



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:11 AM UTC

PDB ID : 5LID / pdb_00005lid
Title : X-ray structure of a pentameric ligand gated ion channel from *Erwinia chrysanthemi* (ELIC) in complex with bromopromazine
Authors : Nys, M.; Wijckmans, E.; Farinha, A.; Brams, M.; Spurny, R.; Ulens, C.
Deposited on : 2016-07-14
Resolution : 4.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

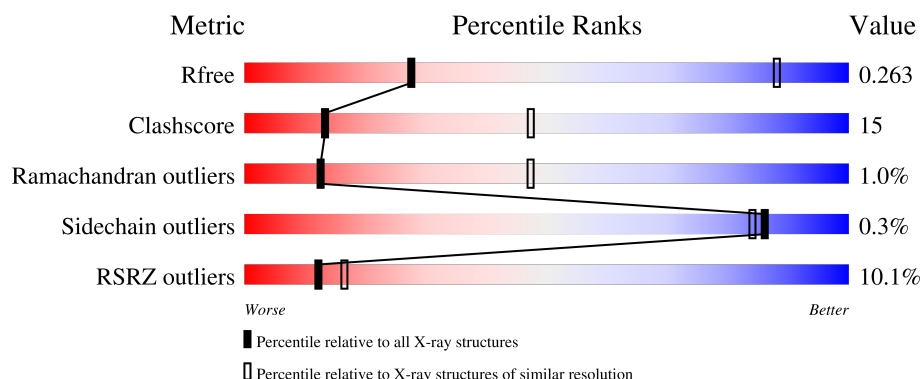
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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	1127 (5.10-3.90)
Clashscore	190562	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)

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	7% 74% 25% .
1	B	307	16% 66% 33% .
1	C	307	8% 66% 33% .
1	D	307	12% 68% 31% .
1	E	307	10% 64% 34% .

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Mol	Chain	Length	Quality of chain
1	F	307	
1	G	307	
1	H	307	
1	I	307	
1	J	307	

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	6XY	B	402	-	-	-	X
2	6XY	D	401	-	-	-	X
2	6XY	H	402	-	-	-	X
2	6XY	J	401	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25070 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
			2505	1633	416	450	6			
1	B	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	C	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	D	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	E	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	F	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	G	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	H	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	I	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	J	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			

There are 20 discrepancies between the modelled and reference sequences:

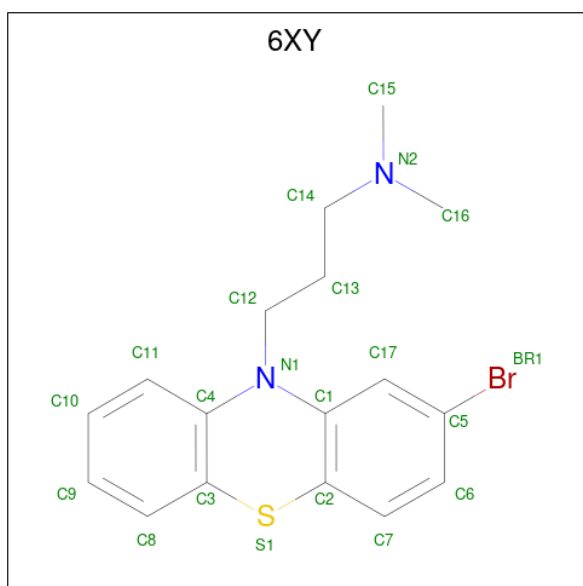
Chain	Residue	Modelled	Actual	Comment	Reference
A	164	GLY	-	insertion	UNP P0C7B7
A	289	ASN	MET	conflict	UNP P0C7B7
B	164	GLY	-	insertion	UNP P0C7B7
B	289	ASN	MET	conflict	UNP P0C7B7
C	164	GLY	-	insertion	UNP P0C7B7
C	289	ASN	MET	conflict	UNP P0C7B7
D	164	GLY	-	insertion	UNP P0C7B7
D	289	ASN	MET	conflict	UNP P0C7B7
E	164	GLY	-	insertion	UNP P0C7B7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	289	ASN	MET	conflict	UNP P0C7B7
F	164	GLY	-	insertion	UNP P0C7B7
F	289	ASN	MET	conflict	UNP P0C7B7
G	164	GLY	-	insertion	UNP P0C7B7
G	289	ASN	MET	conflict	UNP P0C7B7
H	164	GLY	-	insertion	UNP P0C7B7
H	289	ASN	MET	conflict	UNP P0C7B7
I	164	GLY	-	insertion	UNP P0C7B7
I	289	ASN	MET	conflict	UNP P0C7B7
J	164	GLY	-	insertion	UNP P0C7B7
J	289	ASN	MET	conflict	UNP P0C7B7

- Molecule 2 is bromopromazine (CCD ID: 6XY) (formula: $C_{17}H_{19}BrN_2S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Br 1 1	0	0
2	A	1	Total Br 1 1	0	0
2	B	1	Total Br 1 1	0	0
2	B	1	Total Br 1 1	0	0
2	C	1	Total Br 1 1	0	0
2	C	1	Total Br 1 1	0	0

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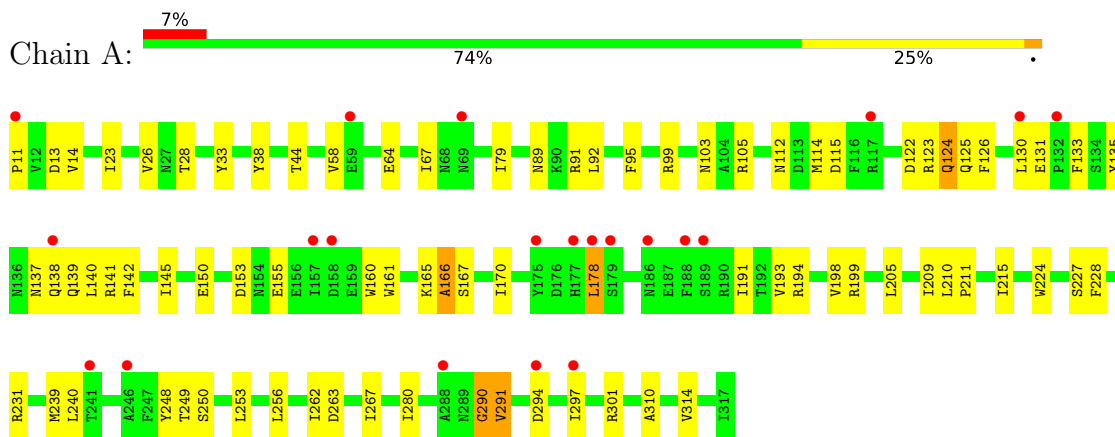
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total 1	Br 1	0	0
2	D	1	Total 1	Br 1	0	0
2	E	1	Total 1	Br 1	0	0
2	E	1	Total 1	Br 1	0	0
2	F	1	Total 1	Br 1	0	0
2	F	1	Total 1	Br 1	0	0
2	G	1	Total 1	Br 1	0	0
2	G	1	Total 1	Br 1	0	0
2	H	1	Total 1	Br 1	0	0
2	H	1	Total 1	Br 1	0	0
2	I	1	Total 1	Br 1	0	0
2	I	1	Total 1	Br 1	0	0
2	J	1	Total 1	Br 1	0	0
2	J	1	Total 1	Br 1	0	0

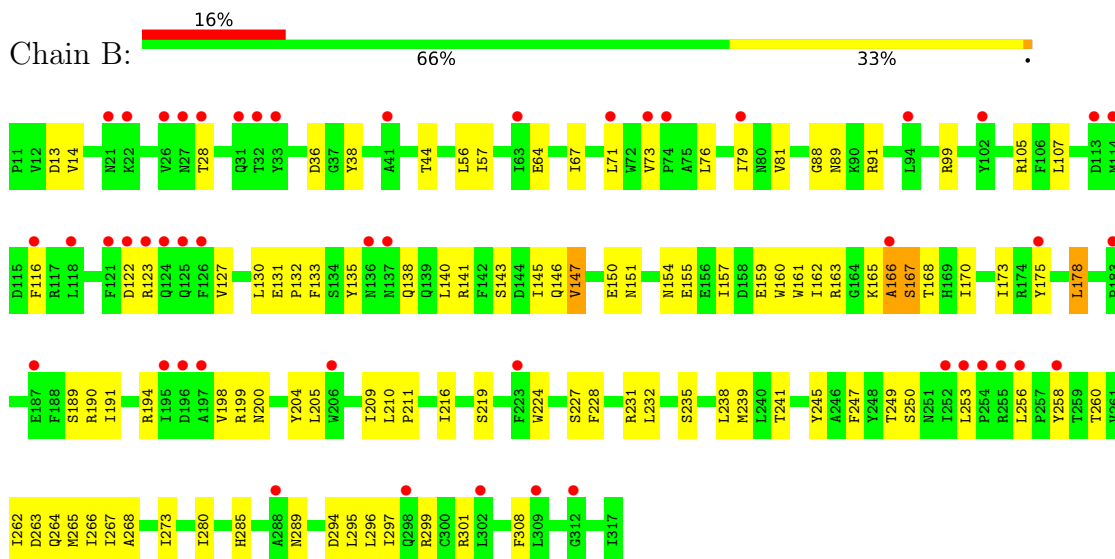
3 Residue-property plots [i](#)

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

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

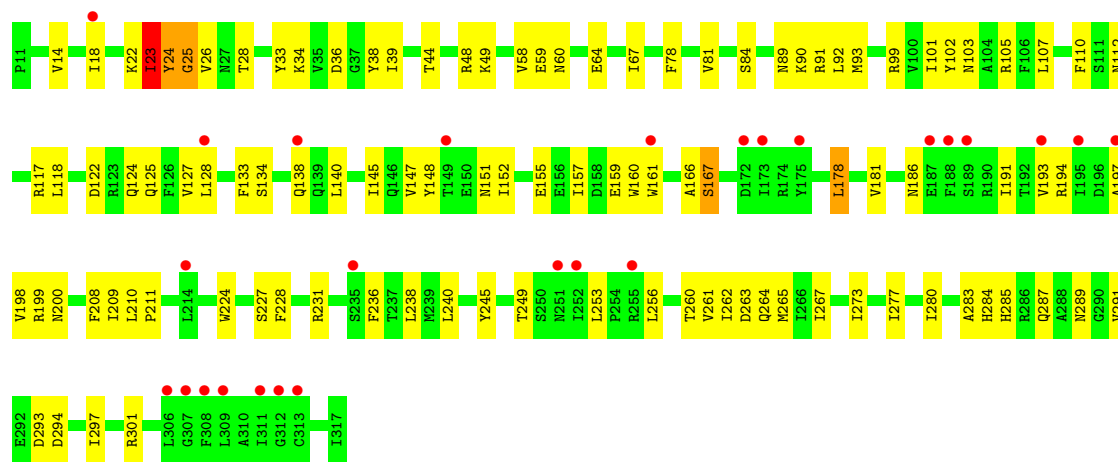


- Molecule 1: Cys-loop ligand-gated ion channel

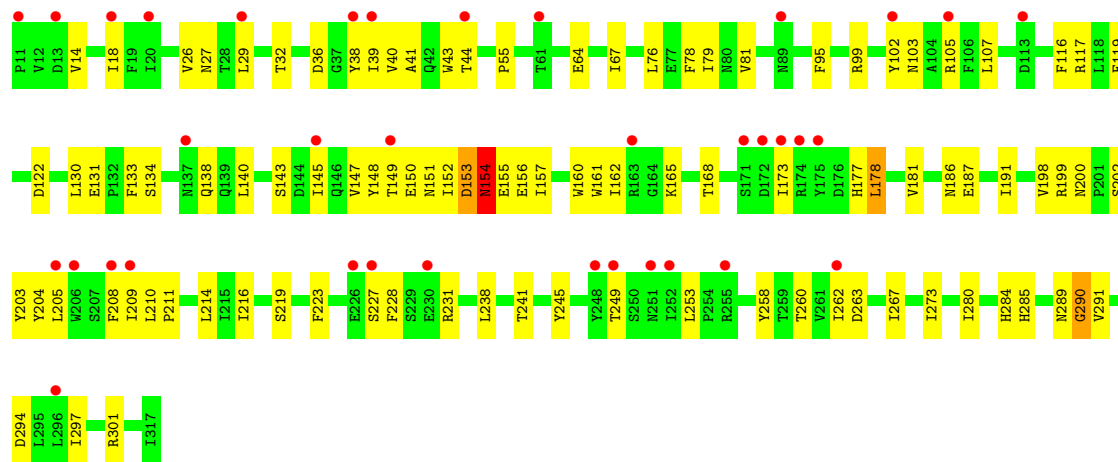


- Molecule 1: Cys-loop ligand-gated ion channel

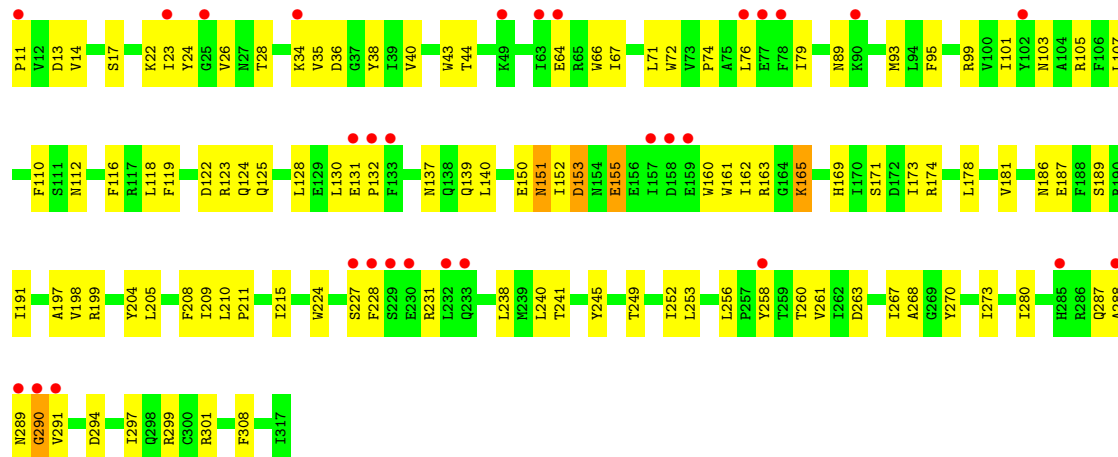




• Molecule 1: Cys-loop ligand-gated ion channel



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



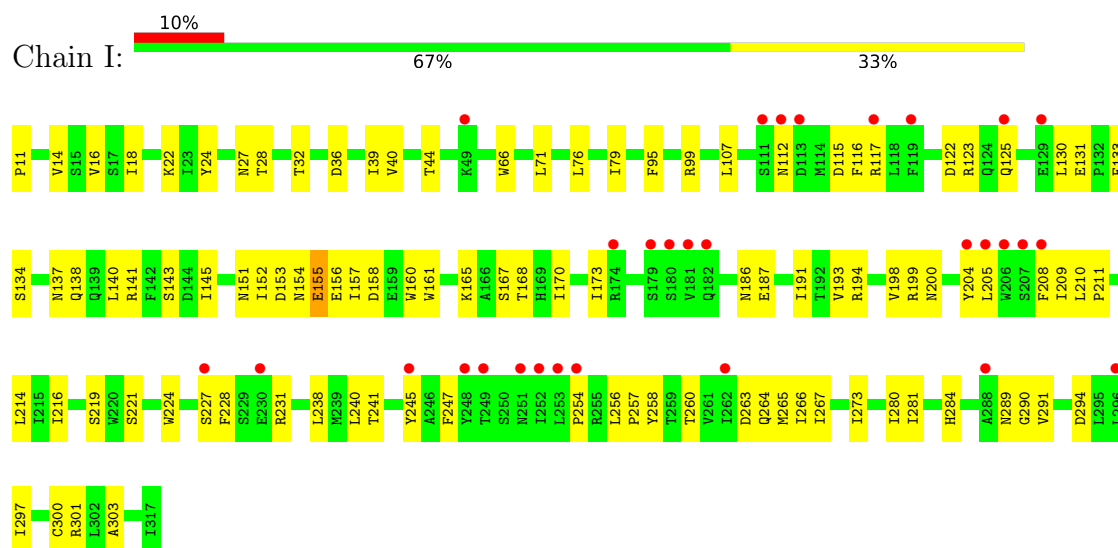
Chain F:

[illegible]

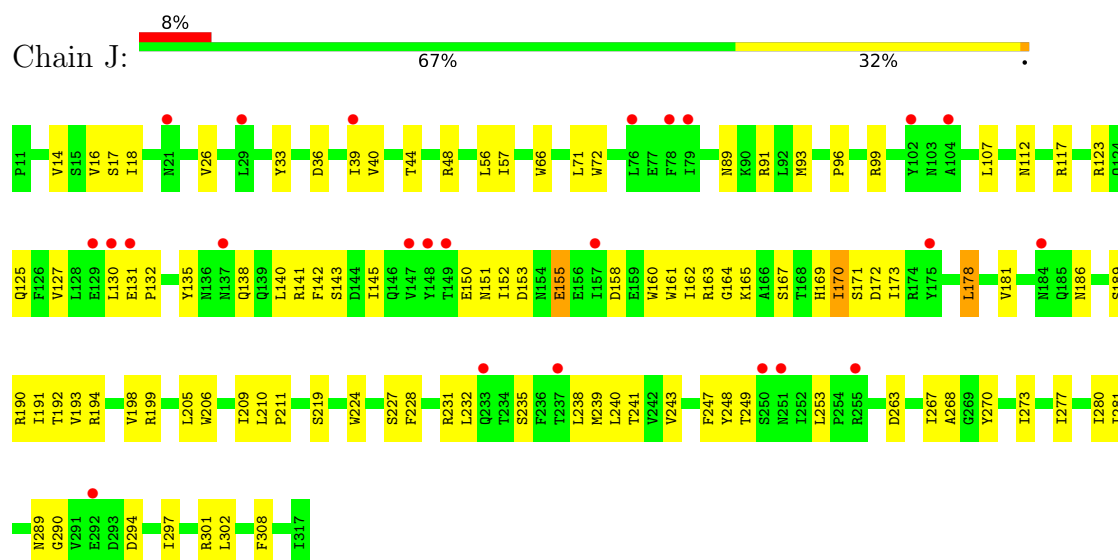
Chain H:

F11	F10	N186	I280
F12	S111	F187	R286
D13	D113	E188	Q287
F14		I191	A288
S15	L118	T192	E292
S17	F119	V193	C300
I18	P120	R194	R301
	F121	V198	L302
I23	R123	R199	A303
C25	Q124	Y204	L309
V26	L128	L205	A310
N27	E129	F208	I311
T28	L130	T209	G312
L29	E131	L210	I317
E30		P211	
Q31	S134	A217	
T32	V135	W220	
F33	N136	S221	
K34	N137	W224	
V35	Q138	L225	
D36	E139	E226	
G37	L140	S227	
F38	R141	F228	
I39	I145	R231	
V40		L232	
A41	T149	F236	
	E150	T237	
T44	M151	L238	
L56	I152	M239	
I57	D153	L240	
V58	M154	T241	
E64	E155	A244	
R65	E156	T249	
W66	I157	L253	
I67	E159	L256	
	V160	T259	
F78	W161	T260	
I79	R162	V261	
	R163	L262	
N89	A166	D263	
R90	S167	Q264	
R91	I170	I273	
L92		L277	
M93	I173		
R99	L178		
V100	S179		
I101	E180		
I102	V181		
N103	P182		
A104	P183		
R105	M184		
L107	E185		
F106			
I108			

• 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	105.72Å 267.91Å 111.33Å 90.00° 106.70° 90.00°	Depositor
Resolution (Å)	49.54 – 4.50 49.54 – 4.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.54-4.50) 99.8 (49.54-4.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.212 , 0.257 0.215 , 0.263	Depositor DCC
R_{free} test set	3118 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	161.1	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 116.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	25070	wwPDB-VP
Average B, all atoms (Å ²)	214.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6XY

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	0.22	0/2573	0.51	0/3507
1	B	0.20	0/2573	0.54	0/3507
1	C	0.22	0/2573	0.56	1/3507 (0.0%)
1	D	0.25	0/2573	0.59	1/3507 (0.0%)
1	E	0.25	0/2573	0.59	2/3507 (0.1%)
1	F	0.20	0/2573	0.50	0/3507
1	G	0.20	0/2573	0.50	0/3507
1	H	0.22	0/2573	0.50	1/3507 (0.0%)
1	I	0.24	0/2573	0.52	0/3507
1	J	0.21	0/2573	0.54	0/3507
All	All	0.22	0/25730	0.54	5/35070 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	I	0	1
1	J	0	2
All	All	0	4

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	154	ASN	N-CA-C	-6.69	96.55	110.80
1	H	166	ALA	N-CA-C	5.28	122.05	110.80
1	C	23	ILE	N-CA-C	-5.05	98.84	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	151	ASN	CA-C-N	5.01	130.71	121.70
1	E	151	ASN	C-N-CA	5.01	130.71	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	290	GLY	Peptide
1	I	155	GLU	Peptide
1	J	155	GLU	Peptide
1	J	164	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2505	0	2478	59	0
1	B	2505	0	2478	78	0
1	C	2505	0	2478	92	0
1	D	2505	0	2478	84	0
1	E	2505	0	2478	89	0
1	F	2505	0	2478	66	0
1	G	2505	0	2478	77	0
1	H	2505	0	2478	82	0
1	I	2505	0	2478	84	0
1	J	2505	0	2478	84	0
2	A	2	0	0	3	0
2	B	2	0	0	0	0
2	C	2	0	0	4	0
2	D	2	0	0	2	0
2	E	2	0	0	6	0
2	F	2	0	0	5	0
2	G	2	0	0	2	0
2	H	2	0	0	3	0
2	I	2	0	0	2	0
2	J	2	0	0	6	0
All	All	25070	0	24780	736	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 (736) 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:J:160:TRP:CZ3	2:J:402:6XY:BR1	2.36	1.33
1:E:160:TRP:CD1	2:E:402:6XY:BR1	2.50	1.19
1:E:160:TRP:NE1	2:E:402:6XY:BR1	2.33	1.16
1:F:160:TRP:NE1	2:F:402:6XY:BR1	2.40	1.08
1:C:24:TYR:HA	2:C:402:6XY:BR1	2.14	1.03
1:H:160:TRP:NE1	2:H:402:6XY:BR1	2.50	0.99
1:J:160:TRP:CH2	2:J:402:6XY:BR1	2.73	0.95
1:H:167:SER:HB2	1:H:194:ARG:HG3	1.53	0.91
1:D:155:GLU:HB3	1:D:156:GLU:HA	1.53	0.89
1:E:151:ASN:HD21	1:E:161:TRP:CD1	1.91	0.87
1:A:140:LEU:HD13	1:A:191:ILE:HG13	1.57	0.87
1:D:18:ILE:HB	1:D:145:ILE:HG22	1.56	0.87
1:G:160:TRP:NE1	2:G:402:6XY:BR1	2.62	0.87
1:I:205:LEU:HD23	1:I:209:ILE:HG13	1.57	0.86
1:G:155:GLU:HG3	1:G:161:TRP:CD1	2.10	0.86
1:D:140:LEU:HD13	1:D:191:ILE:HG13	1.55	0.86
1:J:169:HIS:CE1	1:J:171:SER:HB2	2.12	0.84
1:B:150:GLU:OE1	1:B:154:ASN:ND2	2.11	0.83
1:D:155:GLU:HB3	1:D:156:GLU:CA	2.08	0.83
1:E:151:ASN:HD21	1:E:161:TRP:HD1	1.26	0.83
1:A:160:TRP:NE1	2:A:401:6XY:BR1	2.67	0.82
1:A:44:THR:HA	1:A:99:ARG:HA	1.60	0.82
1:E:38:TYR:HE1	1:E:105:ARG:HD2	1.42	0.82
1:I:140:LEU:HD13	1:I:191:ILE:HG13	1.60	0.82
1:D:122:ASP:HB2	1:D:199:ARG:HG3	1.62	0.81
1:G:160:TRP:CD1	2:G:402:6XY:BR1	2.89	0.81
1:F:79:ILE:HD11	1:F:131:GLU:HB3	1.64	0.79
1:H:160:TRP:CD1	2:H:402:6XY:BR1	2.92	0.78
1:C:24:TYR:CA	2:C:402:6XY:BR1	2.87	0.78
1:E:160:TRP:HD1	2:E:402:6XY:BR1	2.17	0.77
1:I:167:SER:OG	1:I:194:ARG:O	2.02	0.77
1:D:44:THR:HA	1:D:99:ARG:HA	1.67	0.77
1:I:36:ASP:HB2	1:I:107:LEU:HD13	1.68	0.76
1:J:231:ARG:HB3	1:J:280:ILE:HD13	1.66	0.76
1:D:154:ASN:HB2	1:D:155:GLU:HA	1.68	0.76
1:B:160:TRP:HB2	1:B:198:VAL:O	1.86	0.76
1:C:44:THR:HG22	1:C:99:ARG:HB3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:14:VAL:HG21	1:I:138:GLN:HE21	1.50	0.76
1:C:26:VAL:HG21	1:C:199:ARG:HH22	1.52	0.74
1:I:112:ASN:ND2	1:I:125:GLN:O	2.21	0.74
1:J:155:GLU:HA	1:J:158:ASP:H	1.53	0.74
1:J:44:THR:HA	1:J:99:ARG:HA	1.69	0.74
1:B:44:THR:HA	1:B:99:ARG:HA	1.68	0.73
1:F:26:VAL:HG23	2:F:402:6XY:BR1	2.43	0.73
1:C:145:ILE:HG21	1:C:193:VAL:HG11	1.68	0.73
1:E:140:LEU:HD13	1:E:191:ILE:HG13	1.69	0.73
1:F:151:ASN:ND2	1:F:162:ILE:O	2.22	0.73
1:A:14:VAL:HG21	1:A:138:GLN:HE21	1.52	0.72
1:G:205:LEU:HD23	1:G:209:ILE:HG13	1.71	0.72
1:J:169:HIS:HE1	1:J:171:SER:HB2	1.51	0.72
1:A:112:ASN:ND2	1:A:125:GLN:O	2.22	0.72
1:E:26:VAL:HG23	2:E:402:6XY:BR1	2.44	0.72
1:H:231:ARG:HB3	1:H:280:ILE:HD13	1.70	0.72
1:H:140:LEU:HD13	1:H:191:ILE:HG13	1.72	0.72
1:E:231:ARG:HB3	1:E:280:ILE:HD13	1.72	0.72
1:D:160:TRP:NE1	2:D:402:6XY:BR1	2.76	0.72
1:E:150:GLU:O	1:E:153:ASP:HB2	1.89	0.71
1:H:241:THR:HA	1:I:240:LEU:HD23	1.71	0.71
1:I:153:ASP:O	1:I:155:GLU:N	2.20	0.71
1:I:44:THR:HA	1:I:99:ARG:HA	1.71	0.71
1:C:140:LEU:HD13	1:C:191:ILE:HG13	1.70	0.71
1:D:205:LEU:HD23	1:D:209:ILE:HG13	1.73	0.71
1:B:238:LEU:HB3	1:B:273:ILE:HD13	1.73	0.70
1:E:122:ASP:HB3	1:E:124:GLN:HE22	1.57	0.70
1:J:155:GLU:HG3	1:J:161:TRP:CD1	2.26	0.70
1:C:160:TRP:HA	1:C:198:VAL:O	1.91	0.70
1:B:14:VAL:HG21	1:B:138:GLN:HE21	1.56	0.69
1:F:36:ASP:HB2	1:F:107:LEU:HD13	1.74	0.69
1:H:44:THR:HA	1:H:99:ARG:HA	1.73	0.69
1:B:151:ASN:HD21	1:B:161:TRP:HB3	1.58	0.69
1:H:157:ILE:HD11	1:I:115:ASP:HA	1.74	0.69
1:D:151:ASN:ND2	1:D:154:ASN:OD1	2.25	0.69
1:J:160:TRP:HZ3	2:J:402:6XY:BR1	2.27	0.69
1:C:44:THR:HA	1:C:99:ARG:HA	1.75	0.68
1:G:231:ARG:HB3	1:G:280:ILE:HD13	1.73	0.68
1:F:44:THR:HA	1:F:99:ARG:HA	1.76	0.68
1:G:140:LEU:HD13	1:G:191:ILE:HG13	1.76	0.68
1:I:160:TRP:CD1	2:I:402:6XY:BR1	3.03	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:171:SER:OG	1:J:172:ASP:N	2.25	0.67
1:E:93:MET:HB2	1:E:101:ILE:HB	1.76	0.67
1:C:160:TRP:NE1	2:C:402:6XY:BR1	2.83	0.67
1:C:249:THR:HG23	1:C:253:LEU:HD22	1.76	0.67
1:G:71:LEU:HD11	1:G:94:LEU:HD21	1.77	0.66
1:D:249:THR:HG23	1:D:253:LEU:HD22	1.77	0.66
1:H:155:GLU:HA	1:H:158:ASP:HB2	1.76	0.66
1:E:26:VAL:CG2	2:E:402:6XY:BR1	2.99	0.66
1:G:143:SER:HB2	1:G:170:ILE:HD11	1.77	0.66
1:B:205:LEU:HD23	1:B:209:ILE:HG13	1.77	0.66
1:C:167:SER:HB2	1:C:194:ARG:HG3	1.77	0.66
1:D:154:ASN:CB	1:D:155:GLU:HA	2.26	0.66
1:E:38:TYR:CE1	1:E:105:ARG:HD2	2.29	0.66
1:A:64:GLU:HA	1:A:67:ILE:HD12	1.79	0.65
1:G:93:MET:HB2	1:G:101:ILE:HB	1.77	0.65
1:I:155:GLU:HG2	1:I:158:ASP:HB3	1.78	0.65
1:J:26:VAL:HG23	2:J:402:6XY:BR1	2.51	0.65
1:D:18:ILE:HG12	1:D:39:ILE:HG13	1.78	0.65
1:B:241:THR:HA	1:C:240:LEU:HD23	1.79	0.65
1:J:26:VAL:CG2	2:J:402:6XY:BR1	3.00	0.65
1:A:205:LEU:HD23	1:A:209:ILE:HG13	1.78	0.65
1:D:14:VAL:HG22	1:D:43:TRP:HB3	1.79	0.65
1:G:238:LEU:HB3	1:G:273:ILE:HD13	1.78	0.65
1:J:36:ASP:HB2	1:J:107:LEU:HD13	1.78	0.65
1:I:22:LYS:HE3	1:I:24:TYR:HB3	1.79	0.64
1:H:14:VAL:HG21	1:H:138:GLN:HE21	1.62	0.64
1:I:44:THR:HG22	1:I:99:ARG:HB3	1.78	0.64
1:A:79:ILE:HD11	1:A:131:GLU:HB3	1.79	0.64
1:C:231:ARG:HB3	1:C:280:ILE:HD13	1.79	0.64
1:J:155:GLU:HG3	1:J:161:TRP:HD1	1.61	0.64
1:D:14:VAL:HG21	1:D:138:GLN:HE21	1.62	0.64
1:E:36:ASP:HB2	1:E:107:LEU:HD13	1.80	0.64
1:G:161:TRP:HB2	1:G:198:VAL:HB	1.80	0.64
1:A:160:TRP:CD1	2:A:401:6XY:BR1	3.06	0.63
1:G:241:THR:HA	1:H:240:LEU:HD23	1.80	0.63
1:E:44:THR:HA	1:E:99:ARG:HA	1.80	0.63
1:D:214:LEU:HD12	1:E:270:TYR:HB3	1.79	0.63
1:E:122:ASP:HB3	1:E:124:GLN:NE2	2.12	0.63
1:B:79:ILE:HD11	1:B:131:GLU:HB3	1.79	0.63
1:E:151:ASN:ND2	1:E:161:TRP:CD1	2.66	0.63
1:F:26:VAL:CG2	2:F:402:6XY:BR1	3.02	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:VAL:HG21	1:B:138:GLN:NE2	2.14	0.63
1:E:23:ILE:HG13	1:E:24:TYR:H	1.64	0.63
1:D:26:VAL:HG21	1:D:160:TRP:HZ2	1.64	0.62
1:F:249:THR:HG23	1:F:253:LEU:HD22	1.80	0.62
1:H:287:GLN:HB2	1:H:292:GLU:HB3	1.81	0.62
1:J:14:VAL:O	1:J:141:ARG:N	2.28	0.62
1:F:240:LEU:HD23	1:J:241:THR:HA	1.81	0.62
1:E:152:ILE:HG12	1:E:161:TRP:HE1	1.65	0.62
1:H:64:GLU:HA	1:H:67:ILE:HD12	1.81	0.62
1:J:238:LEU:HB3	1:J:273:ILE:HD13	1.81	0.62
1:E:151:ASN:ND2	1:E:161:TRP:HD1	1.96	0.62
1:A:150:GLU:HG2	1:A:153:ASP:HB2	1.82	0.62
1:F:14:VAL:HG21	1:F:138:GLN:NE2	2.15	0.62
1:B:170:ILE:HG12	1:B:191:ILE:HG12	1.82	0.62
1:E:152:ILE:HG12	1:E:161:TRP:NE1	2.15	0.62
1:E:173:ILE:O	1:E:187:GLU:HA	2.00	0.62
1:F:238:LEU:HB3	1:F:273:ILE:HD13	1.81	0.61
1:G:14:VAL:HG21	1:G:138:GLN:HE21	1.66	0.61
1:I:241:THR:HA	1:J:240:LEU:HD23	1.80	0.61
1:D:149:THR:HB	1:D:162:ILE:HG21	1.82	0.61
1:D:103:ASN:HB3	2:D:401:6XY:BR1	2.55	0.61
1:J:140:LEU:HD13	1:J:191:ILE:HG13	1.83	0.61
1:B:260:THR:O	1:B:264:GLN:HG3	2.00	0.61
1:G:64:GLU:HA	1:G:67:ILE:HD12	1.82	0.61
1:H:205:LEU:HD23	1:H:209:ILE:HG13	1.80	0.61
1:C:166:ALA:O	1:C:167:SER:OG	2.17	0.61
1:E:205:LEU:HD23	1:E:209:ILE:HG13	1.83	0.60
1:A:253:LEU:HD21	1:A:262:ILE:HD12	1.82	0.60
1:H:238:LEU:HB3	1:H:273:ILE:HD13	1.84	0.60
1:J:150:GLU:HG2	1:J:153:ASP:HB2	1.83	0.60
1:C:26:VAL:HG21	1:C:199:ARG:NH2	2.16	0.60
1:F:93:MET:HB2	1:F:101:ILE:HB	1.82	0.60
1:A:210:LEU:HB3	1:A:211:PRO:HD3	1.83	0.60
1:H:28:THR:HB	1:H:256:LEU:HD21	1.83	0.60
1:E:249:THR:HG23	1:E:253:LEU:HD22	1.84	0.60
1:E:289:ASN:O	1:E:291:VAL:N	2.33	0.60
1:I:231:ARG:HB3	1:I:280:ILE:HD13	1.84	0.60
1:J:160:TRP:CE3	2:J:402:6XY:BR1	3.06	0.60
1:J:151:ASN:ND2	1:J:155:GLU:OE2	2.35	0.60
1:C:22:LYS:HG2	1:C:23:ILE:O	2.02	0.59
1:C:24:TYR:HE2	1:C:34:LYS:HD2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:18:ILE:HG12	1:G:39:ILE:HG13	1.84	0.59
1:I:157:ILE:HD11	1:J:117:ARG:HG3	1.84	0.59
1:A:290:GLY:O	1:A:291:VAL:HG12	2.03	0.59
1:A:13:ASP:OD2	1:A:139:GLN:NE2	2.35	0.59
1:E:224:TRP:NE1	1:E:301:ARG:HB3	2.17	0.59
1:I:145:ILE:HD13	1:I:193:VAL:HG13	1.83	0.59
1:I:238:LEU:HB3	1:I:273:ILE:HD13	1.84	0.59
1:E:151:ASN:ND2	1:E:155:GLU:OE2	2.36	0.59
1:H:161:TRP:O	1:H:198:VAL:N	2.23	0.59
1:F:289:ASN:CG	1:F:290:GLY:H	2.09	0.59
1:A:105:ARG:NH2	1:B:81:VAL:O	2.35	0.59
1:B:145:ILE:HG22	1:B:146:GLN:H	1.68	0.59
1:J:169:HIS:HB3	1:J:192:THR:HB	1.84	0.59
1:C:22:LYS:HE3	1:C:24:TYR:CD1	2.38	0.59
1:C:284:HIS:CE1	1:C:291:VAL:HG13	2.38	0.59
1:D:156:GLU:C	1:D:157:ILE:HG13	2.26	0.59
1:F:253:LEU:HD21	1:F:262:ILE:HD12	1.84	0.59
1:G:44:THR:HA	1:G:99:ARG:HA	1.84	0.59
1:F:105:ARG:NH2	1:G:81:VAL:O	2.36	0.58
1:J:160:TRP:CD1	1:J:199:ARG:HA	2.36	0.58
1:F:134:SER:HB3	1:J:91:ARG:HH11	1.67	0.58
1:H:91:ARG:HD3	1:I:134:SER:HB3	1.85	0.58
1:F:14:VAL:HG21	1:F:138:GLN:HE21	1.67	0.58
1:G:151:ASN:OD1	1:G:162:ILE:N	2.34	0.58
1:I:204:TYR:O	1:I:208:PHE:HB2	2.03	0.58
1:E:79:ILE:HD11	1:E:131:GLU:HB3	1.84	0.58
1:G:36:ASP:HB2	1:G:107:LEU:HD13	1.85	0.58
1:I:161:TRP:N	1:I:198:VAL:O	2.35	0.58
1:I:151:ASN:OD1	1:I:152:ILE:HA	2.03	0.58
1:J:18:ILE:HG12	1:J:39:ILE:HG13	1.85	0.58
1:F:241:THR:HA	1:G:240:LEU:HD23	1.85	0.58
1:C:260:THR:O	1:C:264:GLN:HG3	2.04	0.58
1:D:151:ASN:HB2	1:D:162:ILE:HG23	1.85	0.58
1:I:209:ILE:HG23	1:I:265:MET:HE1	1.85	0.58
1:D:238:LEU:HB3	1:D:273:ILE:HD13	1.86	0.58
1:J:14:VAL:HG21	1:J:138:GLN:HE21	1.68	0.58
1:H:157:ILE:CD1	1:I:115:ASP:HA	2.34	0.58
1:I:28:THR:HB	1:I:256:LEU:HD21	1.85	0.58
1:I:155:GLU:HA	1:I:158:ASP:H	1.69	0.58
1:B:38:TYR:CZ	1:B:105:ARG:HD2	2.39	0.57
1:G:14:VAL:HG21	1:G:138:GLN:NE2	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:249:THR:HG23	1:H:253:LEU:HD22	1.85	0.57
1:A:103:ASN:HB3	2:A:402:6XY:BR1	2.59	0.57
1:F:136:ASN:ND2	1:F:185:GLN:OE1	2.37	0.57
1:I:161:TRP:O	1:I:198:VAL:N	2.28	0.57
1:E:299:ARG:HA	1:E:301:ARG:HG3	1.86	0.57
1:I:155:GLU:HA	1:I:158:ASP:HB3	1.86	0.57
1:I:155:GLU:O	1:I:200:ASN:ND2	2.38	0.57
1:E:28:THR:HB	1:E:256:LEU:HD21	1.86	0.57
1:G:284:HIS:CE1	1:G:291:VAL:HG13	2.40	0.57
1:D:178:LEU:O	1:D:181:VAL:HG22	2.05	0.57
1:H:36:ASP:HB2	1:H:107:LEU:HD13	1.87	0.56
1:C:22:LYS:HE3	1:C:24:TYR:HD1	1.70	0.56
1:F:110:PHE:CE2	1:F:128:LEU:HG	2.40	0.56
1:B:36:ASP:HB2	1:B:107:LEU:HD13	1.87	0.56
1:C:155:GLU:HG2	1:C:161:TRP:HD1	1.70	0.56
1:H:136:ASN:ND2	1:H:187:GLU:O	2.38	0.56
1:H:260:THR:O	1:H:264:GLN:HG3	2.05	0.56
1:H:103:ASN:HB3	2:H:401:6XY:BR1	2.61	0.56
1:I:14:VAL:HG21	1:I:138:GLN:NE2	2.17	0.56
1:C:64:GLU:HA	1:C:67:ILE:HD12	1.85	0.56
1:F:27:ASN:HB3	1:F:32:THR:HB	1.87	0.56
1:F:167:SER:HB3	1:F:194:ARG:HG3	1.87	0.56
1:F:294:ASP:HB3	1:F:297:ILE:HG22	1.88	0.56
1:A:240:LEU:HD23	1:E:241:THR:HA	1.88	0.56
1:C:36:ASP:HB2	1:C:107:LEU:HD13	1.86	0.56
1:D:263:ASP:O	1:D:267:ILE:HG12	2.06	0.56
1:G:122:ASP:HB2	1:G:199:ARG:HB2	1.87	0.56
1:B:145:ILE:HG22	1:B:146:GLN:N	2.20	0.56
1:F:226:GLU:OE2	1:G:284:HIS:NE2	2.38	0.56
1:G:263:ASP:O	1:G:267:ILE:HG12	2.06	0.56
1:H:204:TYR:O	1:H:208:PHE:HB2	2.06	0.56
1:D:156:GLU:HA	1:D:156:GLU:OE1	2.04	0.55
1:E:178:LEU:HD12	1:E:181:VAL:HG23	1.88	0.55
1:C:294:ASP:HB3	1:C:297:ILE:HG22	1.87	0.55
1:E:268:ALA:HB1	1:E:308:PHE:CE1	2.41	0.55
1:A:167:SER:HB2	1:A:194:ARG:HG3	1.87	0.55
1:B:210:LEU:HB3	1:B:211:PRO:HD3	1.89	0.55
1:E:210:LEU:HB3	1:E:211:PRO:HD3	1.88	0.55
1:F:260:THR:O	1:F:264:GLN:HG3	2.07	0.55
1:B:140:LEU:HD13	1:B:191:ILE:HG13	1.88	0.55
1:D:231:ARG:HB3	1:D:280:ILE:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:160:TRP:CD1	2:F:402:6XY:BR1	3.15	0.55
1:G:161:TRP:N	1:G:198:VAL:O	2.38	0.55
1:F:259:THR:HG21	1:J:206:TRP:HE3	1.72	0.55
1:G:40:VAL:HG13	1:G:103:ASN:HD21	1.71	0.55
1:A:123:ARG:O	1:A:124:GLN:HB2	2.07	0.55
1:B:127:VAL:HG12	1:B:194:ARG:HB3	1.89	0.55
1:D:241:THR:HA	1:E:240:LEU:HD23	1.87	0.55
1:E:204:TYR:O	1:E:208:PHE:HB2	2.06	0.55
1:H:27:ASN:HB3	1:H:32:THR:HB	1.87	0.54
1:C:24:TYR:HD2	1:C:25:GLY:N	2.06	0.54
1:C:18:ILE:HG12	1:C:39:ILE:HG13	1.90	0.54
1:E:64:GLU:HA	1:E:67:ILE:HD12	1.90	0.54
1:J:205:LEU:HD23	1:J:209:ILE:HG13	1.89	0.54
1:D:79:ILE:HD11	1:D:131:GLU:HB3	1.89	0.54
1:E:163:ARG:HG2	1:E:197:ALA:HA	1.88	0.54
1:F:210:LEU:HB3	1:F:211:PRO:HD3	1.88	0.54
1:F:298:GLN:NE2	1:F:299:ARG:HH21	2.06	0.54
1:G:289:ASN:HD21	1:G:292:GLU:HB2	1.72	0.54
1:F:59:GLU:OE2	1:G:134:SER:OG	2.25	0.54
1:A:23:ILE:HG21	1:A:126:PHE:CD2	2.43	0.54
1:B:231:ARG:HB3	1:B:280:ILE:HD13	1.88	0.54
1:C:91:ARG:HH11	1:D:134:SER:HB3	1.73	0.54
1:A:28:THR:HB	1:A:256:LEU:HD21	1.90	0.54
1:F:299:ARG:HA	1:F:301:ARG:HG3	1.90	0.54
1:J:249:THR:HG23	1:J:253:LEU:HD22	1.89	0.54
1:A:263:ASP:O	1:A:267:ILE:HG12	2.08	0.54
1:C:159:GLU:HB3	1:C:160:TRP:CD1	2.42	0.54
1:G:152:ILE:HA	1:G:155:GLU:OE2	2.07	0.54
1:B:253:LEU:HD21	1:B:262:ILE:HD12	1.89	0.53
1:C:60:ASN:HA	1:C:90:LYS:HG3	1.91	0.53
1:I:122:ASP:OD1	1:I:199:ARG:HB2	2.07	0.53
1:J:224:TRP:NE1	1:J:301:ARG:HB3	2.23	0.53
1:E:151:ASN:HB2	1:E:162:ILE:HG23	1.90	0.53
1:I:224:TRP:NE1	1:I:301:ARG:HB3	2.24	0.53
1:C:38:TYR:CZ	1:C:105:ARG:HD2	2.44	0.53
1:J:151:ASN:ND2	1:J:162:ILE:H	2.07	0.53
1:C:59:GLU:OE2	1:D:134:SER:OG	2.27	0.53
1:E:289:ASN:O	1:E:290:GLY:C	2.51	0.53
1:D:27:ASN:HB3	1:D:32:THR:HB	1.90	0.53
1:J:178:LEU:HD12	1:J:181:VAL:HG23	1.89	0.53
1:A:224:TRP:NE1	1:A:301:ARG:HB3	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:11:PRO:HA	1:I:137:ASN:O	2.09	0.53
1:C:23:ILE:HG22	1:C:24:TYR:H	1.72	0.53
1:D:64:GLU:HA	1:D:67:ILE:HD12	1.91	0.53
1:A:115:ASP:O	1:A:124:GLN:NE2	2.41	0.53
1:F:47:PRO:HB3	1:F:96:PRO:O	2.08	0.53
1:B:294:ASP:HB3	1:B:297:ILE:CG2	2.39	0.53
1:A:133:PHE:CE1	1:E:89:ASN:HB2	2.44	0.52
1:H:136:ASN:O	1:H:138:GLN:N	2.36	0.52
1:B:155:GLU:HG3	1:B:161:TRP:CD1	2.45	0.52
1:G:128:LEU:HB2	1:G:193:VAL:CG2	2.39	0.52
1:B:165:LYS:HG3	1:B:166:ALA:H	1.73	0.52
1:J:169:HIS:ND1	1:J:169:HIS:C	2.68	0.52
1:A:130:LEU:HD23	1:A:191:ILE:HD12	1.91	0.52
1:F:18:ILE:HG12	1:F:39:ILE:HG13	1.92	0.52
1:B:209:ILE:HG23	1:B:265:MET:HE1	1.90	0.52
1:D:26:VAL:HG21	1:D:160:TRP:CZ2	2.44	0.52
1:G:161:TRP:O	1:G:198:VAL:N	2.36	0.52
1:J:112:ASN:ND2	1:J:125:GLN:O	2.38	0.52
1:H:145:ILE:HG12	1:H:193:VAL:HG11	1.91	0.52
1:B:167:SER:HB2	1:B:194:ARG:O	2.10	0.52
1:E:26:VAL:HG21	1:E:160:TRP:HE1	1.75	0.52
1:A:26:VAL:HG12	1:A:33:TYR:HB3	1.92	0.52
1:C:253:LEU:HD21	1:C:262:ILE:HD12	1.92	0.52
1:I:173:ILE:O	1:I:187:GLU:HA	2.09	0.52
1:J:210:LEU:HB3	1:J:211:PRO:HD3	1.91	0.52
1:J:227:SER:O	1:J:231:ARG:HD3	2.10	0.52
1:C:58:VAL:HB	1:C:92:LEU:HB2	1.92	0.51
1:F:150:GLU:HG2	1:F:153:ASP:HB2	1.92	0.51
1:C:210:LEU:HB3	1:C:211:PRO:HD3	1.91	0.51
1:C:238:LEU:HB3	1:C:273:ILE:HD13	1.93	0.51
1:J:16:VAL:O	1:J:143:SER:HA	2.10	0.51
1:J:72:TRP:HZ3	1:J:135:TYR:CZ	2.28	0.51
1:C:118:LEU:HA	1:C:261:VAL:HG23	1.92	0.51
1:D:36:ASP:HB2	1:D:107:LEU:HD13	1.91	0.51
1:B:122:ASP:HB2	1:B:199:ARG:HB2	1.91	0.51
1:C:145:ILE:HD12	1:C:145:ILE:O	2.11	0.51
1:H:167:SER:CB	1:H:194:ARG:HG3	2.32	0.51
1:H:173:ILE:O	1:H:187:GLU:HA	2.11	0.51
1:H:178:LEU:HB3	1:H:181:VAL:HG23	1.93	0.51
1:B:227:SER:O	1:B:231:ARG:HD3	2.10	0.51
1:C:260:THR:H	1:C:263:ASP:HB2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:91:ARG:HD3	1:H:134:SER:HB3	1.92	0.51
1:J:160:TRP:HD1	1:J:199:ARG:HA	1.76	0.51
1:B:245:TYR:HD2	1:B:266:ILE:HD11	1.75	0.51
1:G:302:LEU:HD13	1:G:305:PRO:HG2	1.92	0.51
1:I:247:PHE:CD2	1:J:247:PHE:HE2	2.29	0.51
1:E:123:ARG:HG3	1:E:198:VAL:HG22	1.92	0.51
1:G:284:HIS:HE1	1:G:291:VAL:HG13	1.75	0.51
1:H:161:TRP:N	1:H:198:VAL:O	2.42	0.51
1:B:123:ARG:HG2	1:B:198:VAL:HG22	1.93	0.50
1:B:173:ILE:HG13	1:B:190:ARG:CZ	2.41	0.50
1:C:151:ASN:ND2	1:C:152:ILE:HG12	2.25	0.50
1:A:145:ILE:HD13	1:A:193:VAL:HG13	1.92	0.50
1:B:135:TYR:HB3	1:B:138:GLN:HB3	1.93	0.50
1:C:260:THR:N	1:C:263:ASP:HB2	2.27	0.50
1:E:152:ILE:HG23	1:E:161:TRP:HZ2	1.76	0.50
1:G:79:ILE:HD11	1:G:131:GLU:HB3	1.93	0.50
1:G:227:SER:O	1:G:231:ARG:HD3	2.11	0.50
1:J:152:ILE:HG13	1:J:163:ARG:HH12	1.76	0.50
1:H:154:ASN:O	1:H:157:ILE:N	2.40	0.50
1:G:143:SER:CB	1:G:170:ILE:HD11	2.41	0.50
1:D:149:THR:OG1	1:D:162:ILE:HG12	2.11	0.50
1:G:44:THR:HG22	1:G:99:ARG:HB3	1.93	0.50
1:H:89:ASN:HB2	1:I:133:PHE:CE1	2.46	0.50
1:C:122:ASP:HB3	1:C:124:GLN:OE1	2.11	0.50
1:F:162:ILE:HA	1:F:197:ALA:HA	1.93	0.50
1:I:210:LEU:HB3	1:I:211:PRO:HD3	1.93	0.50
1:C:289:ASN:OD1	1:C:289:ASN:N	2.44	0.50
1:E:155:GLU:CD	1:E:155:GLU:H	2.18	0.50
1:H:122:ASP:HB3	1:H:124:GLN:OE1	2.11	0.50
1:H:226:GLU:OE2	1:I:284:HIS:NE2	2.43	0.50
1:C:155:GLU:N	1:C:155:GLU:OE1	2.45	0.50
1:C:14:VAL:HG21	1:C:138:GLN:HE21	1.77	0.50
1:I:16:VAL:HA	1:I:40:VAL:O	2.12	0.49
1:A:155:GLU:HG2	1:A:161:TRP:HD1	1.77	0.49
1:E:268:ALA:HB1	1:E:308:PHE:HE1	1.76	0.49
1:F:91:ARG:HD3	1:G:134:SER:HB3	1.95	0.49
1:I:160:TRP:NE1	2:I:402:6XY:BR1	3.01	0.49
1:J:232:LEU:HD12	1:J:277:ILE:HD13	1.94	0.49
1:E:132:PRO:HD2	1:E:189:SER:O	2.12	0.49
1:E:76:LEU:HB3	1:E:130:LEU:HD11	1.94	0.49
1:I:263:ASP:O	1:I:267:ILE:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:TRP:NE1	1:C:301:ARG:HB3	2.27	0.49
1:G:212:LEU:HD11	1:G:266:ILE:HG12	1.95	0.49
1:C:24:TYR:CE2	1:C:34:LYS:HD2	2.47	0.49
1:C:273:ILE:O	1:C:277:ILE:HG13	2.13	0.49
1:E:118:LEU:HA	1:E:261:VAL:HG23	1.94	0.49
1:E:169:HIS:CE1	1:E:171:SER:HB3	2.48	0.49
1:J:151:ASN:HD21	1:J:161:TRP:HA	1.77	0.49
1:A:38:TYR:CZ	1:A:105:ARG:HD2	2.48	0.49
1:B:238:LEU:HD21	1:C:236:PHE:CD2	2.48	0.49
1:C:160:TRP:HB3	1:C:197:ALA:HB1	1.95	0.49
1:E:110:PHE:CE2	1:E:128:LEU:HG	2.47	0.49
1:E:208:PHE:O	1:E:245:TYR:OH	2.27	0.49
1:E:227:SER:O	1:E:231:ARG:HD3	2.12	0.49
1:E:122:ASP:HB2	1:E:199:ARG:HB2	1.94	0.49
1:E:238:LEU:HB3	1:E:273:ILE:HD13	1.95	0.49
1:C:287:GLN:OE1	1:C:287:GLN:N	2.44	0.48
1:H:120:PRO:HG3	1:H:262:ILE:HG13	1.95	0.48
1:J:227:SER:OG	1:J:228:PHE:N	2.46	0.48
1:A:231:ARG:HB3	1:A:280:ILE:HD13	1.95	0.48
1:E:14:VAL:HG22	1:E:43:TRP:HB3	1.96	0.48
1:A:145:ILE:CD1	1:A:193:VAL:HG13	2.43	0.48
1:F:14:VAL:HG13	1:F:43:TRP:HD1	1.79	0.48
1:D:153:ASP:C	1:D:155:GLU:HG2	2.38	0.48
1:D:284:HIS:CE1	1:D:291:VAL:HG13	2.48	0.48
1:H:150:GLU:HG2	1:H:153:ASP:HB2	1.95	0.48
1:I:256:LEU:HD12	1:I:260:THR:HG22	1.94	0.48
1:E:294:ASP:HB3	1:E:297:ILE:HG22	1.95	0.48
1:H:217:ALA:HA	1:H:220:TRP:CE3	2.49	0.48
1:I:284:HIS:CE1	1:I:291:VAL:HG13	2.48	0.48
1:D:150:GLU:HG2	1:D:153:ASP:OD1	2.13	0.48
1:H:38:TYR:HA	1:H:105:ARG:HA	1.94	0.48
1:H:79:ILE:HD11	1:H:131:GLU:HB3	1.95	0.48
1:J:33:TYR:HH	1:J:127:VAL:H	1.56	0.48
1:J:123:ARG:HG3	1:J:198:VAL:HG22	1.95	0.48
1:B:28:THR:HB	1:B:256:LEU:HD21	1.96	0.48
1:C:24:TYR:C	2:C:402:6XY:BR1	3.12	0.48
1:D:204:TYR:O	1:D:208:PHE:HB2	2.13	0.48
1:I:145:ILE:CD1	1:I:193:VAL:HG13	2.43	0.48
1:A:122:ASP:OD2	1:A:199:ARG:NE	2.35	0.48
1:A:301:ARG:HH12	1:B:285:HIS:HE2	1.61	0.48
1:D:160:TRP:CZ3	1:D:199:ARG:HG2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:VAL:CG2	1:E:160:TRP:HE1	2.27	0.48
1:B:122:ASP:OD2	1:B:199:ARG:NE	2.41	0.48
1:C:14:VAL:HG21	1:C:138:GLN:NE2	2.29	0.48
1:I:245:TYR:HD2	1:I:266:ILE:HD11	1.79	0.48
1:J:173:ILE:HG13	1:J:190:ARG:CZ	2.44	0.48
1:J:294:ASP:HB3	1:J:297:ILE:HG22	1.95	0.48
1:C:157:ILE:HD11	1:D:117:ARG:NE	2.29	0.48
1:E:227:SER:OG	1:E:228:PHE:N	2.47	0.48
1:G:169:HIS:HB3	1:G:192:THR:HB	1.95	0.48
1:B:160:TRP:HA	1:B:200:ASN:HB2	1.94	0.47
1:B:167:SER:HB3	1:B:194:ARG:HG3	1.95	0.47
1:B:249:THR:HG23	1:B:253:LEU:HD22	1.96	0.47
1:D:156:GLU:O	1:D:157:ILE:HG13	2.14	0.47
1:D:210:LEU:HB3	1:D:211:PRO:HD3	1.95	0.47
1:D:284:HIS:HB3	1:D:285:HIS:ND1	2.29	0.47
1:J:263:ASP:O	1:J:267:ILE:HG12	2.14	0.47
1:F:114:MET:HB3	1:F:124:GLN:OE1	2.14	0.47
1:I:22:LYS:HE3	1:I:24:TYR:CB	2.43	0.47
1:D:155:GLU:CB	1:D:156:GLU:HA	2.37	0.47
1:J:14:VAL:HG21	1:J:138:GLN:NE2	2.29	0.47
1:E:103:ASN:HB3	2:E:401:6XY:BR1	2.70	0.47
1:E:163:ARG:HG2	1:E:197:ALA:CA	2.44	0.47
1:F:250:SER:OG	1:J:248:TYR:HE1	1.96	0.47
1:C:263:ASP:O	1:C:267:ILE:HG12	2.14	0.47
1:H:31:GLN:OE1	1:H:113:ASP:HA	2.14	0.47
1:F:145:ILE:HG12	1:F:193:VAL:HG11	1.97	0.47
1:G:170:ILE:HA	1:G:190:ARG:O	2.15	0.47
1:I:79:ILE:HD11	1:I:131:GLU:HB3	1.97	0.47
1:I:208:PHE:O	1:I:245:TYR:OH	2.30	0.47
1:B:289:ASN:OD1	1:B:289:ASN:N	2.48	0.47
1:F:42:GLN:HA	1:F:100:VAL:O	2.14	0.47
1:G:178:LEU:HD13	1:G:178:LEU:HA	1.75	0.47
1:J:167:SER:HB2	1:J:194:ARG:HG3	1.97	0.47
1:C:178:LEU:HD22	1:C:181:VAL:HG21	1.96	0.47
1:E:112:ASN:ND2	1:E:125:GLN:O	2.47	0.47
1:H:14:VAL:HG21	1:H:138:GLN:NE2	2.28	0.47
1:C:24:TYR:CD2	1:C:25:GLY:N	2.82	0.47
1:D:294:ASP:HB3	1:D:297:ILE:HG22	1.96	0.47
1:F:38:TYR:CZ	1:F:105:ARG:HD2	2.50	0.47
1:I:28:THR:HA	1:I:116:PHE:CE1	2.50	0.47
1:B:143:SER:CB	1:B:170:ILE:HD11	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:289:ASN:CG	1:D:290:GLY:H	2.24	0.46
1:F:135:TYR:HB3	1:F:138:GLN:HB3	1.95	0.46
1:F:247:PHE:CD2	1:G:247:PHE:HE2	2.33	0.46
1:G:167:SER:HB2	1:G:194:ARG:O	2.14	0.46
1:I:294:ASP:HB3	1:I:297:ILE:HG22	1.96	0.46
1:C:186:ASN:OD1	1:C:186:ASN:N	2.48	0.46
1:H:78:PHE:CE2	1:H:130:LEU:HD13	2.50	0.46
1:C:209:ILE:HG23	1:C:265:MET:HE1	1.96	0.46
1:C:285:HIS:HA	1:C:287:GLN:NE2	2.30	0.46
1:D:116:PHE:HB2	1:D:258:TYR:HE1	1.81	0.46
1:F:235:SER:O	1:F:239:MET:N	2.36	0.46
1:G:141:ARG:HD2	1:G:142:PHE:CE2	2.50	0.46
1:G:210:LEU:HB3	1:G:211:PRO:HD3	1.97	0.46
1:H:18:ILE:HD13	1:H:128:LEU:HD23	1.96	0.46
1:J:44:THR:HG23	1:J:99:ARG:HB3	1.98	0.46
1:J:219:SER:HA	1:J:238:LEU:HG	1.98	0.46
1:A:167:SER:CB	1:A:194:ARG:HG3	2.45	0.46
1:B:227:SER:OG	1:B:228:PHE:N	2.49	0.46
1:C:112:ASN:ND2	1:C:125:GLN:O	2.48	0.46
1:D:151:ASN:ND2	1:D:161:TRP:HA	2.31	0.46
1:G:253:LEU:HD21	1:G:262:ILE:HD12	1.98	0.46
1:I:27:ASN:N	1:I:32:THR:O	2.37	0.46
1:A:89:ASN:HB2	1:B:133:PHE:CE1	2.50	0.46
1:E:23:ILE:HG22	1:E:35:VAL:HG22	1.97	0.46
1:F:205:LEU:HD23	1:F:209:ILE:HG13	1.97	0.46
1:I:156:GLU:HA	1:I:200:ASN:ND2	2.30	0.46
1:I:300:CYS:HA	1:I:303:ALA:HB3	1.97	0.46
1:D:147:VAL:O	1:D:148:TYR:CG	2.68	0.46
1:H:41:ALA:O	1:H:101:ILE:HA	2.16	0.46
1:I:153:ASP:C	1:I:155:GLU:H	2.15	0.46
1:J:268:ALA:HB1	1:J:308:PHE:CE1	2.50	0.46
1:C:157:ILE:HD11	1:D:117:ARG:CZ	2.46	0.46
1:D:227:SER:OG	1:D:228:PHE:N	2.48	0.46
1:E:95:PHE:CD1	1:E:99:ARG:HG3	2.51	0.46
1:E:23:ILE:CG1	1:E:24:TYR:H	2.28	0.46
1:F:294:ASP:HB3	1:F:297:ILE:CG2	2.45	0.46
1:H:186:ASN:OD1	1:H:186:ASN:N	2.49	0.46
1:I:227:SER:OG	1:I:228:PHE:N	2.48	0.46
1:J:48:ARG:O	1:J:96:PRO:HA	2.15	0.46
1:G:209:ILE:HG23	1:G:265:MET:HE1	1.97	0.45
1:G:227:SER:OG	1:G:228:PHE:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:TYR:OH	1:C:127:VAL:O	2.33	0.45
1:C:227:SER:OG	1:C:228:PHE:N	2.49	0.45
1:D:78:PHE:O	1:D:81:VAL:HG12	2.17	0.45
1:J:14:VAL:HB	1:J:140:LEU:HD23	1.98	0.45
1:J:66:TRP:HB3	1:J:71:LEU:HD12	1.98	0.45
1:B:147:VAL:HG12	1:B:165:LYS:NZ	2.31	0.45
1:B:157:ILE:HD11	1:C:117:ARG:NE	2.31	0.45
1:C:155:GLU:CG	1:C:161:TRP:HD1	2.30	0.45
1:C:294:ASP:HB3	1:C:297:ILE:CG2	2.46	0.45
1:G:22:LYS:HE3	1:G:24:TYR:HB3	1.97	0.45
1:H:178:LEU:HD13	1:H:178:LEU:HA	1.76	0.45
1:H:260:THR:H	1:H:263:ASP:HB2	1.82	0.45
1:I:27:ASN:HB3	1:I:32:THR:HB	1.98	0.45
1:A:250:SER:HB3	1:E:252:ILE:HG13	1.99	0.45
1:A:294:ASP:HB3	1:A:297:ILE:HG22	1.98	0.45
1:C:91:ARG:HG3	1:C:103:ASN:HB2	1.98	0.45
1:E:150:GLU:O	1:E:150:GLU:HG2	2.17	0.45
1:F:17:SER:O	1:F:40:VAL:HG22	2.17	0.45
1:G:136:ASN:ND2	1:G:185:GLN:OE1	2.50	0.45
1:H:119:PHE:HB2	1:H:260:THR:HB	1.97	0.45
1:H:152:ILE:HA	1:H:155:GLU:OE2	2.17	0.45
1:H:224:TRP:NE1	1:H:301:ARG:HB3	2.31	0.45
1:B:76:LEU:HB3	1:B:130:LEU:HD11	1.99	0.45
1:B:295:LEU:O	1:B:296:LEU:HB3	2.16	0.45
1:C:48:ARG:HG2	1:C:49:LYS:H	1.81	0.45
1:D:173:ILE:O	1:D:187:GLU:HA	2.16	0.45
1:F:91:ARG:CD	1:G:134:SER:HB3	2.47	0.45
1:A:294:ASP:HB3	1:A:297:ILE:CG2	2.46	0.45
1:D:14:VAL:HG21	1:D:138:GLN:NE2	2.29	0.45
1:D:249:THR:O	1:D:253:LEU:HB2	2.17	0.45
1:E:178:LEU:HD13	1:E:178:LEU:HA	1.81	0.45
1:J:131:GLU:OE1	1:J:190:ARG:NH2	2.45	0.45
1:D:95:PHE:CD1	1:D:99:ARG:HG3	2.51	0.45
1:E:23:ILE:HA	1:E:34:LYS:O	2.16	0.45
1:A:248:TYR:HE1	1:B:250:SER:OG	2.00	0.44
1:B:88:GLY:HA2	1:C:84:SER:HB3	1.99	0.44
1:A:227:SER:O	1:A:231:ARG:HD3	2.18	0.44
1:F:116:PHE:HB2	1:F:258:TYR:OH	2.17	0.44
1:G:132:PRO:HD2	1:G:189:SER:O	2.17	0.44
1:H:163:ARG:HD2	1:H:163:ARG:C	2.42	0.44
1:A:11:PRO:HA	1:A:137:ASN:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ILE:HG12	1:B:239:MET:HE3	1.99	0.44
1:I:76:LEU:HB3	1:I:130:LEU:HD11	1.98	0.44
1:A:141:ARG:HD2	1:A:142:PHE:CE2	2.52	0.44
1:A:178:LEU:HD13	1:A:178:LEU:HA	1.87	0.44
1:D:41:ALA:HB3	1:D:102:TYR:HB3	1.99	0.44
1:J:219:SER:OG	1:J:273:ILE:HG12	2.17	0.44
1:B:71:LEU:HD22	1:B:73:VAL:HG22	1.98	0.44
1:C:23:ILE:O	1:C:24:TYR:CD1	2.71	0.44
1:D:151:ASN:HB2	1:D:162:ILE:CG2	2.46	0.44
1:D:186:ASN:N	1:D:186:ASN:OD1	2.50	0.44
1:H:210:LEU:HB3	1:H:211:PRO:HD3	1.98	0.44
1:E:13:ASP:OD2	1:E:139:GLN:NE2	2.41	0.44
1:F:136:ASN:ND2	1:F:185:GLN:HB2	2.33	0.44
1:G:170:ILE:HG12	1:G:191:ILE:HA	1.99	0.44
1:G:238:LEU:HD21	1:H:236:PHE:CD2	2.53	0.44
1:G:300:CYS:HB2	1:G:303:ALA:HB3	2.00	0.44
1:H:221:SER:HB2	1:I:281:ILE:HD11	2.00	0.44
1:A:227:SER:OG	1:A:228:PHE:N	2.51	0.44
1:B:160:TRP:HB3	1:B:200:ASN:H	1.83	0.44
1:D:253:LEU:HD21	1:D:262:ILE:HD12	2.00	0.44
1:E:294:ASP:HB3	1:E:297:ILE:CG2	2.47	0.44
1:B:56:LEU:HD13	1:B:57:ILE:N	2.32	0.44
1:H:227:SER:O	1:H:231:ARG:HD3	2.18	0.44
1:J:39:ILE:HD11	1:J:130:LEU:HD22	1.99	0.44
1:J:56:LEU:HD13	1:J:57:ILE:N	2.32	0.44
1:E:162:ILE:HD11	1:E:165:LYS:HG2	2.00	0.44
1:F:133:PHE:CE1	1:J:89:ASN:HB2	2.52	0.44
1:G:268:ALA:HB1	1:G:308:PHE:CE1	2.52	0.44
1:E:23:ILE:O	1:E:24:TYR:CG	2.71	0.43
1:E:155:GLU:HG3	1:E:161:TRP:CD2	2.53	0.43
1:H:260:THR:N	1:H:263:ASP:HB2	2.33	0.43
1:I:95:PHE:CD1	1:I:99:ARG:HG3	2.52	0.43
1:I:123:ARG:HG3	1:I:198:VAL:HG22	1.99	0.43
1:A:135:TYR:HB3	1:A:138:GLN:HB3	2.00	0.43
1:A:239:MET:HE3	1:E:215:ILE:HG12	2.00	0.43
1:J:72:TRP:CZ3	1:J:135:TYR:CZ	3.06	0.43
1:C:227:SER:O	1:C:231:ARG:HD3	2.19	0.43
1:I:221:SER:HB2	1:J:281:ILE:HD11	2.01	0.43
1:J:145:ILE:HG12	1:J:193:VAL:HG11	1.99	0.43
1:D:165:LYS:HB3	1:D:165:LYS:HE3	1.71	0.43
1:H:16:VAL:HA	1:H:40:VAL:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:227:SER:OG	1:H:228:PHE:N	2.50	0.43
1:I:123:ARG:CG	1:I:198:VAL:HG22	2.48	0.43
1:J:239:MET:O	1:J:243:VAL:HG23	2.18	0.43
1:A:95:PHE:CD1	1:A:99:ARG:HG3	2.53	0.43
1:A:122:ASP:O	1:A:198:VAL:HG13	2.18	0.43
1:B:64:GLU:HA	1:B:67:ILE:HD12	2.00	0.43
1:D:119:PHE:O	1:D:199:ARG:HD2	2.18	0.43
1:H:300:CYS:HA	1:H:303:ALA:HB3	2.00	0.43
1:D:119:PHE:HB3	1:D:260:THR:HB	2.01	0.43
1:F:227:SER:OG	1:F:228:PHE:N	2.50	0.43
1:I:116:PHE:HB2	1:I:258:TYR:OH	2.19	0.43
1:J:140:LEU:O	1:J:170:ILE:HD11	2.18	0.43
1:E:263:ASP:O	1:E:267:ILE:HG12	2.18	0.43
1:G:239:MET:O	1:G:243:VAL:HG23	2.19	0.43
1:H:13:ASP:HB3	1:H:141:ARG:HE	1.82	0.43
1:I:165:LYS:HA	1:I:165:LYS:HD2	1.90	0.43
1:J:132:PRO:HD2	1:J:189:SER:O	2.19	0.43
1:B:263:ASP:O	1:B:267:ILE:HG12	2.19	0.43
1:C:208:PHE:O	1:C:245:TYR:OH	2.35	0.43
1:F:140:LEU:HD13	1:F:191:ILE:HG13	2.01	0.43
1:F:236:PHE:CD2	1:J:238:LEU:HD21	2.54	0.43
1:H:23:ILE:HA	1:H:34:LYS:O	2.19	0.43
1:H:232:LEU:HD12	1:H:277:ILE:HD13	2.01	0.43
1:I:186:ASN:OD1	1:I:186:ASN:N	2.51	0.43
1:A:58:VAL:HB	1:A:92:LEU:HB2	2.01	0.43
1:D:95:PHE:HD1	1:D:99:ARG:HG3	1.84	0.43
1:H:136:ASN:OD1	1:H:136:ASN:C	2.61	0.43
1:I:18:ILE:HG12	1:I:39:ILE:HG13	2.01	0.43
1:A:91:ARG:NE	1:A:103:ASN:HD22	2.16	0.42
1:C:249:THR:O	1:C:253:LEU:HB2	2.19	0.42
1:D:151:ASN:OD1	1:D:152:ILE:HA	2.18	0.42
1:E:66:TRP:HB3	1:E:71:LEU:HD12	2.00	0.42
1:H:145:ILE:HG12	1:H:193:VAL:CG1	2.49	0.42
1:H:159:GLU:HG3	1:I:257:PRO:HB3	2.00	0.42
1:I:216:ILE:O	1:I:219:SER:HB3	2.19	0.42
1:J:123:ARG:CG	1:J:198:VAL:HG22	2.49	0.42
1:B:151:ASN:ND2	1:B:161:TRP:HB3	2.30	0.42
1:G:150:GLU:HG2	1:G:153:ASP:CB	2.49	0.42
1:A:114:MET:HE3	1:A:126:PHE:HE1	1.84	0.42
1:B:116:PHE:HB2	1:B:258:TYR:OH	2.20	0.42
1:B:123:ARG:CG	1:B:198:VAL:HG22	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:LEU:HD13	1:B:178:LEU:HA	1.82	0.42
1:B:268:ALA:HB1	1:B:308:PHE:CZ	2.54	0.42
1:C:78:PHE:O	1:C:81:VAL:HG12	2.19	0.42
1:C:231:ARG:HH22	1:C:293:ASP:CG	2.27	0.42
1:E:287:GLN:OE1	1:E:288:ALA:C	2.62	0.42
1:G:153:ASP:H	1:G:155:GLU:CD	2.28	0.42
1:H:118:LEU:HA	1:H:261:VAL:HG23	2.02	0.42
1:F:103:ASN:HB3	2:F:401:6XY:BR1	2.74	0.42
1:G:66:TRP:HB3	1:G:71:LEU:HD12	2.00	0.42
1:C:24:TYR:C	1:C:24:TYR:CD2	2.97	0.42
1:D:38:TYR:CZ	1:D:105:ARG:HD2	2.55	0.42
1:D:76:LEU:HB3	1:D:130:LEU:HD11	2.02	0.42
1:D:177:HIS:O	1:D:178:LEU:HB2	2.18	0.42
1:F:13:ASP:OD2	1:F:139:GLN:NE2	2.36	0.42
1:I:115:ASP:OD1	1:I:117:ARG:NH2	2.48	0.42
1:A:249:THR:HG23	1:A:253:LEU:HD22	2.01	0.42
1:C:155:GLU:CD	1:C:155:GLU:H	2.27	0.42
1:D:157:ILE:HG23	1:D:200:ASN:HD21	1.85	0.42
1:G:27:ASN:N	1:G:32:THR:O	2.43	0.42
1:I:28:THR:OG1	1:I:254:PRO:HB2	2.19	0.42
1:I:214:LEU:HD12	1:J:270:TYR:HB3	2.02	0.42
1:J:289:ASN:CG	1:J:290:GLY:H	2.26	0.42
1:C:283:ALA:O	1:C:293:ASP:HA	2.19	0.42
1:E:72:TRP:CZ3	1:E:74:PRO:HB3	2.55	0.42
1:E:116:PHE:HB2	1:E:258:TYR:OH	2.19	0.42
1:B:232:LEU:O	1:B:235:SER:HB2	2.20	0.42
1:C:93:MET:HB2	1:C:101:ILE:HB	2.02	0.42
1:E:174:ARG:O	1:E:186:ASN:ND2	2.53	0.42
1:H:287:GLN:OE1	1:H:287:GLN:N	2.49	0.42
1:B:216:ILE:O	1:B:219:SER:HB3	2.19	0.42
1:E:287:GLN:OE1	1:E:289:ASN:N	2.53	0.42
1:G:72:TRP:CZ3	1:G:74:PRO:HB3	2.54	0.42
1:G:217:ALA:HA	1:G:220:TRP:CE3	2.55	0.42
1:H:154:ASN:O	1:H:157:ILE:HG22	2.20	0.42
1:I:66:TRP:HB3	1:I:71:LEU:HD12	2.00	0.42
1:C:28:THR:HB	1:C:256:LEU:HD21	2.02	0.42
1:D:40:VAL:HG13	1:D:103:ASN:OD1	2.20	0.42
1:I:143:SER:HB3	1:I:168:THR:HG21	2.01	0.42
1:B:91:ARG:CD	1:C:134:SER:HB3	2.50	0.41
1:C:92:LEU:HD23	1:C:102:TYR:HA	2.00	0.41
1:D:153:ASP:CA	1:D:155:GLU:HG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:95:PHE:HD1	1:I:99:ARG:HG3	1.84	0.41
1:J:186:ASN:OD1	1:J:186:ASN:N	2.53	0.41
1:A:310:ALA:O	1:A:314:VAL:HG23	2.20	0.41
1:B:162:ILE:H	1:B:162:ILE:HG13	1.74	0.41
1:G:179:SER:HB2	1:G:186:ASN:ND2	2.35	0.41
1:I:125:GLN:NE2	1:I:194:ARG:HD3	2.35	0.41
1:J:235:SER:O	1:J:239:MET:N	2.37	0.41
1:D:223:PHE:HB3	1:D:301:ARG:HG2	2.01	0.41
1:F:178:LEU:HD13	1:F:178:LEU:HA	1.87	0.41
1:G:155:GLU:HA	1:G:158:ASP:H	1.84	0.41
1:H:93:MET:O	1:H:100:VAL:HA	2.20	0.41
1:A:14:VAL:HG21	1:A:138:GLN:NE2	2.28	0.41
1:A:165:LYS:O	1:A:166:ALA:CB	2.69	0.41
1:B:238:LEU:HD13	1:B:238:LEU:HA	1.94	0.41
1:C:24:TYR:HD2	1:C:25:GLY:HA3	1.86	0.41
1:I:155:GLU:OE1	1:I:161:TRP:HA	2.20	0.41
1:I:211:PRO:HB3	1:J:270:TYR:CD1	2.55	0.41
1:B:13:ASP:HB3	1:B:141:ARG:HE	1.86	0.41
1:B:161:TRP:CD1	1:B:161:TRP:N	2.89	0.41
1:D:119:PHE:CB	1:D:260:THR:HB	2.50	0.41
1:D:150:GLU:O	1:D:153:ASP:O	2.38	0.41
1:D:208:PHE:O	1:D:245:TYR:OH	2.35	0.41
1:G:27:ASN:HB3	1:G:32:THR:HB	2.01	0.41
1:H:58:VAL:O	1:H:91:ARG:HA	2.20	0.41
1:H:178:LEU:HB3	1:H:181:VAL:CG2	2.50	0.41
1:J:17:SER:O	1:J:40:VAL:HG22	2.19	0.41
1:D:143:SER:HB3	1:D:168:THR:HG21	2.02	0.41
1:D:160:TRP:HA	1:D:198:VAL:O	2.20	0.41
1:F:247:PHE:HA	1:J:248:TYR:HD1	1.86	0.41
1:G:169:HIS:CB	1:G:192:THR:HB	2.51	0.41
1:F:157:ILE:HD11	1:G:117:ARG:NE	2.35	0.41
1:G:204:TYR:O	1:G:208:PHE:HB2	2.20	0.41
1:H:18:ILE:O	1:H:145:ILE:HA	2.21	0.41
1:I:14:VAL:O	1:I:141:ARG:N	2.39	0.41
1:J:294:ASP:HB3	1:J:297:ILE:CG2	2.50	0.41
1:B:204:TYR:O	1:B:209:ILE:HG12	2.21	0.41
1:D:55:PRO:HB3	1:D:95:PHE:CD2	2.56	0.41
1:D:154:ASN:CB	1:D:155:GLU:CA	2.98	0.41
1:H:122:ASP:OD2	1:H:199:ARG:NE	2.41	0.41
1:B:132:PRO:HD2	1:B:189:SER:O	2.21	0.41
1:B:168:THR:O	1:I:167:SER:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:ARG:HA	1:B:301:ARG:HG3	2.03	0.41
1:C:89:ASN:HB2	1:D:133:PHE:CE1	2.56	0.41
1:D:216:ILE:O	1:D:219:SER:HB3	2.21	0.41
1:E:11:PRO:HA	1:E:137:ASN:O	2.21	0.41
1:E:17:SER:O	1:E:40:VAL:HG22	2.21	0.41
1:F:58:VAL:HB	1:F:92:LEU:HB2	2.02	0.41
1:H:56:LEU:HD13	1:H:57:ILE:N	2.36	0.41
1:I:153:ASP:C	1:I:155:GLU:N	2.78	0.41
1:I:156:GLU:HA	1:I:200:ASN:HD21	1.85	0.41
1:I:289:ASN:OD1	1:I:289:ASN:N	2.54	0.41
1:J:224:TRP:HZ2	1:J:302:LEU:HD13	1.86	0.41
1:A:165:LYS:O	1:A:166:ALA:HB2	2.20	0.41
1:B:89:ASN:HB2	1:C:133:PHE:CE1	2.56	0.41
1:B:175:TYR:OH	1:B:190:ARG:NH2	2.54	0.41
1:C:110:PHE:CE2	1:C:128:LEU:HG	2.56	0.41
1:E:119:PHE:CB	1:E:260:THR:HB	2.51	0.41
1:F:182:GLN:CD	1:J:93:MET:HE1	2.46	0.41
1:G:170:ILE:HD13	1:G:170:ILE:HG21	1.78	0.41
1:G:206:TRP:HE3	1:H:259:THR:HG21	1.87	0.41
1:H:119:PHE:HB3	1:H:120:PRO:HD3	2.03	0.41
1:B:159:GLU:O	1:B:200:ASN:HB3	2.21	0.40
1:B:224:TRP:NE1	1:B:301:ARG:HB3	2.35	0.40
1:C:147:VAL:O	1:C:148:TYR:CG	2.74	0.40
1:F:56:LEU:HD13	1:F:57:ILE:N	2.36	0.40
1:H:65:ARG:HE	1:H:65:ARG:HB3	1.73	0.40
1:H:128:LEU:HB2	1:H:193:VAL:HB	2.02	0.40
1:B:91:ARG:HD3	1:C:134:SER:HB3	2.03	0.40
1:C:24:TYR:HD2	1:C:25:GLY:CA	2.33	0.40
1:C:147:VAL:HG23	1:C:148:TYR:H	1.86	0.40
1:E:287:GLN:OE1	1:E:287:GLN:C	2.63	0.40
1:F:284:HIS:HB3	1:F:285:HIS:ND1	2.36	0.40
1:G:38:TYR:CE1	1:G:105:ARG:HD2	2.55	0.40
1:G:55:PRO:HB3	1:G:95:PHE:CD2	2.56	0.40
1:G:260:THR:O	1:G:264:GLN:HG3	2.21	0.40
1:H:155:GLU:HG3	1:H:158:ASP:HB2	2.02	0.40
1:I:260:THR:O	1:I:264:GLN:HG3	2.21	0.40
1:D:29:LEU:HD23	1:D:29:LEU:HA	1.89	0.40
1:F:224:TRP:NE1	1:F:301:ARG:HB3	2.36	0.40
1:J:141:ARG:HD2	1:J:142:PHE:CE2	2.57	0.40
1:A:248:TYR:HA	1:B:247:PHE:CE1	2.56	0.40
1:D:202:SER:OG	1:D:203:TYR:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:22:LYS:HG2	1:E:24:TYR:HD1	1.87	0.40
1:F:13:ASP:HB3	1:F:141:ARG:HE	1.87	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%)	268 (88%)	33 (11%)	4 (1%)	9	41
1	B	305/307 (99%)	269 (88%)	32 (10%)	4 (1%)	9	41
1	C	305/307 (99%)	268 (88%)	32 (10%)	5 (2%)	7	37
1	D	305/307 (99%)	268 (88%)	34 (11%)	3 (1%)	12	47
1	E	305/307 (99%)	267 (88%)	34 (11%)	4 (1%)	9	41
1	F	305/307 (99%)	270 (88%)	33 (11%)	2 (1%)	18	55
1	G	305/307 (99%)	270 (88%)	34 (11%)	1 (0%)	36	71
1	H	305/307 (99%)	266 (87%)	36 (12%)	3 (1%)	12	47
1	I	305/307 (99%)	269 (88%)	33 (11%)	3 (1%)	12	47
1	J	305/307 (99%)	275 (90%)	28 (9%)	2 (1%)	18	55
All	All	3050/3070 (99%)	2690 (88%)	329 (11%)	31 (1%)	12	47

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	166	ALA
1	A	291	VAL
1	B	166	ALA
1	C	24	TYR

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Mol	Chain	Res	Type
1	D	153	ASP
1	D	154	ASN
1	E	290	GLY
1	H	166	ALA
1	I	154	ASN
1	J	165	LYS
1	B	167	SER
1	E	165	LYS
1	C	167	SER
1	D	290	GLY
1	B	147	VAL
1	B	163	ARG
1	C	200	ASN
1	E	153	ASP
1	E	155	GLU
1	G	153	ASP
1	C	25	GLY
1	J	170	ILE
1	C	23	ILE
1	F	170	ILE
1	I	290	GLY
1	A	170	ILE
1	F	291	VAL
1	H	157	ILE
1	I	170	ILE
1	H	170	ILE

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	275/275 (100%)	274 (100%)	1 (0%)	84	82
1	B	275/275 (100%)	274 (100%)	1 (0%)	84	82
1	C	275/275 (100%)	274 (100%)	1 (0%)	84	82
1	D	275/275 (100%)	274 (100%)	1 (0%)	84	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	275/275 (100%)	275 (100%)	0	100	100
1	F	275/275 (100%)	274 (100%)	1 (0%)	84	82
1	G	275/275 (100%)	275 (100%)	0	100	100
1	H	275/275 (100%)	274 (100%)	1 (0%)	84	82
1	I	275/275 (100%)	275 (100%)	0	100	100
1	J	275/275 (100%)	274 (100%)	1 (0%)	84	82
All	All	2750/2750 (100%)	2743 (100%)	7 (0%)	86	84

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	LEU
1	B	178	LEU
1	C	178	LEU
1	D	178	LEU
1	F	178	LEU
1	H	178	LEU
1	J	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	GLN
1	A	177	HIS
1	B	151	ASN
1	B	154	ASN
1	B	182	GLN
1	C	62	GLN
1	C	138	GLN
1	C	200	ASN
1	D	138	GLN
1	D	200	ASN
1	E	62	GLN
1	E	124	GLN
1	E	151	ASN
1	F	151	ASN
1	F	177	HIS
1	F	298	GLN
1	G	103	ASN

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Mol	Chain	Res	Type
1	G	124	GLN
1	G	138	GLN
1	H	138	GLN
1	H	177	HIS
1	H	284	HIS
1	J	124	GLN
1	J	138	GLN
1	J	151	ASN
1	J	284	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 20 are modelled with single atom - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	307/307 (100%)	0.37	21 (6%)	23 25	140, 202, 313, 418	0
1	B	307/307 (100%)	0.85	48 (15%)	5 10	126, 193, 323, 428	0
1	C	307/307 (100%)	0.44	26 (8%)	16 20	132, 191, 340, 497	0
1	D	307/307 (100%)	0.59	36 (11%)	9 13	126, 185, 315, 451	0
1	E	307/307 (100%)	0.53	30 (9%)	13 17	125, 196, 316, 412	0
1	F	307/307 (100%)	0.44	20 (6%)	25 26	154, 215, 342, 427	0
1	G	307/307 (100%)	0.76	45 (14%)	6 10	135, 198, 313, 424	0
1	H	307/307 (100%)	0.54	29 (9%)	14 18	129, 206, 361, 413	0
1	I	307/307 (100%)	0.56	30 (9%)	13 17	118, 197, 330, 459	0
1	J	307/307 (100%)	0.42	24 (7%)	19 22	144, 212, 337, 400	0
All	All	3070/3070 (100%)	0.55	309 (10%)	12 16	118, 200, 329, 497	0

All (309) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	290	GLY	16.8
1	E	291	VAL	15.6
1	G	255	ARG	13.4
1	D	226	GLU	9.7
1	F	89	ASN	8.5
1	B	116	PHE	7.6
1	E	289	ASN	7.4
1	H	185	GLN	7.4
1	I	252	ILE	7.4
1	I	251	ASN	6.7
1	I	248	TYR	6.7
1	B	28	THR	6.4
1	F	252	ILE	6.3

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Mol	Chain	Res	Type	RSRZ
1	I	49	LYS	6.1
1	B	126	PHE	6.0
1	H	184	ASN	5.9
1	B	254	PRO	5.8
1	B	256	LEU	5.8
1	I	208	PHE	5.7
1	G	256	LEU	5.7
1	A	297	ILE	5.7
1	A	175	TYR	5.6
1	B	114	MET	5.4
1	F	88	GLY	5.4
1	J	39	ILE	5.4
1	J	104	ALA	5.3
1	E	77	GLU	5.3
1	H	138	GLN	5.2
1	F	60	ASN	5.1
1	F	59	GLU	5.0
1	B	255	ARG	4.9
1	B	26	VAL	4.9
1	I	230	GLU	4.8
1	C	173	ILE	4.7
1	G	254	PRO	4.6
1	D	38	TYR	4.5
1	F	61	THR	4.5
1	D	149	THR	4.4
1	G	232	LEU	4.4
1	E	64	GLU	4.4
1	H	182	GLN	4.4
1	H	13	ASP	4.4
1	D	230	GLU	4.3
1	B	125	GLN	4.3
1	J	79	ILE	4.2
1	D	171	SER	4.2
1	G	102	TYR	4.2
1	D	208	PHE	4.2
1	I	253	LEU	4.2
1	E	233	GLN	4.2
1	J	233	GLN	4.2
1	J	131	GLU	4.1
1	B	196	ASP	4.1
1	I	262	ILE	4.1
1	D	89	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	251	ASN	4.1
1	G	41	ALA	4.0
1	E	232	LEU	4.0
1	H	198	VAL	4.0
1	J	102	TYR	4.0
1	J	148	TYR	3.9
1	C	188	PHE	3.9
1	C	306	LEU	3.9
1	A	186	ASN	3.9
1	G	251	ASN	3.9
1	F	179	SER	3.9
1	C	309	LEU	3.9
1	B	206	TRP	3.8
1	B	31	GLN	3.8
1	B	302	LEU	3.8
1	F	90	LYS	3.8
1	C	161	TRP	3.8
1	G	75	ALA	3.7
1	D	248	TYR	3.7
1	F	175	TYR	3.7
1	J	251	ASN	3.6
1	I	181	VAL	3.6
1	A	59	GLU	3.6
1	F	253	LEU	3.6
1	G	90	LYS	3.5
1	C	312	GLY	3.5
1	B	124	GLN	3.5
1	H	106	PHE	3.5
1	B	195	ILE	3.5
1	B	123	ARG	3.5
1	E	49	LYS	3.5
1	H	149	THR	3.5
1	B	136	ASN	3.4
1	J	157	ILE	3.4
1	J	21	ASN	3.4
1	B	288	ALA	3.4
1	C	255	ARG	3.3
1	A	288	ALA	3.3
1	A	157	ILE	3.3
1	H	311	ILE	3.3
1	C	18	ILE	3.2
1	E	11	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	313	CYS	3.2
1	J	255	ARG	3.2
1	G	63	ILE	3.2
1	D	205	LEU	3.2
1	D	39	ILE	3.2
1	B	175	TYR	3.1
1	E	78	PHE	3.1
1	E	63	ILE	3.1
1	E	229	SER	3.1
1	I	113	ASP	3.1
1	G	73	VAL	3.1
1	H	12	VAL	3.1
1	B	63	ILE	3.1
1	G	116	PHE	3.1
1	F	141	ARG	3.1
1	D	105	ARG	3.1
1	E	90	LYS	3.1
1	D	206	TRP	3.1
1	A	69	ASN	3.1
1	I	249	THR	3.0
1	B	71	LEU	3.0
1	F	182	GLN	3.0
1	B	41	ALA	3.0
1	G	176	ASP	3.0
1	G	74	PRO	3.0
1	A	294	ASP	3.0
1	I	180	SER	3.0
1	A	138	GLN	3.0
1	A	188	PHE	3.0
1	C	197	ALA	3.0
1	C	195	ILE	3.0
1	G	213	GLY	3.0
1	G	28	THR	2.9
1	G	174	ARG	2.9
1	H	312	GLY	2.9
1	I	119	PHE	2.9
1	B	309	LEU	2.9
1	C	307	GLY	2.9
1	D	174	ARG	2.9
1	F	23	ILE	2.9
1	G	177	HIS	2.9
1	B	253	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	I	111	SER	2.9
1	J	237	THR	2.9
1	E	76	LEU	2.9
1	D	20	ILE	2.9
1	J	147	VAL	2.9
1	B	122	ASP	2.9
1	F	117	ARG	2.8
1	E	227	SER	2.8
1	B	94	LEU	2.8
1	B	187	GLU	2.8
1	J	76	LEU	2.8
1	E	132	PRO	2.8
1	B	21	ASN	2.8
1	D	163	ARG	2.8
1	C	172	ASP	2.8
1	C	175	TYR	2.8
1	G	258	TYR	2.8
1	A	178	LEU	2.8
1	C	149	THR	2.8
1	H	288	ALA	2.8
1	D	209	ILE	2.7
1	I	179	SER	2.7
1	I	207	SER	2.7
1	C	187	GLU	2.7
1	D	175	TYR	2.7
1	H	302	LEU	2.7
1	A	177	HIS	2.7
1	I	112	ASN	2.7
1	D	113	ASP	2.7
1	B	102	TYR	2.7
1	H	161	TRP	2.7
1	F	176	ASP	2.6
1	D	11	PRO	2.6
1	B	118	LEU	2.6
1	G	138	GLN	2.6
1	C	189	SER	2.6
1	H	139	GLN	2.6
1	B	223	PHE	2.6
1	J	149	THR	2.6
1	D	172	ASP	2.6
1	H	187	GLU	2.6
1	E	228	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	214	LEU	2.6
1	I	204	TYR	2.6
1	F	177	HIS	2.6
1	A	179	SER	2.6
1	D	252	ILE	2.6
1	E	288	ALA	2.6
1	F	237	THR	2.6
1	G	126	PHE	2.5
1	H	309	LEU	2.5
1	G	64	GLU	2.5
1	B	197	ALA	2.5
1	B	298	GLN	2.5
1	B	74	PRO	2.5
1	E	158	ASP	2.5
1	E	157	ILE	2.5
1	B	73	VAL	2.5
1	I	182	GLN	2.5
1	G	257	PRO	2.5
1	C	251	ASN	2.5
1	A	189	SER	2.5
1	A	246	ALA	2.5
1	D	18	ILE	2.5
1	B	137	ASN	2.5
1	D	173	ILE	2.4
1	H	179	SER	2.4
1	A	158	ASP	2.4
1	D	255	ARG	2.4
1	H	286	ARG	2.4
1	C	308	PHE	2.4
1	G	306	LEU	2.4
1	A	241	THR	2.4
1	D	61	THR	2.4
1	E	159	GLU	2.4
1	F	11	PRO	2.4
1	F	251	ASN	2.4
1	H	32	THR	2.4
1	D	227	SER	2.4
1	E	258	TYR	2.4
1	D	102	TYR	2.4
1	G	76	LEU	2.4
1	I	254	PRO	2.4
1	J	130	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	113	ASP	2.4
1	B	27	ASN	2.4
1	J	129	GLU	2.3
1	J	250	SER	2.3
1	H	29	LEU	2.3
1	I	125	GLN	2.3
1	J	78	PHE	2.3
1	B	183	PRO	2.3
1	I	288	ALA	2.3
1	B	252	ILE	2.3
1	B	32	THR	2.3
1	H	241	THR	2.3
1	E	102	TYR	2.3
1	I	245	TYR	2.3
1	D	145	ILE	2.3
1	C	138	GLN	2.3
1	C	252	ILE	2.3
1	D	262	ILE	2.3
1	A	117	ARG	2.3
1	G	233	GLN	2.3
1	I	206	TRP	2.2
1	E	34	LYS	2.2
1	B	166	ALA	2.2
1	D	296	LEU	2.2
1	G	51	PRO	2.2
1	I	174	ARG	2.2
1	H	156	GLU	2.2
1	J	175	TYR	2.2
1	C	128	LEU	2.2
1	I	296	LEU	2.2
1	G	189	SER	2.2
1	C	311	ILE	2.2
1	F	240	LEU	2.2
1	G	133	PHE	2.2
1	E	131	GLU	2.2
1	E	230	GLU	2.2
1	H	244	ALA	2.2
1	J	137	ASN	2.2
1	G	149	THR	2.2
1	G	40	VAL	2.2
1	G	156	GLU	2.2
1	B	121	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	249	THR	2.1
1	E	285	HIS	2.1
1	C	235	SER	2.1
1	J	292	GLU	2.1
1	D	13	ASP	2.1
1	A	130	LEU	2.1
1	G	22	LYS	2.1
1	H	111	SER	2.1
1	H	25	GLY	2.1
1	E	133	PHE	2.1
1	G	271	GLY	2.1
1	A	132	PRO	2.1
1	G	67	ILE	2.1
1	G	157	ILE	2.1
1	G	163	ARG	2.1
1	B	33	TYR	2.1
1	G	52	GLY	2.1
1	G	139	GLN	2.1
1	G	53	ASP	2.1
1	I	205	LEU	2.1
1	J	184	ASN	2.1
1	E	23	ILE	2.1
1	H	287	GLN	2.1
1	B	22	LYS	2.1
1	D	29	LEU	2.1
1	B	79	ILE	2.1
1	E	25	GLY	2.1
1	A	11	PRO	2.1
1	I	227	SER	2.1
1	C	193	VAL	2.1
1	G	39	ILE	2.0
1	G	29	LEU	2.0
1	G	71	LEU	2.0
1	H	188	PHE	2.0
1	D	137	ASN	2.0
1	I	117	ARG	2.0
1	H	109	SER	2.0
1	J	29	LEU	2.0
1	B	258	TYR	2.0
1	B	312	GLY	2.0
1	D	44	THR	2.0
1	G	65	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	129	GLU	2.0
1	G	180	SER	2.0

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

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

6.3 Carbohydrates [i](#)

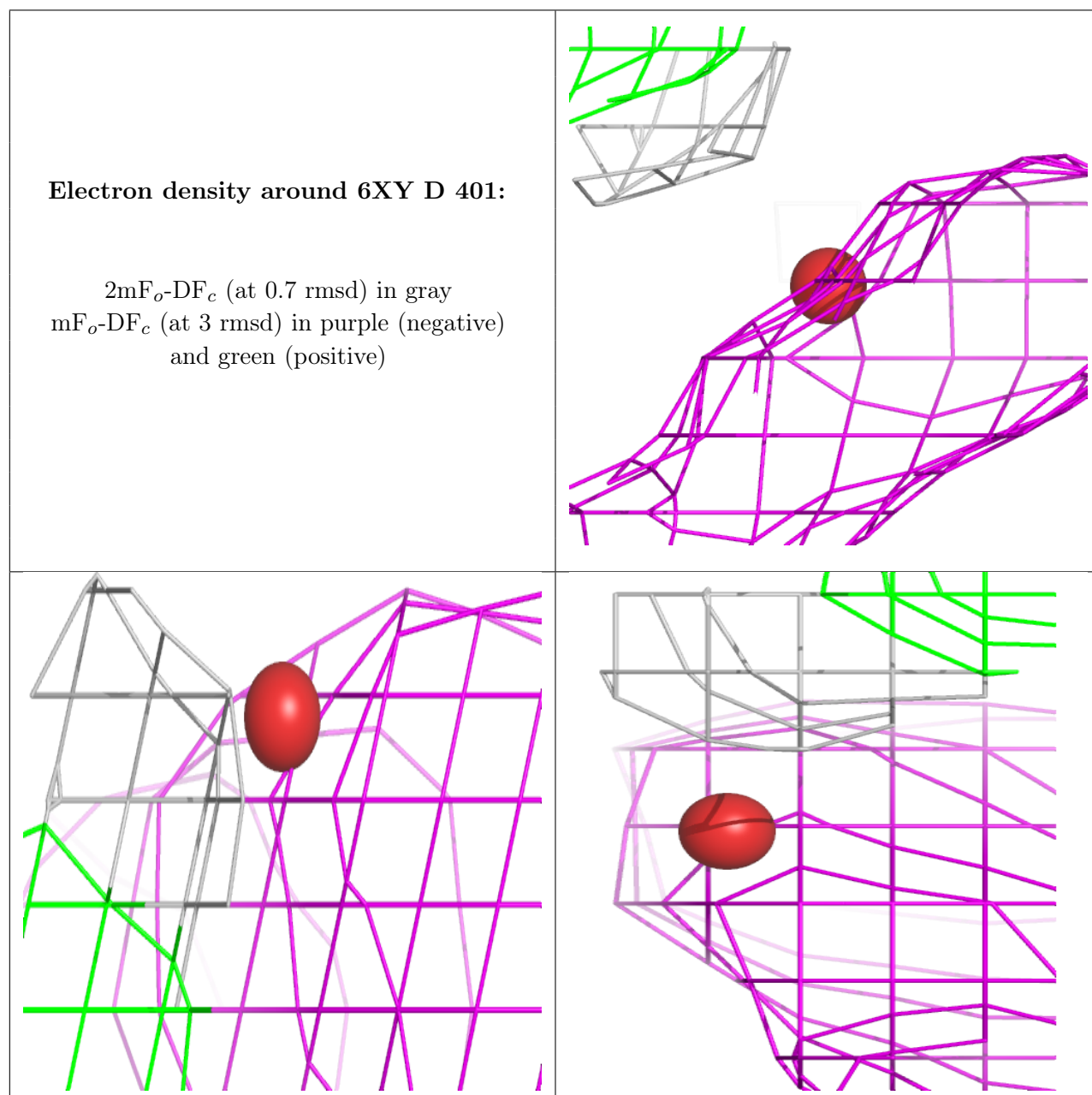
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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.

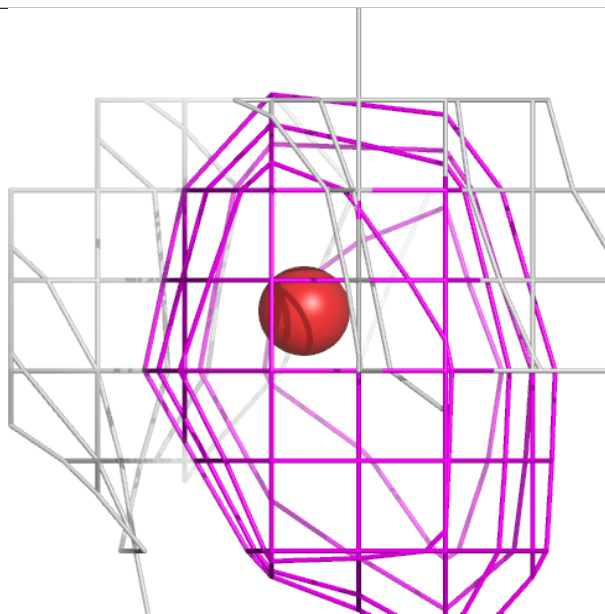
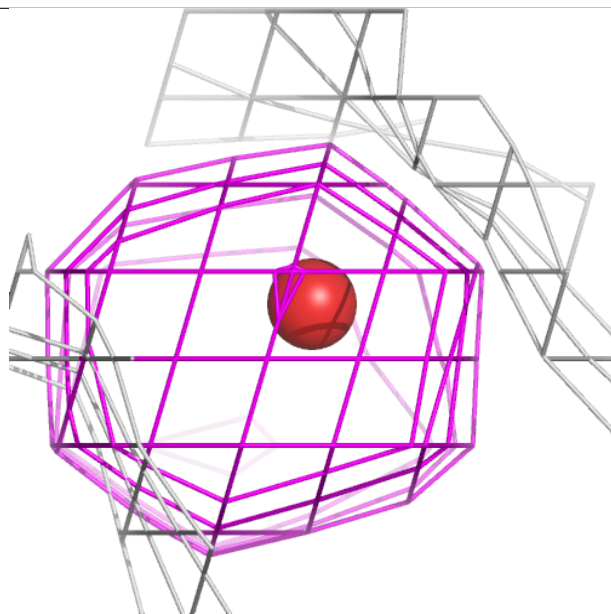
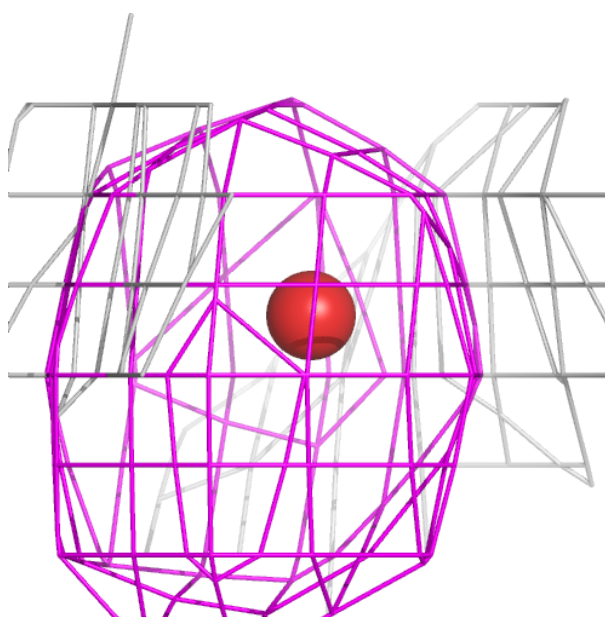
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	6XY	A	402	1/21	0.13	0.25	244,244,244,244	0
2	6XY	B	401	1/21	0.19	0.28	241,241,241,241	0
2	6XY	I	402	1/21	0.21	0.34	235,235,235,235	0
2	6XY	C	402	1/21	0.22	0.22	308,308,308,308	0
2	6XY	C	401	1/21	0.29	0.27	242,242,242,242	0
2	6XY	D	402	1/21	0.37	0.23	276,276,276,276	0
2	6XY	I	401	1/21	0.38	0.25	212,212,212,212	0
2	6XY	G	401	1/21	0.38	0.31	233,233,233,233	0
2	6XY	D	401	1/21	0.40	0.51	238,238,238,238	0
2	6XY	H	402	1/21	0.42	0.40	213,213,213,213	0
2	6XY	J	401	1/21	0.43	0.60	223,223,223,223	0
2	6XY	F	401	1/21	0.44	0.24	250,250,250,250	0
2	6XY	H	401	1/21	0.45	0.29	249,249,249,249	0
2	6XY	J	402	1/21	0.58	0.20	329,329,329,329	0
2	6XY	A	401	1/21	0.60	0.15	439,439,439,439	0
2	6XY	B	402	1/21	0.66	0.52	697,697,697,697	0
2	6XY	E	402	1/21	0.66	0.15	338,338,338,338	0
2	6XY	F	402	1/21	0.72	0.11	318,318,318,318	0
2	6XY	G	402	1/21	0.86	0.31	431,431,431,431	0
2	6XY	E	401	1/21	0.89	0.27	438,438,438,438	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



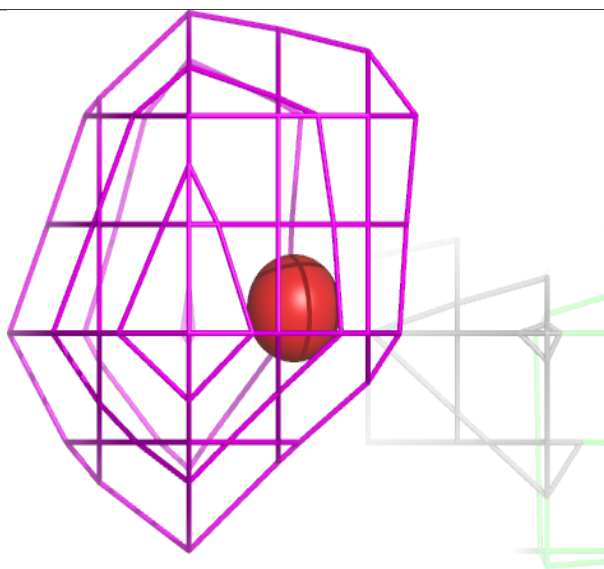
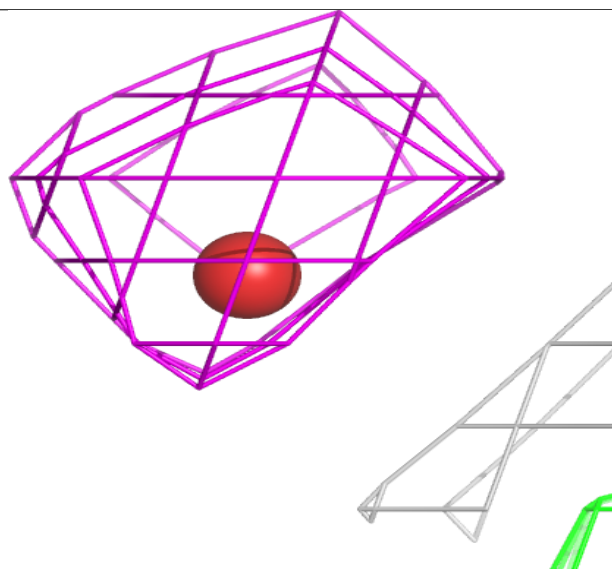
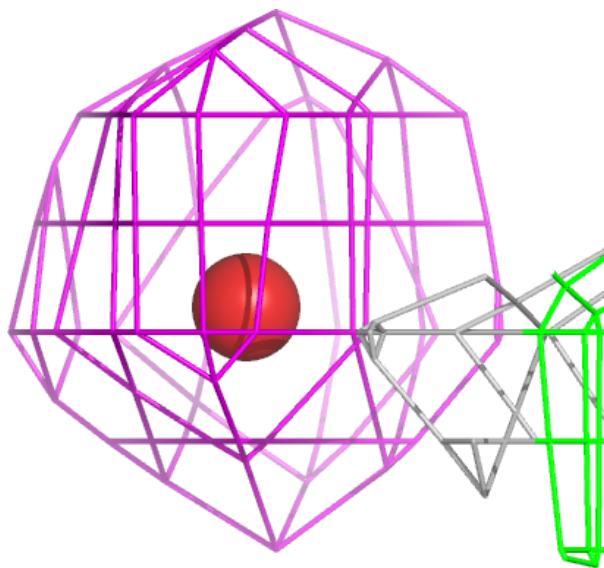
Electron density around 6XY H 402:

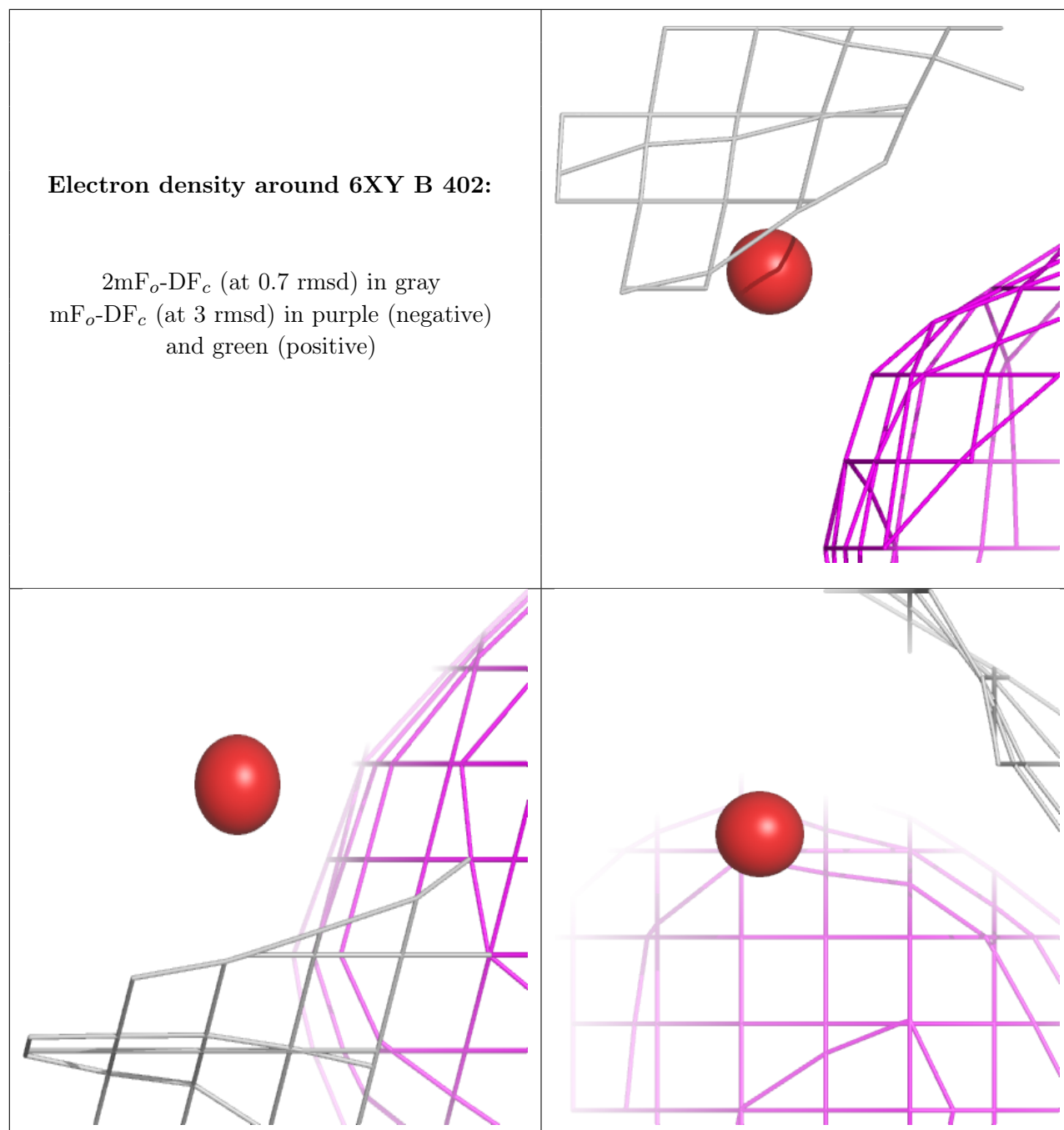
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 6XY J 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.