



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:29 AM UTC

PDB ID : 4TWD / pdb_00004twd
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

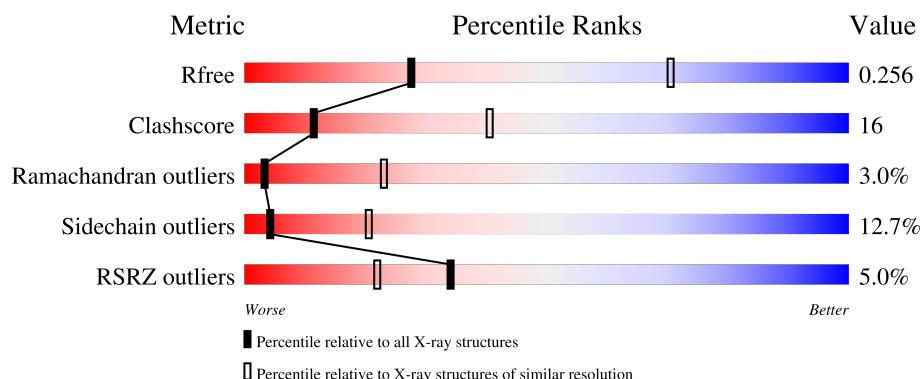
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	307	2% 59% 33% 8%
1	B	307	6% 60% 31% 8%
1	C	307	5% 54% 39% 7%
1	D	307	3% 56% 35% 9%
1	E	307	5% 55% 36% 9%

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Mol	Chain	Length	Quality of chain
1	F	307	5% 55% 37% 8%
1	G	307	8% 55% 37% 7%
1	H	307	5% 57% 35% 7%
1	I	307	6% 59% 33% 6%
1	J	307	5% 59% 35% 6%

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:

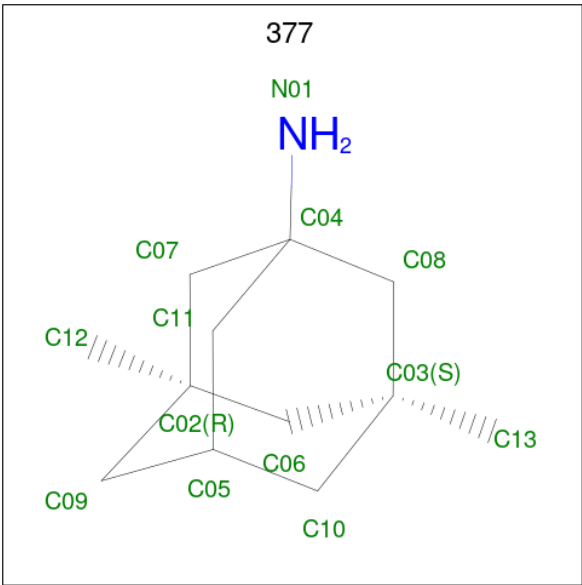
Chain	Residue	Modelled	Actual	Comment	Reference
A	152	ALA	ILE	conflict	UNP P0C7B7
A	164	GLY	-	insertion	UNP P0C7B7
A	247	SER	PHE	engineered mutation	UNP P0C7B7
A	289	ASN	MET	conflict	UNP P0C7B7
B	152	ALA	ILE	conflict	UNP P0C7B7
B	164	GLY	-	insertion	UNP P0C7B7
B	247	SER	PHE	engineered mutation	UNP P0C7B7
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 (CCD ID: 377) (formula: C₁₂H₂₁N).

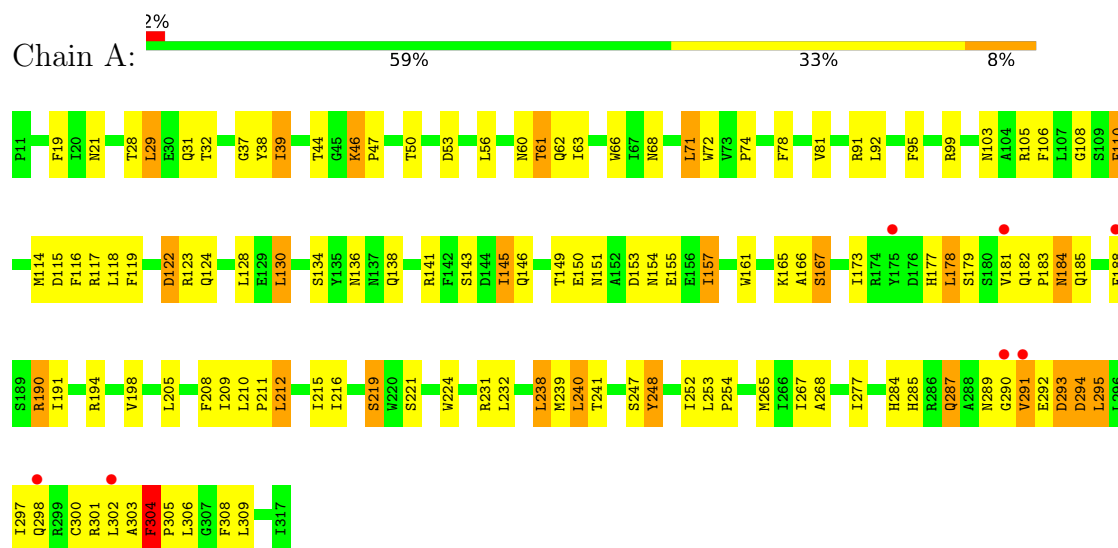


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			13	12	1		
2	A	1	Total	C	N	0	0
			13	12	1		
2	B	1	Total	C	N	0	0
			13	12	1		
2	C	1	Total	C	N	0	0
			13	12	1		
2	C	1	Total	C	N	0	0
			13	12	1		
2	E	1	Total	C	N	0	0
			13	12	1		
2	F	1	Total	C	N	0	0
			13	12	1		
2	F	1	Total	C	N	0	0
			13	12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

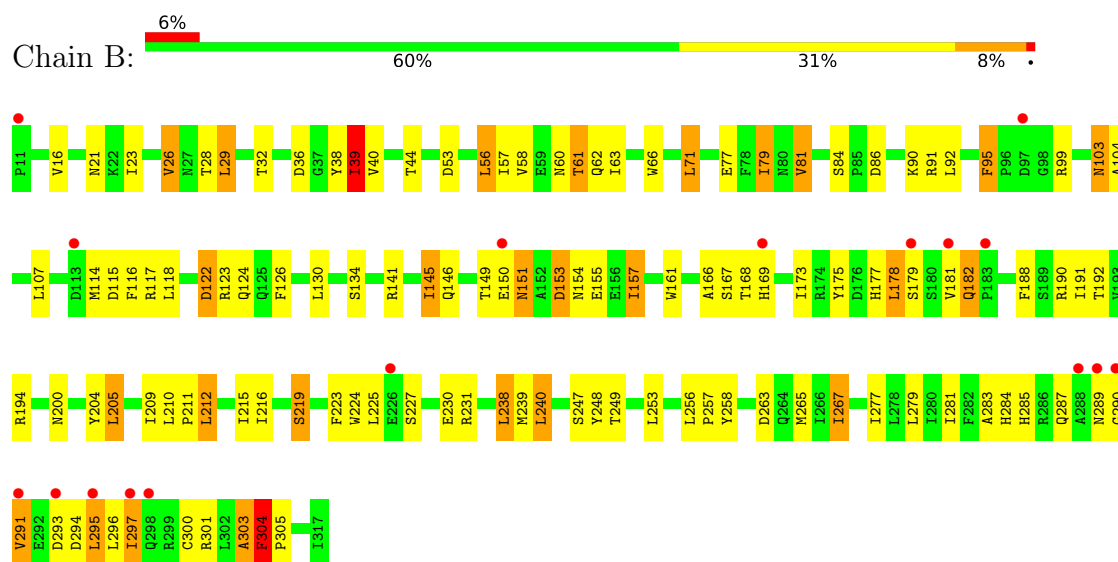
3 Residue-property plots

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

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

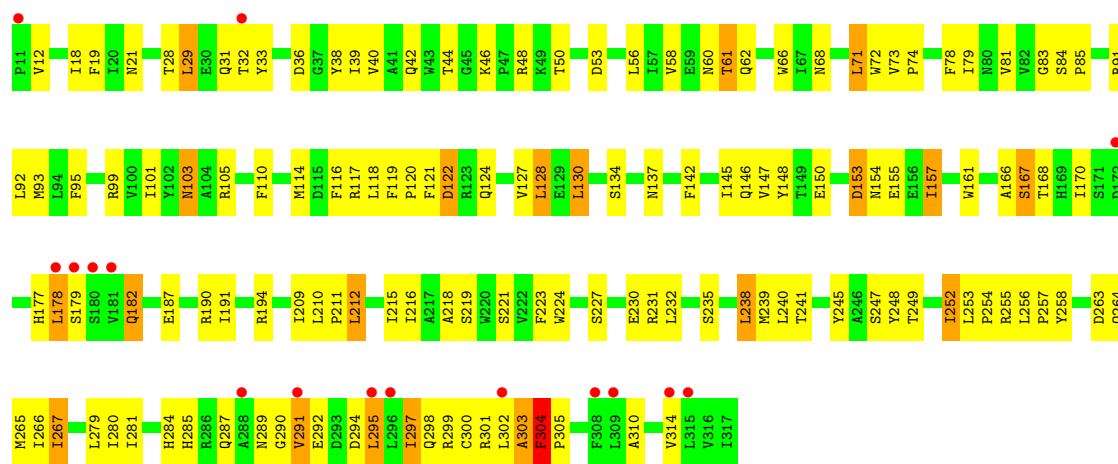


• Molecule 1: Cys-loop ligand-gated ion channel

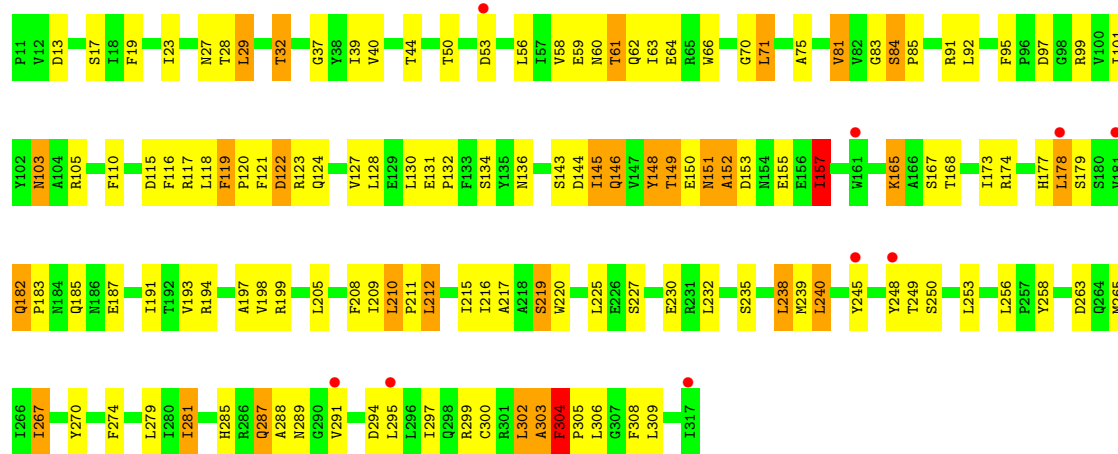


• Molecule 1: Cys-loop ligand-gated ion channel

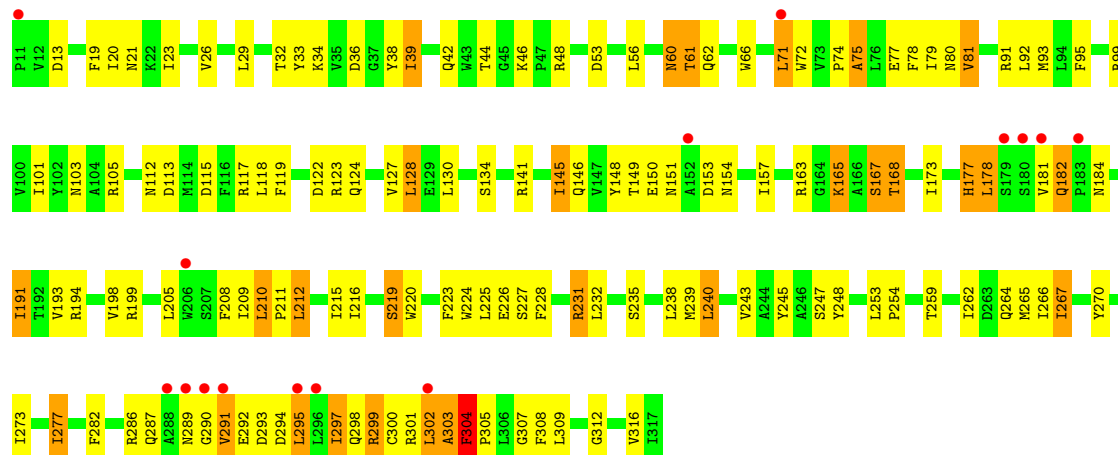




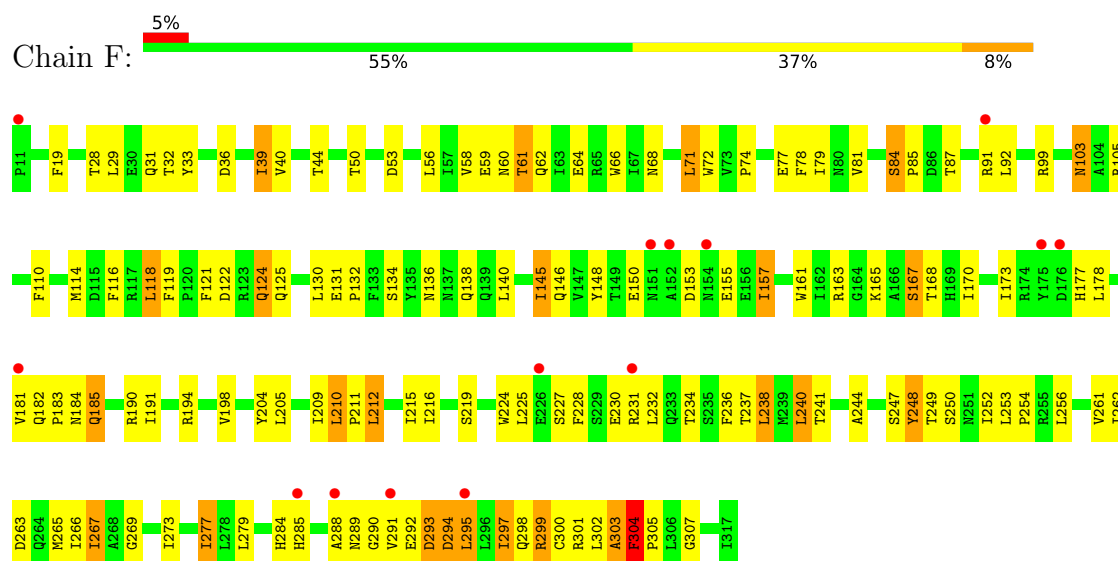
• Molecule 1: Cys-loop ligand-gated ion channel



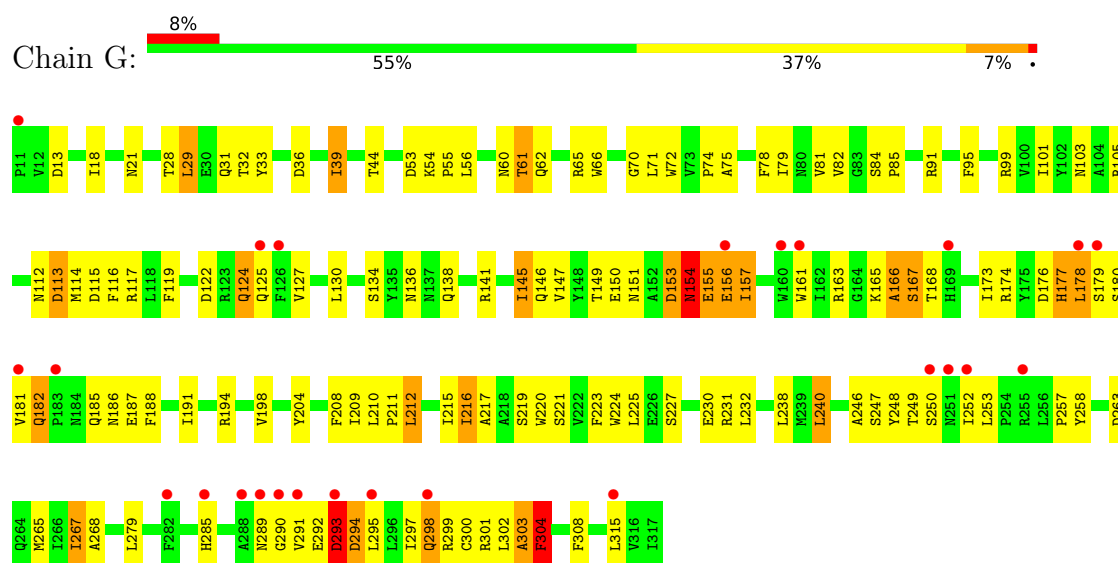
• Molecule 1: Cys-loop ligand-gated ion channel



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

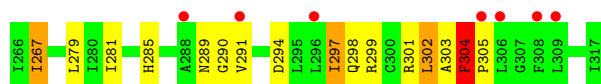


• Molecule 1: Cys-loop ligand-gated ion channel

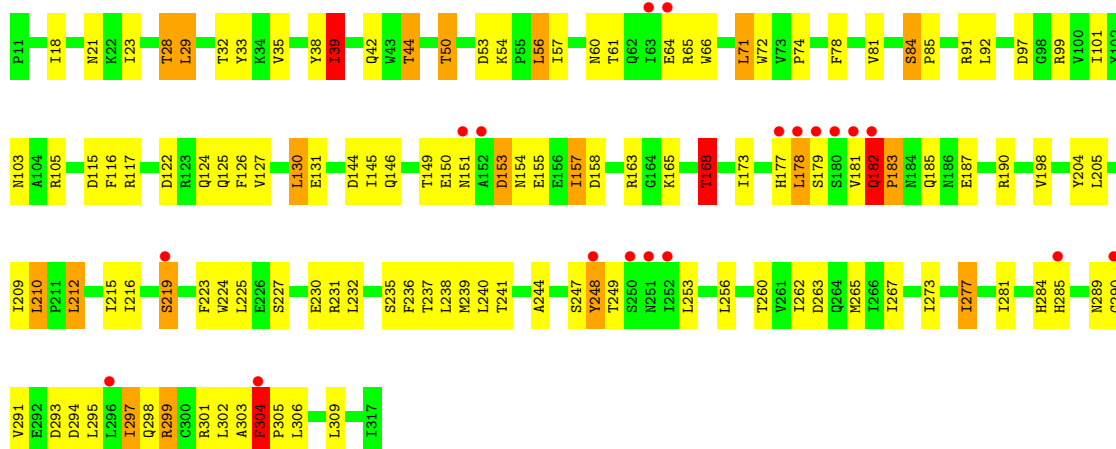


• Molecule 1: Cys-loop ligand-gated ion channel

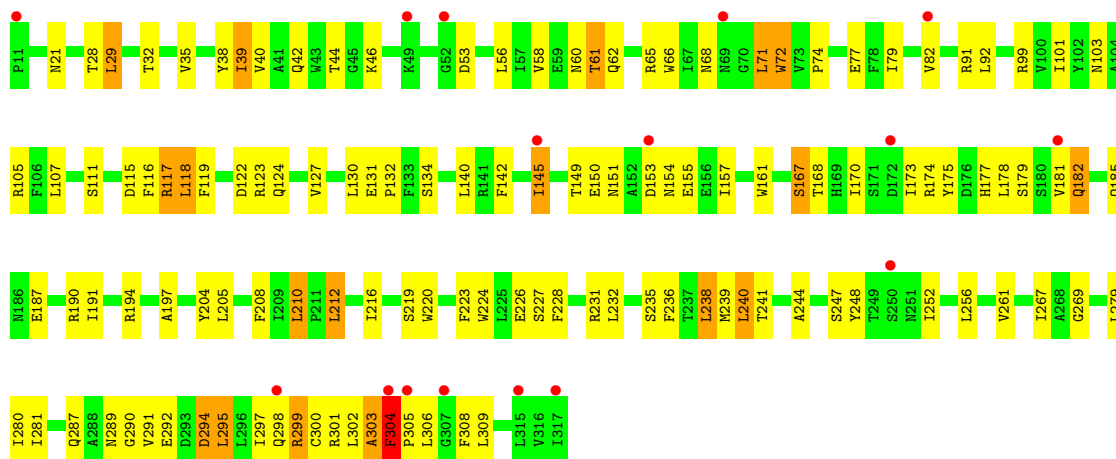




• Molecule 1: Cys-loop ligand-gated ion channel



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



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.199 , 0.252 0.205 , 0.256	Depositor DCC
R_{free} test set	4705 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	84.2	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 59.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	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 3.17% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.73	1/2564 (0.0%)	1.14	6/3495 (0.2%)
1	B	0.84	1/2564 (0.0%)	1.28	16/3495 (0.5%)
1	C	0.85	1/2564 (0.0%)	1.22	10/3495 (0.3%)
1	D	0.85	1/2564 (0.0%)	1.24	20/3495 (0.6%)
1	E	0.74	0/2564	1.18	15/3495 (0.4%)
1	F	0.69	0/2564	1.11	9/3495 (0.3%)
1	G	0.82	0/2564	1.25	21/3495 (0.6%)
1	H	0.75	0/2564	1.16	15/3495 (0.4%)
1	I	0.76	0/2564	1.16	13/3495 (0.4%)
1	J	0.71	0/2564	1.09	7/3495 (0.2%)
All	All	0.78	4/25640 (0.0%)	1.19	132/34950 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	81	VAL	CA-C	5.42	1.58	1.52
1	B	26	VAL	CA-CB	-5.32	1.47	1.54
1	A	252	ILE	CA-CB	-5.22	1.48	1.54
1	C	266	ILE	CA-CB	-5.18	1.48	1.54

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	84	SER	CA-C-N	9.32	129.27	119.85
1	I	84	SER	C-N-CA	9.32	129.27	119.85
1	G	84	SER	CA-C-N	9.20	128.96	119.76
1	G	84	SER	C-N-CA	9.20	128.96	119.76
1	E	165	LYS	N-CA-C	-9.11	101.31	108.78
1	D	155	GLU	N-CA-C	8.80	120.88	111.28
1	F	304	PHE	CA-C-N	-8.70	109.37	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	304	PHE	C-N-CA	-8.70	109.37	118.85
1	A	39	ILE	CB-CA-C	-8.48	99.02	110.98
1	E	304	PHE	CA-C-N	-8.07	110.05	118.85
1	E	304	PHE	C-N-CA	-8.07	110.05	118.85
1	G	153	ASP	N-CA-C	7.93	123.91	109.32
1	G	153	ASP	CB-CA-C	-7.80	106.51	115.79
1	F	165	LYS	N-CA-C	-7.70	97.71	109.95
1	G	163	ARG	CA-C-N	-7.53	114.81	122.27
1	G	163	ARG	C-N-CA	-7.53	114.81	122.27
1	F	84	SER	CA-C-N	7.36	127.28	119.85
1	F	84	SER	C-N-CA	7.36	127.28	119.85
1	C	12	VAL	N-CA-C	7.34	118.84	108.93
1	J	39	ILE	CB-CA-C	-7.15	100.51	111.31
1	C	287	GLN	N-CA-C	7.10	118.54	108.74
1	A	252	ILE	N-CA-C	7.09	117.64	111.90
1	C	46	LYS	N-CA-C	-7.05	101.18	109.93
1	E	287	GLN	N-CA-C	6.85	119.17	108.96
1	C	50	THR	CA-C-N	6.82	127.22	119.93
1	C	50	THR	C-N-CA	6.82	127.22	119.93
1	D	84	SER	CA-C-N	6.79	126.70	119.85
1	D	84	SER	C-N-CA	6.79	126.70	119.85
1	D	165	LYS	N-CA-C	-6.69	102.51	110.41
1	A	46	LYS	CA-C-N	6.58	126.61	119.90
1	A	46	LYS	C-N-CA	6.58	126.61	119.90
1	B	84	SER	CA-C-N	6.47	126.39	119.85
1	B	84	SER	C-N-CA	6.47	126.39	119.85
1	I	210	LEU	CA-C-N	-6.40	111.94	119.05
1	I	210	LEU	C-N-CA	-6.40	111.94	119.05
1	B	249	THR	N-CA-C	6.36	117.88	111.07
1	I	39	ILE	CB-CA-C	-6.30	101.79	111.31
1	H	302	LEU	N-CA-C	-6.29	106.14	113.88
1	I	168	THR	N-CA-C	6.29	118.98	109.23
1	B	95	PHE	CA-C-N	6.28	125.84	119.19
1	B	95	PHE	C-N-CA	6.28	125.84	119.19
1	G	168	THR	N-CA-C	6.23	118.88	109.23
1	J	72	TRP	CA-C-N	-6.23	116.40	123.25
1	J	72	TRP	C-N-CA	-6.23	116.40	123.25
1	E	210	LEU	CA-C-N	-6.22	112.44	119.28
1	E	210	LEU	C-N-CA	-6.22	112.44	119.28
1	E	60	ASN	N-CA-C	6.07	123.72	110.80
1	J	226	GLU	N-CA-C	6.03	117.65	111.14
1	B	39	ILE	CB-CA-C	-6.00	102.52	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	298	GLN	N-CA-C	-5.96	105.27	112.54
1	E	302	LEU	N-CA-C	-5.95	106.35	113.97
1	G	285	HIS	N-CA-C	5.94	120.81	113.50
1	G	253	LEU	CA-C-N	5.92	125.68	119.76
1	G	253	LEU	C-N-CA	5.92	125.68	119.76
1	C	153	ASP	N-CA-C	5.86	123.28	110.80
1	G	298	GLN	N-CA-C	-5.78	105.48	112.54
1	D	287	GLN	N-CA-C	5.75	117.71	109.14
1	E	39	ILE	CB-CA-C	-5.71	102.93	110.98
1	I	237	THR	N-CA-C	-5.70	105.06	111.28
1	B	200	ASN	CA-C-N	5.68	126.55	120.47
1	B	200	ASN	C-N-CA	5.68	126.55	120.47
1	E	81	VAL	N-CA-C	5.65	116.72	108.58
1	B	151	ASN	N-CA-C	5.61	118.84	110.14
1	D	70	GLY	N-CA-C	5.61	125.22	116.01
1	D	308	PHE	N-CA-C	-5.61	105.31	111.82
1	C	73	VAL	CA-C-N	-5.61	114.01	119.90
1	C	73	VAL	C-N-CA	-5.61	114.01	119.90
1	B	153	ASP	N-CA-C	5.53	122.58	110.80
1	H	117	ARG	N-CA-C	5.51	118.21	111.82
1	D	23	ILE	N-CA-C	-5.44	99.80	107.75
1	C	252	ILE	N-CA-C	5.44	116.49	111.81
1	B	123	ARG	N-CA-C	-5.41	100.89	109.59
1	E	46	LYS	CA-C-N	5.37	125.36	119.89
1	E	46	LYS	C-N-CA	5.37	125.36	119.89
1	J	46	LYS	N-CA-C	-5.37	103.28	109.93
1	G	70	GLY	N-CA-C	5.36	123.81	115.72
1	G	188	PHE	CA-C-N	-5.34	114.19	122.09
1	G	188	PHE	C-N-CA	-5.34	114.19	122.09
1	H	253	LEU	CA-C-N	5.33	125.25	119.76
1	H	253	LEU	C-N-CA	5.33	125.25	119.76
1	H	124	GLN	CA-C-N	-5.32	115.27	122.77
1	H	124	GLN	C-N-CA	-5.32	115.27	122.77
1	I	304	PHE	CA-C-N	-5.32	113.15	119.05
1	I	304	PHE	C-N-CA	-5.32	113.15	119.05
1	H	54	LYS	CA-C-N	5.27	125.27	119.89
1	H	54	LYS	C-N-CA	5.27	125.27	119.89
1	D	37	GLY	N-CA-C	5.27	118.23	110.80
1	H	153	ASP	N-CA-C	5.27	122.02	110.80
1	E	259	THR	N-CA-C	5.24	118.24	110.48
1	I	153	ASP	N-CA-C	5.24	118.96	109.32
1	J	210	LEU	CA-C-N	-5.24	113.24	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	210	LEU	C-N-CA	-5.24	113.24	119.05
1	D	119	PHE	N-CA-C	-5.24	102.99	109.64
1	C	190	ARG	N-CA-C	5.21	117.39	108.90
1	E	75	ALA	N-CA-C	5.21	116.65	109.15
1	F	185	GLN	N-CA-C	5.21	118.77	110.70
1	D	288	ALA	N-CA-C	-5.20	105.65	112.41
1	A	287	GLN	N-CA-C	5.18	115.89	108.74
1	H	304	PHE	CA-C-N	-5.18	113.20	118.85
1	H	304	PHE	C-N-CA	-5.18	113.20	118.85
1	B	188	PHE	CA-C-N	-5.18	114.88	122.19
1	B	188	PHE	C-N-CA	-5.18	114.88	122.19
1	D	151	ASN	N-CA-C	5.18	118.03	109.85
1	G	293	ASP	N-CA-C	-5.16	102.01	109.59
1	E	80	ASN	N-CA-C	5.14	118.58	112.72
1	F	210	LEU	CA-C-N	-5.14	113.34	119.05
1	F	210	LEU	C-N-CA	-5.14	113.34	119.05
1	I	44	THR	N-CA-C	5.14	116.78	108.41
1	H	210	LEU	CA-C-N	-5.13	113.63	119.28
1	H	210	LEU	C-N-CA	-5.13	113.63	119.28
1	G	156	GLU	CA-C-N	5.13	128.76	121.02
1	G	156	GLU	C-N-CA	5.13	128.76	121.02
1	G	154	ASN	N-CA-C	5.12	121.71	110.80
1	D	197	ALA	N-CA-C	5.11	117.01	108.99
1	D	75	ALA	CA-C-N	-5.09	116.22	122.84
1	D	75	ALA	C-N-CA	-5.09	116.22	122.84
1	B	253	LEU	CA-C-N	5.08	124.84	119.76
1	B	253	LEU	C-N-CA	5.08	124.84	119.76
1	D	157	ILE	N-CA-C	-5.08	105.44	112.50
1	I	125	GLN	N-CA-C	5.08	117.06	108.02
1	D	302	LEU	N-CA-C	-5.07	107.78	114.31
1	G	124	GLN	CA-C-N	-5.06	115.63	122.77
1	G	124	GLN	C-N-CA	-5.06	115.63	122.77
1	I	249	THR	N-CA-C	5.05	117.17	111.11
1	D	50	THR	CA-C-N	5.05	125.33	119.93
1	D	50	THR	C-N-CA	5.05	125.33	119.93
1	H	297	ILE	N-CA-C	5.04	117.39	111.09
1	D	304	PHE	N-CA-C	5.02	120.91	109.81
1	G	216	ILE	CB-CA-C	-5.02	105.46	111.88
1	B	90	LYS	N-CA-C	-5.01	101.71	109.72
1	A	190	ARG	N-CA-C	5.01	117.06	108.90
1	F	293	ASP	N-CA-C	-5.00	101.59	109.25

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	2497	0	2468	80	0
1	B	2497	0	2468	89	0
1	C	2497	0	2468	95	0
1	D	2497	0	2468	96	0
1	E	2497	0	2468	92	0
1	F	2497	0	2468	95	0
1	G	2497	0	2468	101	0
1	H	2497	0	2468	91	0
1	I	2497	0	2468	82	0
1	J	2497	0	2468	83	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	804	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 16.

All (804) 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:B:215:ILE:HD13	1:C:239:MET:HE3	1.53	0.87
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:HIS:HE1	1:C:291:VAL:HG13	1.45	0.81
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:B:62:GLN:NE2	1:C:68:ASN:OD1	2.22	0.71
1:F:99:ARG:HH12	1:G:180:SER:HB2	1.54	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:264:GLN:HA	1:E:267:ILE:HG13	1.75	0.69
1:E:289:ASN:OD1	1:E:290:GLY:N	2.23	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:B:167:SER:HB3	1:B:194:ARG:HB2	1.76	0.68
1:F:66:TRP:HB3	1:F:71:LEU:HD12	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:H:212:LEU:O	1:H:216:ILE:HG12	1.94	0.67
1:I:216:ILE:O	1:I:219:SER:HB3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:66:TRP:HB3	1:J:71:LEU:HD12	1.76	0.67
1:C:294:ASP:HB2	1:C:297:ILE:HG22	1.74	0.67
1:D:205:LEU:HD23	1:D:209:ILE:HG13	1.75	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:B:175:TYR:CE1	2:B:401:377:H9	2.32	0.65
1:F:36:ASP:OD2	1:F:105:ARG:NH2	2.29	0.65
1:D:148:TYR:HE1	1:E:177:HIS:HB2	1.61	0.64
1:A:215:ILE:HD13	1:B:239:MET:HE3	1.79	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:F:225:LEU:HD21	1:G:232:LEU:HD22	1.80	0.63
1:I:205:LEU:HD23	1:I:209:ILE:HG13	1.80	0.63
1:H:28:THR:HG22	1:H:116:PHE:CE1	2.34	0.63
1:C:44:THR:HA	1:C:99:ARG:HA	1.80	0.63
1:G:211:PRO:O	1:G:215:ILE:HG12	1.99	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:B:169:HIS:HB3	1:B:192:THR:HB	1.81	0.63
1:I:212:LEU:O	1:I:216:ILE:HG12	1.98	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:C:248:TYR:HE1	1:D:250:SER:HG	1.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:G:248:TYR:HE1	1:H:250:SER:HG	1.47	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:B:212:LEU:HD12	1:B:265:MET:HB3	1.82	0.61
1:D:216:ILE:O	1:D:219:SER:HB3	2.00	0.61
1:D:17:SER:HB2	1:D:40:VAL:HB	1.81	0.61
1:E:38:TYR:CZ	1:E:105:ARG:HD2	2.36	0.61
1:J:212:LEU:O	1:J:216:ILE:HG12	2.00	0.60
1:A:68:ASN:OD1	1:E:62:GLN:NE2	2.31	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:C:263:ASP:O	1:C:267:ILE:HG12	2.01	0.60
1:F:44:THR:HA	1:F:99:ARG:HA	1.83	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:E:300:CYS:HB2	1:E:303:ALA:HB3	1.83	0.60
1:J:127:VAL:HG22	1:J:194:ARG:HG2	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:B:212:LEU:O	1:B:216:ILE:HG12	2.03	0.59
1:C:284:HIS:CE1	1:C:291:VAL:HG13	2.32	0.59
1:F:295:LEU:O	1:F:299:ARG:HG3	2.02	0.59
1:G:212:LEU:O	1:G:216:ILE:HG12	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:I:289:ASN:OD1	1:I:290:GLY:N	2.36	0.59
1:J:145:ILE:HD12	1:J:191:ILE:CG2	2.33	0.59
1:D:97:ASP:OD2	1:D:99:ARG:NH1	2.35	0.59
1:B:284:HIS:NE2	1:B:291:VAL:HG13	2.18	0.59
1:C:289:ASN:OD1	1:C:290:GLY:N	2.34	0.59
1:G:31:GLN:HG2	1:G:114:MET:HB2	1.85	0.58
1:E:13:ASP:OD2	1:E:141:ARG:HD3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:99:ARG:NH1	1:G:180:SER:HB2	2.17	0.58
1:A:248:TYR:HB2	1:B:247:SER:HB3	1.84	0.58
1:C:157:ILE:HD11	1:D:115:ASP:CG	2.28	0.58
1:D:91:ARG:HD2	1:E:134:SER:HB3	1.86	0.58
2:F:402:377:H19	1:J:244:ALA:HA	1.84	0.58
1:E:128:LEU:HB2	1:E:193:VAL:HB	1.85	0.58
1:F:136:ASN:H	1:F:136:ASN:HD22	1.50	0.58
1:H:289:ASN:OD1	1:H:290:GLY:N	2.37	0.58
1:C:209:ILE:HG23	1:C:265:MET:HE1	1.85	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:A:173:ILE:HD13	1:A:190:ARG:HB3	1.85	0.57
1:I:91:ARG:HD2	1:J:134:SER:HB3	1.85	0.57
1:I:181:VAL:HG21	1:I:185:GLN:HB2	1.85	0.57
1:A:221:SER:HB2	1:B:281:ILE:HD11	1.85	0.57
1:F:31:GLN:HG2	1:F:114:MET:HB2	1.85	0.57
1:H:114:MET:HE2	1:H:116:PHE:HZ	1.69	0.57
1:J:145:ILE:HD12	1:J:191:ILE:HG21	1.86	0.57
1:G:136:ASN:HD21	1:G:138:GLN:HB2	1.68	0.57
1:A:66:TRP:HB3	1:A:71:LEU:HD12	1.85	0.57
1:A:167:SER:HB3	1:A:194:ARG:HB2	1.86	0.57
1:B:107:LEU:HD22	1:C:83:GLY:CA	2.33	0.57
1:B:248:TYR:HB2	1:C:247:SER:HB3	1.85	0.57
1:C:38:TYR:CE2	1:C:105:ARG:HD2	2.40	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: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:215:ILE:HD13	1:J:239:MET:HE3	1.86	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:A:122:ASP:OD1	1:A:122:ASP:N	2.31	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:212:LEU:O	1:A:216:ILE:HG12	2.05	0.56
1:B:209:ILE:HG23	1:B:265:MET:HE1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:PRO:O	1:B:215:ILE:HG12	2.05	0.56
1:F:39:ILE:HD11	1:F:78:PHE:CZ	2.40	0.56
1:H:225:LEU:HD21	1:I:232:LEU:HD22	1.86	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:A:285:HIS:O	1:A:287:GLN:HG3	2.05	0.56
1:D:146:GLN:HB2	1:D:148:TYR:HE2	1.70	0.56
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:C:227:SER:HB3	1:C:230:GLU:CD	2.31	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:A:157:ILE:HD11	1:B:115:ASP:CG	2.32	0.55
1:C:212:LEU:HD12	1:C:265:MET:HB3	1.89	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:I:227:SER:HB3	1:I:230:GLU:HG3	1.88	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:F:19:PHE:CE2	1:F:148:TYR:HD2	2.25	0.55
1:C:31:GLN:HG2	1:C:114:MET:HB2	1.89	0.54
1:G:13:ASP:CG	1:G:141:ARG:NH1	2.65	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:E:262:ILE:O	1:E:266:ILE:HG12	2.08	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:F:211:PRO:O	1:F:215:ILE:HG12	2.07	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:H:38:TYR:CZ	1:H:105:ARG:HD2	2.42	0.54
1:C:117:ARG:HG2	1:C:258:TYR:CD1	2.42	0.54
1:D:294:ASP:HB2	1:D:297:ILE:HG22	1.89	0.54
1:F:294:ASP:HB2	1:F:297:ILE:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:112:ASN:OD1	1:G:113:ASP:N	2.41	0.54
1:I:301:ARG:O	1:I:305:PRO:HG2	2.08	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:B:107:LEU:HD22	1:C:83:GLY:HA2	1.89	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:F:167:SER:CB	1:F:194:ARG:HB2	2.38	0.53
1:H:114:MET:HE2	1:H:116:PHE:CZ	2.43	0.53
1:B:179:SER:HB2	1:B:181:VAL:HG12	1.91	0.53
1:E:301:ARG:O	1:E:305:PRO:HG2	2.08	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:G:209:ILE:HG23	1:G:265:MET:HE1	1.90	0.53
1:D:28:THR:HG22	1:D:116:PHE:CZ	2.43	0.53
1:E:66:TRP:HB3	1:E:71:LEU:HD12	1.91	0.53
1:E:145:ILE:HD12	1:E:191:ILE:CG2	2.38	0.53
1:E:289:ASN:OD1	1:E:291:VAL:N	2.42	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:A:284:HIS:HE1	1:E:226:GLU:OE2	1.92	0.53
1:C:264:GLN:HA	1:C:267:ILE:HG13	1.89	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:C:215:ILE:HD13	1:D:239:MET:HE3	1.90	0.52
1:G:72:TRP:CZ2	1:G:74:PRO:HB3	2.44	0.52
1:G:173:ILE:O	1:G:187:GLU:HA	2.08	0.52
1:H:136:ASN:H	1:H:136:ASN:HD22	1.57	0.52
1:I:204:TYR:O	1:I:209:ILE:HG12	2.09	0.52
1:E:26:VAL:HG22	1:E:33:TYR:HB3	1.91	0.52
1:G:54:LYS:HB3	1:G:55:PRO:HD2	1.90	0.52
1:I:294:ASP:HB2	1:I:297:ILE:HG22	1.91	0.52
1:A:211:PRO:O	1:A:215:ILE:HG12	2.09	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:B:38:TYR:CE2	2:C:401:377:H1	2.45	0.52
1:J:181:VAL:HG21	1:J:185:GLN:HB2	1.91	0.52
1:A:188:PHE:CZ	2:A:401:377:H17	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:401:377:H1	1:E:38:TYR:CD2	2.45	0.52
1:D:300:CYS:HB2	1:D:303:ALA:HB3	1.92	0.52
1:I:224:TRP:CH2	1:I:301:ARG:HB3	2.45	0.52
1:E:115:ASP:OD1	1:E:117:ARG:HG3	2.09	0.52
1:F:91:ARG:NH2	1:F:103:ASN:OD1	2.43	0.52
1:H:294:ASP:HB2	1:H:297:ILE:HG22	1.92	0.52
1:B:28:THR:HG22	1:B:116:PHE:CZ	2.45	0.52
1:B:149:THR:O	1:B:151:ASN:N	2.43	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:H:157:ILE:HD11	1:I:117:ARG:NE	2.24	0.52
1:B:212:LEU:CD1	1:B:265:MET:HB3	2.40	0.52
1:B:227:SER:HB3	1:B:230:GLU:HG3	1.92	0.52
1:E:273:ILE:O	1:E:277:ILE:HG12	2.10	0.52
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: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:B:39:ILE:HG13	1:B:104:ALA:HB3	1.92	0.51
1:B:294:ASP:HB2	1:B:297:ILE:CG2	2.40	0.51
1:J:208:PHE:HE2	1:J:248:TYR:CE1	2.27	0.51
1:B:173:ILE:HD13	1:B:190:ARG:HB3	1.92	0.51
1:C:78:PHE:CE2	1:C:128:LEU:HD23	2.45	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:F:295:LEU:HA	1:F:298:GLN:CD	2.36	0.51
1:A:141:ARG:NH1	1:A:143:SER:HA	2.26	0.51
1:C:48:ARG:NH1	1:C:48:ARG:HB2	2.26	0.51
1:C:58:VAL:O	1:C:91:ARG:HA	2.11	0.51
1:D:217:ALA:HA	1:D:220:TRP:CE3	2.46	0.51
1:E:216:ILE:O	1:E:219:SER:HB3	2.11	0.51
1:G:224:TRP:CZ3	1:G:301:ARG:HB3	2.46	0.51
1:A:241:THR:HA	1:B:240:LEU:HD23	1.93	0.51
1:A:247:SER:HA	1:E:248:TYR:CD1	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:PHE:HD1	1:A:38:TYR:HB2	1.76	0.50
1:E:312:GLY:O	1:E:316:VAL:HG23	2.11	0.50
1:F:36:ASP:CG	1:F:105:ARG:HH21	2.17	0.50
1:G:294:ASP:HB2	1:G:297:ILE:HG22	1.93	0.50
1:D:249:THR:HG23	1:D:253:LEU:HD22	1.93	0.50
1:G:248:TYR:HE1	1:H:250:SER:OG	1.94	0.50
1:H:110:PHE:CE2	1:H:128:LEU:HG	2.46	0.50
1:I:299:ARG:C	1:I:301:ARG:H	2.19	0.50
1:C:211:PRO:O	1:C:215:ILE:HG12	2.11	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:A:155:GLU:HB3	1:A:161:TRP:CD1	2.45	0.50
1:B:61:THR:HG22	1:B:62:GLN:NE2	2.26	0.50
1:C:40:VAL:HG13	1:C:103:ASN:OD1	2.12	0.50
1:F:145:ILE:HD12	1:F:191:ILE:HG23	1.93	0.50
1:I:78:PHE:O	1:I:81:VAL:HG12	2.11	0.50
1:F:91:ARG:HD2	1:G:134:SER:HB3	1.92	0.50
1:A:123:ARG:HD2	1:A:198:VAL:HG22	1.93	0.50
1:A:304:PHE:HD1	1:A:305:PRO:HD3	1.77	0.50
1:E:78:PHE:O	1:E:81:VAL:HG12	2.11	0.50
1:A:44:THR:HA	1:A:99:ARG:HA	1.92	0.50
1:A:302:LEU:C	1:A:305:PRO:HD2	2.37	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:C:18:ILE:HB	1:C:147:VAL:HG22	1.93	0.50
1:C:122:ASP:OD1	1:C:122:ASP:N	2.41	0.49
1:F:300:CYS:HB2	1:F:303:ALA:HB3	1.94	0.49
1:J:289:ASN:OD1	1:J:290:GLY:N	2.44	0.49
1:A:61:THR:HG22	1:A:62:GLN:NE2	2.26	0.49
1:C:212:LEU:CD1	1:C:265:MET:HB3	2.42	0.49
1:G:18:ILE:HD13	1:G:39:ILE:HG12	1.95	0.49
1:G:18:ILE:HB	1:G:147:VAL:HG22	1.94	0.49
1:H:145:ILE:HD12	1:H:191:ILE:HG21	1.93	0.49
1:I:232:LEU:O	1:I:235:SER:OG	2.29	0.49
1:B:61:THR:HG22	1:B:62:GLN:HE21	1.78	0.49
1:D:27:ASN:HB3	1:D:32:THR:HB	1.94	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:C:127:VAL:HG22	1:C:194:ARG:HG2	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:THR:HB	1:D:256:LEU:HD21	1.95	0.49
1:F:224:TRP:CZ3	1:F:301:ARG:HB3	2.47	0.49
1:I:253:LEU:HD21	1:I:262:ILE:HD12	1.95	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:G:28:THR:HG22	1:G:116:PHE:CZ	2.47	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:119:PHE:CE1	1:C:254:PRO:HG3	2.47	0.49
1:C:257:PRO:HG2	1:C:258:TYR:CD2	2.48	0.49
1:G:136:ASN:CG	1:G:185:GLN:HG3	2.37	0.49
1:F:249:THR:HG23	1:F:253:LEU:HD22	1.94	0.49
1:I:28:THR:HB	1:I:256:LEU:HD21	1.95	0.49
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:A:300:CYS:HB2	1:A:303:ALA:HB3	1.94	0.48
1:C:167:SER:HB3	1:C:194:ARG:HB2	1.95	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:C:28:THR:HB	1:C:256:LEU:CD2	2.43	0.48
1:C:72:TRP:CZ2	1:C:74:PRO:HB3	2.48	0.48
1:E:19:PHE:HD2	1:E:148:TYR:HB2	1.78	0.48
1:I:306:LEU:HA	1:I:309:LEU:HB2	1.95	0.48
1:A:285:HIS:C	1:A:287:GLN:HG3	2.39	0.48
1:E:227:SER:OG	1:E:228:PHE:N	2.46	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:G:149:THR:HB	1:G:151:ASN:CG	2.38	0.48
1:G:215:ILE:HA	1:H:239:MET:HE3	1.95	0.48
1:J:123:ARG:HG2	1:J:197:ALA:O	2.13	0.48
1:A:63:ILE:HG23	1:A:92:LEU:HD12	1.95	0.48
1:C:19:PHE:CE2	1:C:148:TYR:CD2	3.02	0.48
1:F:61:THR:HG22	1:F:62:GLN:NE2	2.29	0.48
1:H:38:TYR:CD2	2:H:402:377:H1	2.48	0.48
1:J:72:TRP:CH2	1:J:74:PRO:HG3	2.48	0.48
1:A:239:MET:HE3	1:E:215:ILE:HD13	1.95	0.48
1:A:295:LEU:HD12	1:A:298:GLN:OE1	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:LEU:HD23	1:B:29:LEU:HA	1.65	0.48
1:G:101:ILE:HD13	1:H:179:SER:HB3	1.96	0.48
1:J:149:THR:O	1:J:151:ASN:N	2.43	0.48
1:J:208:PHE:HE2	1:J:248:TYR:CZ	2.31	0.48
1:J:279:LEU:HD22	1:J:297:ILE:HD11	1.95	0.48
1:H:294:ASP:HB2	1:H:297:ILE:CG2	2.42	0.48
1:C:19:PHE:CE2	1:C:148:TYR:HD2	2.32	0.48
1:F:232:LEU:CD2	1:F:236:PHE:HE1	2.27	0.48
1:G:115:ASP:OD1	1:G:117:ARG:HG3	2.13	0.48
1:J:299:ARG:C	1:J:301:ARG:H	2.21	0.48
1:A:232:LEU:HD22	1:E:225:LEU:HD21	1.96	0.47
1:G:44:THR:HA	1:G:99:ARG:HA	1.95	0.47
1:G:221:SER:HB2	1:H:281:ILE:HD11	1.96	0.47
1:I:299:ARG:HD3	1:I:301:ARG:HD2	1.95	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
1:G:55:PRO:HB3	1:G:95:PHE:CD2	2.48	0.47
1:I:42:GLN:HG3	1:I:101:ILE:HG12	1.96	0.47
1:I:223:PHE:HE1	1:I:304:PHE:CE1	2.32	0.47
1:B:91:ARG:HD2	1:C:134:SER:HB3	1.95	0.47
1:B:285:HIS:C	1:B:287:GLN:HG3	2.39	0.47
1:D:127:VAL:HG22	1:D:194:ARG:HG2	1.97	0.47
1:E:291:VAL:HG12	1:E:293:ASP:OD2	2.14	0.47
1:H:157:ILE:HD13	1:H:157:ILE:HA	1.62	0.47
1:D:227:SER:HB3	1:D:230:GLU:HG3	1.96	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:H:215:ILE:HD13	1:I:239:MET:HE3	1.96	0.47
1:B:204:TYR:O	1:B:209:ILE:HG12	2.15	0.47
1:C:211:PRO:HB3	1:D:270:TYR:CD1	2.49	0.47
1:J:232:LEU:HD23	1:J:236:PHE:HE1	1.80	0.47
1:D:148:TYR:N	1:D:148:TYR:CD2	2.83	0.47
1:H:145:ILE:HD12	1:H:191:ILE:CG2	2.45	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:B:294:ASP:HB2	1:B:297:ILE:HG22	1.96	0.47
1:D:59:GLU:OE2	1:E:75:ALA:HB3	2.15	0.47
1:D:185:GLN:OE1	1:D:185:GLN:N	2.48	0.47
1:E:20:ILE:HB	1:E:149:THR:HG22	1.96	0.47
1:F:145:ILE:HD12	1:F:191:ILE:CG2	2.43	0.47
1:F:227:SER:HB3	1:F:230:GLU:CD	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:217:ALA:HA	1:H:220:TRP:CE3	2.50	0.47
1:I:157:ILE:HD13	1:I:157:ILE:HA	1.50	0.47
1:I:248:TYR:HB2	1:J:247:SER:CB	2.44	0.47
1:J:79:ILE:HD13	1:J:79:ILE:HA	1.71	0.47
1:C:257:PRO:HD2	1:C:258:TYR:CE2	2.49	0.47
1:D:29:LEU:HD23	1:D:29:LEU:HA	1.65	0.47
1:F:72:TRP:CH2	1:F:74:PRO:HG3	2.50	0.47
1:F:244:ALA:HB1	2:F:402:377:H21	1.95	0.47
1:H:173:ILE:O	1:H:187:GLU:HA	2.14	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: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:B:86:ASP:HB3	1:B:107:LEU:HB3	1.97	0.46
1:E:223:PHE:CZ	1:E:304:PHE:HE1	2.33	0.46
1:G:21:ASN:HB2	1:G:36:ASP:O	2.15	0.46
1:G:267:ILE:HG12	1:G:267:ILE:H	1.53	0.46
1:J:216:ILE:HD12	1:J:269:GLY:HA2	1.96	0.46
1:A:119:PHE:CE1	1:A:254:PRO:HG3	2.51	0.46
1:D:178:LEU:HB2	1:D:179:SER:H	1.43	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:E:163:ARG:HA	1:E:163:ARG:HD3	1.68	0.46
1:E:304:PHE:HA	1:E:307:GLY:H	1.80	0.46
1:G:61:THR:HG22	1:G:62:GLN:NE2	2.30	0.46
1:H:248:TYR:HB2	1:I:247:SER:CB	2.44	0.46
1:B:23:ILE:HG21	1:B:126:PHE:CD1	2.50	0.46
1:B:92:LEU:HD23	1:B:92:LEU:HA	1.74	0.46
1:F:227:SER:HB3	1:F:230:GLU:CG	2.45	0.46
1:F:285:HIS:CD2	1:J:224:TRP:HD1	2.32	0.46
1:I:72:TRP:CH2	1:I:74:PRO:HG3	2.51	0.46
1:I:157:ILE:HD11	1:J:117:ARG:CG	2.45	0.46
1:I:273:ILE:O	1:I:277:ILE:HG12	2.15	0.46
1:B:169:HIS:ND1	1:I:168:THR:HG22	2.31	0.46
1:E:92:LEU:HD23	1:E:92:LEU:HA	1.73	0.46
1:E:145:ILE:HD12	1:E:191:ILE:HG23	1.98	0.46
1:D:84:SER:HA	1:D:85:PRO:HD3	1.73	0.46
1:D:148:TYR:N	1:D:148:TYR:HD2	2.13	0.46
1:D:205:LEU:HD23	1:D:205:LEU:HA	1.47	0.46
1:G:176:ASP:HB2	1:G:177:HIS:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:185:GLN:OE1	1:G:185:GLN:N	2.49	0.46
1:H:93:MET:HG2	1:H:95:PHE:CE1	2.51	0.46
1:A:105:ARG:NH2	1:B:81:VAL:O	2.49	0.46
1:B:95:PHE:CD1	1:B:99:ARG:HG3	2.50	0.46
1:D:145:ILE:HD12	1:D:191:ILE:CG2	2.46	0.46
1:B:157:ILE:HD11	1:C:117:ARG:HE	1.80	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:D:61:THR:HG22	1:D:62:GLN:NE2	2.31	0.46
1:G:157:ILE:HD13	1:G:157:ILE:HA	1.66	0.46
1:J:115:ASP:OD1	1:J:117:ARG:HG3	2.16	0.46
1:J:220:TRP:HZ2	1:J:308:PHE:CD2	2.34	0.46
1:A:72:TRP:CH2	1:A:74:PRO:HG3	2.51	0.46
1:A:291:VAL:O	1:A:293:ASP:N	2.49	0.46
1:C:58:VAL:HB	1:C:92:LEU:HB2	1.98	0.46
1:D:144:ASP:OD2	1:D:146:GLN:NE2	2.49	0.46
1:D:157:ILE:HD13	1:D:157:ILE:HA	1.51	0.46
1:I:38:TYR:CD2	2:J:401:377:H1	2.50	0.46
1:J:131:GLU:OE1	1:J:190:ARG:NH2	2.41	0.46
1:J:145:ILE:HG23	1:J:168:THR:CG2	2.46	0.46
1:A:145:ILE:HD12	1:A:191:ILE:CG2	2.46	0.45
1:D:210:LEU:HB3	1:D:211:PRO:HD3	1.98	0.45
1:G:33:TYR:HH	1:G:127:VAL:H	1.64	0.45
1:G:279:LEU:HD23	1:G:279:LEU:HA	1.76	0.45
1:I:144:ASP:OD1	1:I:144:ASP:N	2.44	0.45
1:J:61:THR:HG22	1:J:62:GLN:HE21	1.81	0.45
1:J:185:GLN:N	1:J:185:GLN:OE1	2.49	0.45
1:B:79:ILE:HD13	1:B:79:ILE:HA	1.76	0.45
1:C:93:MET:HG2	1:C:95:PHE:CE1	2.51	0.45
1:F:64:GLU:CG	1:J:61:THR:HG21	2.45	0.45
1:F:77:GLU:OE2	1:J:105:ARG:HD3	2.17	0.45
1:B:155:GLU:HB3	1:B:161:TRP:NE1	2.32	0.45
1:D:28:THR:HB	1:D:256:LEU:CD2	2.47	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: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:C:93:MET:HE2	1:C:95:PHE:CZ	2.52	0.45
1:I:38:TYR:CE2	2:J:401:377:H1	2.51	0.45
1:F:212:LEU:HD12	1:F:265:MET:HB3	1.99	0.45
1:H:39:ILE:HG12	1:H:106:PHE:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:ASN:ND2	1:C:36:ASP:OD2	2.30	0.45
1:C:120:PRO:HD2	1:C:121:PHE:CE1	2.52	0.45
1:H:27:ASN:HB3	1:H:32:THR:HB	1.98	0.45
1:H:263:ASP:O	1:H:267:ILE:HG12	2.17	0.45
1:I:56:LEU:HD22	1:I:57:ILE:N	2.31	0.45
1:J:295:LEU:HA	1:J:298:GLN:OE1	2.17	0.45
1:A:224:TRP:CE2	1:A:301:ARG:HD3	2.51	0.45
1:B:205:LEU:HD23	1:B:205:LEU:HA	1.68	0.45
1:C:61:THR:HG21	1:D:64:GLU:CG	2.47	0.45
1:C:279:LEU:HA	1:C:279:LEU:HD23	1.75	0.45
1:C:294:ASP:HB2	1:C:297:ILE:CG2	2.44	0.45
1:J:173:ILE:O	1:J:187:GLU:HA	2.14	0.45
1:B:40:VAL:HG13	1:B:103:ASN:OD1	2.16	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: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:D:263:ASP:O	1:D:267:ILE:HG12	2.17	0.45
1:E:149:THR:C	1:E:151:ASN:H	2.22	0.45
1:F:33:TYR:CE2	1:F:110:PHE:HB2	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:J:224:TRP:CZ3	1:J:301:ARG:HB3	2.52	0.45
1:B:21:ASN:HB2	1:B:36:ASP:O	2.16	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:I:227:SER:HB3	1:I:230:GLU:CG	2.47	0.45
1:A:29:LEU:HD23	1:A:29:LEU:HA	1.62	0.44
1:B:58:VAL:HG12	1:B:63:ILE:HG12	2.00	0.44
1:B:168:THR:HG22	1:B:169:HIS:N	2.30	0.44
1:B:238:LEU:HD12	1:B:238:LEU:HA	1.72	0.44
1:B:304:PHE:CD1	1:B:304:PHE:C	2.95	0.44
1:H:221:SER:HB2	1:I:281:ILE:HD11	1.99	0.44
1:J:227:SER:OG	1:J:228:PHE:N	2.50	0.44
1:D:58:VAL:HG12	1:D:63:ILE:HG12	1.99	0.44
1:F:84:SER:HA	1:F:85:PRO:HD3	1.74	0.44
1:J:82:VAL:CG2	1:J:111:SER:HB2	2.47	0.44
1:A:205:LEU:HD23	1:A:209:ILE:HG13	1.98	0.44
1:B:289:ASN:OD1	1:B:290:GLY:N	2.48	0.44
1:C:119:PHE:C	1:C:119:PHE:CD2	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:23:ILE:HA	1:E:34:LYS:O	2.17	0.44
1:A:145:ILE:HD12	1:A:191:ILE:HG21	1.98	0.44
1:C:29:LEU:HD23	1:C:255:ARG:O	2.17	0.44
1:F:228:PHE:CG	1:F:284:HIS:CD2	3.05	0.44
1:F:299:ARG:C	1:F:301:ARG:H	2.25	0.44
1:I:299:ARG:NH1	1:I:302:LEU:HB2	2.32	0.44
1:A:110:PHE:CE2	1:A:128:LEU:HG	2.53	0.44
1:A:240:LEU:HD13	1:B:240:LEU:HD21	1.98	0.44
1:B:66:TRP:HB3	1:B:71:LEU:HD12	1.99	0.44
1:B:227:SER:HB3	1:B:230:GLU:CG	2.48	0.44
1:E:282:PHE:CE1	1:E:286:ARG:HB2	2.53	0.44
1:B:267:ILE:HG12	1:B:267:ILE:H	1.63	0.44
1:C:253:LEU:HG	1:C:254:PRO:HD2	2.00	0.44
1:D:287:GLN:HB2	1:D:289:ASN:H	1.81	0.44
1:E:223:PHE:CZ	1:E:304:PHE:CE1	3.06	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:J:28:THR:HG22	1:J:116:PHE:CZ	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:23:ILE:HG21	1:I:126:PHE:CD1	2.52	0.44
1:I:115:ASP:OD2	1:I:117:ARG:NH2	2.42	0.44
1:B:223:PHE:HE1	1:B:304:PHE:CE1	2.36	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:G:212:LEU:O	1:G:212:LEU:HD22	2.18	0.44
1:H:216:ILE:O	1:H:219:SER:HB3	2.16	0.44
1:H:221:SER:OG	1:I:236:PHE:HZ	2.01	0.44
1:I:65:ARG:HD2	1:J:68:ASN:ND2	2.33	0.44
1:A:92:LEU:HD23	1:A:92:LEU:HA	1.70	0.44
1:A:61:THR:HG22	1:A:62:GLN:HE21	1.82	0.43
1:B:178:LEU:HB2	1:B:179:SER:H	1.55	0.43
1:C:235:SER:HA	1:C:238:LEU:HB2	2.00	0.43
1:F:216:ILE:HD12	1:F:269:GLY:HA2	2.00	0.43
1:H:136:ASN:ND2	1:H:139:GLN:OE1	2.51	0.43
1:H:224:TRP:CE2	1:H:301:ARG:HD3	2.52	0.43
1:J:244:ALA:O	1:J:247:SER:OG	2.23	0.43
1:A:31:GLN:HG2	1:A:114:MET:HB2	2.00	0.43
1:B:38:TYR:HA	1:B:104:ALA:O	2.17	0.43
1:C:249:THR:CG2	1:C:253:LEU:HD22	2.48	0.43
1:D:66:TRP:HB3	1:D:71:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:21:ASN:HD21	1:H:38:TYR:HE1	1.64	0.43
1:A:149:THR:O	1:A:151:ASN:N	2.46	0.43
1:B:122:ASP:OD1	1:B:122:ASP:N	2.49	0.43
1:C:33:TYR:CE2	1:C:110:PHE:HB2	2.54	0.43
1:C:248:TYR:HE1	1:D:250:SER:OG	2.01	0.43
1:F:114:MET:HE2	1:F:116:PHE:CZ	2.53	0.43
1:G:79:ILE:HD13	1:G:79:ILE:HA	1.83	0.43
1:C:157:ILE:HD13	1:C:157:ILE:HA	1.58	0.43
1:E:266:ILE:HG22	1:E:270:TYR:CE1	2.52	0.43
1:F:132:PRO:HG3	1:F:140:LEU:HD22	2.00	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:A:247:SER:CB	1:E:248:TYR:HB2	2.41	0.43
1:E:294:ASP:O	1:E:298:GLN:HG2	2.18	0.43
1:F:170:ILE:HA	1:F:190:ARG:O	2.18	0.43
1:F:302:LEU:C	1:F:305:PRO:HD2	2.43	0.43
1:G:178:LEU:HD21	1:G:186:ASN:HA	2.01	0.43
1:H:136:ASN:O	1:H:139:GLN:N	2.44	0.43
1:I:50:THR:OG1	1:I:54:LYS:O	2.32	0.43
1:J:155:GLU:HB3	1:J:161:TRP:CD1	2.52	0.43
1:A:108:GLY:HA3	1:A:110:PHE:HE1	1.83	0.43
1:C:295:LEU:HA	1:C:298:GLN:OE1	2.19	0.43
1:F:238:LEU:HD12	1:F:238:LEU:HA	1.79	0.43
1:G:29:LEU:HD23	1:G:29:LEU:HA	1.87	0.43
1:G:155:GLU:HB3	1:G:161:TRP:NE1	2.34	0.43
1:H:155:GLU:HB3	1:H:161:TRP:CD1	2.54	0.43
1:B:26:VAL:HG13	1:B:114:MET:HE1	2.01	0.43
1:C:84:SER:HA	1:C:85:PRO:HD3	1.83	0.43
1:F:118:LEU:HA	1:F:261:VAL:HG23	1.99	0.43
1:G:208:PHE:CE2	1:G:249:THR:HA	2.54	0.43
1:A:138:GLN:OE1	1:A:184:ASN:HB3	2.19	0.43
1:D:81:VAL:HG13	1:D:83:GLY:O	2.19	0.43
1:F:79:ILE:HD13	1:F:79:ILE:HA	1.87	0.43
1:E:299:ARG:C	1:E:301:ARG:H	2.26	0.43
1:F:28:THR:HG22	1:F:116:PHE:CZ	2.54	0.43
1:F:299:ARG:HD3	1:F:301:ARG:NH2	2.33	0.43
1:G:95:PHE:CD1	1:G:99:ARG:HG3	2.53	0.43
1:H:204:TYR:HD2	1:H:208:PHE:CD1	2.36	0.43
1:J:295:LEU:HD12	1:J:298:GLN:OE1	2.19	0.43
1:A:306:LEU:HA	1:A:309:LEU:HB2	2.00	0.43
1:D:215:ILE:HD13	1:E:239:MET:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:SER:HA	1:D:238:LEU:HD22	2.01	0.43
1:D:267:ILE:HG12	1:D:267:ILE:H	1.64	0.43
1:H:35:VAL:HG21	1:H:128:LEU:HD11	2.00	0.43
1:I:130:LEU:HA	1:I:130:LEU:HD23	1.70	0.43
1:J:142:PHE:O	1:J:170:ILE:HD13	2.19	0.43
1:D:119:PHE:HA	1:D:122:ASP:OD1	2.19	0.42
1:E:19:PHE:CE2	1:E:148:TYR:CD2	3.07	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:F:227:SER:HB3	1:F:230:GLU:HG3	2.01	0.42
1:G:224:TRP:CE2	1:G:301:ARG:HD3	2.53	0.42
1:G:294:ASP:HB3	1:G:297:ILE:H	1.84	0.42
1:H:205:LEU:HA	1:H:205:LEU:HD23	1.58	0.42
1:I:33:TYR:OH	1:I:127:VAL:N	2.41	0.42
1:J:208:PHE:CE2	1:J:248:TYR:CZ	3.06	0.42
1:J:304:PHE:HD1	1:J:305:PRO:HD3	1.84	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:I:225:LEU:CD2	1:J:232:LEU:HD22	2.50	0.42
1:A:115:ASP:OD1	1:A:117:ARG:HG3	2.18	0.42
1:A:134:SER:HB3	1:E:91:ARG:HD2	2.00	0.42
1:B:28:THR:HB	1:B:256:LEU:CD2	2.50	0.42
1:B:145:ILE:HD12	1:B:191:ILE:CG2	2.45	0.42
1:B:287:GLN:HB2	1:B:289:ASN:H	1.84	0.42
1:C:223:PHE:HE2	1:C:280:ILE:HG13	1.85	0.42
1:D:122:ASP:OD1	1:D:122:ASP:N	2.42	0.42
1:E:223:PHE:CE1	1:E:304:PHE:CE1	3.07	0.42
1:H:304:PHE:HD1	1:H:305:PRO:HD3	1.83	0.42
1:I:92:LEU:HD23	1:I:92:LEU:HA	1.83	0.42
1:I:105:ARG:HD3	1:J:77:GLU:OE2	2.19	0.42
1:J:132:PRO:HG3	1:J:140:LEU:HD22	2.01	0.42
1:B:216:ILE:O	1:B:219:SER:HB3	2.20	0.42
1:D:40:VAL:HG13	1:D:103:ASN:HD22	1.83	0.42
1:D:97:ASP:CG	1:D:99:ARG:NH1	2.77	0.42
1:F:205:LEU:HD23	1:F:209:ILE:HG13	2.01	0.42
1:G:293:ASP:O	1:G:295:LEU:HD12	2.19	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:A:212:LEU:CD1	1:A:265:MET:HB3	2.49	0.42
1:B:301:ARG:O	1:B:305:PRO:HG2	2.18	0.42
1:C:72:TRP:CH2	1:C:74:PRO:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:112:ASN:ND2	1:G:125:GLN:O	2.51	0.42
1:G:212:LEU:HD12	1:G:265:MET:HB3	2.00	0.42
1:H:140:LEU:HD23	1:H:140:LEU:C	2.44	0.42
1:I:97:ASP:OD1	1:I:99:ARG:HG2	2.19	0.42
1:I:163:ARG:HA	1:I:163:ARG:HD3	1.37	0.42
1:J:145:ILE:HD12	1:J:191:ILE:HG23	2.02	0.42
1:D:285:HIS:O	1:D:287:GLN:HG3	2.19	0.42
1:E:79:ILE:HA	1:E:79:ILE:HD13	1.78	0.42
1:E:119:PHE:HE1	1:E:199:ARG:NH1	2.17	0.42
1:E:178:LEU:HD13	1:E:181:VAL:HG13	2.02	0.42
1:H:110:PHE:CD1	1:H:110:PHE:N	2.86	0.42
1:I:84:SER:HA	1:I:85:PRO:HD3	1.57	0.42
1:I:149:THR:C	1:I:151:ASN:N	2.77	0.42
1:J:119:PHE:CD2	1:J:119:PHE:C	2.97	0.42
1:J:145:ILE:HG21	1:J:191:ILE:HG12	2.00	0.42
1:A:130:LEU:HD23	1:A:130:LEU:HA	1.89	0.42
1:A:248:TYR:HB2	1:B:247:SER:CB	2.50	0.42
1:A:268:ALA:HB1	1:A:308:PHE:CE1	2.55	0.42
1:B:296:LEU:HD23	1:B:296:LEU:HA	1.81	0.42
1:D:95:PHE:HE1	1:D:101:ILE:CD1	2.33	0.42
1:H:209:ILE:HD11	1:H:262:ILE:HG12	2.01	0.42
1:A:216:ILE:O	1:A:219:SER:HB3	2.18	0.42
1:D:240:LEU:HD13	1:E:240:LEU:HD21	2.02	0.42
1:F:125:GLN:O	1:F:125:GLN:HG3	2.19	0.42
1:H:61:THR:HG21	1:I:64:GLU:HG3	2.01	0.42
1:B:56:LEU:HD22	1:B:57:ILE:N	2.35	0.42
1:C:310:ALA:O	1:C:314:VAL:HG23	2.20	0.42
1:D:305:PRO:O	1:D:309:LEU:HD13	2.19	0.42
1:E:145:ILE:HD13	1:E:168:THR:HG22	2.01	0.42
1:E:209:ILE:HG23	1:E:265:MET:HE1	2.02	0.42
1:G:268:ALA:HB1	1:G:308:PHE:CE1	2.54	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:A:106:PHE:CD1	1:A:106:PHE:C	2.98	0.42
1:C:28:THR:HB	1:C:256:LEU:HD21	2.02	0.42
1:D:128:LEU:HB2	1:D:193:VAL:HB	2.02	0.42
1:D:302:LEU:C	1:D:305:PRO:HD2	2.44	0.42
1:F:68:ASN:ND2	1:J:65:ARG:HD2	2.35	0.42
1:F:204:TYR:O	1:F:209:ILE:HG12	2.20	0.42
1:G:246:ALA:O	1:G:249:THR:HB	2.20	0.42
1:J:35:VAL:O	1:J:107:LEU:HD12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:58:VAL:HB	1:J:92:LEU:HB2	2.02	0.42
1:A:157:ILE:HD13	1:A:157:ILE:HA	1.65	0.41
1:B:248:TYR:HD1	1:C:247:SER:HA	1.85	0.41
1:C:28:THR:HA	1:C:116:PHE:CE1	2.55	0.41
1:E:33:TYR:OH	1:E:127:VAL:N	2.37	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:72:TRP:CH2	1:H:140:LEU:HD12	2.55	0.41
1:H:136:ASN:H	1:H:136:ASN:ND2	2.17	0.41
1:A:238:LEU:O	1:A:241:THR:HB	2.20	0.41
1:E:48:ARG:NH1	1:E:48:ARG:HB2	2.35	0.41
1:F:224:TRP:CH2	1:F:301:ARG:HB3	2.55	0.41
1:F:304:PHE:HA	1:F:307:GLY:H	1.84	0.41
1:G:145:ILE:HD12	1:G:191:ILE:HG23	2.02	0.41
1:H:212:LEU:O	1:H:212:LEU:HD22	2.20	0.41
1:I:178:LEU:HB2	1:I:179:SER:H	1.45	0.41
1:I:260:THR:H	1:I:263:ASP:HB2	1.85	0.41
1:I:277:ILE:HG22	1:I:281:ILE:HD12	2.02	0.41
1:C:218:ALA:HB2	1:D:274:PHE:CD1	2.54	0.41
1:D:19:PHE:HD2	1:D:148:TYR:HB2	1.86	0.41
1:D:136:ASN:HD21	1:D:185:GLN:HG3	1.84	0.41
1:G:62:GLN:O	1:G:66:TRP:HD1	2.04	0.41
1:H:84:SER:HA	1:H:85:PRO:HD3	1.93	0.41
1:J:204:TYR:HD2	1:J:208:PHE:HD1	1.67	0.41
1:J:205:LEU:HA	1:J:205:LEU:HD23	1.57	0.41
1:D:32:THR:HA	1:D:110:PHE:O	2.20	0.41
1:F:212:LEU:CD1	1:F:265:MET:HB3	2.50	0.41
1:F:241:THR:HA	1:G:240:LEU:HD23	2.02	0.41
1:G:65:ARG:NH1	1:H:68:ASN:O	2.53	0.41
1:G:119:PHE:CD2	1:G:119:PHE:C	2.97	0.41
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:C:178:LEU:HB2	1:C:179:SER:H	1.39	0.41
1:F:138:GLN:OE1	1:F:184:ASN:HB3	2.21	0.41
1:G:105:ARG:HD3	1:H:77:GLU:OE2	2.20	0.41
1:G:165:LYS:O	1:G:166:ALA:CB	2.68	0.41
1:G:217:ALA:HA	1:G:220:TRP:CE3	2.55	0.41
1:I:173:ILE:O	1:I:187:GLU:HA	2.20	0.41
1:A:136:ASN:HD21	1:A:185:GLN:HG3	1.84	0.41
1:A:285:HIS:CE1	1:E:224:TRP:HD1	2.38	0.41
1:C:212:LEU:HD23	1:C:245:TYR:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:279:LEU:HA	1:D:279:LEU:HD23	1.67	0.41
1:E:93:MET:HG2	1:E:95:PHE:CE1	2.56	0.41
1:E:145:ILE:HD12	1:E:191:ILE:HG21	2.02	0.41
1:F:262:ILE:O	1:F:266:ILE:HG12	2.21	0.41
1:G:62:GLN:OE1	1:G:65:ARG:HD3	2.20	0.41
1:I:39:ILE:HD13	1:I:39:ILE:HG21	1.87	0.41
1:J:306:LEU:O	1:J:309:LEU:HB2	2.20	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:A:208:PHE:HE2	1:A:248:TYR:CE2	2.39	0.41
1:C:142:PHE:HB3	1:C:170:ILE:HD13	2.02	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:H:29:LEU:HA	1:H:29:LEU:HD23	1.69	0.41
1:H:279:LEU:HD23	1:H:279:LEU:HA	1.75	0.41
1:I:29:LEU:HD23	1:I:29:LEU:HA	1.91	0.41
1:D:122:ASP:CG	1:D:199:ARG:HE	2.29	0.41
1:D:146:GLN:HB2	1:D:148:TYR:CE2	2.53	0.41
1:E:61:THR:HG22	1:E:62:GLN:HE21	1.86	0.41
1:E:253:LEU:HG	1:E:254:PRO:HD2	2.03	0.41
1:G:39:ILE:HD11	1:G:78:PHE:CZ	2.56	0.41
1:G:173:ILE:N	1:G:173:ILE:HD12	2.36	0.41
1:H:31:GLN:HB3	1:H:112:ASN:O	2.21	0.41
1:H:33:TYR:OH	1:H:127:VAL:O	2.31	0.41
1:H:72:TRP:HH2	1:H:140:LEU:HD12	1.86	0.41
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:D:136:ASN:HB2	1:D:187:GLU:O	2.21	0.41
1:D:151:ASN:O	1:D:152:ALA:HB2	2.21	0.41
1:F:234:THR:O	1:F:237:THR:HB	2.21	0.41
1:F:249:THR:CG2	1:F:253:LEU:HD22	2.51	0.41
1:G:252:ILE:HD13	1:G:252:ILE:HA	1.85	0.41
1:G:294:ASP:HB2	1:G:297:ILE:CG2	2.51	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:D:105:ARG:HD3	1:E:77:GLU:OE2	2.21	0.40
1:D:256:LEU:HD13	1:D:258:TYR:CE1	2.56	0.40
1:F:157:ILE:HD13	1:F:157:ILE:HA	1.71	0.40
1:F:279:LEU:HD23	1:F:279:LEU:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:153:ASP:HB3	1:G:154:ASN:H	1.42	0.40
1:H:149:THR:C	1:H:151:ASN:H	2.28	0.40
1:B:146:GLN:CD	1:B:146:GLN:N	2.79	0.40
1:D:116:PHE:HB2	1:D:258:TYR:OH	2.20	0.40
1:D:131:GLU:HA	1:D:132:PRO:HD3	1.95	0.40
1:D:145:ILE:HD12	1:D:191:ILE:HG23	2.03	0.40
1:G:153:ASP:O	1:G:155:GLU:N	2.55	0.40
1:H:41:ALA:HB3	1:H:102:TYR:HB3	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: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:A:46:LYS:HA	1:A:47:PRO:HD3	1.89	0.40
1:C:252:ILE:HA	1:C:252:ILE:HD13	1.51	0.40
1:D:13:ASP:HB3	1:D:143:SER:HB3	2.04	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%)	3	23
1	B	305/307 (99%)	275 (90%)	19 (6%)	11 (4%)	2	19
1	C	305/307 (99%)	274 (90%)	23 (8%)	8 (3%)	4	26
1	D	305/307 (99%)	278 (91%)	18 (6%)	9 (3%)	3	23
1	E	305/307 (99%)	280 (92%)	16 (5%)	9 (3%)	3	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	305/307 (99%)	278 (91%)	18 (6%)	9 (3%)	3	23
1	G	305/307 (99%)	278 (91%)	17 (6%)	10 (3%)	3	21
1	H	305/307 (99%)	277 (91%)	19 (6%)	9 (3%)	3	23
1	I	305/307 (99%)	276 (90%)	22 (7%)	7 (2%)	5	29
1	J	305/307 (99%)	279 (92%)	17 (6%)	9 (3%)	3	23
All	All	3050/3070 (99%)	2774 (91%)	186 (6%)	90 (3%)	3	23

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
1	I	60	ASN
1	J	60	ASN
1	A	166	ALA
1	A	294	ASP
1	B	53	ASP
1	B	154	ASN

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Mol	Chain	Res	Type
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
1	E	304	PHE
1	G	304	PHE
1	H	304	PHE
1	I	53	ASP
1	J	154	ASN
1	C	304	PHE

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Mol	Chain	Res	Type
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 ⓘ

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%)	236 (86%)	38 (14%)	3	17
1	B	274/274 (100%)	243 (89%)	31 (11%)	5	24
1	C	274/274 (100%)	238 (87%)	36 (13%)	4	19
1	D	274/274 (100%)	240 (88%)	34 (12%)	4	21
1	E	274/274 (100%)	236 (86%)	38 (14%)	3	17
1	F	274/274 (100%)	239 (87%)	35 (13%)	4	20
1	G	274/274 (100%)	240 (88%)	34 (12%)	4	21
1	H	274/274 (100%)	240 (88%)	34 (12%)	4	21
1	I	274/274 (100%)	239 (87%)	35 (13%)	4	20
1	J	274/274 (100%)	241 (88%)	33 (12%)	5	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2740/2740 (100%)	2392 (87%)	348 (13%)	4 20

All (348) 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	50	THR
1	A	56	LEU
1	A	61	THR
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	231	ARG
1	A	238	LEU
1	A	240	LEU
1	A	248	TYR
1	A	253	LEU
1	A	267	ILE
1	A	277	ILE
1	A	291	VAL
1	A	293	ASP
1	A	294	ASP
1	A	295	LEU
1	A	297	ILE

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Mol	Chain	Res	Type
1	A	304	PHE
1	B	29	LEU
1	B	32	THR
1	B	39	ILE
1	B	56	LEU
1	B	61	THR
1	B	71	LEU
1	B	79	ILE
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	157	ILE
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	231	ARG
1	B	238	LEU
1	B	240	LEU
1	B	267	ILE
1	B	277	ILE
1	B	279	LEU
1	B	291	VAL
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	79	ILE
1	C	103	ASN
1	C	118	LEU
1	C	122	ASP

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Mol	Chain	Res	Type
1	C	124	GLN
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	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	231	ARG
1	C	238	LEU
1	C	240	LEU
1	C	267	ILE
1	C	281	ILE
1	C	291	VAL
1	C	295	LEU
1	C	297	ILE
1	C	299	ARG
1	C	302	LEU
1	C	304	PHE
1	D	29	LEU
1	D	32	THR
1	D	39	ILE
1	D	56	LEU
1	D	61	THR
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

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Mol	Chain	Res	Type
1	D	157	ILE
1	D	167	SER
1	D	168	THR
1	D	174	ARG
1	D	177	HIS
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	267	ILE
1	D	281	ILE
1	D	291	VAL
1	D	295	LEU
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	61	THR
1	E	71	LEU
1	E	103	ASN
1	E	118	LEU
1	E	122	ASP
1	E	124	GLN
1	E	128	LEU
1	E	130	LEU
1	E	145	ILE
1	E	146	GLN
1	E	157	ILE
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	184	ASN
1	E	191	ILE
1	E	210	LEU

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Mol	Chain	Res	Type
1	E	212	LEU
1	E	219	SER
1	E	231	ARG
1	E	238	LEU
1	E	240	LEU
1	E	243	VAL
1	E	267	ILE
1	E	277	ILE
1	E	291	VAL
1	E	295	LEU
1	E	297	ILE
1	E	299	ARG
1	E	302	LEU
1	E	309	LEU
1	F	29	LEU
1	F	32	THR
1	F	39	ILE
1	F	40	VAL
1	F	50	THR
1	F	56	LEU
1	F	61	THR
1	F	71	LEU
1	F	87	THR
1	F	103	ASN
1	F	118	LEU
1	F	122	ASP
1	F	124	GLN
1	F	130	LEU
1	F	145	ILE
1	F	146	GLN
1	F	157	ILE
1	F	167	SER
1	F	168	THR
1	F	177	HIS
1	F	178	LEU
1	F	210	LEU
1	F	212	LEU
1	F	219	SER
1	F	231	ARG
1	F	238	LEU
1	F	240	LEU
1	F	248	TYR

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Mol	Chain	Res	Type
1	F	267	ILE
1	F	277	ILE
1	F	291	VAL
1	F	295	LEU
1	F	297	ILE
1	F	299	ARG
1	F	304	PHE
1	G	29	LEU
1	G	32	THR
1	G	39	ILE
1	G	56	LEU
1	G	61	THR
1	G	71	LEU
1	G	82	VAL
1	G	103	ASN
1	G	113	ASP
1	G	122	ASP
1	G	124	GLN
1	G	130	LEU
1	G	145	ILE
1	G	146	GLN
1	G	157	ILE
1	G	167	SER
1	G	174	ARG
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	231	ARG
1	G	238	LEU
1	G	240	LEU
1	G	267	ILE
1	G	291	VAL
1	G	293	ASP
1	G	299	ARG
1	G	302	LEU
1	G	304	PHE
1	G	315	LEU
1	H	18	ILE

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Mol	Chain	Res	Type
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	157	ILE
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	231	ARG
1	H	238	LEU
1	H	240	LEU
1	H	267	ILE
1	H	291	VAL
1	H	299	ARG
1	H	302	LEU
1	H	304	PHE
1	I	18	ILE
1	I	28	THR
1	I	29	LEU
1	I	32	THR
1	I	39	ILE
1	I	50	THR
1	I	56	LEU
1	I	61	THR
1	I	71	LEU

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Mol	Chain	Res	Type
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	231	ARG
1	I	238	LEU
1	I	240	LEU
1	I	248	TYR
1	I	267	ILE
1	I	277	ILE
1	I	291	VAL
1	I	295	LEU
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	40	VAL
1	J	56	LEU
1	J	61	THR
1	J	71	LEU
1	J	103	ASN
1	J	117	ARG
1	J	118	LEU
1	J	122	ASP
1	J	124	GLN
1	J	130	LEU
1	J	145	ILE
1	J	157	ILE
1	J	167	SER

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Mol	Chain	Res	Type
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	231	ARG
1	J	238	LEU
1	J	240	LEU
1	J	267	ILE
1	J	281	ILE
1	J	291	VAL
1	J	295	LEU
1	J	299	ARG
1	J	302	LEU
1	J	304	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	ASN
1	A	251	ASN
1	B	42	GLN
1	B	184	ASN
1	B	233	GLN
1	B	251	ASN
1	B	264	GLN
1	C	124	GLN
1	C	184	ASN
1	C	233	GLN
1	C	251	ASN
1	C	284	HIS
1	D	103	ASN
1	D	138	GLN
1	D	184	ASN
1	D	233	GLN
1	E	136	ASN
1	E	139	GLN
1	E	177	HIS
1	E	233	GLN
1	E	287	GLN

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Mol	Chain	Res	Type
1	E	298	GLN
1	F	136	ASN
1	F	169	HIS
1	F	182	GLN
1	F	233	GLN
1	F	284	HIS
1	F	285	HIS
1	G	136	ASN
1	G	177	HIS
1	G	184	ASN
1	G	298	GLN
1	H	136	ASN
1	H	298	GLN
1	I	31	GLN
1	I	89	ASN
1	I	124	GLN
1	I	125	GLN
1	I	284	HIS
1	J	138	GLN
1	J	233	GLN
1	J	285	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	H	402	-	13,15,15	2.37	8 (61%)	22,27,27	2.68	12 (54%)
2	377	J	401	-	13,15,15	2.48	9 (69%)	22,27,27	2.96	9 (40%)
2	377	G	401	-	13,15,15	2.32	8 (61%)	22,27,27	2.45	8 (36%)
2	377	C	401	-	13,15,15	2.56	8 (61%)	22,27,27	3.38	9 (40%)
2	377	F	402	-	13,15,15	2.98	9 (69%)	22,27,27	2.48	8 (36%)
2	377	F	401	-	13,15,15	2.33	7 (53%)	22,27,27	2.37	6 (27%)
2	377	A	401	-	13,15,15	2.45	8 (61%)	22,27,27	2.77	6 (27%)
2	377	B	401	-	13,15,15	2.37	9 (69%)	22,27,27	2.92	7 (31%)
2	377	A	402	-	13,15,15	2.96	9 (69%)	22,27,27	3.66	12 (54%)
2	377	C	402	-	13,15,15	2.04	6 (46%)	22,27,27	2.68	8 (36%)
2	377	H	401	-	13,15,15	2.38	8 (61%)	22,27,27	3.37	6 (27%)
2	377	E	401	-	13,15,15	2.65	10 (76%)	22,27,27	2.97	9 (40%)

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	H	402	-	-	-	0/4/3/3
2	377	J	401	-	-	-	0/4/3/3
2	377	G	401	-	-	-	0/4/3/3
2	377	C	401	-	-	-	0/4/3/3
2	377	F	402	-	-	-	0/4/3/3
2	377	F	401	-	-	-	0/4/3/3
2	377	A	401	-	-	-	0/4/3/3
2	377	B	401	-	-	-	0/4/3/3
2	377	A	402	-	-	-	0/4/3/3
2	377	C	402	-	-	-	0/4/3/3
2	377	H	401	-	-	-	0/4/3/3
2	377	E	401	-	-	-	0/4/3/3

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	402	377	C06-C02	-4.50	1.47	1.53
2	A	402	377	C08-C03	-4.36	1.47	1.53
2	A	402	377	C06-C03	-3.89	1.48	1.53
2	F	402	377	C09-C02	-3.87	1.49	1.53
2	F	402	377	C07-C02	-3.84	1.48	1.53
2	F	402	377	C06-C03	-3.82	1.48	1.53
2	A	402	377	C09-C02	-3.71	1.49	1.53
2	J	401	377	C08-C03	-3.66	1.48	1.53
2	C	401	377	C07-C02	-3.63	1.48	1.53
2	F	402	377	C10-C03	-3.60	1.49	1.53
2	H	401	377	C08-C03	-3.56	1.48	1.53
2	E	401	377	C07-C02	-3.55	1.48	1.53
2	C	401	377	C06-C03	-3.50	1.49	1.53
2	F	402	377	C06-C02	-3.46	1.49	1.53
2	C	401	377	C08-C03	-3.41	1.49	1.53
2	E	401	377	C08-C03	-3.36	1.49	1.53
2	F	401	377	C06-C03	-3.36	1.49	1.53
2	B	401	377	C06-C02	-3.33	1.49	1.53
2	E	401	377	C06-C03	-3.33	1.49	1.53
2	H	402	377	C06-C03	-3.30	1.49	1.53
2	G	401	377	C12-C02	-3.30	1.47	1.54
2	F	402	377	C08-C03	-3.28	1.49	1.53
2	A	401	377	C06-C03	-3.23	1.49	1.53
2	A	401	377	C07-C02	-3.17	1.49	1.53
2	E	401	377	C06-C02	-3.16	1.49	1.53
2	C	401	377	C06-C02	-3.15	1.49	1.53
2	A	402	377	C13-C03	-3.14	1.47	1.54
2	F	402	377	C12-C02	-3.12	1.47	1.54
2	C	402	377	C06-C03	-3.08	1.49	1.53
2	H	401	377	C06-C03	-3.08	1.49	1.53
2	C	401	377	C12-C02	-3.08	1.47	1.54
2	F	401	377	C06-C02	-3.07	1.49	1.53
2	A	401	377	C09-C02	-3.05	1.50	1.53
2	A	401	377	C12-C02	-3.03	1.47	1.54
2	G	401	377	C06-C03	-3.03	1.49	1.53
2	H	402	377	C10-C03	-3.03	1.50	1.53
2	B	401	377	C12-C02	-3.01	1.47	1.54
2	G	401	377	C06-C02	-3.01	1.49	1.53
2	H	402	377	C13-C03	-3.01	1.47	1.54
2	J	401	377	C07-C02	-3.00	1.49	1.53
2	J	401	377	C06-C02	-2.99	1.49	1.53
2	A	401	377	C06-C02	-2.97	1.49	1.53
2	E	401	377	C09-C02	-2.96	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	377	C12-C02	-2.96	1.48	1.54
2	J	401	377	C06-C03	-2.96	1.49	1.53
2	B	401	377	C07-C02	-2.91	1.49	1.53
2	H	402	377	C08-C03	-2.90	1.49	1.53
2	F	401	377	C07-C02	-2.90	1.49	1.53
2	A	402	377	C12-C02	-2.89	1.48	1.54
2	H	401	377	C12-C02	-2.88	1.48	1.54
2	B	401	377	C09-C02	-2.82	1.50	1.53
2	J	401	377	C12-C02	-2.82	1.48	1.54
2	H	402	377	C12-C02	-2.80	1.48	1.54
2	G	401	377	C10-C03	-2.75	1.50	1.53
2	F	401	377	C12-C02	-2.72	1.48	1.54
2	F	402	377	C13-C03	-2.70	1.48	1.54
2	C	402	377	C06-C02	-2.66	1.50	1.53
2	F	401	377	C09-C02	-2.66	1.50	1.53
2	A	401	377	C10-C03	-2.65	1.50	1.53
2	J	401	377	C13-C03	-2.62	1.48	1.54
2	A	402	377	C10-C03	-2.61	1.50	1.53
2	H	401	377	C09-C02	-2.60	1.50	1.53
2	J	401	377	C10-C03	-2.58	1.50	1.53
2	G	401	377	C13-C03	-2.56	1.48	1.54
2	B	401	377	C08-C03	-2.56	1.50	1.53
2	A	401	377	C08-C03	-2.55	1.50	1.53
2	H	402	377	C06-C02	-2.54	1.50	1.53
2	H	401	377	C06-C02	-2.51	1.50	1.53
2	F	401	377	C10-C03	-2.51	1.50	1.53
2	C	402	377	C12-C02	-2.47	1.49	1.54
2	E	401	377	C13-C03	-2.44	1.49	1.54
2	H	401	377	C07-C02	-2.42	1.50	1.53
2	C	402	377	C07-C02	-2.40	1.50	1.53
2	G	401	377	C09-C02	-2.39	1.50	1.53
2	B	401	377	C10-C03	-2.39	1.50	1.53
2	H	402	377	C09-C02	-2.39	1.50	1.53
2	A	401	377	C13-C03	-2.38	1.49	1.54
2	G	401	377	C07-C02	-2.36	1.50	1.53
2	E	401	377	C10-C03	-2.35	1.50	1.53
2	F	402	377	C09-C05	-2.34	1.48	1.54
2	J	401	377	C09-C05	-2.33	1.48	1.54
2	B	401	377	C13-C03	-2.32	1.49	1.54
2	G	401	377	C08-C03	-2.31	1.50	1.53
2	A	402	377	C09-C05	-2.31	1.48	1.54
2	H	402	377	C07-C02	-2.28	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	402	377	C13-C03	-2.26	1.49	1.54
2	C	401	377	C09-C02	-2.25	1.51	1.53
2	C	401	377	C11-C05	-2.25	1.48	1.54
2	H	401	377	C09-C05	-2.24	1.48	1.54
2	E	401	377	C04-N01	-2.23	1.42	1.49
2	H	401	377	C10-C03	-2.20	1.51	1.53
2	B	401	377	C06-C03	-2.20	1.50	1.53
2	C	401	377	C09-C05	-2.20	1.48	1.54
2	C	402	377	C10-C03	-2.17	1.51	1.53
2	A	402	377	C10-C05	-2.12	1.48	1.54
2	E	401	377	C09-C05	-2.12	1.48	1.54
2	F	401	377	C11-C05	-2.12	1.48	1.54
2	B	401	377	C09-C05	-2.11	1.48	1.54
2	J	401	377	C11-C05	-2.08	1.48	1.54

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	401	377	C04-C07-C02	-11.76	104.52	110.73
2	C	401	377	C04-C07-C02	-8.51	106.24	110.73
2	E	401	377	C04-C07-C02	-8.07	106.47	110.73
2	A	402	377	C07-C02-C09	8.06	113.60	108.59
2	A	401	377	C04-C07-C02	-7.76	106.64	110.73
2	A	402	377	C04-C08-C03	-7.53	106.75	110.73
2	C	401	377	C06-C02-C09	6.98	112.93	108.59
2	B	401	377	C07-C02-C09	6.91	112.88	108.59
2	C	402	377	C04-C07-C02	-6.63	107.23	110.73
2	C	402	377	C08-C03-C10	6.58	112.68	108.59
2	H	402	377	C06-C02-C09	6.55	112.66	108.59
2	A	402	377	C06-C03-C10	6.36	112.55	108.59
2	F	402	377	C04-C07-C02	-6.25	107.43	110.73
2	J	401	377	C04-C07-C02	-6.21	107.45	110.73
2	A	402	377	C12-C02-C09	-6.11	103.23	110.49
2	B	401	377	C06-C03-C10	6.11	112.39	108.59
2	B	401	377	C04-C07-C02	-6.05	107.54	110.73
2	F	401	377	C04-C07-C02	-6.05	107.54	110.73
2	H	401	377	C07-C02-C09	6.03	112.34	108.59
2	E	401	377	C04-C08-C03	-5.96	107.58	110.73
2	G	401	377	C04-C07-C02	-5.90	107.61	110.73
2	C	401	377	C04-C08-C03	-5.79	107.67	110.73
2	F	401	377	C06-C02-C09	5.58	112.06	108.59
2	J	401	377	C04-C08-C03	-5.49	107.83	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	401	377	C07-C02-C09	5.33	111.91	108.59
2	F	402	377	C07-C02-C09	5.19	111.82	108.59
2	J	401	377	C06-C02-C09	5.08	111.75	108.59
2	H	402	377	C04-C07-C02	-4.99	108.09	110.73
2	A	401	377	C06-C02-C09	4.94	111.67	108.59
2	A	401	377	C08-C03-C10	4.87	111.62	108.59
2	C	401	377	C08-C03-C10	4.77	111.56	108.59
2	B	401	377	C12-C02-C09	-4.62	105.00	110.49
2	A	401	377	C04-C08-C03	-4.38	108.42	110.73
2	B	401	377	C04-C08-C03	-4.31	108.46	110.73
2	E	401	377	C07-C02-C09	4.14	111.17	108.59
2	C	401	377	C09-C05-C11	-4.07	104.56	109.41
2	A	402	377	C06-C02-C09	4.06	111.11	108.59
2	H	401	377	C08-C03-C10	4.03	111.10	108.59
2	A	402	377	C02-C09-C05	-4.00	107.74	110.51
2	G	401	377	C04-C08-C03	-3.90	108.67	110.73
2	F	402	377	C12-C02-C07	-3.86	105.31	110.55
2	E	401	377	C09-C05-C10	-3.81	104.87	109.41
2	E	401	377	C08-C03-C10	3.80	110.95	108.59
2	G	401	377	C07-C02-C09	3.71	110.90	108.59
2	J	401	377	C08-C03-C10	3.66	110.87	108.59
2	H	401	377	C09-C05-C11	-3.64	105.07	109.41
2	J	401	377	C13-C03-C08	-3.60	105.67	110.55
2	H	402	377	C12-C02-C06	-3.51	105.79	110.55
2	C	401	377	C13-C03-C08	-3.50	105.81	110.55
2	G	401	377	C06-C02-C09	3.49	110.76	108.59
2	A	401	377	C12-C02-C06	-3.49	105.81	110.55
2	A	402	377	C04-C07-C02	-3.48	108.89	110.73
2	J	401	377	C12-C02-C09	-3.48	106.36	110.49
2	A	402	377	C03-C06-C02	-3.46	104.75	111.63
2	C	402	377	C07-C02-C09	3.44	110.73	108.59
2	F	401	377	C13-C03-C06	-3.44	105.89	110.55
2	H	401	377	C07-C02-C06	3.41	111.72	108.54
2	G	401	377	C02-C09-C05	-3.41	108.15	110.51
2	H	402	377	C08-C03-C06	3.38	111.69	108.54
2	C	402	377	C06-C03-C10	3.35	110.67	108.59
2	G	401	377	C08-C03-C10	3.27	110.63	108.59
2	E	401	377	C12-C02-C07	-3.24	106.16	110.55
2	C	401	377	C13-C03-C10	3.15	114.23	110.49
2	H	402	377	C08-C03-C10	3.12	110.53	108.59
2	F	401	377	C12-C02-C06	-3.10	106.35	110.55
2	H	402	377	C09-C05-C10	-3.07	105.75	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	402	377	C13-C03-C08	-3.00	106.48	110.55
2	C	402	377	C08-C03-C06	-2.98	105.77	108.54
2	F	401	377	C04-C08-C03	-2.94	109.18	110.73
2	C	401	377	C12-C02-C06	-2.93	106.58	110.55
2	F	402	377	C07-C02-C06	2.90	111.24	108.54
2	H	402	377	C04-C08-C03	-2.89	109.21	110.73
2	E	401	377	C13-C03-C08	-2.87	106.65	110.55
2	J	401	377	C09-C05-C11	-2.81	106.06	109.41
2	F	402	377	C02-C09-C05	-2.81	108.56	110.51
2	F	402	377	C04-C08-C03	-2.81	109.25	110.73
2	G	401	377	C12-C02-C06	-2.76	106.81	110.55
2	H	402	377	C13-C03-C08	-2.75	106.82	110.55
2	C	402	377	C07-C02-C06	2.70	111.06	108.54
2	J	401	377	C03-C10-C05	2.69	112.38	110.51
2	G	401	377	C12-C02-C09	-2.61	107.39	110.49
2	H	401	377	C12-C02-C07	-2.57	107.07	110.55
2	B	401	377	C13-C03-C10	-2.54	107.47	110.49
2	H	402	377	C06-C03-C10	-2.47	107.06	108.59
2	C	401	377	C06-C03-C10	-2.45	107.07	108.59
2	A	402	377	C13-C03-C10	-2.45	107.58	110.49
2	H	402	377	C03-C06-C02	-2.43	106.79	111.63
2	E	401	377	C07-C02-C06	2.41	110.78	108.54
2	C	402	377	C12-C02-C06	-2.40	107.30	110.55
2	H	402	377	C07-C02-C06	2.38	110.76	108.54
2	A	401	377	C03-C10-C05	-2.36	108.88	110.51
2	A	402	377	C09-C05-C10	-2.34	106.61	109.41
2	B	401	377	C03-C06-C02	-2.23	107.20	111.63
2	C	402	377	C03-C10-C05	-2.20	108.99	110.51
2	F	402	377	C03-C06-C02	-2.19	107.27	111.63
2	F	401	377	C06-C03-C10	2.18	109.95	108.59
2	F	402	377	C08-C03-C06	2.16	110.55	108.54
2	H	402	377	C12-C02-C09	-2.14	107.95	110.49
2	A	402	377	C08-C03-C06	2.07	110.47	108.54
2	E	401	377	C12-C02-C09	-2.02	108.09	110.49

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	H	402	377	2	0
2	J	401	377	3	0
2	C	401	377	1	0
2	F	402	377	3	0
2	A	401	377	2	0
2	B	401	377	1	0
2	C	402	377	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	307/307 (100%)	0.08	7 (2%) 61 41	74, 118, 193, 267	0
1	B	307/307 (100%)	0.02	17 (5%) 30 19	74, 103, 203, 322	0
1	C	307/307 (100%)	0.09	16 (5%) 33 21	66, 102, 199, 249	0
1	D	307/307 (100%)	-0.01	9 (2%) 53 35	69, 101, 200, 262	0
1	E	307/307 (100%)	0.14	15 (4%) 35 22	77, 113, 191, 247	0
1	F	307/307 (100%)	0.10	14 (4%) 37 23	76, 116, 204, 258	0
1	G	307/307 (100%)	0.25	25 (8%) 18 11	69, 105, 188, 269	0
1	H	307/307 (100%)	0.10	14 (4%) 37 23	72, 110, 216, 256	0
1	I	307/307 (100%)	0.18	19 (6%) 26 17	70, 107, 203, 302	0
1	J	307/307 (100%)	0.13	16 (5%) 33 21	80, 119, 214, 266	0
All	All	3070/3070 (100%)	0.11	152 (4%) 34 22	66, 110, 204, 322	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	291	VAL	9.7
1	E	290	GLY	7.8
1	A	175	TYR	6.7
1	B	291	VAL	5.9
1	G	291	VAL	5.1
1	G	288	ALA	4.9
1	C	309	LEU	4.7
1	C	172	ASP	4.4
1	H	291	VAL	4.3
1	B	295	LEU	4.3
1	J	305	PRO	4.1
1	D	245	TYR	4.1
1	I	64	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	176	ASP	4.0
1	E	289	ASN	4.0
1	G	125	GLN	4.0
1	G	126	PHE	4.0
1	D	317	ILE	3.9
1	E	180	SER	3.9
1	B	289	ASN	3.8
1	C	181	VAL	3.8
1	F	175	TYR	3.8
1	H	309	LEU	3.7
1	A	188	PHE	3.7
1	B	290	GLY	3.7
1	I	182	GLN	3.5
1	G	255	ARG	3.5
1	D	248	TYR	3.5
1	J	69	ASN	3.5
1	D	181	VAL	3.5
1	G	285	HIS	3.4
1	I	250	SER	3.3
1	J	82	VAL	3.3
1	I	178	LEU	3.3
1	C	302	LEU	3.2
1	B	179	SER	3.2
1	C	291	VAL	3.2
1	F	285	HIS	3.2
1	B	293	ASP	3.2
1	G	290	GLY	3.2
1	E	295	LEU	3.2
1	I	251	ASN	3.2
1	B	181	VAL	3.2
1	B	183	PRO	3.1
1	G	298	GLN	3.1
1	F	11	PRO	3.1
1	J	315	LEU	3.1
1	J	11	PRO	3.1
1	E	179	SER	3.1
1	C	11	PRO	3.0
1	G	160	TRP	3.0
1	G	293	ASP	3.0
1	J	317	ILE	3.0
1	B	288	ALA	2.9
1	G	179	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	I	290	GLY	2.9
1	A	302	LEU	2.9
1	H	179	SER	2.9
1	H	180	SER	2.9
1	G	169	HIS	2.9
1	G	11	PRO	2.9
1	I	248	TYR	2.9
1	I	179	SER	2.9
1	I	219	SER	2.9
1	B	169	HIS	2.8
1	G	250	SER	2.8
1	E	181	VAL	2.8
1	C	179	SER	2.8
1	G	181	VAL	2.8
1	D	161	TRP	2.7
1	E	206	TRP	2.7
1	I	296	LEU	2.7
1	H	150	GLU	2.7
1	G	156	GLU	2.7
1	J	250	SER	2.7
1	A	181	VAL	2.7
1	G	251	ASN	2.7
1	E	152	ALA	2.7
1	C	308	PHE	2.6
1	E	183	PRO	2.6
1	F	154	ASN	2.6
1	E	296	LEU	2.6
1	H	306	LEU	2.6
1	A	291	VAL	2.6
1	C	314	VAL	2.6
1	B	226	GLU	2.6
1	J	49	LYS	2.6
1	G	252	ILE	2.6
1	I	180	SER	2.6
1	G	315	LEU	2.5
1	D	53	ASP	2.5
1	B	11	PRO	2.5
1	C	178	LEU	2.5
1	I	304	PHE	2.5
1	J	153	ASP	2.5
1	H	308	PHE	2.4
1	F	295	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	181	VAL	2.4
1	J	304	PHE	2.4
1	I	252	ILE	2.4
1	J	181	VAL	2.4
1	C	32	THR	2.3
1	C	296	LEU	2.3
1	J	298	GLN	2.3
1	I	152	ALA	2.3
1	F	291	VAL	2.3
1	E	11	PRO	2.3
1	E	71	LEU	2.3
1	I	285	HIS	2.3
1	F	151	ASN	2.3
1	E	288	ALA	2.3
1	C	180	SER	2.2
1	F	231	ARG	2.2
1	G	289	ASN	2.2
1	B	97	ASP	2.2
1	G	178	LEU	2.2
1	H	183	PRO	2.2
1	B	150	GLU	2.2
1	H	188	PHE	2.2
1	G	161	TRP	2.2
1	F	226	GLU	2.2
1	H	288	ALA	2.2
1	H	11	PRO	2.2
1	B	298	GLN	2.1
1	H	305	PRO	2.1
1	C	315	LEU	2.1
1	H	296	LEU	2.1
1	J	307	GLY	2.1
1	B	297	ILE	2.1
1	J	145	ILE	2.1
1	G	282	PHE	2.1
1	I	181	VAL	2.1
1	H	91	ARG	2.1
1	C	288	ALA	2.1
1	F	288	ALA	2.1
1	A	290	GLY	2.1
1	J	52	GLY	2.1
1	D	291	VAL	2.1
1	D	178	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	152	ALA	2.1
1	A	298	GLN	2.1
1	D	295	LEU	2.0
1	I	151	ASN	2.0
1	I	177	HIS	2.0
1	G	183	PRO	2.0
1	E	302	LEU	2.0
1	G	295	LEU	2.0
1	B	113	ASP	2.0
1	J	172	ASP	2.0
1	F	91	ARG	2.0
1	C	295	LEU	2.0
1	I	63	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	377	F	401	13/13	0.93	0.15	111,115,119,121	0
2	377	H	401	13/13	0.93	0.13	106,113,120,120	0
2	377	A	402	13/13	0.94	0.21	95,102,109,113	0
2	377	H	402	13/13	0.94	0.13	96,101,107,107	0
2	377	F	402	13/13	0.96	0.18	116,119,130,134	0
2	377	C	402	13/13	0.96	0.10	84,88,91,91	0
2	377	A	401	13/13	0.96	0.14	130,135,138,138	0
2	377	B	401	13/13	0.97	0.11	101,105,109,115	0
2	377	G	401	13/13	0.97	0.13	105,108,116,117	0
2	377	E	401	13/13	0.97	0.13	92,97,104,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	377	C	401	13/13	0.97	0.11	92,97,106,108	0
2	377	J	401	13/13	0.97	0.09	91,97,98,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.