



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:05 PM GMT

PDB ID : 3W14
Title : Insulin receptor ectodomain construct comprising domains L1,CR,L2, FNIII-1 and alphact peptide in complex with bovine insulin and FAB 83-14
Authors : Lawrence, M.C.; Smith, B.J.
Deposited on : 2012-11-06
Resolution : 4.40 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

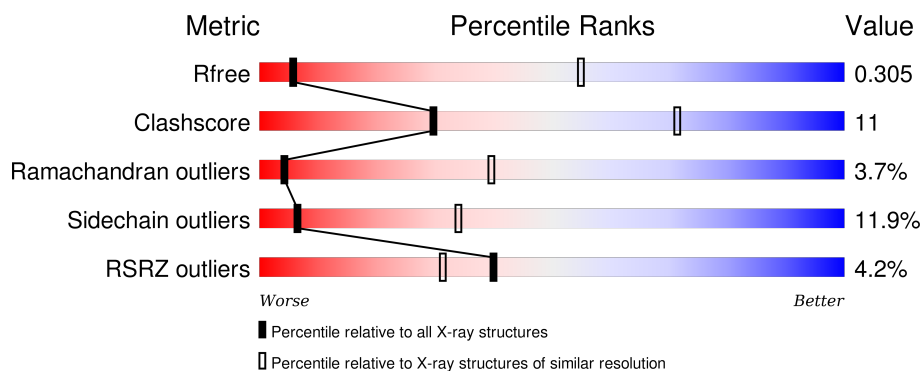
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.40 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}	91344	1067 (5.20-3.60)
Clashscore	102246	1175 (5.20-3.60)
Ramachandran outliers	100387	1114 (5.20-3.60)
Sidechain outliers	100360	1096 (5.20-3.60)
RSRZ outliers	91569	1071 (5.20-3.60)

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 ≥ 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.

Mol	Chain	Length	Quality of chain
1	A	21	<div> <div>57%</div> <div>33%</div> <div>10%</div> </div>
1	I	21	<div> <div>67%</div> <div>33%</div> </div>
2	B	30	<div> <div>27%</div> <div>23%</div> <div>7%</div> <div>43%</div> </div>
2	J	30	<div> <div>30%</div> <div>23%</div> <div>•</div> <div>43%</div> </div>
3	C	207	<div> <div>%</div> <div>65%</div> <div>24%</div> <div>•</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
3	P	207	<div><div></div><div>3%</div><div>68%</div><div>20%</div><div>5%</div><div>7%</div></div>
4	D	214	<div><div></div><div>7%</div><div>71%</div><div>25%</div><div></div><div></div></div>
4	Q	214	<div><div></div><div>3%</div><div>71%</div><div>24%</div><div>5%</div><div></div></div>
5	E	609	<div><div></div><div>4%</div><div>70%</div><div>19%</div><div>5%</div><div>5%</div></div>
5	F	609	<div><div></div><div>5%</div><div>69%</div><div>20%</div><div>6%</div><div>5%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16158 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 Insulin A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	21	Total	C	N	O	S	0	0	0
			160	97	25	34	4			
1	I	21	Total	C	N	O	S	0	0	0
			160	97	25	34	4			

- Molecule 2 is a protein called Insulin B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	17	Total	C	N	O	S	0	0	0
			127	81	21	23	2			
2	J	17	Total	C	N	O	S	0	0	0
			127	81	21	23	2			

- Molecule 3 is a protein called MONOCLONAL ANTIBODY FAB 83-14 - HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	193	Total	C	N	O	S	0	0	0
			1468	940	239	284	5			
3	P	193	Total	C	N	O	S	0	0	0
			1468	940	239	284	5			

- Molecule 4 is a protein called MONOCLONAL ANTIBODY FAB 83-14 - LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	214	Total	C	N	O	S	0	0	0
			1652	1025	278	342	7			
4	Q	214	Total	C	N	O	S	0	0	0
			1652	1025	278	342	7			

- Molecule 5 is a protein called INSULIN RECEPTOR DOMAINS L1-CR-L2-(FNIII-1)-ALP HACT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	580	Total	C	N	O	S	0	0	0
			4672	2962	812	857	41			
5	F	580	Total	C	N	O	S	0	0	0
			4672	2962	812	857	41			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	144	HIS	TYR	SEE REMARK 999	UNP P06213
F	144	HIS	TYR	SEE REMARK 999	UNP P06213

3 Residue-property plots [i](#)

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.

- Molecule 1: Insulin A chain

Chain A: 




- Molecule 1: Insulin A chain

Chain I: 

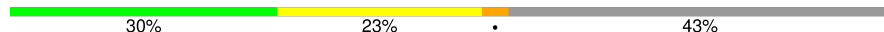


- Molecule 2: Insulin B chain

Chain B: 



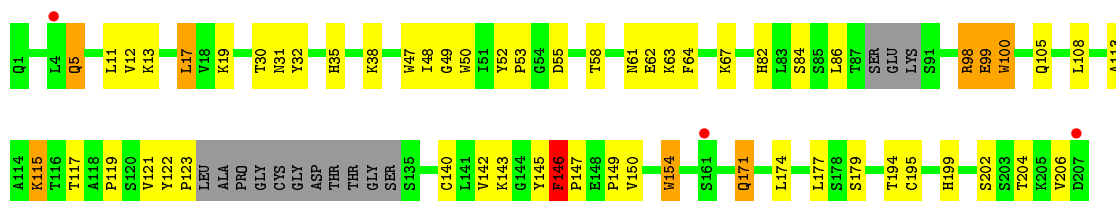
- Molecule 2: Insulin B chain

Chain J: 

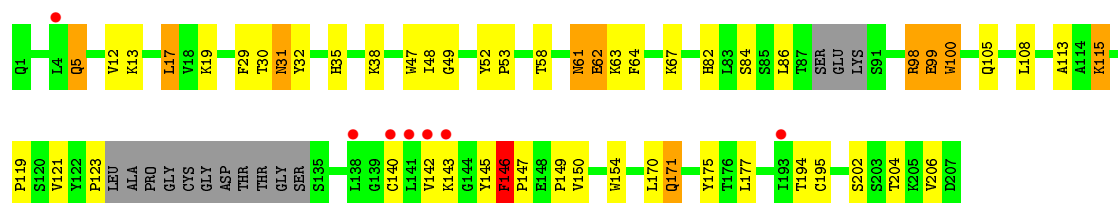


- Molecule 3: MONOCLONAL ANTIBODY FAB 83-14 - HEAVY CHAIN

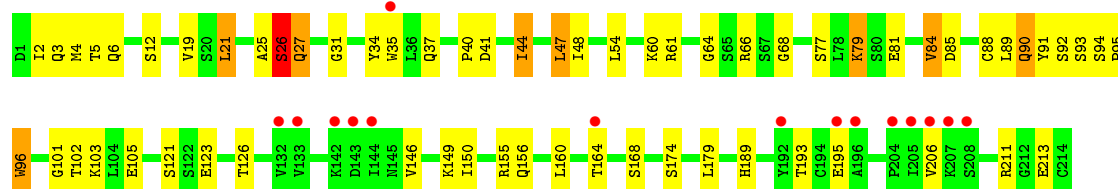
Chain C: 



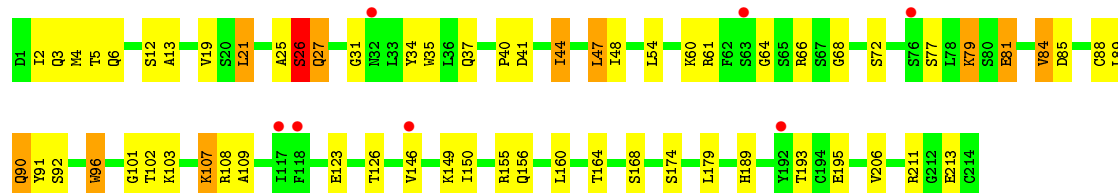
- Molecule 3: MONOCLONAL ANTIBODY FAB 83-14 - HEAVY CHAIN



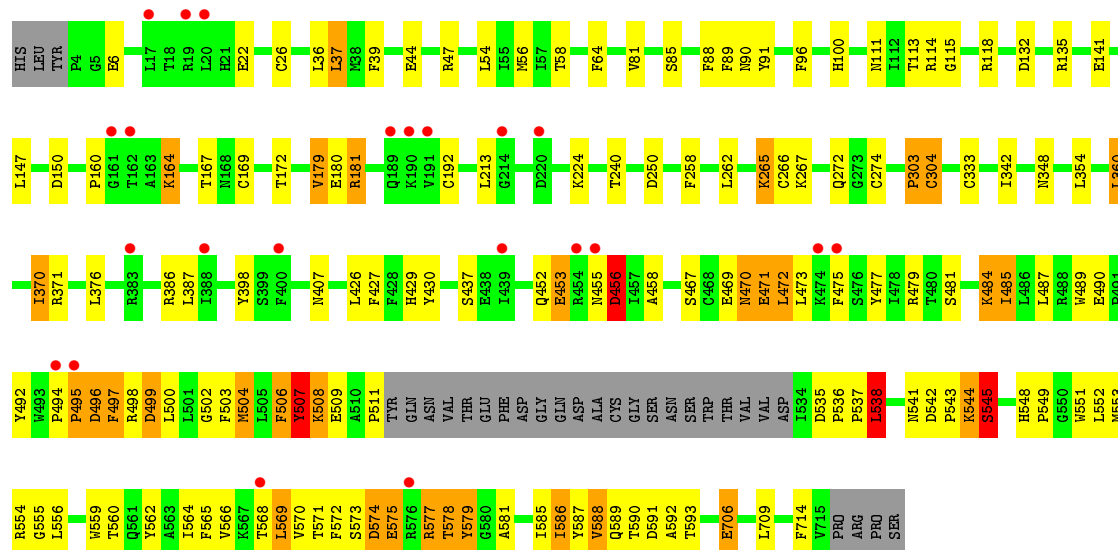
• Molecule 4: MONOCLONAL ANTIBODY FAB 83-14 - LIGHT CHAIN



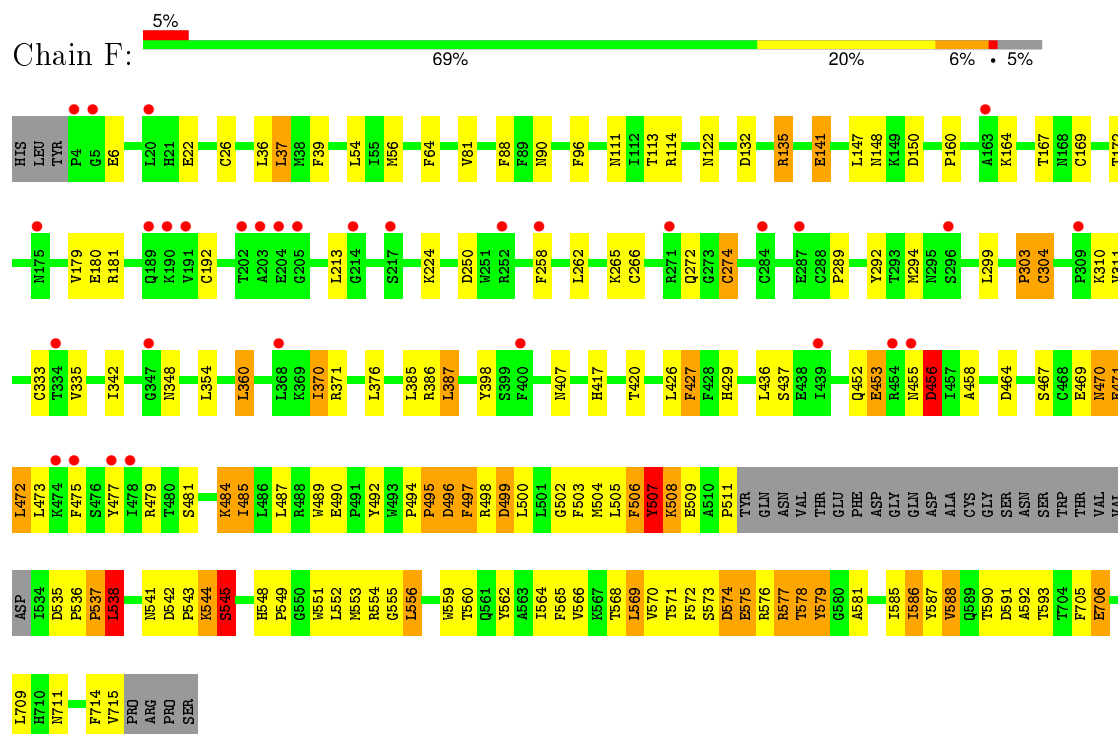
• Molecule 4: MONOCLONAL ANTIBODY FAB 83-14 - LIGHT CHAIN



• Molecule 5: INSULIN RECEPTOR DOMAINS L1-CR-L2-(FNIII-1)-ALPHA CT



• Molecule 5: INSULIN RECEPTOR DOMAINS L1-CR-L2-(FNIII-1)-ALPHACT



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	118.15Å 140.10Å 190.02Å 90.00° 95.04° 90.00°	Depositor
Resolution (Å)	42.49 – 4.40 56.31 – 4.40	Depositor EDS
% Data completeness (in resolution range)	88.1 (42.49-4.40) 88.0 (56.31-4.40)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 4.46Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.245 , 0.262 0.271 , 0.305	Depositor DCC
R_{free} test set	885 reflections (5.11%)	DCC
Wilson B-factor (Å ²)	172.2	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 197.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 17335 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	16158	wwPDB-VP
Average B, all atoms (Å ²)	230.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.37% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.70	0/161	1.05	0/216
1	I	0.66	0/161	1.03	0/216
2	B	0.60	0/129	0.81	0/174
2	J	0.58	0/129	0.80	0/174
3	C	0.51	0/1509	0.90	1/2062 (0.0%)
3	P	0.52	0/1509	0.91	1/2062 (0.0%)
4	D	0.47	0/1688	0.83	3/2287 (0.1%)
4	Q	0.48	0/1688	0.84	3/2287 (0.1%)
5	E	0.50	0/4784	0.83	4/6479 (0.1%)
5	F	0.49	0/4784	0.84	4/6479 (0.1%)
All	All	0.50	0/16542	0.85	16/22436 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	303	PRO	N-CA-C	7.02	130.35	112.10
5	E	538	LEU	CA-CB-CG	6.83	131.00	115.30
5	F	538	LEU	CA-CB-CG	6.80	130.95	115.30
5	E	303	PRO	N-CA-C	6.77	129.71	112.10
4	D	31	GLY	C-N-CA	6.40	137.70	121.70
4	D	44	ILE	CB-CA-C	6.36	124.32	111.60
5	E	456	ASP	N-CA-C	6.00	127.20	111.00
5	F	456	ASP	N-CA-C	5.95	127.07	111.00
4	Q	31	GLY	C-N-CA	5.93	136.53	121.70
5	E	509	GLU	N-CA-C	5.69	126.37	111.00
5	F	509	GLU	N-CA-C	5.66	126.29	111.00
4	Q	26	SER	C-N-CA	5.63	135.77	121.70
4	D	26	SER	C-N-CA	5.48	135.39	121.70
3	P	146	PHE	N-CA-CB	5.23	120.01	110.60
3	C	146	PHE	N-CA-CB	5.20	119.97	110.60
4	Q	44	ILE	CB-CA-C	5.18	121.96	111.60

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	160	0	145	7	0
1	I	160	0	145	1	0
2	B	127	0	120	4	0
2	J	127	0	120	2	0
3	C	1468	0	1433	44	0
3	P	1468	0	1433	37	0
4	D	1652	0	1582	36	0
4	Q	1652	0	1582	40	0
5	E	4672	0	4560	107	1
5	F	4672	0	4560	111	1
All	All	16158	0	15680	355	1

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 11.

All (355) 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)
5:F:487:LEU:HD11	5:F:564:ILE:HD12	1.41	0.99
5:E:487:LEU:HD11	5:E:564:ILE:HD12	1.42	0.98
5:F:502:GLY:CA	5:F:538:LEU:HG	1.98	0.93
5:E:502:GLY:CA	5:E:538:LEU:HG	1.99	0.93
5:E:498:ARG:CZ	5:E:570:VAL:HA	2.01	0.91
5:F:498:ARG:CZ	5:F:570:VAL:HA	2.01	0.90
5:E:504:MET:O	5:E:536:PRO:HD2	1.70	0.89
5:F:502:GLY:HA3	5:F:538:LEU:HG	1.55	0.89
5:F:544:LYS:HD3	5:F:545:SER:H	1.39	0.87
4:Q:37:GLN:HB2	4:Q:47:LEU:HD21	1.57	0.86
5:F:504:MET:O	5:F:536:PRO:HD2	1.75	0.85
5:E:544:LYS:HD3	5:E:545:SER:H	1.39	0.85
5:E:502:GLY:HA3	5:E:538:LEU:HG	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:100:TRP:CB	4:D:34:TYR:HE2	1.92	0.82
5:E:498:ARG:NH2	5:E:570:VAL:HA	1.95	0.82
5:F:559:TRP:CE3	5:F:592:ALA:HB2	2.16	0.80
4:D:37:GLN:HB2	4:D:47:LEU:HD21	1.65	0.79
5:E:559:TRP:CE3	5:E:592:ALA:HB2	2.18	0.79
5:F:498:ARG:NH2	5:F:570:VAL:HA	1.97	0.79
5:E:452:GLN:HG3	5:E:456:ASP:OD2	1.81	0.79
3:C:100:TRP:HB2	4:D:34:TYR:HE2	1.48	0.78
5:E:503:PHE:HD2	5:E:565:PHE:CZ	2.02	0.78
3:P:100:TRP:CB	4:Q:34:TYR:HE2	1.97	0.78
5:E:544:LYS:HD3	5:E:545:SER:N	1.98	0.77
5:F:489:TRP:O	5:F:549:PRO:HD2	1.86	0.76
5:E:485:ILE:HD12	5:E:588:VAL:HG21	1.66	0.76
3:P:30:THR:O	3:P:31:ASN:HB2	1.85	0.75
4:Q:84:VAL:HG13	4:Q:85:ASP:H	1.52	0.75
5:F:503:PHE:HD2	5:F:565:PHE:CZ	2.04	0.74
5:F:544:LYS:HD3	5:F:545:SER:N	2.00	0.74
2:B:6:LEU:HD13	2:B:11:LEU:HA	1.68	0.74
5:E:568:THR:HG23	5:E:581:ALA:O	1.88	0.73
4:Q:48:ILE:HG22	4:Q:54:LEU:HA	1.69	0.73
4:D:2:ILE:HG22	4:D:4:MET:HE2	1.71	0.73
5:F:452:GLN:HG3	5:F:456:ASP:OD2	1.89	0.72
5:F:502:GLY:HA3	5:F:538:LEU:CG	2.18	0.72
4:Q:2:ILE:HG22	4:Q:4:MET:HE2	1.72	0.71
5:F:487:LEU:HD11	5:F:564:ILE:CD1	2.19	0.71
3:C:31:ASN:HA	3:C:52:TYR:OH	1.91	0.71
5:E:342:ILE:HB	5:E:370:ILE:HD12	1.73	0.71
5:E:489:TRP:O	5:E:549:PRO:HD2	1.90	0.70
5:E:487:LEU:HD11	5:E:564:ILE:CD1	2.20	0.70
4:D:4:MET:HE1	4:D:25:ALA:HA	1.73	0.70
5:E:503:PHE:CD2	5:E:565:PHE:CZ	2.79	0.69
5:E:502:GLY:HA3	5:E:538:LEU:CG	2.21	0.69
3:C:63:LYS:HA	5:F:147:LEU:HD21	1.73	0.69
5:F:503:PHE:CD2	5:F:565:PHE:CZ	2.81	0.68
5:F:485:ILE:HD12	5:F:588:VAL:HG21	1.73	0.68
3:C:17:LEU:HB2	3:C:82:HIS:CE1	2.28	0.68
3:P:17:LEU:HB2	3:P:82:HIS:CE1	2.29	0.68
3:P:35:HIS:HD2	3:P:47:TRP:HE1	1.39	0.68
5:F:559:TRP:HE3	5:F:592:ALA:HB2	1.56	0.68
5:F:568:THR:HG23	5:F:581:ALA:O	1.94	0.68
4:D:150:ILE:HD11	4:D:179:LEU:HD21	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:100:TRP:HB2	4:Q:34:TYR:HE2	1.60	0.67
3:C:30:THR:O	3:C:31:ASN:HB2	1.94	0.67
5:E:498:ARG:NH1	5:E:571:THR:H	1.91	0.67
3:P:31:ASN:HA	3:P:52:TYR:OH	1.96	0.66
5:F:498:ARG:NH1	5:F:571:THR:H	1.93	0.66
5:E:467:SER:HA	5:E:579:TYR:HB3	1.78	0.66
4:D:84:VAL:HG13	4:D:85:ASP:H	1.58	0.66
4:Q:4:MET:HE1	4:Q:25:ALA:HA	1.76	0.66
5:E:511:PRO:HG3	5:E:587:TYR:OH	1.96	0.65
5:E:553:MET:HB3	5:E:556:LEU:HD21	1.78	0.65
4:Q:150:ILE:HD11	4:Q:179:LEU:HD21	1.76	0.65
4:D:2:ILE:HG22	4:D:4:MET:CE	2.25	0.65
5:F:506:PHE:CE2	5:F:560:THR:HG21	2.32	0.65
4:Q:84:VAL:CG1	4:Q:85:ASP:H	2.10	0.65
5:F:559:TRP:CE3	5:F:592:ALA:CB	2.79	0.65
4:Q:84:VAL:CG1	4:Q:85:ASP:N	2.60	0.65
3:P:121:VAL:HG22	3:P:142:VAL:HG13	1.78	0.65
5:E:494:PRO:HB3	5:E:578:THR:HG21	1.77	0.65
3:C:35:HIS:HD2	3:C:47:TRP:HE1	1.44	0.64
5:E:469:GLU:HB3	5:E:579:TYR:HB2	1.78	0.64
4:Q:26:SER:HB3	4:Q:27:GLN:HG3	1.79	0.64
4:D:21:LEU:HD22	4:D:102:THR:HG21	1.80	0.64
4:D:48:ILE:HG22	4:D:54:LEU:HA	1.80	0.63
4:D:84:VAL:CG1	4:D:85:ASP:H	2.12	0.63
2:J:6:LEU:HD13	2:J:11:LEU:HA	1.80	0.63
5:E:499:ASP:HB2	5:E:569:LEU:HB3	1.80	0.63
4:Q:21:LEU:HD22	4:Q:102:THR:HG21	1.81	0.63
5:E:559:TRP:CE3	5:E:592:ALA:CB	2.81	0.63
4:D:40:PRO:HD3	4:D:84:VAL:HG22	1.81	0.62
5:F:553:MET:HB3	5:F:556:LEU:HD21	1.82	0.62
5:F:499:ASP:HB2	5:F:569:LEU:HB3	1.81	0.61
5:E:559:TRP:HE3	5:E:592:ALA:HB2	1.62	0.61
4:Q:40:PRO:HD3	4:Q:84:VAL:HG22	1.81	0.61
5:F:494:PRO:HB3	5:F:578:THR:HG21	1.82	0.61
5:E:494:PRO:O	5:E:495:PRO:C	2.39	0.61
5:F:132:ASP:HB2	5:F:181:ARG:HD2	1.83	0.60
5:F:503:PHE:HB3	5:F:535:ASP:HB3	1.83	0.60
3:P:100:TRP:HB3	4:Q:34:TYR:HE2	1.67	0.60
4:D:84:VAL:CG1	4:D:85:ASP:N	2.63	0.60
4:D:6:GLN:NE2	4:D:101:GLY:H	2.00	0.60
3:C:17:LEU:HD13	3:C:82:HIS:HE1	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:132:ASP:HB2	5:E:181:ARG:HD2	1.84	0.60
3:C:115:LYS:H	3:C:115:LYS:HE3	1.67	0.59
4:Q:91:TYR:HB2	4:Q:96:TRP:CZ3	2.37	0.59
5:F:342:ILE:HB	5:F:370:ILE:HD12	1.83	0.59
3:C:115:LYS:NZ	3:C:174:LEU:HD21	2.17	0.59
5:F:494:PRO:O	5:F:495:PRO:C	2.42	0.58
5:F:499:ASP:HB2	5:F:569:LEU:CB	2.33	0.58
5:E:556:LEU:HD22	5:E:562:TYR:CE2	2.38	0.58
3:P:98:ARG:O	3:P:100:TRP:N	2.37	0.58
5:E:485:ILE:HD12	5:E:588:VAL:CG2	2.34	0.57
5:F:552:LEU:HD12	5:F:553:MET:N	2.19	0.57
5:F:492:TYR:CE2	5:F:494:PRO:HG3	2.40	0.57
5:E:552:LEU:HD12	5:E:553:MET:N	2.19	0.57
3:C:100:TRP:HB3	4:D:34:TYR:HE2	1.69	0.57
5:F:556:LEU:HD22	5:F:562:TYR:CE2	2.39	0.57
5:F:511:PRO:HG3	5:F:587:TYR:OH	2.04	0.57
5:E:499:ASP:HB2	5:E:569:LEU:CB	2.35	0.57
3:C:98:ARG:O	3:C:100:TRP:N	2.38	0.57
4:Q:4:MET:CE	4:Q:25:ALA:HA	2.34	0.57
5:F:553:MET:O	5:F:555:GLY:N	2.35	0.57
5:F:556:LEU:HB3	5:F:562:TYR:CZ	2.39	0.57
5:E:706:GLU:HG2	5:F:96:PHE:HZ	1.69	0.57
5:F:36:LEU:HD12	5:F:37:LEU:CD2	2.35	0.56
5:E:706:GLU:HG2	5:F:96:PHE:CZ	2.40	0.56
3:C:98:ARG:HG2	3:C:98:ARG:HH11	1.70	0.56
3:C:115:LYS:HZ1	3:C:174:LEU:HD21	1.70	0.56
4:D:48:ILE:CD1	4:D:64:GLY:HA3	2.35	0.56
5:E:503:PHE:HB3	5:E:535:ASP:HB3	1.86	0.56
4:Q:2:ILE:HG22	4:Q:4:MET:CE	2.34	0.56
5:E:498:ARG:NE	5:E:569:LEU:O	2.40	0.55
5:F:469:GLU:HB3	5:F:579:TYR:HB2	1.89	0.55
3:C:119:PRO:HB3	3:C:145:TYR:HB3	1.89	0.55
3:C:121:VAL:HG22	3:C:142:VAL:HG13	1.89	0.55
5:E:492:TYR:CE2	5:E:494:PRO:HG3	2.42	0.54
3:P:12:VAL:HG21	3:P:86:LEU:HD13	1.89	0.54
5:F:360:LEU:H	5:F:360:LEU:HD22	1.72	0.54
4:Q:164:THR:HG22	4:Q:174:SER:H	1.70	0.54
5:E:398:TYR:OH	5:E:455:ASN:HB2	2.06	0.54
5:E:96:PHE:CZ	5:F:706:GLU:HG2	2.43	0.54
5:F:560:THR:H	5:F:590:THR:HG23	1.73	0.54
5:E:37:LEU:HD12	5:E:39:PHE:CZ	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:119:PRO:HB3	3:P:145:TYR:HB3	1.90	0.54
5:F:370:ILE:HD11	5:F:376:LEU:HD12	1.89	0.53
5:E:96:PHE:HZ	5:F:706:GLU:HG2	1.74	0.53
5:F:485:ILE:HD12	5:F:588:VAL:CG2	2.38	0.53
3:P:123:PRO:HG2	4:Q:123:GLU:OE1	2.08	0.53
5:E:370:ILE:HD11	5:E:376:LEU:HD12	1.90	0.53
5:E:556:LEU:HB3	5:E:562:TYR:CZ	2.43	0.53
5:E:169:CYS:HB2	5:E:180:GLU:HG2	1.91	0.53
5:F:497:PHE:O	5:F:498:ARG:HG2	2.09	0.53
3:C:98:ARG:NH1	3:C:98:ARG:HG2	2.24	0.53
5:E:111:ASN:HD22	5:E:213:LEU:HD21	1.74	0.53
4:D:90:GLN:HG2	4:D:92:SER:H	1.74	0.52
3:C:121:VAL:HB	3:C:206:VAL:HG11	1.91	0.52
5:E:551:TRP:HA	5:E:551:TRP:CE3	2.44	0.52
3:C:50:TRP:CZ2	5:E:479:ARG:HD2	2.45	0.52
4:D:26:SER:HB3	4:D:27:GLN:HG3	1.92	0.52
5:E:499:ASP:O	5:E:569:LEU:N	2.34	0.52
3:P:100:TRP:HB3	4:Q:34:TYR:CE2	2.45	0.52
5:F:499:ASP:O	5:F:569:LEU:N	2.32	0.52
5:E:258:PHE:O	5:E:262:LEU:HD13	2.10	0.52
5:F:565:PHE:HB3	5:F:585:ILE:HA	1.92	0.51
5:E:553:MET:O	5:E:555:GLY:N	2.37	0.51
5:F:258:PHE:O	5:F:262:LEU:HD13	2.11	0.51
5:F:472:LEU:HD12	5:F:472:LEU:O	2.10	0.51
3:P:19:LYS:NZ	3:P:82:HIS:HB2	2.26	0.51
5:E:506:PHE:CE2	5:E:560:THR:HG21	2.46	0.51
3:C:47:TRP:CZ2	3:C:49:GLY:HA2	2.46	0.51
5:E:179:VAL:HG12	5:E:181:ARG:CZ	2.40	0.51
5:F:551:TRP:CE3	5:F:551:TRP:HA	2.45	0.51
5:E:360:LEU:HD22	5:E:360:LEU:H	1.76	0.51
5:E:497:PHE:O	5:E:498:ARG:HG2	2.11	0.51
2:J:19:CYS:C	2:J:21:GLU:H	2.14	0.51
5:F:311:VAL:HB	5:F:335:VAL:HB	1.92	0.51
5:F:498:ARG:NE	5:F:569:LEU:O	2.44	0.51
3:P:98:ARG:HG2	3:P:98:ARG:HH11	1.75	0.51
3:P:98:ARG:O	3:P:99:GLU:C	2.50	0.51
3:C:12:VAL:HG21	3:C:86:LEU:HD13	1.92	0.51
1:A:1:GLY:HA3	5:F:711:ASN:HA	1.93	0.51
5:E:565:PHE:HB3	5:E:585:ILE:HA	1.92	0.50
5:F:502:GLY:N	5:F:538:LEU:HG	2.26	0.50
5:E:36:LEU:HD12	5:E:37:LEU:CD2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:48:ILE:CD1	4:Q:64:GLY:HA3	2.41	0.50
5:F:56:MET:HG3	5:F:81:VAL:HB	1.92	0.50
3:C:98:ARG:O	3:C:99:GLU:C	2.49	0.50
5:F:111:ASN:HD22	5:F:213:LEU:HD21	1.76	0.50
1:A:12:SER:O	1:A:16:LEU:HD12	2.11	0.50
3:C:100:TRP:HB3	4:D:34:TYR:CE2	2.46	0.50
3:C:171:GLN:HB2	4:D:160:LEU:HD21	1.93	0.50
3:C:100:TRP:HB2	4:D:34:TYR:CE2	2.38	0.50
4:Q:195:GLU:HG2	4:Q:206:VAL:HG22	1.94	0.49
4:Q:6:GLN:NE2	4:Q:101:GLY:H	2.10	0.49
5:F:560:THR:H	5:F:590:THR:CG2	2.26	0.49
5:E:147:LEU:HD21	3:P:63:LYS:HA	1.94	0.49
5:E:502:GLY:HA2	5:E:566:VAL:HA	1.95	0.49
3:P:98:ARG:HG2	3:P:98:ARG:NH1	2.27	0.49
4:D:4:MET:CE	4:D:25:ALA:HA	2.41	0.49
4:Q:91:TYR:HB2	4:Q:96:TRP:HZ3	1.76	0.49
5:E:538:LEU:HD22	5:E:553:MET:CE	2.43	0.49
5:F:311:VAL:CG1	5:F:335:VAL:HB	2.42	0.49
5:F:429:HIS:CD2	5:F:458:ALA:HB2	2.48	0.49
5:F:477:TYR:OH	5:F:479:ARG:HB2	2.13	0.48
4:Q:90:GLN:HG2	4:Q:92:SER:H	1.78	0.48
4:D:91:TYR:HB2	4:D:96:TRP:CZ3	2.48	0.48
5:E:502:GLY:N	5:E:538:LEU:HG	2.28	0.48
5:F:426:LEU:O	5:F:456:ASP:OD2	2.32	0.48
4:Q:2:ILE:HD12	4:Q:90:GLN:NE2	2.28	0.48
5:E:88:PHE:CZ	5:F:709:LEU:HD12	2.49	0.48
4:D:195:GLU:HG2	4:D:206:VAL:HG22	1.94	0.48
5:F:289:PRO:HG2	5:F:292:TYR:CD2	2.49	0.48
5:F:179:VAL:HG12	5:F:181:ARG:CZ	2.44	0.48
5:E:467:SER:HA	5:E:579:TYR:CD2	2.49	0.48
5:F:169:CYS:HB2	5:F:180:GLU:HG2	1.96	0.47
4:Q:108:ARG:NH1	4:Q:109:ALA:O	2.46	0.47
3:P:47:TRP:CZ2	3:P:49:GLY:HA2	2.49	0.47
5:F:36:LEU:HD12	5:F:37:LEU:HD22	1.95	0.47
5:E:548:HIS:HA	5:E:549:PRO:HD3	1.81	0.47
1:I:13:LEU:H	1:I:13:LEU:HD12	1.78	0.47
5:E:503:PHE:HD2	5:E:565:PHE:CE1	2.32	0.47
5:F:489:TRP:HE1	5:F:500:LEU:HD13	1.80	0.47
3:C:13:LYS:HD3	3:C:113:ALA:HA	1.95	0.47
5:F:398:TYR:OH	5:F:455:ASN:HB2	2.14	0.47
1:A:13:LEU:H	1:A:13:LEU:HD12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:38:LYS:HB2	3:C:48:ILE:HD11	1.97	0.47
5:F:464:ASP:O	5:F:577:ARG:NH2	2.48	0.47
5:E:56:MET:HG3	5:E:81:VAL:HB	1.96	0.47
5:F:470:ASN:HB3	5:F:471:GLU:H	1.51	0.47
3:C:17:LEU:HD13	3:C:82:HIS:CE1	2.49	0.46
3:P:35:HIS:HD2	3:P:47:TRP:NE1	2.11	0.46
5:E:181:ARG:HD3	5:E:181:ARG:HA	1.76	0.46
3:C:19:LYS:NZ	3:C:82:HIS:HB2	2.30	0.46
3:C:32:TYR:O	3:C:53:PRO:HD2	2.15	0.46
5:E:429:HIS:CD2	5:E:458:ALA:HB2	2.51	0.46
5:E:502:GLY:HA3	5:E:566:VAL:HG12	1.98	0.46
5:E:472:LEU:HD12	5:E:472:LEU:O	2.15	0.46
3:P:64:PHE:HA	3:P:67:LYS:HD2	1.97	0.46
5:F:495:PRO:O	5:F:496:ASP:HB2	2.15	0.46
4:D:149:LYS:HB2	4:D:193:THR:HB	1.98	0.46
5:F:507:TYR:CG	5:F:508:LYS:N	2.83	0.46
5:F:311:VAL:HG11	5:F:335:VAL:HB	1.97	0.46
3:C:64:PHE:HA	3:C:67:LYS:HD2	1.96	0.46
4:Q:91:TYR:CB	4:Q:96:TRP:CE3	2.99	0.46
3:P:29:PHE:CE2	3:P:53:PRO:HB3	2.51	0.46
3:C:5:GLN:OE1	3:C:105:GLN:NE2	2.49	0.46
4:Q:2:ILE:HD12	4:Q:90:GLN:HE21	1.81	0.46
3:C:52:TYR:HB3	3:C:55:ASP:OD1	2.15	0.46
5:E:489:TRP:HE1	5:E:500:LEU:HD13	1.81	0.46
3:P:32:TYR:O	3:P:53:PRO:HD2	2.15	0.46
5:E:536:PRO:HA	5:E:537:PRO:HD3	1.83	0.45
4:D:121:SER:HB2	4:D:123:GLU:OE2	2.16	0.45
4:D:26:SER:HB3	4:D:27:GLN:H	1.36	0.45
4:D:189:HIS:O	4:D:211:ARG:NH1	2.50	0.45
5:E:560:THR:H	5:E:590:THR:HG23	1.80	0.45
3:P:13:LYS:HD3	3:P:113:ALA:HA	1.97	0.45
2:B:13:GLU:O	2:B:15:LEU:N	2.48	0.45
3:C:100:TRP:CB	4:D:34:TYR:CE2	2.84	0.45
5:E:467:SER:HA	5:E:579:TYR:HD2	1.81	0.45
3:P:121:VAL:HB	3:P:206:VAL:HG11	1.99	0.45
5:E:477:TYR:OH	5:E:479:ARG:HB2	2.17	0.45
4:Q:79:LYS:HA	4:Q:79:LYS:HD2	1.86	0.45
5:E:44:GLU:HB2	5:E:47:ARG:HH11	1.81	0.45
3:C:63:LYS:HG3	5:F:147:LEU:HD21	1.99	0.45
5:E:467:SER:CA	5:E:579:TYR:HB3	2.45	0.45
5:E:551:TRP:HA	5:E:551:TRP:HE3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:311:VAL:CB	5:F:335:VAL:HB	2.47	0.45
5:E:503:PHE:O	5:E:564:ILE:HA	2.17	0.45
5:F:502:GLY:HA2	5:F:566:VAL:HA	1.98	0.45
4:Q:48:ILE:HG22	4:Q:54:LEU:CA	2.42	0.45
5:F:387:LEU:HD22	5:F:420:THR:HB	1.99	0.45
5:E:507:TYR:CG	5:E:508:LYS:N	2.84	0.45
1:A:2:ILE:CG2	2:B:11:LEU:HD21	2.47	0.45
5:F:551:TRP:HA	5:F:551:TRP:HE3	1.81	0.45
5:F:294:MET:SD	5:F:299:LEU:HA	2.57	0.45
1:A:19:TYR:CE1	5:F:715:VAL:HA	2.52	0.45
5:E:467:SER:HB2	5:E:579:TYR:O	2.16	0.44
5:E:575:GLU:O	5:E:577:ARG:HG2	2.17	0.44
3:C:98:ARG:HG3	3:C:99:GLU:N	2.31	0.44
3:C:63:LYS:HA	5:F:147:LEU:HD11	1.99	0.44
5:F:484:LYS:HB2	5:F:552:LEU:HD11	1.99	0.44
3:C:154:TRP:CZ3	3:C:179:SER:HB3	2.52	0.44
3:P:61:ASN:HD22	3:P:62:GLU:N	2.15	0.44
5:E:36:LEU:HD12	5:E:37:LEU:HD22	1.99	0.44
4:Q:149:LYS:HD2	4:Q:195:GLU:OE1	2.17	0.44
4:Q:79:LYS:HE3	4:Q:81:GLU:OE1	2.17	0.44
4:Q:91:TYR:CB	4:Q:96:TRP:HE3	2.30	0.44
5:E:64:PHE:HA	5:E:96:PHE:O	2.17	0.44
5:F:475:PHE:CE2	5:F:586:ILE:HD11	2.53	0.44
5:E:484:LYS:HB2	5:E:552:LEU:HD11	2.00	0.44
5:F:64:PHE:HA	5:F:96:PHE:O	2.18	0.44
3:P:146:PHE:O	3:P:147:PRO:C	2.56	0.44
3:P:38:LYS:HB2	3:P:48:ILE:HD11	1.98	0.44
5:F:37:LEU:HD12	5:F:39:PHE:CZ	2.52	0.43
3:C:50:TRP:CE2	5:E:479:ARG:HD2	2.53	0.43
4:D:149:LYS:HD2	4:D:195:GLU:OE1	2.18	0.43
5:E:502:GLY:C	5:E:538:LEU:HG	2.39	0.43
4:D:79:LYS:HD2	4:D:79:LYS:HA	1.88	0.43
5:F:503:PHE:O	5:F:564:ILE:HA	2.18	0.43
3:P:19:LYS:HZ3	3:P:82:HIS:HB2	1.81	0.43
4:Q:91:TYR:HB2	4:Q:96:TRP:CE3	2.53	0.43
5:F:572:PHE:CZ	5:F:579:TYR:HA	2.53	0.43
5:E:147:LEU:HD21	3:P:63:LYS:HG3	1.99	0.43
4:D:164:THR:HG22	4:D:174:SER:H	1.83	0.43
5:F:575:GLU:O	5:F:577:ARG:HG2	2.18	0.43
3:P:171:GLN:HB2	4:Q:160:LEU:HD21	2.01	0.43
3:C:35:HIS:HD2	3:C:47:TRP:NE1	2.14	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:266:CYS:HB3	5:E:274:CYS:HB3	1.85	0.43
3:C:122:TYR:HA	3:C:123:PRO:HD3	1.88	0.43
5:E:585:ILE:HD11	5:E:587:TYR:CE2	2.54	0.43
5:E:265:LYS:HB3	5:E:267:LYS:HE3	2.01	0.43
3:C:11:LEU:HD23	3:C:146:PHE:CE2	2.53	0.43
5:E:538:LEU:HD22	5:E:553:MET:HE3	2.00	0.43
5:E:426:LEU:O	5:E:456:ASP:OD2	2.35	0.43
5:E:495:PRO:O	5:E:496:ASP:HB2	2.18	0.42
4:Q:149:LYS:HB2	4:Q:193:THR:HB	1.99	0.42
5:F:560:THR:O	5:F:590:THR:HG22	2.19	0.42
5:E:560:THR:H	5:E:590:THR:CG2	2.32	0.42
3:C:146:PHE:O	3:C:147:PRO:C	2.55	0.42
2:B:19:CYS:C	2:B:21:GLU:H	2.23	0.42
5:F:536:PRO:HA	5:F:537:PRO:HD3	1.83	0.42
3:P:35:HIS:CD2	3:P:47:TRP:HE1	2.28	0.42
3:P:170:LEU:HB3	3:P:175:TYR:CE1	2.53	0.42
4:D:27:GLN:NE2	5:F:141:GLU:O	2.52	0.42
5:F:492:TYR:HE2	5:F:494:PRO:HG3	1.84	0.42
5:F:266:CYS:HB3	5:F:274:CYS:HB3	1.80	0.42
3:P:98:ARG:HG3	3:P:99:GLU:N	2.34	0.42
3:P:5:GLN:OE1	3:P:105:GLN:NE2	2.53	0.42
5:F:181:ARG:HA	5:F:181:ARG:HD3	1.77	0.42
5:F:135:ARG:HA	5:F:135:ARG:HH11	1.85	0.42
5:E:89:PHE:CE2	5:F:705:PHE:HA	2.55	0.42
5:F:503:PHE:HD2	5:F:565:PHE:CE1	2.37	0.42
5:F:548:HIS:HA	5:F:549:PRO:HD3	1.80	0.42
4:Q:35:TRP:CZ3	4:Q:88:CYS:HB3	2.55	0.42
4:D:94:SER:HB3	4:D:95:PRO:HD3	2.02	0.41
5:E:58:THR:HG22	5:E:85:SER:OG	2.20	0.41
5:F:427:PHE:CD1	5:F:427:PHE:C	2.93	0.41
5:E:470:ASN:HB3	5:E:471:GLU:H	1.54	0.41
5:E:572:PHE:CZ	5:E:579:TYR:HA	2.56	0.41
1:A:19:TYR:CE2	5:F:715:VAL:HG22	2.55	0.41
5:E:89:PHE:HE2	5:F:705:PHE:HA	1.85	0.41
3:C:117:THR:O	3:C:199:HIS:HE1	2.03	0.41
5:E:475:PHE:CE2	5:E:586:ILE:HD11	2.56	0.41
5:F:502:GLY:HA3	5:F:566:VAL:HG12	2.02	0.41
4:Q:189:HIS:O	4:Q:211:ARG:NH1	2.53	0.41
5:F:505:LEU:HB3	5:F:506:PHE:H	1.64	0.41
3:P:119:PRO:HB2	3:P:142:VAL:HG12	2.03	0.41
5:E:91:TYR:CE2	5:E:118:ARG:HD3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:585:ILE:HD11	5:F:587:TYR:CE2	2.56	0.41
5:F:122:ASN:HD22	5:F:148:ASN:ND2	2.19	0.41
4:Q:13:ALA:HA	4:Q:107:LYS:HE3	2.03	0.41
5:E:164:LYS:HB3	5:E:164:LYS:HE2	1.96	0.41
5:F:502:GLY:C	5:F:538:LEU:HG	2.41	0.40
5:F:385:LEU:O	5:F:417:HIS:NE2	2.41	0.40
5:E:709:LEU:HD12	5:F:88:PHE:CZ	2.56	0.40
4:D:35:TRP:CZ3	4:D:88:CYS:HB3	2.55	0.40
5:E:560:THR:O	5:E:589:GLN:HA	2.21	0.40
1:A:19:TYR:CZ	5:F:715:VAL:HA	2.56	0.40
3:P:115:LYS:HG3	3:P:115:LYS:H	1.78	0.40
4:D:2:ILE:CG2	4:D:4:MET:CE	2.97	0.40
5:E:494:PRO:CB	5:E:578:THR:HG21	2.49	0.40
5:E:265:LYS:HB3	5:E:267:LYS:NZ	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:430:TYR:OH	5:F:571:THR:OG1[2_655]	1.86	0.34

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	19/21 (90%)	15 (79%)	4 (21%)	0	100	100
1	I	19/21 (90%)	16 (84%)	2 (10%)	1 (5%)	2	30
2	B	15/30 (50%)	11 (73%)	2 (13%)	2 (13%)	0	7
2	J	15/30 (50%)	11 (73%)	2 (13%)	2 (13%)	0	7
3	C	187/207 (90%)	170 (91%)	12 (6%)	5 (3%)	6	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	P	187/207 (90%)	171 (91%)	10 (5%)	6 (3%)	5	43
4	D	212/214 (99%)	199 (94%)	8 (4%)	5 (2%)	7	49
4	Q	212/214 (99%)	197 (93%)	10 (5%)	5 (2%)	7	49
5	E	576/609 (95%)	505 (88%)	47 (8%)	24 (4%)	3	35
5	F	576/609 (95%)	497 (86%)	55 (10%)	24 (4%)	3	35
All	All	2018/2162 (93%)	1792 (89%)	152 (8%)	74 (4%)	4	39

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	14	ALA
3	C	99	GLU
3	C	149	PRO
4	D	27	GLN
4	D	77	SER
4	D	213	GLU
5	E	164	LYS
5	E	304	CYS
5	E	456	ASP
5	E	470	ASN
5	E	495	PRO
5	E	541	ASN
5	E	543	PRO
5	E	545	SER
5	E	554	ARG
5	F	164	LYS
5	F	304	CYS
5	F	456	ASP
5	F	495	PRO
5	F	541	ASN
5	F	543	PRO
5	F	545	SER
5	F	554	ARG
3	P	99	GLU
3	P	149	PRO
4	Q	27	GLN
4	Q	77	SER
4	Q	213	GLU
2	B	13	GLU
3	C	100	TRP

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Mol	Chain	Res	Type
3	C	146	PHE
3	C	150	VAL
4	D	68	GLY
5	E	115	GLY
5	E	160	PRO
5	E	167	THR
5	E	303	PRO
5	E	407	ASN
5	E	507	TYR
5	E	579	TYR
5	F	114	ARG
5	F	160	PRO
5	F	167	THR
5	F	303	PRO
5	F	407	ASN
5	F	507	TYR
5	F	579	TYR
2	J	14	ALA
3	P	146	PHE
3	P	150	VAL
4	Q	68	GLY
4	D	26	SER
5	E	114	ARG
5	E	496	ASP
5	E	577	ARG
5	F	470	ASN
5	F	496	ASP
5	F	577	ARG
3	P	100	TRP
4	Q	26	SER
5	E	453	GLU
5	E	591	ASP
5	F	453	GLU
5	F	591	ASP
1	I	15	GLN
2	J	13	GLU
5	E	6	GLU
5	E	100	HIS
5	E	574	ASP
5	F	574	ASP
5	F	576	ARG
3	P	31	ASN

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Mol	Chain	Res	Type
5	F	6	GLU
5	F	537	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	19/19 (100%)	14 (74%)	5 (26%)	0	6
1	I	19/19 (100%)	14 (74%)	5 (26%)	0	6
2	B	14/25 (56%)	11 (79%)	3 (21%)	1	10
2	J	14/25 (56%)	11 (79%)	3 (21%)	1	10
3	C	164/174 (94%)	146 (89%)	18 (11%)	8	37
3	P	164/174 (94%)	146 (89%)	18 (11%)	8	37
4	D	190/190 (100%)	165 (87%)	25 (13%)	5	30
4	Q	190/190 (100%)	165 (87%)	25 (13%)	5	30
5	E	527/553 (95%)	470 (89%)	57 (11%)	8	38
5	F	527/553 (95%)	469 (89%)	58 (11%)	8	37
All	All	1828/1922 (95%)	1611 (88%)	217 (12%)	6	34

All (217) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	3	VAL
1	A	5	GLN
1	A	10	VAL
1	A	16	LEU
2	B	5	HIS
2	B	7	CYS
2	B	19	CYS
3	C	5	GLN
3	C	17	LEU
3	C	58	THR

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Mol	Chain	Res	Type
3	C	61	ASN
3	C	62	GLU
3	C	84	SER
3	C	98	ARG
3	C	108	LEU
3	C	115	LYS
3	C	140	CYS
3	C	143	LYS
3	C	154	TRP
3	C	171	GLN
3	C	177	LEU
3	C	194	THR
3	C	195	CYS
3	C	202	SER
3	C	204	THR
4	D	3	GLN
4	D	5	THR
4	D	12	SER
4	D	19	VAL
4	D	21	LEU
4	D	41	ASP
4	D	44	ILE
4	D	47	LEU
4	D	60	LYS
4	D	61	ARG
4	D	66	ARG
4	D	79	LYS
4	D	81	GLU
4	D	84	VAL
4	D	89	LEU
4	D	90	GLN
4	D	93	SER
4	D	96	TRP
4	D	103	LYS
4	D	105	GLU
4	D	126	THR
4	D	146	VAL
4	D	155	ARG
4	D	156	GLN
4	D	168	SER
5	E	22	GLU
5	E	26	CYS

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Mol	Chain	Res	Type
5	E	37	LEU
5	E	54	LEU
5	E	90	ASN
5	E	113	THR
5	E	135	ARG
5	E	141	GLU
5	E	150	ASP
5	E	172	THR
5	E	179	VAL
5	E	181	ARG
5	E	192	CYS
5	E	224	LYS
5	E	240	THR
5	E	250	ASP
5	E	265	LYS
5	E	272	GLN
5	E	304	CYS
5	E	333	CYS
5	E	348	ASN
5	E	354	LEU
5	E	360	LEU
5	E	370	ILE
5	E	371	ARG
5	E	386	ARG
5	E	387	LEU
5	E	427	PHE
5	E	437	SER
5	E	453	GLU
5	E	471	GLU
5	E	472	LEU
5	E	473	LEU
5	E	481	SER
5	E	484	LYS
5	E	485	ILE
5	E	490	GLU
5	E	497	PHE
5	E	499	ASP
5	E	504	MET
5	E	506	PHE
5	E	507	TYR
5	E	508	LYS
5	E	538	LEU

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Mol	Chain	Res	Type
5	E	542	ASP
5	E	544	LYS
5	E	545	SER
5	E	569	LEU
5	E	573	SER
5	E	574	ASP
5	E	575	GLU
5	E	578	THR
5	E	586	ILE
5	E	588	VAL
5	E	593	THR
5	E	706	GLU
5	E	714	PHE
5	F	22	GLU
5	F	26	CYS
5	F	37	LEU
5	F	54	LEU
5	F	90	ASN
5	F	113	THR
5	F	135	ARG
5	F	141	GLU
5	F	150	ASP
5	F	172	THR
5	F	192	CYS
5	F	224	LYS
5	F	250	ASP
5	F	265	LYS
5	F	272	GLN
5	F	274	CYS
5	F	304	CYS
5	F	310	LYS
5	F	333	CYS
5	F	348	ASN
5	F	354	LEU
5	F	360	LEU
5	F	370	ILE
5	F	371	ARG
5	F	386	ARG
5	F	387	LEU
5	F	427	PHE
5	F	436	LEU
5	F	437	SER

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Mol	Chain	Res	Type
5	F	453	GLU
5	F	467	SER
5	F	471	GLU
5	F	472	LEU
5	F	473	LEU
5	F	481	SER
5	F	484	LYS
5	F	485	ILE
5	F	490	GLU
5	F	497	PHE
5	F	499	ASP
5	F	506	PHE
5	F	507	TYR
5	F	508	LYS
5	F	538	LEU
5	F	542	ASP
5	F	544	LYS
5	F	545	SER
5	F	556	LEU
5	F	569	LEU
5	F	573	SER
5	F	574	ASP
5	F	575	GLU
5	F	578	THR
5	F	586	ILE
5	F	588	VAL
5	F	593	THR
5	F	706	GLU
5	F	714	PHE
1	I	2	ILE
1	I	3	VAL
1	I	5	GLN
1	I	10	VAL
1	I	16	LEU
2	J	5	HIS
2	J	7	CYS
2	J	19	CYS
3	P	5	GLN
3	P	17	LEU
3	P	58	THR
3	P	61	ASN
3	P	62	GLU

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Mol	Chain	Res	Type
3	P	84	SER
3	P	98	ARG
3	P	108	LEU
3	P	115	LYS
3	P	140	CYS
3	P	143	LYS
3	P	154	TRP
3	P	171	GLN
3	P	177	LEU
3	P	194	THR
3	P	195	CYS
3	P	202	SER
3	P	204	THR
4	Q	3	GLN
4	Q	5	THR
4	Q	12	SER
4	Q	19	VAL
4	Q	21	LEU
4	Q	41	ASP
4	Q	44	ILE
4	Q	47	LEU
4	Q	60	LYS
4	Q	61	ARG
4	Q	66	ARG
4	Q	72	SER
4	Q	79	LYS
4	Q	81	GLU
4	Q	84	VAL
4	Q	89	LEU
4	Q	90	GLN
4	Q	96	TRP
4	Q	103	LYS
4	Q	107	LYS
4	Q	126	THR
4	Q	146	VAL
4	Q	155	ARG
4	Q	156	GLN
4	Q	168	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	35	HIS
3	C	61	ASN
3	C	82	HIS
4	D	6	GLN
4	D	27	GLN
4	D	124	GLN
4	D	156	GLN
4	D	190	ASN
5	E	32	HIS
5	E	111	ASN
5	E	148	ASN
5	E	175	ASN
5	E	264	HIS
5	F	15	ASN
5	F	32	HIS
5	F	34	GLN
5	F	111	ASN
5	F	148	ASN
5	F	175	ASN
5	F	218	GLN
5	F	264	HIS
5	F	710	HIS
3	P	35	HIS
3	P	61	ASN
3	P	82	HIS
4	Q	6	GLN
4	Q	124	GLN
4	Q	190	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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 ⓘ

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	21/21 (100%)	-0.46	0 100 100	186, 211, 225, 231	0
1	I	21/21 (100%)	-0.54	0 100 100	172, 195, 205, 216	0
2	B	17/30 (56%)	-0.17	0 100 100	178, 207, 219, 246	0
2	J	17/30 (56%)	-0.29	0 100 100	164, 191, 204, 222	0
3	C	193/207 (93%)	0.04	3 (1%) 74 65	149, 217, 273, 289	0
3	P	193/207 (93%)	-0.01	7 (3%) 46 37	134, 205, 260, 297	0
4	D	214/214 (100%)	0.08	15 (7%) 19 14	151, 226, 276, 295	0
4	Q	214/214 (100%)	-0.09	7 (3%) 50 39	135, 206, 274, 299	0
5	E	580/609 (95%)	0.08	22 (3%) 44 35	159, 238, 302, 327	0
5	F	580/609 (95%)	0.15	32 (5%) 29 22	156, 249, 325, 341	0
All	All	2050/2162 (94%)	0.05	86 (4%) 40 31	134, 229, 306, 341	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	4	PRO	7.9
5	E	161	GLY	7.7
5	F	204	GLU	6.2
5	F	203	ALA	4.9
5	E	162	THR	4.5
5	F	190	LYS	4.4
5	E	17	LEU	4.3
5	E	190	LYS	4.0
5	F	454	ARG	3.9
3	P	141	LEU	3.6
5	F	202	THR	3.6
5	F	474	LYS	3.5
5	E	454	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
4	D	206	VAL	3.4
3	C	207	ASP	3.4
5	F	252	ARG	3.3
5	F	189	GLN	3.3
5	E	455	ASN	3.3
5	E	495	PRO	3.2
5	F	475	PHE	3.2
5	E	19	ARG	3.1
5	F	5	GLY	3.1
5	E	400	PHE	3.0
4	D	196	ALA	3.0
3	P	142	VAL	3.0
3	P	143	LYS	3.0
5	E	474	LYS	3.0
5	F	334	THR	3.0
5	F	347	GLY	2.9
5	F	309	PRO	2.9
5	E	220	ASP	2.8
5	F	368	LEU	2.8
5	F	217	SER	2.8
5	E	576	ARG	2.8
4	Q	63	SER	2.7
5	F	287	GLU	2.7
4	D	164	THR	2.7
5	F	214	GLY	2.7
5	F	205	GLY	2.7
5	F	20	LEU	2.7
5	F	191	VAL	2.7
5	E	475	PHE	2.6
3	P	140	CYS	2.6
5	F	284	CYS	2.6
5	F	175	ASN	2.6
5	F	296	SER	2.6
5	F	455	ASN	2.6
3	C	4	LEU	2.6
4	Q	117	ILE	2.5
4	Q	192	TYR	2.5
4	D	205	ILE	2.5
3	C	161	SER	2.5
4	D	35	TRP	2.5
4	Q	146	VAL	2.4
3	P	138	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
4	D	204	PRO	2.4
4	D	142	LYS	2.3
5	E	191	VAL	2.3
5	E	439	ILE	2.3
5	F	258	PHE	2.3
4	D	132	VAL	2.3
3	P	193	ILE	2.2
4	D	207	LYS	2.2
5	E	214	GLY	2.2
4	D	192	TYR	2.2
5	F	478	ILE	2.2
4	D	208	SER	2.2
5	F	163	ALA	2.2
5	F	400	PHE	2.2
5	F	477	TYR	2.2
4	Q	76	SER	2.2
3	P	4	LEU	2.2
4	D	144	ILE	2.1
5	E	189	GLN	2.1
4	D	143	ASP	2.1
5	E	494	PRO	2.1
4	D	133	VAL	2.1
5	E	383	ARG	2.1
5	E	20	LEU	2.1
4	D	195	GLU	2.1
5	E	568	THR	2.1
4	Q	32	ASN	2.0
5	E	388	ILE	2.0
4	Q	118	PHE	2.0
5	F	439	ILE	2.0
5	F	271	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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.