZ	1:A:661:GLN:HB3	2.50	0.47
1:A:508:TYR:CE1	1:A:545:ARG:HA	2.50	0.47
2:B:1071:LEU:HD11	3:C:2077:PHE:HB3	1.95	0.47
3:C:2002:CYS:SG	3:C:2007:SER:O	2.73	0.47
1:A:522:SER:HA	1:A:589:SER:H	1.79	0.47
4:D:164:PRO:HB2	4:D:167:LEU:HB2	1.97	0.47
3:C:2014:TYR:HA	3:C:2121:CYS:O	2.15	0.47
1:A:519:LEU:HD12	1:A:519:LEU:N	2.30	0.47
4:D:254:PHE:CD2	4:D:254:PHE:N	2.82	0.47
4:D:233:GLY:C	4:D:235:ASP:H	2.17	0.46
4:D:121:ARG:HA	4:D:146:PRO:CG	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2040:VAL:CG1	3:C:2066:ILE:HG22	2.45	0.46
2:B:1122:GLN:HG2	2:B:1124:ASN:ND2	2.30	0.46
2:B:1023:TRP:CH2	2:B:1072:ARG:HD2	2.50	0.46
1:A:603:PHE:O	1:A:607:SER:HB3	2.16	0.46
1:A:499:ILE:HG23	1:A:500:SER:N	2.31	0.46
4:D:139:LEU:HD11	4:D:155:LEU:CD1	2.45	0.46
4:D:118:GLY:HA2	4:D:121:ARG:HB2	1.98	0.46
1:A:647:ILE:HD12	1:A:647:ILE:N	2.30	0.46
1:A:632:ARG:NH1	3:C:2114:THR:HG21	2.17	0.46
1:A:532:VAL:HG11	1:A:680:VAL:HG23	1.97	0.46
4:D:1:HIS:HB3	4:D:4:CYS:O	2.16	0.46
4:D:14:GLU:HG3	4:D:35:ILE:HG12	1.97	0.46
2:B:1022:ASN:N	2:B:1022:ASN:HD22	1.99	0.46
4:D:42:LEU:O	4:D:43:LEU:C	2.53	0.46
4:D:197:LEU:CD2	4:D:200:ALA:HB2	2.45	0.46
1:A:557:GLU:OE2	1:A:559:HIS:CE1	2.69	0.46
4:D:193:GLY:HA3	4:D:195:HIS:ND1	2.31	0.46
3:C:2023:TRP:CZ2	3:C:2069:SER:HB3	2.51	0.46
1:A:532:VAL:HB	1:A:680:VAL:HB	1.97	0.46
4:D:139:LEU:HD11	4:D:155:LEU:HD13	1.97	0.46
1:A:522:SER:C	1:A:588:GLY:HA2	2.36	0.46
3:C:2072:TRP:CE3	3:C:2072:TRP:HA	2.51	0.46
4:D:52:MET:C	4:D:54:TYR:H	2.19	0.46
4:D:18:ASP:HB3	4:D:39:SER:OG	2.16	0.46
1:A:642:LYS:HE3	1:A:669:ALA:HB2	1.97	0.46
4:D:49:ALA:O	4:D:51:LEU:N	2.49	0.45
1:A:642:LYS:HD2	1:A:669:ALA:HB2	1.98	0.45
4:D:120:LEU:HA	4:D:123:LEU:HD12	1.97	0.45
1:A:509:CYS:HB3	1:A:544:LEU:HD23	1.98	0.45
4:D:56:ARG:HA	4:D:78:VAL:HG21	1.98	0.45
1:A:501:GLU:OE2	1:A:575:SER:HB3	2.15	0.45
2:B:1066:TYR:HA	2:B:1106:LEU:O	2.16	0.45
4:D:107:VAL:HG23	4:D:131:LEU:HD23	1.99	0.45
1:A:702:PRO:N	1:A:703:PRO:CD	2.78	0.45
1:A:649:ILE:HD11	1:A:693:TYR:HE2	1.80	0.45
4:D:144:LEU:HD22	4:D:150:LEU:HD22	1.99	0.45
4:D:201:PHE:HZ	4:D:239:MET:CE	2.30	0.45
1:A:702:PRO:HG2	1:A:703:PRO:HD3	1.98	0.45
1:A:665:ILE:HG22	1:A:672:ASN:HD22	1.82	0.45
4:D:202:LEU:HB2	4:D:246:VAL:CG2	2.46	0.45
1:A:579:ARG:HG2	1:A:579:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2039:LEU:CD2	3:C:2119:PHE:HB2	2.47	0.45
4:D:42:LEU:O	4:D:44:TYR:N	2.49	0.44
3:C:2086:ASP:O	3:C:2088:ASP:N	2.50	0.44
4:D:231:LYS:HD3	4:D:231:LYS:O	2.17	0.44
4:D:245:SER:O	4:D:247:GLN:HG2	2.17	0.44
1:A:537:VAL:O	1:A:541:MET:HG3	2.17	0.44
2:B:1068:TRP:HB2	2:B:1126:PHE:HB3	1.98	0.44
2:B:1074:GLU:HB3	3:C:2076:ARG:O	2.17	0.44
1:A:663:ARG:HH12	2:B:1045:TYR:HE2	1.66	0.44
2:B:1084:TRP:CD2	3:C:2041:SER:HB2	2.52	0.44
2:B:1044:ILE:HG12	2:B:1115:TRP:CH2	2.53	0.44
2:B:1086:ASP:C	2:B:1086:ASP:OD1	2.55	0.44
4:D:101:ALA:O	4:D:103:THR:HG23	2.16	0.44
4:D:60:LEU:HD23	4:D:82:LEU:HD11	1.96	0.44
4:D:127:GLN:HA	4:D:150:LEU:HA	2.00	0.44
4:D:164:PRO:O	4:D:165:ALA:C	2.55	0.44
2:B:1065:LEU:O	2:B:1108:LYS:N	2.51	0.44
4:D:25:LEU:HD11	4:D:29:LEU:HD11	1.99	0.44
4:D:18:ASP:HA	4:D:39:SER:O	2.18	0.44
1:A:559:HIS:HA	1:A:592:ALA:HA	2.00	0.44
4:D:94:LEU:N	4:D:94:LEU:CD2	2.80	0.44
4:D:72:VAL:O	4:D:72:VAL:HG23	2.18	0.44
4:D:52:MET:N	4:D:53:PRO:CD	2.81	0.44
4:D:22:LEU:HD13	4:D:26:PRO:CG	2.47	0.44
1:A:498:ASP:OD2	1:A:499:ILE:HG22	2.19	0.43
1:A:703:PRO:CB	1:A:704:PRO:C	2.86	0.43
4:D:167:LEU:HD12	4:D:167:LEU:O	2.18	0.43
4:D:105:LEU:HD23	4:D:129:LEU:CD1	2.48	0.43
4:D:177:LEU:HB3	4:D:197:LEU:HD21	1.99	0.43
2:B:1100:VAL:HG13	3:C:2072:TRP:HH2	1.82	0.43
3:C:2015:ARG:HG2	3:C:2015:ARG:NH1	2.33	0.43
1:A:574:PRO:O	1:A:578:ARG:HB2	2.19	0.43
2:B:1041:SER:HA	3:C:2079:TRP:CE3	2.53	0.43
1:A:543:ARG:HG3	1:A:543:ARG:NH1	2.33	0.43
1:A:546:ILE:CD1	1:A:577:LEU:CD1	2.95	0.43
4:D:70:LEU:HD23	4:D:93:PRO:CB	2.49	0.43
3:C:2009:TYR:HB2	3:C:2050:PHE:CE2	2.54	0.43
4:D:58:THR:HA	4:D:78:VAL:O	2.18	0.43
4:D:120:LEU:CA	4:D:123:LEU:HD12	2.48	0.43
4:D:192:PHE:O	4:D:195:HIS:ND1	2.51	0.43
4:D:132:LYS:HA	4:D:156:ALA:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:ARG:HG2	1:A:688:ASP:N	2.34	0.43
4:D:84:LEU:CB	4:D:107:VAL:HG12	2.34	0.43
4:D:201:PHE:CZ	4:D:239:MET:CE	3.02	0.43
4:D:213:ILE:CD1	4:D:256:VAL:HG13	2.49	0.43
3:C:2020:TRP:CE3	4:D:221:GLN:NE2	2.86	0.43
1:A:541:MET:HA	1:A:544:LEU:HD12	2.01	0.43
4:D:210:ASN:OD1	4:D:211:CYS:N	2.52	0.43
3:C:2098:CYS:N	3:C:2113:CYS:SG	2.92	0.43
3:C:2066:ILE:O	3:C:2068:LEU:N	2.52	0.43
3:C:2050:PHE:CZ	3:C:2054:LEU:HD21	2.54	0.43
4:D:5:GLU:O	4:D:15:VAL:HA	2.18	0.42
4:D:56:ARG:CA	4:D:78:VAL:HG21	2.49	0.42
1:A:524:ARG:HA	1:A:524:ARG:HD2	1.65	0.42
4:D:6:VAL:CG2	4:D:15:VAL:HG22	2.35	0.42
1:A:546:ILE:HD12	1:A:553:VAL:CG1	2.49	0.42
4:D:81:THR:HA	4:D:104:VAL:CG2	2.48	0.42
4:D:95:LEU:HD12	4:D:105:LEU:HD11	2.01	0.42
2:B:1110:LEU:HD23	2:B:1114:LEU:HD11	2.00	0.42
4:D:144:LEU:CD1	4:D:153:LEU:HD22	2.49	0.42
4:D:95:LEU:HB3	4:D:99:LEU:HB2	2.01	0.42
1:A:703:PRO:HG2	1:A:704:PRO:O	2.20	0.42
2:B:1059:ASN:C	2:B:1061:GLN:N	2.72	0.42
3:C:2009:TYR:HB3	3:C:2014:TYR:HE1	1.84	0.42
4:D:80:GLY:HA2	4:D:102:LEU:CA	2.41	0.42
2:B:1096:VAL:O	2:B:1097:GLU:C	2.58	0.42
2:B:1028:ARG:O	2:B:1031:SER:OG	2.26	0.42
4:D:47:SER:CA	4:D:71:GLN:HB2	2.29	0.42
1:A:604:GLN:HE21	4:D:239:MET:HE3	1.83	0.42
4:D:128:GLU:HG2	4:D:152:LYS:HG2	2.01	0.42
1:A:658:ASN:OD1	1:A:661:GLN:HG3	2.20	0.42
4:D:14:GLU:CA	4:D:35:ILE:HD11	2.49	0.42
1:A:663:ARG:C	1:A:663:ARG:HD2	2.40	0.42
4:D:135:GLU:O	4:D:137:LYS:HD2	2.19	0.42
2:B:1043:LYS:HB3	2:B:1046:SER:OG	2.19	0.42
4:D:34:THR:HG1	4:D:35:ILE:HD13	1.83	0.42
1:A:522:SER:C	1:A:524:ARG:N	2.73	0.42
1:A:565:TYR:CE2	4:D:236:VAL:CG2	3.03	0.42
1:A:663:ARG:NH2	3:C:2089:ASP:HA	2.30	0.42
3:C:2016:PHE:CD1	3:C:2017:PHE:N	2.88	0.42
4:D:128:GLU:OE1	4:D:130:TYR:OH	2.27	0.42
3:C:2037:ALA:CB	3:C:2123:PHE:HB3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:167:LEU:HG	4:D:168:LEU:HD23	2.00	0.42
2:B:1055:LEU:HA	2:B:1055:LEU:HD12	1.86	0.42
1:A:619:LEU:HD12	1:A:619:LEU:HA	1.85	0.42
1:A:500:SER:O	1:A:501:GLU:HB2	2.19	0.42
3:C:2004:PRO:C	3:C:2006:TRP:H	2.24	0.42
1:A:686:GLN:O	1:A:690:ILE:HD13	2.20	0.42
3:C:2124:GLN:HB2	3:C:2124:GLN:HE21	1.54	0.41
4:D:247:GLN:HB3	4:D:255:PRO:HA	2.03	0.41
1:A:559:HIS:HB3	1:A:589:SER:OG	2.20	0.41
3:C:2020:TRP:N	3:C:2020:TRP:CD1	2.88	0.41
2:B:1075:ASN:HD21	3:C:2076:ARG:CB	2.33	0.41
4:D:14:GLU:HB2	4:D:35:ILE:HD11	2.00	0.41
1:A:604:GLN:NE2	4:D:239:MET:HE3	2.36	0.41
1:A:499:ILE:HD11	1:A:573:ARG:HA	2.02	0.41
1:A:644:LYS:O	1:A:645:LYS:HB2	2.21	0.41
4:D:8:LYS:HG2	4:D:13:LEU:HD12	2.00	0.41
4:D:39:SER:CB	4:D:63:ASP:OD1	2.65	0.41
4:D:180:GLN:O	4:D:181:GLU:HB2	2.21	0.41
1:A:642:LYS:CE	1:A:669:ALA:HB2	2.50	0.41
1:A:631:SER:HB2	3:C:2092:LEU:CD1	2.50	0.41
4:D:80:GLY:CA	4:D:102:LEU:HA	2.42	0.41
4:D:49:ALA:C	4:D:51:LEU:N	2.73	0.41
2:B:1021:MET:HA	2:B:1123:LYS:HZ3	1.85	0.41
4:D:6:VAL:HG13	4:D:15:VAL:HG22	2.02	0.41
1:A:701:ALA:HB1	1:A:703:PRO:HD2	2.02	0.41
2:B:1056:VAL:O	2:B:1058:LYS:N	2.53	0.41
2:B:1056:VAL:O	2:B:1059:ASN:N	2.53	0.41
1:A:663:ARG:C	1:A:663:ARG:CD	2.89	0.41
3:C:2091:TYR:O	3:C:2092:LEU:C	2.59	0.41
1:A:703:PRO:CG	1:A:704:PRO:C	2.88	0.41
1:A:606:PHE:CD1	1:A:616:ARG:HD2	2.56	0.41
3:C:2040:VAL:HG21	3:C:2042:PHE:CE2	2.56	0.41
2:B:1122:GLN:HB2	2:B:1122:GLN:HE21	1.62	0.41
1:A:499:ILE:HG23	1:A:500:SER:H	1.86	0.41
4:D:63:ASP:HA	4:D:85:SER:O	2.21	0.41
2:B:1070:GLY:O	3:C:2080:THR:HG23	2.21	0.41
2:B:1077:GLU:CD	2:B:1077:GLU:N	2.74	0.41
2:B:1084:TRP:C	2:B:1086:ASP:H	2.23	0.40
4:D:182:ASN:HB3	4:D:183:SER:H	1.80	0.40
4:D:92:LEU:HD22	4:D:115:LEU:HD22	2.03	0.40
3:C:2097:GLU:HB3	3:C:2111:ILE:C	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:GLN:HG3	1:A:658:ASN:ND2	2.36	0.40
2:B:1103:CYS:O	2:B:1117:ASN:HA	2.22	0.40
4:D:52:MET:C	4:D:54:TYR:N	2.73	0.40
2:B:1093:GLU:HA	3:C:2108:TRP:CZ3	2.57	0.40
2:B:1099:THR:CG2	3:C:2110:ILE:H	2.27	0.40
1:A:636:ARG:NH1	1:A:636:ARG:HG3	2.36	0.40
1:A:531:GLU:O	1:A:532:VAL:C	2.60	0.40
1:A:690:ILE:N	1:A:690:ILE:HD12	2.36	0.40
3:C:2018:LYS:HD2	3:C:2118:ASN:OD1	2.20	0.40
4:D:262:LYS:HB2	4:D:262:LYS:NZ	2.36	0.40
3:C:2044:SER:O	3:C:2047:GLU:HB3	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	206/208 (99%)	183 (89%)	19 (9%)	4 (2%)	10	40
2	B	131/133 (98%)	107 (82%)	18 (14%)	6 (5%)	3	15
3	C	123/125 (98%)	94 (76%)	20 (16%)	9 (7%)	1	5
4	D	263/265 (99%)	216 (82%)	36 (14%)	11 (4%)	3	17
All	All	723/731 (99%)	600 (83%)	93 (13%)	30 (4%)	3	17

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1061	GLN
3	C	2055	THR
3	C	2057	GLU
3	C	2067	GLY

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Mol	Chain	Res	Type
4	D	43	LEU
4	D	56	ARG
4	D	195	HIS
4	D	250	ASN
1	A	703	PRO
2	B	1044	ILE
2	B	1057	THR
3	C	2056	SER
3	C	2087	TYR
4	D	50	THR
4	D	165	ALA
1	A	500	SER
2	B	1059	ASN
4	D	100	PRO
4	D	164	PRO
4	D	234	VAL
1	A	501	GLU
2	B	1097	GLU
4	D	157	ASN
4	D	249	ASP
1	A	670	PRO
3	C	2092	LEU
2	B	1099	THR
3	C	2042	PHE
3	C	2104	THR
3	C	2004	PRO

### 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	185/186 (100%)	174 (94%)	11 (6%)	24	61
2	B	118/119 (99%)	108 (92%)	10 (8%)	13	42
3	C	114/114 (100%)	111 (97%)	3 (3%)	54	84
4	D	238/238 (100%)	224 (94%)	14 (6%)	24	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	655/657 (100%)	617 (94%)	38 (6%)	25	62

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	499	ILE
1	A	524	ARG
1	A	559	HIS
1	A	562	SER
1	A	573	ARG
1	A	590	GLN
1	A	596	GLU
1	A	611	ARG
1	A	663	ARG
1	A	682	GLU
1	A	691	VAL
2	B	1010	GLU
2	B	1022	ASN
2	B	1058	LYS
2	B	1074	GLU
2	B	1075	ASN
2	B	1076	LYS
2	B	1083	GLU
2	B	1094	ASN
2	B	1099	THR
2	B	1110	LEU
3	C	2081	ASP
3	C	2093	ILE
3	C	2124	GLN
4	D	5	GLU
4	D	20	ARG
4	D	21	GLN
4	D	35	ILE
4	D	68	THR
4	D	75	THR
4	D	79	LEU
4	D	94	LEU
4	D	121	ARG
4	D	137	LYS
4	D	143	LEU
4	D	232	GLN
4	D	248	CYS

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Mol	Chain	Res	Type
4	D	252	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	505	HIS
1	A	628	GLN
1	A	639	GLN
1	A	672	ASN
1	A	685	GLN
2	B	1022	ASN
2	B	1061	GLN
2	B	1075	ASN
2	B	1094	ASN
2	B	1122	GLN
3	C	2124	GLN
4	D	59	GLN
4	D	86	HIS
4	D	159	GLN
4	D	226	ASN
4	D	232	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.