Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:38 PM GMT

PDB ID	:	4TWD
Title	:	X-ray structure of a pentameric ligand gated ion channel from Erwinia chrysanthemi (ELIC) in complex with memantine
Authors	:	Ulens, C.; Spurny, R.; Thompson, A.J.; Alqazzaz, M.; Debaveye, S.; Lu, H.; Price, K.; Villalgordo, J.M.; Tresadern, G.; Lynch, J.W.; Lummis, S.C.R.
Deposited on	:	2014-06-30
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

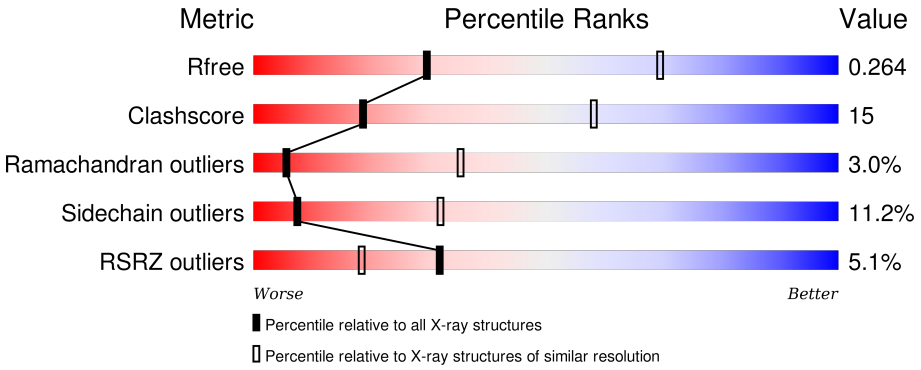
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	307	5% 61% 32% 6%
1	B	307	3% 63% 30% 6% •
1	C	307	7% 58% 37% 5%
1	D	307	3% 60% 33% 7%
1	E	307	4% 58% 36% 5% •

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Mol	Chain	Length	Quality of chain
1	F	307	6% 57% 38% 5%
1	G	307	7% 59% 35% 6%
1	H	307	7% 60% 34% 6%
1	I	307	5% 63% 32% 5%
1	J	307	4% 61% 33% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	377	A	401	-	-	-	X
2	377	A	402	-	-	-	X
2	377	C	401	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25126 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 Cys-loop ligand-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	B	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	C	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	D	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	E	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	F	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	G	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	H	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	I	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			
1	J	307	Total	C	N	O	S	0	0	0
			2497	1624	416	451	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	ALA	ILE	conflict	UNP P0C7B7
A	164	GLY	-	insertion	UNP P0C7B7
A	247	SER	PHE	engineered mutation	UNP P0C7B7
A	289	ASN	MET	conflict	UNP P0C7B7
B	152	ALA	ILE	conflict	UNP P0C7B7
B	164	GLY	-	insertion	UNP P0C7B7
B	247	SER	PHE	engineered mutation	UNP P0C7B7
B	289	ASN	MET	conflict	UNP P0C7B7
C	152	ALA	ILE	conflict	UNP P0C7B7

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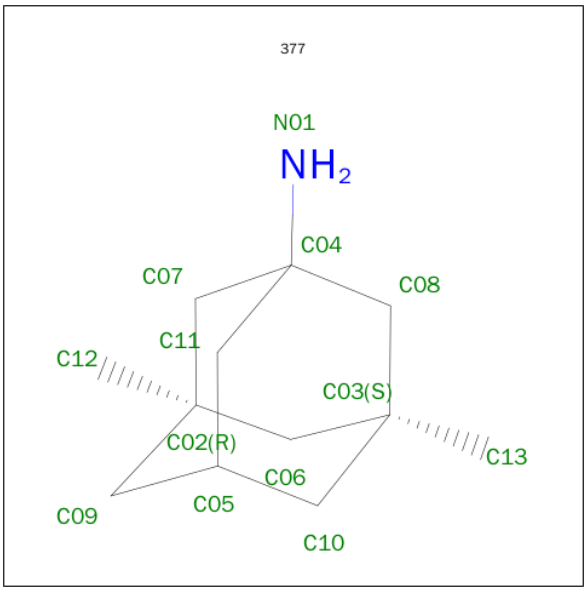
Chain	Residue	Modelled	Actual	Comment	Reference
C	164	GLY	-	insertion	UNP P0C7B7
C	247	SER	PHE	engineered mutation	UNP P0C7B7
C	289	ASN	MET	conflict	UNP P0C7B7
D	152	ALA	ILE	conflict	UNP P0C7B7
D	164	GLY	-	insertion	UNP P0C7B7
D	247	SER	PHE	engineered mutation	UNP P0C7B7
D	289	ASN	MET	conflict	UNP P0C7B7
E	152	ALA	ILE	conflict	UNP P0C7B7
E	164	GLY	-	insertion	UNP P0C7B7
E	247	SER	PHE	engineered mutation	UNP P0C7B7
E	289	ASN	MET	conflict	UNP P0C7B7
F	152	ALA	ILE	conflict	UNP P0C7B7
F	164	GLY	-	insertion	UNP P0C7B7
F	247	SER	PHE	engineered mutation	UNP P0C7B7
F	289	ASN	MET	conflict	UNP P0C7B7
G	152	ALA	ILE	conflict	UNP P0C7B7
G	164	GLY	-	insertion	UNP P0C7B7
G	247	SER	PHE	engineered mutation	UNP P0C7B7
G	289	ASN	MET	conflict	UNP P0C7B7
H	152	ALA	ILE	conflict	UNP P0C7B7
H	164	GLY	-	insertion	UNP P0C7B7
H	247	SER	PHE	engineered mutation	UNP P0C7B7
H	289	ASN	MET	conflict	UNP P0C7B7
I	152	ALA	ILE	conflict	UNP P0C7B7
I	164	GLY	-	insertion	UNP P0C7B7
I	247	SER	PHE	engineered mutation	UNP P0C7B7
I	289	ASN	MET	conflict	UNP P0C7B7
J	152	ALA	ILE	conflict	UNP P0C7B7
J	164	GLY	-	insertion	UNP P0C7B7
J	247	SER	PHE	engineered mutation	UNP P0C7B7
J	289	ASN	MET	conflict	UNP P0C7B7

- Molecule 2 is Memantine (three-letter code: 377) (formula: $C_{12}H_{21}N$).



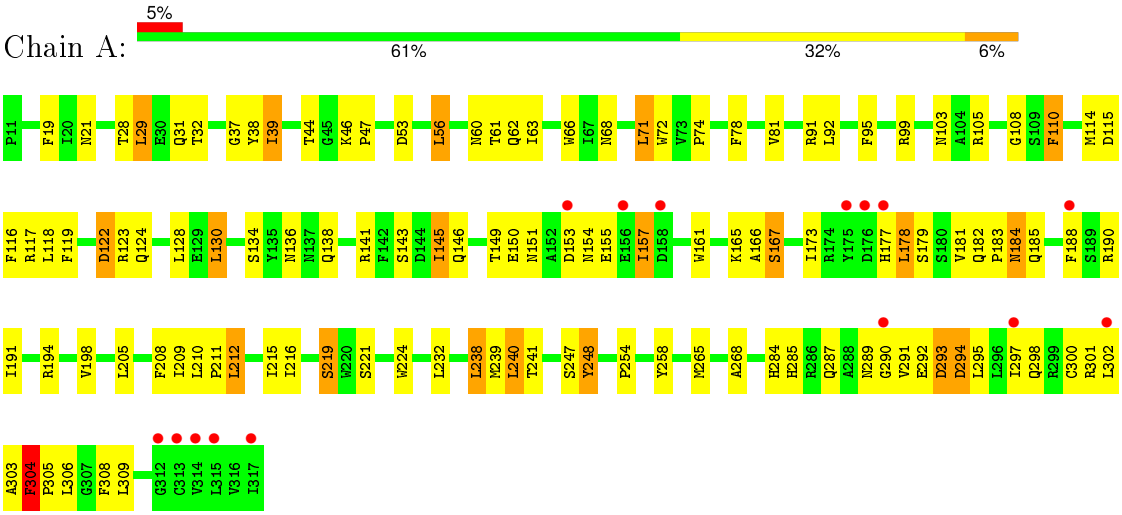
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N 13 12 1	0	0
2	A	1	Total C N 13 12 1	0	0
2	B	1	Total C N 13 12 1	0	0
2	C	1	Total C N 13 12 1	0	0
2	C	1	Total C N 13 12 1	0	0
2	E	1	Total C N 13 12 1	0	0
2	F	1	Total C N 13 12 1	0	0
2	F	1	Total C N 13 12 1	0	0
2	G	1	Total C N 13 12 1	0	0
2	H	1	Total C N 13 12 1	0	0
2	H	1	Total C N 13 12 1	0	0
2	J	1	Total C N 13 12 1	0	0

3 Residue-property plots (i)

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

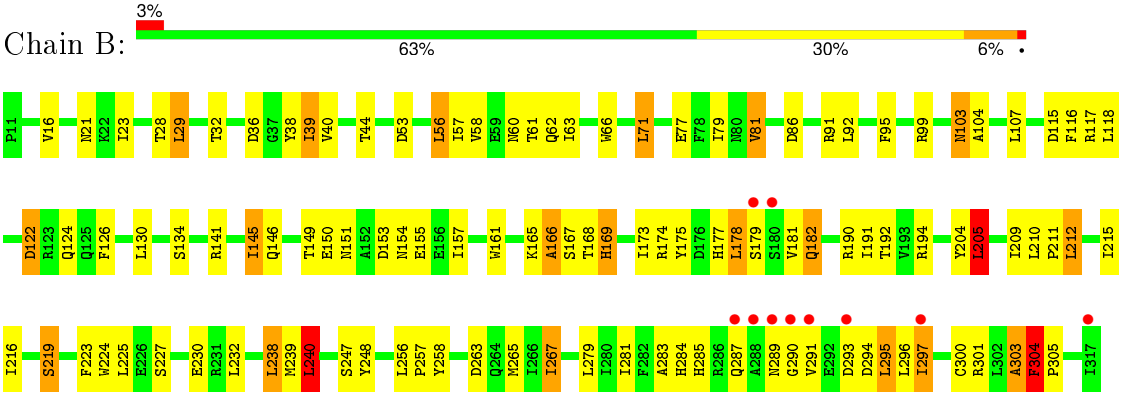
- Molecule 1: Cys-loop ligand-gated ion channel

Chain A:



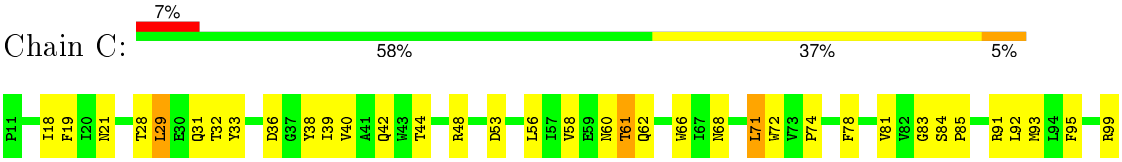
- Molecule 1: Cys-loop ligand-gated ion channel

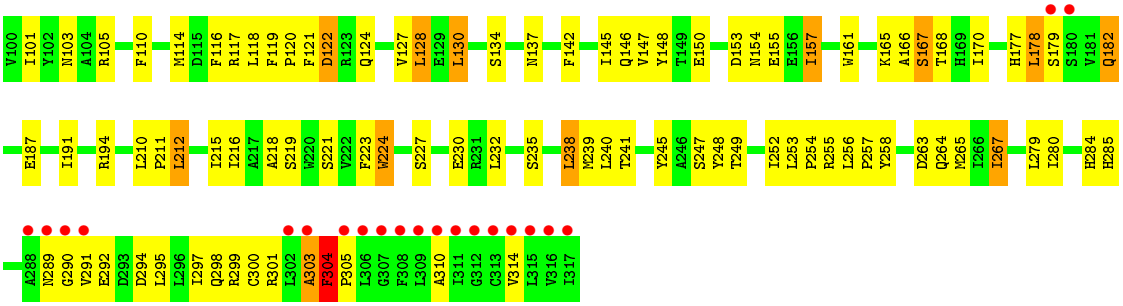
Chain B:



- Molecule 1: Cys-loop ligand-gated ion channel

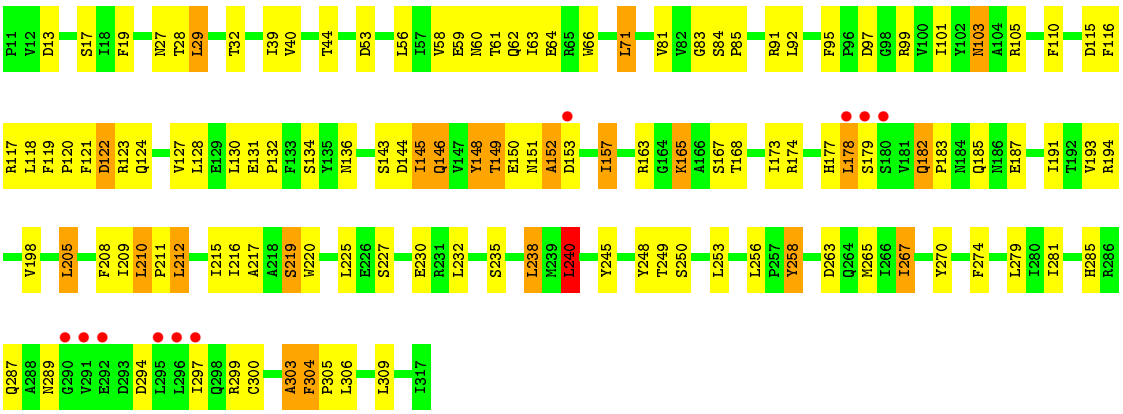
Chain C:





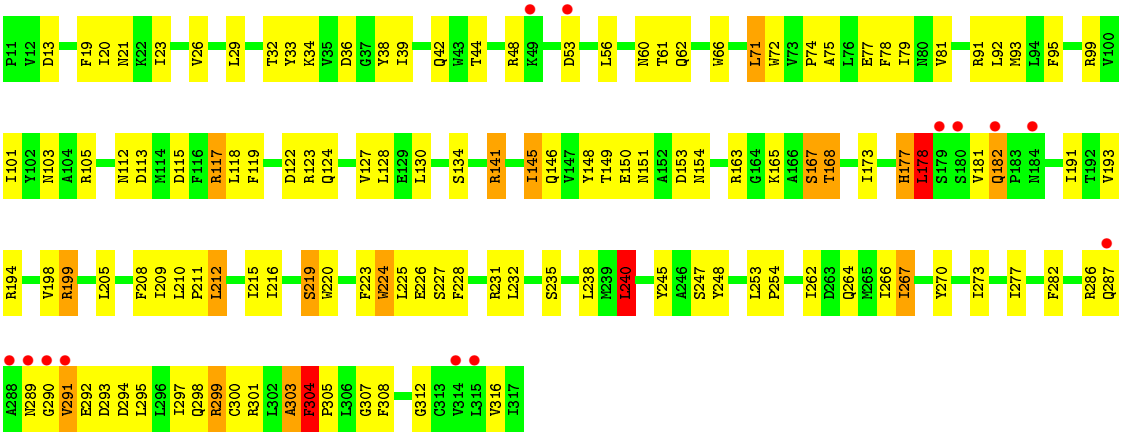
• Molecule 1: Cys-loop ligand-gated ion channel

Chain D:



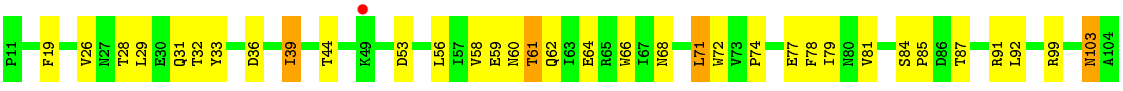
• Molecule 1: Cys-loop ligand-gated ion channel

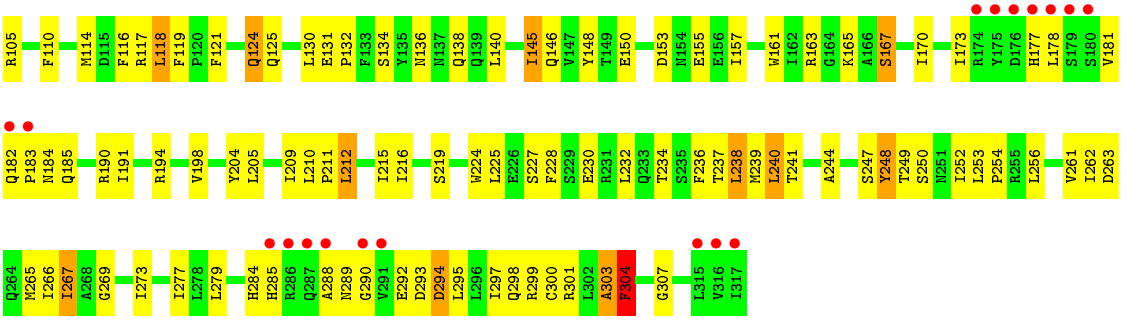
Chain E:



• Molecule 1: Cys-loop ligand-gated ion channel

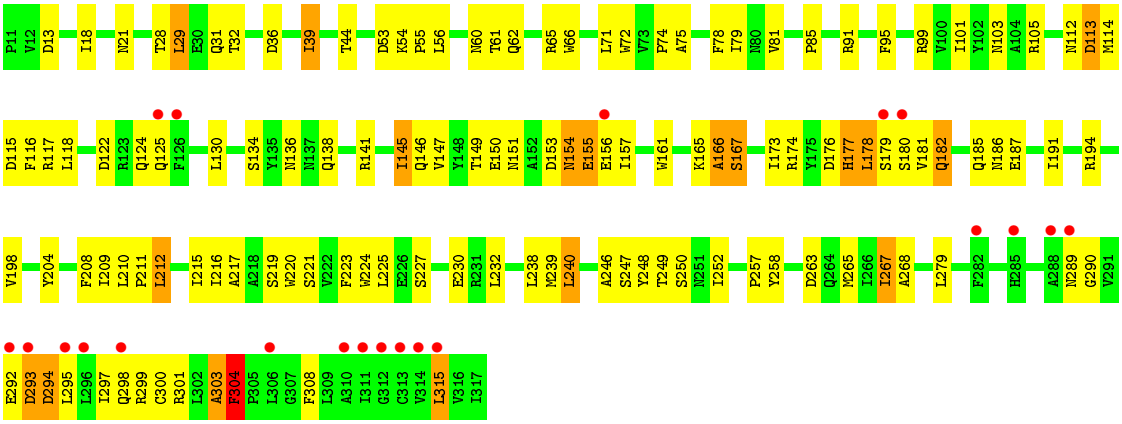
Chain F:





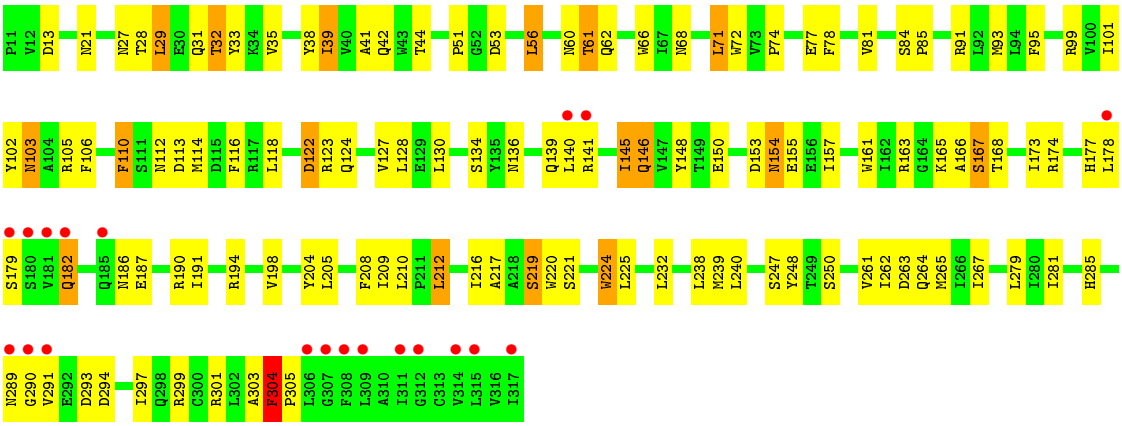
• Molecule 1: Cys-loop ligand-gated ion channel

Chain G:



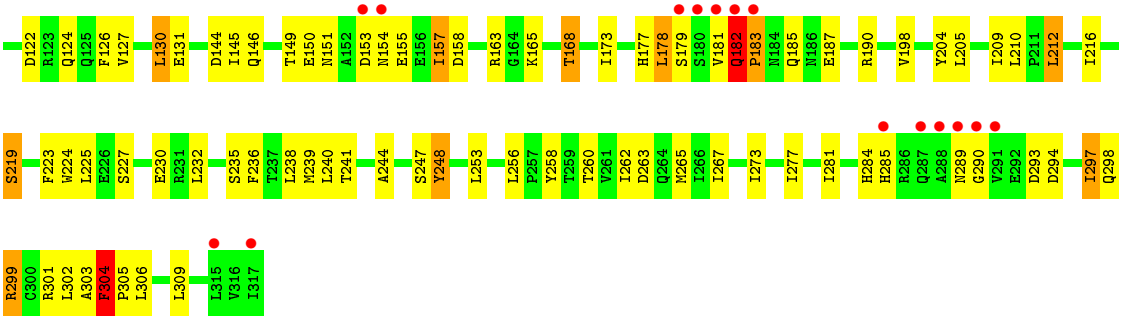
• Molecule 1: Cys-loop ligand-gated ion channel

Chain H:

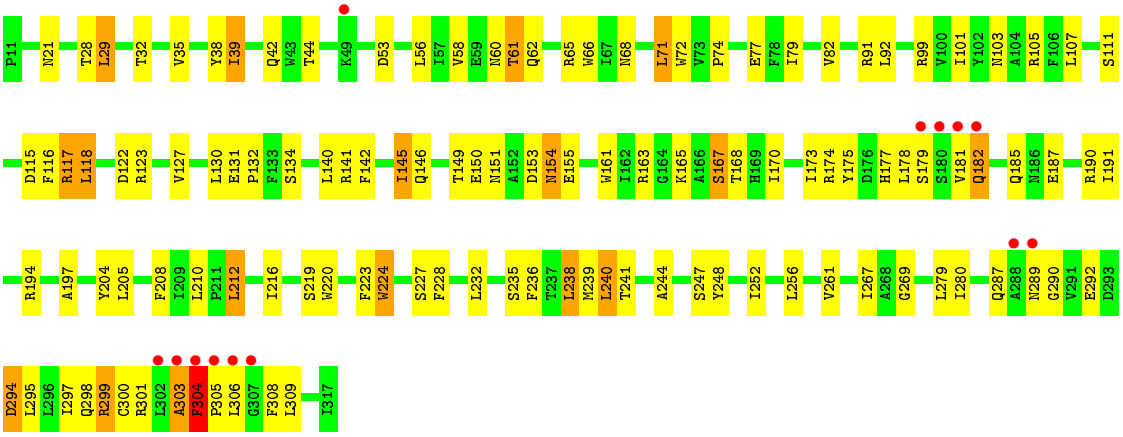


• Molecule 1: Cys-loop ligand-gated ion channel

Chain I:



- Molecule 1: Cys-loop ligand-gated ion channel



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	105.48Å 265.28Å 111.10Å 90.00° 110.28° 90.00°	Depositor
Resolution (Å)	48.63 – 3.20 48.63 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.63-3.20) 91.0 (48.63-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.199 , 0.252 0.209 , 0.264	Depositor DCC
R_{free} test set	4705 reflections (5.79%)	DCC
Wilson B-factor (Å^2)	85.6	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 73.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 93784 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	25126	wwPDB-VP
Average B, all atoms (Å^2)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 377

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	0.56	0/2564	0.80	2/3495 (0.1%)
1	B	0.66	0/2564	0.90	3/3495 (0.1%)
1	C	0.67	0/2564	0.86	0/3495
1	D	0.68	0/2564	0.87	2/3495 (0.1%)
1	E	0.58	0/2564	0.80	3/3495 (0.1%)
1	F	0.53	0/2564	0.77	0/3495
1	G	0.65	0/2564	0.87	1/3495 (0.0%)
1	H	0.60	0/2564	0.79	0/3495
1	I	0.61	0/2564	0.81	0/3495
1	J	0.54	0/2564	0.76	1/3495 (0.0%)
All	All	0.61	0/25640	0.82	12/34950 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	56	LEU	CB-CG-CD1	-6.60	99.78	111.00
1	A	39	ILE	CB-CA-C	-6.29	99.02	111.60
1	B	240	LEU	CA-CB-CG	6.11	129.34	115.30
1	D	205	LEU	CA-CB-CG	-5.98	101.55	115.30
1	E	178	LEU	CA-CB-CG	5.98	129.04	115.30
1	J	39	ILE	CB-CA-C	-5.54	100.51	111.60
1	D	240	LEU	CA-CB-CG	5.49	127.93	115.30
1	E	240	LEU	CA-CB-CG	5.29	127.47	115.30
1	B	205	LEU	CB-CG-CD1	-5.11	102.32	111.00
1	G	315	LEU	CA-CB-CG	5.09	127.01	115.30
1	E	199	ARG	NE-CZ-NH1	-5.09	117.76	120.30
1	B	166	ALA	N-CA-CB	5.00	117.10	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2497	0	2468	77	0
1	B	2497	0	2468	84	0
1	C	2497	0	2468	90	0
1	D	2497	0	2468	90	0
1	E	2497	0	2468	87	0
1	F	2497	0	2468	94	0
1	G	2497	0	2468	98	0
1	H	2497	0	2468	85	0
1	I	2497	0	2468	78	0
1	J	2497	0	2468	81	0
2	A	26	0	42	2	0
2	B	13	0	21	1	0
2	C	26	0	42	2	0
2	E	13	0	21	0	0
2	F	26	0	42	3	0
2	G	13	0	21	0	0
2	H	26	0	42	2	0
2	J	13	0	21	3	0
All	All	25126	0	24932	771	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (771) 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:294:ASP:HB2	1:E:297:ILE:HG22	1.46	0.93
1:G:13:ASP:OD2	1:G:141:ARG:NH1	2.05	0.89
1:G:154:ASN:O	1:G:156:GLU:N	2.10	0.84
1:A:224:TRP:CH2	1:A:301:ARG:HB3	2.13	0.84
1:E:293:ASP:O	1:E:298:GLN:NE2	2.12	0.82
1:C:284:HIS:HE1	1:C:291:VAL:HG13	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:VAL:HG21	1:C:85:PRO:HG3	1.63	0.80
1:D:248:TYR:HB2	1:E:247:SER:HB3	1.63	0.79
1:A:247:SER:HB3	1:E:248:TYR:HB2	1.64	0.79
1:F:248:TYR:HB2	1:G:247:SER:HB3	1.66	0.77
1:E:205:LEU:HD23	1:E:209:ILE:HG13	1.67	0.77
1:E:21:ASN:HD21	1:E:38:TYR:HE1	1.32	0.76
1:J:294:ASP:HB2	1:J:297:ILE:HG22	1.67	0.76
1:G:81:VAL:HG21	1:G:85:PRO:HG3	1.66	0.75
1:I:149:THR:O	1:I:151:ASN:N	2.20	0.75
1:D:306:LEU:HA	1:D:309:LEU:HB2	1.69	0.75
1:B:145:ILE:HD12	1:B:191:ILE:HG21	1.68	0.75
1:F:167:SER:HB3	1:F:194:ARG:HB2	1.68	0.74
1:A:289:ASN:OD1	1:A:290:GLY:N	2.20	0.73
1:C:155:GLU:OE2	1:C:161:TRP:HB3	1.89	0.72
1:G:289:ASN:OD1	1:G:290:GLY:N	2.21	0.72
1:J:167:SER:HB3	1:J:194:ARG:HB2	1.71	0.72
1:F:99:ARG:HH12	1:G:180:SER:HB2	1.54	0.71
1:B:62:GLN:NE2	1:C:68:ASN:OD1	2.22	0.71
1:H:13:ASP:OD2	1:H:141:ARG:NH1	2.23	0.71
1:F:247:SER:HB3	1:J:248:TYR:HB2	1.73	0.71
1:C:137:ASN:ND2	1:C:187:GLU:HB3	2.06	0.70
1:H:61:THR:HG22	1:H:62:GLN:HE21	1.57	0.69
1:D:123:ARG:HD2	1:D:198:VAL:HG22	1.73	0.69
1:E:289:ASN:OD1	1:E:290:GLY:N	2.23	0.69
1:E:264:GLN:HA	1:E:267:ILE:HG13	1.75	0.69
1:H:248:TYR:HB2	1:I:247:SER:HB3	1.75	0.69
1:F:240:LEU:HD23	1:J:241:THR:HA	1.75	0.69
1:F:181:VAL:HG21	1:F:185:GLN:HB2	1.74	0.69
1:F:212:LEU:O	1:F:216:ILE:HG12	1.93	0.69
1:G:248:TYR:HB2	1:H:247:SER:HB3	1.74	0.68
1:C:61:THR:HG22	1:C:62:GLN:HE21	1.58	0.68
1:D:212:LEU:O	1:D:216:ILE:HG12	1.94	0.68
1:E:295:LEU:O	1:E:299:ARG:HB2	1.93	0.68
1:F:66:TRP:HB3	1:F:71:LEU:HD12	1.76	0.68
1:B:167:SER:HB3	1:B:194:ARG:HB2	1.76	0.68
1:D:149:THR:O	1:D:151:ASN:N	2.25	0.68
1:G:224:TRP:CH2	1:G:301:ARG:HB3	2.29	0.68
1:J:224:TRP:CH2	1:J:301:ARG:HB3	2.28	0.67
1:I:216:ILE:O	1:I:219:SER:HB3	1.95	0.67
1:J:66:TRP:HB3	1:J:71:LEU:HD12	1.76	0.67
1:H:212:LEU:O	1:H:216:ILE:HG12	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:LEU:HD23	1:D:209:ILE:HG13	1.75	0.67
1:C:294:ASP:HB2	1:C:297:ILE:HG22	1.74	0.67
1:D:211:PRO:O	1:D:215:ILE:HG12	1.95	0.67
1:A:181:VAL:HG21	1:A:185:GLN:HB2	1.77	0.66
1:A:224:TRP:CZ3	1:A:301:ARG:HB3	2.29	0.66
1:I:248:TYR:HB2	1:J:247:SER:HB3	1.78	0.66
1:F:131:GLU:OE1	1:F:190:ARG:NH2	2.29	0.66
1:C:241:THR:HA	1:D:240:LEU:HD23	1.77	0.66
1:E:294:ASP:HB2	1:E:297:ILE:CG2	2.25	0.66
1:E:123:ARG:HD2	1:E:198:VAL:HG22	1.77	0.66
1:H:44:THR:HA	1:H:99:ARG:HA	1.78	0.65
1:G:181:VAL:HG21	1:G:185:GLN:HB2	1.78	0.65
1:F:36:ASP:OD2	1:F:105:ARG:NH2	2.29	0.65
1:B:175:TYR:CE1	2:B:401:377:H9	2.32	0.65
1:D:148:TYR:HE1	1:E:177:HIS:HB2	1.61	0.64
1:I:23:ILE:HG12	1:I:35:VAL:HG22	1.78	0.64
1:D:44:THR:HA	1:D:99:ARG:HA	1.80	0.64
1:H:61:THR:HG22	1:H:62:GLN:NE2	2.12	0.64
1:H:38:TYR:CE2	2:H:402:377:H1	2.31	0.64
1:D:40:VAL:HG13	1:D:103:ASN:ND2	2.12	0.64
1:B:300:CYS:HB2	1:B:303:ALA:HB3	1.78	0.64
1:E:167:SER:HB3	1:E:194:ARG:HB2	1.80	0.63
1:I:293:ASP:O	1:I:298:GLN:NE2	2.31	0.63
1:I:205:LEU:HD23	1:I:209:ILE:HG13	1.80	0.63
1:F:225:LEU:HD21	1:G:232:LEU:HD22	1.80	0.63
1:H:28:THR:HG22	1:H:116:PHE:CE1	2.34	0.63
1:G:211:PRO:O	1:G:215:ILE:HG12	1.99	0.63
1:C:44:THR:HA	1:C:99:ARG:HA	1.80	0.63
1:I:163:ARG:HE	1:I:198:VAL:HG21	1.64	0.63
1:J:179:SER:HB2	1:J:181:VAL:HG12	1.80	0.63
1:H:127:VAL:HG22	1:H:194:ARG:HG2	1.80	0.63
1:I:212:LEU:O	1:I:216:ILE:HG12	1.98	0.63
1:B:169:HIS:HB3	1:B:192:THR:HB	1.81	0.63
1:J:21:ASN:HD21	1:J:38:TYR:HE1	1.47	0.63
1:D:148:TYR:CE1	1:E:177:HIS:HB2	2.34	0.62
1:G:248:TYR:HE1	1:H:250:SER:HG	1.46	0.62
1:B:224:TRP:CH2	1:B:301:ARG:HB3	2.35	0.62
1:F:263:ASP:O	1:F:267:ILE:HG12	1.98	0.62
1:I:182:GLN:HG3	1:I:183:PRO:HD3	1.80	0.62
1:H:42:GLN:HG3	1:H:101:ILE:HG12	1.81	0.62
1:F:68:ASN:OD1	1:J:62:GLN:NE2	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ARG:HD2	1:D:134:SER:HB3	1.81	0.61
1:J:42:GLN:HG3	1:J:101:ILE:HG12	1.82	0.61
1:B:283:ALA:O	1:B:293:ASP:HA	2.01	0.61
1:E:112:ASN:OD1	1:E:113:ASP:N	2.33	0.61
1:E:208:PHE:O	1:E:245:TYR:OH	2.19	0.61
1:I:155:GLU:O	1:I:158:ASP:N	2.26	0.61
1:J:28:THR:HB	1:J:256:LEU:HD21	1.81	0.61
1:D:216:ILE:O	1:D:219:SER:HB3	2.00	0.61
1:B:212:LEU:HD12	1:B:265:MET:HB3	1.82	0.61
1:E:38:TYR:CZ	1:E:105:ARG:HD2	2.36	0.61
1:D:17:SER:HB2	1:D:40:VAL:HB	1.81	0.61
1:J:212:LEU:O	1:J:216:ILE:HG12	2.00	0.60
1:A:247:SER:HA	1:E:248:TYR:HD1	1.66	0.60
1:C:224:TRP:CZ3	1:C:301:ARG:HB3	2.36	0.60
1:A:68:ASN:OD1	1:E:62:GLN:NE2	2.31	0.60
1:F:44:THR:HA	1:F:99:ARG:HA	1.83	0.60
1:C:263:ASP:O	1:C:267:ILE:HG12	2.01	0.60
1:C:300:CYS:HB2	1:C:303:ALA:HB3	1.83	0.60
1:J:235:SER:HA	1:J:238:LEU:HB2	1.81	0.60
1:J:127:VAL:HG22	1:J:194:ARG:HG2	1.83	0.60
1:E:300:CYS:HB2	1:E:303:ALA:HB3	1.83	0.60
1:D:225:LEU:HD21	1:E:232:LEU:HD22	1.82	0.60
1:H:31:GLN:HG2	1:H:114:MET:HB2	1.83	0.59
1:F:99:ARG:HH12	1:G:180:SER:CB	2.16	0.59
1:C:284:HIS:CE1	1:C:291:VAL:HG13	2.32	0.59
1:B:212:LEU:O	1:B:216:ILE:HG12	2.03	0.59
1:G:212:LEU:O	1:G:216:ILE:HG12	2.02	0.59
1:F:295:LEU:O	1:F:299:ARG:HG3	2.02	0.59
1:C:221:SER:HB2	1:D:281:ILE:HD11	1.84	0.59
1:C:212:LEU:O	1:C:216:ILE:HG12	2.02	0.59
1:D:81:VAL:HG21	1:D:85:PRO:HG3	1.84	0.59
1:J:145:ILE:HD12	1:J:191:ILE:CG2	2.33	0.59
1:I:289:ASN:OD1	1:I:290:GLY:N	2.36	0.59
1:D:97:ASP:OD2	1:D:99:ARG:NH1	2.35	0.59
1:C:289:ASN:OD1	1:C:290:GLY:N	2.34	0.59
1:B:284:HIS:NE2	1:B:291:VAL:HG13	2.18	0.59
1:G:31:GLN:HG2	1:G:114:MET:HB2	1.85	0.58
1:F:99:ARG:NH1	1:G:180:SER:HB2	2.17	0.58
1:E:13:ASP:OD2	1:E:141:ARG:HD3	2.03	0.58
1:A:248:TYR:HB2	1:B:247:SER:HB3	1.84	0.58
2:F:402:377:H19	1:J:244:ALA:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:ARG:HD2	1:E:134:SER:HB3	1.86	0.58
1:E:128:LEU:HB2	1:E:193:VAL:HB	1.85	0.58
1:H:289:ASN:OD1	1:H:290:GLY:N	2.37	0.58
1:F:136:ASN:H	1:F:136:ASN:HD22	1.50	0.58
1:D:212:LEU:CD1	1:D:265:MET:HB3	2.34	0.58
1:H:72:TRP:CZ2	1:H:74:PRO:HB3	2.38	0.58
1:I:91:ARG:HD2	1:J:134:SER:HB3	1.85	0.57
1:A:173:ILE:HD13	1:A:190:ARG:HB3	1.85	0.57
1:I:181:VAL:HG21	1:I:185:GLN:HB2	1.85	0.57
1:J:145:ILE:HD12	1:J:191:ILE:HG21	1.86	0.57
1:F:31:GLN:HG2	1:F:114:MET:HB2	1.85	0.57
1:A:221:SER:HB2	1:B:281:ILE:HD11	1.85	0.57
1:G:136:ASN:HD21	1:G:138:GLN:HB2	1.68	0.57
1:B:107:LEU:HD22	1:C:83:GLY:CA	2.33	0.57
1:A:167:SER:HB3	1:A:194:ARG:HB2	1.86	0.57
1:A:66:TRP:HB3	1:A:71:LEU:HD12	1.85	0.57
1:B:248:TYR:HB2	1:C:247:SER:HB3	1.85	0.57
1:C:279:LEU:HD13	1:C:300:CYS:SG	2.44	0.57
1:J:44:THR:HA	1:J:99:ARG:HA	1.85	0.57
1:C:38:TYR:CE2	1:C:105:ARG:HD2	2.40	0.57
1:D:149:THR:HG23	1:D:165:LYS:HE2	1.87	0.57
2:F:402:377:H17	1:I:244:ALA:HB1	1.85	0.57
1:G:62:GLN:NE2	1:H:68:ASN:OD1	2.36	0.57
1:I:131:GLU:OE1	1:I:190:ARG:NH2	2.35	0.57
1:E:232:LEU:O	1:E:235:SER:OG	2.22	0.57
1:J:287:GLN:HB3	1:J:292:GLU:HB3	1.87	0.56
1:G:91:ARG:HD2	1:H:134:SER:HB3	1.87	0.56
1:C:38:TYR:CE1	2:C:402:377:H22	2.40	0.56
1:F:28:THR:HB	1:F:256:LEU:HD21	1.86	0.56
1:I:21:ASN:HD21	1:I:38:TYR:HE1	1.52	0.56
1:J:175:TYR:CE1	2:J:401:377:H12	2.40	0.56
1:A:122:ASP:N	1:A:122:ASP:OD1	2.31	0.56
1:H:225:LEU:HD21	1:I:232:LEU:HD22	1.86	0.56
1:A:212:LEU:O	1:A:216:ILE:HG12	2.05	0.56
1:F:39:ILE:HD11	1:F:78:PHE:CZ	2.40	0.56
1:B:211:PRO:O	1:B:215:ILE:HG12	2.05	0.56
1:G:263:ASP:O	1:G:267:ILE:HG12	2.05	0.56
1:B:284:HIS:HE2	1:B:291:VAL:HG13	1.70	0.56
1:G:117:ARG:HG2	1:G:258:TYR:CD1	2.40	0.56
1:D:146:GLN:HB2	1:D:148:TYR:HE2	1.70	0.56
1:A:285:HIS:O	1:A:287:GLN:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ASN:OD1	1:A:292:GLU:N	2.36	0.56
1:E:149:THR:O	1:E:151:ASN:N	2.32	0.56
1:F:250:SER:HB3	1:J:252:ILE:HD11	1.86	0.55
1:H:122:ASP:OD1	1:H:122:ASP:N	2.34	0.55
1:F:81:VAL:HG21	1:F:85:PRO:HG3	1.88	0.55
1:A:78:PHE:O	1:A:81:VAL:HG12	2.07	0.55
1:C:66:TRP:HB3	1:C:71:LEU:HD12	1.88	0.55
1:F:289:ASN:OD1	1:F:290:GLY:N	2.38	0.55
1:F:252:ILE:HD11	1:G:250:SER:HB3	1.88	0.55
1:H:167:SER:HB3	1:H:194:ARG:HB2	1.88	0.55
1:C:212:LEU:HD12	1:C:265:MET:HB3	1.89	0.55
1:I:227:SER:HB3	1:I:230:GLU:HG3	1.88	0.55
1:F:19:PHE:CE2	1:F:148:TYR:HD2	2.25	0.55
1:E:72:TRP:CZ2	1:E:74:PRO:HB3	2.42	0.55
1:E:212:LEU:O	1:E:216:ILE:HG12	2.07	0.55
1:C:31:GLN:HG2	1:C:114:MET:HB2	1.89	0.54
1:G:145:ILE:HD12	1:G:191:ILE:CG2	2.36	0.54
1:I:44:THR:HA	1:I:99:ARG:HA	1.89	0.54
1:B:16:VAL:HG12	1:B:145:ILE:HG13	1.89	0.54
1:A:28:THR:HG22	1:A:116:PHE:CE1	2.42	0.54
1:F:58:VAL:HB	1:F:92:LEU:HB2	1.90	0.54
1:J:118:LEU:HA	1:J:261:VAL:HG23	1.89	0.54
1:E:262:ILE:O	1:E:266:ILE:HG12	2.08	0.54
1:G:289:ASN:HD21	1:G:292:GLU:HB2	1.73	0.54
1:H:212:LEU:HD12	1:H:265:MET:HB3	1.90	0.54
1:F:211:PRO:O	1:F:215:ILE:HG12	2.07	0.54
1:H:38:TYR:CZ	1:H:105:ARG:HD2	2.42	0.54
1:D:294:ASP:HB2	1:D:297:ILE:HG22	1.89	0.54
1:I:301:ARG:O	1:I:305:PRO:HG2	2.08	0.54
1:F:294:ASP:HB2	1:F:297:ILE:HG22	1.89	0.54
1:C:117:ARG:HG2	1:C:258:TYR:CD1	2.42	0.54
1:G:112:ASN:OD1	1:G:113:ASP:N	2.41	0.54
1:E:227:SER:O	1:E:231:ARG:NH1	2.41	0.54
1:G:227:SER:HB3	1:G:230:GLU:HG3	1.89	0.54
1:F:167:SER:CB	1:F:194:ARG:HB2	2.38	0.53
1:B:224:TRP:HD1	1:C:285:HIS:CD2	2.25	0.53
1:C:289:ASN:OD1	1:C:292:GLU:N	2.40	0.53
1:F:114:MET:HG2	1:F:124:GLN:HG3	1.90	0.53
1:B:107:LEU:HD22	1:C:83:GLY:HA2	1.89	0.53
1:C:157:ILE:HD11	1:D:115:ASP:CG	2.28	0.53
1:E:301:ARG:O	1:E:305:PRO:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:SER:HB2	1:B:181:VAL:HG12	1.91	0.53
1:G:300:CYS:HB2	1:G:303:ALA:HB3	1.89	0.53
1:B:294:ASP:O	1:B:296:LEU:N	2.42	0.53
1:E:289:ASN:OD1	1:E:291:VAL:N	2.42	0.53
1:E:66:TRP:HB3	1:E:71:LEU:HD12	1.91	0.53
1:D:28:THR:HG22	1:D:116:PHE:CZ	2.43	0.53
1:E:145:ILE:HD12	1:E:191:ILE:CG2	2.38	0.53
1:I:224:TRP:CE2	1:I:301:ARG:HD3	2.44	0.53
1:E:42:GLN:HG3	1:E:101:ILE:HG12	1.89	0.53
1:I:294:ASP:HB2	1:I:297:ILE:CG2	2.38	0.53
1:G:227:SER:HB3	1:G:230:GLU:CG	2.39	0.53
1:F:248:TYR:HE1	1:G:250:SER:HG	1.57	0.53
1:C:264:GLN:HA	1:C:267:ILE:HG13	1.89	0.53
1:A:284:HIS:HE1	1:E:226:GLU:OE2	1.92	0.53
1:C:249:THR:HG23	1:C:253:LEU:HD22	1.90	0.53
1:F:232:LEU:HD23	1:F:236:PHE:HE1	1.73	0.53
1:I:204:TYR:O	1:I:209:ILE:HG12	2.09	0.52
1:H:136:ASN:HD22	1:H:136:ASN:H	1.57	0.52
1:G:173:ILE:O	1:G:187:GLU:HA	2.08	0.52
1:G:72:TRP:CZ2	1:G:74:PRO:HB3	2.44	0.52
1:E:26:VAL:HG22	1:E:33:TYR:HB3	1.91	0.52
1:I:294:ASP:HB2	1:I:297:ILE:HG22	1.91	0.52
1:G:54:LYS:HB3	1:G:55:PRO:HD2	1.90	0.52
1:C:61:THR:HG21	1:D:64:GLU:HG3	1.91	0.52
1:H:146:GLN:HG3	1:H:148:TYR:OH	2.08	0.52
1:A:211:PRO:O	1:A:215:ILE:HG12	2.09	0.52
1:J:181:VAL:HG21	1:J:185:GLN:HB2	1.91	0.52
1:B:38:TYR:CE2	2:C:401:377:H1	2.45	0.52
1:A:188:PHE:CZ	2:A:401:377:H17	2.44	0.52
2:A:401:377:H1	1:E:38:TYR:CD2	2.45	0.52
1:I:224:TRP:CH2	1:I:301:ARG:HB3	2.45	0.52
1:D:300:CYS:HB2	1:D:303:ALA:HB3	1.92	0.52
1:F:91:ARG:NH2	1:F:103:ASN:OD1	2.43	0.52
1:E:115:ASP:OD1	1:E:117:ARG:HG3	2.09	0.52
1:H:294:ASP:HB2	1:H:297:ILE:HG22	1.92	0.52
1:B:149:THR:O	1:B:151:ASN:N	2.43	0.52
1:H:157:ILE:HD11	1:I:117:ARG:NE	2.24	0.52
1:G:167:SER:HB3	1:G:194:ARG:HB2	1.92	0.52
1:H:123:ARG:HD2	1:H:198:VAL:HG22	1.91	0.52
1:B:28:THR:HG22	1:B:116:PHE:CZ	2.45	0.52
1:B:212:LEU:CD1	1:B:265:MET:HB3	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:119:PHE:CE1	1:F:254:PRO:HG3	2.44	0.52
1:F:163:ARG:HE	1:F:198:VAL:HG21	1.75	0.52
1:E:273:ILE:O	1:E:277:ILE:HG12	2.10	0.52
1:B:227:SER:HB3	1:B:230:GLU:HG3	1.92	0.52
1:H:173:ILE:HD13	1:H:190:ARG:HB3	1.92	0.52
1:A:155:GLU:OE2	1:A:161:TRP:HB3	2.10	0.51
1:I:225:LEU:HD21	1:J:232:LEU:HD22	1.92	0.51
1:J:208:PHE:HE2	1:J:248:TYR:CE1	2.27	0.51
1:B:294:ASP:HB2	1:B:297:ILE:CG2	2.40	0.51
1:B:39:ILE:HG13	1:B:104:ALA:HB3	1.92	0.51
1:C:78:PHE:CE2	1:C:128:LEU:HD23	2.45	0.51
1:B:173:ILE:HD13	1:B:190:ARG:HB3	1.92	0.51
1:J:223:PHE:CE2	1:J:280:ILE:HG13	2.44	0.51
1:H:78:PHE:O	1:H:81:VAL:HG12	2.10	0.51
1:D:210:LEU:HB3	1:D:211:PRO:CD	2.41	0.51
1:H:161:TRP:HE3	1:H:163:ARG:HH21	1.59	0.51
1:C:137:ASN:HD21	1:C:187:GLU:HB3	1.73	0.51
1:F:273:ILE:O	1:F:277:ILE:HG12	2.11	0.51
1:G:224:TRP:CZ3	1:G:301:ARG:HB3	2.46	0.51
1:C:58:VAL:O	1:C:91:ARG:HA	2.11	0.51
1:E:216:ILE:O	1:E:219:SER:HB3	2.11	0.51
1:A:141:ARG:NH1	1:A:143:SER:HA	2.26	0.51
1:D:217:ALA:HA	1:D:220:TRP:CE3	2.46	0.51
1:C:48:ARG:NH1	1:C:48:ARG:HB2	2.26	0.51
1:A:247:SER:HA	1:E:248:TYR:CD1	2.45	0.51
1:A:241:THR:HA	1:B:240:LEU:HD23	1.93	0.51
1:C:227:SER:HB3	1:C:230:GLU:CD	2.31	0.51
1:F:134:SER:HB3	1:J:91:ARG:HD2	1.93	0.51
1:F:293:ASP:O	1:F:295:LEU:N	2.44	0.51
1:A:19:PHE:HD1	1:A:38:TYR:HB2	1.76	0.50
1:G:294:ASP:HB2	1:G:297:ILE:HG22	1.93	0.50
1:E:312:GLY:O	1:E:316:VAL:HG23	2.11	0.50
1:G:248:TYR:HE1	1:H:250:SER:OG	1.94	0.50
1:D:249:THR:HG23	1:D:253:LEU:HD22	1.93	0.50
1:H:110:PHE:CE2	1:H:128:LEU:HG	2.46	0.50
1:D:212:LEU:HD11	1:D:265:MET:HB3	1.93	0.50
1:F:61:THR:HG22	1:F:62:GLN:HE21	1.77	0.50
1:C:211:PRO:O	1:C:215:ILE:HG12	2.11	0.50
1:B:61:THR:HG22	1:B:62:GLN:NE2	2.26	0.50
1:A:155:GLU:HB3	1:A:161:TRP:CD1	2.45	0.50
1:I:78:PHE:O	1:I:81:VAL:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ILE:HD11	1:B:115:ASP:CG	2.32	0.50
1:F:145:ILE:HD12	1:F:191:ILE:HG23	1.93	0.50
1:C:40:VAL:HG13	1:C:103:ASN:OD1	2.12	0.50
1:F:91:ARG:HD2	1:G:134:SER:HB3	1.92	0.50
1:A:304:PHE:HD1	1:A:305:PRO:HD3	1.77	0.50
1:A:123:ARG:HD2	1:A:198:VAL:HG22	1.93	0.50
1:E:78:PHE:O	1:E:81:VAL:HG12	2.11	0.50
1:G:13:ASP:CG	1:G:141:ARG:NH1	2.65	0.50
1:E:127:VAL:HG22	1:E:194:ARG:HG2	1.94	0.50
1:I:66:TRP:HB3	1:I:71:LEU:HD12	1.94	0.50
1:A:44:THR:HA	1:A:99:ARG:HA	1.92	0.50
1:C:18:ILE:HB	1:C:147:VAL:HG22	1.93	0.50
1:F:300:CYS:HB2	1:F:303:ALA:HB3	1.94	0.49
1:C:122:ASP:N	1:C:122:ASP:OD1	2.41	0.49
1:J:289:ASN:OD1	1:J:290:GLY:N	2.44	0.49
1:C:212:LEU:CD1	1:C:265:MET:HB3	2.42	0.49
1:I:232:LEU:O	1:I:235:SER:OG	2.29	0.49
1:G:18:ILE:HB	1:G:147:VAL:HG22	1.94	0.49
1:G:18:ILE:HD13	1:G:39:ILE:HG12	1.95	0.49
1:H:145:ILE:HD12	1:H:191:ILE:HG21	1.93	0.49
1:A:61:THR:HG22	1:A:62:GLN:NE2	2.26	0.49
1:B:61:THR:HG22	1:B:62:GLN:HE21	1.78	0.49
1:F:136:ASN:H	1:F:136:ASN:ND2	2.10	0.49
1:F:288:ALA:N	1:F:292:GLU:OE2	2.44	0.49
1:D:27:ASN:HB3	1:D:32:THR:HB	1.94	0.49
1:F:299:ARG:HA	1:F:301:ARG:HG3	1.95	0.49
1:G:268:ALA:HB1	1:G:308:PHE:HE1	1.76	0.49
1:C:127:VAL:HG22	1:C:194:ARG:HG2	1.93	0.49
1:F:224:TRP:CZ3	1:F:301:ARG:HB3	2.47	0.49
1:D:28:THR:HB	1:D:256:LEU:HD21	1.95	0.49
1:I:253:LEU:HD21	1:I:262:ILE:HD12	1.95	0.49
1:G:28:THR:HG22	1:G:116:PHE:CZ	2.47	0.49
1:B:263:ASP:O	1:B:267:ILE:HG12	2.13	0.49
1:D:58:VAL:HB	1:D:92:LEU:HB2	1.93	0.49
1:C:38:TYR:CZ	1:C:105:ARG:HD2	2.48	0.49
1:D:208:PHE:O	1:D:245:TYR:OH	2.30	0.49
1:G:208:PHE:HE2	1:G:249:THR:HA	1.78	0.49
1:C:257:PRO:HG2	1:C:258:TYR:CD2	2.48	0.49
1:C:119:PHE:CE1	1:C:254:PRO:HG3	2.47	0.49
1:I:28:THR:HB	1:I:256:LEU:HD21	1.95	0.49
1:F:249:THR:HG23	1:F:253:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:LEU:HD21	1:C:232:LEU:HD22	1.95	0.49
1:E:211:PRO:O	1:E:215:ILE:HG12	2.13	0.49
1:E:220:TRP:HZ2	1:E:308:PHE:CG	2.31	0.49
1:C:167:SER:HB3	1:C:194:ARG:HB2	1.95	0.48
1:A:300:CYS:HB2	1:A:303:ALA:HB3	1.94	0.48
1:F:59:GLU:OE2	1:G:75:ALA:HB3	2.12	0.48
1:J:29:LEU:HD23	1:J:29:LEU:HA	1.72	0.48
1:E:19:PHE:HD2	1:E:148:TYR:HB2	1.78	0.48
1:C:72:TRP:CZ2	1:C:74:PRO:HB3	2.48	0.48
1:I:306:LEU:HA	1:I:309:LEU:HB2	1.95	0.48
1:C:28:THR:HB	1:C:256:LEU:CD2	2.43	0.48
1:G:136:ASN:ND2	1:G:185:GLN:HG3	2.27	0.48
1:G:145:ILE:HD12	1:G:191:ILE:HG21	1.96	0.48
1:E:227:SER:OG	1:E:228:PHE:N	2.46	0.48
1:J:123:ARG:HG2	1:J:197:ALA:O	2.13	0.48
1:C:19:PHE:CE2	1:C:148:TYR:CD2	3.02	0.48
1:A:63:ILE:HG23	1:A:92:LEU:HD12	1.95	0.48
1:H:38:TYR:CD2	2:H:402:377:H1	2.48	0.48
1:F:61:THR:HG22	1:F:62:GLN:NE2	2.29	0.48
1:J:72:TRP:CH2	1:J:74:PRO:HG3	2.48	0.48
1:C:301:ARG:O	1:C:305:PRO:HG2	2.14	0.48
1:G:295:LEU:HA	1:G:298:GLN:NE2	2.29	0.48
1:A:295:LEU:HD12	1:A:298:GLN:OE1	2.14	0.48
1:J:279:LEU:HD22	1:J:297:ILE:HD11	1.95	0.48
1:J:208:PHE:HE2	1:J:248:TYR:CZ	2.31	0.48
1:J:149:THR:O	1:J:151:ASN:N	2.43	0.48
1:G:101:ILE:HD13	1:H:179:SER:HB3	1.96	0.48
1:B:29:LEU:HD23	1:B:29:LEU:HA	1.65	0.48
1:H:294:ASP:HB2	1:H:297:ILE:CG2	2.42	0.48
1:G:115:ASP:OD1	1:G:117:ARG:HG3	2.13	0.48
1:F:232:LEU:CD2	1:F:236:PHE:HE1	2.27	0.48
1:C:19:PHE:CE2	1:C:148:TYR:HD2	2.32	0.48
1:B:215:ILE:HD13	1:C:239:MET:CE	2.43	0.47
1:I:299:ARG:HD3	1:I:301:ARG:HD2	1.95	0.47
1:G:44:THR:HA	1:G:99:ARG:HA	1.95	0.47
1:A:232:LEU:HD22	1:E:225:LEU:HD21	1.96	0.47
1:G:221:SER:HB2	1:H:281:ILE:HD11	1.96	0.47
1:G:55:PRO:HB3	1:G:95:PHE:CD2	2.48	0.47
1:I:223:PHE:HE1	1:I:304:PHE:CE1	2.32	0.47
1:E:44:THR:HA	1:E:99:ARG:HA	1.95	0.47
1:E:173:ILE:N	1:E:173:ILE:HD12	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:42:GLN:HG3	1:I:101:ILE:HG12	1.96	0.47
1:E:291:VAL:HG12	1:E:293:ASP:OD2	2.14	0.47
1:H:157:ILE:HA	1:H:157:ILE:HD13	1.62	0.47
1:B:91:ARG:HD2	1:C:134:SER:HB3	1.95	0.47
1:D:127:VAL:HG22	1:D:194:ARG:HG2	1.97	0.47
1:G:61:THR:HG22	1:G:62:GLN:HE21	1.79	0.47
1:G:257:PRO:HG2	1:G:258:TYR:CD2	2.49	0.47
1:D:227:SER:HB3	1:D:230:GLU:HG3	1.96	0.47
1:J:232:LEU:HD23	1:J:236:PHE:HE1	1.80	0.47
1:C:211:PRO:HB3	1:D:270:TYR:CD1	2.49	0.47
1:B:204:TYR:O	1:B:209:ILE:HG12	2.15	0.47
1:D:148:TYR:CD2	1:D:148:TYR:N	2.83	0.47
1:H:145:ILE:HD12	1:H:191:ILE:CG2	2.45	0.47
1:I:144:ASP:OD1	1:I:144:ASP:N	2.44	0.47
1:I:248:TYR:HB2	1:J:247:SER:CB	2.44	0.47
1:E:20:ILE:HB	1:E:149:THR:HG22	1.96	0.47
1:B:294:ASP:HB2	1:B:297:ILE:HG22	1.96	0.47
1:F:145:ILE:HD12	1:F:191:ILE:CG2	2.43	0.47
1:A:95:PHE:HB2	1:A:99:ARG:HG2	1.97	0.47
1:A:295:LEU:HA	1:A:298:GLN:OE1	2.14	0.47
1:H:217:ALA:HA	1:H:220:TRP:CE3	2.50	0.47
1:J:79:ILE:HD13	1:J:79:ILE:HA	1.71	0.47
1:D:185:GLN:N	1:D:185:GLN:OE1	2.48	0.47
1:D:59:GLU:OE2	1:E:75:ALA:HB3	2.15	0.47
1:I:157:ILE:HD13	1:I:157:ILE:HA	1.50	0.47
1:F:244:ALA:HB1	2:F:402:377:H21	1.95	0.47
1:C:257:PRO:HD2	1:C:258:TYR:CE2	2.49	0.47
1:H:173:ILE:O	1:H:187:GLU:HA	2.14	0.47
1:F:72:TRP:CH2	1:F:74:PRO:HG3	2.50	0.47
1:D:29:LEU:HA	1:D:29:LEU:HD23	1.65	0.47
1:H:38:TYR:CE1	1:H:105:ARG:HD2	2.50	0.47
1:J:38:TYR:CZ	1:J:105:ARG:HD2	2.49	0.47
1:C:304:PHE:HD1	1:C:305:PRO:HD3	1.78	0.47
1:F:28:THR:HB	1:F:256:LEU:CD2	2.45	0.47
1:G:225:LEU:HD21	1:H:232:LEU:HD22	1.96	0.47
1:J:216:ILE:HD12	1:J:269:GLY:HA2	1.96	0.46
1:E:223:PHE:CZ	1:E:304:PHE:HE1	2.33	0.46
1:B:86:ASP:HB3	1:B:107:LEU:HB3	1.97	0.46
1:G:267:ILE:H	1:G:267:ILE:HG12	1.53	0.46
1:G:21:ASN:HB2	1:G:36:ASP:O	2.15	0.46
1:D:178:LEU:HB2	1:D:179:SER:H	1.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:PHE:CE1	1:A:254:PRO:HG3	2.51	0.46
1:G:223:PHE:HE1	1:G:304:PHE:CE1	2.33	0.46
1:J:181:VAL:CG2	1:J:185:GLN:HB2	2.44	0.46
1:H:248:TYR:HB2	1:I:247:SER:CB	2.44	0.46
1:E:304:PHE:HA	1:E:307:GLY:H	1.80	0.46
1:F:295:LEU:HA	1:F:298:GLN:CD	2.36	0.46
1:G:61:THR:HG22	1:G:62:GLN:NE2	2.30	0.46
1:I:299:ARG:C	1:I:301:ARG:H	2.19	0.46
1:E:163:ARG:HA	1:E:163:ARG:HD3	1.68	0.46
1:F:285:HIS:CD2	1:J:224:TRP:HD1	2.32	0.46
1:I:157:ILE:HD11	1:J:117:ARG:CG	2.45	0.46
1:I:72:TRP:CH2	1:I:74:PRO:HG3	2.51	0.46
1:F:227:SER:HB3	1:F:230:GLU:CG	2.45	0.46
1:B:23:ILE:HG21	1:B:126:PHE:CD1	2.50	0.46
1:I:273:ILE:O	1:I:277:ILE:HG12	2.15	0.46
1:B:92:LEU:HD23	1:B:92:LEU:HA	1.74	0.46
1:B:169:HIS:ND1	1:I:168:THR:HG22	2.31	0.46
1:E:145:ILE:HD12	1:E:191:ILE:HG23	1.98	0.46
1:E:92:LEU:HA	1:E:92:LEU:HD23	1.73	0.46
1:D:205:LEU:HA	1:D:205:LEU:HD23	1.47	0.46
1:G:185:GLN:OE1	1:G:185:GLN:N	2.49	0.46
1:D:148:TYR:HD2	1:D:148:TYR:N	2.13	0.46
1:B:168:THR:HG22	1:B:169:HIS:N	2.30	0.46
1:D:84:SER:HA	1:D:85:PRO:HD3	1.73	0.46
1:H:93:MET:HG2	1:H:95:PHE:CE1	2.51	0.46
1:G:176:ASP:HB2	1:G:177:HIS:CE1	2.51	0.46
1:F:36:ASP:CG	1:F:105:ARG:HH21	2.17	0.46
1:B:95:PHE:CD1	1:B:99:ARG:HG3	2.50	0.46
1:A:105:ARG:NH2	1:B:81:VAL:O	2.49	0.46
1:D:145:ILE:HD12	1:D:191:ILE:CG2	2.46	0.46
1:B:224:TRP:CE2	1:B:301:ARG:HD3	2.50	0.46
1:B:293:ASP:O	1:B:295:LEU:N	2.49	0.46
1:B:157:ILE:HD11	1:C:117:ARG:HE	1.80	0.46
1:J:115:ASP:OD1	1:J:117:ARG:HG3	2.16	0.46
1:D:61:THR:HG22	1:D:62:GLN:NE2	2.31	0.46
1:J:220:TRP:HZ2	1:J:308:PHE:CD2	2.34	0.46
1:G:157:ILE:HD13	1:G:157:ILE:HA	1.66	0.46
1:D:144:ASP:OD2	1:D:146:GLN:NE2	2.49	0.46
1:C:58:VAL:HB	1:C:92:LEU:HB2	1.98	0.46
1:J:145:ILE:HG23	1:J:168:THR:CG2	2.46	0.46
1:I:38:TYR:CD2	2:J:401:377:H1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:131:GLU:OE1	1:J:190:ARG:NH2	2.41	0.46
1:A:291:VAL:O	1:A:293:ASP:N	2.49	0.46
1:D:157:ILE:HA	1:D:157:ILE:HD13	1.51	0.46
1:A:72:TRP:CH2	1:A:74:PRO:HG3	2.51	0.46
1:D:210:LEU:HB3	1:D:211:PRO:HD3	1.98	0.45
1:J:185:GLN:OE1	1:J:185:GLN:N	2.49	0.45
1:J:61:THR:HG22	1:J:62:GLN:HE21	1.81	0.45
1:A:145:ILE:HD12	1:A:191:ILE:CG2	2.46	0.45
1:G:279:LEU:HA	1:G:279:LEU:HD23	1.76	0.45
1:F:77:GLU:OE2	1:J:105:ARG:HD3	2.17	0.45
1:F:64:GLU:CG	1:J:61:THR:HG21	2.45	0.45
1:C:93:MET:HG2	1:C:95:PHE:CE1	2.51	0.45
1:B:79:ILE:HD13	1:B:79:ILE:HA	1.76	0.45
1:D:28:THR:HB	1:D:256:LEU:CD2	2.47	0.45
1:B:155:GLU:HB3	1:B:161:TRP:NE1	2.32	0.45
1:I:284:HIS:HD2	1:I:285:HIS:CE1	2.34	0.45
1:A:66:TRP:O	1:A:71:LEU:HB2	2.16	0.45
1:I:38:TYR:CE2	2:J:401:377:H1	2.51	0.45
1:A:91:ARG:HD2	1:B:134:SER:HB3	1.98	0.45
1:C:42:GLN:HG3	1:C:101:ILE:HG12	1.99	0.45
1:F:212:LEU:HD12	1:F:265:MET:HB3	1.99	0.45
1:A:302:LEU:C	1:A:305:PRO:HD2	2.37	0.45
1:H:39:ILE:HG12	1:H:106:PHE:CD2	2.51	0.45
1:J:295:LEU:HA	1:J:298:GLN:OE1	2.17	0.45
1:C:120:PRO:HD2	1:C:121:PHE:CE1	2.52	0.45
1:J:227:SER:OG	1:J:228:PHE:N	2.50	0.45
1:H:263:ASP:O	1:H:267:ILE:HG12	2.17	0.45
1:H:27:ASN:HB3	1:H:32:THR:HB	1.98	0.45
1:C:21:ASN:ND2	1:C:36:ASP:OD2	2.30	0.45
1:I:56:LEU:HD22	1:I:57:ILE:N	2.31	0.45
1:A:224:TRP:CE2	1:A:301:ARG:HD3	2.51	0.45
1:C:61:THR:HG21	1:D:64:GLU:CG	2.47	0.45
1:C:294:ASP:HB2	1:C:297:ILE:CG2	2.44	0.45
1:C:279:LEU:HD23	1:C:279:LEU:HA	1.75	0.45
1:B:205:LEU:HA	1:B:205:LEU:HD23	1.68	0.45
1:J:173:ILE:O	1:J:187:GLU:HA	2.14	0.45
1:E:19:PHE:HD1	1:E:38:TYR:HB2	1.80	0.45
1:I:212:LEU:HD12	1:I:265:MET:HB3	1.98	0.45
1:B:115:ASP:OD1	1:B:117:ARG:HG3	2.17	0.45
1:B:257:PRO:HD2	1:B:258:TYR:CE2	2.52	0.45
1:B:40:VAL:HG13	1:B:103:ASN:OD1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:224:TRP:CZ3	1:J:301:ARG:HB3	2.52	0.45
1:F:173:ILE:HD13	1:F:190:ARG:HB3	1.99	0.45
1:I:28:THR:HG22	1:I:116:PHE:CZ	2.51	0.45
1:I:157:ILE:HD11	1:J:117:ARG:HG3	1.98	0.45
1:D:263:ASP:O	1:D:267:ILE:HG12	2.17	0.45
1:F:33:TYR:CE2	1:F:110:PHE:HB2	2.52	0.45
1:I:227:SER:HB3	1:I:230:GLU:CG	2.47	0.45
1:D:173:ILE:O	1:D:187:GLU:HA	2.16	0.45
1:G:165:LYS:O	1:G:166:ALA:HB3	2.16	0.45
1:B:21:ASN:HB2	1:B:36:ASP:O	2.16	0.45
1:H:221:SER:HB2	1:I:281:ILE:HD11	1.99	0.44
1:B:58:VAL:HG12	1:B:63:ILE:HG12	2.00	0.44
1:B:238:LEU:HD12	1:B:238:LEU:HA	1.72	0.44
1:A:29:LEU:HD23	1:A:29:LEU:HA	1.62	0.44
1:F:84:SER:HA	1:F:85:PRO:HD3	1.74	0.44
1:D:58:VAL:HG12	1:D:63:ILE:HG12	1.99	0.44
1:J:82:VAL:CG2	1:J:111:SER:HB2	2.47	0.44
1:G:136:ASN:CG	1:G:185:GLN:HG3	2.37	0.44
1:B:289:ASN:OD1	1:B:290:GLY:N	2.48	0.44
1:A:205:LEU:HD23	1:A:209:ILE:HG13	1.98	0.44
1:E:23:ILE:HA	1:E:34:LYS:O	2.17	0.44
1:I:299:ARG:NH1	1:I:302:LEU:HB2	2.32	0.44
1:A:145:ILE:HD12	1:A:191:ILE:HG21	1.98	0.44
1:F:228:PHE:CG	1:F:284:HIS:CD2	3.05	0.44
1:C:29:LEU:HD23	1:C:255:ARG:O	2.17	0.44
1:B:227:SER:HB3	1:B:230:GLU:CG	2.48	0.44
1:A:240:LEU:HD13	1:B:240:LEU:HD21	1.98	0.44
1:E:282:PHE:CE1	1:E:286:ARG:HB2	2.53	0.44
1:A:110:PHE:CE2	1:A:128:LEU:HG	2.53	0.44
1:B:66:TRP:HB3	1:B:71:LEU:HD12	1.99	0.44
1:J:28:THR:HG22	1:J:116:PHE:CZ	2.52	0.44
1:E:223:PHE:CZ	1:E:304:PHE:CE1	3.06	0.44
1:C:253:LEU:HG	1:C:254:PRO:HD2	2.00	0.44
1:B:267:ILE:H	1:B:267:ILE:HG12	1.63	0.44
1:F:155:GLU:OE2	1:F:161:TRP:HB3	2.17	0.44
1:H:224:TRP:CH2	1:H:301:ARG:HB3	2.53	0.44
1:D:287:GLN:HB2	1:D:289:ASN:H	1.81	0.44
1:I:23:ILE:HG21	1:I:126:PHE:CD1	2.52	0.44
1:E:61:THR:HG22	1:E:62:GLN:NE2	2.31	0.44
1:E:303:ALA:O	1:E:307:GLY:N	2.50	0.44
1:I:115:ASP:OD2	1:I:117:ARG:NH2	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:216:ILE:O	1:H:219:SER:HB3	2.16	0.44
1:G:212:LEU:O	1:G:212:LEU:HD22	2.18	0.44
1:H:221:SER:OG	1:I:236:PHE:HZ	2.01	0.44
1:B:223:PHE:HE1	1:B:304:PHE:CE1	2.36	0.44
1:I:65:ARG:HD2	1:J:68:ASN:ND2	2.33	0.44
1:C:130:LEU:HB3	1:C:191:ILE:HB	1.99	0.44
1:G:178:LEU:HB2	1:G:179:SER:H	1.42	0.44
1:A:285:HIS:C	1:A:287:GLN:HG3	2.39	0.44
1:A:92:LEU:HA	1:A:92:LEU:HD23	1.70	0.44
1:C:248:TYR:HE1	1:D:250:SER:OG	2.01	0.44
1:F:216:ILE:HD12	1:F:269:GLY:HA2	2.00	0.43
1:J:244:ALA:O	1:J:247:SER:OG	2.23	0.43
1:B:178:LEU:HB2	1:B:179:SER:H	1.55	0.43
1:H:136:ASN:ND2	1:H:139:GLN:OE1	2.51	0.43
1:A:61:THR:HG22	1:A:62:GLN:HE21	1.82	0.43
1:H:224:TRP:CE2	1:H:301:ARG:HD3	2.52	0.43
1:C:235:SER:HA	1:C:238:LEU:HB2	2.00	0.43
1:H:21:ASN:HD21	1:H:38:TYR:HE1	1.64	0.43
1:C:249:THR:CG2	1:C:253:LEU:HD22	2.48	0.43
1:B:38:TYR:HA	1:B:104:ALA:O	2.17	0.43
1:D:66:TRP:HB3	1:D:71:LEU:HD12	1.99	0.43
1:A:31:GLN:HG2	1:A:114:MET:HB2	2.00	0.43
1:A:149:THR:O	1:A:151:ASN:N	2.46	0.43
1:C:33:TYR:CE2	1:C:110:PHE:HB2	2.54	0.43
1:G:79:ILE:HD13	1:G:79:ILE:HA	1.83	0.43
1:B:122:ASP:N	1:B:122:ASP:OD1	2.49	0.43
1:G:289:ASN:ND2	1:G:292:GLU:HB2	2.33	0.43
1:H:212:LEU:CD1	1:H:265:MET:HB3	2.48	0.43
1:F:26:VAL:HG13	1:F:114:MET:HE1	1.99	0.43
1:E:266:ILE:HG22	1:E:270:TYR:CE1	2.52	0.43
1:C:157:ILE:HD13	1:C:157:ILE:HA	1.58	0.43
1:G:149:THR:HB	1:G:151:ASN:CG	2.38	0.43
1:F:132:PRO:HG3	1:F:140:LEU:HD22	2.00	0.43
1:E:294:ASP:O	1:E:298:GLN:HG2	2.18	0.43
1:A:247:SER:CB	1:E:248:TYR:HB2	2.41	0.43
1:F:170:ILE:HA	1:F:190:ARG:O	2.18	0.43
1:H:136:ASN:O	1:H:139:GLN:N	2.44	0.43
1:G:178:LEU:HD21	1:G:186:ASN:HA	2.01	0.43
1:J:155:GLU:HB3	1:J:161:TRP:CD1	2.52	0.43
1:G:155:GLU:HB3	1:G:161:TRP:NE1	2.34	0.43
1:J:299:ARG:C	1:J:301:ARG:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:155:GLU:HB3	1:H:161:TRP:CD1	2.54	0.43
1:A:108:GLY:HA3	1:A:110:PHE:HE1	1.83	0.43
1:F:238:LEU:HD12	1:F:238:LEU:HA	1.79	0.43
1:G:29:LEU:HA	1:G:29:LEU:HD23	1.87	0.43
1:C:295:LEU:HA	1:C:298:GLN:OE1	2.19	0.43
1:C:84:SER:HA	1:C:85:PRO:HD3	1.83	0.43
1:G:208:PHE:CE2	1:G:249:THR:HA	2.54	0.43
1:F:118:LEU:HA	1:F:261:VAL:HG23	1.99	0.43
1:D:81:VAL:HG13	1:D:83:GLY:O	2.19	0.43
1:A:138:GLN:OE1	1:A:184:ASN:HB3	2.19	0.43
1:F:79:ILE:HA	1:F:79:ILE:HD13	1.87	0.43
1:F:299:ARG:HD3	1:F:301:ARG:NH2	2.33	0.43
1:F:28:THR:HG22	1:F:116:PHE:CZ	2.54	0.43
1:G:95:PHE:CD1	1:G:99:ARG:HG3	2.53	0.43
1:J:295:LEU:HD12	1:J:298:GLN:OE1	2.19	0.43
1:H:204:TYR:HD2	1:H:208:PHE:CD1	2.36	0.43
1:H:35:VAL:HG21	1:H:128:LEU:HD11	2.00	0.43
1:D:267:ILE:H	1:D:267:ILE:HG12	1.64	0.43
1:B:285:HIS:C	1:B:287:GLN:HG3	2.39	0.43
1:A:306:LEU:HA	1:A:309:LEU:HB2	2.00	0.43
1:D:235:SER:HA	1:D:238:LEU:HD22	2.01	0.43
1:J:142:PHE:O	1:J:170:ILE:HD13	2.19	0.43
1:I:130:LEU:HA	1:I:130:LEU:HD23	1.70	0.43
1:E:19:PHE:CE2	1:E:148:TYR:CD2	3.07	0.42
1:J:208:PHE:CE2	1:J:248:TYR:CZ	3.06	0.42
1:G:224:TRP:CE2	1:G:301:ARG:HD3	2.53	0.42
1:E:224:TRP:CE2	1:E:301:ARG:HD3	2.54	0.42
1:F:58:VAL:O	1:F:91:ARG:HA	2.18	0.42
1:G:294:ASP:HB3	1:G:297:ILE:H	1.84	0.42
1:F:227:SER:HB3	1:F:230:GLU:HG3	2.01	0.42
1:D:119:PHE:HA	1:D:122:ASP:OD1	2.19	0.42
1:J:304:PHE:HD1	1:J:305:PRO:HD3	1.84	0.42
1:I:33:TYR:OH	1:I:127:VAL:N	2.41	0.42
1:H:205:LEU:HD23	1:H:205:LEU:HA	1.58	0.42
1:I:225:LEU:CD2	1:J:232:LEU:HD22	2.50	0.42
1:B:117:ARG:HG2	1:B:258:TYR:CD1	2.54	0.42
1:H:66:TRP:HB3	1:H:71:LEU:HD12	2.01	0.42
1:B:145:ILE:HD12	1:B:191:ILE:CG2	2.45	0.42
1:E:223:PHE:CE1	1:E:304:PHE:CE1	3.07	0.42
1:B:28:THR:HB	1:B:256:LEU:CD2	2.50	0.42
1:J:132:PRO:HG3	1:J:140:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:GLN:HB2	1:B:289:ASN:H	1.84	0.42
1:D:122:ASP:N	1:D:122:ASP:OD1	2.42	0.42
1:C:223:PHE:HE2	1:C:280:ILE:HG13	1.85	0.42
1:A:134:SER:HB3	1:E:91:ARG:HD2	2.00	0.42
1:A:115:ASP:OD1	1:A:117:ARG:HG3	2.18	0.42
1:I:92:LEU:HA	1:I:92:LEU:HD23	1.83	0.42
1:I:105:ARG:HD3	1:J:77:GLU:OE2	2.19	0.42
1:H:304:PHE:HD1	1:H:305:PRO:HD3	1.83	0.42
1:D:40:VAL:HG13	1:D:103:ASN:HD22	1.83	0.42
1:B:216:ILE:O	1:B:219:SER:HB3	2.20	0.42
1:H:112:ASN:OD1	1:H:113:ASP:N	2.53	0.42
1:H:163:ARG:HA	1:H:163:ARG:HD3	1.69	0.42
1:G:293:ASP:O	1:G:295:LEU:HD12	2.19	0.42
1:F:227:SER:HB3	1:F:230:GLU:CD	2.40	0.42
1:F:205:LEU:HD23	1:F:209:ILE:HG13	2.01	0.42
1:I:163:ARG:HD3	1:I:163:ARG:HA	1.37	0.42
1:B:301:ARG:O	1:B:305:PRO:HG2	2.18	0.42
1:G:212:LEU:HD12	1:G:265:MET:HB3	2.00	0.42
1:J:145:ILE:HD12	1:J:191:ILE:HG23	2.02	0.42
1:A:212:LEU:CD1	1:A:265:MET:HB3	2.49	0.42
1:I:97:ASP:OD1	1:I:99:ARG:HG2	2.19	0.42
1:G:112:ASN:ND2	1:G:125:GLN:O	2.51	0.42
1:C:72:TRP:CH2	1:C:74:PRO:HG3	2.54	0.42
1:J:145:ILE:HG21	1:J:191:ILE:HG12	2.00	0.42
1:H:110:PHE:N	1:H:110:PHE:CD1	2.86	0.42
1:D:285:HIS:O	1:D:287:GLN:HG3	2.19	0.42
1:E:178:LEU:HD13	1:E:181:VAL:HG13	2.02	0.42
1:E:119:PHE:HE1	1:E:199:ARG:NH1	2.17	0.42
1:I:84:SER:HA	1:I:85:PRO:HD3	1.57	0.42
1:E:79:ILE:HA	1:E:79:ILE:HD13	1.78	0.42
1:A:248:TYR:HB2	1:B:247:SER:CB	2.50	0.42
1:B:296:LEU:HD23	1:B:296:LEU:HA	1.81	0.42
1:A:268:ALA:HB1	1:A:308:PHE:CE1	2.55	0.42
1:D:95:PHE:HE1	1:D:101:ILE:CD1	2.33	0.42
1:A:130:LEU:HA	1:A:130:LEU:HD23	1.89	0.42
1:H:209:ILE:HD11	1:H:262:ILE:HG12	2.01	0.42
1:H:61:THR:HG21	1:I:64:GLU:HG3	2.01	0.42
1:D:240:LEU:HD13	1:E:240:LEU:HD21	2.02	0.42
1:A:216:ILE:O	1:A:219:SER:HB3	2.18	0.42
1:F:125:GLN:HG3	1:F:125:GLN:O	2.19	0.42
1:D:305:PRO:O	1:D:309:LEU:HD13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:145:ILE:HD13	1:E:168:THR:HG22	2.01	0.42
1:G:268:ALA:HB1	1:G:308:PHE:CE1	2.54	0.42
1:C:310:ALA:O	1:C:314:VAL:HG23	2.20	0.42
1:H:174:ARG:HA	1:H:186:ASN:O	2.20	0.42
1:I:241:THR:HA	1:J:240:LEU:HD23	2.01	0.42
1:B:56:LEU:HD22	1:B:57:ILE:N	2.35	0.42
1:F:68:ASN:ND2	1:J:65:ARG:HD2	2.35	0.42
1:G:246:ALA:O	1:G:249:THR:HB	2.20	0.42
1:C:28:THR:HB	1:C:256:LEU:HD21	2.02	0.42
1:F:204:TYR:O	1:F:209:ILE:HG12	2.20	0.42
1:J:35:VAL:O	1:J:107:LEU:HD12	2.20	0.42
1:J:58:VAL:HB	1:J:92:LEU:HB2	2.02	0.42
1:D:128:LEU:HB2	1:D:193:VAL:HB	2.02	0.42
1:E:33:TYR:OH	1:E:127:VAL:N	2.37	0.41
1:H:72:TRP:CH2	1:H:140:LEU:HD12	2.55	0.41
1:B:248:TYR:HD1	1:C:247:SER:HA	1.85	0.41
1:H:136:ASN:ND2	1:H:136:ASN:H	2.17	0.41
1:A:157:ILE:HA	1:A:157:ILE:HD13	1.65	0.41
1:C:28:THR:HA	1:C:116:PHE:CE1	2.55	0.41
1:G:204:TYR:O	1:G:209:ILE:HG12	2.20	0.41
1:H:51:PRO:HD2	1:H:56:LEU:HG	2.02	0.41
1:H:212:LEU:O	1:H:212:LEU:HD22	2.20	0.41
1:F:224:TRP:CH2	1:F:301:ARG:HB3	2.55	0.41
1:G:145:ILE:HD12	1:G:191:ILE:HG23	2.02	0.41
1:A:238:LEU:O	1:A:241:THR:HB	2.20	0.41
1:I:277:ILE:HG22	1:I:281:ILE:HD12	2.02	0.41
1:I:260:THR:H	1:I:263:ASP:HB2	1.85	0.41
1:I:178:LEU:HB2	1:I:179:SER:H	1.45	0.41
1:F:304:PHE:HA	1:F:307:GLY:H	1.84	0.41
1:E:48:ARG:HB2	1:E:48:ARG:NH1	2.35	0.41
1:J:204:TYR:HD2	1:J:208:PHE:HD1	1.67	0.41
1:D:19:PHE:HD2	1:D:148:TYR:HB2	1.86	0.41
1:G:62:GLN:O	1:G:66:TRP:HD1	2.04	0.41
1:D:136:ASN:HD21	1:D:185:GLN:HG3	1.84	0.41
1:H:84:SER:HA	1:H:85:PRO:HD3	1.93	0.41
1:J:205:LEU:HD23	1:J:205:LEU:HA	1.57	0.41
1:C:218:ALA:HB2	1:D:274:PHE:CD1	2.54	0.41
1:F:212:LEU:CD1	1:F:265:MET:HB3	2.50	0.41
1:G:65:ARG:NH1	1:H:68:ASN:O	2.53	0.41
1:D:32:THR:HA	1:D:110:PHE:O	2.20	0.41
1:F:241:THR:HA	1:G:240:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:261:VAL:O	1:H:264:GLN:HB2	2.20	0.41
1:B:295:LEU:HD12	1:B:295:LEU:HA	1.76	0.41
1:G:165:LYS:O	1:G:166:ALA:CB	2.68	0.41
1:G:105:ARG:HD3	1:H:77:GLU:OE2	2.20	0.41
1:C:178:LEU:HB2	1:C:179:SER:H	1.39	0.41
1:I:173:ILE:O	1:I:187:GLU:HA	2.20	0.41
1:F:138:GLN:OE1	1:F:184:ASN:HB3	2.21	0.41
1:G:217:ALA:HA	1:G:220:TRP:CE3	2.55	0.41
1:A:136:ASN:HD21	1:A:185:GLN:HG3	1.84	0.41
1:C:212:LEU:HD23	1:C:245:TYR:CD2	2.55	0.41
1:A:285:HIS:CE1	1:E:224:TRP:HD1	2.38	0.41
1:G:62:GLN:OE1	1:G:65:ARG:HD3	2.20	0.41
1:E:145:ILE:HD12	1:E:191:ILE:HG21	2.02	0.41
1:B:44:THR:HA	1:B:99:ARG:HA	2.03	0.41
1:D:145:ILE:O	1:D:145:ILE:HG23	2.21	0.41
1:F:262:ILE:O	1:F:266:ILE:HG12	2.21	0.41
1:J:306:LEU:O	1:J:309:LEU:HB2	2.20	0.41
1:E:93:MET:HG2	1:E:95:PHE:CE1	2.56	0.41
1:D:279:LEU:HD23	1:D:279:LEU:HA	1.67	0.41
1:I:39:ILE:HD13	1:I:39:ILE:HG21	1.87	0.41
1:E:21:ASN:HB2	1:E:36:ASP:OD2	2.19	0.41
1:G:224:TRP:HD1	1:H:285:HIS:CE1	2.38	0.41
1:A:208:PHE:HE2	1:A:248:TYR:CE2	2.39	0.41
1:A:105:ARG:HD3	1:B:77:GLU:OE2	2.21	0.41
1:A:178:LEU:HB2	1:A:179:SER:H	1.61	0.41
1:C:142:PHE:HB3	1:C:170:ILE:HD13	2.02	0.41
1:H:29:LEU:HD23	1:H:29:LEU:HA	1.69	0.41
1:H:279:LEU:HD23	1:H:279:LEU:HA	1.75	0.41
1:I:29:LEU:HA	1:I:29:LEU:HD23	1.91	0.41
1:D:146:GLN:HB2	1:D:148:TYR:CE2	2.53	0.41
1:H:33:TYR:OH	1:H:127:VAL:O	2.31	0.41
1:E:61:THR:HG22	1:E:62:GLN:HE21	1.86	0.41
1:H:31:GLN:HB3	1:H:112:ASN:O	2.21	0.41
1:H:72:TRP:HH2	1:H:140:LEU:HD12	1.86	0.41
1:G:173:ILE:N	1:G:173:ILE:HD12	2.36	0.41
1:G:39:ILE:HD11	1:G:78:PHE:CZ	2.56	0.41
1:E:253:LEU:HG	1:E:254:PRO:HD2	2.03	0.41
1:D:151:ASN:O	1:D:152:ALA:HB2	2.21	0.41
1:G:294:ASP:HB2	1:G:297:ILE:CG2	2.51	0.41
1:F:249:THR:CG2	1:F:253:LEU:HD22	2.51	0.41
1:D:136:ASN:HB2	1:D:187:GLU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ASN:ND2	1:A:37:GLY:HA2	2.36	0.41
1:D:120:PRO:HD2	1:D:121:PHE:CD1	2.56	0.41
1:F:234:THR:O	1:F:237:THR:HB	2.21	0.41
1:G:252:ILE:HA	1:G:252:ILE:HD13	1.85	0.41
1:F:118:LEU:O	1:F:121:PHE:N	2.45	0.40
1:H:91:ARG:NH2	1:H:103:ASN:OD1	2.54	0.40
1:G:153:ASP:HB3	1:G:154:ASN:H	1.42	0.40
1:D:256:LEU:HD13	1:D:258:TYR:CE1	2.56	0.40
1:D:105:ARG:HD3	1:E:77:GLU:OE2	2.21	0.40
1:F:157:ILE:HA	1:F:157:ILE:HD13	1.71	0.40
1:F:279:LEU:HD23	1:F:279:LEU:HA	1.91	0.40
1:G:153:ASP:O	1:G:155:GLU:N	2.55	0.40
1:D:116:PHE:HB2	1:D:258:TYR:OH	2.20	0.40
1:D:145:ILE:HD12	1:D:191:ILE:HG23	2.03	0.40
1:J:131:GLU:HA	1:J:132:PRO:HD3	1.99	0.40
1:J:300:CYS:HB2	1:J:303:ALA:HB3	2.03	0.40
1:H:41:ALA:HB3	1:H:102:TYR:HB3	2.03	0.40
1:D:131:GLU:HA	1:D:132:PRO:HD3	1.95	0.40
1:C:61:THR:CG2	1:C:62:GLN:HE21	2.32	0.40
1:D:149:THR:O	1:D:149:THR:OG1	2.26	0.40
1:D:232:LEU:HD12	1:D:281:ILE:HG13	2.03	0.40
1:D:256:LEU:HD13	1:D:258:TYR:HE1	1.87	0.40
1:I:28:THR:HB	1:I:256:LEU:CD2	2.52	0.40
1:I:153:ASP:HB3	1:I:154:ASN:H	1.64	0.40
1:D:13:ASP:HB3	1:D:143:SER:HB3	2.04	0.40
1:A:46:LYS:HA	1:A:47:PRO:HD3	1.89	0.40
1:C:252:ILE:HD13	1:C:252:ILE:HA	1.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	305/307 (99%)	279 (92%)	17 (6%)	9 (3%)	5	35
1	B	305/307 (99%)	275 (90%)	19 (6%)	11 (4%)	4	30
1	C	305/307 (99%)	274 (90%)	23 (8%)	8 (3%)	7	40
1	D	305/307 (99%)	278 (91%)	18 (6%)	9 (3%)	5	35
1	E	305/307 (99%)	280 (92%)	16 (5%)	9 (3%)	5	35
1	F	305/307 (99%)	278 (91%)	18 (6%)	9 (3%)	5	35
1	G	305/307 (99%)	278 (91%)	17 (6%)	10 (3%)	5	32
1	H	305/307 (99%)	277 (91%)	19 (6%)	9 (3%)	5	35
1	I	305/307 (99%)	276 (90%)	22 (7%)	7 (2%)	8	44
1	J	305/307 (99%)	279 (92%)	17 (6%)	9 (3%)	5	35
All	All	3050/3070 (99%)	2774 (91%)	186 (6%)	90 (3%)	5	35

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	153	ASP
1	B	166	ALA
1	C	153	ASP
1	C	166	ALA
1	G	154	ASN
1	G	155	GLU
1	I	150	GLU
1	J	153	ASP
1	A	60	ASN
1	A	153	ASP
1	B	60	ASN
1	B	150	GLU
1	B	295	LEU
1	C	53	ASP
1	D	150	GLU
1	E	150	GLU
1	F	150	GLU
1	F	153	ASP
1	F	294	ASP
1	G	166	ALA
1	G	303	ALA
1	H	60	ASN
1	H	153	ASP
1	H	166	ALA

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Mol	Chain	Res	Type
1	I	60	ASN
1	J	60	ASN
1	A	166	ALA
1	A	294	ASP
1	B	53	ASP
1	B	154	ASN
1	B	303	ALA
1	C	60	ASN
1	C	150	GLU
1	D	53	ASP
1	D	60	ASN
1	D	153	ASP
1	E	53	ASP
1	E	60	ASN
1	F	53	ASP
1	F	60	ASN
1	G	53	ASP
1	G	60	ASN
1	G	150	GLU
1	H	53	ASP
1	H	150	GLU
1	H	303	ALA
1	I	303	ALA
1	J	150	GLU
1	A	53	ASP
1	A	150	GLU
1	E	303	ALA
1	F	303	ALA
1	G	294	ASP
1	H	154	ASN
1	J	53	ASP
1	J	303	ALA
1	A	184	ASN
1	A	304	PHE
1	B	297	ILE
1	C	182	GLN
1	C	303	ALA
1	D	152	ALA
1	D	303	ALA
1	E	153	ASP
1	E	154	ASN
1	E	292	GLU

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Mol	Chain	Res	Type
1	E	304	PHE
1	G	304	PHE
1	H	304	PHE
1	I	53	ASP
1	J	154	ASN
1	C	304	PHE
1	D	182	GLN
1	D	183	PRO
1	D	304	PHE
1	E	182	GLN
1	F	304	PHE
1	I	304	PHE
1	J	294	ASP
1	J	304	PHE
1	A	183	PRO
1	F	182	GLN
1	G	182	GLN
1	H	182	GLN
1	I	183	PRO
1	J	182	GLN
1	B	304	PHE
1	B	182	GLN
1	I	182	GLN
1	F	183	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	274/274 (100%)	242 (88%)	32 (12%)	7	30
1	B	274/274 (100%)	243 (89%)	31 (11%)	7	31
1	C	274/274 (100%)	244 (89%)	30 (11%)	8	33
1	D	274/274 (100%)	242 (88%)	32 (12%)	7	30
1	E	274/274 (100%)	243 (89%)	31 (11%)	7	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	274/274 (100%)	247 (90%)	27 (10%)	10 38
1	G	274/274 (100%)	244 (89%)	30 (11%)	8 33
1	H	274/274 (100%)	242 (88%)	32 (12%)	7 30
1	I	274/274 (100%)	245 (89%)	29 (11%)	8 34
1	J	274/274 (100%)	242 (88%)	32 (12%)	7 30
All	All	2740/2740 (100%)	2434 (89%)	306 (11%)	7 32

All (306) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	32	THR
1	A	39	ILE
1	A	56	LEU
1	A	71	LEU
1	A	103	ASN
1	A	110	PHE
1	A	118	LEU
1	A	122	ASP
1	A	124	GLN
1	A	130	LEU
1	A	145	ILE
1	A	146	GLN
1	A	154	ASN
1	A	157	ILE
1	A	165	LYS
1	A	167	SER
1	A	177	HIS
1	A	178	LEU
1	A	182	GLN
1	A	210	LEU
1	A	212	LEU
1	A	219	SER
1	A	238	LEU
1	A	239	MET
1	A	240	LEU
1	A	248	TYR
1	A	258	TYR
1	A	293	ASP
1	A	294	ASP

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Mol	Chain	Res	Type
1	A	297	ILE
1	A	304	PHE
1	B	29	LEU
1	B	32	THR
1	B	39	ILE
1	B	56	LEU
1	B	71	LEU
1	B	81	VAL
1	B	103	ASN
1	B	118	LEU
1	B	122	ASP
1	B	124	GLN
1	B	130	LEU
1	B	141	ARG
1	B	145	ILE
1	B	146	GLN
1	B	165	LYS
1	B	169	HIS
1	B	174	ARG
1	B	177	HIS
1	B	178	LEU
1	B	182	GLN
1	B	205	LEU
1	B	210	LEU
1	B	212	LEU
1	B	219	SER
1	B	232	LEU
1	B	238	LEU
1	B	239	MET
1	B	240	LEU
1	B	267	ILE
1	B	279	LEU
1	B	304	PHE
1	C	29	LEU
1	C	32	THR
1	C	39	ILE
1	C	56	LEU
1	C	61	THR
1	C	71	LEU
1	C	118	LEU
1	C	122	ASP
1	C	124	GLN

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Mol	Chain	Res	Type
1	C	128	LEU
1	C	130	LEU
1	C	145	ILE
1	C	146	GLN
1	C	154	ASN
1	C	157	ILE
1	C	165	LYS
1	C	167	SER
1	C	168	THR
1	C	177	HIS
1	C	178	LEU
1	C	182	GLN
1	C	210	LEU
1	C	212	LEU
1	C	219	SER
1	C	224	TRP
1	C	238	LEU
1	C	240	LEU
1	C	267	ILE
1	C	299	ARG
1	C	304	PHE
1	D	29	LEU
1	D	39	ILE
1	D	56	LEU
1	D	71	LEU
1	D	103	ASN
1	D	117	ARG
1	D	118	LEU
1	D	122	ASP
1	D	124	GLN
1	D	130	LEU
1	D	145	ILE
1	D	146	GLN
1	D	148	TYR
1	D	149	THR
1	D	157	ILE
1	D	163	ARG
1	D	165	LYS
1	D	167	SER
1	D	168	THR
1	D	174	ARG
1	D	177	HIS

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Mol	Chain	Res	Type
1	D	178	LEU
1	D	182	GLN
1	D	210	LEU
1	D	212	LEU
1	D	219	SER
1	D	238	LEU
1	D	240	LEU
1	D	258	TYR
1	D	267	ILE
1	D	299	ARG
1	D	304	PHE
1	E	29	LEU
1	E	32	THR
1	E	39	ILE
1	E	56	LEU
1	E	71	LEU
1	E	103	ASN
1	E	117	ARG
1	E	118	LEU
1	E	122	ASP
1	E	124	GLN
1	E	130	LEU
1	E	141	ARG
1	E	145	ILE
1	E	146	GLN
1	E	165	LYS
1	E	167	SER
1	E	168	THR
1	E	177	HIS
1	E	178	LEU
1	E	182	GLN
1	E	210	LEU
1	E	212	LEU
1	E	219	SER
1	E	224	TRP
1	E	238	LEU
1	E	240	LEU
1	E	267	ILE
1	E	287	GLN
1	E	291	VAL
1	E	299	ARG
1	E	304	PHE

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Mol	Chain	Res	Type
1	F	29	LEU
1	F	32	THR
1	F	39	ILE
1	F	56	LEU
1	F	61	THR
1	F	71	LEU
1	F	87	THR
1	F	103	ASN
1	F	117	ARG
1	F	118	LEU
1	F	124	GLN
1	F	130	LEU
1	F	145	ILE
1	F	146	GLN
1	F	165	LYS
1	F	167	SER
1	F	177	HIS
1	F	178	LEU
1	F	210	LEU
1	F	212	LEU
1	F	219	SER
1	F	238	LEU
1	F	239	MET
1	F	240	LEU
1	F	248	TYR
1	F	267	ILE
1	F	304	PHE
1	G	29	LEU
1	G	32	THR
1	G	39	ILE
1	G	56	LEU
1	G	71	LEU
1	G	103	ASN
1	G	113	ASP
1	G	118	LEU
1	G	122	ASP
1	G	124	GLN
1	G	130	LEU
1	G	145	ILE
1	G	146	GLN
1	G	167	SER
1	G	174	ARG

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Mol	Chain	Res	Type
1	G	177	HIS
1	G	178	LEU
1	G	182	GLN
1	G	198	VAL
1	G	210	LEU
1	G	212	LEU
1	G	219	SER
1	G	238	LEU
1	G	239	MET
1	G	240	LEU
1	G	267	ILE
1	G	293	ASP
1	G	299	ARG
1	G	304	PHE
1	G	315	LEU
1	H	29	LEU
1	H	32	THR
1	H	39	ILE
1	H	56	LEU
1	H	61	THR
1	H	71	LEU
1	H	103	ASN
1	H	110	PHE
1	H	118	LEU
1	H	122	ASP
1	H	124	GLN
1	H	130	LEU
1	H	145	ILE
1	H	146	GLN
1	H	154	ASN
1	H	165	LYS
1	H	167	SER
1	H	168	THR
1	H	177	HIS
1	H	178	LEU
1	H	182	GLN
1	H	210	LEU
1	H	212	LEU
1	H	219	SER
1	H	224	TRP
1	H	238	LEU
1	H	239	MET

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Mol	Chain	Res	Type
1	H	240	LEU
1	H	291	VAL
1	H	293	ASP
1	H	299	ARG
1	H	304	PHE
1	I	29	LEU
1	I	32	THR
1	I	39	ILE
1	I	56	LEU
1	I	71	LEU
1	I	103	ASN
1	I	122	ASP
1	I	124	GLN
1	I	130	LEU
1	I	145	ILE
1	I	146	GLN
1	I	157	ILE
1	I	165	LYS
1	I	168	THR
1	I	177	HIS
1	I	178	LEU
1	I	182	GLN
1	I	210	LEU
1	I	212	LEU
1	I	219	SER
1	I	238	LEU
1	I	239	MET
1	I	240	LEU
1	I	248	TYR
1	I	258	TYR
1	I	267	ILE
1	I	297	ILE
1	I	299	ARG
1	I	304	PHE
1	J	29	LEU
1	J	32	THR
1	J	39	ILE
1	J	56	LEU
1	J	61	THR
1	J	71	LEU
1	J	103	ASN
1	J	117	ARG

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Mol	Chain	Res	Type
1	J	118	LEU
1	J	122	ASP
1	J	130	LEU
1	J	141	ARG
1	J	145	ILE
1	J	146	GLN
1	J	154	ASN
1	J	163	ARG
1	J	165	LYS
1	J	167	SER
1	J	174	ARG
1	J	177	HIS
1	J	178	LEU
1	J	182	GLN
1	J	210	LEU
1	J	212	LEU
1	J	219	SER
1	J	224	TRP
1	J	238	LEU
1	J	239	MET
1	J	240	LEU
1	J	267	ILE
1	J	299	ARG
1	J	304	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	284	HIS
1	A	285	HIS
1	B	42	GLN
1	C	284	HIS
1	D	103	ASN
1	E	177	HIS
1	E	298	GLN
1	F	136	ASN
1	F	284	HIS
1	F	285	HIS
1	F	298	GLN
1	G	136	ASN
1	H	136	ASN
1	I	89	ASN

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Mol	Chain	Res	Type
1	I	284	HIS
1	I	298	GLN
1	J	285	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 carbohydrates in this entry.

5.6 Ligand geometry

12 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	377	A	401	-	13,15,15	2.47	9 (69%)	22,27,27	1.67	4 (18%)
2	377	A	402	-	13,15,15	3.01	10 (76%)	22,27,27	3.03	11 (50%)
2	377	B	401	-	13,15,15	2.41	10 (76%)	22,27,27	2.05	4 (18%)
2	377	C	401	-	13,15,15	2.58	9 (69%)	22,27,27	2.27	9 (40%)
2	377	C	402	-	13,15,15	2.05	6 (46%)	22,27,27	1.85	5 (22%)
2	377	E	401	-	13,15,15	2.66	11 (84%)	22,27,27	1.78	6 (27%)
2	377	F	401	-	13,15,15	2.39	8 (61%)	22,27,27	1.70	4 (18%)
2	377	F	402	-	13,15,15	3.06	10 (76%)	22,27,27	1.63	3 (13%)
2	377	G	401	-	13,15,15	2.35	9 (69%)	22,27,27	1.59	6 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	377	H	401	-	13,15,15	2.45	9 (69%)	22,27,27	1.85	6 (27%)
2	377	H	402	-	13,15,15	2.36	8 (61%)	22,27,27	1.96	7 (31%)
2	377	J	401	-	13,15,15	2.48	9 (69%)	22,27,27	2.00	7 (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	377	A	401	-	-	0/0/33/33	0/0/3/3
2	377	A	402	-	-	0/0/33/33	0/0/3/3
2	377	B	401	-	-	0/0/33/33	0/0/3/3
2	377	C	401	-	-	0/0/33/33	0/0/3/3
2	377	C	402	-	-	0/0/33/33	0/0/3/3
2	377	E	401	-	-	0/0/33/33	0/0/3/3
2	377	F	401	-	-	0/0/33/33	0/0/3/3
2	377	F	402	-	-	0/0/33/33	0/0/3/3
2	377	G	401	-	-	0/0/33/33	0/0/3/3
2	377	H	401	-	-	0/0/33/33	0/0/3/3
2	377	H	402	-	-	0/0/33/33	0/0/3/3
2	377	J	401	-	-	0/0/33/33	0/0/3/3

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	402	377	C06-C02	-4.49	1.47	1.53
2	A	402	377	C08-C03	-4.34	1.47	1.53
2	A	402	377	C06-C03	-3.86	1.48	1.53
2	F	402	377	C07-C02	-3.81	1.48	1.53
2	F	402	377	C06-C03	-3.80	1.48	1.53
2	F	402	377	C09-C02	-3.76	1.49	1.53
2	F	402	377	C11-C04	-3.63	1.49	1.53
2	J	401	377	C08-C03	-3.63	1.48	1.53
2	A	402	377	C09-C02	-3.60	1.49	1.53
2	C	401	377	C07-C02	-3.60	1.48	1.53
2	H	401	377	C08-C03	-3.53	1.48	1.53
2	E	401	377	C07-C02	-3.52	1.48	1.53
2	F	402	377	C10-C03	-3.49	1.49	1.53
2	C	401	377	C06-C03	-3.47	1.49	1.53
2	F	402	377	C06-C02	-3.43	1.49	1.53
2	C	401	377	C08-C03	-3.38	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	377	C08-C03	-3.33	1.49	1.53
2	F	401	377	C06-C03	-3.32	1.49	1.53
2	B	401	377	C06-C02	-3.30	1.49	1.53
2	E	401	377	C06-C03	-3.29	1.49	1.53
2	H	402	377	C06-C03	-3.27	1.49	1.53
2	G	401	377	C12-C02	-3.27	1.47	1.54
2	F	402	377	C08-C03	-3.24	1.49	1.53
2	A	401	377	C06-C03	-3.19	1.49	1.53
2	A	401	377	C07-C02	-3.13	1.49	1.53
2	E	401	377	C06-C02	-3.12	1.49	1.53
2	H	401	377	C11-C04	-3.12	1.50	1.53
2	C	401	377	C06-C02	-3.11	1.49	1.53
2	A	402	377	C13-C03	-3.11	1.47	1.54
2	F	402	377	C12-C02	-3.09	1.47	1.54
2	C	401	377	C12-C02	-3.05	1.47	1.54
2	C	402	377	C06-C03	-3.04	1.49	1.53
2	H	401	377	C06-C03	-3.04	1.49	1.53
2	A	402	377	C11-C04	-3.03	1.50	1.53
2	F	401	377	C06-C02	-3.03	1.49	1.53
2	A	401	377	C12-C02	-3.01	1.47	1.54
2	B	401	377	C12-C02	-2.99	1.47	1.54
2	G	401	377	C06-C03	-2.99	1.49	1.53
2	H	402	377	C13-C03	-2.99	1.47	1.54
2	G	401	377	C06-C02	-2.97	1.49	1.53
2	J	401	377	C07-C02	-2.96	1.49	1.53
2	A	401	377	C09-C02	-2.95	1.50	1.53
2	J	401	377	C06-C02	-2.94	1.49	1.53
2	E	401	377	C12-C02	-2.94	1.48	1.54
2	H	402	377	C10-C03	-2.93	1.50	1.53
2	A	401	377	C06-C02	-2.93	1.49	1.53
2	F	401	377	C11-C04	-2.93	1.50	1.53
2	J	401	377	C06-C03	-2.91	1.49	1.53
2	E	401	377	C09-C02	-2.87	1.50	1.53
2	A	402	377	C12-C02	-2.87	1.48	1.54
2	B	401	377	C07-C02	-2.86	1.49	1.53
2	H	401	377	C12-C02	-2.86	1.48	1.54
2	H	402	377	C08-C03	-2.86	1.49	1.53
2	F	401	377	C07-C02	-2.85	1.49	1.53
2	J	401	377	C12-C02	-2.80	1.48	1.54
2	H	402	377	C12-C02	-2.78	1.48	1.54
2	B	401	377	C09-C02	-2.73	1.50	1.53
2	F	401	377	C12-C02	-2.70	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	402	377	C13-C03	-2.69	1.48	1.54
2	G	401	377	C10-C03	-2.66	1.50	1.53
2	C	402	377	C06-C02	-2.61	1.50	1.53
2	J	401	377	C13-C03	-2.61	1.48	1.54
2	F	401	377	C09-C02	-2.57	1.50	1.53
2	A	401	377	C10-C03	-2.56	1.50	1.53
2	G	401	377	C13-C03	-2.56	1.48	1.54
2	A	402	377	C10-C03	-2.53	1.50	1.53
2	H	401	377	C09-C02	-2.52	1.50	1.53
2	B	401	377	C11-C04	-2.52	1.51	1.53
2	B	401	377	C08-C03	-2.51	1.50	1.53
2	A	401	377	C08-C03	-2.50	1.50	1.53
2	J	401	377	C10-C03	-2.49	1.50	1.53
2	H	402	377	C06-C02	-2.49	1.50	1.53
2	C	402	377	C12-C02	-2.46	1.49	1.54
2	H	401	377	C06-C02	-2.46	1.50	1.53
2	E	401	377	C13-C03	-2.43	1.49	1.54
2	F	401	377	C10-C03	-2.43	1.50	1.53
2	A	401	377	C13-C03	-2.38	1.49	1.54
2	G	401	377	C11-C04	-2.37	1.51	1.53
2	H	401	377	C07-C02	-2.37	1.50	1.53
2	A	401	377	C11-C04	-2.36	1.51	1.53
2	C	402	377	C07-C02	-2.34	1.50	1.53
2	B	401	377	C13-C03	-2.32	1.49	1.54
2	G	401	377	C09-C02	-2.31	1.50	1.53
2	B	401	377	C10-C03	-2.31	1.50	1.53
2	H	402	377	C09-C02	-2.31	1.50	1.53
2	G	401	377	C07-C02	-2.30	1.50	1.53
2	E	401	377	C11-C04	-2.29	1.51	1.53
2	E	401	377	C10-C03	-2.27	1.50	1.53
2	F	402	377	C09-C05	-2.26	1.48	1.54
2	C	402	377	C13-C03	-2.26	1.49	1.54
2	G	401	377	C08-C03	-2.26	1.50	1.53
2	J	401	377	C09-C05	-2.25	1.48	1.54
2	A	402	377	C09-C05	-2.24	1.48	1.54
2	C	401	377	C11-C04	-2.23	1.51	1.53
2	H	402	377	C07-C02	-2.22	1.50	1.53
2	C	401	377	C09-C02	-2.18	1.51	1.53
2	C	401	377	C11-C05	-2.17	1.48	1.54
2	H	401	377	C09-C05	-2.17	1.48	1.54
2	B	401	377	C06-C03	-2.14	1.50	1.53
2	H	401	377	C10-C03	-2.13	1.51	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	377	C09-C05	-2.13	1.48	1.54
2	E	401	377	C04-N01	-2.11	1.42	1.49
2	C	402	377	C10-C03	-2.10	1.51	1.53
2	A	402	377	C10-C05	-2.05	1.48	1.54
2	F	401	377	C11-C05	-2.05	1.48	1.54
2	E	401	377	C09-C05	-2.05	1.48	1.54
2	B	401	377	C09-C05	-2.04	1.48	1.54
2	J	401	377	C11-C05	-2.01	1.48	1.54

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	402	377	C12-C02-C09	-5.83	103.23	110.36
2	B	401	377	C12-C02-C09	-4.39	105.00	110.36
2	A	402	377	C08-C04-N01	-4.30	102.28	110.10
2	C	401	377	C11-C05-C09	-3.74	104.56	109.44
2	A	402	377	C02-C09-C05	-3.65	107.74	110.48
2	E	401	377	C10-C05-C09	-3.50	104.87	109.44
2	F	402	377	C12-C02-C07	-3.44	105.31	110.69
2	H	401	377	C11-C05-C09	-3.35	105.07	109.44
2	J	401	377	C12-C02-C09	-3.28	106.36	110.36
2	J	401	377	C13-C03-C08	-3.21	105.67	110.69
2	H	402	377	C12-C02-C06	-3.14	105.79	110.69
2	C	401	377	C13-C03-C08	-3.12	105.81	110.69
2	A	401	377	C12-C02-C06	-3.12	105.81	110.69
2	G	401	377	C02-C09-C05	-3.11	108.15	110.48
2	F	401	377	C13-C03-C06	-3.07	105.89	110.69
2	E	401	377	C12-C02-C07	-2.90	106.16	110.69
2	H	402	377	C10-C05-C09	-2.83	105.75	109.44
2	F	401	377	C12-C02-C06	-2.78	106.35	110.69
2	F	401	377	C07-C04-N01	-2.73	105.14	110.10
2	A	402	377	C13-C03-C08	-2.70	106.48	110.69
2	C	402	377	C08-C03-C06	-2.65	105.77	109.06
2	C	401	377	C12-C02-C06	-2.63	106.58	110.69
2	J	401	377	C11-C05-C09	-2.60	106.06	109.44
2	E	401	377	C13-C03-C08	-2.58	106.65	110.69
2	F	402	377	C02-C09-C05	-2.55	108.56	110.48
2	G	401	377	C12-C02-C06	-2.49	106.81	110.69
2	H	402	377	C13-C03-C08	-2.48	106.82	110.69
2	C	401	377	C07-C04-N01	-2.45	105.63	110.10
2	G	401	377	C12-C02-C09	-2.43	107.39	110.36
2	H	402	377	C06-C03-C10	-2.38	107.06	108.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	377	C13-C03-C10	-2.37	107.47	110.36
2	C	401	377	C06-C03-C10	-2.36	107.07	108.82
2	A	402	377	C03-C06-C02	-2.34	104.75	111.85
2	H	401	377	C12-C02-C07	-2.32	107.07	110.69
2	A	402	377	C13-C03-C10	-2.28	107.58	110.36
2	C	402	377	C12-C02-C06	-2.17	107.30	110.69
2	A	402	377	C10-C05-C09	-2.17	106.61	109.44
2	A	401	377	C03-C10-C05	-2.13	108.88	110.48
2	E	401	377	C07-C04-N01	-2.05	106.37	110.10
2	H	401	377	C11-C04-N01	-2.03	106.41	110.10
2	C	401	377	C04-C11-C05	2.03	112.28	109.92
2	H	402	377	C08-C03-C06	2.12	111.69	109.06
2	H	401	377	C06-C02-C07	2.14	111.72	109.06
2	H	402	377	C08-C03-C10	2.30	110.53	108.82
2	G	401	377	C08-C03-C10	2.44	110.63	108.82
2	C	402	377	C06-C03-C10	2.50	110.67	108.82
2	J	401	377	C03-C10-C05	2.54	112.38	110.48
2	C	402	377	C07-C02-C09	2.58	110.73	108.82
2	G	401	377	C06-C02-C09	2.62	110.76	108.82
2	J	401	377	C08-C03-C10	2.76	110.87	108.82
2	G	401	377	C07-C02-C09	2.80	110.90	108.82
2	E	401	377	C08-C03-C10	2.87	110.95	108.82
2	H	401	377	C08-C03-C10	3.07	111.10	108.82
2	A	402	377	C06-C02-C09	3.09	111.11	108.82
2	E	401	377	C07-C02-C09	3.16	111.17	108.82
2	C	401	377	C13-C03-C10	3.17	114.23	110.36
2	C	401	377	C08-C03-C10	3.69	111.56	108.82
2	A	401	377	C08-C03-C10	3.77	111.62	108.82
2	A	401	377	C06-C02-C09	3.83	111.67	108.82
2	J	401	377	C06-C02-C09	3.95	111.75	108.82
2	F	402	377	C07-C02-C09	4.04	111.82	108.82
2	J	401	377	C07-C02-C09	4.16	111.91	108.82
2	F	401	377	C06-C02-C09	4.36	112.06	108.82
2	H	401	377	C07-C02-C09	4.74	112.34	108.82
2	B	401	377	C06-C03-C10	4.81	112.39	108.82
2	A	402	377	C07-C04-N01	4.93	119.07	110.10
2	A	402	377	C06-C03-C10	5.02	112.55	108.82
2	H	402	377	C06-C02-C09	5.18	112.66	108.82
2	C	402	377	C08-C03-C10	5.21	112.68	108.82
2	B	401	377	C07-C02-C09	5.48	112.88	108.82
2	C	401	377	C06-C02-C09	5.54	112.93	108.82
2	A	402	377	C07-C02-C09	6.44	113.60	108.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	377	2	0
2	B	401	377	1	0
2	C	401	377	1	0
2	C	402	377	1	0
2	F	402	377	3	0
2	H	402	377	2	0
2	J	401	377	3	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, 95^{th} 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	307/307 (100%)	-0.10	15 (4%)	33	20	74, 118, 193, 267	0
1	B	307/307 (100%)	0.03	10 (3%)	50	35	74, 103, 203, 322	0
1	C	307/307 (100%)	-0.07	21 (6%)	20	11	66, 102, 199, 249	0
1	D	307/307 (100%)	-0.20	10 (3%)	50	35	69, 101, 200, 262	0
1	E	307/307 (100%)	-0.18	13 (4%)	40	26	77, 113, 191, 247	0
1	F	307/307 (100%)	-0.08	19 (6%)	24	13	76, 116, 204, 258	0
1	G	307/307 (100%)	-0.04	21 (6%)	20	11	69, 105, 188, 269	0
1	H	307/307 (100%)	-0.09	20 (6%)	22	12	72, 110, 216, 256	0
1	I	307/307 (100%)	-0.15	15 (4%)	33	20	70, 107, 203, 302	0
1	J	307/307 (100%)	-0.20	13 (4%)	40	26	80, 119, 214, 266	0
All	All	3070/3070 (100%)	-0.11	157 (5%)	32	18	66, 110, 204, 322	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	290	GLY	15.8
1	C	180	SER	12.7
1	E	290	GLY	12.5
1	I	180	SER	9.5
1	I	182	GLN	8.8
1	E	291	VAL	8.0
1	H	180	SER	7.9
1	I	290	GLY	7.8
1	I	181	VAL	7.6
1	B	291	VAL	7.6
1	B	289	ASN	7.3
1	C	314	VAL	7.3
1	A	175	TYR	7.0

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Mol	Chain	Res	Type	RSRZ
1	H	179	SER	6.9
1	C	316	VAL	6.7
1	C	317	ILE	6.6
1	I	289	ASN	6.5
1	H	181	VAL	6.3
1	C	306	LEU	6.3
1	I	179	SER	6.1
1	B	179	SER	5.9
1	E	180	SER	5.8
1	B	180	SER	5.8
1	G	288	ALA	5.8
1	A	176	ASP	5.7
1	C	309	LEU	5.6
1	F	176	ASP	5.6
1	F	288	ALA	5.5
1	D	180	SER	5.4
1	F	182	GLN	5.3
1	I	288	ALA	5.1
1	C	313	CYS	5.0
1	E	289	ASN	4.9
1	C	179	SER	4.9
1	C	315	LEU	4.8
1	F	287	GLN	4.8
1	C	289	ASN	4.7
1	C	291	VAL	4.6
1	F	291	VAL	4.6
1	F	179	SER	4.4
1	A	177	HIS	4.3
1	D	179	SER	4.2
1	G	289	ASN	4.2
1	H	289	ASN	4.2
1	F	178	LEU	4.2
1	B	293	ASP	4.0
1	E	287	GLN	4.0
1	J	306	LEU	3.9
1	F	175	TYR	3.9
1	G	313	CYS	3.9
1	F	285	HIS	3.8
1	E	179	SER	3.7
1	A	153	ASP	3.7
1	I	291	VAL	3.6
1	C	290	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	288	ALA	3.6
1	F	177	HIS	3.6
1	H	312	GLY	3.5
1	H	140	LEU	3.5
1	H	306	LEU	3.5
1	G	298	GLN	3.5
1	D	297	ILE	3.5
1	G	295	LEU	3.5
1	H	314	VAL	3.4
1	E	49	LYS	3.4
1	H	178	LEU	3.3
1	H	317	ILE	3.3
1	J	179	SER	3.3
1	C	308	PHE	3.3
1	G	179	SER	3.3
1	F	49	LYS	3.2
1	E	53	ASP	3.2
1	J	289	ASN	3.2
1	G	282	PHE	3.2
1	C	288	ALA	3.1
1	F	317	ILE	3.1
1	A	297	ILE	3.1
1	A	156	GLU	3.1
1	J	305	PRO	3.0
1	G	314	VAL	3.0
1	H	141	ARG	3.0
1	F	180	SER	3.0
1	J	307	GLY	3.0
1	G	293	ASP	3.0
1	I	154	ASN	2.9
1	G	296	LEU	2.9
1	H	315	LEU	2.9
1	I	153	ASP	2.9
1	F	183	PRO	2.9
1	D	291	VAL	2.9
1	H	307	GLY	2.9
1	F	290	GLY	2.8
1	C	307	GLY	2.8
1	H	309	LEU	2.8
1	C	310	ALA	2.8
1	B	297	ILE	2.7
1	D	296	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	317	ILE	2.7
1	E	182	GLN	2.7
1	A	313	CYS	2.7
1	G	312	GLY	2.7
1	J	302	LEU	2.7
1	J	182	GLN	2.7
1	G	180	SER	2.7
1	A	302	LEU	2.6
1	C	303	ALA	2.6
1	H	308	PHE	2.6
1	A	315	LEU	2.6
1	H	291	VAL	2.6
1	G	285	HIS	2.6
1	F	286	ARG	2.5
1	C	302	LEU	2.5
1	I	315	LEU	2.5
1	J	303	ALA	2.5
1	G	315	LEU	2.5
1	A	290	GLY	2.5
1	H	311	ILE	2.5
1	G	126	PHE	2.5
1	F	316	VAL	2.4
1	C	312	GLY	2.4
1	D	290	GLY	2.4
1	J	304	PHE	2.4
1	I	287	GLN	2.4
1	G	292	GLU	2.4
1	C	311	ILE	2.4
1	F	174	ARG	2.4
1	H	182	GLN	2.3
1	H	185	GLN	2.3
1	E	315	LEU	2.3
1	I	285	HIS	2.3
1	A	158	ASP	2.3
1	D	178	LEU	2.3
1	G	311	ILE	2.3
1	A	188	PHE	2.3
1	J	288	ALA	2.3
1	I	183	PRO	2.3
1	B	317	ILE	2.3
1	A	312	GLY	2.2
1	F	315	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	314	VAL	2.2
1	G	156	GLU	2.2
1	G	310	ALA	2.2
1	G	306	LEU	2.1
1	E	184	ASN	2.1
1	J	49	LYS	2.1
1	J	181	VAL	2.1
1	G	125	GLN	2.1
1	D	292	GLU	2.1
1	H	290	GLY	2.1
1	D	153	ASP	2.1
1	C	305	PRO	2.1
1	E	288	ALA	2.1
1	I	317	ILE	2.0
1	D	295	LEU	2.0
1	J	180	SER	2.0
1	B	287	GLN	2.0
1	E	314	VAL	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	377	C	401	13/13	0.98	0.43	2.90	92,97,106,108	0
2	377	A	402	13/13	0.94	0.34	2.00	95,102,109,113	0
2	377	F	402	13/13	0.95	0.27	1.45	116,119,130,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	377	E	401	13/13	0.96	0.31	1.34	92,97,104,105	0
2	377	J	401	13/13	0.97	0.31	1.05	91,97,98,99	0
2	377	G	401	13/13	0.96	0.22	0.81	105,108,116,117	0
2	377	A	401	13/13	0.95	0.49	0.81	130,135,138,138	0
2	377	F	401	13/13	0.94	0.38	0.59	111,115,119,121	0
2	377	C	402	13/13	0.96	0.26	0.38	84,88,91,91	0
2	377	H	401	13/13	0.93	0.27	0.19	106,113,120,120	0
2	377	B	401	13/13	0.95	0.23	0.14	101,105,109,115	0
2	377	H	402	13/13	0.95	0.22	0.06	96,101,107,107	0

6.5 Other polymers (i)

There are no such residues in this entry.