



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:37 PM UTC

PDB ID : 5TGH / pdb_00005tgh
Title : Structure of the SNX5 PX domain in complex with chlamydial protein IncE
in space group P32
Authors : Collins, B.; Paul, B.
Deposited on : 2016-09-27
Resolution : 2.80 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:

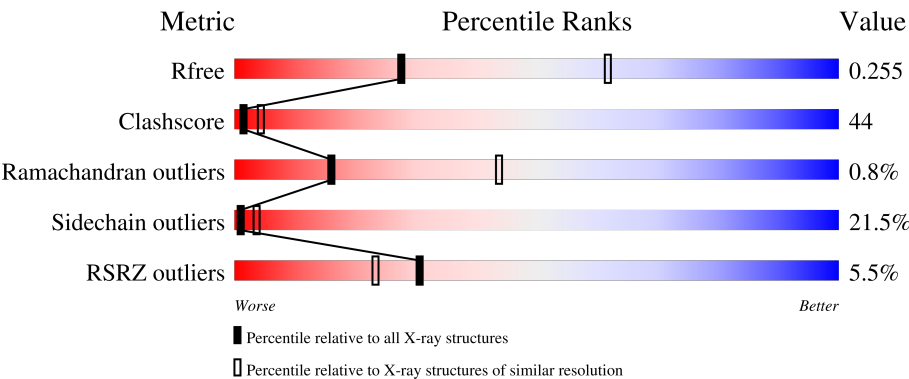
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	152	4% 49%39%5% • 7%
1	C	152	3% 55%29%9%7%
1	E	152	8% 39%41%13% • 6%
1	G	152	7% 39%37%17% • 6%
2	B	23	4% 35%30%22% • 9%

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Mol	Chain	Length	Quality of chain
2	D	23	48%35%9%9%
2	F	23	4% 52%35%13%
2	H	23	4% 22%48%17%13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5190 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 Sorting nexin-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	S	0	0	0
			1141	738	180	220	3			
1	C	142	Total	C	N	O	S	0	0	0
			1141	738	180	220	3			
1	E	143	Total	C	N	O	S	0	0	0
			1146	741	181	221	3			
1	G	143	Total	C	N	O	S	0	0	0
			1146	741	181	221	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLY	-	expression tag	UNP Q9Y5X3
A	171	PRO	-	expression tag	UNP Q9Y5X3
A	172	ALA	-	expression tag	UNP Q9Y5X3
C	21	GLY	-	expression tag	UNP Q9Y5X3
C	171	PRO	-	expression tag	UNP Q9Y5X3
C	172	ALA	-	expression tag	UNP Q9Y5X3
E	21	GLY	-	expression tag	UNP Q9Y5X3
E	171	PRO	-	expression tag	UNP Q9Y5X3
E	172	ALA	-	expression tag	UNP Q9Y5X3
G	21	GLY	-	expression tag	UNP Q9Y5X3
G	171	PRO	-	expression tag	UNP Q9Y5X3
G	172	ALA	-	expression tag	UNP Q9Y5X3

- Molecule 2 is a protein called IncE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	21	Total	C	N	O	0	0	0
			159	102	27	30			
2	D	21	Total	C	N	O	0	0	0
			158	102	27	29			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	20	Total	C	N	O	0	0	0
			149	97	25	27			
2	H	20	Total	C	N	O	0	0	0
			149	97	25	27			

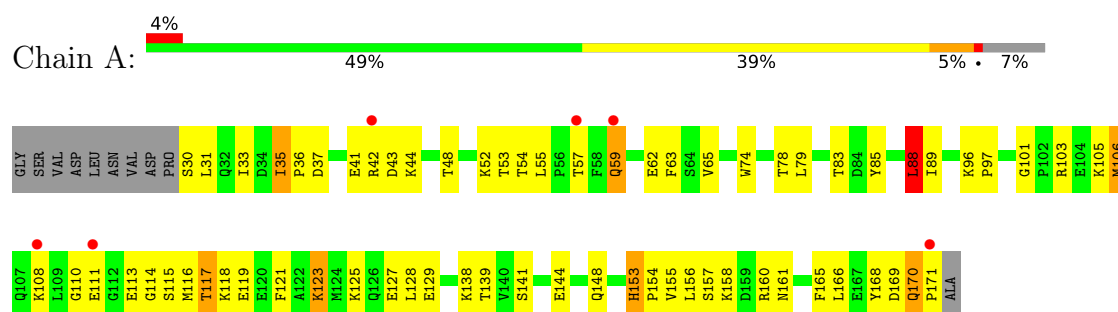
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		

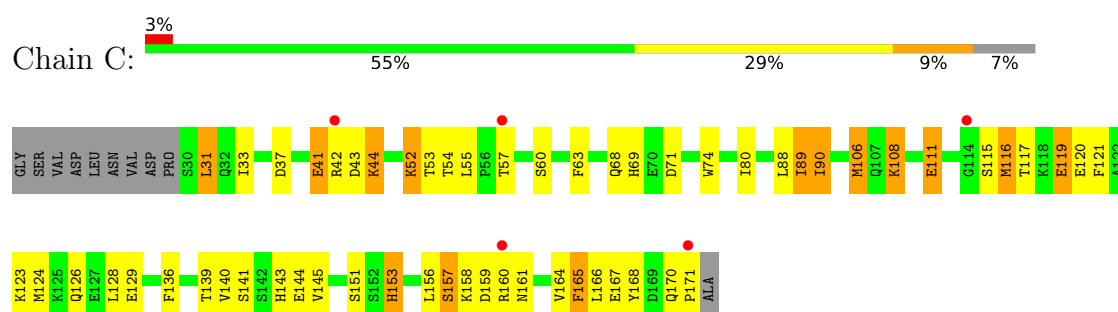
3 Residue-property plots [i](#)

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.

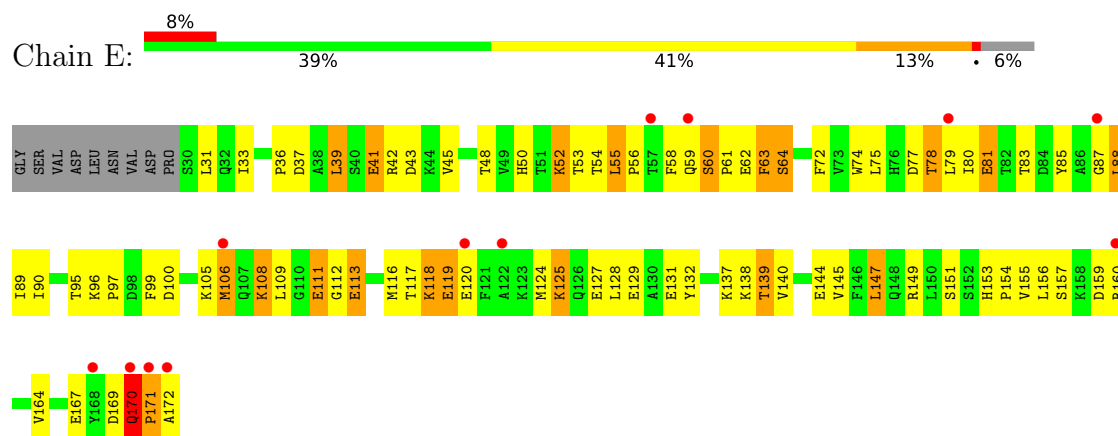
• Molecule 1: Sorting nexin-5



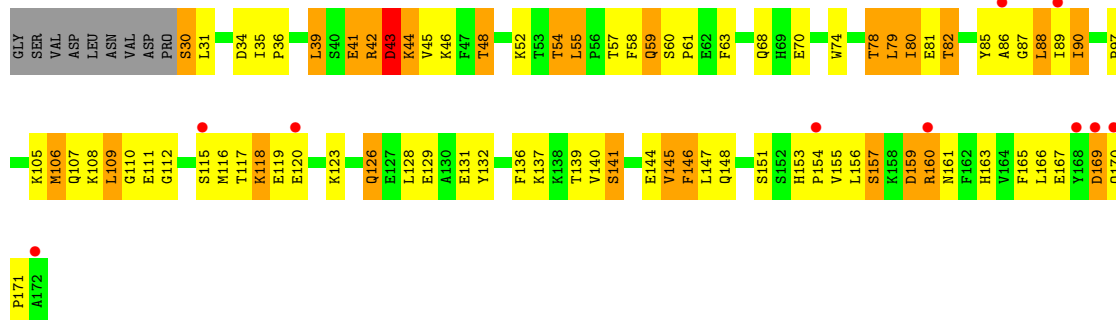
• Molecule 1: Sorting nexin-5



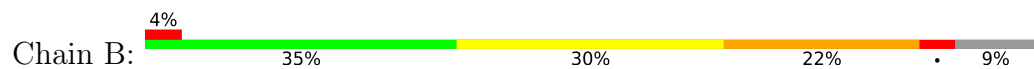
• Molecule 1: Sorting nexin-5



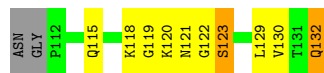
• Molecule 1: Sorting nexin-5



• Molecule 2: IncE



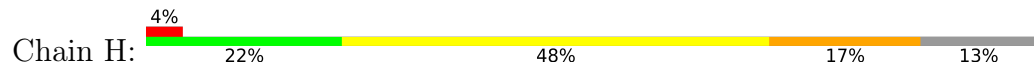
• Molecule 2: IncE



• Molecule 2: IncE



• Molecule 2: IncE



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	100.64Å 100.64Å 71.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.18 – 2.80 41.18 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (41.18-2.80) 96.4 (41.18-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.236 , 0.254 0.240 , 0.255	Depositor DCC
R_{free} test set	1972 reflections (9.87%)	wwPDB-VP
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l 0.037 for h,-h-k,-l 0.026 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5190	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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	1.18	1/1170 (0.1%)	1.04	5/1580 (0.3%)
1	C	1.21	3/1170 (0.3%)	0.96	1/1580 (0.1%)
1	E	1.17	0/1175	1.01	3/1587 (0.2%)
1	G	1.13	0/1175	1.00	2/1587 (0.1%)
2	B	1.01	0/161	1.05	1/214 (0.5%)
2	D	0.98	0/160	0.86	0/214
2	F	1.02	0/151	0.93	0/202
2	H	1.02	0/151	0.84	0/202
All	All	1.15	4/5313 (0.1%)	1.00	12/7166 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	HIS	CG-ND1	-5.31	1.32	1.38
1	C	143	HIS	CG-ND1	-5.24	1.32	1.38
1	C	69	HIS	CG-ND1	-5.07	1.32	1.38
1	C	153	HIS	CG-ND1	-5.01	1.32	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	130	VAL	N-CA-C	9.01	119.69	112.12
1	A	155	VAL	N-CA-C	7.78	117.84	110.53
1	G	111	GLU	N-CA-C	-7.36	104.04	112.87
1	A	117	THR	N-CA-C	-6.42	101.62	110.35
1	A	110	GLY	N-CA-C	-6.34	104.93	113.24
1	A	83	THR	N-CA-C	6.26	118.18	111.36
1	E	155	VAL	N-CA-C	5.82	116.00	110.53
1	A	88	LEU	N-CA-C	-5.80	100.44	109.72
1	G	43	ASP	N-CA-C	5.67	117.47	111.28
1	E	42	ARG	CB-CA-C	-5.34	109.97	117.23
1	E	88	LEU	N-CA-C	-5.05	103.86	110.53
1	C	166	LEU	N-CA-C	5.04	116.85	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1141	0	1103	80	0
1	C	1141	0	1104	71	1
1	E	1146	0	1108	114	1
1	G	1146	0	1106	139	0
2	B	159	0	161	18	0
2	D	158	0	162	27	0
2	F	149	0	154	10	0
2	H	149	0	153	44	0
3	A	1	0	0	0	0
All	All	5190	0	5051	446	2

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 44.

All (446) 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:E:170:GLN:CG	1:E:171:PRO:HD3	1.29	1.59
2:H:119:GLY:C	2:H:123:SER:CB	1.78	1.54
2:H:119:GLY:CA	2:H:123:SER:HB2	1.43	1.46
2:H:119:GLY:C	2:H:123:SER:HB2	1.37	1.41
1:G:170:GLN:OE1	1:G:171:PRO:CD	1.75	1.33
1:A:105:LYS:CB	1:A:108:LYS:NZ	1.92	1.33
1:A:42:ARG:HD2	2:B:132:GLN:OE1	1.16	1.26
1:A:105:LYS:CA	1:A:108:LYS:NZ	2.00	1.24
1:C:42:ARG:HG3	2:D:132:GLN:OE1	1.12	1.24
1:A:105:LYS:HA	1:A:108:LYS:NZ	1.51	1.23
1:E:170:GLN:CG	1:E:171:PRO:CD	2.15	1.22
1:G:87:GLY:C	1:G:88:LEU:HD23	1.65	1.21
1:A:105:LYS:HB3	1:A:108:LYS:NZ	1.49	1.19
1:G:87:GLY:C	1:G:88:LEU:CD2	2.15	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:LYS:HE2	1:E:118:LYS:CA	1.71	1.18
1:E:118:LYS:HA	1:E:118:LYS:CE	1.70	1.18
1:A:105:LYS:CB	1:A:108:LYS:HZ3	1.50	1.17
1:C:89:ILE:N	1:C:89:ILE:HD12	1.54	1.16
1:G:87:GLY:O	1:G:88:LEU:HD22	1.45	1.14
1:E:170:GLN:HG3	1:E:171:PRO:CD	1.75	1.12
1:G:79:LEU:HD23	1:G:79:LEU:N	1.51	1.11
2:H:120:LYS:N	2:H:123:SER:CB	2.09	1.11
1:E:55:LEU:N	1:E:55:LEU:HD23	1.53	1.11
1:E:111:GLU:OE1	1:E:111:GLU:HA	1.46	1.11
1:E:112:GLY:O	1:E:116:MET:HE3	1.51	1.11
1:E:170:GLN:CB	1:E:171:PRO:CD	2.26	1.10
1:G:170:GLN:OE1	1:G:171:PRO:HD3	0.95	1.10
2:H:119:GLY:HA3	2:H:123:SER:HB2	1.17	1.10
1:G:170:GLN:CD	1:G:171:PRO:HD3	1.78	1.09
1:C:117:THR:OG1	1:C:120:GLU:HB2	1.51	1.09
1:E:170:GLN:HE21	1:E:170:GLN:CA	1.66	1.08
1:E:60:SER:OG	1:E:61:PRO:HD2	1.54	1.07
1:A:105:LYS:HA	1:A:108:LYS:HZ2	0.96	1.07
1:E:74:TRP:O	1:E:78:THR:OG1	1.72	1.06
1:E:170:GLN:HB3	1:E:171:PRO:HD2	1.32	1.06
1:E:170:GLN:HA	1:E:170:GLN:NE2	1.61	1.05
1:G:39:LEU:HD12	2:H:115:GLN:NE2	1.71	1.05
1:A:108:LYS:O	1:A:111:GLU:HB3	1.56	1.05
1:E:170:GLN:CD	1:E:171:PRO:HD3	1.82	1.05
2:H:119:GLY:CA	2:H:123:SER:CB	2.19	1.04
1:C:42:ARG:CG	2:D:132:GLN:OE1	2.05	1.04
1:G:30:SER:N	1:G:54:THR:HG1	1.54	1.03
1:C:89:ILE:HD12	1:C:89:ILE:H	0.92	1.03
1:G:167:GLU:O	1:G:169:ASP:OD1	1.77	1.03
1:C:89:ILE:H	1:C:89:ILE:CD1	1.68	1.03
1:E:118:LYS:CA	1:E:118:LYS:CE	2.30	1.02
1:C:161:ASN:OD1	1:E:59:GLN:NE2	1.92	1.02
2:B:120:LYS:O	2:B:123:SER:N	1.89	1.01
1:C:74:TRP:CZ2	1:C:74:TRP:CZ3	2.43	1.00
1:A:74:TRP:CZ2	1:A:74:TRP:CZ3	2.43	1.00
1:G:39:LEU:CD1	2:H:115:GLN:NE2	2.24	0.99
1:C:153:HIS:O	1:C:157:SER:OG	1.77	0.99
1:A:144:GLU:O	1:A:148:GLN:HG3	1.63	0.99
1:A:105:LYS:CA	1:A:108:LYS:HZ3	1.66	0.98
1:E:74:TRP:CZ2	1:E:74:TRP:CZ3	2.45	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:88:LEU:HD23	1:G:88:LEU:N	1.74	0.98
1:E:170:GLN:HB3	1:E:171:PRO:CD	1.88	0.98
1:G:63:PHE:CE2	1:G:167:GLU:HB3	1.99	0.98
1:A:105:LYS:HB3	1:A:108:LYS:HZ3	1.03	0.98
1:G:74:TRP:O	1:G:78:THR:OG1	1.81	0.98
1:G:74:TRP:CZ3	1:G:74:TRP:CZ2	2.43	0.97
1:A:170:GLN:C	1:A:170:GLN:CD	2.30	0.96
1:A:42:ARG:CD	2:B:132:GLN:OE1	2.12	0.96
1:A:105:LYS:CA	1:A:108:LYS:HZ2	1.66	0.96
1:E:170:GLN:HE21	1:E:170:GLN:HA	0.80	0.95
1:E:170:GLN:HG3	1:E:171:PRO:HD3	0.95	0.94
1:G:30:SER:N	1:G:54:THR:OG1	2.00	0.94
1:C:119:GLU:OE1	1:C:119:GLU:HA	1.69	0.93
1:E:53:THR:HG21	1:E:58:PHE:CD1	2.03	0.93
1:G:79:LEU:N	1:G:79:LEU:CD2	2.30	0.93
1:G:39:LEU:CD1	2:H:115:GLN:HE21	1.81	0.92
1:C:42:ARG:HG3	2:D:132:GLN:CD	1.94	0.92
1:G:87:GLY:O	1:G:88:LEU:CD2	2.13	0.91
1:E:170:GLN:CB	1:E:171:PRO:HD3	1.96	0.91
1:E:55:LEU:N	1:E:55:LEU:CD2	2.30	0.90
1:A:41:GLU:O	1:A:41:GLU:HG3	1.72	0.90
1:E:117:THR:HG22	1:E:120:GLU:HG2	1.52	0.89
1:C:170:GLN:CD	1:C:171:PRO:HD2	1.98	0.88
1:E:112:GLY:O	1:E:116:MET:CE	2.20	0.88
1:E:41:GLU:O	1:E:41:GLU:HG2	1.71	0.88
1:E:77:ASP:O	1:E:81:GLU:HG2	1.71	0.88
1:A:30:SER:HB3	1:A:54:THR:HG23	1.55	0.88
1:C:80:ILE:HD13	1:C:90:ILE:HG12	1.54	0.88
1:G:39:LEU:HD12	2:H:115:GLN:HE21	1.35	0.88
2:H:119:GLY:HA3	2:H:123:SER:CB	1.95	0.87
1:E:118:LYS:N	1:E:118:LYS:HE3	1.90	0.86
1:G:153:HIS:O	1:G:157:SER:OG	1.91	0.86
1:C:90:ILE:N	1:C:90:ILE:HD13	1.89	0.86
1:E:105:LYS:HB3	1:E:128:LEU:HD11	1.54	0.86
1:A:105:LYS:O	1:A:108:LYS:HG2	1.76	0.86
2:D:120:LYS:O	2:D:123:SER:OG	1.93	0.86
1:E:39:LEU:HD12	2:F:115:GLN:OE1	1.74	0.86
1:A:42:ARG:HD2	2:B:132:GLN:CD	2.01	0.85
2:B:130:VAL:O	2:B:131:THR:CB	2.25	0.85
2:B:130:VAL:O	2:B:131:THR:HB	1.74	0.85
1:A:105:LYS:CB	1:A:108:LYS:HZ1	1.90	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:LYS:O	1:E:111:GLU:HB2	1.77	0.85
1:G:87:GLY:C	1:G:88:LEU:HD22	1.92	0.83
2:H:120:LYS:O	2:H:123:SER:N	2.11	0.83
1:E:118:LYS:HE2	1:E:118:LYS:HA	0.87	0.82
1:G:36:PRO:HD2	1:G:48:THR:O	1.78	0.82
1:A:65:VAL:HG12	1:A:169:ASP:HB2	1.62	0.82
1:E:106:MET:HE3	1:E:106:MET:HA	1.59	0.81
1:E:60:SER:OG	1:E:61:PRO:CD	2.28	0.81
1:A:59:GLN:OE1	1:A:59:GLN:HA	1.79	0.81
2:H:121:ASN:HA	2:H:123:SER:H	1.45	0.81
1:A:105:LYS:HB3	1:A:108:LYS:HZ1	1.42	0.80
1:C:161:ASN:CG	1:E:59:GLN:HE22	1.88	0.80
1:C:170:GLN:OE1	1:C:171:PRO:CD	2.30	0.80
1:G:137:LYS:HE3	2:H:125:ASP:OD2	1.82	0.80
1:G:80:ILE:CD1	1:G:90:ILE:HG21	2.12	0.79
1:A:144:GLU:OE2	2:B:118:LYS:NZ	2.14	0.79
1:E:105:LYS:HB3	1:E:128:LEU:CD1	2.12	0.79
1:E:170:GLN:CA	1:E:170:GLN:NE2	2.30	0.79
1:A:108:LYS:O	1:A:111:GLU:CB	2.30	0.79
1:C:170:GLN:OE1	1:C:170:GLN:HA	1.84	0.78
1:E:55:LEU:HD23	1:E:55:LEU:H	1.45	0.78
1:C:168:TYR:CZ	1:C:170:GLN:HB3	2.19	0.78
2:H:119:GLY:C	2:H:123:SER:OG	1.81	0.77
1:E:109:LEU:HD13	1:E:124:MET:HG3	1.67	0.77
2:H:119:GLY:O	2:H:123:SER:OG	2.02	0.77
1:C:170:GLN:OE1	1:C:171:PRO:HD2	1.85	0.76
1:A:35:ILE:O	1:A:35:ILE:HG22	1.84	0.76
1:G:86:ALA:O	1:G:88:LEU:HD23	1.86	0.76
1:A:168:TYR:CE1	1:A:170:GLN:HB3	2.20	0.76
2:B:120:LYS:N	2:B:123:SER:OG	2.18	0.76
1:E:53:THR:OG1	1:E:55:LEU:HG	1.86	0.76
2:H:120:LYS:N	2:H:123:SER:HB3	2.01	0.75
1:E:111:GLU:OE1	1:E:111:GLU:CA	2.30	0.75
1:C:129:GLU:OE2	2:D:129:LEU:HD13	1.86	0.75
2:D:115:GLN:NE2	2:H:130:VAL:HG13	2.01	0.75
2:D:115:GLN:HE22	2:H:131:THR:H	1.31	0.75
1:E:118:LYS:CE	1:E:118:LYS:N	2.47	0.75
1:A:170:GLN:OE1	1:A:171:PRO:C	2.30	0.74
1:E:41:GLU:O	1:E:41:GLU:CG	2.35	0.74
2:D:115:GLN:HE21	2:H:130:VAL:HG13	1.52	0.74
1:A:169:ASP:O	1:A:169:ASP:CG	2.30	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:170:GLN:OE1	1:G:170:GLN:C	2.30	0.74
1:A:170:GLN:C	1:A:170:GLN:OE1	2.30	0.74
1:E:145:VAL:O	1:E:149:ARG:HG3	1.87	0.74
2:D:130:VAL:HG13	1:G:39:LEU:HD13	1.70	0.73
1:E:171:PRO:O	1:E:172:ALA:HB3	1.86	0.73
1:E:85:TYR:O	1:E:88:LEU:HB2	1.87	0.73
2:B:119:GLY:HA3	2:B:123:SER:O	1.89	0.72
1:E:169:ASP:O	1:E:170:GLN:O	2.07	0.72
1:C:90:ILE:N	1:C:90:ILE:CD1	2.51	0.72
1:E:117:THR:HG23	1:E:120:GLU:H	1.54	0.72
1:E:53:THR:HG21	1:E:58:PHE:HD1	1.54	0.72
1:G:79:LEU:HD23	1:G:79:LEU:H	1.50	0.72
1:G:44:LYS:HZ2	1:G:46:LYS:HE3	1.55	0.72
1:G:80:ILE:HD11	1:G:90:ILE:HG21	1.73	0.71
1:C:161:ASN:CG	1:E:59:GLN:NE2	2.48	0.71
1:C:153:HIS:HB3	1:C:156:LEU:HB2	1.71	0.71
1:C:136:PHE:O	1:C:140:VAL:HG23	1.91	0.71
1:E:63:PHE:CE2	1:E:167:GLU:HB3	2.25	0.70
1:G:39:LEU:HD13	2:H:115:GLN:NE2	2.04	0.69
1:G:44:LYS:NZ	1:G:46:LYS:NZ	2.39	0.69
1:A:170:GLN:NE2	1:A:171:PRO:HD2	2.08	0.69
1:G:90:ILE:HG22	1:G:90:ILE:O	1.92	0.69
2:H:119:GLY:CA	2:H:123:SER:HB3	2.22	0.69
2:H:119:GLY:O	2:H:123:SER:CB	2.37	0.69
1:G:41:GLU:O	1:G:42:ARG:C	2.36	0.68
1:C:161:ASN:HD21	1:E:59:GLN:NE2	1.92	0.68
1:G:153:HIS:CE1	1:G:155:VAL:H	2.12	0.67
2:D:115:GLN:OE1	2:H:131:THR:HG22	1.93	0.67
2:H:121:ASN:CA	2:H:123:SER:H	2.07	0.67
1:A:105:LYS:O	1:A:108:LYS:CG	2.42	0.67
1:A:168:TYR:CZ	1:A:170:GLN:HB3	2.29	0.67
1:E:153:HIS:ND1	1:E:154:PRO:HD2	2.10	0.67
1:C:42:ARG:HG2	2:D:132:GLN:HE22	1.59	0.66
1:G:44:LYS:HZ1	1:G:46:LYS:NZ	1.91	0.66
1:E:117:THR:CG2	1:E:120:GLU:HG2	2.23	0.66
1:E:119:GLU:HG3	1:E:120:GLU:N	2.11	0.66
2:H:119:GLY:O	2:H:123:SER:HB2	1.92	0.66
1:C:119:GLU:OE1	1:C:119:GLU:CA	2.43	0.66
1:E:89:ILE:HG23	1:E:89:ILE:O	1.95	0.66
1:E:109:LEU:HD13	1:E:124:MET:CG	2.25	0.65
1:G:60:SER:OG	1:G:61:PRO:HD2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:LYS:O	1:E:111:GLU:N	2.29	0.65
2:F:120:LYS:O	2:F:123:SER:N	2.20	0.65
1:A:105:LYS:CG	1:A:108:LYS:NZ	2.59	0.65
1:G:132:TYR:CE2	2:H:114:VAL:HG21	2.32	0.65
1:G:36:PRO:CD	1:G:48:THR:O	2.44	0.65
1:C:161:ASN:ND2	1:E:59:GLN:NE2	2.44	0.65
1:G:85:TYR:O	1:G:88:LEU:HG	1.97	0.65
1:G:86:ALA:O	1:G:88:LEU:CD2	2.44	0.65
1:G:44:LYS:HZ2	1:G:46:LYS:CE	2.09	0.64
1:G:170:GLN:HG2	1:G:171:PRO:HA	1.80	0.64
1:C:144:GLU:OE1	2:D:118:LYS:NZ	2.29	0.64
1:A:170:GLN:CD	1:A:171:PRO:N	2.56	0.63
1:C:106:MET:HE3	1:C:106:MET:HA	1.79	0.63
1:E:39:LEU:CD1	2:F:115:GLN:OE1	2.45	0.63
1:E:75:LEU:O	1:E:75:LEU:HD12	1.98	0.63
1:G:44:LYS:NZ	1:G:46:LYS:HE3	2.11	0.63
1:A:41:GLU:O	1:A:41:GLU:CG	2.45	0.63
1:G:108:LYS:O	1:G:110:GLY:N	2.30	0.63
1:G:63:PHE:CE2	1:G:167:GLU:CB	2.80	0.63
1:G:55:LEU:N	1:G:55:LEU:HD23	2.14	0.63
1:G:70:GLU:N	1:G:70:GLU:OE2	2.30	0.63
1:G:39:LEU:HD23	1:G:41:GLU:HG2	1.79	0.62
1:A:59:GLN:OE1	1:A:59:GLN:CA	2.47	0.62
1:C:170:GLN:OE1	1:C:171:PRO:HD3	1.99	0.62
1:E:54:THR:C	1:E:55:LEU:HD23	2.22	0.62
1:C:31:LEU:HB3	1:C:151:SER:HB2	1.82	0.62
1:G:86:ALA:C	1:G:88:LEU:HD23	2.24	0.62
1:A:170:GLN:NE2	1:A:171:PRO:CD	2.63	0.61
1:E:144:GLU:OE2	2:F:118:LYS:NZ	2.32	0.61
1:A:85:TYR:O	1:A:88:LEU:HB2	2.01	0.61
1:G:160:ARG:O	1:G:163:HIS:HB2	2.00	0.61
2:D:115:GLN:OE1	2:H:131:THR:CG2	2.50	0.60
1:E:80:ILE:HD13	1:E:90:ILE:HG13	1.84	0.60
1:E:170:GLN:CD	1:E:171:PRO:CD	2.62	0.60
1:A:105:LYS:CG	1:A:108:LYS:HZ1	2.13	0.60
2:B:130:VAL:HG13	1:E:39:LEU:HD13	1.83	0.60
2:H:119:GLY:C	2:H:123:SER:HB3	2.11	0.60
2:B:121:ASN:OD1	2:B:121:ASN:N	2.30	0.60
1:E:171:PRO:O	1:E:172:ALA:CB	2.50	0.60
1:A:123:LYS:O	1:A:127:GLU:HG3	2.01	0.60
1:G:34:ASP:C	1:G:34:ASP:OD2	2.43	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:121:ASN:HA	2:H:123:SER:N	2.13	0.60
1:G:153:HIS:ND1	1:G:153:HIS:C	2.60	0.59
1:G:97:PRO:HG3	1:G:139:THR:OG1	2.01	0.59
1:G:109:LEU:O	1:G:109:LEU:HD12	2.03	0.59
1:E:63:PHE:N	1:E:63:PHE:CD1	2.68	0.59
1:G:31:LEU:HD23	1:G:31:LEU:H	1.66	0.59
1:G:78:THR:C	1:G:79:LEU:HD23	2.24	0.59
1:G:106:MET:O	1:G:107:GLN:C	2.45	0.59
1:E:52:LYS:HG2	1:E:62:GLU:HG3	1.84	0.59
1:G:153:HIS:CG	1:G:156:LEU:HD12	2.37	0.59
1:C:161:ASN:HD21	1:E:59:GLN:HE21	1.50	0.59
1:E:108:LYS:O	1:E:111:GLU:CB	2.50	0.59
1:G:41:GLU:O	1:G:42:ARG:O	2.20	0.59
1:G:153:HIS:ND1	1:G:154:PRO:N	2.50	0.59
1:G:110:GLY:C	1:G:112:GLY:H	2.09	0.58
1:E:140:VAL:O	1:E:144:GLU:HG3	2.03	0.58
1:C:117:THR:HG1	1:C:120:GLU:HB2	1.61	0.58
1:E:169:ASP:C	1:E:170:GLN:O	2.47	0.58
1:G:55:LEU:HB3	1:G:57:THR:HG22	1.86	0.58
1:C:41:GLU:O	1:C:41:GLU:HG2	2.04	0.58
1:E:117:THR:HG22	1:E:120:GLU:CG	2.30	0.57
1:E:105:LYS:O	1:E:108:LYS:HB2	2.05	0.57
1:A:170:GLN:NE2	1:A:171:PRO:N	2.52	0.57
1:G:110:GLY:C	1:G:112:GLY:N	2.59	0.57
1:C:90:ILE:HD13	1:C:90:ILE:H	1.68	0.57
1:C:170:GLN:CD	1:C:171:PRO:CD	2.75	0.57
1:C:41:GLU:O	1:C:42:ARG:C	2.47	0.57
1:E:117:THR:CG2	1:E:120:GLU:H	2.16	0.57
1:G:44:LYS:NZ	1:G:46:LYS:CE	2.66	0.57
1:C:42:ARG:CG	2:D:132:GLN:HE22	2.17	0.56
1:G:153:HIS:CE1	1:G:155:VAL:HB	2.40	0.56
1:G:44:LYS:CD	1:G:46:LYS:HE3	2.35	0.56
1:G:85:TYR:O	1:G:88:LEU:CG	2.53	0.56
1:G:44:LYS:NZ	1:G:46:LYS:HZ1	2.01	0.56
1:E:125:LYS:HE2	1:E:129:GLU:OE2	2.05	0.56
1:G:129:GLU:OE2	2:H:129:LEU:HD11	2.06	0.56
1:C:165:PHE:CD1	1:C:165:PHE:C	2.84	0.55
1:G:169:ASP:OD1	1:G:169:ASP:N	2.38	0.55
1:G:170:GLN:OE1	1:G:171:PRO:N	2.35	0.55
1:G:31:LEU:O	1:G:31:LEU:HG	2.05	0.55
1:G:159:ASP:OD1	1:G:159:ASP:C	2.49	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:165:PHE:CD1	1:G:165:PHE:C	2.85	0.55
2:D:115:GLN:NE2	2:H:131:THR:H	2.03	0.55
1:C:42:ARG:CG	2:D:132:GLN:NE2	2.69	0.54
1:E:79:LEU:CD2	1:E:159:ASP:OD2	2.56	0.54
1:E:106:MET:CE	1:E:106:MET:CA	2.86	0.54
1:E:106:MET:HE3	1:E:106:MET:CA	2.34	0.54
1:E:106:MET:HA	1:E:106:MET:CE	2.34	0.54
1:A:105:LYS:C	1:A:108:LYS:HG2	2.33	0.54
1:G:85:TYR:O	1:G:88:LEU:HB2	2.08	0.54
1:C:42:ARG:CG	2:D:132:GLN:CD	2.69	0.54
1:G:31:LEU:HA	1:G:52:LYS:O	2.08	0.54
1:G:44:LYS:CE	1:G:46:LYS:HE3	2.37	0.54
1:A:113:GLU:OE1	1:E:64:SER:OG	2.24	0.53
1:E:36:PRO:HD2	1:E:48:THR:O	2.08	0.53
1:G:153:HIS:CD2	1:G:156:LEU:HD12	2.44	0.53
1:G:118:LYS:CE	1:G:118:LYS:HA	2.39	0.52
1:C:129:GLU:OE2	2:D:129:LEU:CD1	2.56	0.52
1:G:118:LYS:HA	1:G:118:LYS:HE2	1.92	0.52
1:E:170:GLN:NE2	1:E:170:GLN:C	2.67	0.52
1:G:70:GLU:H	1:G:70:GLU:CD	2.16	0.52
1:G:117:THR:HG23	1:G:120:GLU:H	1.74	0.52
1:A:106:MET:HG2	1:A:128:LEU:HD13	1.90	0.52
1:A:108:LYS:O	1:A:111:GLU:N	2.42	0.52
1:G:108:LYS:O	1:G:109:LEU:C	2.49	0.52
1:A:105:LYS:HA	1:A:108:LYS:HG2	1.92	0.52
2:B:129:LEU:N	2:B:129:LEU:HD22	2.25	0.51
2:D:119:GLY:HA3	2:D:123:SER:O	2.10	0.51
1:E:33:ILE:HG21	1:E:147:LEU:HD13	1.92	0.51
1:A:170:GLN:HE22	1:A:171:PRO:HD2	1.74	0.51
2:F:115:GLN:O	2:F:127:VAL:HA	2.11	0.51
1:G:43:ASP:OD2	1:G:43:ASP:N	2.43	0.50
1:G:118:LYS:HE2	1:G:118:LYS:CA	2.41	0.50
1:A:169:ASP:O	1:A:169:ASP:OD1	2.30	0.50
1:G:34:ASP:OD2	1:G:34:ASP:O	2.30	0.50
1:C:68:GLN:O	1:C:71:ASP:HB2	2.11	0.50
1:G:58:PHE:CZ	1:G:163:HIS:CD2	3.00	0.50
1:G:132:TYR:CZ	2:H:114:VAL:HG21	2.46	0.50
1:A:170:GLN:OE1	1:A:170:GLN:O	2.30	0.50
2:B:130:VAL:O	2:F:115:GLN:OE1	2.30	0.50
1:E:89:ILE:O	1:E:89:ILE:CG2	2.60	0.50
1:G:105:LYS:HD2	1:G:128:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:108:LYS:C	1:G:110:GLY:N	2.70	0.50
2:F:121:ASN:OD1	2:F:121:ASN:O	2.30	0.50
1:C:80:ILE:HD13	1:C:90:ILE:CG1	2.34	0.49
2:H:115:GLN:O	2:H:127:VAL:HA	2.12	0.49
1:A:62:GLU:HG2	1:E:113:GLU:HG2	1.94	0.49
1:A:41:GLU:O	1:A:42:ARG:HB2	2.11	0.49
1:G:81:GLU:HA	1:G:81:GLU:OE1	2.13	0.49
1:G:41:GLU:CD	1:G:44:LYS:HE3	2.37	0.49
1:C:108:LYS:O	1:C:111:GLU:HB2	2.13	0.49
1:E:50:HIS:NE2	1:E:62:GLU:OE2	2.46	0.49
1:C:168:TYR:CE1	1:C:170:GLN:HB3	2.47	0.49
1:E:31:LEU:HD13	1:E:53:THR:HB	1.94	0.49
1:G:109:LEU:O	1:G:109:LEU:CD1	2.60	0.49
1:G:118:LYS:HE2	1:G:118:LYS:N	2.27	0.49
2:B:115:GLN:O	2:B:127:VAL:HA	2.13	0.48
1:G:42:ARG:HG2	1:G:43:ASP:OD2	2.13	0.48
1:E:108:LYS:HD2	1:E:108:LYS:HA	1.41	0.48
1:G:36:PRO:CG	1:G:48:THR:HG22	2.44	0.48
1:E:77:ASP:O	1:E:81:GLU:CG	2.53	0.48
1:A:101:GLY:O	1:A:105:LYS:HG3	2.14	0.48
1:A:153:HIS:ND1	1:A:154:PRO:HD2	2.29	0.48
1:A:165:PHE:CD1	1:A:165:PHE:C	2.91	0.48
1:C:144:GLU:CD	2:D:118:LYS:NZ	2.72	0.48
1:E:60:SER:CB	1:E:61:PRO:CD	2.90	0.48
1:C:170:GLN:OE1	1:C:170:GLN:CA	2.55	0.48
1:E:99:PHE:CD2	1:E:132:TYR:CE2	3.02	0.48
1:G:35:ILE:O	1:G:35:ILE:HG22	2.14	0.48
1:G:44:LYS:HZ1	1:G:46:LYS:HZ1	1.62	0.48
1:G:109:LEU:O	1:G:109:LEU:CG	2.58	0.48
1:G:146:PHE:CE2	1:G:147:LEU:HD23	2.49	0.48
1:C:37:ASP:OD1	2:H:131:THR:HB	2.14	0.47
1:A:41:GLU:O	1:A:43:ASP:N	2.48	0.47
1:G:80:ILE:HG22	1:G:81:GLU:N	2.27	0.47
1:C:80:ILE:CD1	1:C:90:ILE:HG12	2.34	0.47
1:E:117:THR:C	1:E:118:LYS:HE3	2.37	0.47
1:A:129:GLU:OE2	2:B:129:LEU:HD23	2.15	0.47
1:E:156:LEU:HD23	1:E:156:LEU:HA	1.64	0.47
1:E:113:GLU:O	1:E:113:GLU:HG3	2.12	0.47
1:G:109:LEU:O	1:G:109:LEU:HG	2.10	0.47
1:C:41:GLU:O	1:C:44:LYS:N	2.48	0.47
2:B:120:LYS:CB	2:B:123:SER:OG	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:LYS:HD3	1:A:62:GLU:CD	2.40	0.46
1:C:156:LEU:N	1:C:156:LEU:HD23	2.30	0.46
1:E:100:ASP:OD1	1:E:100:ASP:N	2.46	0.46
2:H:120:LYS:C	2:H:123:SER:H	2.23	0.46
1:A:121:PHE:C	1:A:121:PHE:CD2	2.92	0.46
1:G:167:GLU:C	1:G:169:ASP:OD1	2.56	0.46
2:F:121:ASN:HA	2:F:122:GLY:HA2	1.68	0.46
1:G:30:SER:CA	1:G:54:THR:OG1	2.63	0.46
1:G:58:PHE:CE2	1:G:163:HIS:CD2	3.03	0.46
1:G:90:ILE:O	1:G:90:ILE:CG2	2.55	0.46
1:G:108:LYS:C	1:G:110:GLY:H	2.24	0.46
1:G:153:HIS:CD2	1:G:156:LEU:CD1	2.99	0.46
1:A:30:SER:HB3	1:A:54:THR:CG2	2.36	0.45
1:C:44:LYS:HD2	1:C:68:GLN:NE2	2.31	0.45
1:E:31:LEU:CD1	1:E:53:THR:HB	2.46	0.45
1:E:97:PRO:HG3	1:E:139:THR:OG1	2.17	0.45
1:C:108:LYS:HE2	1:C:108:LYS:HB2	1.59	0.45
1:C:37:ASP:OD1	2:H:131:THR:CG2	2.65	0.45
1:G:63:PHE:CD1	1:G:63:PHE:N	2.84	0.45
1:A:156:LEU:HA	1:A:156:LEU:HD23	1.66	0.45
1:G:39:LEU:HD13	2:H:115:GLN:HE22	1.77	0.45
1:G:90:ILE:HD12	1:G:90:ILE:HA	1.78	0.45
1:A:161:ASN:OD1	1:G:59:GLN:NE2	2.50	0.44
1:A:158:LYS:HE2	1:A:158:LYS:HB2	1.87	0.44
1:E:63:PHE:CE2	1:E:167:GLU:CB	2.97	0.44
1:G:141:SER:O	1:G:145:VAL:HB	2.18	0.44
2:B:121:ASN:HA	2:B:122:GLY:HA2	1.77	0.44
1:E:108:LYS:C	1:E:111:GLU:HB2	2.40	0.44
1:E:153:HIS:HA	1:E:154:PRO:HD3	1.74	0.44
1:G:166:LEU:HD23	1:G:166:LEU:HA	1.78	0.44
1:E:88:LEU:HD23	1:E:88:LEU:HA	1.85	0.44
1:G:63:PHE:CD2	1:G:167:GLU:CB	3.00	0.44
1:G:123:LYS:O	1:G:126:GLN:HG2	2.18	0.44
1:C:106:MET:CA	1:C:106:MET:CE	2.95	0.44
1:C:159:ASP:OD1	1:C:159:ASP:C	2.61	0.44
1:E:79:LEU:HD23	1:E:159:ASP:OD2	2.16	0.44
1:A:52:LYS:HD3	1:A:62:GLU:OE1	2.18	0.44
1:G:44:LYS:HZ1	1:G:46:LYS:HZ2	1.65	0.44
1:A:96:LYS:HA	1:A:97:PRO:HD3	1.83	0.43
1:E:55:LEU:HA	1:E:56:PRO:HD3	1.77	0.43
1:G:153:HIS:ND1	1:G:154:PRO:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ILE:O	1:A:148:GLN:NE2	2.43	0.43
1:C:42:ARG:O	1:C:43:ASP:HB3	2.18	0.43
1:C:80:ILE:HD13	1:C:80:ILE:HA	1.83	0.43
1:G:85:TYR:O	1:G:88:LEU:CB	2.65	0.43
2:D:121:ASN:HA	2:D:122:GLY:HA2	1.73	0.43
1:G:82:THR:HG22	1:G:85:TYR:H	1.82	0.43
1:G:116:MET:HG3	1:G:117:THR:O	2.18	0.43
2:D:120:LYS:O	2:D:123:SER:N	2.49	0.43
1:G:136:PHE:O	1:G:139:THR:HG22	2.18	0.43
1:G:39:LEU:CD1	2:H:115:GLN:HE22	2.26	0.43
1:G:144:GLU:O	1:G:148:GLN:HG3	2.19	0.43
1:G:153:HIS:ND1	1:G:154:PRO:CD	2.81	0.43
2:H:129:LEU:N	2:H:129:LEU:HD12	2.34	0.43
1:E:105:LYS:HB3	1:E:128:LEU:HD13	1.99	0.43
1:C:42:ARG:HE	2:D:132:GLN:NE2	2.17	0.43
1:G:139:THR:HG23	1:G:140:VAL:N	2.33	0.43
1:E:109:LEU:CD1	1:E:124:MET:CG	2.96	0.43
1:G:132:TYR:CD2	2:H:114:VAL:HG21	2.54	0.43
1:G:139:THR:CG2	1:G:140:VAL:N	2.81	0.43
1:A:79:LEU:HD23	1:A:79:LEU:HA	1.83	0.42
1:A:88:LEU:HD13	1:A:153:HIS:NE2	2.35	0.42
1:C:52:LYS:HE2	1:C:52:LYS:HB2	1.89	0.42
1:G:159:ASP:OD1	1:G:161:ASN:N	2.51	0.42
1:A:114:GLY:HA2	1:E:62:GLU:HB3	2.00	0.42
1:A:166:LEU:HA	1:A:166:LEU:HD23	1.78	0.42
1:G:36:PRO:HG2	1:G:48:THR:CG2	2.50	0.42
2:D:130:VAL:HG13	1:G:39:LEU:CD1	2.46	0.42
1:E:108:LYS:HA	1:E:111:GLU:HB2	2.00	0.42
2:F:120:LYS:O	2:F:121:ASN:C	2.63	0.42
1:A:36:PRO:HD2	1:A:48:THR:O	2.19	0.42
2:D:115:GLN:HE22	2:H:131:THR:HG23	1.85	0.42
1:G:153:HIS:HA	1:G:154:PRO:HD3	1.70	0.42
1:G:60:SER:OG	1:G:61:PRO:CD	2.66	0.42
1:A:153:HIS:HB3	1:A:156:LEU:HB2	2.02	0.42
1:C:53:THR:OG1	1:C:54:THR:N	2.53	0.41
2:B:129:LEU:N	2:B:129:LEU:CD2	2.83	0.41
2:D:130:VAL:HG13	2:H:115:GLN:NE2	2.35	0.41
1:E:53:THR:OG1	1:E:55:LEU:CG	2.65	0.41
1:G:44:LYS:HZ2	1:G:46:LYS:NZ	2.14	0.41
1:E:159:ASP:OD1	1:E:160:ARG:N	2.53	0.41
1:C:63:PHE:CE2	1:C:167:GLU:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:121:ASN:OD1	2:F:121:ASN:N	2.50	0.41
1:G:36:PRO:CG	1:G:48:THR:CG2	2.99	0.41
1:A:116:MET:HG2	1:A:117:THR:O	2.20	0.41
1:A:170:GLN:OE1	1:A:171:PRO:N	2.53	0.41
1:E:72:PHE:N	1:E:72:PHE:CD1	2.89	0.41
1:A:37:ASP:OD1	1:A:48:THR:OG1	2.36	0.41
1:E:75:LEU:HD12	1:E:75:LEU:C	2.44	0.41
1:A:63:PHE:CD1	1:A:63:PHE:N	2.88	0.41
1:C:144:GLU:OE2	2:D:118:LYS:NZ	2.53	0.41
1:A:123:LYS:O	1:A:127:GLU:CG	2.68	0.41
1:A:30:SER:O	1:A:53:THR:HA	2.21	0.41
1:C:156:LEU:HD23	1:C:156:LEU:HA	1.69	0.41
1:C:116:MET:HG2	1:C:121:PHE:HB2	2.03	0.40
1:C:139:THR:CG2	1:C:140:VAL:N	2.84	0.40
1:A:35:ILE:HA	1:A:36:PRO:HD3	1.92	0.40
1:A:105:LYS:HD3	1:A:108:LYS:HZ1	1.86	0.40
1:G:170:GLN:CD	1:G:171:PRO:CD	2.63	0.40
2:H:121:ASN:HA	2:H:122:GLY:HA2	1.83	0.40
1:C:106:MET:HE3	1:C:106:MET:CA	2.50	0.40
1:G:116:MET:HE2	1:G:116:MET:HB3	1.88	0.40
1:C:88:LEU:C	1:C:89:ILE:HD12	2.37	0.40
1:C:124:MET:O	1:C:128:LEU:HG	2.21	0.40

All (2) 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:C:89:ILE:CG2	1:C:108:LYS:NZ[2_674]	1.94	0.26
1:E:87:GLY:O	1:E:120:GLU:OE1[3_474]	2.12	0.08

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	140/152 (92%)	137 (98%)	3 (2%)	0	100	100
1	C	140/152 (92%)	139 (99%)	1 (1%)	0	100	100
1	E	141/152 (93%)	135 (96%)	4 (3%)	2 (1%)	9	30
1	G	141/152 (93%)	136 (96%)	3 (2%)	2 (1%)	9	30
2	B	19/23 (83%)	17 (90%)	1 (5%)	1 (5%)	1	5
2	D	19/23 (83%)	19 (100%)	0	0	100	100
2	F	18/23 (78%)	17 (94%)	1 (6%)	0	100	100
2	H	18/23 (78%)	18 (100%)	0	0	100	100
All	All	636/700 (91%)	618 (97%)	13 (2%)	5 (1%)	16	44

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	131	THR
1	E	170	GLN
1	G	42	ARG
1	G	109	LEU
1	E	171	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	131/139 (94%)	109 (83%)	22 (17%)	2	8
1	C	131/139 (94%)	106 (81%)	25 (19%)	1	5
1	E	131/139 (94%)	99 (76%)	32 (24%)	1	2
1	G	131/139 (94%)	99 (76%)	32 (24%)	1	2
2	B	17/18 (94%)	11 (65%)	6 (35%)	0	0
2	D	17/18 (94%)	15 (88%)	2 (12%)	5	17
2	F	16/18 (89%)	15 (94%)	1 (6%)	16	45
2	H	16/18 (89%)	9 (56%)	7 (44%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	590/628 (94%)	463 (78%)	127 (22%)	1 4

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	35	ILE
1	A	44	LYS
1	A	55	LEU
1	A	57	THR
1	A	59	GLN
1	A	78	THR
1	A	88	LEU
1	A	89	ILE
1	A	103	ARG
1	A	106	MET
1	A	115	SER
1	A	118	LYS
1	A	119	GLU
1	A	123	LYS
1	A	125	LYS
1	A	138	LYS
1	A	139	THR
1	A	141	SER
1	A	157	SER
1	A	160	ARG
1	A	170	GLN
2	B	120	LYS
2	B	121	ASN
2	B	123	SER
2	B	128	ILE
2	B	130	VAL
2	B	132	GLN
1	C	31	LEU
1	C	33	ILE
1	C	41	GLU
1	C	44	LYS
1	C	52	LYS
1	C	55	LEU
1	C	57	THR
1	C	60	SER
1	C	89	ILE

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Mol	Chain	Res	Type
1	C	90	ILE
1	C	106	MET
1	C	108	LYS
1	C	111	GLU
1	C	115	SER
1	C	116	MET
1	C	119	GLU
1	C	123	LYS
1	C	126	GLN
1	C	141	SER
1	C	145	VAL
1	C	157	SER
1	C	158	LYS
1	C	160	ARG
1	C	164	VAL
1	C	165	PHE
2	D	123	SER
2	D	132	GLN
1	E	37	ASP
1	E	39	LEU
1	E	41	GLU
1	E	43	ASP
1	E	45	VAL
1	E	52	LYS
1	E	55	LEU
1	E	60	SER
1	E	63	PHE
1	E	64	SER
1	E	78	THR
1	E	81	GLU
1	E	83	THR
1	E	95	THR
1	E	96	LYS
1	E	106	MET
1	E	108	LYS
1	E	111	GLU
1	E	113	GLU
1	E	118	LYS
1	E	119	GLU
1	E	125	LYS
1	E	127	GLU
1	E	131	GLU

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Mol	Chain	Res	Type
1	E	137	LYS
1	E	138	LYS
1	E	139	THR
1	E	147	LEU
1	E	151	SER
1	E	157	SER
1	E	164	VAL
1	E	170	GLN
2	F	128	ILE
1	G	30	SER
1	G	39	LEU
1	G	41	GLU
1	G	43	ASP
1	G	44	LYS
1	G	45	VAL
1	G	48	THR
1	G	54	THR
1	G	55	LEU
1	G	59	GLN
1	G	68	GLN
1	G	78	THR
1	G	79	LEU
1	G	80	ILE
1	G	82	THR
1	G	88	LEU
1	G	89	ILE
1	G	90	ILE
1	G	106	MET
1	G	115	SER
1	G	118	LYS
1	G	119	GLU
1	G	126	GLN
1	G	131	GLU
1	G	141	SER
1	G	145	VAL
1	G	146	PHE
1	G	151	SER
1	G	157	SER
1	G	159	ASP
1	G	160	ARG
1	G	169	ASP
2	H	114	VAL

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Mol	Chain	Res	Type
2	H	118	LYS
2	H	121	ASN
2	H	123	SER
2	H	126	GLN
2	H	128	ILE
2	H	131	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	GLN
1	A	161	ASN
1	C	107	GLN
2	D	115	GLN
1	E	59	GLN
1	E	68	GLN
1	E	170	GLN
1	G	59	GLN
1	G	76	HIS
1	G	126	GLN
1	G	148	GLN
1	G	163	HIS
2	H	115	GLN
2	H	121	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	142/152 (93%)	0.33	6 (4%)	40	32	29, 48, 76, 110	0
1	C	142/152 (93%)	0.17	5 (3%)	47	38	27, 46, 76, 110	0
1	E	143/152 (94%)	0.63	12 (8%)	17	12	37, 59, 82, 116	0
1	G	143/152 (94%)	0.60	10 (6%)	22	16	39, 62, 80, 109	0
2	B	21/23 (91%)	0.64	1 (4%)	35	28	34, 49, 81, 97	0
2	D	21/23 (91%)	0.26	0	100	100	35, 46, 86, 96	0
2	F	20/23 (86%)	0.66	1 (5%)	34	26	35, 53, 73, 93	0
2	H	20/23 (86%)	0.56	1 (5%)	34	26	32, 50, 97, 107	0
All	All	652/700 (93%)	0.44	36 (5%)	30	23	27, 55, 82, 116	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	111	GLU	4.4
1	G	172	ALA	4.2
1	E	172	ALA	3.9
1	A	171	PRO	3.8
2	H	112	PRO	3.7
1	G	170	GLN	3.6
1	E	120	GLU	3.4
1	E	160	ARG	3.4
1	C	171	PRO	3.3
1	C	160	ARG	3.2
2	B	112	PRO	3.2
1	A	42	ARG	3.2
1	A	108	LYS	3.1
1	G	160	ARG	3.0
1	C	42	ARG	3.0
2	F	121	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	114	GLY	2.7
1	E	170	GLN	2.6
1	E	106	MET	2.5
1	E	171	PRO	2.5
1	E	79	LEU	2.4
1	A	59	GLN	2.4
1	G	89	ILE	2.4
1	E	122	ALA	2.3
1	E	57	THR	2.3
1	G	168	TYR	2.3
1	E	168	TYR	2.3
1	G	154	PRO	2.3
1	E	59	GLN	2.2
1	G	169	ASP	2.2
1	C	57	THR	2.2
1	E	87	GLY	2.2
1	G	115	SER	2.1
1	A	57	THR	2.0
1	G	120	GLU	2.0
1	G	86	ALA	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.