



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:11 PM UTC

PDB ID : 1PFC / pdb_00001pfc
Title : MOLECULAR-REPLACEMENT STRUCTURE OF GUINEA PIG IGG1
P*FC(PRIME) REFINED AT 3.1 ANGSTROMS RESOLUTION
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Deposited on : 1981-10-28
Resolution : 3.12 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

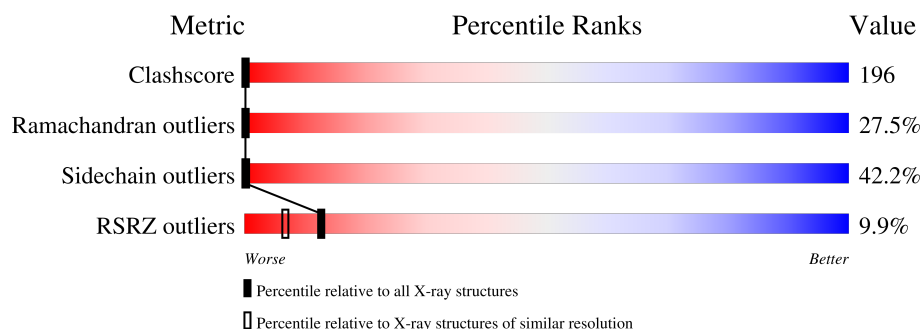
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.12 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))
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)

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	113	10% 10% 40% 49% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 878 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.

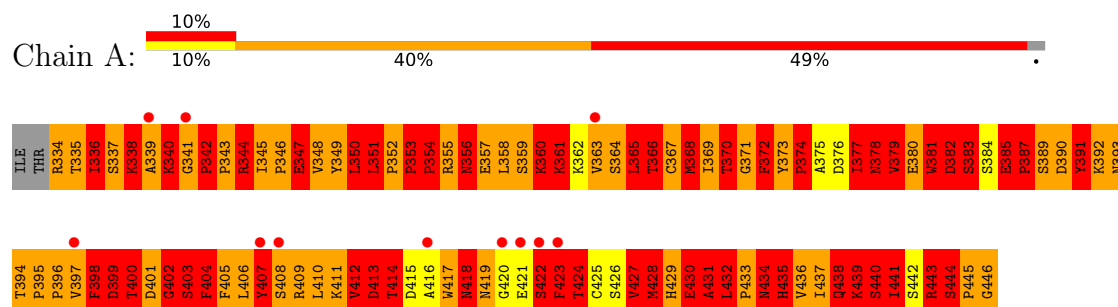
- Molecule 1 is a protein called IGG1 PFC' FC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	111	Total	C	N	O	S	0	0	0
			878	558	147	169	4			

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: IGG1 PFC' FC



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	60.57Å 60.57Å 136.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 3.12 5.00 – 3.13	Depositor EDS
% Data completeness (in resolution range)	(Not available) (5.00-3.12) 69.6 (5.00-3.13)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	0.303 , (Not available) 0.359 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	47.7	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	28.09 , 999.0	EDS
L-test for twinning ¹	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	878	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	3.35	84/904 (9.3%)	5.59	283/1230 (23.0%)

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	11

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	403	SER	C-O	28.02	1.59	1.24
1	A	398	PHE	C-O	27.86	1.55	1.24
1	A	402	GLY	C-O	27.66	1.61	1.23
1	A	370	THR	C-O	19.49	1.47	1.23
1	A	402	GLY	C-N	-16.82	1.10	1.33
1	A	392	LYS	C-O	16.53	1.44	1.23
1	A	398	PHE	C-N	-15.81	1.10	1.33
1	A	392	LYS	C-N	-12.16	1.16	1.33
1	A	418	ASN	C-O	11.76	1.38	1.24
1	A	394	THR	CA-C	11.26	1.64	1.52
1	A	370	THR	CA-C	-9.93	1.42	1.53
1	A	370	THR	C-N	-9.77	1.19	1.33
1	A	392	LYS	N-CA	9.55	1.57	1.45
1	A	399	ASP	N-CA	-9.34	1.34	1.46
1	A	398	PHE	CA-C	-8.98	1.42	1.52
1	A	418	ASN	C-N	-8.84	1.21	1.34
1	A	419	ASN	N-CA	-8.71	1.35	1.46
1	A	351	LEU	N-CA	8.04	1.55	1.46
1	A	335	THR	CA-CB	7.96	1.67	1.53
1	A	434	ASN	N-CA	7.89	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	423	PHE	N-CA	-7.73	1.36	1.45
1	A	349	TYR	C-O	7.67	1.33	1.23
1	A	422	SER	N-CA	7.50	1.55	1.46
1	A	381	TRP	N-CA	7.42	1.55	1.46
1	A	428	MET	CA-CB	-7.34	1.40	1.53
1	A	390	ASP	CA-CB	7.26	1.64	1.53
1	A	378	ASN	CA-C	7.25	1.61	1.52
1	A	349	TYR	CA-CB	7.09	1.67	1.54
1	A	366	THR	N-CA	-7.06	1.36	1.45
1	A	368	MET	N-CA	6.85	1.54	1.46
1	A	379	VAL	CA-CB	6.83	1.62	1.54
1	A	405	PHE	N-CA	6.80	1.54	1.46
1	A	394	THR	C-O	-6.77	1.16	1.24
1	A	435	HIS	CE1-NE2	-6.75	1.25	1.32
1	A	384	SER	N-CA	6.65	1.53	1.45
1	A	409	ARG	CZ-NH2	6.57	1.42	1.33
1	A	422	SER	C-N	-6.52	1.24	1.33
1	A	366	THR	CA-CB	6.46	1.67	1.54
1	A	393	ASN	N-CA	-6.43	1.38	1.45
1	A	392	LYS	CA-C	-6.30	1.45	1.52
1	A	334	ARG	CD-NE	-6.28	1.37	1.46
1	A	334	ARG	NE-CZ	-6.27	1.26	1.33
1	A	371	GLY	CA-C	6.19	1.60	1.51
1	A	336	ILE	C-O	6.16	1.31	1.24
1	A	373	TYR	CA-C	6.13	1.60	1.52
1	A	390	ASP	CA-C	-6.09	1.47	1.53
1	A	381	TRP	CA-CB	-6.09	1.44	1.53
1	A	404	PHE	C-N	6.08	1.41	1.33
1	A	359	SER	C-O	6.07	1.31	1.23
1	A	380	GLU	N-CA	6.06	1.53	1.45
1	A	341	GLY	N-CA	-6.04	1.36	1.44
1	A	370	THR	CA-CB	5.95	1.60	1.52
1	A	398	PHE	N-CA	5.89	1.53	1.46
1	A	355	ARG	C-O	5.76	1.31	1.24
1	A	369	ILE	CA-CB	5.67	1.61	1.54
1	A	339	ALA	CA-CB	5.65	1.63	1.53
1	A	385	GLU	CA-C	-5.60	1.45	1.52
1	A	424	THR	CA-CB	5.50	1.65	1.54
1	A	389	SER	C-N	-5.49	1.26	1.33
1	A	389	SER	C-O	5.47	1.30	1.24
1	A	393	ASN	CA-C	5.38	1.59	1.52
1	A	409	ARG	CD-NE	-5.37	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	416	ALA	N-CA	5.35	1.53	1.46
1	A	433	PRO	N-CA	-5.34	1.40	1.47
1	A	361	LYS	C-O	5.34	1.30	1.24
1	A	390	ASP	N-CA	-5.32	1.39	1.46
1	A	435	HIS	N-CA	5.31	1.52	1.46
1	A	433	PRO	CA-CB	5.30	1.61	1.53
1	A	343	PRO	CA-CB	5.24	1.61	1.53
1	A	413	ASP	C-O	5.20	1.30	1.24
1	A	383	SER	N-CA	-5.18	1.39	1.46
1	A	365	LEU	C-N	-5.16	1.26	1.33
1	A	436	VAL	N-CA	-5.16	1.40	1.46
1	A	373	TYR	CA-CB	-5.15	1.45	1.53
1	A	370	THR	CB-OG1	5.13	1.51	1.43
1	A	401	ASP	N-CA	5.12	1.52	1.46
1	A	431	ALA	N-CA	5.12	1.52	1.46
1	A	397	VAL	N-CA	5.08	1.52	1.46
1	A	336	ILE	N-CA	5.07	1.52	1.46
1	A	446	GLY	N-CA	5.07	1.53	1.45
1	A	375	ALA	N-CA	5.04	1.52	1.46
1	A	347	GLU	C-O	5.04	1.29	1.23
1	A	403	SER	CA-CB	-5.01	1.45	1.53
1	A	400	THR	N-CA	-5.01	1.39	1.46

All (283) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	THR	O-C-N	-33.39	85.67	123.40
1	A	402	GLY	O-C-N	-30.46	83.10	122.70
1	A	392	LYS	CA-C-N	29.30	170.04	122.87
1	A	392	LYS	C-N-CA	29.30	170.04	122.87
1	A	402	GLY	CA-C-N	29.28	177.47	121.54
1	A	402	GLY	C-N-CA	29.28	177.47	121.54
1	A	398	PHE	O-C-N	-27.43	91.45	123.27
1	A	418	ASN	CA-C-N	25.95	159.75	120.31
1	A	418	ASN	C-N-CA	25.95	159.75	120.31
1	A	392	LYS	O-C-N	-25.62	93.55	123.27
1	A	422	SER	CA-C-N	24.16	160.74	122.81
1	A	422	SER	C-N-CA	24.16	160.74	122.81
1	A	365	LEU	CA-C-N	23.80	159.95	122.59
1	A	365	LEU	C-N-CA	23.80	159.95	122.59
1	A	394	THR	O-C-N	23.66	142.45	121.39
1	A	370	THR	CA-C-O	-22.76	92.05	120.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	PHE	CA-C-N	22.58	156.81	122.94
1	A	398	PHE	C-N-CA	22.58	156.81	122.94
1	A	403	SER	CA-C-O	-21.23	90.16	120.51
1	A	414	THR	CA-C-N	20.70	151.11	122.34
1	A	414	THR	C-N-CA	20.70	151.11	122.34
1	A	398	PHE	CA-C-O	-19.76	99.16	120.30
1	A	334	ARG	CD-NE-CZ	19.41	151.58	124.40
1	A	394	THR	N-CA-CB	18.71	143.35	110.23
1	A	435	HIS	CA-CB-CG	17.54	131.34	113.80
1	A	347	GLU	CA-C-N	17.04	151.30	122.67
1	A	347	GLU	C-N-CA	17.04	151.30	122.67
1	A	385	GLU	CB-CG-CD	16.38	140.44	112.60
1	A	409	ARG	CD-NE-CZ	15.91	146.68	124.40
1	A	372	PHE	CA-CB-CG	15.40	129.20	113.80
1	A	402	GLY	CA-C-O	-15.34	93.89	120.57
1	A	424	THR	N-CA-C	15.07	132.59	109.23
1	A	376	ASP	CA-CB-CG	14.59	127.19	112.60
1	A	356	ASN	CA-CB-CG	14.45	127.05	112.60
1	A	349	TYR	N-CA-C	14.45	131.06	109.24
1	A	418	ASN	CA-CB-CG	14.36	126.96	112.60
1	A	390	ASP	N-CA-C	14.04	129.50	109.71
1	A	428	MET	CB-CA-C	13.45	129.88	110.24
1	A	346	PRO	N-CA-C	13.01	130.04	112.48
1	A	382	ASP	CA-C-N	12.94	146.25	121.54
1	A	382	ASP	C-N-CA	12.94	146.25	121.54
1	A	350	LEU	CA-C-N	-12.66	110.60	122.37
1	A	350	LEU	C-N-CA	-12.66	110.60	122.37
1	A	418	ASN	O-C-N	-12.54	105.92	122.59
1	A	339	ALA	N-CA-C	12.31	137.03	110.80
1	A	419	ASN	CA-CB-CG	-12.27	100.33	112.60
1	A	371	GLY	N-CA-C	-12.04	84.66	113.18
1	A	385	GLU	CA-CB-CG	12.02	138.15	114.10
1	A	366	THR	N-CA-C	11.94	128.03	109.52
1	A	377	ILE	CA-C-O	-11.79	111.05	120.96
1	A	403	SER	CA-CB-OG	11.77	134.63	111.10
1	A	423	PHE	N-CA-C	11.70	128.43	109.72
1	A	352	PRO	N-CA-C	11.51	124.74	110.70
1	A	394	THR	N-CA-C	-11.41	91.14	109.40
1	A	424	THR	CA-CB-OG1	-11.31	92.64	109.60
1	A	443	ARG	NE-CZ-NH1	-11.29	110.21	121.50
1	A	369	ILE	CA-C-N	-11.29	104.34	121.72
1	A	369	ILE	C-N-CA	-11.29	104.34	121.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	PRO	N-CA-C	11.20	128.77	113.65
1	A	403	SER	N-CA-C	-11.13	87.09	110.80
1	A	399	ASP	CA-CB-CG	-10.96	101.64	112.60
1	A	381	TRP	CA-CB-CG	10.71	133.95	113.60
1	A	381	TRP	CB-CA-C	10.58	126.07	110.62
1	A	389	SER	CA-C-N	10.52	136.68	122.06
1	A	389	SER	C-N-CA	10.52	136.68	122.06
1	A	358	LEU	CA-C-O	10.43	132.97	121.40
1	A	363	VAL	N-CA-CB	-10.28	99.41	110.82
1	A	385	GLU	N-CA-C	10.20	132.36	109.81
1	A	403	SER	O-C-N	-10.19	109.04	122.59
1	A	443	ARG	NH1-CZ-NH2	9.94	132.22	119.30
1	A	392	LYS	CA-CB-CG	9.86	133.81	114.10
1	A	401	ASP	N-CA-C	-9.81	99.62	111.69
1	A	361	LYS	CG-CD-CE	9.77	133.76	111.30
1	A	353	PRO	N-CA-C	9.76	122.61	110.70
1	A	418	ASN	CA-C-O	-9.75	106.56	120.51
1	A	347	GLU	CB-CG-CD	9.73	129.15	112.60
1	A	378	ASN	CA-C-O	9.71	132.47	121.11
1	A	400	THR	O-C-N	9.71	135.50	122.59
1	A	344	ARG	CA-C-N	9.65	139.98	122.13
1	A	344	ARG	C-N-CA	9.65	139.98	122.13
1	A	433	PRO	CA-C-N	-9.62	108.15	122.39
1	A	433	PRO	C-N-CA	-9.62	108.15	122.39
1	A	407	TYR	CA-C-O	-9.51	108.58	120.28
1	A	399	ASP	O-C-N	9.37	135.41	123.23
1	A	334	ARG	NE-CZ-NH1	9.27	130.76	121.50
1	A	427	VAL	CB-CA-C	-9.25	96.26	110.50
1	A	404	PHE	N-CA-C	9.10	124.23	109.85
1	A	390	ASP	N-CA-CB	-9.09	100.17	110.35
1	A	340	LYS	N-CA-C	-9.01	101.86	113.12
1	A	378	ASN	CA-C-N	9.00	135.07	123.10
1	A	378	ASN	C-N-CA	9.00	135.07	123.10
1	A	359	SER	CA-C-O	-8.99	110.94	121.46
1	A	341	GLY	N-CA-C	8.93	130.56	112.34
1	A	339	ALA	N-CA-CB	-8.84	95.55	110.49
1	A	398	PHE	CA-CB-CG	8.79	122.59	113.80
1	A	399	ASP	N-CA-CB	8.79	126.12	110.83
1	A	439	LYS	N-CA-C	8.73	122.35	109.07
1	A	338	LYS	N-CA-C	8.70	129.34	110.80
1	A	434	ASN	OD1-CG-ND2	8.69	131.28	122.60
1	A	379	VAL	CB-CA-C	-8.68	98.44	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	347	GLU	O-C-N	-8.66	114.16	123.42
1	A	344	ARG	CA-CB-CG	8.63	131.36	114.10
1	A	426	SER	CA-C-O	8.56	129.95	120.70
1	A	434	ASN	CA-C-O	-8.53	109.80	120.20
1	A	433	PRO	O-C-N	8.49	134.10	122.64
1	A	340	LYS	CA-C-O	8.43	129.98	119.78
1	A	344	ARG	CB-CG-CD	8.40	130.62	111.30
1	A	367	CYS	CA-C-N	-8.32	109.92	122.74
1	A	367	CYS	C-N-CA	-8.32	109.92	122.74
1	A	415	ASP	CA-CB-CG	8.32	120.92	112.60
1	A	348	VAL	CB-CA-C	-8.31	98.02	110.82
1	A	418	ASN	N-CA-CB	-8.29	96.48	110.49
1	A	361	LYS	N-CA-C	8.23	128.32	110.80
1	A	370	THR	N-CA-C	8.21	120.93	107.23
1	A	342	PRO	CA-C-N	8.19	128.29	119.28
1	A	342	PRO	C-N-CA	8.19	128.29	119.28
1	A	441	ILE	CB-CA-C	8.13	124.63	111.29
1	A	394	THR	CB-CA-C	-8.02	98.60	109.42
1	A	415	ASP	N-CA-CB	7.98	124.04	111.91
1	A	362	LYS	N-CA-C	7.92	123.40	113.43
1	A	397	VAL	N-CA-C	-7.87	96.06	107.78
1	A	404	PHE	CA-C-N	-7.69	111.92	122.77
1	A	404	PHE	C-N-CA	-7.69	111.92	122.77
1	A	391	TYR	O-C-N	7.66	133.24	123.12
1	A	334	ARG	NE-CZ-NH2	-7.65	112.31	119.20
1	A	422	SER	O-C-N	-7.64	112.42	122.59
1	A	349	TYR	CA-CB-CG	-7.62	100.18	113.90
1	A	370	THR	CA-CB-OG1	-7.59	98.21	109.60
1	A	383	SER	N-CA-CB	7.57	123.28	110.49
1	A	338	LYS	CA-C-O	7.56	131.32	120.51
1	A	355	ARG	NE-CZ-NH2	7.56	126.00	119.20
1	A	362	LYS	N-CA-CB	-7.55	97.68	110.51
1	A	390	ASP	CA-C-O	-7.54	112.41	122.51
1	A	366	THR	CA-C-O	7.51	130.22	121.44
1	A	378	ASN	CA-CB-CG	7.48	120.08	112.60
1	A	444	SER	CA-CB-OG	7.46	126.03	111.10
1	A	404	PHE	O-C-N	7.44	133.08	123.11
1	A	384	SER	CB-CA-C	7.42	123.07	109.71
1	A	405	PHE	CA-C-O	7.42	128.11	120.24
1	A	335	THR	N-CA-CB	-7.34	98.08	110.49
1	A	434	ASN	O-C-N	7.34	132.67	123.28
1	A	438	GLN	OE1-CD-NE2	7.30	129.90	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381	TRP	CA-C-O	7.21	129.34	120.25
1	A	411	LYS	CA-C-N	7.21	134.94	121.97
1	A	411	LYS	C-N-CA	7.21	134.94	121.97
1	A	377	ILE	O-C-N	7.19	129.23	122.97
1	A	369	ILE	N-CA-CB	-7.17	102.93	112.10
1	A	348	VAL	N-CA-C	7.15	119.86	108.85
1	A	431	ALA	CA-C-O	7.15	130.74	120.51
1	A	379	VAL	N-CA-C	7.14	118.17	107.75
1	A	412	VAL	CA-C-N	7.13	135.17	121.54
1	A	412	VAL	C-N-CA	7.13	135.17	121.54
1	A	424	THR	N-CA-CB	-7.10	98.33	111.53
1	A	415	ASP	O-C-N	7.07	131.07	122.58
1	A	437	ILE	O-C-N	7.04	130.68	123.07
1	A	446	GLY	CA-C-O	-7.04	99.89	121.00
1	A	431	ALA	N-CA-C	-7.00	95.88	110.80
1	A	363	VAL	N-CA-C	7.00	118.08	108.84
1	A	376	ASP	N-CA-C	6.93	120.96	108.48
1	A	419	ASN	N-CA-C	6.87	119.79	111.82
1	A	438	GLN	CG-CD-NE2	-6.83	106.16	116.40
1	A	364	SER	N-CA-CB	6.82	122.67	111.62
1	A	357	GLU	CA-C-N	6.81	133.49	122.53
1	A	357	GLU	C-N-CA	6.81	133.49	122.53
1	A	427	VAL	N-CA-CB	6.81	122.60	111.44
1	A	401	ASP	O-C-N	6.79	131.05	122.23
1	A	435	HIS	ND1-CG-CD2	-6.77	99.33	106.10
1	A	353	PRO	CA-C-N	6.77	128.30	119.84
1	A	353	PRO	C-N-CA	6.77	128.30	119.84
1	A	395	PRO	N-CA-C	6.73	118.91	110.70
1	A	391	TYR	N-CA-CB	6.73	121.28	110.65
1	A	382	ASP	CA-CB-CG	-6.70	105.90	112.60
1	A	424	THR	OG1-CB-CG2	6.67	122.64	109.30
1	A	394	THR	CA-C-O	-6.66	112.89	119.69
1	A	355	ARG	NE-CZ-NH1	-6.64	114.86	121.50
1	A	403	SER	CB-CA-C	6.61	123.57	110.42
1	A	436	VAL	CB-CA-C	-6.60	100.66	110.82
1	A	446	GLY	N-CA-C	-6.59	94.19	113.30
1	A	355	ARG	O-C-N	6.57	131.33	122.59
1	A	373	TYR	N-CA-CB	6.55	122.03	110.37
1	A	370	THR	CA-CB-CG2	6.54	121.62	110.50
1	A	434	ASN	CA-CB-CG	-6.53	106.07	112.60
1	A	408	SER	CA-C-O	6.48	128.69	121.11
1	A	434	ASN	N-CA-C	-6.46	97.54	108.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	429	HIS	O-C-N	6.40	131.57	123.12
1	A	356	ASN	N-CA-C	6.39	119.77	107.44
1	A	336	ILE	CB-CA-C	6.32	121.65	111.29
1	A	425	CYS	O-C-N	6.30	130.79	123.30
1	A	356	ASN	OD1-CG-ND2	-6.29	116.31	122.60
1	A	373	TYR	CA-CB-CG	6.27	125.18	113.90
1	A	435	HIS	CB-CG-CD2	6.26	139.34	131.20
1	A	350	LEU	O-C-N	6.25	130.93	123.24
1	A	347	GLU	CG-CD-OE1	6.23	132.72	118.40
1	A	412	VAL	CA-C-O	6.23	128.56	120.78
1	A	400	THR	CA-CB-OG1	-6.22	100.27	109.60
1	A	415	ASP	CA-C-O	-6.20	114.40	121.65
1	A	376	ASP	CA-C-N	6.20	130.27	121.96
1	A	376	ASP	C-N-CA	6.20	130.27	121.96
1	A	356	ASN	CA-C-O	6.18	128.82	120.47
1	A	347	GLU	CA-C-O	6.17	127.83	121.23
1	A	428	MET	N-CA-C	-6.13	97.59	108.13
1	A	373	TYR	N-CA-C	-6.11	96.32	109.81
1	A	378	ASN	N-CA-CB	6.03	122.35	111.37
1	A	433	PRO	N-CA-C	6.03	124.89	112.47
1	A	390	ASP	CB-CA-C	-6.01	103.17	112.07
1	A	392	LYS	CG-CD-CE	5.94	124.96	111.30
1	A	350	LEU	CA-C-O	-5.92	114.18	121.11
1	A	356	ASN	CA-C-N	5.91	132.82	121.54
1	A	356	ASN	C-N-CA	5.91	132.82	121.54
1	A	347	GLU	N-CA-C	5.90	117.81	108.79
1	A	381	TRP	N-CA-CB	-5.86	101.76	110.90
1	A	335	THR	CA-CB-OG1	5.83	118.35	109.60
1	A	357	GLU	N-CA-CB	-5.82	100.65	110.49
1	A	393	ASN	N-CA-C	-5.82	100.69	109.95
1	A	430	GLU	N-CA-CB	5.82	119.26	110.42
1	A	432	LEU	CB-CA-C	5.80	121.59	110.17
1	A	389	SER	CA-CB-OG	-5.78	99.54	111.10
1	A	410	LEU	CA-C-O	5.78	127.64	120.54
1	A	370	THR	CB-CA-C	-5.73	103.92	111.42
1	A	344	ARG	N-CA-C	5.68	117.68	108.41
1	A	351	LEU	CB-CA-C	5.67	118.18	111.15
1	A	425	CYS	CB-CA-C	-5.67	99.33	109.71
1	A	427	VAL	O-C-N	5.67	129.16	123.10
1	A	371	GLY	CA-C-N	-5.67	110.72	121.54
1	A	371	GLY	C-N-CA	-5.67	110.72	121.54
1	A	385	GLU	CG-CD-OE2	5.65	131.39	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	418	ASN	OD1-CG-ND2	-5.64	116.95	122.60
1	A	438	GLN	CB-CG-CD	-5.63	103.04	112.60
1	A	433	PRO	CB-CA-C	-5.61	102.30	111.56
1	A	416	ALA	CA-C-O	5.57	128.47	120.51
1	A	407	TYR	O-C-N	5.55	130.13	123.36
1	A	422	SER	N-CA-C	-5.54	98.99	110.80
1	A	360	LYS	CB-CG-CD	5.54	124.03	111.30
1	A	428	MET	CA-C-O	5.54	127.69	120.11
1	A	347	GLU	CB-CA-C	5.53	120.90	110.62
1	A	389	SER	CB-CA-C	5.51	121.39	110.42
1	A	365	LEU	CB-CA-C	5.51	122.96	110.67
1	A	408	SER	CA-CB-OG	-5.51	100.09	111.10
1	A	357	GLU	N-CA-C	5.50	122.50	110.80
1	A	435	HIS	CA-C-O	5.49	126.17	120.40
1	A	409	ARG	NE-CZ-NH2	-5.48	114.27	119.20
1	A	383	SER	CA-C-N	-5.48	113.28	122.92
1	A	383	SER	C-N-CA	-5.48	113.28	122.92
1	A	436	VAL	CA-C-O	5.47	128.54	121.32
1	A	392	LYS	CB-CA-C	5.47	121.69	109.56
1	A	429	HIS	N-CA-CB	-5.47	102.53	110.84
1	A	409	ARG	N-CA-C	5.46	118.48	109.85
1	A	356	ASN	O-C-N	-5.44	116.18	123.14
1	A	380	GLU	CA-C-N	-5.42	114.57	122.44
1	A	380	GLU	C-N-CA	-5.42	114.57	122.44
1	A	401	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	393	ASN	CA-CB-CG	5.42	118.02	112.60
1	A	411	LYS	CG-CD-CE	5.39	123.69	111.30
1	A	411	LYS	CB-CG-CD	5.38	123.66	111.30
1	A	409	ARG	NE-CZ-NH1	5.36	126.86	121.50
1	A	350	LEU	CA-CB-CG	5.34	135.01	116.30
1	A	366	THR	CA-C-N	5.34	130.97	122.74
1	A	366	THR	C-N-CA	5.34	130.97	122.74
1	A	385	GLU	CA-C-N	5.34	126.51	119.84
1	A	385	GLU	C-N-CA	5.34	126.51	119.84
1	A	387	PRO	CA-C-O	5.34	130.31	120.60
1	A	365	LEU	O-C-N	-5.33	116.25	122.96
1	A	361	LYS	O-C-N	-5.32	115.51	122.59
1	A	435	HIS	N-CA-CB	5.24	118.93	110.65
1	A	437	ILE	CB-CA-C	5.23	118.55	110.28
1	A	356	ASN	CB-CG-ND2	5.20	124.20	116.40
1	A	423	PHE	CA-C-O	5.18	126.96	121.11
1	A	428	MET	CA-C-N	-5.17	115.52	122.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	428	MET	C-N-CA	-5.17	115.52	122.86
1	A	354	PRO	CA-C-O	5.15	129.97	120.60
1	A	400	THR	CA-C-N	-5.12	111.82	120.58
1	A	400	THR	C-N-CA	-5.12	111.82	120.58
1	A	351	LEU	CA-C-O	-5.10	116.54	121.34
1	A	346	PRO	N-CA-CB	-5.10	98.68	102.25
1	A	380	GLU	CA-CB-CG	5.09	124.29	114.10
1	A	352	PRO	CA-C-N	5.09	125.62	120.38
1	A	352	PRO	C-N-CA	5.09	125.62	120.38
1	A	389	SER	CA-C-O	-5.09	113.24	120.51
1	A	430	GLU	N-CA-C	-5.04	103.28	110.59
1	A	391	TYR	CA-CB-CG	5.03	122.95	113.90
1	A	374	PRO	CA-C-N	-5.01	114.78	122.60
1	A	374	PRO	C-N-CA	-5.01	114.78	122.60
1	A	359	SER	CB-CA-C	5.00	119.37	109.66

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	370	THR	Mainchain,Peptide
1	A	392	LYS	Mainchain,Peptide
1	A	398	PHE	Mainchain
1	A	402	GLY	Mainchain,Peptide
1	A	403	SER	Mainchain,Peptide
1	A	418	ASN	Mainchain
1	A	422	SER	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	878	0	848	339	5
All	All	878	0	848	339	5

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 196.

All (339) 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:A:361:LYS:N	1:A:414:THR:HG21	1.38	1.33
1:A:381:TRP:NE1	1:A:410:LEU:HB2	1.41	1.32
1:A:381:TRP:HE1	1:A:410:LEU:CB	1.44	1.31
1:A:444:SER:HB2	1:A:445:PRO:CD	1.66	1.24
1:A:372:PHE:N	1:A:404:PHE:H	1.36	1.23
1:A:377:ILE:CG2	1:A:429:HIS:HD2	1.52	1.20
1:A:377:ILE:HG21	1:A:429:HIS:HD2	1.06	1.20
1:A:344:ARG:NH1	1:A:344:ARG:H	1.38	1.20
1:A:373:TYR:HB3	1:A:374:PRO:CA	1.73	1.18
1:A:346:PRO:O	1:A:347:GLU:HG3	1.44	1.16
1:A:342:PRO:CA	1:A:373:TYR:HB2	1.74	1.16
1:A:443:ARG:O	1:A:444:SER:OG	1.63	1.13
1:A:427:VAL:HG12	1:A:436:VAL:HG22	1.14	1.11
1:A:381:TRP:CZ2	1:A:410:LEU:HB3	1.85	1.10
1:A:411:LYS:HD2	1:A:413:ASP:CA	1.80	1.10
1:A:370:THR:HG22	1:A:406:LEU:H	1.17	1.09
1:A:444:SER:HB2	1:A:445:PRO:HD2	1.22	1.09
1:A:377:ILE:CG2	1:A:429:HIS:CD2	2.35	1.08
1:A:349:TYR:CB	1:A:368:MET:HG3	1.85	1.07
1:A:342:PRO:HA	1:A:373:TYR:CB	1.84	1.07
1:A:379:VAL:HG12	1:A:379:VAL:O	1.54	1.06
1:A:361:LYS:H	1:A:414:THR:CG2	1.69	1.05
1:A:411:LYS:HD2	1:A:413:ASP:HA	1.11	1.05
1:A:404:PHE:HD1	1:A:405:PHE:N	1.53	1.04
1:A:342:PRO:HA	1:A:373:TYR:HB2	1.04	1.03
1:A:421:GLU:O	1:A:422:SER:C	2.00	1.02
1:A:338:LYS:HB2	1:A:342:PRO:HG3	1.39	1.02
1:A:335:THR:O	1:A:336:ILE:HG13	1.59	1.01
1:A:342:PRO:CG	1:A:343:PRO:HD2	1.89	1.01
1:A:439:LYS:O	1:A:440:SER:HB2	1.61	1.00
1:A:417:TRP:HE3	1:A:417:TRP:C	1.70	1.00
1:A:361:LYS:N	1:A:414:THR:CG2	2.24	0.99
1:A:370:THR:HB	1:A:405:PHE:HA	1.45	0.99
1:A:344:ARG:H	1:A:344:ARG:HH11	1.00	0.98
1:A:373:TYR:HB3	1:A:374:PRO:HA	0.99	0.98
1:A:381:TRP:NE1	1:A:410:LEU:CB	2.13	0.97
1:A:372:PHE:H	1:A:404:PHE:N	1.61	0.96
1:A:394:THR:OG1	1:A:407:TYR:HB2	1.65	0.96
1:A:379:VAL:O	1:A:379:VAL:CG1	2.14	0.95
1:A:406:LEU:C	1:A:407:TYR:HD2	1.73	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:TRP:HZ2	1:A:410:LEU:HB3	1.28	0.94
1:A:427:VAL:CG1	1:A:436:VAL:HG22	1.96	0.94
1:A:349:TYR:HB2	1:A:368:MET:HG3	1.44	0.93
1:A:340:LYS:HD2	1:A:373:TYR:OH	1.68	0.93
1:A:370:THR:HG22	1:A:406:LEU:N	1.85	0.92
1:A:377:ILE:HG21	1:A:429:HIS:CD2	1.99	0.92
1:A:444:SER:CB	1:A:445:PRO:CD	2.47	0.92
1:A:421:GLU:HB3	1:A:423:PHE:CD2	2.04	0.92
1:A:373:TYR:CB	1:A:374:PRO:HA	1.95	0.91
1:A:344:ARG:NH1	1:A:344:ARG:N	2.18	0.91
1:A:404:PHE:CD1	1:A:405:PHE:N	2.38	0.91
1:A:380:GLU:HA	1:A:391:TYR:OH	1.70	0.90
1:A:339:ALA:HB1	1:A:340:LYS:HE2	1.54	0.90
1:A:372:PHE:H	1:A:404:PHE:H	0.91	0.88
1:A:417:TRP:C	1:A:417:TRP:CE3	2.51	0.88
1:A:434:ASN:HD21	1:A:436:VAL:HG13	1.37	0.88
1:A:342:PRO:HG2	1:A:343:PRO:HD2	1.55	0.88
1:A:402:GLY:O	1:A:405:PHE:CE1	2.26	0.88
1:A:406:LEU:O	1:A:407:TYR:CD2	2.26	0.87
1:A:364:SER:OG	1:A:365:LEU:N	2.02	0.87
1:A:372:PHE:N	1:A:404:PHE:N	2.19	0.86
1:A:381:TRP:NE1	1:A:410:LEU:HD22	1.90	0.86
1:A:360:LYS:O	1:A:361:LYS:HB2	1.75	0.86
1:A:381:TRP:NE1	1:A:410:LEU:CD2	2.40	0.85
1:A:352:PRO:O	1:A:354:PRO:HD3	1.77	0.84
1:A:421:GLU:O	1:A:423:PHE:N	2.09	0.84
1:A:434:ASN:ND2	1:A:436:VAL:HG13	1.93	0.84
1:A:377:ILE:HG22	1:A:429:HIS:CD2	2.10	0.84
1:A:443:ARG:C	1:A:444:SER:HG	1.84	0.83
1:A:351:LEU:HD11	1:A:366:THR:HG22	1.61	0.83
1:A:381:TRP:CE2	1:A:410:LEU:HB3	2.14	0.82
1:A:342:PRO:CD	1:A:343:PRO:HD2	2.08	0.82
1:A:353:PRO:HB2	1:A:444:SER:HA	1.61	0.82
1:A:404:PHE:CD1	1:A:404:PHE:C	2.58	0.82
1:A:366:THR:OG1	1:A:409:ARG:HG3	1.80	0.81
1:A:411:LYS:HD2	1:A:413:ASP:N	1.96	0.81
1:A:351:LEU:O	1:A:365:LEU:HG	1.82	0.80
1:A:377:ILE:HD13	1:A:404:PHE:CZ	2.16	0.80
1:A:406:LEU:C	1:A:407:TYR:CD2	2.60	0.79
1:A:352:PRO:C	1:A:354:PRO:HD3	2.06	0.78
1:A:353:PRO:O	1:A:443:ARG:HG3	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:PHE:O	1:A:404:PHE:CD2	2.35	0.78
1:A:381:TRP:HE1	1:A:410:LEU:HB2	0.62	0.78
1:A:336:ILE:HG22	1:A:337:SER:H	1.48	0.78
1:A:364:SER:HB2	1:A:411:LYS:HB2	1.67	0.77
1:A:377:ILE:HG23	1:A:404:PHE:HE2	1.47	0.77
1:A:377:ILE:CD1	1:A:404:PHE:CZ	2.67	0.77
1:A:381:TRP:CE2	1:A:410:LEU:CB	2.67	0.77
1:A:402:GLY:HA2	1:A:405:PHE:CZ	2.18	0.77
1:A:351:LEU:CD1	1:A:366:THR:HG22	2.14	0.77
1:A:439:LYS:O	1:A:440:SER:CB	2.33	0.77
1:A:349:TYR:HB3	1:A:368:MET:HG3	1.66	0.77
1:A:369:ILE:HG21	1:A:427:VAL:HG21	1.68	0.76
1:A:377:ILE:HD13	1:A:404:PHE:HZ	1.49	0.76
1:A:377:ILE:CD1	1:A:404:PHE:HZ	1.99	0.76
1:A:402:GLY:O	1:A:403:SER:C	2.28	0.76
1:A:351:LEU:HD11	1:A:366:THR:CG2	2.16	0.76
1:A:342:PRO:CG	1:A:343:PRO:CD	2.65	0.75
1:A:360:LYS:CB	1:A:414:THR:HB	2.16	0.75
1:A:427:VAL:HG12	1:A:436:VAL:CG2	2.08	0.75
1:A:377:ILE:HB	1:A:429:HIS:CB	2.18	0.74
1:A:421:GLU:HB3	1:A:423:PHE:HD2	1.51	0.74
1:A:338:LYS:HB2	1:A:342:PRO:CG	2.18	0.74
1:A:342:PRO:HG2	1:A:343:PRO:CD	2.17	0.74
1:A:432:LEU:HD23	1:A:433:PRO:HD2	1.67	0.74
1:A:342:PRO:HA	1:A:373:TYR:CA	2.18	0.74
1:A:370:THR:HG21	1:A:405:PHE:HB3	1.69	0.74
1:A:402:GLY:HA2	1:A:405:PHE:HZ	1.51	0.73
1:A:344:ARG:HH11	1:A:344:ARG:N	1.83	0.73
1:A:351:LEU:CG	1:A:366:THR:HG22	2.18	0.73
1:A:404:PHE:C	1:A:405:PHE:HD1	1.96	0.73
1:A:351:LEU:O	1:A:365:LEU:CG	2.36	0.73
1:A:364:SER:OG	1:A:410:LEU:O	2.05	0.72
1:A:444:SER:C	1:A:446:GLY:H	1.97	0.72
1:A:419:ASN:OD1	1:A:419:ASN:O	2.06	0.72
1:A:352:PRO:O	1:A:354:PRO:CD	2.36	0.72
1:A:342:PRO:CB	1:A:343:PRO:CD	2.67	0.72
1:A:421:GLU:CB	1:A:423:PHE:CE2	2.74	0.71
1:A:345:ILE:HB	1:A:371:GLY:O	1.90	0.71
1:A:443:ARG:O	1:A:444:SER:CB	2.39	0.71
1:A:432:LEU:CD2	1:A:433:PRO:HD2	2.20	0.71
1:A:397:VAL:O	1:A:405:PHE:HB2	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:GLY:HA2	1:A:404:PHE:O	1.91	0.70
1:A:381:TRP:CD1	1:A:410:LEU:HD22	2.26	0.70
1:A:404:PHE:C	1:A:405:PHE:CD1	2.70	0.70
1:A:406:LEU:O	1:A:407:TYR:HD2	1.65	0.70
1:A:377:ILE:HB	1:A:429:HIS:HB2	1.72	0.70
1:A:401:ASP:O	1:A:402:GLY:C	2.35	0.70
1:A:370:THR:CG2	1:A:405:PHE:HA	2.22	0.69
1:A:402:GLY:O	1:A:403:SER:O	2.10	0.69
1:A:417:TRP:HE3	1:A:417:TRP:O	1.75	0.69
1:A:430:GLU:O	1:A:431:ALA:CB	2.40	0.69
1:A:337:SER:O	1:A:338:LYS:CB	2.40	0.69
1:A:411:LYS:CD	1:A:413:ASP:H	2.05	0.69
1:A:349:TYR:HD1	1:A:368:MET:O	1.75	0.69
1:A:360:LYS:O	1:A:361:LYS:CB	2.41	0.69
1:A:342:PRO:CB	1:A:373:TYR:HB2	2.23	0.68
1:A:404:PHE:O	1:A:405:PHE:HD1	1.76	0.68
1:A:430:GLU:O	1:A:431:ALA:HB2	1.94	0.67
1:A:360:LYS:HB2	1:A:414:THR:HB	1.75	0.67
1:A:381:TRP:HE1	1:A:410:LEU:CG	2.08	0.67
1:A:396:PRO:CB	1:A:398:PHE:HE2	2.07	0.67
1:A:417:TRP:CH2	1:A:441:ILE:HG23	2.30	0.66
1:A:404:PHE:HD1	1:A:405:PHE:CA	2.09	0.66
1:A:411:LYS:CD	1:A:413:ASP:N	2.59	0.66
1:A:402:GLY:CA	1:A:405:PHE:CZ	2.79	0.66
1:A:404:PHE:CE1	1:A:406:LEU:HB2	2.31	0.65
1:A:370:THR:HG21	1:A:407:TYR:HE2	1.62	0.65
1:A:372:PHE:O	1:A:404:PHE:HD2	1.79	0.65
1:A:413:ASP:O	1:A:414:THR:HG23	1.96	0.65
1:A:370:THR:CB	1:A:405:PHE:HA	2.23	0.65
1:A:380:GLU:OE2	1:A:383:SER:OG	2.14	0.64
1:A:335:THR:C	1:A:336:ILE:HG13	2.23	0.64
1:A:399:ASP:O	1:A:402:GLY:N	2.30	0.64
1:A:382:ASP:HA	1:A:424:THR:HG22	1.79	0.64
1:A:410:LEU:HD12	1:A:411:LYS:O	1.97	0.64
1:A:341:GLY:O	1:A:344:ARG:NH2	2.31	0.64
1:A:361:LYS:O	1:A:361:LYS:CD	2.46	0.63
1:A:421:GLU:HB3	1:A:423:PHE:CE2	2.32	0.63
1:A:345:ILE:N	1:A:372:PHE:CE1	2.67	0.63
1:A:360:LYS:CA	1:A:414:THR:HB	2.28	0.63
1:A:417:TRP:O	1:A:418:ASN:O	2.17	0.63
1:A:370:THR:HB	1:A:405:PHE:CA	2.26	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:GLY:HA3	1:A:344:ARG:CZ	2.29	0.63
1:A:337:SER:O	1:A:338:LYS:HB2	1.97	0.63
1:A:351:LEU:HG	1:A:366:THR:HG22	1.81	0.63
1:A:427:VAL:CG1	1:A:427:VAL:O	2.38	0.62
1:A:396:PRO:HB2	1:A:398:PHE:HE2	1.64	0.62
1:A:374:PRO:CG	1:A:431:ALA:HB1	2.30	0.62
1:A:399:ASP:O	1:A:402:GLY:CA	2.47	0.62
1:A:358:LEU:HD12	1:A:363:VAL:HB	1.80	0.62
1:A:421:GLU:HB2	1:A:423:PHE:HE2	1.64	0.62
1:A:444:SER:CB	1:A:445:PRO:HD3	2.29	0.62
1:A:421:GLU:O	1:A:423:PHE:CD2	2.53	0.61
1:A:404:PHE:HE1	1:A:406:LEU:N	1.97	0.61
1:A:361:LYS:O	1:A:361:LYS:HD2	1.98	0.61
1:A:366:THR:CB	1:A:409:ARG:HG3	2.30	0.61
1:A:337:SER:O	1:A:338:LYS:CG	2.49	0.61
1:A:374:PRO:CD	1:A:431:ALA:HB1	2.31	0.61
1:A:345:ILE:N	1:A:372:PHE:HE1	1.99	0.61
1:A:349:TYR:CD1	1:A:368:MET:O	2.53	0.61
1:A:372:PHE:O	1:A:404:PHE:HB3	1.99	0.61
1:A:385:GLU:O	1:A:387:PRO:C	2.44	0.61
1:A:345:ILE:H	1:A:372:PHE:HE1	1.49	0.60
1:A:434:ASN:CG	1:A:434:ASN:O	2.44	0.60
1:A:417:TRP:HE1	1:A:444:SER:HB3	1.67	0.60
1:A:444:SER:C	1:A:446:GLY:N	2.57	0.60
1:A:338:LYS:HD2	1:A:339:ALA:HB2	1.82	0.60
1:A:424:THR:OG1	1:A:439:LYS:HB3	2.01	0.60
1:A:346:PRO:C	1:A:347:GLU:HG3	2.23	0.59
1:A:427:VAL:HG12	1:A:427:VAL:O	2.01	0.59
1:A:366:THR:HG23	1:A:367:CYS:N	2.16	0.59
1:A:370:THR:HG22	1:A:405:PHE:HA	1.83	0.59
1:A:394:THR:HG1	1:A:407:TYR:HB2	1.65	0.59
1:A:411:LYS:HD3	1:A:413:ASP:H	1.67	0.59
1:A:390:ASP:CG	1:A:390:ASP:O	2.39	0.59
1:A:341:GLY:C	1:A:344:ARG:NH1	2.61	0.58
1:A:411:LYS:HD3	1:A:412:VAL:H	1.67	0.58
1:A:367:CYS:HB2	1:A:381:TRP:CZ3	2.39	0.58
1:A:341:GLY:O	1:A:344:ARG:NH1	2.37	0.57
1:A:372:PHE:H	1:A:404:PHE:CA	2.17	0.57
1:A:399:ASP:HB2	1:A:405:PHE:CE2	2.39	0.57
1:A:363:VAL:O	1:A:363:VAL:HG13	2.02	0.57
1:A:344:ARG:O	1:A:345:ILE:HG13	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:GLU:HB2	1:A:423:PHE:CE2	2.39	0.57
1:A:377:ILE:CG2	1:A:404:PHE:HE2	2.18	0.56
1:A:444:SER:O	1:A:446:GLY:N	2.39	0.56
1:A:361:LYS:HA	1:A:414:THR:HG1	1.70	0.56
1:A:434:ASN:ND2	1:A:434:ASN:C	2.63	0.56
1:A:385:GLU:O	1:A:387:PRO:O	2.24	0.56
1:A:424:THR:OG1	1:A:439:LYS:CB	2.53	0.56
1:A:377:ILE:HG23	1:A:404:PHE:CE2	2.37	0.56
1:A:364:SER:O	1:A:365:LEU:HD13	2.05	0.55
1:A:337:SER:O	1:A:338:LYS:HG2	2.06	0.55
1:A:343:PRO:O	1:A:372:PHE:CE1	2.60	0.55
1:A:417:TRP:HZ2	1:A:441:ILE:HG12	1.72	0.55
1:A:444:SER:C	1:A:446:GLY:O	2.49	0.55
1:A:342:PRO:HB2	1:A:343:PRO:CD	2.37	0.55
1:A:371:GLY:CA	1:A:404:PHE:O	2.55	0.55
1:A:399:ASP:HB2	1:A:405:PHE:HE2	1.72	0.55
1:A:361:LYS:H	1:A:414:THR:HG21	0.73	0.55
1:A:374:PRO:CD	1:A:431:ALA:CB	2.85	0.54
1:A:366:THR:HG1	1:A:409:ARG:HG3	1.73	0.54
1:A:417:TRP:HH2	1:A:441:ILE:HG23	1.72	0.54
1:A:377:ILE:HD11	1:A:406:LEU:HD12	1.90	0.54
1:A:431:ALA:O	1:A:432:LEU:HB2	2.07	0.54
1:A:438:GLN:HG2	1:A:439:LYS:N	2.22	0.54
1:A:381:TRP:CE2	1:A:410:LEU:CD2	2.90	0.54
1:A:361:LYS:N	1:A:414:THR:CB	2.71	0.53
1:A:365:LEU:C	1:A:409:ARG:HG2	2.33	0.53
1:A:396:PRO:HB3	1:A:398:PHE:HE2	1.73	0.53
1:A:404:PHE:HE1	1:A:406:LEU:HB2	1.72	0.53
1:A:351:LEU:O	1:A:365:LEU:CD2	2.57	0.53
1:A:354:PRO:HB2	1:A:356:ASN:ND2	2.24	0.53
1:A:397:VAL:O	1:A:405:PHE:CB	2.57	0.53
1:A:417:TRP:CE3	1:A:418:ASN:N	2.77	0.53
1:A:417:TRP:CH2	1:A:441:ILE:CG2	2.91	0.53
1:A:431:ALA:O	1:A:432:LEU:CB	2.57	0.53
1:A:365:LEU:O	1:A:409:ARG:HG2	2.09	0.52
1:A:377:ILE:HB	1:A:429:HIS:HA	1.90	0.52
1:A:381:TRP:NE1	1:A:410:LEU:CG	2.69	0.52
1:A:341:GLY:O	1:A:344:ARG:CZ	2.57	0.52
1:A:381:TRP:CE2	1:A:410:LEU:HD23	2.45	0.52
1:A:421:GLU:C	1:A:423:PHE:CD2	2.87	0.52
1:A:349:TYR:HB2	1:A:368:MET:CG	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:PHE:CE1	1:A:406:LEU:N	2.78	0.52
1:A:344:ARG:HA	1:A:372:PHE:HE1	1.75	0.52
1:A:368:MET:C	1:A:369:ILE:HG13	2.35	0.52
1:A:354:PRO:O	1:A:356:ASN:N	2.42	0.52
1:A:361:LYS:O	1:A:361:LYS:HD3	2.09	0.52
1:A:361:LYS:HA	1:A:414:THR:OG1	2.10	0.52
1:A:395:PRO:O	1:A:396:PRO:C	2.53	0.52
1:A:344:ARG:CZ	1:A:344:ARG:O	2.58	0.51
1:A:351:LEU:HD12	1:A:365:LEU:HG	1.91	0.51
1:A:396:PRO:HA	1:A:405:PHE:O	2.09	0.51
1:A:428:MET:HB2	1:A:435:HIS:CD2	2.45	0.51
1:A:377:ILE:CB	1:A:429:HIS:CD2	2.95	0.50
1:A:370:THR:C	1:A:404:PHE:O	2.54	0.50
1:A:404:PHE:CD1	1:A:405:PHE:CA	2.92	0.50
1:A:370:THR:CG2	1:A:405:PHE:CA	2.89	0.50
1:A:404:PHE:CD1	1:A:405:PHE:C	2.90	0.50
1:A:373:TYR:CB	1:A:374:PRO:CA	2.59	0.50
1:A:342:PRO:HB3	1:A:373:TYR:HB2	1.93	0.49
1:A:353:PRO:HD3	1:A:365:LEU:HD23	1.95	0.49
1:A:341:GLY:O	1:A:403:SER:OG	2.31	0.49
1:A:373:TYR:HA	1:A:374:PRO:O	2.12	0.49
1:A:394:THR:O	1:A:406:LEU:CD2	2.60	0.49
1:A:413:ASP:O	1:A:414:THR:CB	2.60	0.49
1:A:427:VAL:CG1	1:A:436:VAL:CG2	2.82	0.49
1:A:381:TRP:CD1	1:A:391:TYR:CD1	3.01	0.49
1:A:342:PRO:C	1:A:344:ARG:HH12	2.21	0.48
1:A:417:TRP:O	1:A:418:ASN:C	2.56	0.48
1:A:399:ASP:O	1:A:402:GLY:HA3	2.14	0.48
1:A:413:ASP:O	1:A:414:THR:CG2	2.61	0.48
1:A:440:SER:C	1:A:441:ILE:HG22	2.38	0.47
1:A:377:ILE:HD13	1:A:404:PHE:CE2	2.49	0.47
1:A:417:TRP:CE3	1:A:418:ASN:CA	2.98	0.47
1:A:394:THR:O	1:A:406:LEU:HD23	2.14	0.47
1:A:421:GLU:CB	1:A:423:PHE:CD2	2.85	0.47
1:A:428:MET:CB	1:A:435:HIS:CD2	2.98	0.47
1:A:377:ILE:HB	1:A:429:HIS:CA	2.44	0.47
1:A:342:PRO:HB3	1:A:373:TYR:CB	2.45	0.47
1:A:370:THR:HG22	1:A:405:PHE:CA	2.45	0.47
1:A:404:PHE:HE1	1:A:406:LEU:CB	2.28	0.46
1:A:351:LEU:O	1:A:365:LEU:HD23	2.14	0.46
1:A:360:LYS:C	1:A:414:THR:CB	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:GLU:HA	1:A:391:TYR:CZ	2.51	0.46
1:A:382:ASP:C	1:A:382:ASP:OD2	2.59	0.46
1:A:412:VAL:O	1:A:413:ASP:HB2	2.16	0.46
1:A:336:ILE:CG2	1:A:337:SER:H	2.24	0.46
1:A:366:THR:OG1	1:A:408:SER:O	2.29	0.46
1:A:404:PHE:HE1	1:A:406:LEU:CA	2.29	0.46
1:A:417:TRP:CE3	1:A:418:ASN:HA	2.51	0.46
1:A:444:SER:O	1:A:446:GLY:O	2.34	0.45
1:A:440:SER:O	1:A:441:ILE:HB	2.17	0.45
1:A:366:THR:HG1	1:A:408:SER:C	2.24	0.45
1:A:342:PRO:HB2	1:A:343:PRO:HD3	1.99	0.45
1:A:342:PRO:HB3	1:A:374:PRO:CA	2.47	0.45
1:A:369:ILE:HD13	1:A:427:VAL:HG23	1.97	0.45
1:A:342:PRO:HA	1:A:373:TYR:N	2.32	0.45
1:A:381:TRP:CD1	1:A:391:TYR:HD1	2.35	0.45
1:A:404:PHE:CE1	1:A:405:PHE:C	2.95	0.45
1:A:338:LYS:HB3	1:A:339:ALA:H	1.31	0.45
1:A:381:TRP:HB3	1:A:391:TYR:CE1	2.52	0.44
1:A:401:ASP:O	1:A:403:SER:N	2.49	0.44
1:A:353:PRO:CB	1:A:444:SER:HA	2.40	0.44
1:A:391:TYR:CD2	1:A:391:TYR:O	2.70	0.44
1:A:364:SER:CB	1:A:411:LYS:HB2	2.43	0.44
1:A:370:THR:HG21	1:A:407:TYR:CE2	2.48	0.44
1:A:432:LEU:HD22	1:A:433:PRO:HD2	1.98	0.44
1:A:396:PRO:HB3	1:A:398:PHE:CE2	2.52	0.43
1:A:377:ILE:C	1:A:378:ASN:HD22	2.25	0.43
1:A:407:TYR:CD2	1:A:407:TYR:N	2.85	0.43
1:A:413:ASP:O	1:A:414:THR:OG1	2.29	0.43
1:A:377:ILE:HB	1:A:429:HIS:CG	2.53	0.43
1:A:341:GLY:C	1:A:344:ARG:CZ	2.92	0.43
1:A:423:PHE:HD1	1:A:441:ILE:HG21	1.84	0.43
1:A:399:ASP:O	1:A:400:THR:C	2.61	0.42
1:A:417:TRP:CZ2	1:A:441:ILE:HD13	2.53	0.42
1:A:338:LYS:HB3	1:A:342:PRO:HD3	2.02	0.42
1:A:344:ARG:CA	1:A:372:PHE:HE1	2.33	0.42
1:A:368:MET:HB2	1:A:368:MET:HE3	1.66	0.42
1:A:340:LYS:H	1:A:340:LYS:HG2	1.64	0.42
1:A:342:PRO:HB3	1:A:374:PRO:CB	2.50	0.42
1:A:340:LYS:HG3	1:A:373:TYR:CE1	2.55	0.41
1:A:360:LYS:C	1:A:414:THR:HG21	2.29	0.41
1:A:417:TRP:CZ3	1:A:423:PHE:CE1	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:ASN:OD1	1:A:419:ASN:C	2.63	0.41
1:A:342:PRO:HD2	1:A:343:PRO:HD2	1.98	0.41
1:A:346:PRO:O	1:A:347:GLU:CG	2.38	0.41
1:A:417:TRP:CZ2	1:A:441:ILE:HG23	2.55	0.41
1:A:423:PHE:CD1	1:A:441:ILE:HG21	2.55	0.41
1:A:334:ARG:C	1:A:335:THR:HG22	2.46	0.41
1:A:360:LYS:HA	1:A:414:THR:CG2	2.51	0.41
1:A:404:PHE:HD1	1:A:405:PHE:C	2.26	0.41
1:A:342:PRO:N	1:A:343:PRO:HD2	2.30	0.40
1:A:405:PHE:N	1:A:405:PHE:CD1	2.89	0.40
1:A:407:TYR:HD2	1:A:407:TYR:N	2.16	0.40
1:A:420:GLY:O	1:A:421:GLU:HG2	2.21	0.40

All (5) 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:350:LEU:CD1	1:A:356:ASN:OD1[2_655]	1.23	0.97
1:A:350:LEU:CD1	1:A:356:ASN:CG[2_655]	1.62	0.58
1:A:344:ARG:CB	1:A:435:HIS:NE2[3_645]	1.82	0.38
1:A:407:TYR:OH	1:A:409:ARG:CZ[2_655]	1.90	0.30
1:A:407:TYR:OH	1:A:409:ARG:NH2[2_655]	2.13	0.07

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	109/113 (96%)	66 (61%)	13 (12%)	30 (28%)	0 0

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	353	PRO
1	A	355	ARG
1	A	361	LYS
1	A	374	PRO
1	A	382	ASP
1	A	383	SER
1	A	387	PRO
1	A	400	THR
1	A	402	GLY
1	A	403	SER
1	A	414	THR
1	A	418	ASN
1	A	432	LEU
1	A	440	SER
1	A	443	ARG
1	A	444	SER
1	A	336	ILE
1	A	389	SER
1	A	413	ASP
1	A	431	ALA
1	A	338	LYS
1	A	345	ILE
1	A	357	GLU
1	A	422	SER
1	A	445	PRO
1	A	337	SER
1	A	342	PRO
1	A	354	PRO
1	A	441	ILE
1	A	396	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	102/104 (98%)	59 (58%)	43 (42%)	0 0

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	340	LYS
1	A	344	ARG
1	A	347	GLU
1	A	348	VAL
1	A	350	LEU
1	A	351	LEU
1	A	356	ASN
1	A	359	SER
1	A	360	LYS
1	A	361	LYS
1	A	365	LEU
1	A	366	THR
1	A	368	MET
1	A	372	PHE
1	A	377	ILE
1	A	378	ASN
1	A	379	VAL
1	A	381	TRP
1	A	383	SER
1	A	385	GLU
1	A	387	PRO
1	A	391	TYR
1	A	393	ASN
1	A	399	ASP
1	A	404	PHE
1	A	406	LEU
1	A	407	TYR
1	A	412	VAL
1	A	413	ASP
1	A	417	TRP
1	A	423	PHE
1	A	424	THR
1	A	427	VAL
1	A	428	MET
1	A	430	GLU
1	A	434	ASN
1	A	435	HIS
1	A	437	ILE
1	A	438	GLN
1	A	439	LYS
1	A	440	SER
1	A	442	SER

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Mol	Chain	Res	Type
1	A	444	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	356	ASN
1	A	378	ASN
1	A	419	ASN
1	A	429	HIS
1	A	434	ASN
1	A	435	HIS
1	A	438	GLN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	370:THR	C	371:GLY	N	1.19
1	A	392:LYS	C	393:ASN	N	1.16
1	A	398:PHE	C	399:ASP	N	1.10
1	A	402:GLY	C	403:SER	N	1.10

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	111/113 (98%)	0.90	11 (9%) 13 7	23, 37, 44, 54	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	341	GLY	4.5
1	A	422	SER	4.4
1	A	363	VAL	3.4
1	A	423	PHE	2.9
1	A	421	GLU	2.8
1	A	397	VAL	2.7
1	A	420	GLY	2.7
1	A	416	ALA	2.2
1	A	407	TYR	2.2
1	A	339	ALA	2.1
1	A	408	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.