



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:23 PM UTC

PDB ID : 3ZKR / pdb_00003zkr
Title : X-ray structure of a pentameric ligand gated ion channel from *Erwinia chrysanthemi* (ELIC) in complex with bromoform
Authors : Spurny, R.; Billen, B.; Howard, R.J.; Brams, M.; Debaveye, S.; Price, K.L.; Weston, D.A.; Strelkov, S.V.; Tytgat, J.; Bertrand, S.; Bertrand, D.; Lummis, S.C.R.; Ulens, C.
Deposited on : 2013-01-24
Resolution : 3.65 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

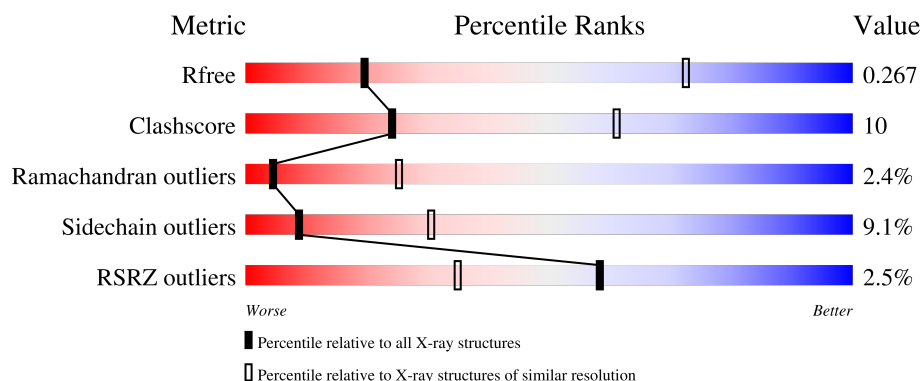
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.65 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.



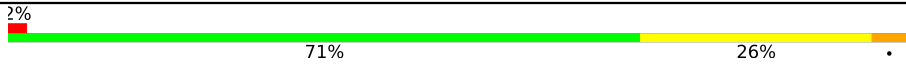
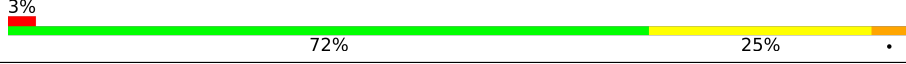
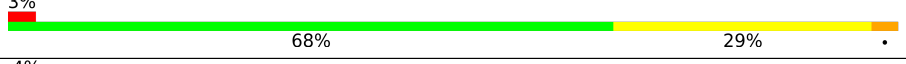
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1132 (3.76-3.52)
Clashscore	190562	1014 (3.74-3.54)
Ramachandran outliers	187476	1123 (3.76-3.52)
Sidechain outliers	187428	1121 (3.76-3.52)
RSRZ outliers	180081	1130 (3.76-3.52)

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	
1	B	307	
1	C	307	
1	D	307	
1	E	307	

Continued on next page...

Continued from previous page...

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	MBR	A	402	-	-	X	-
2	MBR	B	402	-	-	X	-
2	MBR	C	402	-	-	X	-
2	MBR	D	402	-	-	X	X
2	MBR	E	401	-	-	X	-
2	MBR	E	402	-	-	X	-
2	MBR	F	401	-	-	X	-
2	MBR	F	402	-	-	X	-
2	MBR	G	402	-	-	X	X
2	MBR	H	402	-	-	X	-
2	MBR	I	402	-	-	X	X
2	MBR	J	402	-	-	X	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25042 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
			2502	1630	416	450	6			
1	B	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	C	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	D	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	E	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	F	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	G	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	H	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	I	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	J	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			

There are 20 discrepancies between the modelled and reference sequences:

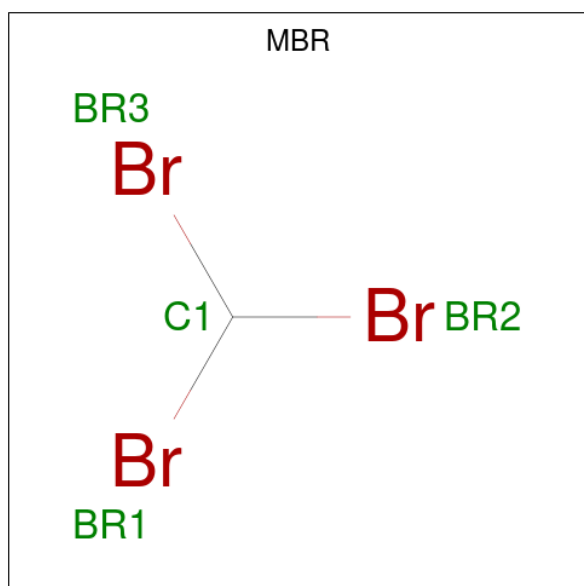
Chain	Residue	Modelled	Actual	Comment	Reference
A	164	GLY	-	insertion	UNP P0C7B7
A	289	ASN	MET	conflict	UNP P0C7B7
B	164	GLY	-	insertion	UNP P0C7B7
B	289	ASN	MET	conflict	UNP P0C7B7
C	164	GLY	-	insertion	UNP P0C7B7
C	289	ASN	MET	conflict	UNP P0C7B7
D	164	GLY	-	insertion	UNP P0C7B7
D	289	ASN	MET	conflict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

Continued on next page...

Continued from previous page...

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 TRIBROMOMETHANE (CCD ID: MBR) (formula: CHBr_3).



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	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

Continued on next page...

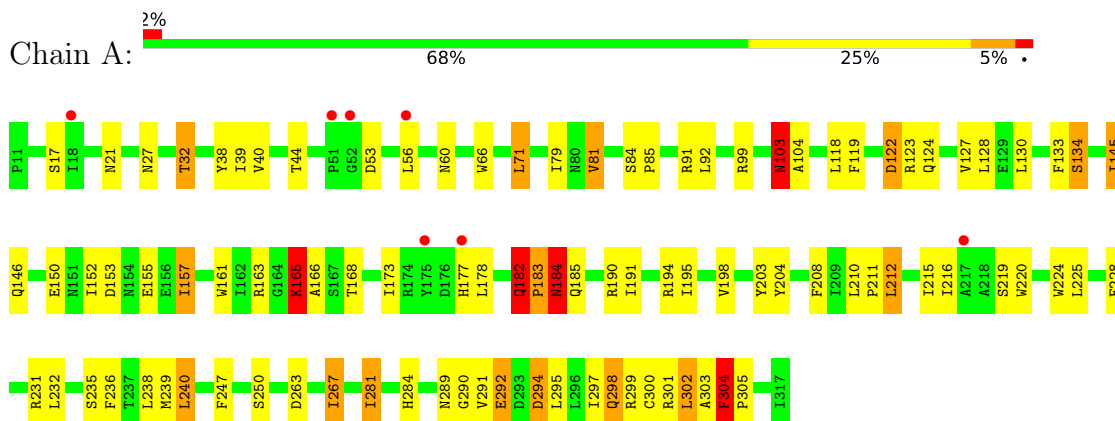
Continued from previous page...

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

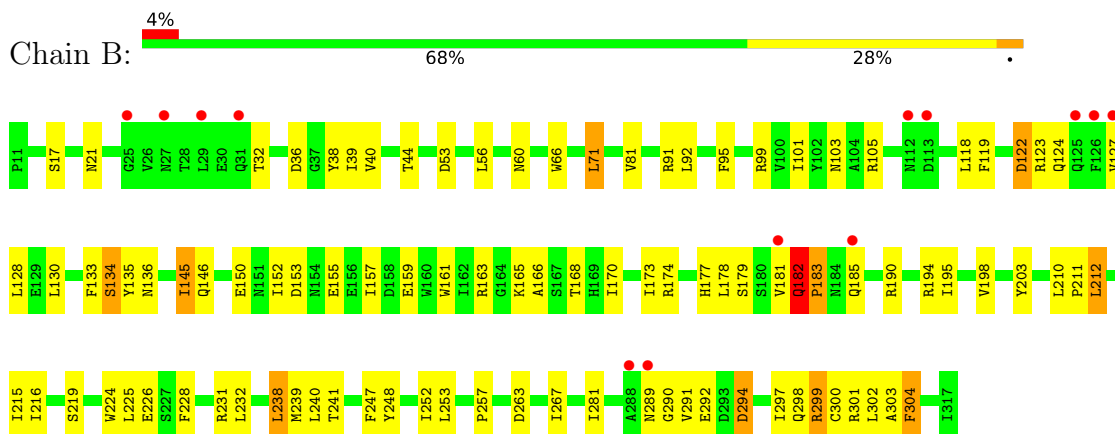
3 Residue-property plots

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.

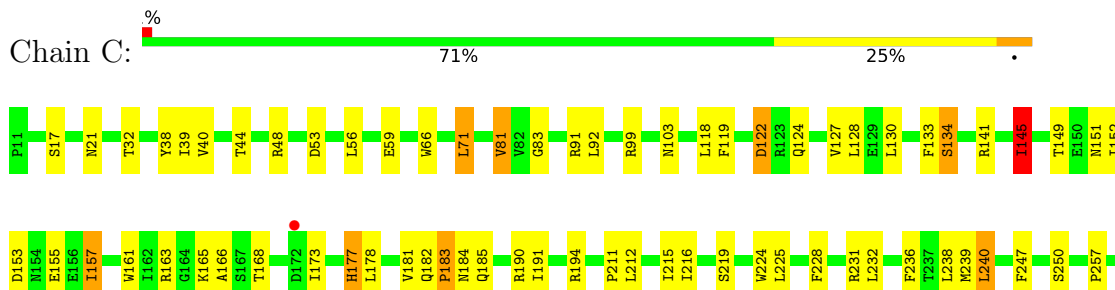
• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL



• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

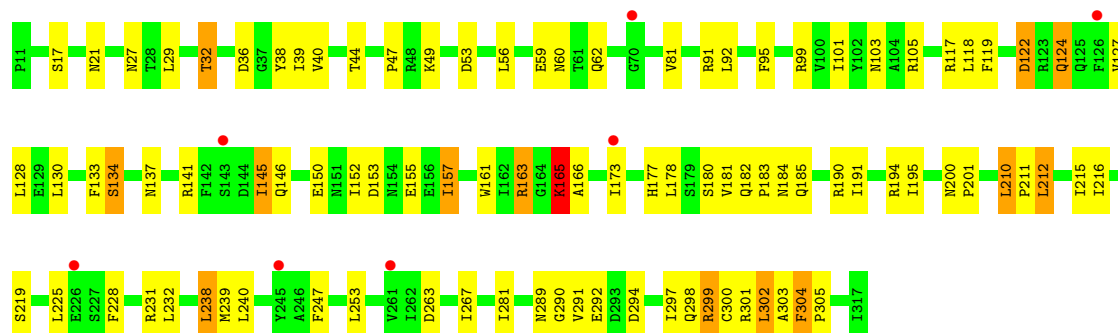


• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

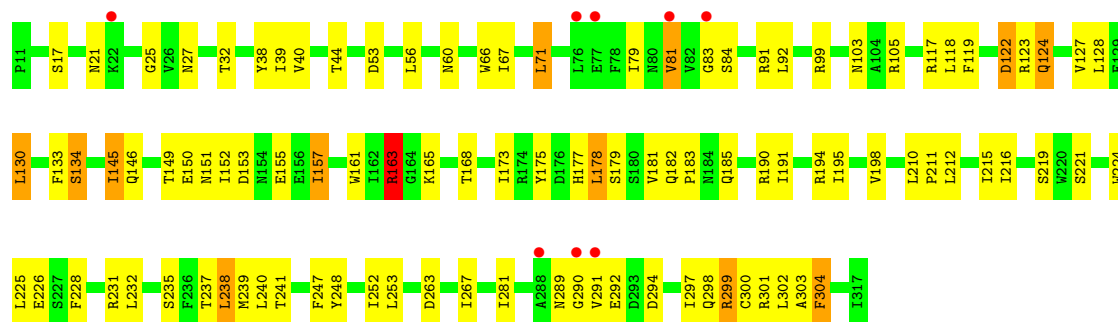




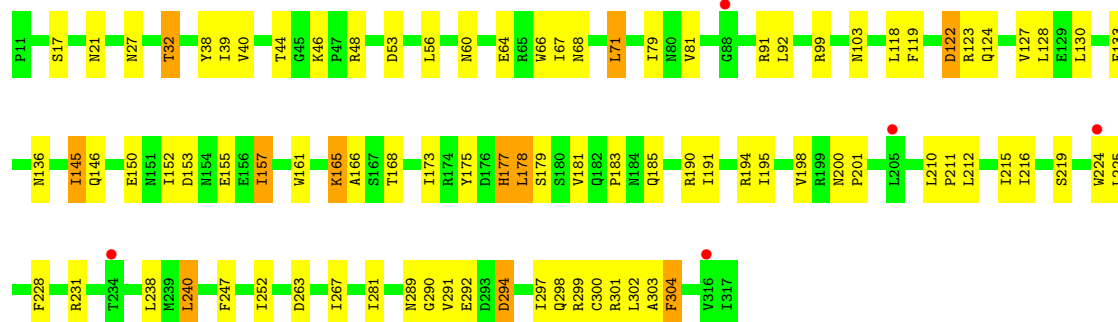
• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL



• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

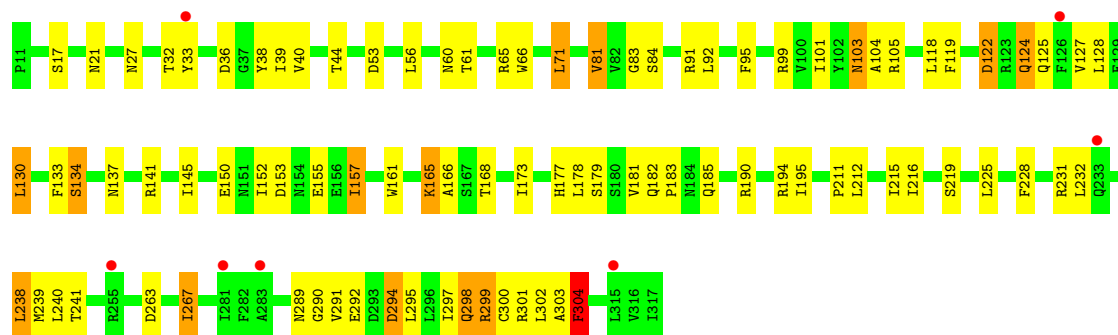


• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

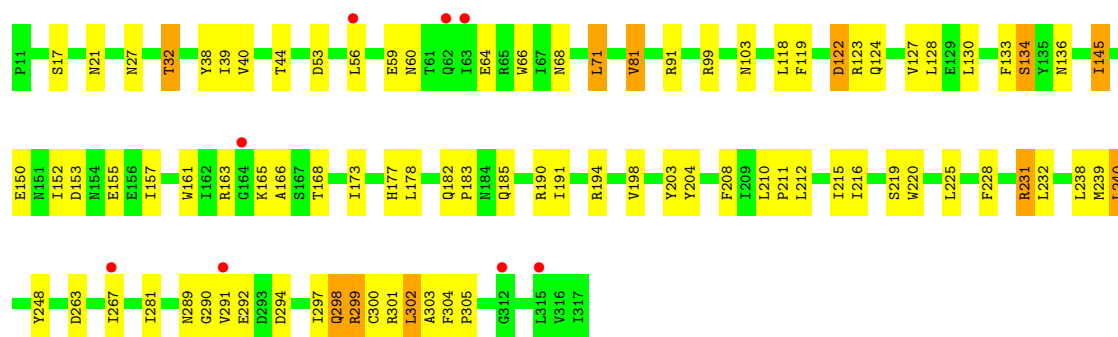


• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

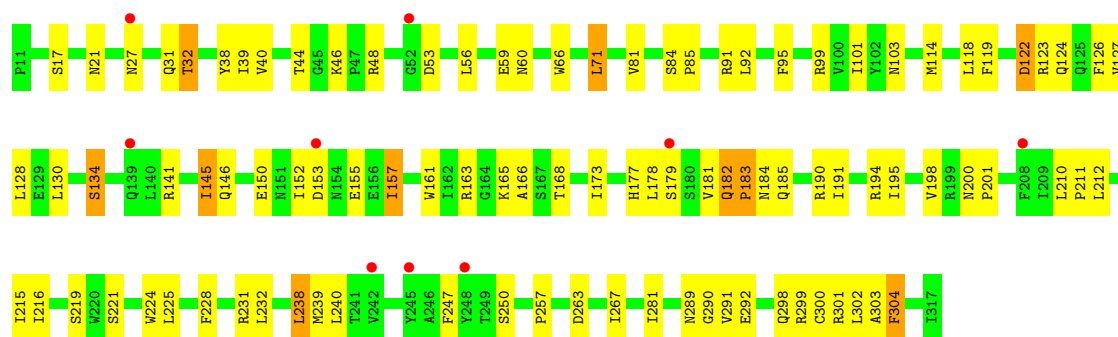




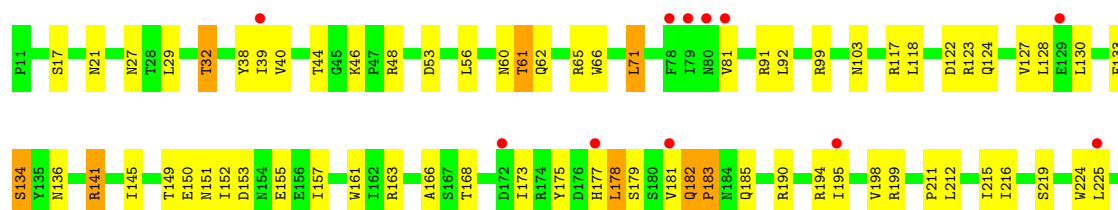
• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL



• 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	105.11Å 266.25Å 110.75Å 90.00° 109.78° 90.00°	Depositor
Resolution (Å)	44.08 – 3.65 44.08 – 3.65	Depositor EDS
% Data completeness (in resolution range)	98.9 (44.08-3.65) 98.8 (44.08-3.65)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 3.66Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.229 , 0.264 0.234 , 0.267	Depositor DCC
R_{free} test set	3189 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	108.2	Xtriage
Anisotropy	0.437	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 62.7	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	0.90	EDS
Total number of atoms	25042	wwPDB-VP
Average B, all atoms (Å ²)	131.0	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

5.1 Standard geometry

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

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	0.52	3/2570 (0.1%)	1.01	8/3503 (0.2%)
1	B	0.51	4/2570 (0.2%)	0.97	5/3503 (0.1%)
1	C	0.48	4/2570 (0.2%)	0.96	3/3503 (0.1%)
1	D	0.58	4/2570 (0.2%)	1.02	8/3503 (0.2%)
1	E	0.52	5/2570 (0.2%)	1.00	11/3503 (0.3%)
1	F	0.53	5/2570 (0.2%)	1.35	7/3503 (0.2%)
1	G	0.56	5/2570 (0.2%)	1.00	8/3503 (0.2%)
1	H	0.50	3/2570 (0.1%)	0.96	0/3503
1	I	0.58	5/2570 (0.2%)	0.99	5/3503 (0.1%)
1	J	0.46	2/2570 (0.1%)	0.94	6/3503 (0.2%)
All	All	0.53	40/25700 (0.2%)	1.03	61/35030 (0.2%)

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	D	0	2
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
All	All	0	7

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	103	ASN	CG-ND2	-9.64	1.13	1.33
1	D	124	GLN	CD-NE2	-9.38	1.13	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	124	GLN	CD-NE2	-8.96	1.14	1.33
1	G	103	ASN	CG-OD1	-8.45	1.07	1.23
1	E	124	GLN	CD-NE2	-8.40	1.15	1.33
1	B	298	GLN	CD-NE2	-8.37	1.15	1.33
1	I	298	GLN	CD-NE2	-8.19	1.16	1.33
1	F	103	ASN	CG-ND2	-7.99	1.16	1.33
1	H	298	GLN	CD-NE2	-7.75	1.17	1.33
1	H	298	GLN	CD-OE1	-7.04	1.10	1.23
1	I	298	GLN	CD-OE1	-7.01	1.10	1.23
1	I	183	PRO	CA-C	6.98	1.62	1.52
1	A	103	ASN	CG-ND2	-6.96	1.18	1.33
1	D	124	GLN	CD-OE1	-6.91	1.10	1.23
1	G	103	ASN	CG-ND2	-6.62	1.19	1.33
1	B	103	ASN	CG-ND2	-6.51	1.19	1.33
1	D	298	GLN	CD-NE2	-6.43	1.19	1.33
1	E	124	GLN	CD-OE1	-6.38	1.11	1.23
1	B	298	GLN	CD-OE1	-6.21	1.11	1.23
1	A	103	ASN	CG-OD1	-6.13	1.11	1.23
1	F	103	ASN	CG-OD1	-5.97	1.12	1.23
1	E	103	ASN	CG-ND2	-5.97	1.20	1.33
1	F	298	GLN	CD-NE2	-5.95	1.20	1.33
1	B	103	ASN	CG-OD1	-5.90	1.12	1.23
1	I	103	ASN	CG-ND2	-5.79	1.21	1.33
1	J	103	ASN	CG-ND2	-5.70	1.21	1.33
1	H	103	ASN	CG-ND2	-5.63	1.21	1.33
1	C	103	ASN	CG-ND2	-5.60	1.21	1.33
1	F	165	LYS	C-O	5.46	1.30	1.23
1	E	298	GLN	CD-NE2	-5.41	1.21	1.33
1	I	184	ASN	N-CA	5.41	1.51	1.47
1	J	298	GLN	CD-NE2	-5.39	1.22	1.33
1	C	298	GLN	CD-NE2	-5.38	1.22	1.33
1	G	298	GLN	CD-NE2	-5.33	1.22	1.33
1	G	124	GLN	CD-OE1	-5.28	1.13	1.23
1	C	177	HIS	CE1-NE2	-5.22	1.27	1.32
1	C	103	ASN	CG-OD1	-5.21	1.13	1.23
1	A	298	GLN	CD-NE2	-5.11	1.22	1.33
1	F	177	HIS	CE1-NE2	-5.10	1.27	1.32
1	E	103	ASN	CG-OD1	-5.09	1.13	1.23

All (61) bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	165	LYS	O-C-N	-38.63	79.38	123.03
1	F	165	LYS	CA-C-O	-34.79	79.22	121.66
1	F	166	ALA	N-CA-C	12.17	127.40	110.24
1	F	165	LYS	CA-C-N	11.99	137.80	120.90
1	F	165	LYS	C-N-CA	11.99	137.80	120.90
1	E	163	ARG	NE-CZ-NH1	8.29	129.79	121.50
1	D	163	ARG	CB-CG-CD	8.13	129.99	111.30
1	A	165	LYS	CA-C-O	-7.62	111.33	120.55
1	E	163	ARG	CG-CD-NE	7.50	128.50	112.00
1	A	182	GLN	CA-C-N	-7.02	111.07	119.84
1	A	182	GLN	C-N-CA	-7.02	111.07	119.84
1	E	163	ARG	NE-CZ-NH2	-6.99	112.91	119.20
1	E	163	ARG	CD-NE-CZ	6.55	133.57	124.40
1	F	166	ALA	N-CA-CB	-6.45	99.43	109.69
1	D	210	LEU	CA-C-N	-6.27	112.55	119.19
1	D	210	LEU	C-N-CA	-6.27	112.55	119.19
1	G	84	SER	CA-C-N	6.15	126.11	119.78
1	G	84	SER	C-N-CA	6.15	126.11	119.78
1	B	145	ILE	N-CA-C	6.08	116.60	108.27
1	G	124	GLN	OE1-CD-NE2	-6.05	116.55	122.60
1	E	84	SER	CA-C-N	6.00	126.01	119.89
1	E	84	SER	C-N-CA	6.00	126.01	119.89
1	I	183	PRO	CA-C-N	5.96	129.35	119.35
1	I	183	PRO	C-N-CA	5.96	129.35	119.35
1	D	163	ARG	NE-CZ-NH1	5.75	127.25	121.50
1	G	304	PHE	N-CA-C	5.66	122.31	109.81
1	D	165	LYS	CA-C-O	-5.59	112.88	119.48
1	G	165	LYS	CA-C-N	5.56	132.15	121.54
1	G	165	LYS	C-N-CA	5.56	132.15	121.54
1	A	79	ILE	N-CA-C	5.53	116.16	110.36
1	D	253	LEU	CA-C-N	5.53	125.28	119.76
1	D	253	LEU	C-N-CA	5.53	125.28	119.76
1	I	182	GLN	N-CA-C	5.52	122.00	109.81
1	A	304	PHE	CA-C-N	-5.50	112.95	119.05
1	A	304	PHE	C-N-CA	-5.50	112.95	119.05
1	E	298	GLN	N-CA-C	-5.47	105.47	111.82
1	E	253	LEU	CA-C-N	5.45	125.21	119.76
1	E	253	LEU	C-N-CA	5.45	125.21	119.76
1	J	61	THR	N-CA-C	5.40	117.87	111.33
1	A	267	ILE	CB-CA-C	-5.34	104.93	112.14
1	C	145	ILE	N-CA-C	5.31	115.55	108.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	141	ARG	CD-NE-CZ	-5.29	117.00	124.40
1	G	267	ILE	CB-CA-C	-5.27	105.14	112.04
1	G	125	GLN	N-CA-C	5.25	116.95	108.34
1	F	252	ILE	N-CA-C	5.22	116.30	111.81
1	J	46	LYS	CA-C-N	5.22	125.51	119.93
1	J	46	LYS	C-N-CA	5.22	125.51	119.93
1	B	298	GLN	N-CA-C	-5.19	106.21	112.54
1	B	135	TYR	N-CA-C	5.18	117.05	108.20
1	E	25	GLY	N-CA-C	5.16	121.02	113.48
1	B	253	LEU	CA-C-N	5.15	124.91	119.76
1	B	253	LEU	C-N-CA	5.15	124.91	119.76
1	I	46	LYS	CA-C-N	5.11	125.39	119.93
1	I	46	LYS	C-N-CA	5.11	125.39	119.93
1	A	184	ASN	N-CA-C	5.05	121.56	110.80
1	J	253	LEU	CA-C-N	5.05	124.81	119.76
1	J	253	LEU	C-N-CA	5.05	124.81	119.76
1	D	117	ARG	N-CA-C	5.03	117.42	111.33
1	E	237	THR	N-CA-C	-5.02	105.89	111.36
1	C	165	LYS	CA-C-N	5.00	131.09	121.54
1	C	165	LYS	C-N-CA	5.00	131.09	121.54

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	LYS	Mainchain
1	D	165	LYS	Mainchain
1	D	47	PRO	Mainchain
1	E	165	LYS	Mainchain
1	F	165	LYS	Mainchain
1	G	165	LYS	Mainchain
1	H	165	LYS	Mainchain

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	2502	0	2469	67	1
1	B	2502	0	2469	57	0
1	C	2502	0	2469	59	0
1	D	2502	0	2469	55	1
1	E	2502	0	2469	71	0
1	F	2502	0	2469	57	0
1	G	2502	0	2469	55	0
1	H	2502	0	2469	52	0
1	I	2502	0	2469	58	0
1	J	2502	0	2469	56	0
2	A	3	0	0	4	0
2	B	2	0	0	3	0
2	C	2	0	0	3	0
2	D	2	0	0	3	0
2	E	2	0	0	8	0
2	F	3	0	0	6	0
2	G	2	0	0	5	0
2	H	2	0	0	4	0
2	I	2	0	0	5	0
2	J	2	0	0	4	0
All	All	25042	0	24690	497	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (497) 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:195:ILE:HD12	2:J:402:MBR:BR1	1.28	1.84
1:E:221:SER:HB3	2:E:401:MBR:BR1	1.37	1.76
1:I:195:ILE:HD12	2:I:402:MBR:BR1	1.57	1.56
1:C:128:LEU:HD13	2:C:402:MBR:BR1	1.61	1.52
1:J:195:ILE:CD1	2:J:402:MBR:BR1	2.19	1.44
1:E:221:SER:CB	2:E:401:MBR:BR1	2.18	1.43
1:G:128:LEU:CD1	2:G:402:MBR:BR1	2.24	1.40
1:H:128:LEU:HD13	2:H:402:MBR:BR1	1.77	1.39
1:H:128:LEU:CD1	2:H:402:MBR:BR1	2.29	1.36
1:D:128:LEU:HD13	2:D:402:MBR:BR1	1.82	1.33
1:A:128:LEU:HD13	2:A:402:MBR:BR1	1.86	1.31
1:G:128:LEU:HD13	2:G:402:MBR:BR1	1.84	1.28
1:C:128:LEU:CD1	2:C:402:MBR:BR1	2.35	1.27
1:F:195:ILE:HD12	2:F:402:MBR:BR1	1.90	1.27

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:ILE:HD12	2:B:402:MBR:BR1	1.96	1.21
1:F:128:LEU:HD13	2:F:402:MBR:BR1	1.96	1.19
1:E:128:LEU:HD13	2:E:402:MBR:BR1	2.02	1.14
1:I:195:ILE:CD1	2:I:402:MBR:BR1	2.53	1.10
1:A:128:LEU:CD1	2:A:402:MBR:BR1	2.56	1.08
1:D:128:LEU:CD1	2:D:402:MBR:BR1	2.59	1.04
1:G:128:LEU:HD12	2:G:402:MBR:BR1	2.14	1.00
1:D:195:ILE:HD12	2:D:402:MBR:BR1	2.18	0.99
1:E:128:LEU:CD1	2:E:402:MBR:BR1	2.65	0.99
1:A:195:ILE:HD12	2:A:402:MBR:BR1	2.17	0.98
1:F:128:LEU:CD1	2:F:402:MBR:BR1	2.72	0.92
1:H:128:LEU:HD11	2:H:402:MBR:BR1	2.27	0.87
1:F:195:ILE:CD1	2:F:402:MBR:BR1	2.78	0.86
1:C:91:ARG:HD2	1:D:134:SER:HB3	1.59	0.84
1:B:128:LEU:HD13	2:B:402:MBR:BR1	2.35	0.81
1:H:91:ARG:HD2	1:I:134:SER:HB3	1.61	0.81
1:E:195:ILE:HD12	2:E:402:MBR:BR1	2.36	0.81
1:C:128:LEU:HD12	2:C:402:MBR:BR1	2.34	0.81
1:D:181:VAL:HG21	1:D:185:GLN:HB2	1.63	0.80
1:G:91:ARG:HD2	1:H:134:SER:HB3	1.62	0.78
1:B:91:ARG:HD2	1:C:134:SER:HB3	1.65	0.77
1:A:91:ARG:HD2	1:B:134:SER:HB3	1.66	0.76
1:E:221:SER:HB2	2:E:401:MBR:BR1	2.37	0.74
1:I:91:ARG:HD2	1:J:134:SER:HB3	1.68	0.74
1:E:221:SER:CA	2:E:401:MBR:BR1	2.90	0.73
1:F:91:ARG:HD2	1:G:134:SER:HB3	1.69	0.73
1:D:91:ARG:HB2	1:E:133:PHE:HE2	1.54	0.71
1:E:155:GLU:OE2	1:E:163:ARG:NH2	2.24	0.71
1:A:219:SER:HA	1:A:238:LEU:HD21	1.73	0.70
1:G:128:LEU:HD11	2:G:402:MBR:BR1	2.41	0.70
1:J:128:LEU:HD13	2:J:402:MBR:BR1	2.46	0.69
1:A:103:ASN:HD22	1:A:104:ALA:N	1.90	0.69
1:B:128:LEU:CD1	2:B:402:MBR:BR1	2.96	0.69
1:C:219:SER:HA	1:C:238:LEU:HD21	1.74	0.69
1:A:133:PHE:HE2	1:E:91:ARG:HB2	1.57	0.69
1:D:155:GLU:OE2	1:D:163:ARG:NH2	2.26	0.68
1:B:219:SER:HA	1:B:238:LEU:HD21	1.75	0.68
1:I:225:LEU:HD21	1:J:232:LEU:HD22	1.74	0.68
1:E:219:SER:HA	1:E:238:LEU:HD21	1.76	0.68
1:J:219:SER:HA	1:J:238:LEU:HD21	1.75	0.67
1:H:219:SER:HA	1:H:238:LEU:HD21	1.74	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:219:SER:HA	1:G:238:LEU:HD21	1.77	0.67
1:I:219:SER:HA	1:I:238:LEU:HD21	1.76	0.67
1:F:219:SER:HA	1:F:238:LEU:HD21	1.77	0.67
1:D:219:SER:HA	1:D:238:LEU:HD21	1.76	0.67
1:D:91:ARG:HD2	1:E:134:SER:HB3	1.76	0.66
1:D:127:VAL:HG22	1:D:194:ARG:HG2	1.77	0.66
1:A:239:MET:HE3	1:E:215:ILE:HD13	1.76	0.66
1:F:215:ILE:HD13	1:G:239:MET:HE3	1.78	0.65
1:I:215:ILE:HD13	1:J:239:MET:HE3	1.77	0.65
1:C:225:LEU:HD21	1:D:232:LEU:HD22	1.79	0.64
1:F:224:TRP:CZ3	2:F:401:MBR:BR1	3.05	0.64
1:F:91:ARG:HB2	1:G:133:PHE:HE2	1.61	0.64
1:A:225:LEU:HD21	1:B:232:LEU:HD22	1.78	0.64
1:A:240:LEU:HD23	1:E:241:THR:HA	1.80	0.63
1:G:294:ASP:HB2	1:G:297:ILE:HG22	1.81	0.62
1:F:44:THR:HA	1:F:99:ARG:HA	1.80	0.62
1:A:119:PHE:HA	1:A:122:ASP:OD1	2.00	0.61
1:G:289:ASN:OD1	1:G:290:GLY:N	2.34	0.61
1:G:91:ARG:HB2	1:H:133:PHE:HE2	1.66	0.61
1:H:128:LEU:HD12	2:H:402:MBR:BR1	2.49	0.61
1:A:134:SER:HB3	1:E:91:ARG:HD2	1.82	0.60
1:A:44:THR:HA	1:A:99:ARG:HA	1.83	0.60
1:A:289:ASN:OD1	1:A:290:GLY:N	2.32	0.60
1:C:212:LEU:O	1:C:216:ILE:HG12	2.02	0.60
1:A:127:VAL:HG22	1:A:194:ARG:HG2	1.84	0.59
1:G:195:ILE:HD12	2:G:402:MBR:BR1	2.58	0.59
1:H:127:VAL:HG22	1:H:194:ARG:HG2	1.84	0.59
1:D:91:ARG:HB2	1:E:133:PHE:CE2	2.37	0.59
1:D:59:GLU:OE2	1:E:134:SER:OG	2.21	0.59
1:H:173:ILE:HD13	1:H:190:ARG:HB3	1.84	0.59
1:E:212:LEU:O	1:E:216:ILE:HG12	2.03	0.59
1:A:263:ASP:O	1:A:267:ILE:HG12	2.03	0.58
1:A:294:ASP:HB2	1:A:297:ILE:HG22	1.84	0.58
1:F:133:PHE:HE2	1:J:91:ARG:HB2	1.67	0.58
1:I:44:THR:HA	1:I:99:ARG:HA	1.85	0.58
1:D:44:THR:HA	1:D:99:ARG:HA	1.85	0.58
1:D:215:ILE:HD13	1:E:239:MET:HE3	1.86	0.58
1:D:212:LEU:O	1:D:216:ILE:HG12	2.03	0.58
1:D:263:ASP:O	1:D:267:ILE:HG12	2.04	0.58
1:F:212:LEU:O	1:F:216:ILE:HG12	2.04	0.58
1:F:175:TYR:HB2	1:F:178:LEU:HD21	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ILE:HD13	1:A:190:ARG:HB3	1.86	0.57
1:C:173:ILE:HD13	1:C:190:ARG:HB3	1.86	0.57
1:J:212:LEU:O	1:J:216:ILE:HG12	2.05	0.57
1:E:127:VAL:HG22	1:E:194:ARG:HG2	1.87	0.57
1:F:179:SER:HB2	1:F:181:VAL:HG12	1.87	0.57
1:H:294:ASP:HB2	1:H:297:ILE:HG22	1.87	0.57
1:I:212:LEU:O	1:I:216:ILE:HG12	2.05	0.57
1:A:185:GLN:N	1:A:185:GLN:OE1	2.38	0.56
1:E:263:ASP:O	1:E:267:ILE:HG12	2.04	0.56
1:J:127:VAL:HG22	1:J:194:ARG:HG2	1.87	0.56
1:F:127:VAL:HG22	1:F:194:ARG:HG2	1.87	0.56
1:B:173:ILE:HD13	1:B:190:ARG:HB3	1.87	0.56
1:J:294:ASP:HB2	1:J:297:ILE:HG22	1.87	0.56
1:J:173:ILE:HD13	1:J:190:ARG:HB3	1.86	0.56
1:A:212:LEU:O	1:A:216:ILE:HG12	2.05	0.56
1:B:212:LEU:O	1:B:216:ILE:HG12	2.05	0.56
1:B:241:THR:HA	1:C:240:LEU:HD23	1.88	0.56
1:C:263:ASP:O	1:C:267:ILE:HG12	2.05	0.56
1:E:44:THR:HA	1:E:99:ARG:HA	1.88	0.56
1:E:289:ASN:OD1	1:E:290:GLY:N	2.35	0.56
1:I:127:VAL:HG22	1:I:194:ARG:HG2	1.86	0.56
1:H:225:LEU:HD21	1:I:232:LEU:HD22	1.87	0.56
1:I:221:SER:HB3	2:I:401:MBR:BR1	2.62	0.56
1:B:44:THR:HA	1:B:99:ARG:HA	1.87	0.55
1:H:212:LEU:O	1:H:216:ILE:HG12	2.05	0.55
1:F:119:PHE:HA	1:F:122:ASP:OD1	2.06	0.55
1:G:173:ILE:HD13	1:G:190:ARG:HB3	1.88	0.55
1:A:103:ASN:HD22	1:A:103:ASN:C	2.13	0.54
1:G:44:THR:HA	1:G:99:ARG:HA	1.88	0.54
1:F:175:TYR:O	1:F:178:LEU:HD11	2.08	0.54
1:I:173:ILE:HD13	1:I:190:ARG:HB3	1.90	0.54
1:B:263:ASP:O	1:B:267:ILE:HG12	2.08	0.54
1:A:215:ILE:HD13	1:B:239:MET:HE3	1.89	0.54
1:F:173:ILE:HD13	1:F:190:ARG:HB3	1.89	0.54
1:C:181:VAL:HG21	1:C:185:GLN:HB2	1.90	0.54
1:B:215:ILE:HD13	1:C:239:MET:HE3	1.90	0.53
1:C:289:ASN:OD1	1:C:290:GLY:N	2.40	0.53
1:G:212:LEU:O	1:G:216:ILE:HG12	2.08	0.53
1:J:155:GLU:O	1:J:161:TRP:NE1	2.41	0.53
1:F:240:LEU:HD23	1:J:241:THR:HA	1.90	0.53
1:C:44:THR:HA	1:C:99:ARG:HA	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:ASP:HB2	1:C:297:ILE:HG22	1.90	0.53
1:D:119:PHE:HA	1:D:122:ASP:OD1	2.09	0.53
1:J:44:THR:HA	1:J:99:ARG:HA	1.88	0.53
1:J:263:ASP:O	1:J:267:ILE:HG12	2.09	0.53
1:B:179:SER:HB2	1:B:181:VAL:HG12	1.90	0.53
1:C:183:PRO:HB2	1:C:185:GLN:OE1	2.09	0.53
1:D:155:GLU:O	1:D:161:TRP:NE1	2.41	0.53
1:H:59:GLU:OE2	1:I:134:SER:OG	2.27	0.53
1:I:91:ARG:HB2	1:J:133:PHE:HE2	1.72	0.53
1:F:123:ARG:HD2	1:F:198:VAL:HG22	1.91	0.53
1:H:263:ASP:O	1:H:267:ILE:HG12	2.09	0.53
1:C:17:SER:HB2	1:C:40:VAL:HB	1.90	0.52
1:H:228:PHE:HA	1:H:231:ARG:NH1	2.23	0.52
1:A:295:LEU:HD12	1:A:298:GLN:OE1	2.09	0.52
1:D:173:ILE:HD13	1:D:190:ARG:HB3	1.91	0.52
1:G:263:ASP:O	1:G:267:ILE:HG12	2.09	0.52
1:A:66:TRP:HB3	1:A:71:LEU:HD12	1.92	0.52
1:G:304:PHE:CD1	1:G:304:PHE:C	2.88	0.52
1:C:127:VAL:HG22	1:C:194:ARG:HG2	1.91	0.52
1:E:173:ILE:HD13	1:E:190:ARG:HB3	1.91	0.52
1:D:21:ASN:HD21	1:D:38:TYR:HE1	1.58	0.52
1:B:225:LEU:HB2	1:B:231:ARG:HG3	1.92	0.52
1:H:44:THR:HA	1:H:99:ARG:HA	1.90	0.52
1:E:123:ARG:HD2	1:E:198:VAL:HG22	1.93	0.51
1:A:155:GLU:O	1:A:161:TRP:NE1	2.40	0.51
1:G:127:VAL:HG22	1:G:194:ARG:HG2	1.92	0.51
1:I:157:ILE:HD11	1:J:117:ARG:HE	1.75	0.51
1:B:248:TYR:HD1	1:C:247:PHE:HA	1.74	0.51
1:A:247:PHE:HE2	1:E:247:PHE:CD2	2.28	0.51
1:B:294:ASP:HB2	1:B:297:ILE:HG22	1.92	0.51
1:E:66:TRP:HB3	1:E:71:LEU:HD12	1.92	0.51
1:F:289:ASN:OD1	1:F:290:GLY:N	2.40	0.51
1:H:119:PHE:HA	1:H:122:ASP:OD1	2.10	0.51
1:G:304:PHE:C	1:G:304:PHE:HD1	2.18	0.51
1:A:225:LEU:HB2	1:A:231:ARG:HG3	1.91	0.50
1:G:225:LEU:HB2	1:G:231:ARG:HG3	1.92	0.50
1:G:36:ASP:OD2	1:G:105:ARG:NH2	2.40	0.50
1:F:225:LEU:HB2	1:F:231:ARG:HG3	1.93	0.50
1:E:228:PHE:HA	1:E:231:ARG:NH1	2.26	0.50
1:A:133:PHE:CE2	1:E:91:ARG:HB2	2.43	0.50
1:F:263:ASP:O	1:F:267:ILE:HG12	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:225:LEU:HD21	1:H:232:LEU:HD22	1.92	0.50
1:I:263:ASP:O	1:I:267:ILE:HG12	2.11	0.50
1:A:128:LEU:HD12	2:A:402:MBR:BR1	2.60	0.50
1:B:123:ARG:HD2	1:B:198:VAL:HG22	1.93	0.50
1:I:119:PHE:HA	1:I:122:ASP:OD1	2.11	0.50
1:D:105:ARG:NH1	1:E:79:ILE:O	2.35	0.49
1:F:66:TRP:HB3	1:F:71:LEU:HD12	1.94	0.49
1:B:66:TRP:HB3	1:B:71:LEU:HD12	1.94	0.49
1:D:17:SER:HB2	1:D:40:VAL:HB	1.94	0.49
1:G:61:THR:HG21	1:H:64:GLU:CG	2.43	0.49
1:I:59:GLU:OE2	1:J:134:SER:OG	2.28	0.49
1:C:119:PHE:HA	1:C:122:ASP:OD1	2.11	0.49
1:G:65:ARG:HD2	1:H:68:ASN:ND2	2.28	0.49
1:C:48:ARG:NH1	1:C:48:ARG:HB2	2.28	0.49
1:H:155:GLU:O	1:H:161:TRP:NE1	2.46	0.49
1:C:228:PHE:HA	1:C:231:ARG:NH1	2.28	0.49
1:G:66:TRP:HB3	1:G:71:LEU:HD12	1.93	0.49
1:A:236:PHE:CD1	1:E:238:LEU:HD13	2.48	0.49
1:F:64:GLU:CG	1:J:61:THR:HG21	2.42	0.49
1:F:145:ILE:HD12	1:F:191:ILE:HG21	1.95	0.48
1:J:228:PHE:HA	1:J:231:ARG:NH1	2.28	0.48
1:E:21:ASN:HD21	1:E:38:TYR:HE1	1.60	0.48
1:G:228:PHE:HA	1:G:231:ARG:NH1	2.28	0.48
1:G:300:CYS:HB2	1:G:303:ALA:HB3	1.95	0.48
1:F:299:ARG:C	1:F:301:ARG:H	2.20	0.48
1:B:300:CYS:HB2	1:B:303:ALA:HB3	1.95	0.48
1:C:185:GLN:OE1	1:C:185:GLN:N	2.47	0.48
1:E:225:LEU:HB2	1:E:231:ARG:HG3	1.95	0.48
1:F:133:PHE:CE2	1:J:91:ARG:HB2	2.48	0.48
1:I:21:ASN:HD21	1:I:38:TYR:HE1	1.61	0.48
1:J:225:LEU:HB2	1:J:231:ARG:HG3	1.96	0.48
1:B:248:TYR:HE1	1:C:250:SER:OG	1.96	0.48
1:E:119:PHE:HA	1:E:122:ASP:OD1	2.14	0.48
1:F:48:ARG:HB2	1:F:48:ARG:NH1	2.28	0.48
1:D:185:GLN:OE1	1:D:185:GLN:N	2.47	0.48
1:D:211:PRO:O	1:D:215:ILE:HG12	2.14	0.48
1:F:91:ARG:HB2	1:G:133:PHE:CE2	2.44	0.48
1:J:216:ILE:O	1:J:219:SER:HB3	2.14	0.48
1:D:145:ILE:HD12	1:D:191:ILE:HG21	1.96	0.48
1:J:21:ASN:HD21	1:J:38:TYR:HE1	1.60	0.48
1:J:181:VAL:HG21	1:J:185:GLN:HB2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:TRP:HB3	1:C:71:LEU:HD12	1.96	0.47
1:E:304:PHE:HD1	1:E:304:PHE:C	2.22	0.47
1:G:215:ILE:HD13	1:H:239:MET:HE3	1.95	0.47
1:J:123:ARG:HD2	1:J:198:VAL:HG22	1.95	0.47
1:C:225:LEU:HB2	1:C:231:ARG:HG3	1.95	0.47
1:E:181:VAL:HG21	1:E:185:GLN:HB2	1.95	0.47
1:J:300:CYS:HB2	1:J:303:ALA:HB3	1.96	0.47
1:D:36:ASP:OD2	1:D:105:ARG:NH2	2.42	0.47
1:E:300:CYS:HB2	1:E:303:ALA:HB3	1.95	0.47
1:B:127:VAL:HG22	1:B:194:ARG:HG2	1.96	0.47
1:D:228:PHE:HA	1:D:231:ARG:NH1	2.30	0.47
1:E:304:PHE:C	1:E:304:PHE:CD1	2.92	0.47
1:F:247:PHE:HE2	1:J:247:PHE:CD2	2.31	0.47
1:F:300:CYS:HB2	1:F:303:ALA:HB3	1.97	0.47
1:H:21:ASN:HD21	1:H:38:TYR:HE1	1.62	0.47
1:G:155:GLU:O	1:G:161:TRP:NE1	2.46	0.47
1:H:66:TRP:HB3	1:H:71:LEU:HD12	1.96	0.47
1:C:155:GLU:O	1:C:161:TRP:NE1	2.44	0.47
1:C:92:LEU:HD23	1:C:92:LEU:HA	1.81	0.47
1:F:155:GLU:O	1:F:161:TRP:NE1	2.44	0.47
1:H:211:PRO:O	1:H:215:ILE:HG12	2.15	0.47
1:H:299:ARG:C	1:H:301:ARG:H	2.23	0.47
1:J:66:TRP:HB3	1:J:71:LEU:HD12	1.95	0.47
1:B:119:PHE:HA	1:B:122:ASP:OD1	2.15	0.47
1:E:232:LEU:O	1:E:235:SER:OG	2.30	0.47
1:H:123:ARG:HD2	1:H:198:VAL:HG22	1.97	0.47
1:A:216:ILE:O	1:A:219:SER:HB3	2.15	0.47
1:I:247:PHE:CD2	1:J:247:PHE:HE2	2.32	0.47
1:C:81:VAL:HG13	1:C:83:GLY:O	2.15	0.47
1:C:299:ARG:C	1:C:301:ARG:H	2.23	0.47
1:D:289:ASN:OD1	1:D:290:GLY:N	2.40	0.47
1:A:211:PRO:O	1:A:215:ILE:HG12	2.15	0.46
1:B:238:LEU:HD13	1:C:236:PHE:HD2	1.80	0.46
1:C:91:ARG:CD	1:D:134:SER:HB3	2.40	0.46
1:C:215:ILE:HD13	1:D:239:MET:HE3	1.96	0.46
1:A:203:TYR:HB2	1:B:257:PRO:C	2.41	0.46
1:J:155:GLU:OE2	1:J:163:ARG:NH1	2.47	0.46
1:A:294:ASP:HB2	1:A:297:ILE:CG2	2.46	0.46
1:F:228:PHE:HA	1:F:231:ARG:NH1	2.29	0.46
1:J:289:ASN:OD1	1:J:290:GLY:N	2.42	0.46
1:E:27:ASN:HB3	1:E:32:THR:HB	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:91:ARG:CD	1:I:134:SER:HB3	2.38	0.46
1:I:145:ILE:HD12	1:I:191:ILE:HG21	1.96	0.46
1:A:204:TYR:O	1:A:208:PHE:HB2	2.15	0.46
1:F:247:PHE:HA	1:J:248:TYR:HD1	1.80	0.46
1:I:211:PRO:O	1:I:215:ILE:HG12	2.15	0.46
1:H:300:CYS:HB2	1:H:303:ALA:HB3	1.98	0.46
1:I:228:PHE:HA	1:I:231:ARG:NH1	2.31	0.46
1:B:36:ASP:OD2	1:B:105:ARG:NH2	2.47	0.46
1:B:225:LEU:HD21	1:C:232:LEU:HD22	1.97	0.46
1:F:46:LYS:H	1:F:46:LYS:HG2	1.53	0.46
1:I:225:LEU:HB2	1:I:231:ARG:HG3	1.97	0.46
1:B:252:ILE:HG13	1:C:250:SER:HB3	1.97	0.46
1:C:59:GLU:OE2	1:D:134:SER:OG	2.34	0.46
1:D:225:LEU:HB2	1:D:231:ARG:HG3	1.98	0.46
1:G:295:LEU:HA	1:G:298:GLN:OE1	2.15	0.46
1:A:247:PHE:CD2	1:B:247:PHE:HE2	2.34	0.46
1:F:67:ILE:HG22	1:J:62:GLN:NE2	2.31	0.46
1:I:155:GLU:O	1:I:161:TRP:NE1	2.46	0.46
1:C:211:PRO:O	1:C:215:ILE:HG12	2.16	0.46
1:J:48:ARG:NH1	1:J:48:ARG:HB2	2.31	0.46
1:B:21:ASN:HD21	1:B:38:TYR:HE1	1.62	0.45
1:D:247:PHE:CD2	1:E:247:PHE:HE2	2.34	0.45
1:D:299:ARG:C	1:D:301:ARG:H	2.24	0.45
1:F:216:ILE:O	1:F:219:SER:HB3	2.16	0.45
1:G:294:ASP:HB2	1:G:297:ILE:CG2	2.46	0.45
1:C:300:CYS:HB2	1:C:303:ALA:HB3	1.97	0.45
1:D:157:ILE:HD11	1:E:117:ARG:HE	1.81	0.45
1:E:175:TYR:HB2	1:E:178:LEU:HD21	1.97	0.45
1:F:68:ASN:ND2	1:J:65:ARG:HD2	2.31	0.45
1:I:66:TRP:HB3	1:I:71:LEU:HD12	1.98	0.45
1:D:216:ILE:O	1:D:219:SER:HB3	2.16	0.45
1:I:163:ARG:HA	1:I:163:ARG:HD3	1.43	0.45
1:A:295:LEU:HA	1:A:298:GLN:OE1	2.17	0.45
1:E:17:SER:HB2	1:E:40:VAL:HB	1.99	0.45
1:E:211:PRO:O	1:E:215:ILE:HG12	2.16	0.45
1:G:216:ILE:O	1:G:219:SER:HB3	2.16	0.45
1:J:295:LEU:HA	1:J:298:GLN:OE1	2.17	0.45
1:A:228:PHE:HA	1:A:231:ARG:NH1	2.32	0.45
1:D:294:ASP:HB2	1:D:297:ILE:HG22	1.97	0.45
1:G:105:ARG:NH2	1:H:81:VAL:O	2.50	0.45
1:G:119:PHE:HA	1:G:122:ASP:OD1	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:27:ASN:HB3	1:H:32:THR:HB	1.98	0.45
1:C:163:ARG:HA	1:C:163:ARG:HD3	1.65	0.45
1:G:17:SER:HB2	1:G:40:VAL:HB	1.99	0.45
1:J:195:ILE:HD11	2:J:402:MBR:BR1	2.51	0.45
1:H:203:TYR:HB2	1:I:257:PRO:C	2.42	0.45
1:C:216:ILE:O	1:C:219:SER:HB3	2.16	0.45
1:D:62:GLN:NE2	1:E:67:ILE:HG22	2.32	0.45
1:F:157:ILE:HD13	1:F:157:ILE:HA	1.80	0.45
1:G:103:ASN:HD22	1:G:104:ALA:N	2.15	0.45
1:I:304:PHE:C	1:I:304:PHE:CD1	2.95	0.45
1:J:179:SER:C	1:J:181:VAL:H	2.25	0.45
1:I:126:PHE:O	2:I:402:MBR:BR1	2.89	0.45
1:I:289:ASN:OD1	1:I:290:GLY:N	2.41	0.45
1:A:299:ARG:C	1:A:301:ARG:H	2.24	0.45
1:A:300:CYS:HB2	1:A:303:ALA:HB3	1.99	0.45
1:C:157:ILE:HD13	1:C:157:ILE:HA	1.81	0.45
1:E:155:GLU:O	1:E:161:TRP:NE1	2.46	0.45
1:I:300:CYS:HB2	1:I:303:ALA:HB3	1.99	0.45
1:F:211:PRO:O	1:F:215:ILE:HG12	2.17	0.44
1:G:137:ASN:N	1:G:137:ASN:OD1	2.49	0.44
1:A:123:ARG:HD2	1:A:198:VAL:HG22	2.00	0.44
1:A:155:GLU:OE2	1:A:163:ARG:NH1	2.50	0.44
1:B:155:GLU:O	1:B:161:TRP:NE1	2.48	0.44
1:C:224:TRP:CH2	1:C:301:ARG:HB3	2.52	0.44
1:I:185:GLN:OE1	1:I:185:GLN:N	2.50	0.44
1:A:21:ASN:HD21	1:A:38:TYR:HE1	1.64	0.44
1:A:304:PHE:CD1	1:A:304:PHE:C	2.96	0.44
1:B:226:GLU:OE2	1:C:284:HIS:HE1	2.01	0.44
1:E:179:SER:C	1:E:181:VAL:H	2.25	0.44
1:G:179:SER:C	1:G:181:VAL:H	2.24	0.44
1:H:216:ILE:O	1:H:219:SER:HB3	2.17	0.44
1:H:294:ASP:HB2	1:H:297:ILE:CG2	2.47	0.44
1:I:216:ILE:O	1:I:219:SER:HB3	2.17	0.44
1:B:216:ILE:O	1:B:219:SER:HB3	2.17	0.44
1:B:299:ARG:C	1:B:301:ARG:H	2.26	0.44
1:I:91:ARG:HB2	1:J:133:PHE:CE2	2.52	0.44
1:C:91:ARG:HB2	1:D:133:PHE:HE2	1.83	0.44
1:E:299:ARG:C	1:E:301:ARG:H	2.25	0.44
1:I:157:ILE:HD13	1:I:157:ILE:HA	1.82	0.44
1:I:299:ARG:C	1:I:301:ARG:H	2.25	0.44
1:C:304:PHE:CD1	1:C:304:PHE:C	2.96	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:PHE:HE1	1:D:101:ILE:HD12	1.82	0.44
1:H:17:SER:HB2	1:H:40:VAL:HB	1.99	0.44
1:J:304:PHE:CD1	1:J:304:PHE:C	2.95	0.44
1:B:228:PHE:HA	1:B:231:ARG:NH1	2.32	0.44
1:C:295:LEU:HA	1:C:298:GLN:OE1	2.18	0.44
1:D:137:ASN:OD1	1:D:137:ASN:N	2.51	0.44
1:D:200:ASN:HA	1:D:201:PRO:HD3	1.86	0.44
1:F:17:SER:HB2	1:F:40:VAL:HB	2.00	0.44
1:G:211:PRO:O	1:G:215:ILE:HG12	2.18	0.44
1:A:210:LEU:HB3	1:A:211:PRO:HD3	1.99	0.43
1:E:224:TRP:CH2	1:E:301:ARG:HB3	2.53	0.43
1:G:241:THR:HA	1:H:240:LEU:HD23	2.00	0.43
1:H:204:TYR:O	1:H:208:PHE:HB2	2.18	0.43
1:A:157:ILE:HD13	1:A:157:ILE:HA	1.85	0.43
1:A:232:LEU:HD22	1:E:225:LEU:HD21	1.99	0.43
1:C:21:ASN:HD21	1:C:38:TYR:HE1	1.65	0.43
1:F:225:LEU:HD21	1:G:232:LEU:HD22	1.99	0.43
1:F:304:PHE:CD1	1:F:304:PHE:C	2.96	0.43
1:H:185:GLN:N	1:H:185:GLN:OE1	2.50	0.43
1:A:17:SER:HB2	1:A:40:VAL:HB	2.00	0.43
1:B:91:ARG:HB2	1:C:133:PHE:HE2	1.84	0.43
1:B:211:PRO:O	1:B:215:ILE:HG12	2.18	0.43
1:F:179:SER:C	1:F:181:VAL:H	2.25	0.43
1:G:157:ILE:HD13	1:G:157:ILE:HA	1.77	0.43
1:J:27:ASN:HB3	1:J:32:THR:HB	2.01	0.43
1:B:17:SER:HB2	1:B:40:VAL:HB	1.99	0.43
1:B:179:SER:C	1:B:181:VAL:H	2.25	0.43
1:C:99:ARG:NH2	1:D:180:SER:HB2	2.33	0.43
1:E:92:LEU:HD23	1:E:92:LEU:HA	1.82	0.43
1:E:157:ILE:HD13	1:E:157:ILE:HA	1.78	0.43
1:H:228:PHE:HA	1:H:231:ARG:HH11	1.83	0.43
1:H:302:LEU:C	1:H:305:PRO:HD2	2.44	0.43
1:A:92:LEU:HD23	1:A:92:LEU:HA	1.81	0.43
1:H:225:LEU:HB2	1:H:231:ARG:HG3	2.00	0.43
1:I:92:LEU:HD23	1:I:92:LEU:HA	1.83	0.43
1:I:304:PHE:C	1:I:304:PHE:HD1	2.26	0.43
1:B:174:ARG:HH22	1:I:141:ARG:HD3	1.84	0.43
1:B:289:ASN:OD1	1:B:290:GLY:N	2.47	0.43
1:E:216:ILE:O	1:E:219:SER:HB3	2.18	0.43
1:I:200:ASN:HA	1:I:201:PRO:HD3	1.86	0.43
1:J:17:SER:HB2	1:J:40:VAL:HB	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:294:ASP:HB2	1:F:297:ILE:HG22	2.01	0.43
1:G:185:GLN:OE1	1:G:185:GLN:N	2.52	0.43
1:A:81:VAL:O	1:E:105:ARG:NH2	2.52	0.43
1:B:163:ARG:HA	1:B:163:ARG:HD3	1.67	0.43
1:B:304:PHE:CD1	1:B:304:PHE:C	2.96	0.43
1:G:95:PHE:HE1	1:G:101:ILE:HD12	1.84	0.43
1:H:289:ASN:OD1	1:H:290:GLY:N	2.45	0.43
1:H:294:ASP:O	1:H:298:GLN:HG2	2.19	0.43
1:A:183:PRO:O	1:A:184:ASN:HB2	2.18	0.43
1:B:203:TYR:HB2	1:C:257:PRO:C	2.44	0.43
1:E:145:ILE:HD12	1:E:191:ILE:HG21	2.01	0.43
1:I:179:SER:C	1:I:181:VAL:H	2.27	0.43
1:D:300:CYS:HB2	1:D:303:ALA:HB3	2.01	0.42
1:H:163:ARG:HA	1:H:163:ARG:HD3	1.58	0.42
1:D:27:ASN:HB3	1:D:32:THR:HB	2.01	0.42
1:D:210:LEU:HB3	1:D:211:PRO:HD3	2.01	0.42
1:E:225:LEU:O	1:E:231:ARG:HD2	2.19	0.42
1:A:145:ILE:HD12	1:A:191:ILE:HG21	2.01	0.42
1:A:232:LEU:O	1:A:235:SER:OG	2.35	0.42
1:A:250:SER:HB3	1:E:252:ILE:HG13	2.01	0.42
1:F:21:ASN:HD21	1:F:38:TYR:HE1	1.66	0.42
1:G:103:ASN:C	1:G:103:ASN:ND2	2.77	0.42
1:C:145:ILE:HD12	1:C:191:ILE:HG21	2.02	0.42
1:C:294:ASP:HB2	1:C:297:ILE:CG2	2.49	0.42
1:D:304:PHE:C	1:D:304:PHE:CD1	2.97	0.42
1:J:149:THR:C	1:J:151:ASN:H	2.28	0.42
1:J:182:GLN:HG3	1:J:183:PRO:HD3	2.01	0.42
1:J:232:LEU:O	1:J:235:SER:OG	2.35	0.42
1:D:157:ILE:HD13	1:D:157:ILE:HA	1.84	0.42
1:G:130:LEU:HD23	1:G:130:LEU:HA	1.89	0.42
1:E:128:LEU:HD11	2:E:402:MBR:BR1	2.68	0.42
1:F:185:GLN:N	1:F:185:GLN:OE1	2.53	0.42
1:I:145:ILE:HG23	1:I:168:THR:HG21	2.02	0.42
1:E:238:LEU:HD12	1:E:238:LEU:HA	1.89	0.42
1:F:224:TRP:HZ3	2:F:401:MBR:BR1	2.57	0.42
1:A:91:ARG:HB2	1:B:133:PHE:HE2	1.85	0.42
1:A:284:HIS:HE1	1:E:226:GLU:OE2	2.03	0.42
1:A:304:PHE:C	1:A:304:PHE:HD1	2.28	0.42
1:B:248:TYR:CD1	1:C:247:PHE:HA	2.52	0.42
1:D:302:LEU:C	1:D:305:PRO:HD2	2.45	0.42
1:I:123:ARG:HD2	1:I:198:VAL:HG22	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:211:PRO:O	1:J:215:ILE:HG12	2.19	0.42
1:J:299:ARG:C	1:J:301:ARG:H	2.27	0.42
1:A:220:TRP:CE3	1:A:305:PRO:HB3	2.55	0.42
1:G:91:ARG:HB2	1:H:133:PHE:CE2	2.49	0.42
1:G:299:ARG:C	1:G:301:ARG:H	2.28	0.42
1:I:17:SER:HB2	1:I:40:VAL:HB	2.01	0.42
1:I:84:SER:HA	1:I:85:PRO:HD3	1.83	0.42
1:I:128:LEU:HD13	2:I:402:MBR:BR1	2.75	0.42
1:J:295:LEU:HD12	1:J:298:GLN:OE1	2.20	0.42
1:A:84:SER:HA	1:A:85:PRO:HD3	1.86	0.41
1:A:224:TRP:CH2	1:A:301:ARG:HB3	2.55	0.41
1:E:210:LEU:HB3	1:E:211:PRO:HD3	2.02	0.41
1:F:92:LEU:HD23	1:F:92:LEU:HA	1.85	0.41
1:F:122:ASP:OD1	1:F:122:ASP:N	2.52	0.41
1:G:27:ASN:HB3	1:G:32:THR:HB	2.02	0.41
1:G:33:TYR:OH	1:G:127:VAL:N	2.47	0.41
1:B:247:PHE:CD2	1:C:247:PHE:HE2	2.37	0.41
1:A:281:ILE:HD11	1:E:221:SER:HB2	2.01	0.41
1:B:224:TRP:CH2	1:B:301:ARG:HB3	2.55	0.41
1:C:224:TRP:CE2	1:C:301:ARG:HD3	2.55	0.41
1:C:304:PHE:C	1:C:304:PHE:HD1	2.28	0.41
1:D:92:LEU:HD23	1:D:92:LEU:HA	1.83	0.41
1:I:27:ASN:HB3	1:I:32:THR:HB	2.02	0.41
1:J:224:TRP:CH2	1:J:301:ARG:HB3	2.55	0.41
1:A:302:LEU:C	1:A:305:PRO:HD2	2.45	0.41
1:B:159:GLU:HG3	1:C:257:PRO:HB3	2.03	0.41
1:B:294:ASP:HB2	1:B:297:ILE:CG2	2.50	0.41
1:D:29:LEU:HD23	1:D:29:LEU:HA	1.85	0.41
1:E:130:LEU:HD23	1:E:130:LEU:HA	1.85	0.41
1:H:231:ARG:HH11	1:H:231:ARG:HD3	1.61	0.41
1:J:304:PHE:C	1:J:304:PHE:HD1	2.27	0.41
1:A:122:ASP:OD1	1:A:122:ASP:N	2.51	0.41
1:B:185:GLN:OE1	1:B:185:GLN:N	2.53	0.41
1:E:185:GLN:N	1:E:185:GLN:OE1	2.53	0.41
1:F:210:LEU:HB3	1:F:211:PRO:HD3	2.03	0.41
1:H:145:ILE:HD12	1:H:191:ILE:HG21	2.03	0.41
1:I:31:GLN:HG2	1:I:114:MET:HB2	2.02	0.41
1:I:238:LEU:HD13	1:J:236:PHE:CD2	2.56	0.41
1:A:182:GLN:O	1:A:183:PRO:C	2.62	0.41
1:A:247:PHE:HA	1:E:248:TYR:HD1	1.86	0.41
1:B:95:PHE:HE1	1:B:101:ILE:HD12	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:ILE:HG12	1:E:117:ARG:HH21	1.86	0.41
1:E:81:VAL:HG13	1:E:83:GLY:O	2.21	0.41
1:F:224:TRP:CH2	1:F:301:ARG:HB3	2.55	0.41
1:A:27:ASN:HB3	1:A:32:THR:HB	2.03	0.41
1:B:92:LEU:HD23	1:B:92:LEU:HA	1.79	0.41
1:D:304:PHE:C	1:D:304:PHE:HD1	2.28	0.41
1:G:21:ASN:HD21	1:G:38:TYR:HE1	1.68	0.41
1:G:81:VAL:HG13	1:G:83:GLY:O	2.21	0.41
1:G:92:LEU:HA	1:G:92:LEU:HD23	1.80	0.41
1:H:210:LEU:HB3	1:H:211:PRO:HD3	2.01	0.41
1:F:200:ASN:HA	1:F:201:PRO:HD3	1.91	0.41
1:F:304:PHE:C	1:F:304:PHE:HD1	2.29	0.41
1:B:182:GLN:O	1:B:183:PRO:C	2.61	0.40
1:E:149:THR:C	1:E:151:ASN:H	2.29	0.40
1:H:248:TYR:HE1	1:I:250:SER:OG	2.05	0.40
1:I:48:ARG:NH1	1:I:48:ARG:HB2	2.36	0.40
1:I:210:LEU:HB3	1:I:211:PRO:HD3	2.03	0.40
1:J:175:TYR:HB2	1:J:178:LEU:HD21	2.03	0.40
1:B:304:PHE:C	1:B:304:PHE:HD1	2.29	0.40
1:D:225:LEU:O	1:D:231:ARG:HD2	2.21	0.40
1:E:294:ASP:HB2	1:E:297:ILE:HG22	2.03	0.40
1:A:247:PHE:CE2	1:E:247:PHE:CG	3.09	0.40
1:C:149:THR:C	1:C:151:ASN:H	2.29	0.40
1:F:27:ASN:HB3	1:F:32:THR:HB	2.03	0.40
1:F:79:ILE:HD13	1:F:79:ILE:HA	1.96	0.40
1:I:95:PHE:HE1	1:I:101:ILE:HD12	1.86	0.40
1:J:92:LEU:HD23	1:J:92:LEU:HA	1.82	0.40
1:B:210:LEU:HB3	1:B:211:PRO:HD3	2.02	0.40
1:H:215:ILE:HD13	1:I:239:MET:HE3	2.03	0.40
1:H:220:TRP:CE3	1:H:305:PRO:HB3	2.56	0.40
1:I:224:TRP:CH2	1:I:301:ARG:HB3	2.56	0.40
1:J:122:ASP:OD2	1:J:199:ARG:NE	2.46	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:GLU:OE1	1:D:49:LYS:NZ[1_556]	2.01	0.19

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	305/307 (99%)	276 (90%)	20 (7%)	9 (3%)	3	21
1	B	305/307 (99%)	275 (90%)	21 (7%)	9 (3%)	3	21
1	C	305/307 (99%)	276 (90%)	23 (8%)	6 (2%)	6	28
1	D	305/307 (99%)	275 (90%)	22 (7%)	8 (3%)	4	23
1	E	305/307 (99%)	273 (90%)	26 (8%)	6 (2%)	6	28
1	F	305/307 (99%)	275 (90%)	23 (8%)	7 (2%)	5	26
1	G	305/307 (99%)	276 (90%)	21 (7%)	8 (3%)	4	23
1	H	305/307 (99%)	273 (90%)	25 (8%)	7 (2%)	5	26
1	I	305/307 (99%)	274 (90%)	24 (8%)	7 (2%)	5	26
1	J	305/307 (99%)	275 (90%)	23 (8%)	7 (2%)	5	26
All	All	3050/3070 (99%)	2748 (90%)	228 (8%)	74 (2%)	4	25

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	B	53	ASP
1	B	60	ASN
1	B	166	ALA
1	C	166	ALA
1	D	53	ASP
1	D	60	ASN
1	E	53	ASP
1	E	60	ASN
1	F	60	ASN
1	G	53	ASP
1	G	60	ASN
1	G	166	ALA
1	H	60	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	60	ASN
1	J	53	ASP
1	J	60	ASN
1	J	166	ALA
1	A	53	ASP
1	A	152	ILE
1	B	152	ILE
1	C	53	ASP
1	C	152	ILE
1	D	152	ILE
1	E	152	ILE
1	F	53	ASP
1	F	152	ILE
1	G	152	ILE
1	G	183	PRO
1	H	53	ASP
1	H	152	ILE
1	H	166	ALA
1	I	53	ASP
1	I	152	ILE
1	J	152	ILE
1	A	183	PRO
1	A	184	ASN
1	A	294	ASP
1	B	150	GLU
1	C	183	PRO
1	D	166	ALA
1	D	183	PRO
1	E	183	PRO
1	H	153	ASP
1	H	183	PRO
1	I	183	PRO
1	B	153	ASP
1	B	294	ASP
1	C	153	ASP
1	D	150	GLU
1	F	153	ASP
1	F	183	PRO
1	F	294	ASP
1	G	150	GLU
1	H	150	GLU
1	I	150	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	166	ALA
1	J	150	GLU
1	J	183	PRO
1	A	150	GLU
1	A	153	ASP
1	A	166	ALA
1	C	184	ASN
1	D	153	ASP
1	D	184	ASN
1	E	150	GLU
1	E	153	ASP
1	F	150	GLU
1	G	294	ASP
1	J	153	ASP
1	G	153	ASP
1	I	153	ASP
1	B	183	PRO
1	B	182	GLN

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	274/275 (100%)	248 (90%)	26 (10%)	8	29
1	B	274/275 (100%)	245 (89%)	29 (11%)	6	26
1	C	274/275 (100%)	249 (91%)	25 (9%)	9	30
1	D	274/275 (100%)	248 (90%)	26 (10%)	8	29
1	E	274/275 (100%)	249 (91%)	25 (9%)	9	30
1	F	274/275 (100%)	252 (92%)	22 (8%)	11	34
1	G	274/275 (100%)	251 (92%)	23 (8%)	10	32
1	H	274/275 (100%)	249 (91%)	25 (9%)	9	30
1	I	274/275 (100%)	250 (91%)	24 (9%)	9	31
1	J	274/275 (100%)	250 (91%)	24 (9%)	9	31

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2740/2750 (100%)	2491 (91%)	249 (9%)	9 30

All (249) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	THR
1	A	39	ILE
1	A	56	LEU
1	A	71	LEU
1	A	81	VAL
1	A	103	ASN
1	A	118	LEU
1	A	122	ASP
1	A	124	GLN
1	A	130	LEU
1	A	134	SER
1	A	145	ILE
1	A	146	GLN
1	A	157	ILE
1	A	165	LYS
1	A	168	THR
1	A	177	HIS
1	A	178	LEU
1	A	182	GLN
1	A	212	LEU
1	A	240	LEU
1	A	281	ILE
1	A	291	VAL
1	A	292	GLU
1	A	302	LEU
1	A	304	PHE
1	B	32	THR
1	B	39	ILE
1	B	56	LEU
1	B	71	LEU
1	B	81	VAL
1	B	118	LEU
1	B	122	ASP
1	B	124	GLN
1	B	130	LEU
1	B	134	SER
1	B	136	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	145	ILE
1	B	146	GLN
1	B	157	ILE
1	B	165	LYS
1	B	168	THR
1	B	170	ILE
1	B	177	HIS
1	B	178	LEU
1	B	182	GLN
1	B	212	LEU
1	B	238	LEU
1	B	240	LEU
1	B	281	ILE
1	B	291	VAL
1	B	292	GLU
1	B	299	ARG
1	B	302	LEU
1	B	304	PHE
1	C	32	THR
1	C	39	ILE
1	C	56	LEU
1	C	71	LEU
1	C	81	VAL
1	C	118	LEU
1	C	122	ASP
1	C	124	GLN
1	C	130	LEU
1	C	134	SER
1	C	141	ARG
1	C	145	ILE
1	C	157	ILE
1	C	168	THR
1	C	177	HIS
1	C	178	LEU
1	C	182	GLN
1	C	240	LEU
1	C	281	ILE
1	C	287	GLN
1	C	291	VAL
1	C	292	GLU
1	C	299	ARG
1	C	302	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	304	PHE
1	D	32	THR
1	D	39	ILE
1	D	56	LEU
1	D	81	VAL
1	D	118	LEU
1	D	122	ASP
1	D	124	GLN
1	D	130	LEU
1	D	134	SER
1	D	141	ARG
1	D	145	ILE
1	D	146	GLN
1	D	157	ILE
1	D	165	LYS
1	D	177	HIS
1	D	178	LEU
1	D	182	GLN
1	D	212	LEU
1	D	238	LEU
1	D	240	LEU
1	D	281	ILE
1	D	291	VAL
1	D	292	GLU
1	D	299	ARG
1	D	302	LEU
1	D	304	PHE
1	E	39	ILE
1	E	56	LEU
1	E	71	LEU
1	E	81	VAL
1	E	118	LEU
1	E	122	ASP
1	E	124	GLN
1	E	130	LEU
1	E	134	SER
1	E	145	ILE
1	E	146	GLN
1	E	157	ILE
1	E	163	ARG
1	E	168	THR
1	E	177	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	178	LEU
1	E	182	GLN
1	E	238	LEU
1	E	240	LEU
1	E	281	ILE
1	E	291	VAL
1	E	292	GLU
1	E	299	ARG
1	E	302	LEU
1	E	304	PHE
1	F	32	THR
1	F	39	ILE
1	F	56	LEU
1	F	71	LEU
1	F	81	VAL
1	F	118	LEU
1	F	122	ASP
1	F	124	GLN
1	F	130	LEU
1	F	136	ASN
1	F	145	ILE
1	F	146	GLN
1	F	157	ILE
1	F	168	THR
1	F	177	HIS
1	F	178	LEU
1	F	240	LEU
1	F	281	ILE
1	F	291	VAL
1	F	292	GLU
1	F	302	LEU
1	F	304	PHE
1	G	39	ILE
1	G	56	LEU
1	G	71	LEU
1	G	81	VAL
1	G	118	LEU
1	G	122	ASP
1	G	124	GLN
1	G	130	LEU
1	G	134	SER
1	G	141	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	145	ILE
1	G	157	ILE
1	G	168	THR
1	G	177	HIS
1	G	178	LEU
1	G	182	GLN
1	G	238	LEU
1	G	240	LEU
1	G	291	VAL
1	G	292	GLU
1	G	299	ARG
1	G	302	LEU
1	G	304	PHE
1	H	32	THR
1	H	39	ILE
1	H	56	LEU
1	H	71	LEU
1	H	81	VAL
1	H	118	LEU
1	H	122	ASP
1	H	124	GLN
1	H	130	LEU
1	H	134	SER
1	H	136	ASN
1	H	145	ILE
1	H	157	ILE
1	H	168	THR
1	H	177	HIS
1	H	178	LEU
1	H	182	GLN
1	H	231	ARG
1	H	240	LEU
1	H	281	ILE
1	H	291	VAL
1	H	292	GLU
1	H	299	ARG
1	H	302	LEU
1	H	304	PHE
1	I	32	THR
1	I	39	ILE
1	I	56	LEU
1	I	71	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	81	VAL
1	I	118	LEU
1	I	122	ASP
1	I	124	GLN
1	I	130	LEU
1	I	134	SER
1	I	145	ILE
1	I	146	GLN
1	I	157	ILE
1	I	165	LYS
1	I	177	HIS
1	I	178	LEU
1	I	182	GLN
1	I	238	LEU
1	I	240	LEU
1	I	281	ILE
1	I	291	VAL
1	I	292	GLU
1	I	302	LEU
1	I	304	PHE
1	J	29	LEU
1	J	32	THR
1	J	39	ILE
1	J	56	LEU
1	J	71	LEU
1	J	81	VAL
1	J	118	LEU
1	J	124	GLN
1	J	130	LEU
1	J	134	SER
1	J	136	ASN
1	J	141	ARG
1	J	145	ILE
1	J	157	ILE
1	J	168	THR
1	J	177	HIS
1	J	178	LEU
1	J	182	GLN
1	J	240	LEU
1	J	281	ILE
1	J	291	VAL
1	J	292	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	302	LEU
1	J	304	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	169	HIS
1	A	233	GLN
1	A	251	ASN
1	B	124	GLN
1	B	184	ASN
1	B	251	ASN
1	B	298	GLN
1	C	89	ASN
1	C	169	HIS
1	C	251	ASN
1	D	103	ASN
1	D	177	HIS
1	D	233	GLN
1	D	251	ASN
1	E	103	ASN
1	E	124	GLN
1	E	169	HIS
1	E	233	GLN
1	E	251	ASN
1	F	103	ASN
1	F	169	HIS
1	F	233	GLN
1	F	251	ASN
1	G	103	ASN
1	G	124	GLN
1	G	169	HIS
1	G	177	HIS
1	G	233	GLN
1	G	251	ASN
1	H	21	ASN
1	H	136	ASN
1	H	169	HIS
1	H	177	HIS
1	H	233	GLN
1	H	251	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	284	HIS
1	I	177	HIS
1	I	251	ASN
1	J	124	GLN
1	J	169	HIS
1	J	233	GLN
1	J	251	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 22 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 [i](#)

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%)	0.04	7 (2%) 61 37	73, 122, 214, 290	0
1	B	307/307 (100%)	0.21	13 (4%) 40 24	73, 118, 212, 284	0
1	C	307/307 (100%)	-0.04	2 (0%) 84 62	74, 117, 214, 284	0
1	D	307/307 (100%)	0.12	7 (2%) 61 37	77, 118, 215, 285	0
1	E	307/307 (100%)	0.13	8 (2%) 57 34	77, 122, 213, 287	0
1	F	307/307 (100%)	0.01	5 (1%) 70 44	80, 122, 214, 285	0
1	G	307/307 (100%)	0.16	7 (2%) 61 37	77, 116, 214, 288	0
1	H	307/307 (100%)	0.03	8 (2%) 57 34	78, 118, 210, 285	0
1	I	307/307 (100%)	0.21	9 (2%) 53 31	73, 118, 214, 304	0
1	J	307/307 (100%)	0.19	12 (3%) 43 26	86, 123, 217, 313	0
All	All	3070/3070 (100%)	0.11	78 (2%) 58 35	73, 119, 215, 313	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	52	GLY	6.3
1	B	113	ASP	5.3
1	G	126	PHE	4.5
1	C	289	ASN	4.5
1	H	315	LEU	4.2
1	H	62	GLN	4.1
1	A	51	PRO	3.9
1	E	291	VAL	3.9
1	A	52	GLY	3.8
1	I	248	TYR	3.8
1	G	281	ILE	3.7
1	F	224	TRP	3.7
1	A	175	TYR	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	172	ASP	3.5
1	J	129	GLU	3.2
1	H	63	ILE	3.2
1	I	208	PHE	3.2
1	A	56	LEU	3.1
1	H	267	ILE	3.1
1	J	225	LEU	3.1
1	I	27	ASN	3.1
1	A	177	HIS	3.0
1	F	205	LEU	3.0
1	E	290	GLY	3.0
1	D	226	GLU	3.0
1	D	245	TYR	2.9
1	I	245	TYR	2.9
1	G	283	ALA	2.8
1	J	78	PHE	2.8
1	H	312	GLY	2.7
1	B	112	ASN	2.7
1	G	233	GLN	2.7
1	E	288	ALA	2.7
1	F	316	VAL	2.6
1	J	39	ILE	2.6
1	G	33	TYR	2.6
1	I	179	SER	2.6
1	D	70	GLY	2.6
1	G	255	ARG	2.5
1	H	56	LEU	2.5
1	B	31	GLN	2.5
1	D	261	VAL	2.5
1	B	127	VAL	2.5
1	J	79	ILE	2.4
1	D	126	PHE	2.4
1	B	27	ASN	2.4
1	B	125	GLN	2.4
1	D	173	ILE	2.4
1	B	289	ASN	2.4
1	B	126	PHE	2.4
1	E	77	GLU	2.4
1	B	25	GLY	2.3
1	B	288	ALA	2.3
1	E	81	VAL	2.3
1	J	177	HIS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	22	LYS	2.2
1	H	291	VAL	2.2
1	J	195	ILE	2.2
1	G	315	LEU	2.2
1	B	181	VAL	2.2
1	J	181	VAL	2.2
1	B	29	LEU	2.2
1	D	143	SER	2.1
1	E	76	LEU	2.1
1	I	139	GLN	2.1
1	F	88	GLY	2.1
1	F	234	THR	2.1
1	I	153	ASP	2.1
1	B	185	GLN	2.1
1	J	81	VAL	2.1
1	A	217	ALA	2.1
1	I	242	VAL	2.1
1	E	83	GLY	2.0
1	A	18	ILE	2.0
1	J	291	VAL	2.0
1	J	80	ASN	2.0
1	H	164	GLY	2.0
1	J	172	ASP	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.

Continued on next page...

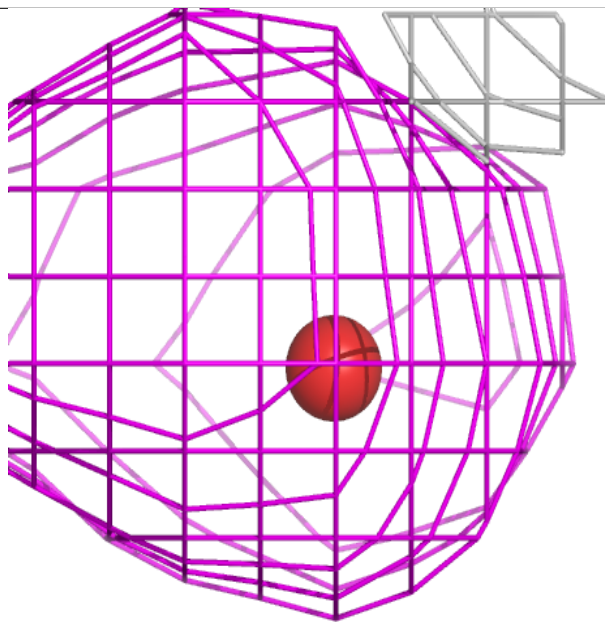
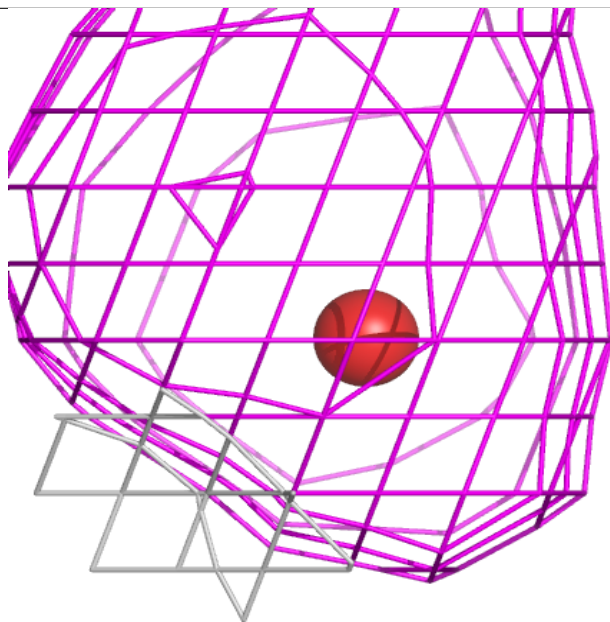
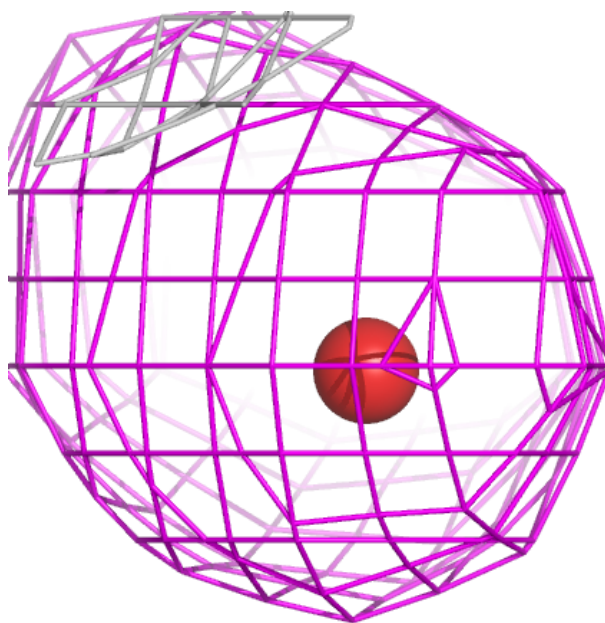
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MBR	F	401	1/4	0.46	0.38	201,201,201,201	0
2	MBR	A	401	1/4	0.56	0.29	210,210,210,210	0
2	MBR	I	401	1/4	0.56	0.22	186,186,186,186	0
2	MBR	D	401	1/4	0.59	0.21	186,186,186,186	0
2	MBR	G	401	1/4	0.66	0.18	190,190,190,190	0
2	MBR	J	401	1/4	0.71	0.24	212,212,212,212	0
2	MBR	E	401	1/4	0.76	0.21	190,190,190,190	0
2	MBR	J	402	1/4	0.76	1.03	202,202,202,202	0
2	MBR	H	401	1/4	0.77	0.19	195,195,195,195	0
2	MBR	I	402	1/4	0.79	0.90	212,212,212,212	0
2	MBR	A	403	1/4	0.79	0.29	154,154,154,154	0
2	MBR	G	402	1/4	0.79	1.04	186,186,186,186	0
2	MBR	D	402	1/4	0.80	1.21	185,185,185,185	0
2	MBR	B	401	1/4	0.80	0.09	200,200,200,200	0
2	MBR	C	402	1/4	0.81	0.55	195,195,195,195	0
2	MBR	E	402	1/4	0.81	0.70	211,211,211,211	0
2	MBR	C	401	1/4	0.84	0.12	193,193,193,193	0
2	MBR	F	403	1/4	0.85	0.20	166,166,166,166	0
2	MBR	F	402	1/4	0.86	0.38	196,196,196,196	0
2	MBR	H	402	1/4	0.89	0.22	198,198,198,198	0
2	MBR	B	402	1/4	0.90	0.54	195,195,195,195	0
2	MBR	A	402	1/4	0.94	0.43	201,201,201,201	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.

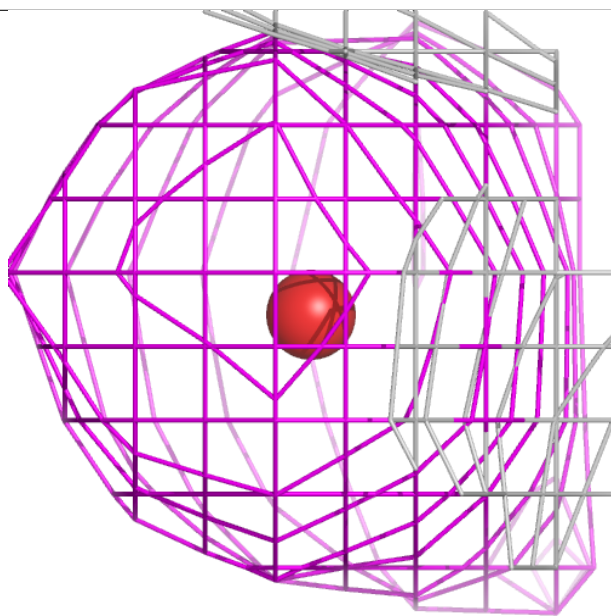
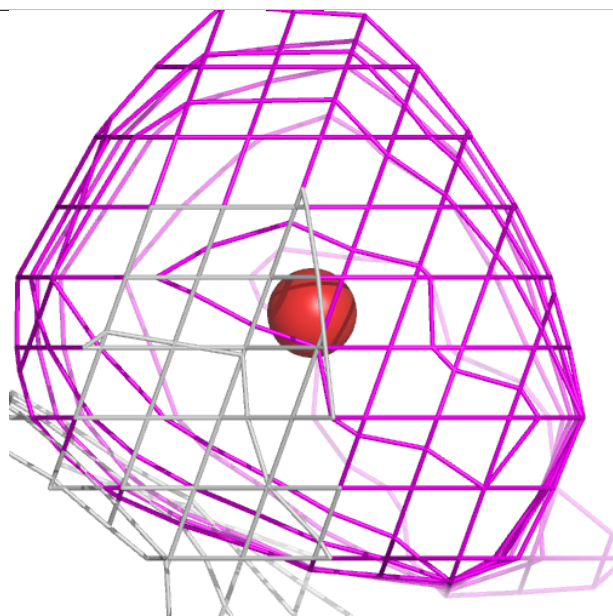
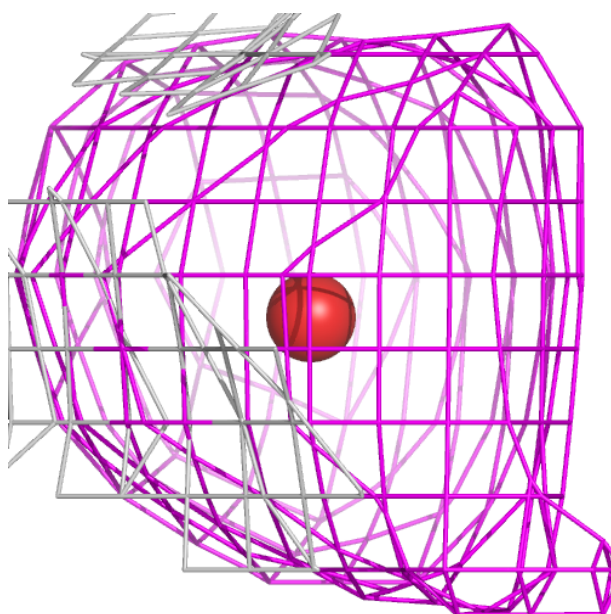
Electron density around MBR J 402:

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



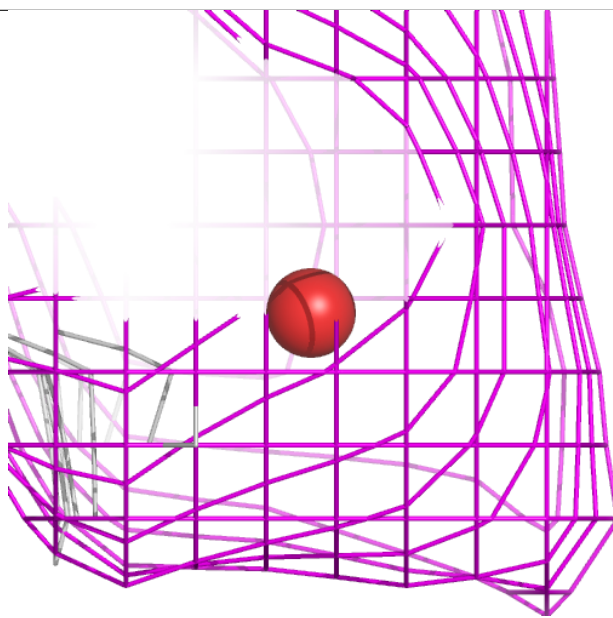
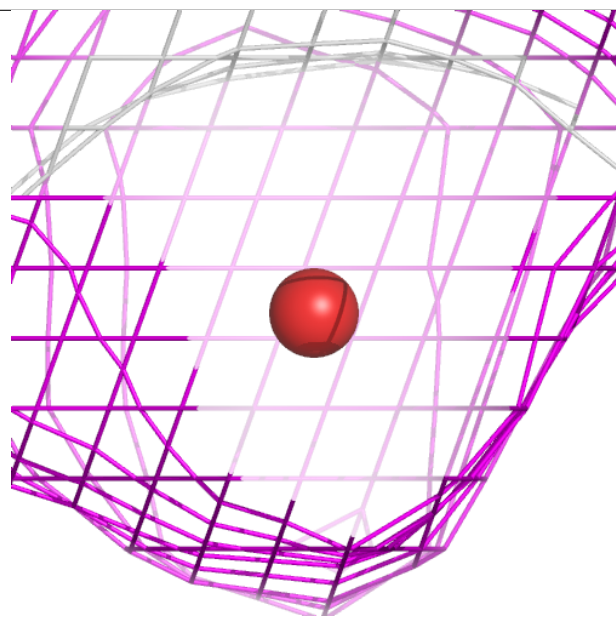
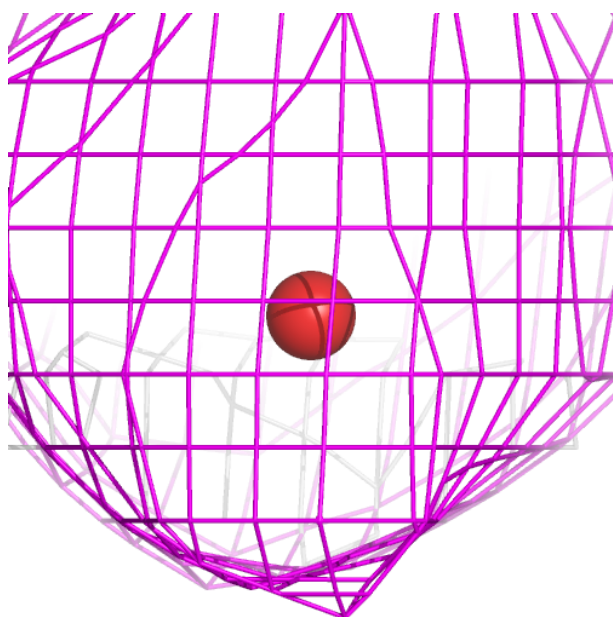
Electron density around MBR I 402:

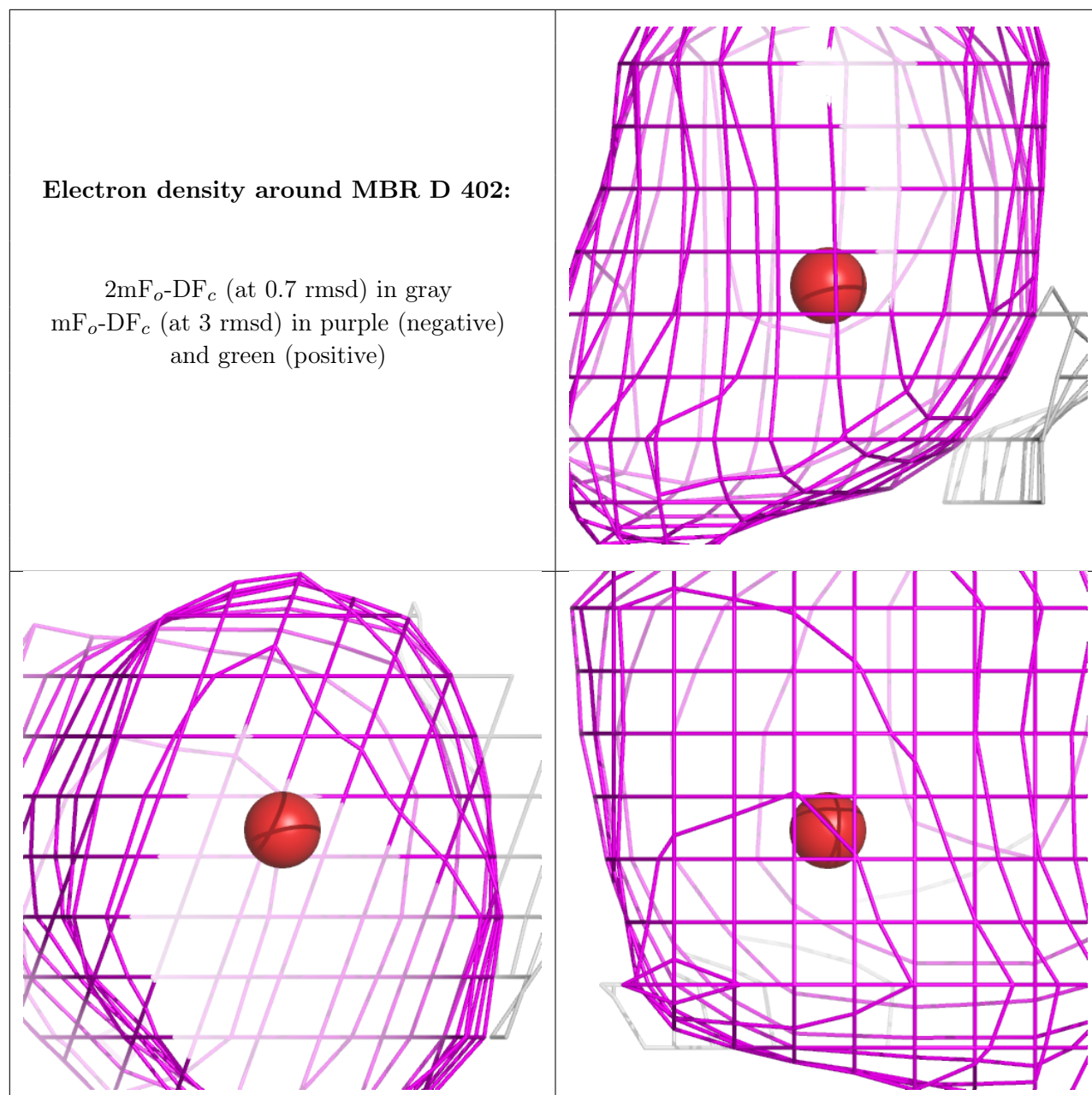
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MBR G 402:

$2mF_o-DF_c$ (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.