



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:30 PM UTC

PDB ID : 4LML / pdb_00004lml
Title : GLIC double mutant I9'A T25'A
Authors : Grosman, C.; Gonzalez-Gutierrez, G.
Deposited on : 2013-07-10
Resolution : 3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

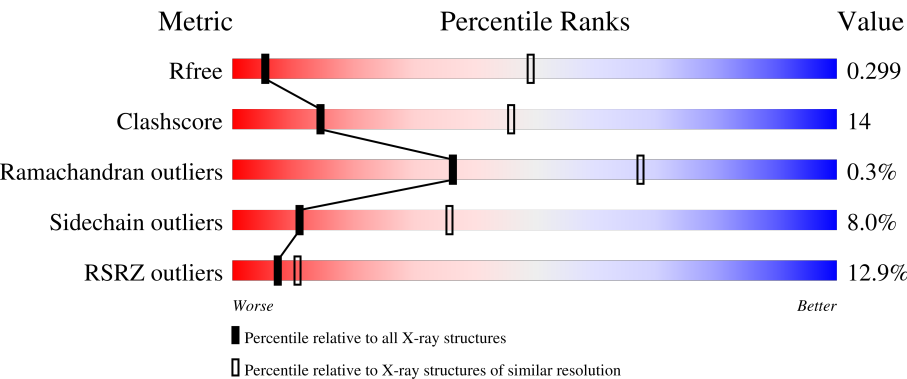
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	318	15% 60% 35% ..
1	B	318	14% 65% 28% ..
1	C	318	13% 63% 31% ..
1	D	318	12% 61% 33% ..
1	E	318	10% 63% 31% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12580 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 Proton-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2516	1658	403	451	4			
1	B	310	Total	C	N	O	S	0	0	0
			2516	1658	403	451	4			
1	C	310	Total	C	N	O	S	0	0	0
			2516	1658	403	451	4			
1	D	310	Total	C	N	O	S	0	0	0
			2516	1658	403	451	4			
1	E	310	Total	C	N	O	S	0	0	0
			2516	1658	403	451	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q7NDN8
A	0	SER	-	expression tag	UNP Q7NDN8
A	232	ALA	ILE	engineered mutation	UNP Q7NDN8
A	248	ALA	THR	engineered mutation	UNP Q7NDN8
B	-1	GLY	-	expression tag	UNP Q7NDN8
B	0	SER	-	expression tag	UNP Q7NDN8
B	232	ALA	ILE	engineered mutation	UNP Q7NDN8
B	248	ALA	THR	engineered mutation	UNP Q7NDN8
C	-1	GLY	-	expression tag	UNP Q7NDN8
C	0	SER	-	expression tag	UNP Q7NDN8
C	232	ALA	ILE	engineered mutation	UNP Q7NDN8
C	248	ALA	THR	engineered mutation	UNP Q7NDN8
D	-1	GLY	-	expression tag	UNP Q7NDN8
D	0	SER	-	expression tag	UNP Q7NDN8
D	232	ALA	ILE	engineered mutation	UNP Q7NDN8
D	248	ALA	THR	engineered mutation	UNP Q7NDN8
E	-1	GLY	-	expression tag	UNP Q7NDN8
E	0	SER	-	expression tag	UNP Q7NDN8
E	232	ALA	ILE	engineered mutation	UNP Q7NDN8

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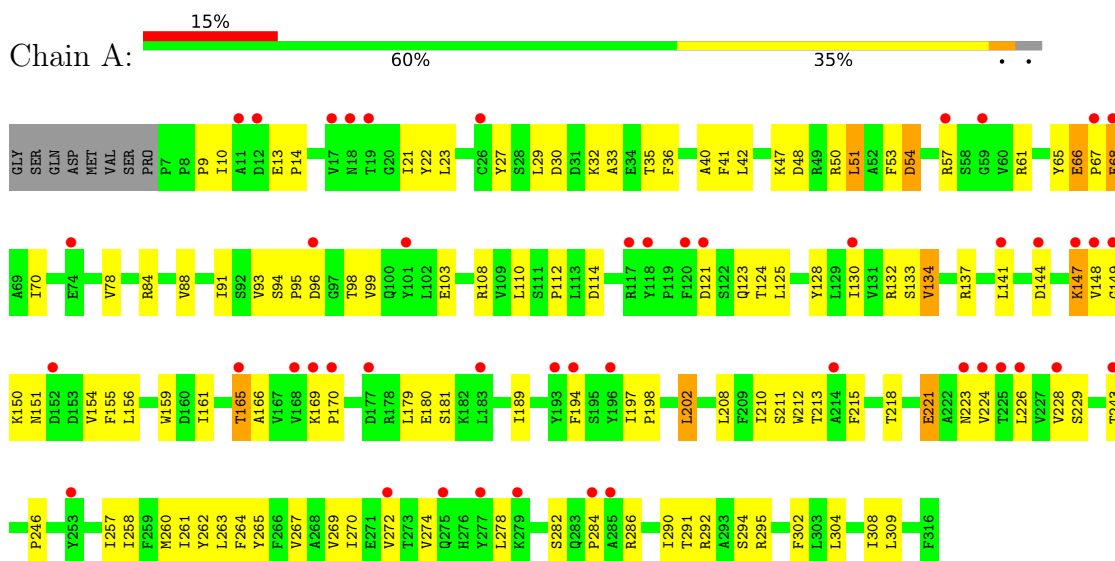
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Chain	Residue	Modelled	Actual	Comment	Reference
E	248	ALA	THR	engineered mutation	UNP Q7NDN8

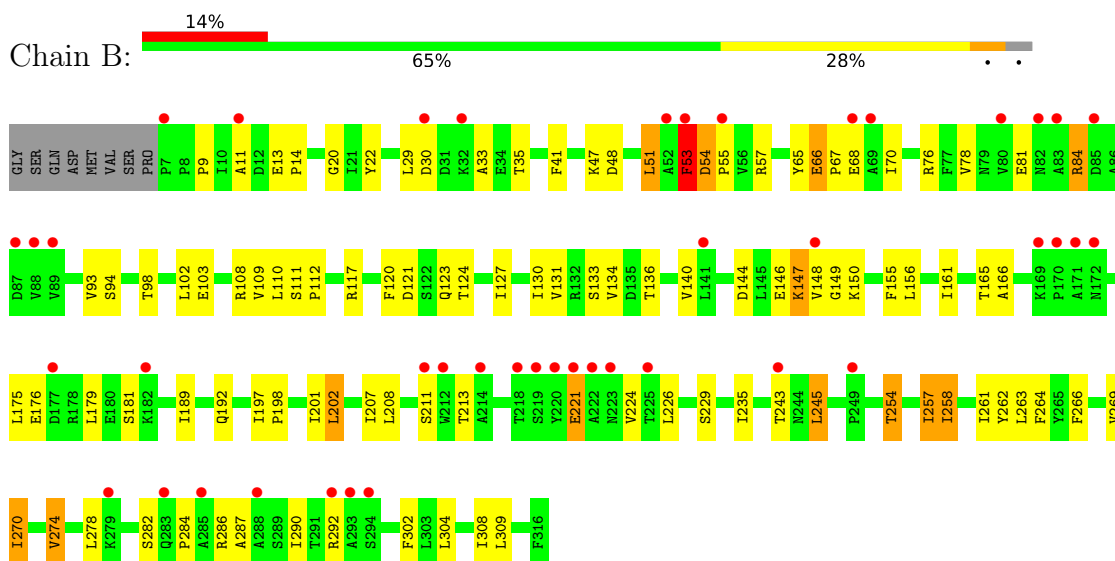
3 Residue-property plots [i](#)

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

- Molecule 1: Proton-gated ion channel



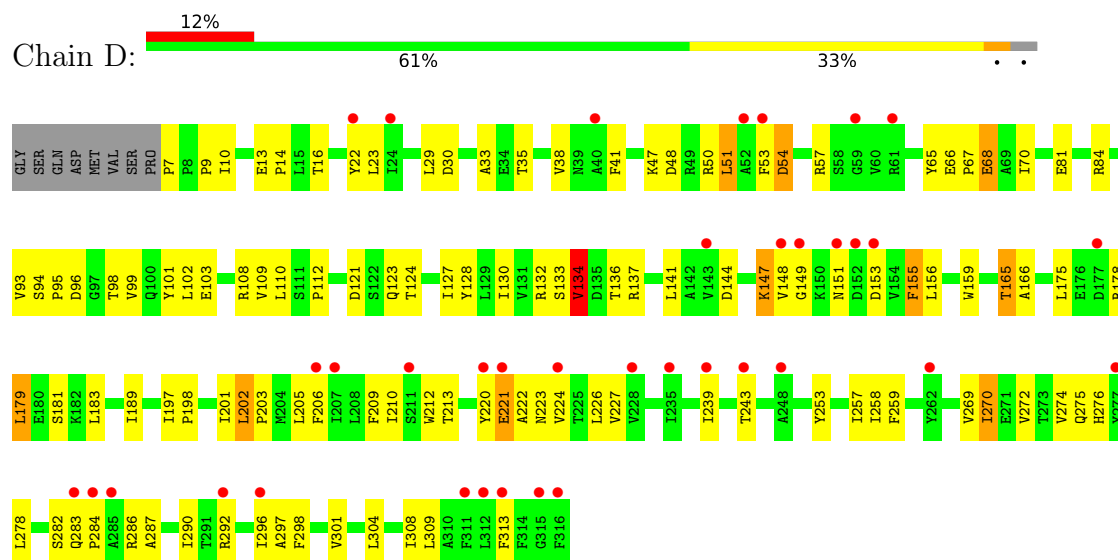
- Molecule 1: Proton-gated ion channel



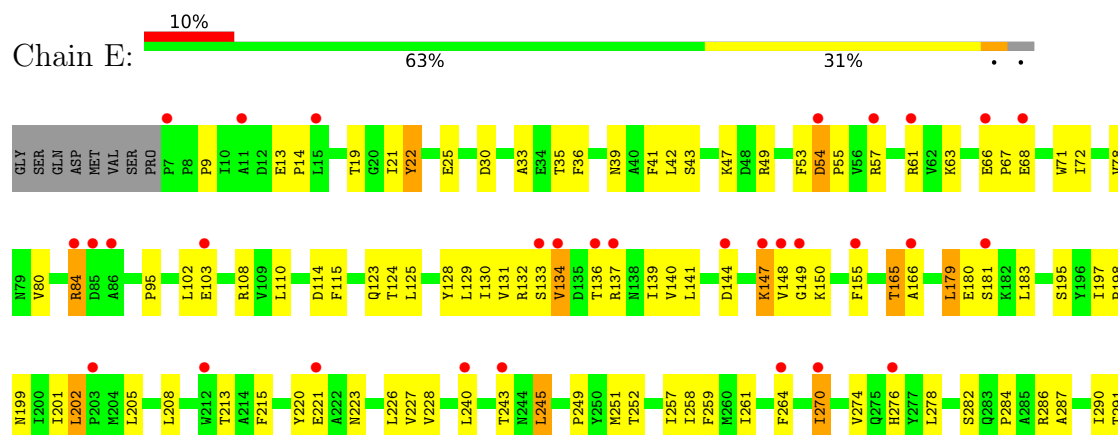
- Molecule 1: Proton-gated ion channel

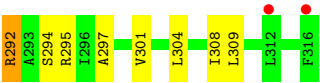


• Molecule 1: Proton-gated ion channel



• Molecule 1: Proton-gated ion channel





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	122.80Å 128.00Å 190.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.93 – 3.80 38.93 – 3.80	Depositor EDS
% Data completeness (in resolution range)	72.2 (38.93-3.80) 71.0 (38.93-3.80)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 3.76Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.246 , 0.302 0.245 , 0.299	Depositor DCC
R_{free} test set	2003 reflections (6.61%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	1.738	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 26.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.032 for k,h,-l	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	12580	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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

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	0.50	0/2584	0.94	3/3528 (0.1%)
1	B	0.51	0/2584	0.93	5/3528 (0.1%)
1	C	0.51	0/2584	0.95	7/3528 (0.2%)
1	D	0.52	0/2584	0.94	2/3528 (0.1%)
1	E	0.52	0/2584	0.97	4/3528 (0.1%)
All	All	0.51	0/12920	0.95	21/17640 (0.1%)

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	1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	149	GLY	N-CA-C	12.04	128.18	112.77
1	E	54	ASP	CA-C-N	8.79	129.67	119.47
1	E	54	ASP	C-N-CA	8.79	129.67	119.47
1	C	56	VAL	N-CA-C	7.79	117.85	110.53
1	D	7	PRO	CA-C-N	7.05	124.74	119.66
1	D	7	PRO	C-N-CA	7.05	124.74	119.66
1	C	130	ILE	N-CA-C	6.65	118.74	109.29
1	B	120	PHE	N-CA-C	6.06	119.78	112.38
1	C	169	LYS	CA-C-N	5.89	125.65	119.76
1	C	169	LYS	C-N-CA	5.89	125.65	119.76
1	C	54	ASP	CA-C-N	5.78	125.15	118.85
1	C	54	ASP	C-N-CA	5.78	125.15	118.85
1	B	111	SER	CA-C-N	5.62	125.57	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111	SER	C-N-CA	5.62	125.57	119.78
1	C	130	ILE	CB-CA-C	-5.34	104.43	111.70
1	A	66	GLU	CA-C-N	5.11	125.39	119.47
1	A	66	GLU	C-N-CA	5.11	125.39	119.47
1	B	66	GLU	CA-C-N	5.04	125.31	119.47
1	B	66	GLU	C-N-CA	5.04	125.31	119.47
1	E	251	MET	N-CA-C	5.01	116.89	108.73
1	A	40	ALA	N-CA-C	5.00	115.64	108.74

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	53	PHE	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	2516	0	2529	77	0
1	B	2516	0	2529	75	1
1	C	2516	0	2529	80	0
1	D	2516	0	2529	79	1
1	E	2516	0	2529	73	0
All	All	12580	0	12645	353	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 14.

All (353) 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:B:121:ASP:OD1	1:B:123:GLN:NE2	2.04	0.90
1:B:117:ARG:HB2	1:B:121:ASP:HB3	1.60	0.83
1:C:22:TYR:HA	1:C:149:GLY:HA3	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:THR:OG1	1:C:108:ARG:NH2	2.12	0.82
1:D:51:LEU:HD12	1:D:93:VAL:HG11	1.63	0.81
1:C:84:ARG:NH1	1:C:103:GLU:OE1	2.15	0.78
1:B:29:LEU:HB2	1:B:156:LEU:HD11	1.68	0.73
1:A:29:LEU:HB2	1:A:156:LEU:HD11	1.69	0.72
1:A:51:LEU:HD12	1:A:93:VAL:HG11	1.72	0.72
1:D:54:ASP:HB2	1:D:57:ARG:HB2	1.71	0.71
1:D:84:ARG:NH1	1:D:103:GLU:OE1	2.15	0.71
1:D:22:TYR:HB3	1:D:41:PHE:HB2	1.73	0.70
1:B:22:TYR:HA	1:B:149:GLY:HA3	1.74	0.69
1:B:208:LEU:HD13	1:B:261:ILE:HG23	1.72	0.69
1:D:121:ASP:OD1	1:D:123:GLN:NE2	2.27	0.68
1:D:257:ILE:HG22	1:D:309:LEU:HD23	1.75	0.67
1:B:144:ASP:HA	1:B:147:LYS:HD2	1.76	0.66
1:E:278:LEU:HD21	1:E:286:ARG:HB3	1.77	0.66
1:A:22:TYR:HB3	1:A:41:PHE:HB2	1.77	0.66
1:D:175:LEU:HD11	1:E:22:TYR:CE1	2.32	0.65
1:C:22:TYR:HB3	1:C:41:PHE:HB2	1.79	0.65
1:E:208:LEU:HD13	1:E:261:ILE:HG23	1.77	0.65
1:B:53:PHE:H	1:B:53:PHE:HD2	1.45	0.65
1:D:94:SER:HB2	1:D:98:THR:HB	1.78	0.64
1:B:257:ILE:HG22	1:B:309:LEU:HD23	1.80	0.64
1:A:78:VAL:HB	1:A:128:TYR:HB2	1.80	0.64
1:A:269:VAL:HG11	1:D:210:ILE:HG23	1.80	0.63
1:E:257:ILE:HG22	1:E:309:LEU:HD23	1.81	0.63
1:C:35:THR:HG22	1:C:110:LEU:HG	1.80	0.63
1:B:94:SER:HB2	1:B:98:THR:HB	1.80	0.62
1:D:112:PRO:HB3	1:E:155:PHE:CZ	2.35	0.62
1:D:165:THR:OG1	1:D:166:ALA:N	2.33	0.62
1:D:278:LEU:HD21	1:D:286:ARG:HB3	1.82	0.61
1:A:210:ILE:HD13	1:C:269:VAL:HG21	1.83	0.61
1:B:208:LEU:O	1:B:211:SER:HB3	2.01	0.60
1:E:22:TYR:HB3	1:E:41:PHE:HB2	1.83	0.60
1:C:208:LEU:HD13	1:C:261:ILE:HG23	1.83	0.60
1:B:54:ASP:HB2	1:B:57:ARG:HB2	1.84	0.59
1:A:30:ASP:HB3	1:A:33:ALA:HB3	1.84	0.59
1:A:66:GLU:HG3	1:A:67:PRO:HD2	1.85	0.59
1:B:197:ILE:HB	1:B:198:PRO:HD3	1.84	0.59
1:C:25:GLU:HB2	1:C:39:ASN:HB3	1.84	0.59
1:A:257:ILE:HG22	1:A:309:LEU:HD23	1.85	0.59
1:B:112:PRO:HB3	1:C:155:PHE:HZ	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:PHE:CE2	1:E:63:LYS:HB3	2.37	0.59
1:E:25:GLU:HB2	1:E:39:ASN:HB3	1.84	0.58
1:A:165:THR:OG1	1:A:166:ALA:N	2.34	0.58
1:B:165:THR:OG1	1:B:166:ALA:N	2.35	0.58
1:D:30:ASP:HB3	1:D:33:ALA:HB3	1.85	0.58
1:E:42:LEU:HB3	1:E:103:GLU:HG2	1.86	0.58
1:B:112:PRO:HB3	1:C:155:PHE:CZ	2.39	0.58
1:C:140:VAL:HG22	1:C:181:SER:HB3	1.86	0.58
1:E:165:THR:OG1	1:E:166:ALA:N	2.34	0.57
1:D:29:LEU:HB2	1:D:156:LEU:HD11	1.85	0.57
1:D:9:PRO:HB3	1:D:48:ASP:CG	2.29	0.57
1:A:278:LEU:HD21	1:A:286:ARG:HB3	1.86	0.57
1:B:53:PHE:HE1	1:B:55:PRO:HG3	1.68	0.57
1:A:144:ASP:O	1:A:148:VAL:HB	2.05	0.57
1:B:22:TYR:HB3	1:B:41:PHE:HB2	1.86	0.57
1:D:134:VAL:O	1:D:178:ARG:NH2	2.38	0.57
1:D:175:LEU:HD11	1:E:22:TYR:HE1	1.68	0.57
1:B:51:LEU:H	1:B:51:LEU:HD23	1.69	0.57
1:C:29:LEU:HB2	1:C:156:LEU:HD11	1.87	0.57
1:C:197:ILE:O	1:C:202:LEU:HB2	2.04	0.57
1:D:227:VAL:HG11	1:D:269:VAL:HG23	1.86	0.57
1:D:147:LYS:O	1:D:147:LYS:HG2	2.03	0.57
1:E:66:GLU:HG3	1:E:67:PRO:HD2	1.87	0.56
1:B:53:PHE:CE1	1:B:55:PRO:HG3	2.40	0.56
1:A:54:ASP:HB2	1:A:57:ARG:HB2	1.88	0.56
1:E:132:ARG:HA	1:E:180:GLU:HG2	1.86	0.56
1:E:140:VAL:HG23	1:E:183:LEU:HG	1.87	0.56
1:B:11:ALA:HB3	1:B:136:THR:HG21	1.88	0.56
1:A:202:LEU:HD12	1:C:259:PHE:CZ	2.41	0.56
1:C:147:LYS:C	1:C:149:GLY:H	2.14	0.56
1:D:22:TYR:HA	1:D:149:GLY:HA3	1.88	0.55
1:D:197:ILE:HA	1:D:201:ILE:HB	1.88	0.55
1:A:114:ASP:O	1:A:123:GLN:NE2	2.39	0.55
1:A:132:ARG:HA	1:A:180:GLU:HG2	1.89	0.55
1:A:32:LYS:HA	1:A:246:PRO:HD3	1.89	0.55
1:E:78:VAL:HB	1:E:128:TYR:HB2	1.88	0.55
1:E:84:ARG:NH2	1:E:103:GLU:OE1	2.19	0.55
1:E:61:ARG:O	1:E:95:PRO:HG3	2.07	0.55
1:A:112:PRO:HB3	1:D:155:PHE:CZ	2.43	0.54
1:B:144:ASP:O	1:B:148:VAL:HG13	2.07	0.54
1:D:147:LYS:C	1:D:149:GLY:H	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:LEU:HD21	1:C:286:ARG:HB3	1.90	0.54
1:B:66:GLU:HG3	1:B:67:PRO:HD2	1.90	0.54
1:C:66:GLU:HG3	1:C:67:PRO:HD2	1.88	0.54
1:B:147:LYS:C	1:B:149:GLY:H	2.16	0.54
1:D:304:LEU:O	1:D:308:ILE:HG12	2.08	0.53
1:E:202:LEU:HD22	1:E:205:LEU:HD12	1.90	0.53
1:E:30:ASP:HB3	1:E:33:ALA:HB3	1.89	0.53
1:E:133:SER:HB3	1:E:136:THR:O	2.08	0.53
1:D:137:ARG:HB3	1:D:179:LEU:HD23	1.89	0.53
1:A:262:TYR:CE1	1:D:203:PRO:HB3	2.44	0.53
1:C:55:PRO:HD3	1:C:95:PRO:HB3	1.91	0.53
1:A:133:SER:HB3	1:A:137:ARG:HA	1.90	0.53
1:A:96:ASP:OD1	1:A:96:ASP:N	2.42	0.53
1:E:197:ILE:HB	1:E:198:PRO:HD3	1.91	0.53
1:E:304:LEU:O	1:E:308:ILE:HG12	2.09	0.52
1:A:161:ILE:HA	1:A:189:ILE:HG22	1.89	0.52
1:E:57:ARG:HE	1:E:57:ARG:HA	1.75	0.52
1:E:144:ASP:O	1:E:148:VAL:HG13	2.09	0.52
1:B:109:VAL:HG11	1:B:127:ILE:HG12	1.92	0.52
1:D:130:ILE:HA	1:D:181:SER:O	2.09	0.52
1:D:197:ILE:HB	1:D:198:PRO:HD3	1.91	0.52
1:D:156:LEU:HD23	1:D:189:ILE:HG21	1.90	0.52
1:E:286:ARG:O	1:E:290:ILE:HG13	2.10	0.52
1:C:30:ASP:HB3	1:C:33:ALA:HB3	1.92	0.52
1:C:197:ILE:HA	1:C:201:ILE:HB	1.92	0.51
1:D:286:ARG:O	1:D:290:ILE:HG13	2.09	0.51
1:A:223:ASN:HB3	1:A:272:VAL:HG11	1.92	0.51
1:C:93:VAL:HG22	1:C:99:VAL:HG22	1.91	0.51
1:C:197:ILE:HB	1:C:198:PRO:HD3	1.91	0.51
1:B:147:LYS:O	1:B:147:LYS:HG2	2.11	0.51
1:A:264:PHE:HA	1:A:267:VAL:HG22	1.93	0.51
1:C:137:ARG:HB3	1:C:179:LEU:HD21	1.93	0.51
1:E:292:ARG:HD2	1:E:295:ARG:HD2	1.91	0.51
1:D:10:ILE:HD12	1:D:50:ARG:HD3	1.92	0.51
1:A:65:TYR:CG	1:A:70:ILE:HD11	2.45	0.51
1:B:284:PRO:HA	1:B:287:ALA:HB3	1.93	0.51
1:B:20:GLY:HA3	1:B:146:GLU:HB3	1.92	0.51
1:E:197:ILE:HA	1:E:201:ILE:HB	1.93	0.50
1:B:269:VAL:HG11	1:C:210:ILE:HG23	1.94	0.50
1:C:118:TYR:O	1:C:254:THR:OG1	2.28	0.50
1:D:144:ASP:O	1:D:148:VAL:HG13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:215:PHE:HB3	1:E:295:ARG:HG2	1.94	0.50
1:D:41:PHE:CD1	1:D:102:LEU:HD11	2.46	0.50
1:D:133:SER:HB3	1:D:136:THR:O	2.12	0.50
1:A:68:GLU:H	1:A:68:GLU:CD	2.20	0.49
1:C:286:ARG:O	1:C:290:ILE:HG13	2.11	0.49
1:A:9:PRO:HB3	1:A:48:ASP:CG	2.37	0.49
1:C:144:ASP:O	1:C:148:VAL:HG13	2.13	0.49
1:E:41:PHE:CD1	1:E:102:LEU:HD11	2.47	0.49
1:A:65:TYR:O	1:A:91:ILE:HB	2.13	0.49
1:D:53:PHE:HB3	1:D:95:PRO:C	2.36	0.49
1:B:35:THR:OG1	1:B:108:ARG:NH2	2.46	0.49
1:C:278:LEU:HD23	1:C:287:ALA:HA	1.95	0.49
1:E:215:PHE:CZ	1:E:294:SER:HB3	2.48	0.49
1:A:291:THR:O	1:A:295:ARG:HG3	2.12	0.49
1:D:66:GLU:HG3	1:D:67:PRO:HD2	1.95	0.49
1:D:93:VAL:HG22	1:D:99:VAL:HG13	1.94	0.48
1:B:13:GLU:HB3	1:B:14:PRO:HD2	1.94	0.48
1:D:94:SER:N	1:D:98:THR:O	2.39	0.48
1:D:275:GLN:HG3	1:D:287:ALA:HB1	1.94	0.48
1:C:80:VAL:HG13	1:C:108:ARG:O	2.14	0.48
1:D:35:THR:OG1	1:D:108:ARG:NH2	2.45	0.48
1:B:266:PHE:HA	1:C:210:ILE:HD11	1.96	0.48
1:B:175:LEU:HD11	1:C:22:TYR:CE1	2.48	0.48
1:D:13:GLU:HB3	1:D:14:PRO:HD2	1.96	0.48
1:E:36:PHE:CD1	1:E:125:LEU:HD13	2.49	0.48
1:A:304:LEU:O	1:A:308:ILE:HG12	2.14	0.48
1:B:304:LEU:O	1:B:308:ILE:HG12	2.13	0.48
1:E:9:PRO:HD3	1:E:71:TRP:CE3	2.49	0.48
1:E:264:PHE:HZ	1:E:301:VAL:HG12	1.78	0.48
1:C:13:GLU:HB3	1:C:14:PRO:HD2	1.96	0.48
1:D:259:PHE:CZ	1:E:202:LEU:HD12	2.48	0.48
1:D:65:TYR:CG	1:D:70:ILE:HD11	2.48	0.47
1:D:239:ILE:HG12	1:E:240:LEU:HD22	1.96	0.47
1:D:253:TYR:HD1	1:D:313:PHE:CD1	2.33	0.47
1:B:35:THR:HG22	1:B:110:LEU:HG	1.96	0.47
1:C:257:ILE:HG22	1:C:309:LEU:HD23	1.96	0.47
1:E:80:VAL:HG13	1:E:108:ARG:O	2.14	0.47
1:B:270:ILE:HD13	1:B:270:ILE:HA	1.79	0.47
1:E:130:ILE:HA	1:E:181:SER:O	2.14	0.47
1:A:263:LEU:HD12	1:D:206:PHE:CE1	2.50	0.47
1:C:284:PRO:HA	1:C:287:ALA:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:PHE:CD2	1:A:96:ASP:HA	2.50	0.47
1:A:197:ILE:HB	1:A:198:PRO:HD3	1.97	0.47
1:B:197:ILE:HG23	1:B:202:LEU:HG	1.96	0.47
1:E:131:VAL:HG11	1:E:140:VAL:HG13	1.96	0.47
1:E:195:SER:O	1:E:199:ASN:ND2	2.48	0.47
1:E:282:SER:C	1:E:284:PRO:HD3	2.40	0.47
1:E:137:ARG:HB3	1:E:179:LEU:HD23	1.97	0.47
1:D:282:SER:C	1:D:284:PRO:HD3	2.40	0.47
1:B:65:TYR:CG	1:B:70:ILE:HD11	2.50	0.47
1:B:76:ARG:HH11	1:C:104:ARG:HH11	1.63	0.47
1:C:311:PHE:CZ	1:C:316:PHE:HB2	2.49	0.47
1:D:101:TYR:OH	1:D:103:GLU:OE2	2.25	0.47
1:B:150:LYS:HB3	1:B:150:LYS:HE2	1.68	0.46
1:C:282:SER:C	1:C:284:PRO:HD3	2.40	0.46
1:B:278:LEU:HD21	1:B:286:ARG:HB3	1.97	0.46
1:D:283:GLN:N	1:D:284:PRO:HD3	2.31	0.46
1:E:19:THR:HA	1:E:43:SER:O	2.14	0.46
1:E:35:THR:HG22	1:E:110:LEU:HG	1.97	0.46
1:A:13:GLU:HB3	1:A:14:PRO:HD2	1.98	0.46
1:B:192:GLN:OE1	1:E:249:PRO:HG3	2.16	0.46
1:D:81:GLU:HG3	1:D:108:ARG:HG3	1.98	0.46
1:E:21:ILE:HD11	1:E:129:LEU:HD11	1.97	0.46
1:E:147:LYS:O	1:E:147:LYS:HG2	2.16	0.46
1:C:304:LEU:O	1:C:308:ILE:HG12	2.15	0.46
1:C:118:TYR:HD1	1:C:191:ARG:NH2	2.13	0.46
1:C:147:LYS:O	1:C:147:LYS:HG2	2.16	0.46
1:A:21:ILE:HA	1:A:41:PHE:O	2.16	0.46
1:A:212:TRP:HB2	1:A:215:PHE:CE1	2.51	0.46
1:B:30:ASP:HB3	1:B:33:ALA:HB3	1.98	0.46
1:B:202:LEU:HD12	1:E:259:PHE:HZ	1.81	0.46
1:E:78:VAL:HG22	1:E:130:ILE:HG12	1.98	0.46
1:E:114:ASP:O	1:E:123:GLN:NE2	2.47	0.46
1:A:93:VAL:HG22	1:A:99:VAL:HG13	1.97	0.45
1:C:147:LYS:HE3	1:C:166:ALA:H	1.80	0.45
1:B:133:SER:HB3	1:B:136:THR:O	2.16	0.45
1:B:274:VAL:O	1:B:278:LEU:HB2	2.16	0.45
1:E:131:VAL:CG1	1:E:140:VAL:HG13	2.47	0.45
1:A:194:PHE:HZ	1:C:251:MET:HE2	1.81	0.45
1:C:309:LEU:HD12	1:C:309:LEU:HA	1.71	0.45
1:E:55:PRO:HD3	1:E:95:PRO:HB3	1.97	0.45
1:E:284:PRO:HA	1:E:287:ALA:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:LEU:HD13	1:A:261:ILE:HG23	1.98	0.45
1:B:9:PRO:HB3	1:B:48:ASP:OD1	2.16	0.45
1:A:151:ASN:O	1:A:154:VAL:HG22	2.16	0.45
1:B:78:VAL:HG22	1:B:130:ILE:HG12	1.99	0.45
1:E:22:TYR:C	1:E:22:TYR:CD2	2.94	0.45
1:A:9:PRO:HB3	1:A:48:ASP:OD1	2.16	0.45
1:B:254:THR:O	1:B:258:ILE:HB	2.17	0.45
1:C:118:TYR:CD1	1:C:119:PRO:HA	2.51	0.45
1:C:221:GLU:O	1:C:224:VAL:HG22	2.17	0.45
1:D:212:TRP:HE3	1:D:298:PHE:HD1	1.64	0.45
1:C:36:PHE:CD1	1:C:125:LEU:HD13	2.51	0.45
1:B:202:LEU:HD12	1:E:259:PHE:CZ	2.52	0.45
1:B:13:GLU:HB3	1:B:14:PRO:CD	2.47	0.45
1:C:197:ILE:HG23	1:C:202:LEU:HD23	1.99	0.45
1:D:159:TRP:CE3	1:D:189:ILE:HD12	2.52	0.44
1:B:41:PHE:CD1	1:B:102:LEU:HD11	2.52	0.44
1:C:80:VAL:HG12	1:C:82:ASN:O	2.18	0.44
1:A:53:PHE:HB3	1:A:95:PRO:C	2.42	0.44
1:B:131:VAL:HG11	1:B:140:VAL:HG13	1.99	0.44
1:E:22:TYR:C	1:E:22:TYR:HD2	2.25	0.44
1:E:291:THR:O	1:E:295:ARG:HG3	2.17	0.44
1:C:165:THR:OG1	1:C:166:ALA:N	2.50	0.44
1:C:277:TYR:O	1:C:281:GLU:HG2	2.18	0.44
1:D:35:THR:HG22	1:D:110:LEU:HG	1.98	0.44
1:E:297:ALA:O	1:E:301:VAL:HG23	2.17	0.44
1:A:260:MET:O	1:A:263:LEU:HB2	2.16	0.44
1:D:175:LEU:HD12	1:D:175:LEU:HA	1.68	0.44
1:A:67:PRO:HG2	1:A:88:VAL:HG21	2.00	0.44
1:B:81:GLU:HG3	1:B:108:ARG:HG3	2.00	0.44
1:E:264:PHE:CZ	1:E:301:VAL:HG12	2.52	0.44
1:B:207:ILE:HG13	1:B:208:LEU:N	2.33	0.44
1:B:286:ARG:O	1:B:290:ILE:HG13	2.18	0.44
1:C:29:LEU:HD12	1:C:125:LEU:HD11	2.00	0.44
1:D:212:TRP:CE3	1:D:298:PHE:HD1	2.36	0.44
1:E:13:GLU:HB3	1:E:14:PRO:HD2	1.99	0.44
1:E:223:ASN:O	1:E:227:VAL:HG23	2.18	0.44
1:A:53:PHE:HD2	1:A:95:PRO:C	2.26	0.44
1:A:221:GLU:OE1	1:D:222:ALA:HA	2.18	0.44
1:D:51:LEU:N	1:D:51:LEU:HD23	2.33	0.44
1:C:274:VAL:O	1:C:278:LEU:HB2	2.18	0.43
1:A:121:ASP:OD1	1:A:123:GLN:NE2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ILE:HA	1:B:181:SER:O	2.18	0.43
1:D:96:ASP:OD1	1:D:96:ASP:N	2.51	0.43
1:A:215:PHE:CE1	1:A:294:SER:HB3	2.54	0.43
1:B:197:ILE:O	1:B:202:LEU:HB2	2.18	0.43
1:A:130:ILE:HA	1:A:181:SER:O	2.18	0.43
1:A:261:ILE:O	1:A:265:TYR:HD1	2.01	0.43
1:B:229:SER:HB3	1:E:228:VAL:HG11	2.00	0.43
1:C:169:LYS:HA	1:C:170:PRO:HD2	1.86	0.43
1:E:220:TYR:CD1	1:E:276:HIS:HB2	2.53	0.43
1:A:10:ILE:HD12	1:A:50:ARG:HD3	2.00	0.43
1:A:286:ARG:O	1:A:290:ILE:HG13	2.18	0.43
1:B:76:ARG:NH2	1:B:130:ILE:HD12	2.34	0.43
1:C:78:VAL:HB	1:C:128:TYR:HB2	2.00	0.43
1:C:94:SER:HB2	1:C:98:THR:HB	2.01	0.43
1:B:51:LEU:HD12	1:B:93:VAL:HG11	2.00	0.43
1:C:34:GLU:OE2	1:C:113:LEU:N	2.39	0.43
1:A:53:PHE:HB3	1:A:95:PRO:CA	2.48	0.43
1:A:159:TRP:CE3	1:A:189:ILE:HD12	2.53	0.43
1:A:224:VAL:O	1:A:228:VAL:HB	2.19	0.43
1:D:223:ASN:HB3	1:D:272:VAL:HG11	2.01	0.43
1:E:215:PHE:CE1	1:E:294:SER:HB3	2.54	0.43
1:B:269:VAL:HG21	1:C:210:ILE:HD13	2.01	0.43
1:A:36:PHE:CD1	1:A:125:LEU:HD13	2.54	0.43
1:A:94:SER:N	1:A:98:THR:O	2.44	0.43
1:A:137:ARG:HA	1:A:137:ARG:HD3	1.73	0.43
1:A:202:LEU:HD12	1:C:259:PHE:HZ	1.82	0.43
1:B:309:LEU:HD12	1:B:309:LEU:HA	1.81	0.43
1:B:156:LEU:HD12	1:B:156:LEU:HA	1.78	0.42
1:C:22:TYR:CD1	1:C:149:GLY:HA2	2.53	0.42
1:B:161:ILE:HA	1:B:189:ILE:HG22	2.00	0.42
1:C:137:ARG:HA	1:C:137:ARG:HD3	1.89	0.42
1:D:202:LEU:HD22	1:D:205:LEU:HD12	1.99	0.42
1:D:259:PHE:HZ	1:E:202:LEU:HD12	1.83	0.42
1:A:208:LEU:O	1:A:211:SER:HB3	2.18	0.42
1:E:139:ILE:HA	1:E:181:SER:OG	2.19	0.42
1:B:53:PHE:N	1:B:53:PHE:CD2	2.82	0.42
1:C:147:LYS:C	1:C:149:GLY:N	2.77	0.42
1:C:151:ASN:O	1:C:154:VAL:HG22	2.20	0.42
1:A:42:LEU:HB3	1:A:103:GLU:HG2	2.01	0.42
1:A:221:GLU:O	1:A:224:VAL:HG22	2.20	0.42
1:B:229:SER:CB	1:E:228:VAL:HG11	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:SER:HB3	1:C:228:VAL:HG11	2.02	0.42
1:B:221:GLU:O	1:B:224:VAL:HG22	2.20	0.42
1:C:144:ASP:HA	1:C:147:LYS:HD2	2.01	0.42
1:D:13:GLU:HB3	1:D:14:PRO:CD	2.49	0.42
1:C:245:LEU:HD12	1:C:245:LEU:HA	1.74	0.42
1:C:261:ILE:O	1:C:265:TYR:HD1	2.02	0.42
1:D:109:VAL:HG11	1:D:127:ILE:HG12	2.02	0.42
1:A:61:ARG:O	1:A:95:PRO:HG3	2.20	0.42
1:C:13:GLU:HB3	1:C:14:PRO:CD	2.49	0.42
1:C:121:ASP:CG	1:C:191:ARG:HH21	2.27	0.42
1:D:297:ALA:O	1:D:301:VAL:HG23	2.20	0.42
1:B:144:ASP:OD1	1:B:147:LYS:NZ	2.33	0.42
1:D:220:TYR:CD1	1:D:276:HIS:HB2	2.55	0.42
1:A:27:TYR:OH	1:C:81:GLU:O	2.36	0.41
1:A:35:THR:HG22	1:A:110:LEU:HG	2.02	0.41
1:B:197:ILE:HA	1:B:201:ILE:HB	2.01	0.41
1:C:220:TYR:CD1	1:C:276:HIS:HB2	2.55	0.41
1:D:84:ARG:HH11	1:D:84:ARG:HD2	1.75	0.41
1:D:155:PHE:HD2	1:D:155:PHE:HA	1.65	0.41
1:B:84:ARG:NH2	1:B:103:GLU:OE1	2.44	0.41
1:B:264:PHE:HE2	1:B:302:PHE:HB2	1.85	0.41
1:C:275:GLN:OE1	1:C:291:THR:OG1	2.28	0.41
1:D:128:TYR:HA	1:D:183:LEU:O	2.20	0.41
1:E:49:ARG:H	1:E:49:ARG:HG2	1.64	0.41
1:E:270:ILE:HD13	1:E:270:ILE:HA	1.86	0.41
1:A:282:SER:C	1:A:284:PRO:HD3	2.45	0.41
1:C:115:PHE:O	1:C:252:THR:HG22	2.20	0.41
1:D:147:LYS:C	1:D:149:GLY:N	2.78	0.41
1:A:35:THR:OG1	1:A:108:ARG:NH2	2.46	0.41
1:E:133:SER:HB3	1:E:137:ARG:HA	2.03	0.41
1:A:68:GLU:CD	1:A:68:GLU:N	2.79	0.41
1:B:245:LEU:HD12	1:B:245:LEU:HA	1.82	0.41
1:D:151:ASN:C	1:D:153:ASP:H	2.28	0.41
1:E:245:LEU:HD12	1:E:245:LEU:HA	1.87	0.41
1:A:264:PHE:CE2	1:A:302:PHE:HD1	2.39	0.41
1:A:27:TYR:HB3	1:C:110:LEU:HD11	2.03	0.41
1:A:147:LYS:C	1:A:149:GLY:H	2.29	0.41
1:A:169:LYS:HA	1:A:170:PRO:HD2	1.98	0.41
1:B:176:GLU:CD	1:C:146:GLU:HG3	2.46	0.41
1:B:282:SER:C	1:B:284:PRO:HD3	2.46	0.41
1:C:9:PRO:HG2	1:C:15:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:LYS:HE2	1:C:165:THR:HA	2.02	0.41
1:D:296:ILE:HD13	1:D:296:ILE:HA	1.91	0.41
1:E:13:GLU:HB3	1:E:14:PRO:CD	2.51	0.41
1:D:23:LEU:HD22	1:D:38:VAL:HG21	2.03	0.41
1:A:53:PHE:HD2	1:A:96:ASP:HA	1.84	0.40
1:C:257:ILE:O	1:C:261:ILE:HG13	2.21	0.40
1:D:132:ARG:NH2	1:D:178:ARG:HB2	2.36	0.40
1:D:209:PHE:HA	1:D:212:TRP:NE1	2.37	0.40
1:D:221:GLU:O	1:D:224:VAL:HG22	2.21	0.40
1:E:130:ILE:HD12	1:E:180:GLU:OE1	2.22	0.40
1:B:235:ILE:HG12	1:B:262:TYR:OH	2.20	0.40
1:C:245:LEU:HG	1:C:246:PRO:HD2	2.02	0.40
1:C:305:ALA:O	1:C:309:LEU:HB2	2.21	0.40
1:D:9:PRO:HB3	1:D:48:ASP:OD1	2.21	0.40
1:D:270:ILE:HA	1:D:270:ILE:HD13	1.82	0.40
1:A:23:LEU:HB2	1:A:150:LYS:HB2	2.02	0.40
1:C:283:GLN:N	1:C:284:PRO:HD3	2.36	0.40
1:D:53:PHE:HB3	1:D:95:PRO:O	2.21	0.40
1:E:115:PHE:O	1:E:252:THR:HG22	2.20	0.40
1:A:202:LEU:HD22	1:A:202:LEU:HA	1.94	0.40
1:A:215:PHE:HB3	1:A:295:ARG:HG2	2.02	0.40
1:D:68:GLU:H	1:D:68:GLU:HG2	1.53	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:B:147:LYS:NZ	1:D:98:THR:OG1[3_554]	2.11	0.09

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	308/318 (97%)	291 (94%)	16 (5%)	1 (0%)	36	67
1	B	308/318 (97%)	290 (94%)	18 (6%)	0	100	100
1	C	308/318 (97%)	286 (93%)	21 (7%)	1 (0%)	36	67
1	D	308/318 (97%)	289 (94%)	18 (6%)	1 (0%)	36	67
1	E	308/318 (97%)	289 (94%)	18 (6%)	1 (0%)	36	67
All	All	1540/1590 (97%)	1445 (94%)	91 (6%)	4 (0%)	36	67

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	VAL
1	C	201	ILE
1	D	134	VAL
1	E	134	VAL

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	276/283 (98%)	254 (92%)	22 (8%)	11	36
1	B	276/283 (98%)	252 (91%)	24 (9%)	9	33
1	C	276/283 (98%)	255 (92%)	21 (8%)	12	37
1	D	276/283 (98%)	255 (92%)	21 (8%)	12	37
1	E	276/283 (98%)	253 (92%)	23 (8%)	10	34
All	All	1380/1415 (98%)	1269 (92%)	111 (8%)	11	36

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LYS
1	A	51	LEU
1	A	54	ASP
1	A	68	GLU

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Mol	Chain	Res	Type
1	A	84	ARG
1	A	124	THR
1	A	134	VAL
1	A	141	LEU
1	A	147	LYS
1	A	155	PHE
1	A	165	THR
1	A	179	LEU
1	A	202	LEU
1	A	213	THR
1	A	218	THR
1	A	221	GLU
1	A	226	LEU
1	A	243	THR
1	A	258	ILE
1	A	270	ILE
1	A	274	VAL
1	A	292	ARG
1	B	47	LYS
1	B	51	LEU
1	B	53	PHE
1	B	54	ASP
1	B	68	GLU
1	B	84	ARG
1	B	124	THR
1	B	134	VAL
1	B	147	LYS
1	B	155	PHE
1	B	179	LEU
1	B	202	LEU
1	B	213	THR
1	B	221	GLU
1	B	226	LEU
1	B	243	THR
1	B	245	LEU
1	B	254	THR
1	B	257	ILE
1	B	258	ILE
1	B	263	LEU
1	B	270	ILE
1	B	274	VAL
1	B	292	ARG

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Mol	Chain	Res	Type
1	C	47	LYS
1	C	54	ASP
1	C	68	GLU
1	C	124	THR
1	C	134	VAL
1	C	147	LYS
1	C	155	PHE
1	C	165	THR
1	C	179	LEU
1	C	202	LEU
1	C	213	THR
1	C	218	THR
1	C	221	GLU
1	C	226	LEU
1	C	243	THR
1	C	257	ILE
1	C	258	ILE
1	C	263	LEU
1	C	270	ILE
1	C	274	VAL
1	C	292	ARG
1	D	16	THR
1	D	47	LYS
1	D	51	LEU
1	D	54	ASP
1	D	68	GLU
1	D	124	THR
1	D	134	VAL
1	D	141	LEU
1	D	147	LYS
1	D	155	PHE
1	D	165	THR
1	D	179	LEU
1	D	202	LEU
1	D	213	THR
1	D	221	GLU
1	D	226	LEU
1	D	243	THR
1	D	258	ILE
1	D	270	ILE
1	D	274	VAL
1	D	292	ARG

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Mol	Chain	Res	Type
1	E	22	TYR
1	E	47	LYS
1	E	54	ASP
1	E	68	GLU
1	E	72	ILE
1	E	84	ARG
1	E	124	THR
1	E	134	VAL
1	E	141	LEU
1	E	147	LYS
1	E	150	LYS
1	E	165	THR
1	E	179	LEU
1	E	202	LEU
1	E	213	THR
1	E	221	GLU
1	E	226	LEU
1	E	243	THR
1	E	245	LEU
1	E	258	ILE
1	E	270	ILE
1	E	274	VAL
1	E	292	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	GLN
1	A	306	ASN
1	B	238	ASN
1	C	18	ASN
1	C	126	HIS
1	C	238	ASN
1	D	18	ASN
1	D	276	HIS
1	E	18	ASN
1	E	238	ASN
1	E	276	HIS
1	E	306	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	310/318 (97%)	0.99	47 (15%) 5 8	13, 48, 116, 160	0
1	B	310/318 (97%)	0.91	43 (13%) 6 9	12, 45, 103, 128	0
1	C	310/318 (97%)	0.89	40 (12%) 7 11	18, 50, 98, 154	0
1	D	310/318 (97%)	0.81	37 (11%) 9 12	14, 45, 107, 130	0
1	E	310/318 (97%)	0.85	33 (10%) 11 14	13, 45, 117, 139	0
All	All	1550/1590 (97%)	0.89	200 (12%) 7 11	12, 46, 108, 160	0

All (200) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	221	GLU	13.7
1	B	223	ASN	7.4
1	E	148	VAL	7.3
1	C	281	GLU	7.1
1	D	292	ARG	6.8
1	D	316	PHE	6.8
1	C	152	ASP	6.7
1	C	280	VAL	6.0
1	B	169	LYS	6.0
1	B	170	PRO	6.0
1	E	84	ARG	5.9
1	D	221	GLU	5.7
1	E	149	GLY	5.7
1	B	222	ALA	5.6
1	A	169	LYS	5.6
1	A	144	ASP	5.6
1	C	153	ASP	5.5
1	E	221	GLU	5.3
1	B	220	TYR	5.3
1	A	253	TYR	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	120	PHE	5.0
1	B	219	SER	4.9
1	B	87	ASP	4.5
1	E	144	ASP	4.4
1	D	296	ILE	4.3
1	A	18	ASN	4.2
1	B	171	ALA	4.2
1	A	141	LEU	4.0
1	A	130	ILE	4.0
1	B	32	LYS	3.9
1	E	57	ARG	3.9
1	E	61	ARG	3.9
1	A	214	ALA	3.9
1	E	147	LYS	3.9
1	B	249	PRO	3.8
1	C	138	ASN	3.8
1	A	152	ASP	3.8
1	A	148	VAL	3.8
1	D	148	VAL	3.8
1	D	315	GLY	3.7
1	E	270	ILE	3.7
1	A	275	GLN	3.7
1	D	152	ASP	3.7
1	A	101	TYR	3.6
1	D	53	PHE	3.6
1	A	228	VAL	3.6
1	A	226	LEU	3.5
1	E	312	LEU	3.5
1	B	52	ALA	3.5
1	C	141	LEU	3.5
1	C	148	VAL	3.4
1	A	177	ASP	3.4
1	B	211	SER	3.4
1	D	52	ALA	3.4
1	A	196	TYR	3.4
1	A	149	GLY	3.3
1	B	283	GLN	3.3
1	D	243	THR	3.3
1	E	136	THR	3.3
1	A	170	PRO	3.2
1	D	228	VAL	3.2
1	A	147	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	213	THR	3.2
1	B	80	VAL	3.2
1	A	12	ASP	3.1
1	A	183	LEU	3.1
1	D	149	GLY	3.1
1	A	193	TYR	3.1
1	B	82	ASN	3.1
1	C	69	ALA	3.1
1	B	182	LYS	3.0
1	D	313	PHE	3.0
1	D	151	ASN	3.0
1	A	243	THR	3.0
1	E	85	ASP	3.0
1	C	66	GLU	3.0
1	E	15	LEU	3.0
1	A	11	ALA	3.0
1	A	118	TYR	3.0
1	B	89	VAL	3.0
1	A	225	THR	2.9
1	B	148	VAL	2.9
1	E	86	ALA	2.9
1	A	121	ASP	2.9
1	B	214	ALA	2.9
1	E	7	PRO	2.9
1	E	134	VAL	2.9
1	B	243	THR	2.9
1	C	282	SER	2.8
1	D	24	ILE	2.8
1	C	216	TRP	2.8
1	E	240	LEU	2.8
1	E	316	PHE	2.8
1	D	61	ARG	2.8
1	D	262	TYR	2.8
1	B	83	ALA	2.8
1	A	279	LYS	2.8
1	A	68	GLU	2.8
1	A	17	VAL	2.8
1	B	172	ASN	2.8
1	C	68	GLU	2.8
1	E	68	GLU	2.8
1	C	287	ALA	2.8
1	D	153	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	284	PRO	2.8
1	E	166	ALA	2.8
1	D	177	ASP	2.7
1	D	248	ALA	2.7
1	C	221	GLU	2.7
1	C	139	ILE	2.7
1	C	220	TYR	2.6
1	A	57	ARG	2.6
1	C	114	ASP	2.6
1	D	277	TYR	2.6
1	C	155	PHE	2.6
1	B	292	ARG	2.6
1	D	207	ILE	2.6
1	A	96	ASP	2.6
1	B	68	GLU	2.6
1	D	311	PHE	2.6
1	C	147	LYS	2.6
1	A	67	PRO	2.6
1	E	276	HIS	2.6
1	C	218	THR	2.6
1	B	293	ALA	2.6
1	D	40	ALA	2.6
1	E	11	ALA	2.6
1	D	312	LEU	2.6
1	E	181	SER	2.5
1	D	283	GLN	2.5
1	C	11	ALA	2.5
1	D	22	TYR	2.5
1	E	203	PRO	2.4
1	E	243	THR	2.4
1	C	250	TYR	2.4
1	E	155	PHE	2.4
1	B	11	ALA	2.4
1	A	224	VAL	2.4
1	D	224	VAL	2.4
1	A	117	ARG	2.4
1	C	277	TYR	2.4
1	C	276	HIS	2.3
1	C	149	GLY	2.3
1	A	74	GLU	2.3
1	D	59	GLY	2.3
1	C	228	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	168	VAL	2.3
1	E	137	ARG	2.3
1	B	69	ALA	2.3
1	C	14	PRO	2.3
1	A	272	VAL	2.3
1	B	212	TRP	2.2
1	B	225	THR	2.2
1	B	7	PRO	2.2
1	C	187	LEU	2.2
1	B	177	ASP	2.2
1	D	143	VAL	2.2
1	D	220	TYR	2.2
1	D	211	SER	2.1
1	B	55	PRO	2.1
1	E	264	PHE	2.1
1	A	285	ALA	2.1
1	C	45	SER	2.1
1	B	30	ASP	2.1
1	B	88	VAL	2.1
1	D	239	ILE	2.1
1	B	279	LYS	2.1
1	D	206	PHE	2.1
1	C	10	ILE	2.1
1	A	277	TYR	2.1
1	C	229	SER	2.1
1	B	53	PHE	2.1
1	C	85	ASP	2.1
1	A	165	THR	2.1
1	C	295	ARG	2.1
1	C	222	ALA	2.1
1	B	85	ASP	2.1
1	D	284	PRO	2.1
1	B	218	THR	2.1
1	B	285	ALA	2.1
1	A	194	PHE	2.1
1	D	235	ILE	2.0
1	E	66	GLU	2.0
1	B	288	ALA	2.0
1	B	294	SER	2.0
1	C	236	ALA	2.0
1	D	285	ALA	2.0
1	B	141	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	224	VAL	2.0
1	C	225	THR	2.0
1	E	54	ASP	2.0
1	E	103	GLU	2.0
1	E	212	TRP	2.0
1	C	15	LEU	2.0
1	A	26	CYS	2.0
1	A	223	ASN	2.0
1	A	59	GLY	2.0
1	A	19	THR	2.0
1	C	12	ASP	2.0
1	E	133	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.