



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2024 – 10:05 AM EDT

PDB ID : 8T9B
Title : Structure of the CK variant of Fab F1 (FabC-F1) in complex with the C-terminal FN3 domain of EphA2
Authors : Singer, A.U.; Bruce, H.A.; Enderle, L.; Blazer, L.; Adams, J.J.; Sicheri, F.; Sidhu, S.S.
Deposited on : 2023-06-23
Resolution : 4.20 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

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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

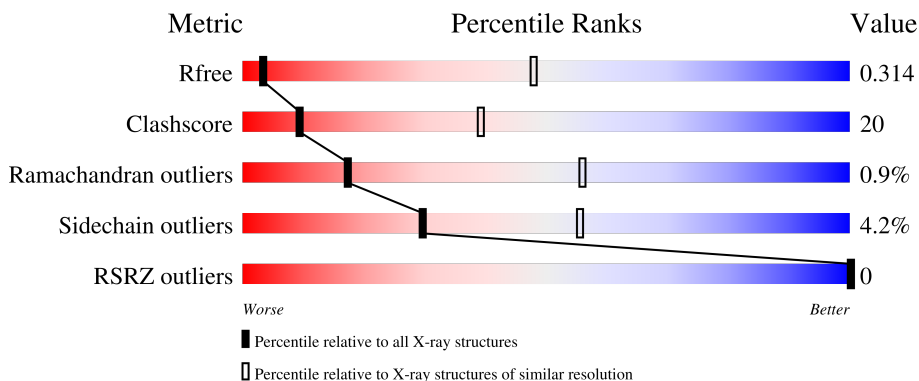
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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}	130704	1005 (4.62-3.78)
Clashscore	141614	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)
RSRZ outliers	127900	1063 (4.70-3.70)

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	237	61% (green), 36% (yellow), .. (grey)
1	C	237	57% (green), 38% (yellow), .. (grey)
1	D	237	62% (green), 32% (yellow), .. (grey)
1	F	237	62% (green), 35% (yellow), . (grey)
2	B	214	62% (green), 35% (yellow), .. (grey)

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Mol	Chain	Length	Quality of chain
2	E	214	 65% 29% . .
2	G	214	 64% 32% . .
2	H	214	 63% 35% .
3	I	98	 59% 30% . 9%
3	J	98	 48% 37% . 11%
3	K	98	 48% 40% . 8%
3	L	98	 48% 39% . 11%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 15657 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 CK variant of Fab F1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	230	Total 1707	C 1086	N 283	O 332	S 6	0	0	0
1	A	232	Total 1719	C 1091	N 284	O 337	S 7	0	0	0
1	D	230	Total 1691	C 1072	N 279	O 334	S 6	0	0	0
1	F	230	Total 1698	C 1079	N 282	O 331	S 6	0	0	0

- Molecule 2 is a protein called CK variant of Fab F1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	G	210	Total 1546	C 965	N 255	O 321	S 5	0	0	0
2	B	210	Total 1565	C 976	N 260	O 324	S 5	0	0	0
2	E	211	Total 1533	C 957	N 251	O 320	S 5	0	0	0
2	H	210	Total 1533	C 957	N 254	O 317	S 5	0	0	0

- Molecule 3 is a protein called Ephrin type-A receptor 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	I	89	Total 654	C 409	N 110	O 135	0	0	0
3	J	87	Total 657	C 413	N 110	O 134	0	0	0
3	K	90	Total 682	C 426	N 119	O 137	0	0	0
3	L	87	Total 672	C 422	N 116	O 134	0	0	0

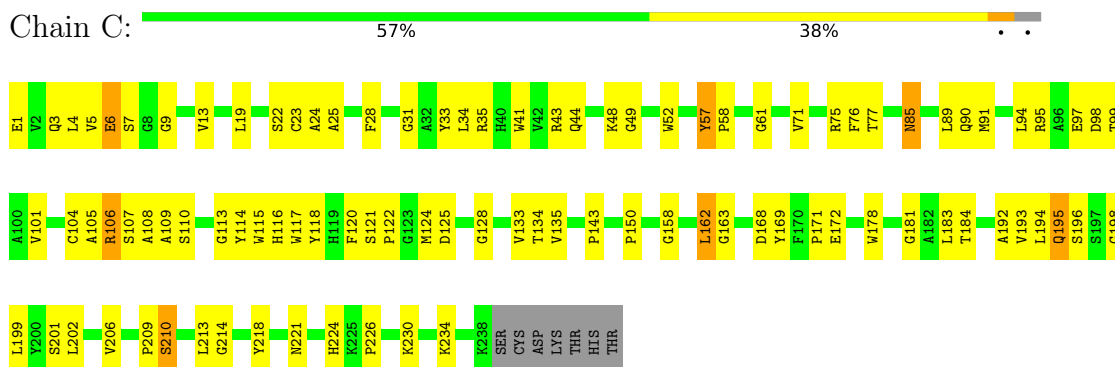
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	530	LEU	-	expression tag	UNP P29317
I	531	THR	-	expression tag	UNP P29317
I	532	PRO	-	expression tag	UNP P29317
I	533	ARG	-	expression tag	UNP P29317
J	530	LEU	-	expression tag	UNP P29317
J	531	THR	-	expression tag	UNP P29317
J	532	PRO	-	expression tag	UNP P29317
J	533	ARG	-	expression tag	UNP P29317
K	530	LEU	-	expression tag	UNP P29317
K	531	THR	-	expression tag	UNP P29317
K	532	PRO	-	expression tag	UNP P29317
K	533	ARG	-	expression tag	UNP P29317
L	530	LEU	-	expression tag	UNP P29317
L	531	THR	-	expression tag	UNP P29317
L	532	PRO	-	expression tag	UNP P29317
L	533	ARG	-	expression tag	UNP P29317

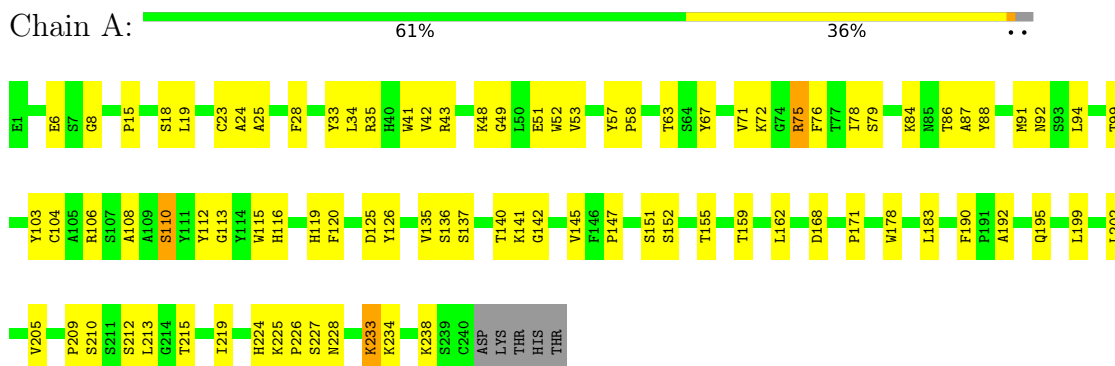
3 Residue-property plots i

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.

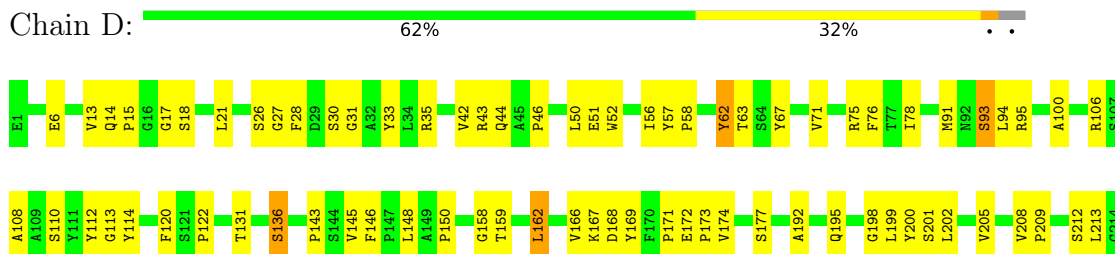
- Molecule 1: CK variant of Fab F1 heavy chain

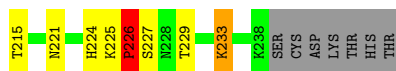


- Molecule 1: CK variant of Fab F1 heavy chain



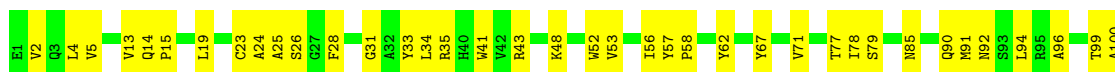
- Molecule 1: CK variant of Fab F1 heavy chain





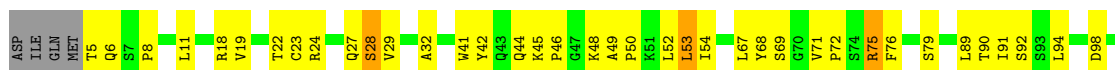
- Molecule 1: CK variant of Fab F1 heavy chain

Chain F: 62% 35%



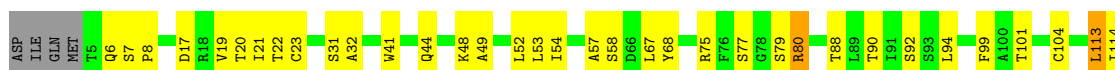
- Molecule 2: CK variant of Fab F1 light chain

Chain G: 64% 32%



- Molecule 2: CK variant of Fab F1 light chain

Chain B: 62% 35%

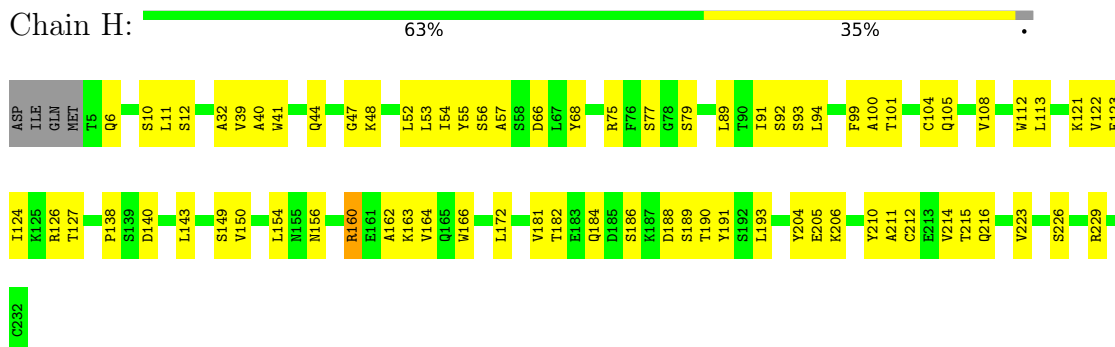


- Molecule 2: CK variant of Fab F1 light chain

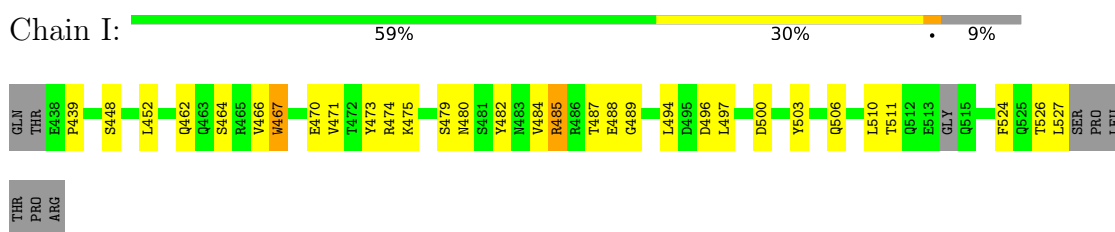
Chain E: 65% 29%



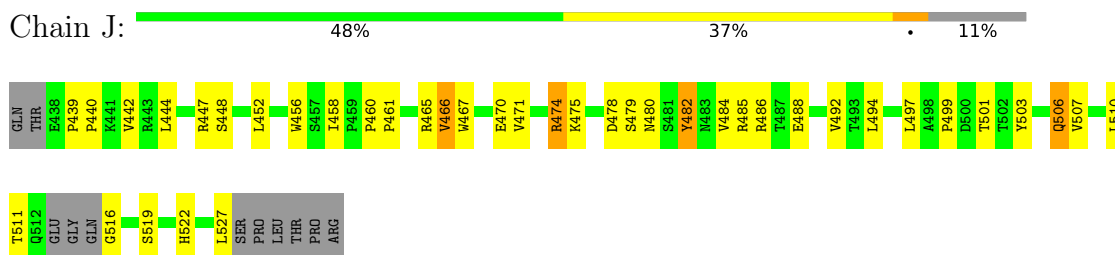
- Molecule 2: CK variant of Fab F1 light chain



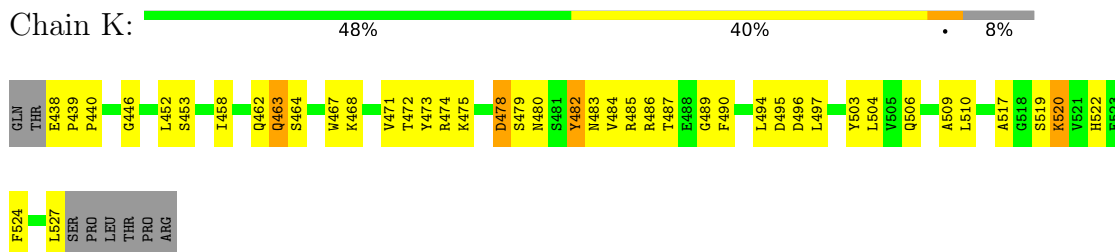
- Molecule 3: Ephrin type-A receptor 2



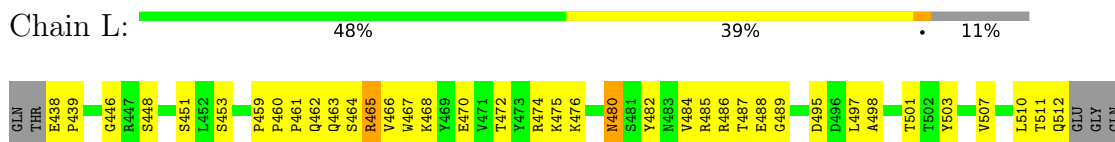
- Molecule 3: Ephrin type-A receptor 2



- Molecule 3: Ephrin type-A receptor 2



- Molecule 3: Ephrin type-A receptor 2



0516	SEF
L527	PRO
	LEU
	THR
	PRO
	ARG

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.66Å 130.65Å 223.00Å 90.00° 89.76° 90.00°	Depositor
Resolution (Å)	66.12 – 4.20 66.12 – 4.20	Depositor EDS
% Data completeness (in resolution range)	96.2 (66.12-4.20) 95.1 (66.12-4.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 4.14Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.296 , 0.315 0.296 , 0.314	Depositor DCC
R_{free} test set	1713 reflections (5.51%)	wwPDB-VP
Wilson B-factor (Å ²)	101.4	Xtrriage
Anisotropy	1.379	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 24.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.347 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	15657	wwPDB-VP
Average B, all atoms (Å ²)	156.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.53 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5258e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.30	0/1770	0.58	0/2424
1	C	0.30	0/1758	0.60	0/2407
1	D	0.32	0/1742	0.64	0/2391
1	F	0.30	0/1749	0.59	0/2397
2	B	0.30	0/1597	0.59	0/2177
2	E	0.33	0/1565	0.61	0/2143
2	G	0.30	0/1578	0.59	0/2154
2	H	0.30	0/1565	0.59	0/2142
3	I	0.31	0/667	0.61	0/915
3	J	0.37	0/672	0.68	0/922
3	K	0.33	0/698	0.64	0/956
3	L	0.35	0/687	0.68	0/939
All	All	0.31	0/16048	0.61	0/21967

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	1
1	D	0	3
3	I	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	75	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	136	SER	Peptide
1	D	35	ARG	Sidechain
1	D	75	ARG	Sidechain
3	I	485	ARG	Sidechain

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	1719	0	1609	68	0
1	C	1707	0	1606	72	0
1	D	1691	0	1558	59	0
1	F	1698	0	1584	67	0
2	B	1565	0	1474	62	0
2	E	1533	0	1404	61	0
2	G	1546	0	1446	54	0
2	H	1533	0	1412	55	0
3	I	654	0	594	20	0
3	J	657	0	604	45	0
3	K	682	0	633	37	0
3	L	672	0	636	46	0
All	All	15657	0	14560	595	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 20.

All (595) 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:E:205:GLU:HA	2:E:229:ARG:HH12	1.16	1.04
2:B:6:GLN:HG3	2:B:119:GLY:H	1.27	1.00
2:G:69:SER:HB3	2:G:72:PRO:HG3	1.43	0.97
2:B:79:SER:HB3	2:B:88:THR:HG23	1.46	0.96
1:D:28:PHE:HE1	1:D:33:TYR:HB2	1.30	0.96
3:L:468:LYS:H	3:L:510:LEU:HD12	1.28	0.95
3:L:482:TYR:HB3	3:L:484:VAL:HG23	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:18:ARG:HG3	2:G:92:SER:HA	1.53	0.91
3:J:444:LEU:HD11	3:J:452:LEU:HD11	1.53	0.91
1:D:28:PHE:CE1	1:D:33:TYR:HB2	2.10	0.86
1:D:224:HIS:HB3	1:D:229:THR:OG1	1.76	0.86
1:D:145:VAL:HG22	1:D:166:VAL:HG12	1.56	0.85
1:F:13:VAL:HG21	1:F:19:LEU:HB2	1.62	0.82
1:F:110:SER:HB2	3:J:484:VAL:HG21	1.62	0.81
3:L:475:LYS:HG3	3:L:476:LYS:H	1.46	0.81
1:F:31:GLY:HA2	1:F:58:PRO:HB2	1.62	0.80
2:G:126:ARG:NH1	2:G:127:THR:O	2.15	0.80
3:L:468:LYS:HG3	3:L:488:GLU:HG2	1.62	0.80
1:A:24:ALA:HA	1:A:86:THR:HG22	1.66	0.78
1:D:56:ILE:HB	1:D:78:ILE:HD12	1.64	0.78
1:C:31:GLY:HA2	1:C:58:PRO:HB2	1.67	0.77
2:G:165:GLN:HB2	2:G:213:GLU:HB3	1.65	0.77
3:L:468:LYS:HB2	3:L:510:LEU:HD11	1.65	0.77
2:E:205:GLU:HA	2:E:229:ARG:NH1	1.98	0.77
2:H:205:GLU:HA	2:H:229:ARG:HH12	1.49	0.77
2:G:6:GLN:HA	2:G:23:CYS:HA	1.66	0.76
3:L:487:THR:HG22	3:L:489:GLY:H	1.51	0.76
3:J:466:VAL:HG22	3:J:488:GLU:HB2	1.69	0.75
2:H:55:TYR:HA	2:H:66:ASP:HA	1.67	0.75
1:D:91:MET:HB3	1:D:94:LEU:HD11	1.66	0.75
2:E:167:LYS:HA	2:E:172:LEU:HA	1.69	0.74
3:I:487:THR:HG22	3:I:489:GLY:H	1.52	0.74
2:G:76:PHE:HA	2:G:91:ILE:HG22	1.70	0.74
2:G:91:ILE:HD11	2:G:94:LEU:HD13	1.68	0.73
1:D:198:GLY:O	1:D:199:LEU:HD22	1.88	0.73
3:L:470:GLU:HA	3:L:486:ARG:HD2	1.70	0.73
2:B:94:LEU:HD22	2:B:99:PHE:CE2	2.24	0.73
3:K:487:THR:HG22	3:K:489:GLY:H	1.54	0.72
3:L:474:ARG:HD2	3:L:475:LYS:N	2.04	0.72
3:I:452:LEU:HD21	3:I:524:PHE:HB2	1.71	0.72
3:J:448:SER:HA	3:J:527:LEU:HD12	1.70	0.72
2:B:48:LYS:HG2	2:B:49:ALA:H	1.53	0.72
1:D:168:ASP:HA	1:D:199:LEU:HB3	1.69	0.71
1:A:23:CYS:SG	1:A:35:ARG:NH2	2.64	0.71
1:C:143:PRO:HB3	1:C:169:TYR:HB3	1.72	0.71
2:B:213:GLU:HA	2:B:224:THR:HA	1.73	0.71
1:A:168:ASP:HA	1:A:199:LEU:HB3	1.73	0.70
3:K:472:THR:HA	3:K:484:VAL:HG12	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:123:GLU:HB3	2:G:184:GLN:HE22	1.55	0.69
1:A:99:THR:HG22	1:A:135:VAL:H	1.55	0.69
3:J:456:TRP:HH2	3:J:492:VAL:HG23	1.56	0.69
3:K:463:GLN:O	3:K:463:GLN:NE2	2.25	0.69
1:C:25:ALA:HB1	1:C:28:PHE:CE1	2.27	0.69
1:A:219:ILE:HG12	1:A:234:LYS:HB2	1.73	0.68
2:E:54:ILE:HG23	2:E:56:SER:H	1.58	0.68
1:A:119:HIS:HD2	1:A:120:PHE:CD1	2.11	0.68
1:D:44:GLN:OE1	1:D:50:LEU:HD22	1.94	0.67
1:F:34:LEU:HB2	1:F:107:SER:HB2	1.75	0.67
1:A:119:HIS:HD2	1:A:120:PHE:HD1	1.43	0.67
2:H:154:LEU:HB2	2:H:193:LEU:HB3	1.76	0.67
2:E:57:ALA:O	2:E:66:ASP:N	2.28	0.67
3:J:442:VAL:HG21	3:J:522:HIS:CE1	2.31	0.66
1:D:158:GLY:HA2	1:D:209:PRO:HA	1.76	0.66
3:J:471:VAL:HG12	3:J:507:VAL:HG22	1.78	0.66
2:H:101:THR:HA	2:H:121:LYS:HA	1.78	0.66
3:L:511:THR:HG23	3:L:516:GLY:HA2	1.78	0.66
2:G:54:ILE:HG22	2:G:67:LEU:O	1.96	0.65
2:B:213:GLU:HB2	2:B:224:THR:HG23	1.79	0.65
2:E:53:LEU:HD13	2:E:66:ASP:HB3	1.79	0.65
2:E:58:SER:OG	2:E:78:GLY:N	2.29	0.65
2:G:75:ARG:NH2	2:G:98:ASP:OD1	2.29	0.65
1:A:43:ARG:NH1	1:A:51:GLU:OE2	2.30	0.65
2:B:207:HIS:O	2:B:229:ARG:NE	2.29	0.65
3:J:478:ASP:OD1	3:J:479:SER:OG	2.12	0.64
1:A:141:LYS:HD2	1:A:142:GLY:N	2.11	0.64
1:D:42:VAL:HG12	1:D:52:TRP:HA	1.80	0.64
1:D:167:LYS:NZ	1:D:168:ASP:OD1	2.18	0.64
1:C:6:GLU:HA	1:C:23:CYS:HA	1.80	0.64
3:L:485:ARG:NH1	3:L:495:ASP:OD1	2.31	0.64
2:B:210:TYR:HE1	2:B:229:ARG:HG3	1.63	0.63
1:D:26:SER:O	1:D:28:PHE:N	2.31	0.63
1:F:159:THR:HA	1:F:209:PRO:HA	1.80	0.63
1:F:91:MET:HB3	1:F:94:LEU:HD11	1.78	0.63
1:C:48:LYS:HG3	1:C:49:GLY:H	1.64	0.63
1:D:63:THR:HA	1:D:78:ILE:HD11	1.81	0.62
1:A:224:HIS:CE1	1:A:226:PRO:HB2	2.34	0.62
3:I:473:TYR:HB3	3:I:494:LEU:HD21	1.80	0.62
2:H:10:SER:O	2:H:11:LEU:HD22	2.00	0.62
2:H:10:SER:CB	2:H:121:LYS:H	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:165:GLN:N	2:G:213:GLU:O	2.31	0.62
2:G:5:THR:O	2:G:24:ARG:N	2.33	0.62
2:E:79:SER:HB3	3:J:527:LEU:HD23	1.81	0.62
1:D:28:PHE:HE1	1:D:33:TYR:CB	2.10	0.61
3:L:474:ARG:HD2	3:L:475:LYS:O	2.00	0.61
1:A:151:SER:O	1:A:155:THR:HG23	2.00	0.61
2:E:179:GLU:N	2:E:179:GLU:OE1	2.33	0.61
1:C:25:ALA:HB1	1:C:28:PHE:HE1	1.66	0.61
1:A:35:ARG:HG3	1:A:87:ALA:HB2	1.82	0.60
1:A:42:VAL:HG23	1:A:103:TYR:HB2	1.83	0.60
1:D:13:VAL:HG11	1:D:17:GLY:HA3	1.83	0.60
1:C:33:TYR:HB3	1:C:106:ARG:HG3	1.83	0.60
1:D:192:ALA:HA	1:D:202:LEU:HB3	1.83	0.60
1:C:125:ASP:HA	2:G:52:LEU:HD12	1.83	0.60
2:E:205:GLU:OE1	2:E:229:ARG:NH1	2.35	0.60
3:J:470:GLU:O	3:J:507:VAL:HA	2.02	0.60
2:H:12:SER:HB2	2:H:123:GLU:HG2	1.83	0.60
3:J:467:TRP:CZ3	3:J:511:THR:HA	2.37	0.60
1:C:19:LEU:O	1:C:91:MET:HB2	2.02	0.60
1:C:104:CYS:O	1:C:128:GLY:N	2.35	0.60
2:E:166:TRP:HD1	2:E:177:SER:HB3	1.66	0.60
3:J:447:ARG:HG3	3:J:527:LEU:HG	1.82	0.60
1:A:34:LEU:HD13	1:A:108:ALA:HB3	1.83	0.59
1:C:85:ASN:O	1:C:85:ASN:ND2	2.35	0.59
2:H:160:ARG:HE	2:H:181:VAL:HG21	1.67	0.59
1:D:33:TYR:HA	1:D:108:ALA:O	2.02	0.59
1:C:118:TYR:CG	2:G:112:TRP:HD1	2.21	0.59
1:D:205:VAL:HG11	2:E:153:LEU:HD22	1.82	0.59
2:H:214:VAL:HB	2:H:223:VAL:HG23	1.85	0.59
1:C:5:VAL:HG23	1:C:24:ALA:HB3	1.84	0.58
2:G:8:PRO:HB3	2:G:11:LEU:HD11	1.85	0.58
1:A:8:GLY:O	1:A:19:LEU:HD21	2.03	0.58
2:E:53:LEU:CD1	2:E:66:ASP:HB3	2.34	0.58
2:B:6:GLN:HA	2:B:23:CYS:HA	1.85	0.58
2:H:10:SER:HB3	2:H:121:LYS:H	1.68	0.58
1:A:63:THR:HA	1:A:78:ILE:HD11	1.86	0.58
2:E:138:PRO:HD3	2:E:150:VAL:HB	1.85	0.57
2:H:55:TYR:O	2:H:57:ALA:N	2.38	0.57
3:J:456:TRP:CH2	3:J:492:VAL:HG23	2.36	0.57
2:G:32:ALA:HA	3:L:480:ASN:OD1	2.04	0.57
2:H:79:SER:HB3	3:I:527:LEU:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:GLN:O	1:C:101:VAL:HG12	2.04	0.57
1:C:224:HIS:CE1	1:C:226:PRO:HB2	2.40	0.57
1:A:42:VAL:HG12	1:A:52:TRP:HA	1.86	0.57
1:A:147:PRO:O	2:B:139:SER:OG	2.23	0.57
2:B:31:SER:H	2:B:80:ARG:HH12	1.52	0.57
1:F:25:ALA:HB1	1:F:28:PHE:CE1	2.40	0.57
2:B:41:TRP:O	2:B:52:LEU:HD12	2.05	0.57
3:J:470:GLU:HG3	3:J:510:LEU:HD11	1.87	0.57
2:G:123:GLU:HB3	2:G:184:GLN:NE2	2.19	0.57
2:B:131:PRO:HB3	2:B:157:PHE:CB	2.35	0.57
3:K:486:ARG:NH2	3:K:510:LEU:HD21	2.20	0.57
1:C:195:GLN:OE1	1:C:196:SER:N	2.38	0.56
3:J:444:LEU:HD21	3:J:447:ARG:HB3	1.85	0.56
3:L:498:ALA:O	3:L:501:THR:OG1	2.23	0.56
1:C:150:PRO:HD3	1:C:162:LEU:HB3	1.87	0.56
1:C:168:ASP:HA	1:C:199:LEU:HB3	1.87	0.56
1:A:71:VAL:HG13	1:A:76:PHE:HB2	1.87	0.56
2:E:136:PHE:O	2:E:150:VAL:HG23	2.06	0.56
2:E:48:LYS:HG2	2:E:49:ALA:H	1.70	0.56
1:D:212:SER:HA	1:D:215:THR:HB	1.86	0.56
2:E:166:TRP:O	2:E:172:LEU:HD12	2.05	0.56
3:K:462:GLN:O	3:K:464:SER:N	2.38	0.56
1:F:160:ALA:N	1:F:208:VAL:O	2.38	0.56
2:B:32:ALA:HA	3:K:480:ASN:HD21	1.70	0.56
2:B:77:SER:HB2	3:L:527:LEU:HB3	1.88	0.56
1:F:23:CYS:SG	1:F:35:ARG:NH2	2.79	0.56
3:L:446:GLY:HA3	3:L:453:SER:HB2	1.88	0.56
1:F:28:PHE:HE2	1:F:33:TYR:HB2	1.70	0.55
2:H:163:LYS:HE3	2:H:163:LYS:HA	1.88	0.55
1:C:183:LEU:HD21	1:C:206:VAL:HG11	1.87	0.55
1:C:110:SER:HB2	3:L:484:VAL:HG11	1.87	0.55
2:G:163:LYS:HE3	2:G:163:LYS:HA	1.88	0.55
3:J:470:GLU:OE2	3:J:486:ARG:NH2	2.36	0.55
1:A:6:GLU:OE2	1:A:104:CYS:N	2.32	0.55
1:F:35:ARG:NH2	1:F:104:CYS:SG	2.79	0.55
3:J:442:VAL:HG21	3:J:522:HIS:ND1	2.21	0.55
1:A:91:MET:HB3	1:A:94:LEU:HD11	1.88	0.55
1:A:152:SER:O	1:A:155:THR:OG1	2.24	0.55
2:G:165:GLN:O	2:G:213:GLU:N	2.37	0.55
3:I:452:LEU:O	3:I:494:LEU:HB2	2.06	0.55
2:G:173:GLN:HB3	2:G:176:ASN:HD21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:56:ILE:HA	1:F:62:TYR:O	2.07	0.55
1:C:168:ASP:HB3	1:C:199:LEU:HD13	1.88	0.55
3:J:442:VAL:CG2	3:J:522:HIS:CE1	2.89	0.55
1:F:33:TYR:HB3	1:F:107:SER:O	2.08	0.54
3:J:440:PRO:HG2	3:J:507:VAL:HG12	1.90	0.54
3:K:467:TRP:CZ3	3:K:510:LEU:HD23	2.42	0.54
1:A:159:THR:HA	1:A:209:PRO:HA	1.90	0.54
2:G:45:LYS:HD2	2:G:46:PRO:HD2	1.89	0.54
3:I:475:LYS:CB	3:I:480:ASN:HB3	2.38	0.54
3:J:440:PRO:HA	3:J:458:ILE:HB	1.89	0.54
1:C:194:LEU:HD21	1:C:198:GLY:HA2	1.89	0.54
1:A:113:GLY:HA2	3:K:482:TYR:CZ	2.42	0.54
1:A:195:GLN:N	1:A:195:GLN:OE1	2.40	0.54
2:E:150:VAL:HG21	2:E:227:PHE:HE2	1.72	0.54
1:F:33:TYR:HD2	1:F:108:ALA:HA	1.70	0.54
3:I:471:VAL:HG11	3:I:494:LEU:HD11	1.89	0.54
3:L:468:LYS:O	3:L:510:LEU:HG	2.07	0.54
1:A:141:LYS:HD2	1:A:142:GLY:H	1.72	0.54
2:B:203:ASP:HA	2:B:206:LYS:HE3	1.90	0.54
1:F:28:PHE:CE2	1:F:33:TYR:HB2	2.43	0.54
1:C:105:ALA:HB1	1:C:124:MET:HB3	1.89	0.54
1:A:168:ASP:HB3	1:A:199:LEU:HD13	1.90	0.54
3:L:468:LYS:H	3:L:510:LEU:CD1	2.13	0.54
1:C:213:LEU:HD12	1:C:214:GLY:N	2.22	0.53
2:G:204:TYR:O	2:G:210:TYR:OH	2.26	0.53
1:D:67:TYR:CE1	1:D:78:ILE:HG12	2.43	0.53
3:L:460:PRO:HA	3:L:463:GLN:CD	2.29	0.53
3:K:458:ILE:HG22	3:K:490:PHE:HE1	1.73	0.53
1:D:28:PHE:CD1	1:D:106:ARG:HD2	2.42	0.53
2:E:41:TRP:HB2	2:E:53:LEU:HD21	1.91	0.53
3:J:497:LEU:HD22	3:J:503:TYR:CZ	2.43	0.53
3:L:467:TRP:HB3	3:L:510:LEU:HD12	1.91	0.53
1:D:43:ARG:HE	1:D:51:GLU:CD	2.12	0.53
3:K:495:ASP:OD1	3:K:495:ASP:N	2.42	0.53
1:A:33:TYR:HB3	1:A:106:ARG:HG2	1.89	0.53
2:B:17:ASP:H	2:B:94:LEU:H	1.55	0.53
2:E:211:ALA:HA	2:E:226:SER:HA	1.89	0.53
1:D:146:PHE:CE2	2:E:142:GLN:HG3	2.44	0.53
2:H:47:GLY:O	2:H:48:LYS:HD2	2.09	0.53
3:K:482:TYR:O	3:K:484:VAL:HG13	2.09	0.53
3:L:472:THR:HA	3:L:484:VAL:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:TYR:CZ	1:A:78:ILE:HG13	2.43	0.53
1:D:145:VAL:HG12	1:D:233:LYS:HE2	1.91	0.53
2:H:40:ALA:HB3	2:H:105:GLN:OE1	2.09	0.53
2:H:41:TRP:O	2:H:53:LEU:HB2	2.09	0.53
1:F:19:LEU:O	1:F:91:MET:HB2	2.09	0.52
1:F:110:SER:OG	1:F:113:GLY:N	2.37	0.52
2:H:205:GLU:O	2:H:229:ARG:NH2	2.21	0.52
1:C:44:GLN:NE2	1:C:48:LYS:O	2.41	0.52
1:A:119:HIS:CD2	1:A:120:PHE:HD1	2.24	0.52
1:F:192:ALA:HA	1:F:202:LEU:HB3	1.91	0.52
1:D:46:PRO:HD3	1:D:100:ALA:HA	1.91	0.52
2:E:67:LEU:HA	2:E:76:PHE:HB2	1.91	0.52
1:F:25:ALA:HB1	1:F:28:PHE:HE1	1.73	0.52
1:F:53:VAL:HG23	1:F:71:VAL:HG11	1.91	0.52
1:C:25:ALA:O	1:C:85:ASN:ND2	2.42	0.52
2:H:138:PRO:HD3	2:H:150:VAL:HG22	1.92	0.52
1:C:71:VAL:HG21	1:C:76:PHE:CD2	2.45	0.52
1:C:210:SER:O	1:C:210:SER:OG	2.27	0.52
1:F:116:HIS:O	1:F:118:TYR:N	2.42	0.52
2:H:204:TYR:HA	2:H:210:TYR:OH	2.09	0.52
3:L:462:GLN:O	3:L:464:SER:N	2.41	0.52
2:B:54:ILE:HG12	2:B:68:TYR:HA	1.90	0.51
1:D:93:SER:O	1:D:95:ARG:NH1	2.43	0.51
2:E:188:ASP:O	2:E:189:SER:C	2.48	0.51
1:F:109:ALA:HB3	3:J:484:VAL:HB	1.93	0.51
3:K:468:LYS:O	3:K:510:LEU:HB2	2.10	0.51
3:K:497:LEU:HD22	3:K:503:TYR:CZ	2.45	0.51
2:G:229:ARG:HE	2:G:230:GLY:N	2.08	0.51
2:H:89:LEU:HD23	2:H:89:LEU:O	2.10	0.51
1:A:205:VAL:HG11	2:B:153:LEU:HD22	1.92	0.51
2:H:92:SER:OG	2:H:93:SER:N	2.44	0.51
1:A:110:SER:HB2	3:K:484:VAL:HG11	1.93	0.51
1:F:5:VAL:HG23	1:F:24:ALA:HB3	1.92	0.51
2:G:69:SER:C	2:G:72:PRO:HD3	2.32	0.51
1:A:48:LYS:CG	1:A:49:GLY:H	2.23	0.51
1:A:79:SER:N	1:A:88:TYR:O	2.44	0.51
2:B:210:TYR:O	2:B:226:SER:HA	2.11	0.51
1:D:71:VAL:HG21	1:D:76:PHE:CD2	2.46	0.51
1:D:172:GLU:HG3	1:D:200:TYR:CD1	2.46	0.51
1:C:110:SER:O	1:C:113:GLY:N	2.44	0.51
2:E:21:ILE:HG23	2:E:120:THR:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:PHE:CD2	3:K:480:ASN:HA	2.46	0.50
2:E:126:ARG:HG3	2:E:127:THR:O	2.11	0.50
2:B:131:PRO:HB3	2:B:157:PHE:HB2	1.92	0.50
1:C:218:TYR:O	1:C:234:LYS:HG2	2.12	0.50
1:D:28:PHE:CE1	1:D:106:ARG:HD2	2.46	0.50
1:A:33:TYR:HA	1:A:108:ALA:O	2.11	0.50
1:A:35:ARG:HG2	1:A:58:PRO:HG3	1.92	0.50
1:D:177:SER:O	1:D:221:ASN:N	2.39	0.50
1:F:120:PHE:CD2	3:J:480:ASN:HA	2.46	0.50
2:H:99:PHE:CE2	2:H:124:ILE:HD13	2.47	0.50
3:L:475:LYS:HG3	3:L:476:LYS:N	2.20	0.50
1:C:77:THR:HB	1:C:90:GLN:HB3	1.93	0.50
2:G:41:TRP:HB2	2:G:53:LEU:HD11	1.94	0.50
2:G:79:SER:HB3	3:K:527:LEU:HA	1.93	0.50
1:A:119:HIS:CD2	1:A:120:PHE:CD1	2.98	0.50
1:C:43:ARG:NH1	1:C:98:ASP:HA	2.27	0.50
3:L:448:SER:N	3:L:451:SER:O	2.45	0.50
1:F:115:TRP:CE2	3:K:439:PRO:HD2	2.47	0.50
2:H:140:ASP:OD1	2:H:143:LEU:HD12	2.12	0.50
2:B:20:THR:HG22	2:B:90:THR:OG1	2.11	0.50
2:E:67:LEU:HD13	2:E:76:PHE:HD2	1.76	0.50
3:L:467:TRP:CB	3:L:510:LEU:HD12	2.42	0.50
1:C:9:GLY:HA2	1:C:133:VAL:HG22	1.94	0.49
1:C:99:THR:HG23	1:C:134:THR:HA	1.94	0.49
1:A:212:SER:HA	1:A:215:THR:HB	1.93	0.49
2:B:215:THR:HA	2:B:220:SER:HA	1.92	0.49
2:B:154:LEU:HB2	2:B:193:LEU:HB3	1.93	0.49
1:D:28:PHE:CZ	1:D:30:SER:HA	2.47	0.49
1:F:112:TYR:HE2	1:F:117:TRP:CH2	2.29	0.49
3:J:475:LYS:HG3	3:J:479:SER:HB2	1.94	0.49
2:G:67:LEU:CB	2:G:72:PRO:HD2	2.42	0.49
1:A:171:PRO:HD2	1:A:226:PRO:HB3	1.93	0.49
1:F:162:LEU:HD21	1:F:218:TYR:CD2	2.47	0.49
3:L:511:THR:CG2	3:L:516:GLY:HA2	2.42	0.49
1:F:227:SER:O	1:F:229:THR:HG23	2.12	0.49
3:K:446:GLY:HA3	3:K:453:SER:HB2	1.94	0.49
2:H:91:ILE:HD11	2:H:94:LEU:HD12	1.93	0.49
3:L:448:SER:HB3	3:L:451:SER:HB3	1.95	0.49
1:A:43:ARG:HG2	1:A:53:VAL:CG1	2.42	0.49
2:B:44:GLN:HB3	2:B:101:THR:OG1	2.12	0.49
2:E:169:ASP:HA	2:E:209:VAL:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:143:PRO:HA	1:F:169:TYR:HB3	1.95	0.49
1:C:172:GLU:OE2	1:C:192:ALA:HB3	2.13	0.49
1:F:115:TRP:NE1	3:K:439:PRO:HD2	2.28	0.49
3:L:475:LYS:HE3	3:L:501:THR:CG2	2.43	0.49
1:C:75:ARG:NH1	1:C:95:ARG:HB2	2.28	0.48
2:B:201:LYS:NZ	2:B:205:GLU:OE2	2.40	0.48
2:H:52:LEU:O	2:H:68:TYR:HE1	1.96	0.48
2:H:211:ALA:HB2	2:H:226:SER:HB2	1.95	0.48
1:A:113:GLY:HA2	3:K:482:TYR:CE2	2.47	0.48
2:E:53:LEU:HA	2:E:68:TYR:CG	2.47	0.48
1:F:179:ASN:ND2	1:F:217:THR:O	2.45	0.48
3:L:438:GLU:HG2	3:L:462:GLN:OE1	2.14	0.48
1:A:140:THR:HG22	1:A:227:SER:HB3	1.95	0.48
3:K:486:ARG:HH21	3:K:510:LEU:HD21	1.77	0.48
2:H:186:SER:O	2:H:189:SER:N	2.47	0.48
2:G:8:PRO:HD3	2:G:22:THR:HB	1.95	0.48
3:I:466:VAL:HG12	3:I:511:THR:HB	1.95	0.48
2:E:176:ASN:ND2	2:E:197:LEU:CD1	2.77	0.48
2:E:178:GLN:O	2:E:195:SER:HA	2.14	0.48
1:F:96:ALA:O	1:F:99:THR:HG22	2.13	0.48
3:J:475:LYS:HD3	3:J:503:TYR:CE2	2.49	0.48
2:E:150:VAL:CG1	2:E:197:LEU:HB3	2.44	0.48
2:H:89:LEU:HD23	2:H:91:ILE:HG23	1.95	0.48
2:B:151:VAL:HG23	2:B:196:THR:HG22	1.96	0.48
3:K:452:LEU:HD21	3:K:524:PHE:HB2	1.96	0.48
1:C:121:SER:HB2	2:G:107:TYR:CD2	2.49	0.47
1:C:158:GLY:HA2	1:C:209:PRO:HA	1.96	0.47
1:F:112:TYR:HE2	1:F:117:TRP:CZ2	2.31	0.47
1:F:112:TYR:O	1:F:116:HIS:HB2	2.14	0.47
2:G:169:ASP:HA	2:G:209:VAL:HB	1.95	0.47
2:B:131:PRO:HB3	2:B:157:PHE:HB3	1.96	0.47
1:F:168:ASP:HB3	1:F:199:LEU:HD13	1.95	0.47
1:A:25:ALA:HB1	1:A:28:PHE:CZ	2.50	0.47
1:F:41:TRP:O	1:F:53:VAL:HG12	2.15	0.47
2:G:71:VAL:N	2:G:72:PRO:HD3	2.30	0.47
2:H:162:ALA:O	2:H:163:LYS:HD2	2.14	0.47
3:L:510:LEU:HB3	3:L:512:GLN:OE1	2.15	0.47
1:C:118:TYR:C	1:C:120:PHE:H	2.17	0.47
1:D:148:LEU:O	1:D:162:LEU:HA	2.15	0.47
1:D:208:VAL:HG22	1:D:209:PRO:HD2	1.97	0.47
1:C:41:TRP:NE1	1:C:89:LEU:HB2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:TRP:O	1:C:117:TRP:N	2.48	0.47
2:G:151:VAL:HG23	2:G:196:THR:HG22	1.95	0.47
2:B:80:ARG:HH21	3:K:478:ASP:HA	1.80	0.47
1:D:110:SER:CB	3:I:484:VAL:HG21	2.45	0.47
2:E:176:ASN:ND2	2:E:197:LEU:HD11	2.29	0.47
2:E:231:GLU:CD	2:E:232:CYS:H	2.15	0.47
3:I:497:LEU:HD22	3:I:503:TYR:CZ	2.50	0.47
2:G:6:GLN:HE22	2:G:103:TYR:HA	1.78	0.47
1:D:108:ALA:HB2	1:D:122:PRO:HD2	1.96	0.47
1:A:192:ALA:HA	1:A:202:LEU:HB3	1.95	0.47
3:I:470:GLU:HB2	3:I:510:LEU:HD11	1.95	0.47
1:F:150:PRO:HD3	1:F:162:LEU:HB3	1.96	0.47
3:K:509:ALA:HB3	3:K:517:ALA:HB3	1.97	0.47
1:D:13:VAL:CG1	1:D:17:GLY:HA3	2.43	0.46
2:B:203:ASP:HA	2:B:206:LYS:HG3	1.97	0.46
3:K:475:LYS:HD2	3:K:479:SER:OG	2.14	0.46
3:K:520:LYS:HE3	3:K:522:HIS:NE2	2.31	0.46
1:C:57:TYR:O	1:C:61:GLY:N	2.41	0.46
1:F:112:TYR:O	1:F:116:HIS:N	2.49	0.46
3:J:470:GLU:HG3	3:J:510:LEU:HD21	1.97	0.46
1:C:181:GLY:O	1:C:184:THR:OG1	2.34	0.46
1:D:150:PRO:HG3	1:D:213:LEU:HD21	1.97	0.46
2:G:19:VAL:O	2:G:90:THR:HA	2.16	0.46
2:H:41:TRP:CG	2:H:89:LEU:HD12	2.50	0.46
3:L:464:SER:OG	3:L:466:VAL:HG13	2.16	0.46
1:A:115:TRP:CZ2	3:J:439:PRO:HD2	2.51	0.46
2:E:150:VAL:HG13	2:E:197:LEU:HB3	1.98	0.46
2:H:205:GLU:HA	2:H:229:ARG:NH1	2.23	0.46
1:C:4:LEU:HD23	1:C:4:LEU:HA	1.76	0.46
1:C:34:LEU:HB2	1:C:107:SER:HB2	1.97	0.46
1:C:95:ARG:NH1	1:C:97:GLU:OE2	2.48	0.46
2:E:30:SER:O	3:I:479:SER:OG	2.33	0.46
1:F:120:PHE:O	3:J:482:TYR:HB2	2.15	0.46
2:G:44:GLN:HG3	2:G:50:PRO:HG3	1.98	0.45
1:A:41:TRP:HB3	1:A:53:VAL:CG2	2.46	0.45
2:B:200:SER:O	2:B:203:ASP:OD1	2.34	0.45
2:B:211:ALA:HA	2:B:226:SER:HA	1.98	0.45
2:G:173:GLN:HB3	2:G:176:ASN:ND2	2.29	0.45
2:E:54:ILE:HG22	2:E:67:LEU:C	2.37	0.45
3:L:438:GLU:OE2	3:L:462:GLN:NE2	2.49	0.45
2:B:20:THR:HA	2:B:90:THR:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:LEU:HD12	2:B:54:ILE:O	2.17	0.45
2:B:101:THR:HA	2:B:121:LYS:HA	1.98	0.45
2:E:214:VAL:O	2:E:223:VAL:N	2.47	0.45
1:F:43:ARG:HB2	1:F:100:ALA:HB3	1.98	0.45
1:F:48:LYS:HB3	2:H:6:GLN:O	2.17	0.45
1:F:67:TYR:CZ	1:F:78:ILE:HG22	2.51	0.45
3:K:452:LEU:O	3:K:494:LEU:HB3	2.17	0.45
2:G:129:ALA:HB3	2:G:158:TYR:H	1.82	0.45
1:A:125:ASP:OD1	1:A:126:TYR:N	2.48	0.45
1:F:34:LEU:HG	1:F:57:TYR:CD1	2.51	0.45
3:L:468:LYS:HB2	3:L:510:LEU:CD1	2.39	0.45
2:E:40:ALA:HB1	2:E:52:LEU:HD13	1.99	0.45
2:H:188:ASP:O	2:H:190:THR:HG23	2.16	0.45
2:B:181:VAL:HG12	2:B:182:THR:O	2.17	0.45
1:F:120:PHE:HD2	3:J:480:ASN:HA	1.81	0.45
2:H:184:GLN:HA	2:H:190:THR:O	2.17	0.45
1:D:110:SER:O	1:D:113:GLY:N	2.50	0.45
2:E:53:LEU:HA	2:E:68:TYR:CD1	2.52	0.45
2:E:100:ALA:O	2:E:122:VAL:HG22	2.17	0.45
1:F:25:ALA:O	1:F:85:ASN:ND2	2.50	0.45
1:D:225:LYS:O	1:D:226:PRO:C	2.55	0.45
1:C:193:VAL:O	1:C:201:SER:N	2.43	0.45
1:A:52:TRP:CD2	2:B:114:ILE:HB	2.52	0.45
2:B:6:GLN:OE1	2:B:117:GLY:HA3	2.17	0.45
1:F:194:LEU:HG	1:F:198:GLY:HA2	1.99	0.45
2:G:75:ARG:O	2:G:91:ILE:HA	2.17	0.44
1:A:145:VAL:HG12	1:A:233:LYS:HD3	1.99	0.44
1:A:225:LYS:O	1:A:226:PRO:C	2.54	0.44
2:B:6:GLN:HG3	2:B:119:GLY:N	2.11	0.44
2:B:212:CYS:N	2:B:225:LYS:O	2.43	0.44
1:F:78:ILE:HD12	1:F:79:SER:H	1.83	0.44
1:C:122:PRO:HD3	3:L:482:TYR:CD2	2.52	0.44
1:D:62:TYR:HD1	1:D:63:THR:N	2.16	0.44
2:E:53:LEU:HD12	2:E:54:ILE:O	2.18	0.44
3:K:474:ARG:NH1	3:K:504:LEU:HD13	2.32	0.44
2:G:28:SER:OG	2:G:29:VAL:N	2.48	0.44
1:A:94:LEU:HD23	1:A:135:VAL:HG22	1.99	0.44
1:A:210:SER:HA	1:A:213:LEU:HG	2.00	0.44
2:E:54:ILE:H	2:E:68:TYR:HA	1.82	0.44
3:J:465:ARG:O	3:J:466:VAL:HB	2.16	0.44
1:A:178:TRP:HB3	1:A:183:LEU:HD23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:507:VAL:O	3:J:519:SER:HB3	2.18	0.44
1:D:171:PRO:HD2	1:D:226:PRO:HB3	1.99	0.44
2:E:169:ASP:OD2	2:E:207:HIS:HB3	2.17	0.44
1:F:144:SER:OG	1:F:167:LYS:O	2.30	0.44
1:F:168:ASP:HA	1:F:199:LEU:HB3	2.00	0.44
3:J:494:LEU:HD23	3:J:494:LEU:HA	1.76	0.44
2:E:77:SER:HB3	3:J:527:LEU:HB3	1.98	0.44
1:F:34:LEU:HD12	1:F:34:LEU:H	1.81	0.44
3:I:467:TRP:O	3:I:488:GLU:HG2	2.17	0.44
3:K:485:ARG:NH1	3:K:495:ASP:OD1	2.51	0.44
1:C:13:VAL:O	1:C:135:VAL:HA	2.18	0.44
2:G:71:VAL:HG12	2:G:71:VAL:O	2.18	0.44
2:G:150:VAL:HG13	2:G:197:LEU:HB3	1.99	0.44
1:A:15:PRO:HD3	1:A:136:SER:O	2.17	0.44
2:E:42:TYR:HE1	2:E:105:GLN:HB3	1.82	0.44
1:F:193:VAL:O	1:F:201:SER:N	2.50	0.44
1:C:115:TRP:CZ2	3:I:439:PRO:HD2	2.52	0.44
1:A:227:SER:O	1:A:228:ASN:C	2.56	0.44
2:E:107:TYR:HE1	2:E:114:ILE:HD13	1.83	0.44
2:E:214:VAL:N	2:E:223:VAL:O	2.40	0.44
1:F:67:TYR:CE2	1:F:77:THR:HA	2.53	0.44
2:H:77:SER:HB2	3:I:527:LEU:HD13	2.00	0.44
1:F:117:TRP:CE2	3:J:474:ARG:NH1	2.86	0.43
3:L:475:LYS:HE3	3:L:501:THR:HG21	2.00	0.43
1:C:48:LYS:HA	1:C:48:LYS:HD2	1.73	0.43
1:C:125:ASP:OD1	1:C:125:ASP:N	2.51	0.43
2:B:7:SER:OG	2:B:8:PRO:HD3	2.18	0.43
1:F:114:TYR:O	2:H:112:TRP:NE1	2.51	0.43
2:H:12:SER:CB	2:H:123:GLU:HG2	2.48	0.43
2:H:39:VAL:H	3:J:480:ASN:ND2	2.16	0.43
3:J:499:PRO:O	3:J:501:THR:HG23	2.18	0.43
3:L:463:GLN:C	3:L:465:ARG:H	2.21	0.43
1:D:195:GLN:NE2	1:D:201:SER:HB3	2.34	0.43
3:L:438:GLU:OE2	3:L:459:PRO:HG2	2.18	0.43
3:L:470:GLU:O	3:L:507:VAL:HA	2.18	0.43
2:G:129:ALA:HB3	2:G:158:TYR:N	2.34	0.43
1:D:6:GLU:HB2	1:D:131:THR:HG23	1.99	0.43
1:D:15:PRO:HD3	1:D:136:SER:O	2.18	0.43
2:B:21:ILE:HG23	2:B:120:THR:HG21	2.01	0.43
2:B:101:THR:HG22	2:B:121:LYS:CB	2.48	0.43
2:B:204:TYR:O	2:B:210:TYR:OH	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:74:SER:O	2:E:75:ARG:HB2	2.18	0.43
3:K:471:VAL:HG12	3:K:485:ARG:O	2.18	0.43
1:C:178:TRP:HB3	1:C:183:LEU:HD23	2.00	0.43
1:A:48:LYS:HG2	1:A:49:GLY:H	1.83	0.43
3:I:474:ARG:HA	3:I:482:TYR:HD1	1.83	0.43
3:J:467:TRP:CE3	3:J:511:THR:HA	2.53	0.43
1:A:238:LYS:HA	1:A:238:LYS:HD2	1.68	0.43
2:B:75:ARG:O	2:B:92:SER:N	2.50	0.43
1:F:2:VAL:HG21	1:F:28:PHE:HB3	2.00	0.43
1:A:190:PHE:CE2	2:B:194:SER:HB3	2.53	0.43
2:B:160:ARG:HD2	2:B:161:GLU:OE2	2.18	0.43
1:D:13:VAL:HG12	1:D:14:GLN:N	2.34	0.43
3:L:474:ARG:HD2	3:L:475:LYS:C	2.39	0.43
1:C:71:VAL:HG21	1:C:76:PHE:CE2	2.53	0.43
2:G:229:ARG:NE	2:G:230:GLY:N	2.66	0.43
2:E:214:VAL:HB	2:E:223:VAL:HG23	2.01	0.43
3:L:459:PRO:HA	3:L:460:PRO:HD3	1.85	0.43
1:C:1:GLU:O	1:C:3:GLN:HG3	2.19	0.43
2:G:108:VAL:HG12	2:G:113:LEU:O	2.19	0.43
2:G:162:ALA:O	2:G:163:LYS:HD2	2.18	0.43
1:D:110:SER:HB3	3:I:484:VAL:HG21	2.00	0.43
1:D:225:LYS:N	1:D:226:PRO:HD2	2.33	0.43
2:H:138:PRO:CD	2:H:150:VAL:HG22	2.49	0.43
1:C:118:TYR:C	1:C:120:PHE:N	2.72	0.42
2:E:173:GLN:HB3	2:E:176:ASN:OD1	2.19	0.42
1:F:14:GLN:HG3	1:F:15:PRO:HD2	2.00	0.42
3:K:473:TYR:CE1	3:K:483:ASN:O	2.72	0.42
1:D:143:PRO:HA	1:D:169:TYR:HB3	2.00	0.42
2:E:71:VAL:HG12	2:E:71:VAL:O	2.18	0.42
1:F:52:TRP:CH2	2:H:113:LEU:HA	2.54	0.42
2:H:160:ARG:HH21	2:H:181:VAL:HG21	1.84	0.42
1:C:52:TRP:CH2	2:G:113:LEU:HA	2.54	0.42
1:C:114:TYR:O	1:C:118:TYR:HB2	2.20	0.42
2:G:41:TRP:CD1	2:G:89:LEU:HD13	2.54	0.42
2:H:100:ALA:O	2:H:122:VAL:HG22	2.19	0.42
3:J:497:LEU:HD22	3:J:503:TYR:CE2	2.54	0.42
2:G:48:LYS:HE2	2:G:49:ALA:O	2.19	0.42
2:B:22:THR:HG22	2:B:23:CYS:N	2.35	0.42
2:E:148:ALA:O	2:E:199:LEU:N	2.26	0.42
1:F:195:GLN:H	1:F:199:LEU:H	1.67	0.42
2:H:182:THR:O	2:H:191:TYR:HD1	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:467:TRP:HZ3	3:J:511:THR:HA	1.82	0.42
1:A:52:TRP:CH2	2:B:113:LEU:HA	2.55	0.42
2:E:45:LYS:NZ	2:E:97:GLU:O	2.51	0.42
1:F:178:TRP:HB3	1:F:183:LEU:HD23	2.01	0.42
3:L:468:LYS:HG3	3:L:488:GLU:CG	2.42	0.42
1:C:163:GLY:HA2	1:C:178:TRP:CZ2	2.53	0.42
3:J:470:GLU:CG	3:J:510:LEU:HD21	2.50	0.42
3:K:467:TRP:HZ3	3:K:510:LEU:HD23	1.83	0.42
1:C:33:TYR:HA	1:C:108:ALA:O	2.20	0.42
1:D:31:GLY:HA2	1:D:58:PRO:HB2	2.01	0.42
2:E:53:LEU:HB2	2:E:67:LEU:O	2.20	0.42
2:H:52:LEU:HD12	2:H:53:LEU:H	1.84	0.42
3:L:460:PRO:N	3:L:461:PRO:HD2	2.34	0.42
1:C:52:TRP:CG	2:G:114:ILE:HB	2.55	0.42
1:A:19:LEU:O	1:A:91:MET:HB2	2.20	0.42
1:C:7:SER:N	1:C:22:SER:O	2.52	0.42
1:C:230:LYS:HA	1:C:230:LYS:HD2	1.92	0.42
1:A:136:SER:OG	1:A:137:SER:N	2.53	0.42
1:D:18:SER:HA	1:D:91:MET:O	2.19	0.42
2:E:15:VAL:HG23	2:E:96:PRO:HD3	2.02	0.42
2:G:133:VAL:HA	2:G:153:LEU:O	2.20	0.42
2:G:213:GLU:OE2	2:G:220:SER:OG	2.36	0.42
2:B:101:THR:HG22	2:B:121:LYS:HB3	2.01	0.42
2:B:211:ALA:HB2	2:B:226:SER:HB3	2.01	0.42
2:B:225:LYS:HA	2:B:225:LYS:HD3	1.82	0.42
1:F:2:VAL:HG23	1:F:26:SER:O	2.20	0.42
1:F:77:THR:OG1	1:F:90:GLN:HB3	2.20	0.42
2:H:181:VAL:HG22	2:H:193:LEU:HD12	2.00	0.42
3:J:506:GLN:HE21	3:J:506:GLN:HB3	1.67	0.42
2:B:203:ASP:OD1	2:B:203:ASP:N	2.53	0.41
2:E:126:ARG:HH21	2:E:127:THR:CG2	2.33	0.41
1:C:91:MET:HB3	1:C:94:LEU:HD21	2.00	0.41
1:C:192:ALA:HA	1:C:202:LEU:HB3	2.00	0.41
1:A:224:HIS:O	1:A:225:LYS:C	2.59	0.41
2:B:57:ALA:O	2:B:58:SER:OG	2.31	0.41
2:B:165:GLN:HB2	2:B:213:GLU:HB3	2.02	0.41
1:D:167:LYS:HG2	1:D:168:ASP:OD1	2.20	0.41
3:I:462:GLN:O	3:I:464:SER:N	2.45	0.41
3:J:460:PRO:N	3:J:461:PRO:HD2	2.35	0.41
1:C:25:ALA:HB3	1:C:85:ASN:O	2.21	0.41
1:C:41:TRP:CD1	1:C:89:LEU:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:ALA:O	1:C:110:SER:HB3	2.19	0.41
1:C:171:PRO:HD2	1:C:226:PRO:HB3	2.01	0.41
1:A:84:LYS:O	1:A:86:THR:HG23	2.20	0.41
2:B:75:ARG:HA	2:B:92:SER:OG	2.20	0.41
3:L:497:LEU:HD22	3:L:503:TYR:CE2	2.55	0.41
1:F:132:LEU:HD21	1:F:134:THR:HG23	2.03	0.41
3:J:467:TRP:HE3	3:J:510:LEU:O	2.03	0.41
3:K:472:THR:OG1	3:K:506:GLN:HB3	2.20	0.41
2:G:136:PHE:O	2:G:150:VAL:HG23	2.20	0.41
1:F:33:TYR:CD2	1:F:108:ALA:HA	2.53	0.41
2:H:164:VAL:HG22	2:H:214:VAL:HG13	2.02	0.41
2:G:69:SER:O	2:G:71:VAL:N	2.49	0.41
1:A:110:SER:HA	3:K:486:ARG:HH12	1.85	0.41
2:B:53:LEU:HD13	2:B:67:LEU:HA	2.03	0.41
2:E:207:HIS:O	2:E:229:ARG:NH2	2.54	0.41
2:G:42:TYR:CE2	2:G:52:LEU:HG	2.56	0.41
2:B:211:ALA:HA	2:B:225:LYS:O	2.20	0.41
2:H:138:PRO:HB3	2:H:149:SER:H	1.85	0.41
2:H:108:VAL:HG12	2:H:113:LEU:O	2.20	0.41
3:K:497:LEU:HD13	3:K:503:TYR:CD2	2.55	0.41
1:A:53:VAL:HB	1:A:71:VAL:HG21	2.02	0.41
1:D:21:LEU:HD23	1:D:21:LEU:HA	1.85	0.41
1:F:147:PRO:HG3	1:F:233:LYS:HE2	2.03	0.41
3:J:511:THR:HG22	3:J:516:GLY:N	2.36	0.41
3:L:438:GLU:HA	3:L:439:PRO:HD3	1.88	0.41
1:D:171:PRO:HB2	1:D:172:GLU:H	1.76	0.41
2:E:133:VAL:HA	2:E:153:LEU:O	2.20	0.41
2:E:149:SER:HA	2:E:198:THR:HA	2.03	0.41
1:D:120:PHE:O	3:I:482:TYR:HB2	2.20	0.40
2:H:44:GLN:HB3	2:H:101:THR:CG2	2.51	0.40
3:L:487:THR:HG22	3:L:489:GLY:N	2.28	0.40
1:C:23:CYS:O	1:C:35:ARG:NH2	2.54	0.40
1:C:28:PHE:CE2	1:C:33:TYR:HB2	2.56	0.40
1:C:122:PRO:HG3	3:L:482:TYR:H	1.86	0.40
2:B:19:VAL:HG21	2:B:94:LEU:HD12	2.02	0.40
2:B:126:ARG:HD3	2:B:127:THR:O	2.21	0.40
1:D:224:HIS:NE2	1:D:226:PRO:HG2	2.36	0.40
1:F:150:PRO:HG3	1:F:162:LEU:HD23	2.03	0.40
1:A:18:SER:HA	1:A:91:MET:O	2.21	0.40
1:A:72:LYS:O	1:A:72:LYS:HD3	2.22	0.40
1:D:177:SER:HB3	1:D:221:ASN:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:500:ASP:N	3:I:526:THR:OG1	2.54	0.40
2:B:169:ASP:HA	2:B:209:VAL:HB	2.03	0.40
1:D:52:TRP:CG	2:E:114:ILE:HB	2.56	0.40
1:D:114:TYR:O	2:E:112:TRP:NE1	2.51	0.40
1:F:110:SER:O	1:F:113:GLY:N	2.54	0.40
2:H:126:ARG:NH2	2:H:127:THR:O	2.54	0.40
2:H:140:ASP:HA	2:H:143:LEU:HB2	2.03	0.40
2:H:150:VAL:HG12	2:H:166:TRP:CH2	2.57	0.40
3:K:440:PRO:HG2	3:K:519:SER:HB3	2.04	0.40
2:B:19:VAL:O	2:B:90:THR:HA	2.22	0.40
1:F:115:TRP:HE1	3:K:438:GLU:CD	2.24	0.40
2:H:32:ALA:HA	3:J:480:ASN:HB3	2.04	0.40
2:H:163:LYS:O	2:H:215:THR:OG1	2.27	0.40
2:H:172:LEU:HD23	2:H:172:LEU:H	1.87	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	230/237 (97%)	202 (88%)	26 (11%)	2 (1%)	17	56
1	C	228/237 (96%)	197 (86%)	30 (13%)	1 (0%)	34	72
1	D	228/237 (96%)	202 (89%)	23 (10%)	3 (1%)	12	48
1	F	228/237 (96%)	204 (90%)	22 (10%)	2 (1%)	17	56
2	B	208/214 (97%)	177 (85%)	31 (15%)	0	100	100
2	E	209/214 (98%)	179 (86%)	29 (14%)	1 (0%)	29	68
2	G	208/214 (97%)	179 (86%)	25 (12%)	4 (2%)	8	41
2	H	208/214 (97%)	178 (86%)	28 (14%)	2 (1%)	15	54
3	I	85/98 (87%)	67 (79%)	17 (20%)	1 (1%)	13	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	J	83/98 (85%)	66 (80%)	16 (19%)	1 (1%)	13	50
3	K	88/98 (90%)	72 (82%)	15 (17%)	1 (1%)	14	52
3	L	83/98 (85%)	70 (84%)	13 (16%)	0	100	100
All	All	2086/2196 (95%)	1793 (86%)	275 (13%)	18 (1%)	17	56

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	116	HIS
1	D	173	PRO
2	H	54	ILE
2	H	56	SER
3	J	466	VAL
1	D	27	GLY
2	E	58	SER
3	I	467	TRP
2	G	75	ARG
1	A	116	HIS
2	G	27	GLN
1	F	117	TRP
1	F	139	SER
2	G	28	SER
2	G	53	LEU
1	A	110	SER
3	K	478	ASP
1	D	226	PRO

5.3.2 Protein sidechains [i](#)

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	182/195 (93%)	176 (97%)	6 (3%)	38	61
1	C	180/195 (92%)	172 (96%)	8 (4%)	28	54
1	D	177/195 (91%)	167 (94%)	10 (6%)	21	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	178/195 (91%)	174 (98%)	4 (2%)	52	70
2	B	173/187 (92%)	166 (96%)	7 (4%)	31	57
2	E	165/187 (88%)	156 (94%)	9 (6%)	21	49
2	G	170/187 (91%)	165 (97%)	5 (3%)	42	64
2	H	165/187 (88%)	158 (96%)	7 (4%)	30	55
3	I	69/89 (78%)	65 (94%)	4 (6%)	20	47
3	J	71/89 (80%)	67 (94%)	4 (6%)	21	48
3	K	73/89 (82%)	69 (94%)	4 (6%)	21	49
3	L	74/89 (83%)	72 (97%)	2 (3%)	44	66
All	All	1677/1884 (89%)	1607 (96%)	70 (4%)	30	55

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	6	GLU
1	C	57	TYR
1	C	85	ASN
1	C	106	ARG
1	C	162	LEU
1	C	195	GLN
1	C	210	SER
1	C	221	ASN
2	G	68	TYR
2	G	104	CYS
2	G	206	LYS
2	G	212	CYS
2	G	220	SER
1	A	57	TYR
1	A	75	ARG
1	A	92	ASN
1	A	112	TYR
1	A	162	LEU
1	A	233	LYS
2	B	80	ARG
2	B	104	CYS
2	B	113	LEU
2	B	116	PHE
2	B	126	ARG
2	B	163	LYS

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Mol	Chain	Res	Type
2	B	227	PHE
1	D	57	TYR
1	D	62	TYR
1	D	93	SER
1	D	112	TYR
1	D	159	THR
1	D	162	LEU
1	D	174	VAL
1	D	226	PRO
1	D	227	SER
1	D	233	LYS
2	E	67	LEU
2	E	68	TYR
2	E	77	SER
2	E	104	CYS
2	E	176	ASN
2	E	188	ASP
2	E	227	PHE
2	E	229	ARG
2	E	232	CYS
1	F	4	LEU
1	F	92	ASN
1	F	184	THR
1	F	221	ASN
2	H	75	ARG
2	H	104	CYS
2	H	156	ASN
2	H	160	ARG
2	H	206	LYS
2	H	212	CYS
2	H	216	GLN
3	I	448	SER
3	I	485	ARG
3	I	496	ASP
3	I	506	GLN
3	J	474	ARG
3	J	482	TYR
3	J	485	ARG
3	J	506	GLN
3	K	463	GLN
3	K	482	TYR
3	K	496	ASP

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Mol	Chain	Res	Type
3	K	520	LYS
3	L	465	ARG
3	L	480	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	40	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	232/237 (97%)	-0.57	0 100 100	121, 156, 216, 248	0
1	C	230/237 (97%)	-0.63	0 100 100	115, 166, 205, 222	0
1	D	230/237 (97%)	-0.60	0 100 100	120, 152, 201, 209	0
1	F	230/237 (97%)	-0.63	0 100 100	118, 149, 200, 216	0
2	B	210/214 (98%)	-0.56	0 100 100	121, 170, 218, 239	0
2	E	211/214 (98%)	-0.61	0 100 100	123, 168, 213, 244	0
2	G	210/214 (98%)	-0.61	0 100 100	114, 159, 191, 210	0
2	H	210/214 (98%)	-0.65	0 100 100	116, 163, 194, 221	0
3	I	89/98 (90%)	-0.62	0 100 100	100, 121, 144, 170	0
3	J	87/98 (88%)	-0.57	0 100 100	100, 130, 185, 202	0
3	K	90/98 (91%)	-0.59	0 100 100	105, 127, 164, 172	0
3	L	87/98 (88%)	-0.64	0 100 100	105, 130, 178, 200	0
All	All	2116/2196 (96%)	-0.61	0 100 100	100, 153, 206, 248	0

There are no RSRZ outliers to report.

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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.