



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:49 PM UTC

PDB ID : 5FJV / pdb_00005fjv
Title : Crystal structure of the extracellular domain of alpha2 nicotinic acetylcholine receptor in pentameric assembly
Authors : Giastas, P.; Kouvatsos, N.; Chroni-Tzartou, D.; Tzartos, S.J.
Deposited on : 2015-10-13
Resolution : 3.20 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

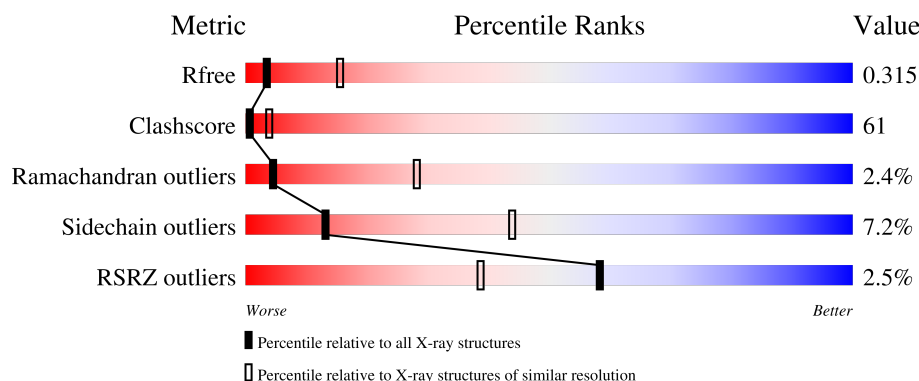
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	213	3% 33% 50% 12% ..
1	B	213	2% 25% 58% 12% ..
1	C	213	35% 54% 9% .
1	D	213	5% 33% 51% 11% ..
1	E	213	2% 31% 53% 11% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8584 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 NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	1
			1702	1099	282	311	10			
1	B	208	Total	C	N	O	S	0	0	1
			1711	1104	283	314	10			
1	C	208	Total	C	N	O	S	0	0	1
			1711	1104	283	314	10			
1	D	205	Total	C	N	O	S	0	0	1
			1679	1080	279	310	10			
1	E	208	Total	C	N	O	S	0	0	1
			1711	1104	283	314	10			

There are 30 discrepancies between the modelled and reference sequences:

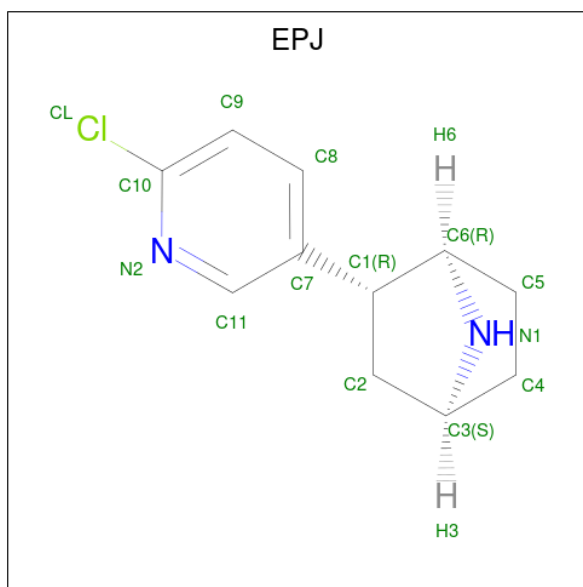
Chain	Residue	Modelled	Actual	Comment	Reference
A	240	HIS	-	expression tag	UNP Q15822
A	241	HIS	-	expression tag	UNP Q15822
A	242	HIS	-	expression tag	UNP Q15822
A	243	HIS	-	expression tag	UNP Q15822
A	244	HIS	-	expression tag	UNP Q15822
A	245	HIS	-	expression tag	UNP Q15822
B	240	HIS	-	expression tag	UNP Q15822
B	241	HIS	-	expression tag	UNP Q15822
B	242	HIS	-	expression tag	UNP Q15822
B	243	HIS	-	expression tag	UNP Q15822
B	244	HIS	-	expression tag	UNP Q15822
B	245	HIS	-	expression tag	UNP Q15822
C	240	HIS	-	expression tag	UNP Q15822
C	241	HIS	-	expression tag	UNP Q15822
C	242	HIS	-	expression tag	UNP Q15822
C	243	HIS	-	expression tag	UNP Q15822
C	244	HIS	-	expression tag	UNP Q15822
C	245	HIS	-	expression tag	UNP Q15822

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Chain	Residue	Modelled	Actual	Comment	Reference
D	240	HIS	-	expression tag	UNP Q15822
D	241	HIS	-	expression tag	UNP Q15822
D	242	HIS	-	expression tag	UNP Q15822
D	243	HIS	-	expression tag	UNP Q15822
D	244	HIS	-	expression tag	UNP Q15822
D	245	HIS	-	expression tag	UNP Q15822
E	240	HIS	-	expression tag	UNP Q15822
E	241	HIS	-	expression tag	UNP Q15822
E	242	HIS	-	expression tag	UNP Q15822
E	243	HIS	-	expression tag	UNP Q15822
E	244	HIS	-	expression tag	UNP Q15822
E	245	HIS	-	expression tag	UNP Q15822

- Molecule 2 is EPIBATIDINE (CCD ID: EPJ) (formula: $C_{11}H_{13}ClN_2$).

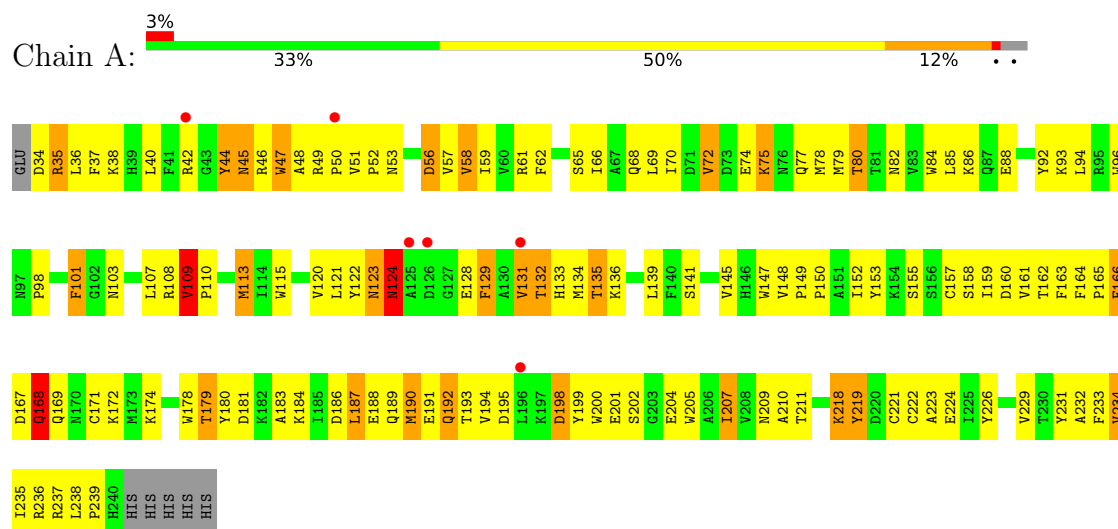


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	0	0
			14	11	1	2		
2	B	1	Total	C	Cl	N	0	0
			14	11	1	2		
2	C	1	Total	C	Cl	N	0	0
			14	11	1	2		
2	D	1	Total	C	Cl	N	0	0
			14	11	1	2		
2	E	1	Total	C	Cl	N	0	0
			14	11	1	2		

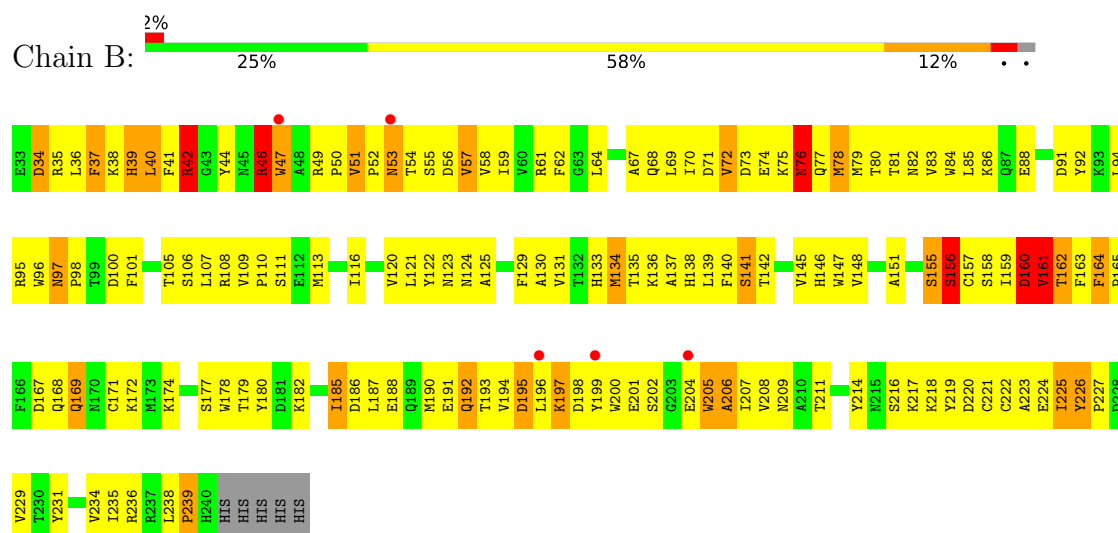
3 Residue-property plots

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

• Molecule 1: NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-2

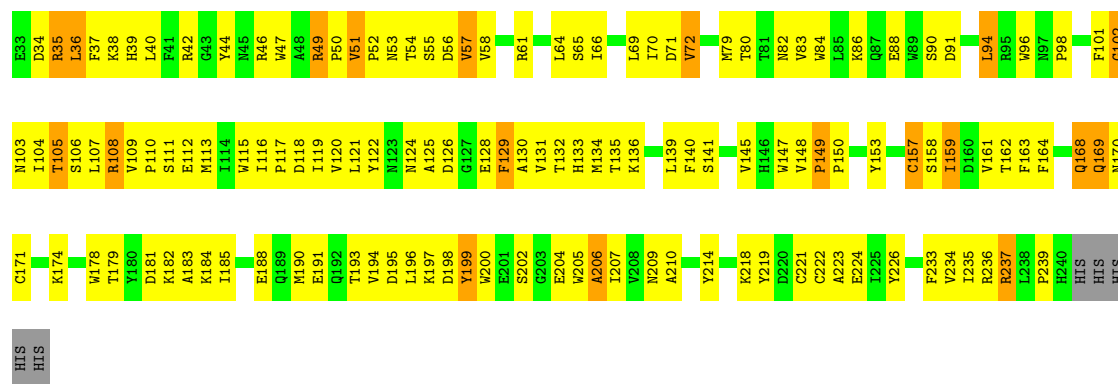


• Molecule 1: NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-2

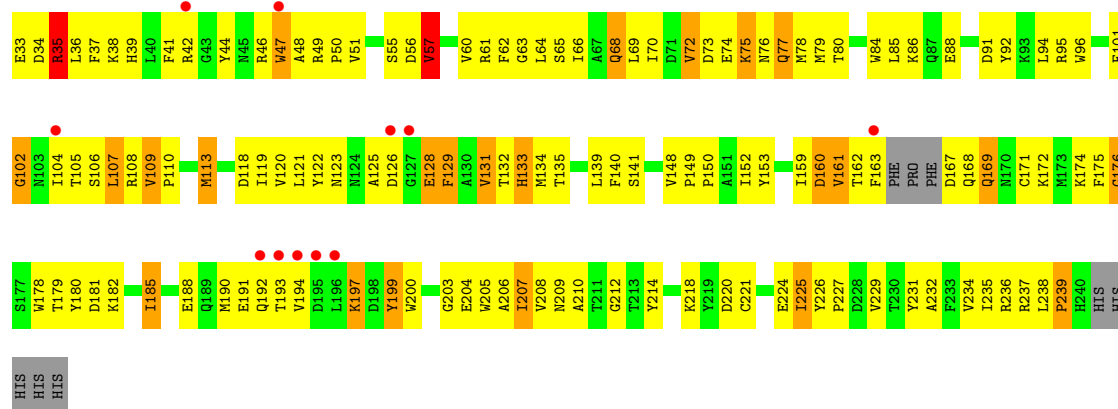


• Molecule 1: NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-2

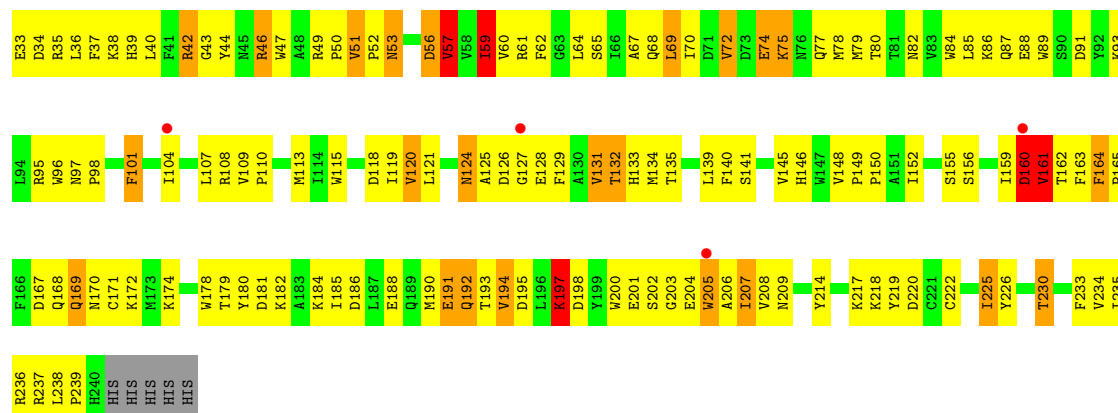




• Molecule 1: NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-2



• Molecule 1: NEURONAL ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.52Å 116.56Å 129.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.26 – 3.20 47.26 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.26-3.20) 99.9 (47.26-3.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 3.12Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.224 , 0.308 0.230 , 0.315	Depositor DCC
R_{free} test set	1442 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	85.1	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 100.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8584	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EPJ

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	0.75	1/1754 (0.1%)	1.27	12/2390 (0.5%)
1	B	0.72	2/1763 (0.1%)	1.37	22/2402 (0.9%)
1	C	0.71	1/1763 (0.1%)	1.26	18/2402 (0.7%)
1	D	0.85	1/1728 (0.1%)	1.32	20/2354 (0.8%)
1	E	0.84	1/1763 (0.1%)	1.29	12/2402 (0.5%)
All	All	0.78	6/8771 (0.1%)	1.30	84/11950 (0.7%)

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	B	0	2
1	D	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	239	PRO	C-N	-7.60	1.22	1.33
1	C	239	PRO	C-N	-7.01	1.23	1.33
1	E	239	PRO	C-N	-6.79	1.23	1.33
1	A	239	PRO	C-N	-6.76	1.23	1.33
1	B	239	PRO	C-N	-6.42	1.24	1.33
1	B	160	ASP	CA-C	5.72	1.60	1.52

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	97	ASN	CA-C-N	11.91	133.28	119.47
1	B	97	ASN	C-N-CA	11.91	133.28	119.47
1	D	190	MET	N-CA-C	-10.62	94.28	110.10
1	B	206	ALA	N-CA-C	9.90	122.65	108.00
1	E	197	LYS	N-CA-C	9.55	126.10	113.30
1	C	237	ARG	N-CA-C	9.02	123.84	113.02
1	B	226	TYR	CA-C-N	8.79	128.72	119.85
1	B	226	TYR	C-N-CA	8.79	128.72	119.85
1	C	164	PHE	N-CA-C	-8.75	98.72	109.83
1	B	78	MET	N-CA-C	8.70	121.13	108.86
1	A	198	ASP	N-CA-C	8.39	121.18	111.11
1	B	156	SER	N-CA-C	-8.38	96.10	109.59
1	E	192	GLN	N-CA-C	-8.38	102.36	112.58
1	B	37	PHE	N-CA-C	-8.28	102.34	111.36
1	E	57	VAL	N-CA-C	8.02	126.02	109.34
1	C	102	GLY	N-CA-C	7.81	131.69	113.18
1	C	159	ILE	N-CA-C	-7.67	103.78	113.22
1	D	128	GLU	N-CA-C	7.48	120.75	107.80
1	B	197	LYS	N-CA-C	7.34	123.14	113.30
1	D	77	GLN	N-CA-C	7.30	121.54	111.90
1	B	205	TRP	N-CA-C	7.17	119.76	108.79
1	B	195	ASP	N-CA-C	7.07	120.63	110.10
1	A	58	VAL	N-CA-C	7.05	118.97	108.54
1	D	176	GLY	N-CA-C	7.03	121.15	110.18
1	C	36	LEU	N-CA-C	-6.75	104.53	112.89
1	A	168	GLN	N-CA-C	6.64	120.34	109.85
1	C	94	LEU	N-CA-C	6.62	121.07	112.92
1	E	46	ARG	N-CA-C	6.60	120.62	110.20
1	B	206	ALA	CB-CA-C	-6.45	107.31	116.34
1	D	192	GLN	N-CA-C	-6.43	105.50	113.15
1	D	107	LEU	N-CA-C	6.35	119.53	109.81
1	D	57	VAL	N-CA-C	6.34	122.54	109.34
1	C	149	PRO	CA-C-N	6.34	126.52	120.31
1	C	149	PRO	C-N-CA	6.34	126.52	120.31
1	C	206	ALA	N-CA-C	6.24	118.09	110.41
1	E	59	ILE	N-CA-C	6.23	117.08	107.99
1	C	35	ARG	N-CA-C	6.22	118.86	111.33
1	C	158	SER	N-CA-C	6.22	119.32	109.50
1	C	105	THR	N-CA-C	6.17	118.84	109.95
1	E	56	ASP	N-CA-C	6.14	118.74	109.23
1	D	129	PHE	N-CA-C	6.05	118.38	111.11
1	D	160	ASP	N-CA-C	5.99	119.47	109.95
1	B	76	ASN	N-CA-C	5.97	119.32	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	THR	N-CA-C	5.97	119.53	112.72
1	E	194	VAL	N-CA-C	-5.97	100.12	108.12
1	B	192	GLN	N-CA-C	-5.87	106.17	113.15
1	B	46	ARG	N-CA-C	5.83	118.97	109.59
1	A	129	PHE	N-CA-C	5.76	118.78	111.69
1	B	34	ASP	N-CA-C	5.73	117.74	108.34
1	E	225	ILE	N-CA-C	5.68	116.12	108.17
1	B	225	ILE	N-CA-C	5.67	116.02	107.80
1	E	60	VAL	N-CA-C	5.67	116.02	107.80
1	B	40	LEU	N-CA-C	-5.57	102.78	110.35
1	D	197	LYS	N-CA-C	5.57	120.18	113.17
1	C	108	ARG	N-CA-C	5.56	117.81	108.96
1	C	157	CYS	N-CA-C	5.51	115.82	108.38
1	D	102	GLY	N-CA-C	-5.47	104.92	112.25
1	D	225	ILE	N-CA-C	5.43	115.68	107.80
1	E	53	ASN	N-CA-C	5.38	118.47	110.14
1	C	49	ARG	CA-C-N	5.36	125.78	119.99
1	C	49	ARG	C-N-CA	5.36	125.78	119.99
1	D	109	VAL	CA-C-N	5.36	125.28	119.76
1	D	109	VAL	C-N-CA	5.36	125.28	119.76
1	A	219	TYR	CA-C-N	-5.35	114.13	122.16
1	A	219	TYR	C-N-CA	-5.35	114.13	122.16
1	E	132	THR	N-CA-C	5.34	118.81	112.72
1	C	202	SER	N-CA-C	-5.30	101.80	109.59
1	A	109	VAL	N-CA-CB	-5.26	108.20	111.83
1	D	175	PHE	N-CA-C	5.23	118.60	110.17
1	E	205	TRP	N-CA-C	5.21	121.89	110.80
1	A	179	THR	CA-C-N	-5.20	115.85	122.77
1	A	179	THR	C-N-CA	-5.20	115.85	122.77
1	D	68	GLN	N-CA-C	5.20	116.98	108.55
1	D	39	HIS	N-CA-C	-5.19	105.52	111.07
1	B	42	ARG	N-CA-C	-5.19	104.55	111.24
1	A	218	LYS	N-CA-C	-5.16	100.83	109.24
1	C	169	GLN	N-CA-C	5.12	117.50	108.75
1	A	166	PHE	N-CA-C	-5.10	106.90	113.02
1	D	44	TYR	N-CA-C	5.08	116.50	110.97
1	D	133	HIS	CA-C-N	5.03	130.76	121.70
1	D	133	HIS	C-N-CA	5.03	130.76	121.70
1	B	155	SER	CA-C-N	-5.03	115.64	122.93
1	B	155	SER	C-N-CA	-5.03	115.64	122.93
1	B	134	MET	CB-CG-SD	-5.03	97.62	112.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	156	SER	Peptide
1	B	76	ASN	Peptide
1	D	126	ASP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1702	0	1635	226	0
1	B	1711	0	1641	254	0
1	C	1711	0	1641	209	0
1	D	1679	0	1612	209	1
1	E	1711	0	1643	211	1
2	A	14	0	13	4	0
2	B	14	0	13	1	0
2	C	14	0	13	1	0
2	D	14	0	13	3	0
2	E	14	0	13	3	0
All	All	8584	0	8237	1019	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 61.

All (1019) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:HIS:HB3	1:C:134:MET:HA	1.30	1.13
1:A:168:GLN:HB3	1:A:236:ARG:NH1	1.63	1.12
1:D:161:VAL:HA	1:D:167:ASP:HB2	1.10	1.10
1:E:74:GLU:HA	1:E:159:ILE:HD12	1.28	1.08
1:B:133:HIS:HB3	1:B:134:MET:HA	1.36	1.07
1:A:195:ASP:HB3	1:A:198:ASP:HB3	1.36	1.05
1:C:121:LEU:HD23	1:C:125:ALA:HB2	1.40	1.03
1:D:33:GLU:HB3	1:D:37:PHE:HD2	1.19	1.03
1:B:195:ASP:OD2	1:B:198:ASP:N	1.90	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:VAL:HG22	1:D:162:THR:H	1.21	1.02
1:D:221:CYS:HB3	1:E:194:VAL:HG23	1.38	1.02
1:A:164:PHE:HB2	1:A:165:PRO:HD3	1.43	1.00
1:C:65:SER:HB3	1:C:199:TYR:HE1	1.26	1.00
1:B:54:THR:HA	1:C:35:ARG:HH12	1.25	1.00
1:E:191:GLU:HB2	1:E:193:THR:HG23	1.43	0.99
1:A:70:ILE:HB	1:A:80:THR:HG22	1.45	0.98
1:A:199:TYR:OH	1:E:220:ASP:N	1.97	0.97
1:C:61:ARG:HB2	1:C:88:GLU:HG2	1.42	0.97
1:E:195:ASP:OD2	1:E:198:ASP:N	1.97	0.97
1:E:124:ASN:ND2	1:E:126:ASP:OD2	1.96	0.97
1:D:161:VAL:CA	1:D:167:ASP:HB2	1.94	0.96
1:C:34:ASP:HB2	1:C:37:PHE:HB2	1.43	0.96
1:D:33:GLU:HB3	1:D:37:PHE:CD2	2.01	0.96
1:B:61:ARG:HB2	1:B:88:GLU:HG2	1.48	0.96
1:C:42:ARG:HE	1:C:42:ARG:HA	1.29	0.96
1:E:133:HIS:HB3	1:E:134:MET:HA	1.45	0.95
1:E:206:ALA:CB	1:E:236:ARG:H	1.78	0.95
1:A:131:VAL:HG21	1:A:149:PRO:HB2	1.49	0.94
1:A:77:GLN:HE22	1:A:159:ILE:HG23	1.29	0.94
1:B:180:TYR:HB3	1:B:185:ILE:HG22	1.46	0.94
1:B:54:THR:HA	1:C:35:ARG:NH1	1.83	0.92
1:E:74:GLU:CA	1:E:159:ILE:HD12	1.98	0.92
1:D:160:ASP:OD1	1:D:169:GLN:HB3	1.71	0.90
1:D:221:CYS:CB	1:E:194:VAL:HG23	2.00	0.90
1:C:51:VAL:HG12	1:C:58:VAL:HG21	1.53	0.90
1:B:169:GLN:NE2	1:B:235:ILE:O	2.05	0.90
1:E:74:GLU:HA	1:E:159:ILE:CD1	2.01	0.90
1:B:123:ASN:HD21	1:B:155:SER:HB2	1.35	0.89
1:B:73:ASP:HB3	1:B:76:ASN:O	1.73	0.89
1:C:103:ASN:N	1:C:104:ILE:HA	1.86	0.88
1:A:209:ASN:O	1:A:234:VAL:HG23	1.74	0.88
1:C:65:SER:HB3	1:C:199:TYR:CE1	2.09	0.88
1:B:205:TRP:HB2	1:B:238:LEU:H	1.39	0.88
1:B:168:GLN:HA	1:B:169:GLN:NE2	1.89	0.87
1:A:221:CYS:HA	1:B:194:VAL:CG2	2.04	0.86
1:A:61:ARG:HB2	1:A:88:GLU:HG2	1.54	0.86
1:A:35:ARG:HG2	1:A:36:LEU:HD12	1.58	0.86
1:A:165:PRO:O	1:A:237:ARG:HB2	1.75	0.85
1:E:77:GLN:HA	1:E:159:ILE:HD13	1.58	0.85
1:B:180:TYR:CD1	1:C:108:ARG:HD2	2.12	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:THR:CA	1:C:35:ARG:HH12	1.90	0.85
1:C:34:ASP:HB2	1:C:37:PHE:CB	2.06	0.84
1:A:46:ARG:HH12	1:A:48:ALA:HA	1.42	0.84
1:B:207:ILE:HA	1:B:235:ILE:HG22	1.60	0.84
1:E:206:ALA:HB2	1:E:236:ARG:H	1.40	0.84
1:D:121:LEU:HD23	1:D:125:ALA:HB2	1.56	0.84
1:E:125:ALA:HB1	1:E:128:GLU:C	2.03	0.83
1:D:50:PRO:HB3	1:E:35:ARG:HD2	1.61	0.83
1:D:96:TRP:CE2	1:D:141:SER:HB3	2.14	0.82
1:C:98:PRO:HB3	1:C:105:THR:HB	1.61	0.82
1:C:133:HIS:HB3	1:C:134:MET:CA	2.09	0.82
1:B:77:GLN:HG3	1:C:71:ASP:HB2	1.62	0.81
1:E:47:TRP:HD1	1:E:50:PRO:HD3	1.44	0.81
1:B:70:ILE:HB	1:B:80:THR:HG22	1.63	0.81
1:B:75:LYS:O	1:B:159:ILE:HG23	1.80	0.81
1:E:167:ASP:OD1	1:E:237:ARG:NH1	2.13	0.81
1:D:169:GLN:CD	1:D:235:ILE:H	1.88	0.81
1:D:169:GLN:OE1	1:D:235:ILE:N	2.14	0.81
1:D:33:GLU:CB	1:D:37:PHE:HB3	2.10	0.80
1:C:98:PRO:O	1:C:104:ILE:HG21	1.80	0.80
1:B:78:MET:HA	1:B:156:SER:HB2	1.63	0.80
1:A:113:MET:HA	1:A:113:MET:HE2	1.64	0.80
1:C:61:ARG:NH1	1:C:188:GLU:OE2	2.15	0.80
1:B:169:GLN:OE1	1:B:235:ILE:N	2.13	0.79
1:D:33:GLU:HB2	1:D:37:PHE:HB3	1.64	0.79
1:B:192:GLN:CD	1:B:196:LEU:HD11	2.06	0.79
1:D:34:ASP:O	1:D:36:LEU:N	2.13	0.79
1:B:74:GLU:H	1:B:75:LYS:C	1.90	0.79
1:C:46:ARG:HH21	1:C:115:TRP:H	1.31	0.79
1:B:169:GLN:N	1:B:169:GLN:CD	2.41	0.79
1:B:238:LEU:HD12	1:B:239:PRO:HD2	1.65	0.79
1:C:161:VAL:HG22	1:C:162:THR:H	1.48	0.78
1:C:117:PRO:HB2	1:C:119:ILE:HG12	1.64	0.78
1:E:190:MET:C	1:E:192:GLN:H	1.91	0.78
1:C:49:ARG:HD2	1:D:110:PRO:HG2	1.64	0.78
1:C:72:VAL:HG21	1:C:237:ARG:HH22	1.49	0.78
1:B:219:TYR:HD2	1:C:199:TYR:HD2	1.31	0.77
1:B:35:ARG:O	1:B:39:HIS:N	2.13	0.77
1:D:209:ASN:O	1:D:234:VAL:HG22	1.83	0.77
1:E:208:VAL:HB	1:E:234:VAL:CG2	2.14	0.77
1:A:163:PHE:O	1:A:167:ASP:HB3	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ARG:HB2	1:A:50:PRO:HD3	1.66	0.77
1:D:47:TRP:HE3	1:D:48:ALA:H	1.30	0.77
1:E:169:GLN:HB2	1:E:235:ILE:HD11	1.64	0.77
1:E:207:ILE:HD12	1:E:233:PHE:HD2	1.50	0.77
1:E:191:GLU:HB2	1:E:193:THR:CG2	2.14	0.77
1:B:156:SER:HA	1:B:157:CYS:HB3	1.65	0.77
1:D:221:CYS:HA	1:E:194:VAL:HA	1.67	0.76
1:E:133:HIS:HB3	1:E:134:MET:CA	2.14	0.76
1:D:60:VAL:HG21	1:D:185:ILE:HD11	1.68	0.76
1:A:179:THR:HG23	2:A:300:EPJ:CL	2.23	0.76
1:E:131:VAL:HG21	1:E:149:PRO:CG	2.16	0.76
1:D:107:LEU:CD1	1:D:109:VAL:HG13	2.16	0.76
1:D:161:VAL:HG22	1:D:162:THR:N	1.99	0.75
1:A:168:GLN:HG2	1:A:236:ARG:CD	2.15	0.75
1:E:174:LYS:HG3	1:E:230:THR:HG22	1.66	0.75
1:B:61:ARG:HD3	1:B:88:GLU:OE2	1.86	0.75
1:D:206:ALA:HB3	1:D:236:ARG:H	1.52	0.75
1:A:108:ARG:HG3	1:A:108:ARG:HH11	1.52	0.75
1:B:110:PRO:HB2	1:B:113:MET:HG3	1.68	0.75
1:E:86:LYS:HD2	1:E:190:MET:SD	2.27	0.75
1:B:53:ASN:O	1:C:35:ARG:NH1	2.19	0.75
1:D:169:GLN:HG2	1:D:235:ILE:HG13	1.68	0.74
1:B:123:ASN:ND2	1:B:155:SER:HB2	2.03	0.74
1:C:133:HIS:CB	1:C:134:MET:HA	2.07	0.74
1:A:74:GLU:N	1:A:75:LYS:HZ3	1.86	0.74
1:A:164:PHE:HB2	1:A:165:PRO:CD	2.17	0.74
1:B:79:MET:CE	1:B:171:CYS:HB3	2.17	0.74
1:B:79:MET:HE1	1:B:171:CYS:HB3	1.67	0.74
1:B:129:PHE:HB2	1:C:133:HIS:NE2	2.02	0.74
1:A:164:PHE:CB	1:A:165:PRO:HD3	2.16	0.74
1:B:197:LYS:O	1:B:197:LYS:HG2	1.87	0.73
1:B:160:ASP:CG	1:B:169:GLN:HB3	2.14	0.73
1:D:106:SER:CB	1:D:140:PHE:HA	2.19	0.73
1:D:205:TRP:HA	1:D:237:ARG:HA	1.70	0.73
1:E:47:TRP:CD1	1:E:50:PRO:HD3	2.23	0.73
1:B:207:ILE:CA	1:B:235:ILE:HG22	2.18	0.73
1:E:107:LEU:CD1	1:E:109:VAL:HG13	2.19	0.73
1:A:77:GLN:HE22	1:A:159:ILE:CG2	2.02	0.73
1:A:162:THR:CB	1:A:168:GLN:HE22	2.02	0.73
1:E:161:VAL:HB	1:E:163:PHE:CD1	2.24	0.72
1:D:47:TRP:HA	1:D:47:TRP:CE3	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:PHE:HB3	1:B:165:PRO:CD	2.20	0.72
1:C:42:ARG:HA	1:C:42:ARG:NE	2.02	0.72
1:A:133:HIS:HB3	1:A:134:MET:O	1.89	0.72
1:D:181:ASP:HB3	1:D:226:TYR:CE2	2.24	0.72
1:C:34:ASP:O	1:C:37:PHE:HB3	1.89	0.71
1:E:70:ILE:HB	1:E:80:THR:HG22	1.72	0.71
1:C:131:VAL:HG13	1:C:134:MET:HE2	1.72	0.71
1:C:174:LYS:NZ	1:C:219:TYR:OH	2.21	0.71
1:A:131:VAL:HG21	1:A:149:PRO:CB	2.21	0.71
1:A:191:GLU:O	1:A:193:THR:N	2.24	0.71
1:A:109:VAL:HG23	1:A:110:PRO:HD2	1.72	0.71
1:C:70:ILE:HD12	1:C:80:THR:HG22	1.72	0.71
1:B:62:PHE:CE1	1:B:85:LEU:HD22	2.26	0.71
1:E:86:LYS:HG2	1:E:148:VAL:HG22	1.73	0.71
1:A:49:ARG:HE	1:B:113:MET:CE	2.04	0.70
1:D:47:TRP:O	1:D:50:PRO:HD2	1.91	0.70
1:D:106:SER:HB3	1:D:140:PHE:HA	1.72	0.70
1:A:47:TRP:HB3	1:A:50:PRO:CD	2.20	0.70
1:D:65:SER:HB2	1:D:84:TRP:HB2	1.71	0.70
1:E:161:VAL:HG11	1:E:163:PHE:CE1	2.26	0.70
1:A:34:ASP:O	1:A:37:PHE:HB3	1.91	0.70
1:E:39:HIS:O	1:E:42:ARG:HG3	1.92	0.70
1:B:206:ALA:O	1:B:207:ILE:HG22	1.91	0.70
1:A:108:ARG:HD2	1:E:180:TYR:CD1	2.27	0.70
1:C:65:SER:CB	1:C:199:TYR:HE1	2.04	0.70
1:E:168:GLN:OE1	1:E:236:ARG:NH1	2.24	0.70
1:D:46:ARG:NH2	1:D:91:ASP:OD2	2.23	0.69
1:D:207:ILE:N	1:D:235:ILE:HG22	2.07	0.69
1:C:157:CYS:CB	1:C:171:CYS:HA	2.23	0.69
1:E:169:GLN:OE1	1:E:170:ASN:N	2.24	0.69
1:E:74:GLU:HG2	1:E:159:ILE:HD12	1.73	0.69
1:A:162:THR:HB	1:A:168:GLN:NE2	2.07	0.69
1:B:133:HIS:HB3	1:B:134:MET:CA	2.20	0.69
1:D:180:TYR:CD1	1:E:108:ARG:HG3	2.27	0.69
1:B:107:LEU:CD1	1:B:109:VAL:HG13	2.23	0.69
1:C:47:TRP:O	1:C:50:PRO:HD2	1.93	0.68
1:A:45:ASN:O	1:A:45:ASN:ND2	2.27	0.68
1:E:133:HIS:CB	1:E:134:MET:HA	2.19	0.68
1:C:131:VAL:HG21	1:C:149:PRO:HB2	1.75	0.68
1:B:157:CYS:SG	1:B:158:SER:N	2.54	0.68
1:C:197:LYS:O	1:C:197:LYS:HG2	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:GLU:H	1:D:75:LYS:HZ3	1.42	0.68
1:D:163:PHE:H	1:D:167:ASP:HA	1.59	0.68
1:E:131:VAL:HG21	1:E:149:PRO:HG3	1.75	0.68
1:B:56:ASP:O	1:B:57:VAL:HG12	1.93	0.68
1:A:168:GLN:HG2	1:A:236:ARG:HD3	1.75	0.67
1:D:169:GLN:O	1:D:169:GLN:NE2	2.27	0.67
1:C:51:VAL:CG1	1:C:58:VAL:HG21	2.23	0.67
1:A:70:ILE:HB	1:A:80:THR:CG2	2.23	0.67
1:A:124:ASN:OD1	1:B:68:GLN:HB2	1.92	0.67
1:A:159:ILE:HG22	1:A:169:GLN:NE2	2.09	0.67
1:D:69:LEU:H	1:D:200:TRP:HZ3	1.40	0.67
1:A:79:MET:HE1	1:A:171:CYS:HB3	1.75	0.67
1:A:192:GLN:OE1	1:A:192:GLN:N	2.21	0.67
1:B:169:GLN:CD	1:B:169:GLN:H	2.02	0.67
1:E:96:TRP:CZ3	1:E:141:SER:HA	2.30	0.67
1:B:180:TYR:HB3	1:B:185:ILE:CG2	2.22	0.66
1:D:207:ILE:H	1:D:235:ILE:HG22	1.60	0.66
1:C:197:LYS:HA	1:C:200:TRP:HB2	1.76	0.66
1:A:45:ASN:O	1:A:46:ARG:HB2	1.94	0.66
1:B:61:ARG:HB2	1:B:88:GLU:CG	2.23	0.66
1:B:72:VAL:HG11	1:B:205:TRP:CH2	2.30	0.66
1:C:72:VAL:HG11	1:C:237:ARG:NH1	2.10	0.66
1:C:72:VAL:HG11	1:C:237:ARG:NH2	2.10	0.66
1:C:205:TRP:CD1	1:C:237:ARG:HD2	2.31	0.66
1:D:107:LEU:C	1:D:107:LEU:HD12	2.21	0.66
1:B:218:LYS:HZ1	1:B:223:ALA:HA	1.58	0.66
1:D:92:TYR:O	1:D:95:ARG:HD3	1.95	0.66
1:E:197:LYS:HZ1	1:E:200:TRP:CB	2.08	0.66
1:A:207:ILE:HD12	1:A:233:PHE:HB3	1.77	0.66
1:A:53:ASN:HA	1:A:92:TYR:CE1	2.29	0.66
1:B:206:ALA:CB	1:B:235:ILE:HB	2.26	0.66
1:A:74:GLU:H	1:A:75:LYS:HZ3	1.43	0.66
1:E:110:PRO:HB2	1:E:113:MET:HG3	1.77	0.65
1:A:79:MET:CE	1:A:171:CYS:HB3	2.25	0.65
1:C:111:SER:OG	1:C:135:THR:O	2.09	0.65
1:D:96:TRP:CE3	1:D:141:SER:HA	2.30	0.65
1:D:119:ILE:HA	1:D:176:GLY:O	1.96	0.65
1:E:51:VAL:HG22	1:E:53:ASN:HB2	1.77	0.65
1:B:139:LEU:HD12	1:B:140:PHE:H	1.62	0.65
1:A:195:ASP:HB3	1:A:198:ASP:CB	2.21	0.65
1:B:64:LEU:HD11	1:B:83:VAL:HB	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:ASP:HB3	1:D:226:TYR:CZ	2.32	0.65
1:A:37:PHE:HD1	1:A:38:LYS:HE2	1.60	0.65
1:B:224:GLU:C	1:B:225:ILE:HD12	2.21	0.65
1:D:63:GLY:HA3	1:D:86:LYS:HE3	1.78	0.65
1:D:73:ASP:OD2	1:D:76:ASN:HB2	1.96	0.65
1:E:209:ASN:H	1:E:234:VAL:HG22	1.62	0.65
1:B:200:TRP:NE1	1:B:207:ILE:HG21	2.12	0.65
1:C:53:ASN:O	1:C:54:THR:OG1	2.11	0.65
1:E:65:SER:HB2	1:E:84:TRP:HB2	1.79	0.64
1:C:168:GLN:HG3	1:C:169:GLN:N	2.13	0.64
1:C:58:VAL:HB	1:C:185:ILE:CD1	2.28	0.64
1:A:62:PHE:C	1:A:190:MET:HB2	2.22	0.64
2:A:300:EPJ:H11	1:B:148:VAL:HB	1.78	0.64
1:B:160:ASP:OD2	1:B:169:GLN:HG3	1.98	0.64
1:B:70:ILE:HB	1:B:80:THR:CG2	2.27	0.64
1:C:61:ARG:HB2	1:C:88:GLU:CG	2.23	0.64
1:E:169:GLN:CB	1:E:235:ILE:HD11	2.28	0.64
1:D:33:GLU:CA	1:D:37:PHE:HB3	2.28	0.64
1:D:208:VAL:CG1	1:D:234:VAL:HG23	2.27	0.64
1:B:46:ARG:HG3	1:B:46:ARG:HH11	1.61	0.64
1:C:182:LYS:NZ	1:C:214:TYR:OH	2.24	0.64
1:A:62:PHE:CE1	1:A:85:LEU:HD22	2.33	0.64
1:B:123:ASN:O	1:C:82:ASN:ND2	2.31	0.64
1:B:168:GLN:OE1	1:B:236:ARG:NE	2.23	0.64
1:D:224:GLU:OE1	1:D:226:TYR:OH	2.15	0.64
1:B:179:THR:HG22	2:B:300:EPJ:CL	2.35	0.64
1:C:168:GLN:HB2	1:C:236:ARG:HG2	1.80	0.64
1:D:128:GLU:OE1	1:D:132:THR:HG21	1.98	0.64
1:A:168:GLN:HB3	1:A:236:ARG:HH11	1.61	0.63
1:C:72:VAL:HG11	1:C:237:ARG:CZ	2.29	0.63
1:D:74:GLU:HB2	1:D:75:LYS:HZ2	1.63	0.63
1:D:101:PHE:CG	1:D:102:GLY:N	2.65	0.63
1:D:120:VAL:HG11	1:D:178:TRP:CE3	2.33	0.63
1:A:66:ILE:HD11	1:A:233:PHE:CZ	2.33	0.63
1:A:82:ASN:HD22	1:E:124:ASN:H	1.44	0.63
1:D:47:TRP:HB3	1:D:50:PRO:CD	2.28	0.63
1:E:208:VAL:HB	1:E:234:VAL:HG21	1.79	0.63
1:A:207:ILE:CD1	1:A:233:PHE:HB3	2.28	0.63
1:B:121:LEU:HD21	1:B:155:SER:HB3	1.80	0.63
1:A:96:TRP:CE3	1:A:141:SER:HA	2.34	0.63
1:B:98:PRO:HA	1:B:105:THR:HG21	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:GLN:HG2	1:D:235:ILE:CG1	2.29	0.63
1:E:238:LEU:HD23	1:E:238:LEU:O	1.99	0.63
1:B:98:PRO:HB3	1:B:105:THR:HG22	1.79	0.63
1:A:113:MET:HA	1:A:113:MET:CE	2.29	0.62
1:A:201:GLU:CD	1:E:172:LYS:HZ1	2.07	0.62
1:C:112:GLU:OE1	1:C:112:GLU:N	2.25	0.62
1:A:57:VAL:HG13	1:A:59:ILE:CD1	2.29	0.62
1:B:74:GLU:N	1:B:75:LYS:C	2.57	0.62
1:B:139:LEU:HD12	1:B:140:PHE:N	2.14	0.62
1:C:98:PRO:HB3	1:C:105:THR:CB	2.28	0.62
1:C:125:ALA:HB1	1:C:129:PHE:H	1.65	0.62
1:D:208:VAL:HG13	1:D:209:ASN:H	1.63	0.62
1:B:46:ARG:NH2	1:B:91:ASP:OD2	2.33	0.62
1:E:197:LYS:HA	1:E:197:LYS:HZ3	1.64	0.62
1:B:49:ARG:HD2	1:C:110:PRO:HG2	1.80	0.62
1:C:61:ARG:O	1:C:190:MET:HE3	1.99	0.62
1:D:169:GLN:HE22	1:D:234:VAL:HA	1.64	0.62
1:A:96:TRP:CZ3	1:A:141:SER:HA	2.35	0.62
1:B:62:PHE:CZ	1:B:85:LEU:HD22	2.35	0.62
1:D:104:ILE:O	1:D:105:THR:OG1	2.15	0.62
1:D:197:LYS:HZ1	1:D:200:TRP:CD1	2.18	0.62
1:D:163:PHE:H	1:D:167:ASP:CA	2.13	0.62
1:A:47:TRP:O	1:A:50:PRO:HD2	1.99	0.62
1:B:74:GLU:HB3	1:B:75:LYS:CB	2.30	0.62
1:A:133:HIS:CD2	1:E:129:PHE:HB2	2.35	0.62
1:B:200:TRP:HE1	1:B:207:ILE:HG21	1.65	0.62
1:B:225:ILE:HD12	1:B:225:ILE:N	2.14	0.62
1:E:68:GLN:HB2	1:E:82:ASN:HB3	1.82	0.62
1:E:86:LYS:HB2	1:E:194:VAL:HG21	1.82	0.62
1:B:221:CYS:HB3	1:C:199:TYR:OH	2.00	0.61
1:C:131:VAL:CG2	1:C:149:PRO:HB2	2.30	0.61
1:D:178:TRP:NE1	1:E:150:PRO:HD3	2.15	0.61
1:C:191:GLU:C	1:C:193:THR:H	2.07	0.61
1:E:77:GLN:NE2	1:E:159:ILE:HD11	2.15	0.61
1:A:123:ASN:ND2	1:A:155:SER:HB2	2.14	0.61
1:A:221:CYS:HA	1:B:194:VAL:HG21	1.80	0.61
1:A:234:VAL:HG12	1:A:236:ARG:NH1	2.15	0.61
1:A:122:TYR:CB	1:A:174:LYS:HD3	2.31	0.61
1:A:134:MET:O	1:A:135:THR:HB	1.99	0.61
1:B:98:PRO:HB3	1:B:105:THR:CG2	2.30	0.61
1:B:200:TRP:NE1	1:B:207:ILE:CG2	2.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:VAL:CG2	1:C:237:ARG:HH22	2.12	0.61
1:E:69:LEU:HD22	1:E:207:ILE:HG12	1.82	0.61
1:C:195:ASP:OD1	1:C:197:LYS:N	2.25	0.61
1:D:180:TYR:HE1	1:E:108:ARG:HB2	1.65	0.61
1:B:161:VAL:HA	1:B:167:ASP:OD2	2.00	0.61
1:D:229:VAL:HG12	1:D:231:TYR:CE1	2.36	0.61
1:A:181:ASP:OD1	1:B:108:ARG:NH2	2.34	0.61
1:D:56:ASP:OD1	1:E:104:ILE:HD11	1.99	0.61
1:D:120:VAL:HG23	1:D:129:PHE:HB3	1.81	0.61
1:E:190:MET:C	1:E:192:GLN:N	2.58	0.61
1:C:157:CYS:HB2	1:C:171:CYS:HA	1.83	0.60
1:D:180:TYR:HB3	1:D:185:ILE:HG22	1.82	0.60
1:A:221:CYS:HA	1:B:194:VAL:HG23	1.84	0.60
1:B:47:TRP:CZ2	1:C:113:MET:HE1	2.36	0.60
1:B:69:LEU:HD22	1:B:207:ILE:HB	1.82	0.60
1:E:47:TRP:HB3	1:E:50:PRO:CD	2.31	0.60
1:A:49:ARG:HE	1:B:113:MET:HE3	1.66	0.60
1:E:62:PHE:CE1	1:E:85:LEU:HD22	2.36	0.60
1:A:35:ARG:HG2	1:A:36:LEU:CD1	2.32	0.60
1:B:179:THR:O	1:C:108:ARG:NE	2.33	0.60
1:C:42:ARG:HE	1:C:42:ARG:CA	2.07	0.60
1:C:170:ASN:ND2	1:C:233:PHE:O	2.35	0.60
1:C:108:ARG:HG3	1:C:108:ARG:HH11	1.67	0.60
1:B:54:THR:HG23	1:B:92:TYR:CE2	2.37	0.59
1:D:33:GLU:HA	1:D:37:PHE:CB	2.33	0.59
1:E:57:VAL:HG13	1:E:57:VAL:O	2.01	0.59
1:A:162:THR:HB	1:A:168:GLN:HE22	1.66	0.59
1:C:161:VAL:HG22	1:C:162:THR:N	2.16	0.59
1:D:50:PRO:HB3	1:E:35:ARG:CD	2.32	0.59
1:D:180:TYR:CB	1:D:185:ILE:HG22	2.32	0.59
1:B:49:ARG:HD2	1:C:110:PRO:CG	2.32	0.59
1:B:218:LYS:NZ	1:B:223:ALA:HA	2.17	0.59
1:B:36:LEU:O	1:B:40:LEU:HD13	2.02	0.59
1:E:127:GLY:C	1:E:128:GLU:HG2	2.27	0.59
1:A:159:ILE:HG13	1:A:159:ILE:O	2.02	0.59
1:B:57:VAL:HG13	1:B:57:VAL:O	2.02	0.59
1:B:192:GLN:NE2	1:B:196:LEU:HD11	2.16	0.59
1:C:53:ASN:OD1	1:C:54:THR:N	2.34	0.59
1:C:72:VAL:HG21	1:C:237:ARG:NH2	2.15	0.59
1:D:34:ASP:C	1:D:36:LEU:H	2.08	0.59
1:D:68:GLN:HA	1:D:200:TRP:CZ3	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:ARG:HH21	1:E:43:GLY:CA	2.16	0.59
1:A:61:ARG:HH11	1:A:88:GLU:CD	2.11	0.59
1:D:68:GLN:HA	1:D:200:TRP:HZ3	1.67	0.59
1:A:131:VAL:CG2	1:A:149:PRO:HB2	2.29	0.59
1:B:47:TRP:CD1	1:B:50:PRO:HD3	2.36	0.59
1:D:69:LEU:N	1:D:200:TRP:CZ3	2.70	0.59
1:E:70:ILE:O	1:E:204:GLU:HG2	2.03	0.59
1:B:36:LEU:O	1:B:40:LEU:HB2	2.03	0.58
1:B:86:LYS:HA	1:B:148:VAL:HG22	1.85	0.58
1:A:53:ASN:HA	1:A:92:TYR:CD1	2.37	0.58
1:C:103:ASN:H	1:C:104:ILE:HA	1.68	0.58
1:E:38:LYS:HG3	1:E:101:PHE:HB2	1.85	0.58
1:E:86:LYS:HE2	1:E:146:HIS:HD2	1.68	0.58
1:B:207:ILE:HG23	1:B:207:ILE:O	2.03	0.58
1:C:96:TRP:HZ2	1:C:106:SER:H	1.51	0.58
1:A:47:TRP:HB3	1:A:50:PRO:HD3	1.84	0.58
1:B:209:ASN:HB3	1:B:234:VAL:HG22	1.86	0.58
1:B:206:ALA:HB1	1:B:235:ILE:CA	2.33	0.58
1:A:51:VAL:HG23	1:B:35:ARG:NH1	2.18	0.58
1:A:36:LEU:HD11	1:E:93:LYS:NZ	2.18	0.58
1:D:66:ILE:HG21	1:D:197:LYS:HE3	1.85	0.58
1:A:167:ASP:OD1	1:A:237:ARG:CD	2.52	0.58
1:B:190:MET:HE2	1:B:194:VAL:HG11	1.85	0.58
1:C:72:VAL:CB	1:C:237:ARG:HH22	2.17	0.58
1:E:34:ASP:H	1:E:37:PHE:HD2	1.47	0.58
1:E:42:ARG:HH21	1:E:43:GLY:HA2	1.68	0.58
1:B:195:ASP:CG	1:B:198:ASP:H	1.99	0.57
1:C:55:SER:OG	1:C:56:ASP:N	2.37	0.57
1:C:120:VAL:HG11	1:C:178:TRP:CE3	2.38	0.57
1:D:218:LYS:HB2	1:D:225:ILE:CD1	2.34	0.57
1:E:197:LYS:HZ1	1:E:200:TRP:CG	2.22	0.57
1:A:82:ASN:ND2	1:E:124:ASN:H	2.01	0.57
1:B:74:GLU:HB3	1:B:76:ASN:N	2.19	0.57
1:B:36:LEU:HB3	1:B:40:LEU:HD13	1.87	0.57
1:D:104:ILE:O	1:D:104:ILE:HG22	2.04	0.57
1:D:122:TYR:HB2	1:D:174:LYS:HD3	1.86	0.57
1:B:91:ASP:HB3	1:B:94:LEU:HD12	1.86	0.57
1:E:206:ALA:HB3	1:E:235:ILE:HA	1.86	0.57
1:B:164:PHE:HB3	1:B:165:PRO:HD2	1.85	0.57
1:D:206:ALA:CB	1:D:236:ARG:H	2.17	0.57
1:D:238:LEU:HG	1:D:239:PRO:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:217:LYS:HG2	1:E:218:LYS:N	2.19	0.57
1:A:74:GLU:H	1:A:75:LYS:NZ	2.01	0.57
2:D:300:EPJ:C11	1:E:148:VAL:HB	2.35	0.57
1:B:47:TRP:HA	1:B:47:TRP:CE3	2.39	0.57
1:A:168:GLN:CG	1:A:236:ARG:HD3	2.34	0.57
1:E:197:LYS:HZ2	1:E:197:LYS:HB3	1.70	0.57
1:A:209:ASN:HB2	1:A:234:VAL:HG21	1.86	0.57
1:D:61:ARG:HB2	1:D:88:GLU:HB3	1.86	0.57
1:D:180:TYR:CE1	1:E:108:ARG:HG3	2.40	0.57
1:A:57:VAL:HG22	1:A:58:VAL:N	2.20	0.56
1:B:160:ASP:OD2	1:B:169:GLN:HB3	2.05	0.56
1:B:67:ALA:HB3	1:B:82:ASN:ND2	2.20	0.56
1:B:107:LEU:C	1:B:107:LEU:HD12	2.30	0.56
1:B:208:VAL:O	1:B:208:VAL:HG22	2.05	0.56
1:C:88:GLU:HA	1:C:145:VAL:O	2.05	0.56
1:E:70:ILE:HB	1:E:80:THR:CG2	2.36	0.56
1:B:72:VAL:CG1	1:B:205:TRP:CH2	2.87	0.56
1:E:169:GLN:H	1:E:235:ILE:HG12	1.70	0.56
1:E:207:ILE:HD12	1:E:233:PHE:CD2	2.36	0.56
1:A:157:CYS:SG	1:A:171:CYS:N	2.78	0.56
1:D:122:TYR:CB	1:D:174:LYS:HD3	2.36	0.56
1:E:164:PHE:HB3	1:E:165:PRO:HD2	1.87	0.56
2:A:300:EPJ:C11	1:B:148:VAL:HB	2.35	0.56
1:C:61:ARG:C	1:C:190:MET:HE3	2.30	0.56
1:D:204:GLU:CD	1:D:204:GLU:N	2.64	0.56
1:A:49:ARG:NE	1:B:113:MET:HE3	2.21	0.56
1:B:229:VAL:HG12	1:B:231:TYR:CE1	2.41	0.56
1:A:122:TYR:N	1:A:174:LYS:O	2.38	0.56
1:A:120:VAL:HG13	1:A:129:PHE:HB3	1.86	0.56
1:A:180:TYR:CE1	1:B:108:ARG:HG3	2.41	0.56
1:A:207:ILE:HA	1:A:234:VAL:O	2.06	0.56
1:C:223:ALA:HB3	1:C:224:GLU:OE2	2.06	0.56
1:D:34:ASP:C	1:D:35:ARG:HG3	2.30	0.56
1:C:157:CYS:HB3	1:C:171:CYS:HA	1.88	0.56
1:D:60:VAL:CG2	1:D:185:ILE:HD11	2.36	0.56
1:D:208:VAL:HG13	1:D:234:VAL:HG23	1.88	0.56
1:D:220:ASP:HB2	1:E:195:ASP:HB2	1.87	0.56
1:E:218:LYS:HB2	1:E:225:ILE:CD1	2.36	0.56
1:A:108:ARG:HG3	1:A:108:ARG:NH1	2.17	0.55
1:D:106:SER:HB3	1:D:139:LEU:O	2.06	0.55
1:A:84:TRP:CZ3	1:A:199:TYR:CD2	2.94	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:THR:OG1	1:C:106:SER:N	2.39	0.55
1:E:36:LEU:HD12	1:E:36:LEU:H	1.71	0.55
1:E:101:PHE:CD1	1:E:101:PHE:C	2.84	0.55
1:B:120:VAL:HG21	1:B:178:TRP:CE3	2.41	0.55
1:C:72:VAL:HG11	1:C:237:ARG:HH12	1.70	0.55
1:C:105:THR:OG1	1:C:141:SER:HB3	2.06	0.55
1:C:107:LEU:HG	1:C:108:ARG:N	2.20	0.55
1:E:125:ALA:HB1	1:E:128:GLU:O	2.06	0.55
1:A:108:ARG:HD2	1:E:180:TYR:CE1	2.42	0.55
1:A:51:VAL:CG1	1:A:58:VAL:HG21	2.37	0.55
1:C:197:LYS:HG2	1:C:200:TRP:HB3	1.87	0.55
1:E:42:ARG:HE	1:E:43:GLY:N	2.04	0.55
1:E:77:GLN:OE1	1:E:159:ILE:HG12	2.07	0.55
1:E:96:TRP:CZ2	1:E:141:SER:HB3	2.41	0.55
1:E:200:TRP:CH2	1:E:202:SER:HA	2.42	0.55
1:B:205:TRP:CB	1:B:238:LEU:H	2.15	0.55
1:C:72:VAL:HG11	1:C:237:ARG:HH22	1.71	0.55
1:B:41:PHE:H	1:B:44:TYR:HB2	1.71	0.55
1:C:139:LEU:HD12	1:C:140:PHE:N	2.21	0.55
1:E:52:PRO:HB2	1:E:91:ASP:OD1	2.06	0.55
1:E:127:GLY:O	1:E:128:GLU:HG2	2.06	0.55
1:C:120:VAL:HG23	1:C:129:PHE:O	2.06	0.55
1:D:96:TRP:HZ2	1:D:106:SER:HA	1.71	0.55
1:D:206:ALA:HB3	1:D:236:ARG:N	2.20	0.55
1:B:156:SER:HA	1:B:157:CYS:CB	2.35	0.54
1:C:70:ILE:HB	1:C:80:THR:HG22	1.89	0.54
1:E:169:GLN:CD	1:E:170:ASN:H	2.14	0.54
1:E:208:VAL:HB	1:E:234:VAL:HG23	1.89	0.54
1:B:54:THR:HG23	1:B:92:TYR:CZ	2.42	0.54
1:D:96:TRP:CZ3	1:D:141:SER:HA	2.41	0.54
1:C:47:TRP:HB3	1:C:50:PRO:HD3	1.90	0.54
1:D:76:ASN:O	1:D:77:GLN:NE2	2.40	0.54
1:E:204:GLU:O	1:E:205:TRP:HD1	1.90	0.54
1:B:180:TYR:HD1	1:C:108:ARG:HD2	1.71	0.54
1:C:39:HIS:CE1	1:C:109:VAL:HG12	2.42	0.54
1:C:135:THR:HG23	1:C:136:LYS:O	2.08	0.54
1:D:33:GLU:HA	1:D:37:PHE:HB3	1.89	0.54
1:A:61:ARG:HD3	1:A:88:GLU:OE2	2.07	0.54
1:B:77:GLN:HA	1:B:159:ILE:HD12	1.89	0.54
1:A:36:LEU:HD12	1:A:36:LEU:N	2.23	0.54
1:A:121:LEU:HD22	1:A:153:TYR:CD1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:GLU:HB2	1:C:205:TRP:CE3	2.42	0.54
1:C:209:ASN:HB2	1:C:234:VAL:CG2	2.38	0.54
1:B:180:TYR:CE1	1:C:108:ARG:HD2	2.43	0.54
1:C:124:ASN:ND2	1:C:126:ASP:OD1	2.41	0.54
1:D:79:MET:CE	1:D:171:CYS:HB3	2.38	0.54
1:A:110:PRO:HB2	1:A:113:MET:HG2	1.90	0.54
1:B:190:MET:CE	1:B:194:VAL:HG11	2.38	0.54
1:C:64:LEU:HD23	1:C:65:SER:N	2.23	0.54
1:D:69:LEU:HB3	1:D:200:TRP:HH2	1.71	0.54
1:E:197:LYS:CA	1:E:197:LYS:NZ	2.71	0.54
1:B:110:PRO:HG2	1:B:113:MET:HE3	1.88	0.54
1:A:161:VAL:HG22	1:A:161:VAL:O	2.08	0.53
1:A:191:GLU:C	1:A:193:THR:H	2.16	0.53
1:C:38:LYS:HZ1	1:C:96:TRP:NE1	2.06	0.53
1:A:38:LYS:HE3	1:A:101:PHE:HB2	1.91	0.53
1:C:58:VAL:HB	1:C:185:ILE:HD13	1.89	0.53
1:B:137:ALA:HB1	1:B:145:VAL:CG1	2.38	0.53
1:E:161:VAL:HG11	1:E:163:PHE:HE1	1.71	0.53
1:E:197:LYS:HA	1:E:197:LYS:NZ	2.23	0.53
1:A:160:ASP:HB3	1:A:168:GLN:HB2	1.89	0.53
1:B:206:ALA:HB3	1:B:235:ILE:HB	1.90	0.53
2:D:300:EPJ:N2	1:E:148:VAL:HB	2.23	0.53
1:E:197:LYS:NZ	1:E:200:TRP:HB2	2.23	0.53
1:E:206:ALA:CB	1:E:236:ARG:N	2.62	0.53
1:A:187:LEU:O	1:A:187:LEU:HD12	2.09	0.53
1:C:98:PRO:HB3	1:C:105:THR:CG2	2.38	0.53
1:A:207:ILE:HD13	1:A:235:ILE:HG23	1.91	0.53
1:B:46:ARG:HH11	1:B:46:ARG:CG	2.20	0.53
1:C:101:PHE:C	1:C:104:ILE:HG23	2.34	0.53
1:D:76:ASN:C	1:D:77:GLN:CD	2.77	0.53
1:B:216:SER:HA	1:B:227:PRO:HA	1.91	0.53
1:C:49:ARG:HD2	1:D:110:PRO:CG	2.37	0.53
1:D:161:VAL:HG23	1:D:167:ASP:OD2	2.09	0.53
1:E:194:VAL:O	1:E:194:VAL:HG13	2.08	0.53
1:A:211:THR:OG1	1:A:232:ALA:HB3	2.09	0.53
1:D:38:LYS:HE3	1:D:96:TRP:CE2	2.44	0.53
1:D:47:TRP:HB3	1:D:50:PRO:HD3	1.90	0.53
1:A:167:ASP:OD1	1:A:237:ARG:HD3	2.09	0.53
1:A:200:TRP:CH2	1:A:202:SER:HA	2.43	0.53
1:B:217:LYS:HD3	1:B:219:TYR:CZ	2.44	0.53
1:C:49:ARG:HE	1:D:113:MET:HE2	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:LYS:HB2	1:D:225:ILE:HD11	1.90	0.53
1:A:77:GLN:O	1:A:77:GLN:HG3	2.08	0.52
1:A:92:TYR:OH	1:A:93:LYS:HE2	2.08	0.52
1:A:36:LEU:HD11	1:E:93:LYS:HZ3	1.74	0.52
1:C:64:LEU:O	1:C:196:LEU:HG	2.08	0.52
1:C:197:LYS:HA	1:C:200:TRP:CB	2.38	0.52
1:A:135:THR:HG22	1:A:147:TRP:HE1	1.75	0.52
1:A:167:ASP:C	1:A:168:GLN:HG3	2.33	0.52
1:A:172:LYS:NZ	1:B:201:GLU:OE2	2.41	0.52
1:B:238:LEU:CD1	1:B:239:PRO:HD2	2.37	0.52
1:E:61:ARG:HB3	1:E:190:MET:HG2	1.92	0.52
1:E:74:GLU:HG2	1:E:159:ILE:CD1	2.37	0.52
1:A:190:MET:O	1:A:191:GLU:HB2	2.10	0.52
1:B:98:PRO:CA	1:B:105:THR:HG21	2.40	0.52
1:C:118:ASP:OD2	1:C:179:THR:OG1	2.27	0.52
1:D:120:VAL:CG2	1:D:129:PHE:HB3	2.38	0.52
1:E:139:LEU:HD12	1:E:140:PHE:H	1.74	0.52
1:A:205:TRP:CH2	1:A:237:ARG:HG2	2.44	0.52
1:B:74:GLU:HB3	1:B:75:LYS:C	2.35	0.52
1:B:116:ILE:HD12	1:B:147:TRP:CZ3	2.44	0.52
1:C:96:TRP:CE2	1:C:141:SER:HB3	2.44	0.52
1:A:70:ILE:CB	1:A:80:THR:HG22	2.30	0.52
1:A:160:ASP:N	1:A:168:GLN:O	2.42	0.52
1:A:70:ILE:HD11	1:A:82:ASN:HB2	1.91	0.52
1:A:168:GLN:HB3	1:A:236:ARG:CZ	2.37	0.52
1:C:57:VAL:HG22	1:C:183:ALA:O	2.09	0.52
1:C:191:GLU:C	1:C:193:THR:N	2.67	0.52
1:E:190:MET:O	1:E:192:GLN:N	2.43	0.52
1:B:206:ALA:HB1	1:B:235:ILE:HB	1.91	0.52
1:A:37:PHE:CD1	1:A:38:LYS:HE2	2.43	0.52
1:A:229:VAL:HG12	1:A:231:TYR:CE1	2.44	0.52
1:A:46:ARG:NH1	1:A:48:ALA:HA	2.20	0.51
1:C:125:ALA:CB	1:C:129:PHE:HA	2.39	0.51
1:E:51:VAL:O	1:E:53:ASN:N	2.42	0.51
1:E:67:ALA:O	1:E:68:GLN:HG2	2.10	0.51
1:A:157:CYS:SG	1:A:158:SER:N	2.83	0.51
1:B:206:ALA:HB2	1:B:236:ARG:O	2.09	0.51
1:D:33:GLU:CB	1:D:37:PHE:CD2	2.86	0.51
1:A:74:GLU:OE2	1:A:169:GLN:NE2	2.42	0.51
1:C:197:LYS:O	1:C:200:TRP:HB3	2.10	0.51
1:D:47:TRP:HE3	1:D:48:ALA:N	2.05	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:SER:OG	1:D:56:ASP:N	2.32	0.51
1:E:161:VAL:HG12	1:E:162:THR:H	1.74	0.51
1:B:47:TRP:CH2	1:C:113:MET:HE1	2.45	0.51
1:B:83:VAL:CG2	1:B:151:ALA:HB3	2.40	0.51
1:C:131:VAL:HG21	1:C:149:PRO:CB	2.39	0.51
1:D:161:VAL:C	1:D:167:ASP:HB2	2.35	0.51
1:E:159:ILE:HG13	1:E:159:ILE:O	2.09	0.51
1:A:51:VAL:HG23	1:B:35:ARG:HH12	1.76	0.51
1:B:101:PHE:CD1	1:B:105:THR:HB	2.46	0.51
1:B:164:PHE:CB	1:B:165:PRO:CD	2.88	0.51
1:C:107:LEU:HD12	1:C:108:ARG:H	1.74	0.51
2:C:300:EPJ:C11	1:D:148:VAL:HB	2.40	0.51
1:D:210:ALA:HA	1:D:232:ALA:O	2.10	0.51
1:E:160:ASP:OD1	1:E:160:ASP:N	2.44	0.51
1:D:49:ARG:NE	1:E:113:MET:CE	2.74	0.51
1:B:169:GLN:HG2	1:B:235:ILE:CG1	2.41	0.51
1:C:207:ILE:HG12	1:C:235:ILE:HG22	1.93	0.51
1:E:46:ARG:HG2	1:E:47:TRP:N	2.26	0.51
1:E:209:ASN:H	1:E:234:VAL:CG2	2.23	0.51
1:A:92:TYR:CZ	1:A:93:LYS:HE2	2.46	0.51
1:C:235:ILE:HD12	1:C:237:ARG:HH21	1.75	0.51
1:D:65:SER:HB3	1:D:199:TYR:CE1	2.45	0.51
1:E:207:ILE:CD1	1:E:233:PHE:HD2	2.21	0.51
1:A:219:TYR:CD2	1:B:199:TYR:CZ	2.99	0.51
1:B:116:ILE:HD12	1:B:147:TRP:CH2	2.46	0.51
1:D:96:TRP:CD2	1:D:141:SER:HA	2.46	0.51
1:E:74:GLU:O	1:E:159:ILE:CD1	2.59	0.51
1:A:162:THR:CB	1:A:168:GLN:NE2	2.68	0.51
1:B:47:TRP:HA	1:B:47:TRP:HE3	1.76	0.51
1:C:116:ILE:HD12	1:C:147:TRP:CZ3	2.46	0.51
1:D:182:LYS:HB2	1:D:227:PRO:HD3	1.92	0.51
1:E:218:LYS:HB2	1:E:225:ILE:HD11	1.93	0.51
1:A:62:PHE:HE1	1:A:85:LEU:HD22	1.74	0.50
1:D:42:ARG:NH1	1:D:94:LEU:HD22	2.26	0.50
1:E:169:GLN:CD	1:E:170:ASN:N	2.69	0.50
1:E:67:ALA:C	1:E:68:GLN:HG2	2.36	0.50
1:A:65:SER:HB2	1:A:84:TRP:HB2	1.92	0.50
1:B:209:ASN:HB3	1:B:234:VAL:CG2	2.41	0.50
1:D:74:GLU:HB2	1:D:75:LYS:HD3	1.94	0.50
1:E:46:ARG:HH21	1:E:115:TRP:H	1.59	0.50
1:E:179:THR:HG22	2:E:300:EPJ:CL	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:TRP:C	1:A:50:PRO:HD2	2.36	0.50
1:C:139:LEU:HD12	1:C:140:PHE:H	1.74	0.50
1:C:179:THR:O	1:D:108:ARG:NE	2.34	0.50
1:E:107:LEU:HD12	1:E:107:LEU:C	2.37	0.50
1:B:138:HIS:HB3	1:B:146:HIS:HB2	1.94	0.50
1:B:180:TYR:CB	1:B:185:ILE:CG2	2.90	0.50
1:E:160:ASP:OD1	1:E:169:GLN:HG2	2.11	0.50
1:B:68:GLN:HG2	1:B:69:LEU:N	2.27	0.50
1:B:131:VAL:O	1:B:134:MET:HE2	2.12	0.50
1:C:58:VAL:HB	1:C:185:ILE:HD12	1.94	0.50
1:C:84:TRP:CZ3	1:C:199:TYR:CD2	2.99	0.50
1:D:123:ASN:ND2	1:D:172:LYS:O	2.44	0.50
1:D:208:VAL:HG12	1:D:234:VAL:HG23	1.94	0.50
1:B:68:GLN:CD	1:B:70:ILE:HD13	2.37	0.50
1:C:96:TRP:NE1	1:C:141:SER:HB3	2.27	0.50
1:E:87:GLN:OE1	1:E:119:ILE:HD12	2.12	0.50
1:A:207:ILE:HD13	1:A:235:ILE:CG2	2.42	0.49
1:B:59:ILE:N	1:B:59:ILE:HD12	2.27	0.49
1:B:204:GLU:N	1:B:204:GLU:OE1	2.44	0.49
1:D:49:ARG:HB2	1:D:50:PRO:HD3	1.93	0.49
1:D:70:ILE:HB	1:D:80:THR:HG22	1.94	0.49
1:D:208:VAL:HG13	1:D:209:ASN:N	2.28	0.49
1:E:197:LYS:NZ	1:E:200:TRP:CB	2.75	0.49
1:A:59:ILE:HA	1:A:186:ASP:O	2.11	0.49
1:A:59:ILE:N	1:A:59:ILE:HD12	2.27	0.49
1:C:70:ILE:HD12	1:C:80:THR:CG2	2.41	0.49
1:D:72:VAL:HG11	1:D:205:TRP:CD2	2.47	0.49
1:D:129:PHE:CZ	1:E:150:PRO:HB2	2.47	0.49
1:A:57:VAL:HG13	1:A:59:ILE:HD11	1.94	0.49
1:B:34:ASP:O	1:B:37:PHE:HB3	2.11	0.49
1:B:121:LEU:HD23	1:B:124:ASN:HA	1.95	0.49
1:D:180:TYR:HD1	1:E:108:ARG:HG3	1.74	0.49
1:A:40:LEU:O	1:A:44:TYR:HB2	2.13	0.49
1:A:131:VAL:HG21	1:A:149:PRO:CG	2.42	0.49
1:C:65:SER:CB	1:C:199:TYR:CE1	2.89	0.49
1:D:118:ASP:OD2	1:D:179:THR:OG1	2.26	0.49
1:A:62:PHE:CZ	1:A:85:LEU:HD22	2.47	0.49
1:A:199:TYR:CZ	1:E:219:TYR:HB3	2.47	0.49
1:B:78:MET:CA	1:B:156:SER:HB2	2.38	0.49
1:C:38:LYS:NZ	1:C:96:TRP:NE1	2.61	0.49
1:A:96:TRP:CE2	1:A:141:SER:HB3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:GLU:C	1:A:193:THR:N	2.71	0.49
1:B:71:ASP:OD1	1:B:72:VAL:N	2.45	0.49
1:D:66:ILE:CG2	1:D:197:LYS:HE3	2.43	0.49
1:E:64:LEU:HD12	1:E:84:TRP:O	2.12	0.49
1:D:96:TRP:CE2	1:D:141:SER:CB	2.92	0.49
1:A:192:GLN:H	1:A:192:GLN:CD	2.12	0.49
1:D:163:PHE:H	1:D:167:ASP:CB	2.25	0.49
1:D:107:LEU:HD13	1:D:109:VAL:HG13	1.94	0.49
1:A:38:LYS:CE	1:A:101:PHE:HB2	2.43	0.48
1:A:75:LYS:H	1:A:75:LYS:CD	2.26	0.48
1:B:185:ILE:HG12	1:B:186:ASP:N	2.28	0.48
1:E:124:ASN:HD21	1:E:126:ASP:CG	2.10	0.48
1:E:82:ASN:HA	1:E:152:ILE:HD13	1.95	0.48
1:E:139:LEU:HD12	1:E:140:PHE:N	2.27	0.48
1:C:96:TRP:NE1	1:C:105:THR:OG1	2.45	0.48
1:A:109:VAL:CG2	1:A:110:PRO:HD2	2.40	0.48
1:A:219:TYR:HA	1:B:199:TYR:OH	2.13	0.48
1:B:98:PRO:CB	1:B:105:THR:HG21	2.44	0.48
1:A:75:LYS:H	1:A:75:LYS:HD3	1.78	0.48
1:B:219:TYR:CD2	1:C:199:TYR:HD2	2.21	0.48
1:C:125:ALA:HB1	1:C:129:PHE:N	2.29	0.48
1:D:207:ILE:H	1:D:235:ILE:HA	1.77	0.48
1:A:53:ASN:CA	1:A:92:TYR:CE1	2.97	0.48
1:C:49:ARG:N	1:C:50:PRO:CD	2.76	0.48
1:C:91:ASP:CG	1:C:94:LEU:HG	2.39	0.48
1:B:122:TYR:CB	1:B:174:LYS:HD3	2.44	0.48
1:C:108:ARG:HG3	1:C:108:ARG:NH1	2.25	0.48
1:D:64:LEU:HD23	1:D:65:SER:N	2.29	0.48
1:E:33:GLU:HG2	1:E:37:PHE:CE2	2.48	0.48
1:A:159:ILE:HA	1:A:169:GLN:HG2	1.94	0.48
1:C:91:ASP:HB3	1:C:94:LEU:HB2	1.96	0.48
1:C:128:GLU:OE1	1:C:132:THR:HG22	2.12	0.48
1:C:128:GLU:O	1:C:129:PHE:HB2	2.13	0.48
1:D:159:ILE:HG13	1:D:159:ILE:O	2.14	0.48
1:A:122:TYR:O	1:A:124:ASN:N	2.47	0.48
1:B:74:GLU:N	1:B:75:LYS:O	2.31	0.48
1:E:53:ASN:HD21	1:E:56:ASP:C	2.21	0.48
1:E:72:VAL:HG11	1:E:205:TRP:CE3	2.48	0.48
1:B:47:TRP:CE2	1:B:49:ARG:CG	2.96	0.47
1:B:200:TRP:HE1	1:B:207:ILE:CG2	2.26	0.47
1:C:69:LEU:C	1:C:69:LEU:HD23	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:VAL:HG21	1:D:149:PRO:CB	2.44	0.47
1:B:78:MET:HA	1:B:156:SER:CB	2.41	0.47
1:D:120:VAL:HG22	1:D:121:LEU:N	2.28	0.47
1:D:163:PHE:H	1:D:167:ASP:HB3	1.80	0.47
1:A:207:ILE:O	1:A:207:ILE:HG22	2.13	0.47
1:B:205:TRP:HB3	1:B:238:LEU:HB3	1.95	0.47
1:C:51:VAL:HG12	1:C:58:VAL:CG2	2.33	0.47
1:C:52:PRO:HB2	1:C:91:ASP:OD1	2.13	0.47
1:E:42:ARG:NH2	1:E:43:GLY:HA2	2.29	0.47
1:E:74:GLU:CG	1:E:159:ILE:HD12	2.42	0.47
1:D:206:ALA:HB3	1:D:235:ILE:HA	1.96	0.47
1:A:40:LEU:HD22	1:A:44:TYR:CE1	2.49	0.47
1:A:88:GLU:HA	1:A:145:VAL:O	2.15	0.47
1:B:54:THR:CG2	1:B:92:TYR:CE2	2.97	0.47
1:C:61:ARG:CB	1:C:88:GLU:HG2	2.30	0.47
1:C:106:SER:HB3	1:C:140:PHE:CD1	2.50	0.47
1:B:55:SER:OG	1:B:56:ASP:N	2.46	0.47
1:C:196:LEU:N	1:C:196:LEU:HD12	2.29	0.47
1:E:34:ASP:HB2	1:E:37:PHE:CE2	2.49	0.47
1:A:57:VAL:HG13	1:A:59:ILE:HD12	1.97	0.47
1:A:136:LYS:HB2	1:E:179:THR:HG21	1.95	0.47
1:B:94:LEU:HB3	1:B:139:LEU:HD21	1.96	0.47
1:B:158:SER:HA	1:C:204:GLU:OE2	2.15	0.47
1:B:159:ILE:O	1:B:160:ASP:HB3	2.12	0.47
1:B:238:LEU:HD12	1:B:239:PRO:CD	2.41	0.47
1:C:96:TRP:CE2	1:C:141:SER:HA	2.50	0.47
1:C:106:SER:HB3	1:C:140:PHE:HD1	1.80	0.47
1:C:197:LYS:HG3	1:C:200:TRP:CE3	2.50	0.47
1:D:96:TRP:NE1	1:D:141:SER:HB3	2.30	0.47
1:D:107:LEU:CD1	1:D:107:LEU:C	2.88	0.47
1:E:120:VAL:CG1	1:E:121:LEU:N	2.78	0.47
1:B:51:VAL:HG23	1:B:52:PRO:HD2	1.95	0.47
1:B:129:PHE:HB2	1:C:133:HIS:HE2	1.75	0.47
1:B:220:ASP:O	1:C:194:VAL:HG13	2.14	0.47
1:B:225:ILE:N	1:B:225:ILE:CD1	2.78	0.47
1:C:72:VAL:CG1	1:C:237:ARG:HH22	2.28	0.47
1:C:157:CYS:HB2	1:C:170:ASN:O	2.14	0.47
1:D:107:LEU:HD12	1:D:107:LEU:O	2.14	0.47
1:D:163:PHE:N	1:D:167:ASP:HA	2.23	0.47
1:B:47:TRP:CE2	1:B:49:ARG:HG2	2.50	0.47
1:B:47:TRP:HD1	1:B:50:PRO:HG3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:TYR:CB	1:B:185:ILE:HG22	2.30	0.47
1:D:57:VAL:O	1:D:57:VAL:HG12	2.15	0.47
1:A:122:TYR:HB2	1:A:174:LYS:HD3	1.98	0.46
1:A:221:CYS:SG	1:A:222:CYS:N	2.88	0.46
1:D:191:GLU:C	1:D:193:THR:H	2.23	0.46
1:A:86:LYS:HZ2	1:A:194:VAL:CG1	2.29	0.46
1:A:162:THR:HB	1:A:168:GLN:CD	2.39	0.46
1:A:207:ILE:CD1	1:A:235:ILE:CG2	2.94	0.46
1:B:220:ASP:HB2	1:C:198:ASP:OD2	2.15	0.46
1:C:102:GLY:CA	1:C:104:ILE:HG12	2.46	0.46
1:E:38:LYS:HA	1:E:38:LYS:HD3	1.66	0.46
1:E:128:GLU:HG3	1:E:132:THR:HG21	1.97	0.46
1:A:45:ASN:HD22	1:A:45:ASN:C	2.22	0.46
1:A:61:ARG:HD3	1:A:88:GLU:CD	2.41	0.46
1:C:46:ARG:HG2	1:C:47:TRP:N	2.29	0.46
1:D:105:THR:OG1	1:D:106:SER:N	2.44	0.46
1:D:168:GLN:HA	1:D:236:ARG:NH1	2.31	0.46
1:E:77:GLN:HA	1:E:159:ILE:CD1	2.39	0.46
1:B:74:GLU:HB2	1:B:76:ASN:O	2.16	0.46
1:C:122:TYR:CB	1:C:174:LYS:HD3	2.45	0.46
1:A:128:GLU:OE1	1:A:132:THR:HG21	2.16	0.46
1:B:169:GLN:CD	1:B:235:ILE:O	2.57	0.46
1:C:40:LEU:O	1:C:44:TYR:HB2	2.16	0.46
1:C:121:LEU:HD23	1:C:125:ALA:CB	2.29	0.46
1:E:89:TRP:CZ2	1:E:145:VAL:HG11	2.51	0.46
1:A:58:VAL:C	1:A:59:ILE:HD12	2.40	0.46
1:D:70:ILE:HD12	1:D:80:THR:HG22	1.96	0.46
1:D:74:GLU:HB2	1:D:75:LYS:NZ	2.31	0.46
1:A:72:VAL:HG23	1:A:78:MET:O	2.16	0.46
1:A:98:PRO:O	1:A:103:ASN:HA	2.15	0.46
1:B:217:LYS:HD3	1:B:219:TYR:CE2	2.51	0.46
1:C:37:PHE:O	1:C:40:LEU:HB2	2.15	0.46
1:D:69:LEU:HB3	1:D:200:TRP:CH2	2.49	0.46
1:D:78:MET:HE2	1:D:78:MET:HB3	1.63	0.46
1:B:221:CYS:SG	1:B:222:CYS:N	2.88	0.46
1:D:169:GLN:CD	1:D:235:ILE:HG12	2.41	0.46
1:E:34:ASP:HB2	1:E:37:PHE:CD2	2.51	0.46
1:E:74:GLU:O	1:E:75:LYS:C	2.59	0.46
1:C:168:GLN:HB2	1:C:236:ARG:CG	2.46	0.46
1:C:237:ARG:HA	1:C:237:ARG:HD3	1.28	0.46
1:A:61:ARG:NH2	1:A:190:MET:HG3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:ASP:OD2	1:B:197:LYS:N	2.49	0.45
1:C:128:GLU:C	1:C:130:ALA:H	2.24	0.45
1:D:161:VAL:O	1:D:162:THR:OG1	2.32	0.45
1:D:133:HIS:HB3	1:D:134:MET:HA	1.98	0.45
1:A:42:ARG:NH2	1:A:107:LEU:HD11	2.31	0.45
1:A:51:VAL:CG2	1:B:35:ARG:NH1	2.80	0.45
1:A:124:ASN:CG	1:B:68:GLN:HB2	2.41	0.45
1:B:156:SER:CA	1:B:157:CYS:HB3	2.40	0.45
1:B:219:TYR:HB3	1:C:199:TYR:HE2	1.81	0.45
1:D:214:TYR:CD1	1:D:214:TYR:C	2.93	0.45
1:A:86:LYS:HE3	1:A:86:LYS:HB2	1.77	0.45
1:B:40:LEU:O	1:B:41:PHE:HB2	2.17	0.45
1:B:47:TRP:CZ2	1:B:49:ARG:HG3	2.51	0.45
1:C:46:ARG:NH1	1:C:91:ASP:OD2	2.50	0.45
1:E:72:VAL:HG11	1:E:205:TRP:CZ3	2.52	0.45
1:E:95:ARG:HB2	1:E:95:ARG:NH1	2.32	0.45
1:B:46:ARG:CG	1:B:46:ARG:NH1	2.77	0.45
1:B:96:TRP:CE2	1:B:141:SER:HB3	2.52	0.45
1:C:101:PHE:O	1:C:104:ILE:HG12	2.16	0.45
1:D:51:VAL:HG22	1:E:35:ARG:CZ	2.46	0.45
1:D:172:LYS:HE3	1:E:201:GLU:OE1	2.17	0.45
1:E:200:TRP:CZ3	1:E:202:SER:HA	2.51	0.45
1:A:51:VAL:CG2	1:B:35:ARG:HH12	2.30	0.45
1:B:106:SER:HB2	1:B:139:LEU:O	2.17	0.45
1:C:70:ILE:HD11	1:C:82:ASN:HB2	1.98	0.45
1:C:131:VAL:O	1:C:132:THR:HG22	2.15	0.45
1:D:47:TRP:HE3	1:D:47:TRP:HA	1.79	0.45
1:D:206:ALA:O	1:D:207:ILE:HB	2.16	0.45
1:A:148:VAL:HB	2:E:300:EPJ:C11	2.47	0.45
1:A:166:PHE:CG	1:A:166:PHE:O	2.68	0.45
1:C:204:GLU:CB	1:C:205:TRP:CE3	3.00	0.45
1:E:68:GLN:HB3	1:E:70:ILE:HD13	1.99	0.45
1:E:107:LEU:HD13	1:E:109:VAL:HG13	1.97	0.45
1:A:70:ILE:HD11	1:A:82:ASN:CB	2.47	0.45
1:C:161:VAL:CG2	1:C:162:THR:H	2.23	0.45
1:E:51:VAL:CG2	1:E:53:ASN:HB2	2.45	0.45
1:E:202:SER:O	1:E:204:GLU:N	2.46	0.45
1:B:76:ASN:HA	1:B:77:GLN:HA	1.80	0.44
1:C:129:PHE:CZ	1:D:150:PRO:HB2	2.52	0.44
1:C:224:GLU:CD	1:C:224:GLU:H	2.25	0.44
1:D:69:LEU:CB	1:D:200:TRP:CH2	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:CYS:HB2	1:E:194:VAL:HG23	1.92	0.44
1:C:72:VAL:CG1	1:C:237:ARG:HH12	2.29	0.44
1:E:36:LEU:HD12	1:E:36:LEU:N	2.31	0.44
1:C:224:GLU:CD	1:C:224:GLU:N	2.75	0.44
1:D:179:THR:HG22	2:D:300:EPJ:CL	2.53	0.44
1:E:160:ASP:OD1	1:E:169:GLN:HB2	2.17	0.44
1:E:197:LYS:NZ	1:E:197:LYS:CB	2.81	0.44
1:D:236:ARG:O	1:D:237:ARG:CG	2.66	0.44
1:A:150:PRO:HD3	1:E:178:TRP:NE1	2.31	0.44
1:B:129:PHE:CZ	1:C:150:PRO:HB2	2.52	0.44
1:C:49:ARG:HB2	1:C:50:PRO:HD3	2.00	0.44
1:A:77:GLN:NE2	1:A:159:ILE:HG23	2.12	0.44
1:A:122:TYR:HB3	1:A:174:LYS:HD3	1.98	0.44
1:D:38:LYS:HE3	1:D:96:TRP:CD2	2.52	0.44
1:E:33:GLU:HG3	1:E:34:ASP:OD1	2.17	0.44
1:E:160:ASP:O	1:E:161:VAL:HG22	2.18	0.44
1:A:36:LEU:HD12	1:A:36:LEU:H	1.83	0.44
1:A:150:PRO:HB2	1:E:129:PHE:CZ	2.53	0.44
1:A:164:PHE:CB	1:A:165:PRO:CD	2.85	0.44
1:A:189:GLN:O	1:A:191:GLU:N	2.51	0.44
1:B:98:PRO:CB	1:B:105:THR:CG2	2.95	0.44
1:B:122:TYR:HB2	1:B:174:LYS:HD3	2.00	0.44
1:D:63:GLY:HA3	1:D:86:LYS:CE	2.47	0.44
1:E:214:TYR:CD1	1:E:214:TYR:C	2.95	0.44
1:E:222:CYS:SG	2:E:300:EPJ:C8	3.06	0.44
1:B:74:GLU:HB3	1:B:75:LYS:CA	2.48	0.44
1:D:49:ARG:HE	1:E:113:MET:HE1	1.83	0.44
1:B:83:VAL:O	1:B:151:ALA:N	2.49	0.44
1:B:206:ALA:HB1	1:B:235:ILE:HA	2.00	0.44
1:E:86:LYS:NZ	1:E:88:GLU:OE1	2.49	0.44
1:A:49:ARG:CB	1:A:50:PRO:HD3	2.40	0.43
1:B:162:THR:HG23	1:B:163:PHE:CD1	2.53	0.43
1:A:47:TRP:CZ3	1:B:39:HIS:HB3	2.53	0.43
1:A:61:ARG:HG2	1:A:188:GLU:OE2	2.18	0.43
1:A:78:MET:HE2	1:A:78:MET:HB3	1.55	0.43
1:A:181:ASP:OD2	1:A:183:ALA:HB3	2.18	0.43
1:A:210:ALA:HA	1:A:232:ALA:O	2.18	0.43
1:B:38:LYS:NZ	1:B:100:ASP:HB2	2.33	0.43
1:E:47:TRP:O	1:E:50:PRO:HD2	2.18	0.43
1:E:62:PHE:C	1:E:190:MET:HG3	2.43	0.43
1:B:47:TRP:CG	1:B:50:PRO:HD3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:ARG:HA	1:E:188:GLU:O	2.19	0.43
1:E:217:LYS:HG2	1:E:218:LYS:O	2.17	0.43
1:B:47:TRP:O	1:B:50:PRO:HD2	2.18	0.43
1:B:164:PHE:HB3	1:B:165:PRO:HD3	1.97	0.43
1:D:133:HIS:ND1	1:D:135:THR:HG22	2.34	0.43
1:D:236:ARG:O	1:D:237:ARG:HG2	2.18	0.43
1:C:148:VAL:HG12	1:C:148:VAL:O	2.17	0.43
1:D:204:GLU:N	1:D:204:GLU:OE1	2.52	0.43
1:D:208:VAL:HG13	1:D:234:VAL:CG2	2.48	0.43
1:E:161:VAL:CG1	1:E:163:PHE:CE1	2.99	0.43
1:A:178:TRP:HH2	1:B:84:TRP:CE2	2.37	0.43
1:C:98:PRO:O	1:C:104:ILE:CG2	2.60	0.43
1:D:46:ARG:HG2	1:D:47:TRP:N	2.32	0.43
1:E:197:LYS:HZ2	1:E:197:LYS:CB	2.30	0.43
1:A:38:LYS:HE3	1:A:101:PHE:CB	2.48	0.43
1:A:52:PRO:HD3	1:A:115:TRP:CE2	2.52	0.43
1:A:68:GLN:HE22	1:E:156:SER:CB	2.28	0.43
1:A:96:TRP:CD2	1:A:141:SER:HA	2.53	0.43
1:A:179:THR:HG22	1:A:179:THR:O	2.18	0.43
1:B:226:TYR:HA	1:B:227:PRO:HD2	1.75	0.43
1:C:66:ILE:HG23	1:C:66:ILE:O	2.18	0.43
1:C:91:ASP:OD2	1:C:94:LEU:HG	2.18	0.43
1:C:98:PRO:C	1:C:104:ILE:HG21	2.43	0.43
1:D:161:VAL:HG13	1:D:162:THR:N	2.33	0.43
1:D:169:GLN:NE2	1:D:169:GLN:C	2.77	0.43
1:A:74:GLU:O	1:A:77:GLN:N	2.51	0.43
1:A:204:GLU:O	1:A:238:LEU:HB3	2.18	0.43
1:A:234:VAL:HG11	1:A:236:ARG:NH2	2.33	0.43
1:B:206:ALA:HB1	1:B:235:ILE:C	2.43	0.43
1:D:62:PHE:HE1	1:D:85:LEU:HD22	1.84	0.43
1:D:96:TRP:CZ2	1:D:141:SER:HB3	2.51	0.43
1:D:161:VAL:C	1:D:167:ASP:CB	2.91	0.43
1:A:37:PHE:CE1	1:A:101:PHE:CG	3.07	0.43
1:B:135:THR:OG1	1:B:136:LYS:N	2.51	0.43
1:B:206:ALA:HB2	1:B:236:ARG:C	2.43	0.43
1:C:101:PHE:O	1:C:104:ILE:HG23	2.17	0.43
1:E:96:TRP:CE3	1:E:141:SER:HA	2.53	0.43
1:A:74:GLU:CD	1:A:169:GLN:HE22	2.27	0.43
1:B:73:ASP:HA	1:B:74:GLU:HA	1.44	0.43
1:C:34:ASP:HB2	1:C:37:PHE:HB3	1.94	0.43
1:C:196:LEU:HD22	1:C:210:ALA:HB1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:GLU:O	1:D:188:GLU:HG3	2.18	0.43
1:D:191:GLU:C	1:D:193:THR:N	2.77	0.43
1:E:169:GLN:N	1:E:235:ILE:HG12	2.34	0.43
1:B:56:ASP:O	1:B:57:VAL:CG1	2.65	0.42
1:E:74:GLU:CB	1:E:159:ILE:HD12	2.48	0.42
1:A:181:ASP:HB3	1:A:226:TYR:CE2	2.54	0.42
1:B:160:ASP:CG	1:B:161:VAL:H	2.27	0.42
1:C:107:LEU:CG	1:C:108:ARG:N	2.81	0.42
1:D:218:LYS:HB2	1:D:225:ILE:HD13	2.00	0.42
1:E:218:LYS:HB2	1:E:225:ILE:HD13	2.01	0.42
1:A:109:VAL:HA	1:A:110:PRO:HD3	1.83	0.42
1:B:96:TRP:HE1	1:B:105:THR:HG21	1.83	0.42
1:C:161:VAL:HG11	1:C:163:PHE:CE2	2.54	0.42
1:D:49:ARG:N	1:D:50:PRO:CD	2.82	0.42
1:E:56:ASP:O	1:E:57:VAL:HG12	2.19	0.42
1:A:180:TYR:CE1	1:B:108:ARG:CG	3.02	0.42
1:B:79:MET:HB3	1:B:79:MET:HE2	1.72	0.42
1:D:180:TYR:HB2	1:D:185:ILE:CG2	2.49	0.42
1:B:42:ARG:HD3	1:B:42:ARG:HA	1.74	0.42
1:B:54:THR:HA	1:C:35:ARG:CZ	2.46	0.42
1:B:163:PHE:HB2	1:B:167:ASP:HB3	2.02	0.42
1:B:207:ILE:N	1:B:235:ILE:HG22	2.34	0.42
1:C:34:ASP:O	1:C:37:PHE:N	2.52	0.42
1:C:120:VAL:HG22	1:C:121:LEU:N	2.35	0.42
1:A:94:LEU:HB3	1:A:139:LEU:HD21	2.01	0.42
1:A:179:THR:HA	2:A:300:EPJ:C9	2.49	0.42
1:B:133:HIS:CB	1:B:134:MET:HA	2.19	0.42
1:B:168:GLN:HG3	1:B:169:GLN:H	1.84	0.42
1:B:177:SER:OG	1:B:180:TYR:HB2	2.20	0.42
1:D:47:TRP:CE3	1:D:47:TRP:CA	3.01	0.42
1:D:194:VAL:HG13	1:D:194:VAL:O	2.20	0.42
1:E:78:MET:HB3	1:E:78:MET:HE2	1.80	0.42
1:E:182:LYS:HA	1:E:185:ILE:O	2.19	0.42
1:A:56:ASP:HA	1:A:57:VAL:HA	1.90	0.42
1:A:75:LYS:HB2	1:A:75:LYS:HE2	1.67	0.42
1:A:184:LYS:HB3	1:A:184:LYS:HE3	1.83	0.42
1:A:218:LYS:HE2	1:A:223:ALA:HA	2.00	0.42
1:D:38:LYS:NZ	1:D:96:TRP:CE2	2.86	0.42
1:E:79:MET:HE3	1:E:155:SER:OG	2.20	0.42
1:E:118:ASP:OD2	1:E:179:THR:OG1	2.23	0.42
1:A:47:TRP:HB3	1:A:50:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:TYR:HA	1:B:95:ARG:NE	2.35	0.42
1:C:204:GLU:OE1	1:C:204:GLU:N	2.40	0.42
1:D:47:TRP:C	1:D:50:PRO:HD2	2.44	0.42
1:E:164:PHE:HB3	1:E:165:PRO:CD	2.49	0.42
1:A:168:GLN:C	1:A:169:GLN:HG3	2.45	0.42
1:D:49:ARG:NE	1:E:113:MET:HE3	2.35	0.42
1:D:94:LEU:HD13	1:D:139:LEU:HD22	2.00	0.42
1:D:96:TRP:CZ2	1:D:106:SER:HA	2.53	0.42
1:D:163:PHE:N	1:D:167:ASP:HB3	2.33	0.42
1:E:59:ILE:CD1	1:E:186:ASP:HB3	2.50	0.42
1:E:86:LYS:HG2	1:E:148:VAL:CG2	2.45	0.42
1:A:57:VAL:CG1	1:A:59:ILE:HD11	2.50	0.42
1:B:96:TRP:CE3	1:B:141:SER:HA	2.55	0.42
1:C:197:LYS:CG	1:C:200:TRP:HB3	2.48	0.42
1:D:125:ALA:HB1	1:D:128:GLU:C	2.45	0.42
1:D:160:ASP:HA	1:D:168:GLN:O	2.20	0.42
1:D:180:TYR:CE1	1:E:108:ARG:CG	3.02	0.42
1:E:70:ILE:HD13	1:E:70:ILE:HA	1.81	0.42
1:A:201:GLU:OE1	1:E:172:LYS:NZ	2.51	0.41
1:B:206:ALA:HB1	1:B:235:ILE:CB	2.49	0.41
1:C:51:VAL:CG1	1:C:58:VAL:CG2	2.95	0.41
1:C:86:LYS:HE3	1:C:86:LYS:HB2	1.78	0.41
1:C:218:LYS:HE2	1:C:223:ALA:HA	2.02	0.41
1:C:221:CYS:SG	1:C:222:CYS:N	2.93	0.41
1:D:37:PHE:O	1:D:41:PHE:N	2.49	0.41
1:E:38:LYS:CG	1:E:101:PHE:HB2	2.49	0.41
1:E:69:LEU:HD22	1:E:207:ILE:CG1	2.48	0.41
1:B:191:GLU:C	1:B:193:THR:H	2.27	0.41
1:D:161:VAL:CG2	1:D:162:THR:N	2.69	0.41
1:D:191:GLU:O	1:D:194:VAL:HG12	2.19	0.41
1:A:79:MET:HE2	1:A:79:MET:HB3	1.87	0.41
1:A:207:ILE:CA	1:A:234:VAL:O	2.68	0.41
1:A:224:GLU:OE1	1:A:226:TYR:OH	2.37	0.41
1:B:214:TYR:CD1	1:B:214:TYR:C	2.99	0.41
1:B:220:ASP:C	1:C:194:VAL:HG13	2.45	0.41
1:C:84:TRP:HZ3	1:C:199:TYR:CD2	2.38	0.41
1:D:207:ILE:CA	1:D:235:ILE:HG22	2.50	0.41
1:D:235:ILE:HG13	1:D:235:ILE:O	2.20	0.41
1:A:42:ARG:HB2	1:A:42:ARG:CZ	2.50	0.41
1:A:51:VAL:CG1	1:A:58:VAL:CG2	2.98	0.41
1:A:198:ASP:OD1	1:A:198:ASP:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:MET:HE2	1:C:79:MET:HB3	1.87	0.41
1:D:38:LYS:CE	1:D:96:TRP:CE2	3.03	0.41
1:B:186:ASP:OD1	1:B:187:LEU:N	2.51	0.41
1:B:219:TYR:HB3	1:C:199:TYR:CE2	2.54	0.41
1:C:181:ASP:HA	1:C:226:TYR:CD1	2.55	0.41
1:D:85:LEU:O	1:D:149:PRO:HD2	2.20	0.41
1:D:180:TYR:HE1	1:E:108:ARG:CB	2.32	0.41
1:E:184:LYS:HE3	1:E:184:LYS:HB3	1.88	0.41
1:C:36:LEU:HD12	1:C:36:LEU:C	2.46	0.41
1:E:97:ASN:HA	1:E:98:PRO:HD3	1.96	0.41
1:A:190:MET:O	1:A:190:MET:HG2	2.20	0.41
1:B:40:LEU:HD12	1:B:40:LEU:N	2.35	0.41
1:C:35:ARG:H	1:C:35:ARG:HG3	1.11	0.41
1:C:61:ARG:HD3	1:C:88:GLU:CD	2.45	0.41
1:D:75:LYS:HB2	1:D:75:LYS:HE2	1.73	0.41
1:E:42:ARG:HH21	1:E:43:GLY:HA3	1.86	0.41
1:E:68:GLN:HB3	1:E:70:ILE:CD1	2.50	0.41
1:A:82:ASN:HA	1:A:152:ILE:HD13	2.02	0.41
1:A:204:GLU:N	1:A:204:GLU:OE1	2.54	0.41
1:B:97:ASN:HA	1:B:98:PRO:HD3	1.57	0.41
1:C:107:LEU:CD1	1:C:108:ARG:H	2.32	0.41
1:A:86:LYS:NZ	1:A:194:VAL:HG12	2.34	0.41
1:B:164:PHE:N	1:B:164:PHE:CD1	2.88	0.41
1:B:172:LYS:HA	1:B:231:TYR:O	2.21	0.41
1:C:184:LYS:O	1:C:185:ILE:HD13	2.21	0.41
1:C:206:ALA:HB3	1:C:236:ARG:O	2.21	0.41
1:D:79:MET:HE2	1:D:79:MET:HB3	1.88	0.41
1:A:133:HIS:HB3	1:A:134:MET:C	2.46	0.41
1:B:38:LYS:HZ2	1:B:100:ASP:HB2	1.85	0.41
1:C:209:ASN:HB2	1:C:234:VAL:HG23	2.01	0.41
1:B:182:LYS:HA	1:B:185:ILE:O	2.21	0.40
1:B:200:TRP:CH2	1:B:202:SER:HA	2.56	0.40
1:B:206:ALA:HB1	1:B:207:ILE:H	1.52	0.40
1:D:180:TYR:HB2	1:D:185:ILE:HG22	2.01	0.40
1:E:49:ARG:HB2	1:E:50:PRO:HD3	2.02	0.40
1:E:181:ASP:HA	1:E:226:TYR:CD2	2.56	0.40
1:A:57:VAL:HG23	1:A:184:LYS:C	2.46	0.40
1:A:168:GLN:HG2	1:A:236:ARG:NE	2.36	0.40
1:B:161:VAL:CG1	1:B:162:THR:H	2.31	0.40
1:C:120:VAL:HG11	1:C:178:TRP:HE3	1.86	0.40
1:D:220:ASP:CB	1:E:195:ASP:HB2	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:LEU:O	1:E:44:TYR:HB2	2.21	0.40
1:B:57:VAL:O	1:B:59:ILE:HD12	2.21	0.40
1:B:96:TRP:CZ3	1:B:141:SER:HA	2.56	0.40
1:C:121:LEU:HD22	1:C:153:TYR:CD1	2.56	0.40
1:D:69:LEU:N	1:D:200:TRP:HZ3	2.10	0.40
1:E:160:ASP:C	1:E:161:VAL:CG2	2.94	0.40
1:E:163:PHE:CD1	1:E:163:PHE:N	2.88	0.40
1:B:108:ARG:NH1	1:B:138:HIS:CE1	2.89	0.40
1:B:111:SER:OG	1:B:135:THR:O	2.29	0.40
1:B:140:PHE:C	1:B:142:THR:N	2.79	0.40
1:C:102:GLY:HA2	1:C:104:ILE:HG12	2.02	0.40
1:D:46:ARG:HG3	1:D:46:ARG:NH1	2.36	0.40
1:D:121:LEU:HD22	1:D:153:TYR:CD1	2.56	0.40
1:D:161:VAL:CG2	1:D:162:THR:H	1.99	0.40
1:D:212:GLY:HA2	1:D:231:TYR:HA	2.03	0.40
1:E:135:THR:H	1:E:135:THR:HG23	1.52	0.40
1:A:124:ASN:HB2	1:B:68:GLN:OE1	2.22	0.40
1:A:169:GLN:HB2	1:A:235:ILE:CG1	2.51	0.40
1:B:98:PRO:O	1:B:101:PHE:HB3	2.21	0.40
1:B:120:VAL:CG2	1:B:178:TRP:CE3	3.04	0.40
1:B:206:ALA:HB1	1:B:236:ARG:N	2.36	0.40
1:B:218:LYS:NZ	1:B:223:ALA:O	2.44	0.40
1:C:126:ASP:OD1	1:C:126:ASP:N	2.54	0.40
1:C:132:THR:O	1:C:132:THR:OG1	2.34	0.40
1:D:46:ARG:HG3	1:D:46:ARG:HH11	1.87	0.40
1:E:74:GLU:CA	1:E:159:ILE:CD1	2.80	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)
1:D:203:GLY:O	1:E:44:TYR:OH[3_544]	2.17	0.03

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	205/213 (96%)	181 (88%)	19 (9%)	5 (2%)	4	28
1	B	206/213 (97%)	182 (88%)	18 (9%)	6 (3%)	3	24
1	C	206/213 (97%)	185 (90%)	20 (10%)	1 (0%)	24	59
1	D	203/213 (95%)	182 (90%)	17 (8%)	4 (2%)	6	31
1	E	206/213 (97%)	178 (86%)	19 (9%)	9 (4%)	2	15
All	All	1026/1065 (96%)	908 (88%)	93 (9%)	25 (2%)	4	28

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	GLN
1	E	161	VAL
1	A	135	THR
1	D	35	ARG
1	D	161	VAL
1	E	191	GLU
1	A	124	ASN
1	B	130	ALA
1	B	161	VAL
1	E	160	ASP
1	E	171	CYS
1	B	164	PHE
1	E	124	ASN
1	B	125	ALA
1	B	160	ASP
1	E	57	VAL
1	A	190	MET
1	C	57	VAL
1	D	57	VAL
1	E	207	ILE
1	B	57	VAL
1	D	207	ILE
1	A	207	ILE
1	E	164	PHE
1	E	203	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	187/194 (96%)	169 (90%)	18 (10%)	8	32
1	B	188/194 (97%)	172 (92%)	16 (8%)	10	37
1	C	188/194 (97%)	180 (96%)	8 (4%)	26	59
1	D	184/194 (95%)	174 (95%)	10 (5%)	20	53
1	E	188/194 (97%)	173 (92%)	15 (8%)	11	40
All	All	935/970 (96%)	868 (93%)	67 (7%)	13	44

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	44	TYR
1	A	45	ASN
1	A	47	TRP
1	A	56	ASP
1	A	69	LEU
1	A	72	VAL
1	A	75	LYS
1	A	80	THR
1	A	101	PHE
1	A	109	VAL
1	A	113	MET
1	A	123	ASN
1	A	124	ASN
1	A	131	VAL
1	A	168	GLN
1	A	187	LEU
1	A	234	VAL
1	B	39	HIS
1	B	42	ARG
1	B	46	ARG
1	B	47	TRP
1	B	51	VAL

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Mol	Chain	Res	Type
1	B	53	ASN
1	B	58	VAL
1	B	72	VAL
1	B	81	THR
1	B	141	SER
1	B	161	VAL
1	B	162	THR
1	B	169	GLN
1	B	185	ILE
1	B	188	GLU
1	B	211	THR
1	C	51	VAL
1	C	72	VAL
1	C	83	VAL
1	C	90	SER
1	C	129	PHE
1	C	159	ILE
1	C	168	GLN
1	C	199	TYR
1	D	35	ARG
1	D	47	TRP
1	D	72	VAL
1	D	75	LYS
1	D	113	MET
1	D	131	VAL
1	D	152	ILE
1	D	169	GLN
1	D	185	ILE
1	D	199	TYR
1	E	42	ARG
1	E	51	VAL
1	E	59	ILE
1	E	69	LEU
1	E	72	VAL
1	E	74	GLU
1	E	75	LYS
1	E	101	PHE
1	E	120	VAL
1	E	131	VAL
1	E	160	ASP
1	E	161	VAL
1	E	169	GLN

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Mol	Chain	Res	Type
1	E	197	LYS
1	E	230	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	77	GLN
1	A	82	ASN
1	A	87	GLN
1	A	169	GLN
1	A	189	GLN
1	A	209	ASN
1	B	87	GLN
1	B	97	ASN
1	B	123	ASN
1	B	170	ASN
1	B	209	ASN
1	C	103	ASN
1	D	39	HIS
1	D	87	GLN
1	D	146	HIS
1	D	215	ASN
1	E	39	HIS
1	E	97	ASN
1	E	146	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	EPJ	A	300	-	16,16,16	1.69	4 (25%)	19,23,23	2.57	7 (36%)
2	EPJ	D	300	-	16,16,16	2.03	6 (37%)	19,23,23	2.12	8 (42%)
2	EPJ	E	300	-	16,16,16	1.55	3 (18%)	19,23,23	1.89	5 (26%)
2	EPJ	B	300	-	16,16,16	1.51	3 (18%)	19,23,23	1.75	5 (26%)
2	EPJ	C	300	-	16,16,16	1.54	2 (12%)	19,23,23	2.04	6 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EPJ	A	300	-	-	0/4/21/21	0/4/3/3
2	EPJ	D	300	-	-	0/4/21/21	0/4/3/3
2	EPJ	E	300	-	-	2/4/21/21	0/4/3/3
2	EPJ	B	300	-	-	1/4/21/21	0/4/3/3
2	EPJ	C	300	-	-	2/4/21/21	0/4/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	300	EPJ	C6-N1	-4.13	1.41	1.48
2	E	300	EPJ	C6-N1	-4.11	1.42	1.48
2	C	300	EPJ	C6-N1	-4.05	1.42	1.48
2	B	300	EPJ	C6-N1	-4.01	1.42	1.48
2	A	300	EPJ	C6-N1	-3.49	1.42	1.48
2	A	300	EPJ	C7-C1	-3.22	1.47	1.51
2	D	300	EPJ	C10-N2	3.16	1.39	1.32
2	D	300	EPJ	C9-C8	-3.05	1.33	1.38
2	C	300	EPJ	C10-CL	2.86	1.80	1.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	300	EPJ	C10-CL	2.83	1.80	1.74
2	A	300	EPJ	C10-CL	2.77	1.80	1.74
2	E	300	EPJ	C10-CL	2.53	1.79	1.74
2	B	300	EPJ	C10-CL	2.51	1.79	1.74
2	D	300	EPJ	C1-C6	-2.36	1.50	1.55
2	A	300	EPJ	C1-C6	-2.34	1.50	1.55
2	B	300	EPJ	C7-C1	-2.30	1.48	1.51
2	D	300	EPJ	C11-N2	2.21	1.38	1.34
2	E	300	EPJ	C1-C6	-2.11	1.51	1.55

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	EPJ	C4-C3-C2	-5.98	103.72	109.58
2	C	300	EPJ	C11-N2-C10	4.65	121.92	116.33
2	E	300	EPJ	C11-N2-C10	4.50	121.73	116.33
2	A	300	EPJ	C5-C6-C1	-4.41	105.14	109.74
2	D	300	EPJ	C7-C11-N2	-4.20	119.36	124.47
2	B	300	EPJ	C11-N2-C10	4.12	121.28	116.33
2	A	300	EPJ	C11-N2-C10	4.03	121.17	116.33
2	C	300	EPJ	C9-C10-N2	-3.89	119.22	124.87
2	A	300	EPJ	C7-C11-N2	-3.62	120.06	124.47
2	A	300	EPJ	C8-C7-C11	3.55	120.55	116.89
2	B	300	EPJ	C9-C10-N2	-3.44	119.87	124.87
2	E	300	EPJ	C9-C10-N2	-3.43	119.88	124.87
2	D	300	EPJ	C5-C6-N1	-3.35	96.98	102.80
2	D	300	EPJ	C8-C9-C10	3.18	120.54	117.36
2	C	300	EPJ	C5-C6-N1	-3.05	97.49	102.80
2	E	300	EPJ	C7-C11-N2	-2.97	120.86	124.47
2	C	300	EPJ	CL-C10-N2	2.91	121.44	115.98
2	E	300	EPJ	CL-C10-N2	2.90	121.42	115.98
2	D	300	EPJ	C4-C3-N1	-2.90	95.17	103.53
2	D	300	EPJ	C9-C10-N2	-2.88	120.69	124.87
2	C	300	EPJ	C7-C11-N2	-2.64	121.26	124.47
2	A	300	EPJ	C9-C10-N2	-2.61	121.08	124.87
2	B	300	EPJ	C7-C11-N2	-2.56	121.35	124.47
2	D	300	EPJ	C11-N2-C10	2.53	119.37	116.33
2	A	300	EPJ	C9-C8-C7	-2.51	118.67	121.18
2	B	300	EPJ	C5-C6-N1	-2.36	98.68	102.80
2	E	300	EPJ	C4-C3-C2	-2.34	107.28	109.58
2	C	300	EPJ	C4-C3-C2	-2.30	107.33	109.58
2	D	300	EPJ	C8-C7-C11	2.15	119.10	116.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	300	EPJ	C4-C3-C2	-2.12	107.50	109.58
2	B	300	EPJ	C8-C9-C10	2.02	119.38	117.36

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	300	EPJ	C6-C1-C7-C11
2	E	300	EPJ	C6-C1-C7-C8
2	C	300	EPJ	C6-C1-C7-C8
2	C	300	EPJ	C6-C1-C7-C11
2	B	300	EPJ	C6-C1-C7-C8

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	EPJ	4	0
2	D	300	EPJ	3	0
2	E	300	EPJ	3	0
2	B	300	EPJ	1	0
2	C	300	EPJ	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	207/213 (97%)	-0.07	6 (2%)	53	35	55, 92, 182, 278	0
1	B	208/213 (97%)	0.00	5 (2%)	59	40	54, 89, 156, 235	0
1	C	208/213 (97%)	0.07	0	100	100	50, 99, 173, 258	0
1	D	205/213 (96%)	-0.01	11 (5%)	31	20	39, 81, 161, 275	0
1	E	208/213 (97%)	-0.12	4 (1%)	66	46	37, 79, 151, 262	0
All	All	1036/1065 (97%)	-0.03	26 (2%)	58	39	37, 88, 167, 278	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	127	GLY	3.4
1	E	104	ILE	3.4
1	D	193	THR	3.2
1	D	104	ILE	3.1
1	D	192	GLN	2.8
1	A	125	ALA	2.8
1	E	160	ASP	2.8
1	D	42	ARG	2.7
1	B	204	GLU	2.7
1	D	126	ASP	2.7
1	A	42	ARG	2.6
1	B	199	TYR	2.6
1	E	205	TRP	2.6
1	B	53	ASN	2.5
1	D	194	VAL	2.5
1	A	131	VAL	2.4
1	A	50	PRO	2.4
1	A	196	LEU	2.3
1	D	196	LEU	2.3
1	B	196	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	126	ASP	2.2
1	D	47	TRP	2.1
1	E	127	GLY	2.1
1	D	163	PHE	2.1
1	D	195	ASP	2.0
1	B	47	TRP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	EPJ	C	300	14/14	0.93	0.19	90,113,130,147	0
2	EPJ	B	300	14/14	0.94	0.13	74,93,115,135	0
2	EPJ	D	300	14/14	0.94	0.19	84,96,124,139	0
2	EPJ	A	300	14/14	0.95	0.12	77,91,106,140	0
2	EPJ	E	300	14/14	0.96	0.12	72,81,90,120	0

6.5 Other polymers [i](#)

There are no such residues in this entry.