



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:37 AM UTC

PDB ID : 5D0Q / pdb_00005d0q
Title : BamACDE complex, outer membrane beta-barrel assembly machinery (BAM) complex
Authors : Gu, Y.; Paterson, N.; Zeng, Y.; Dong, H.; Wang, W.; Dong, C.
Deposited on : 2015-08-03
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

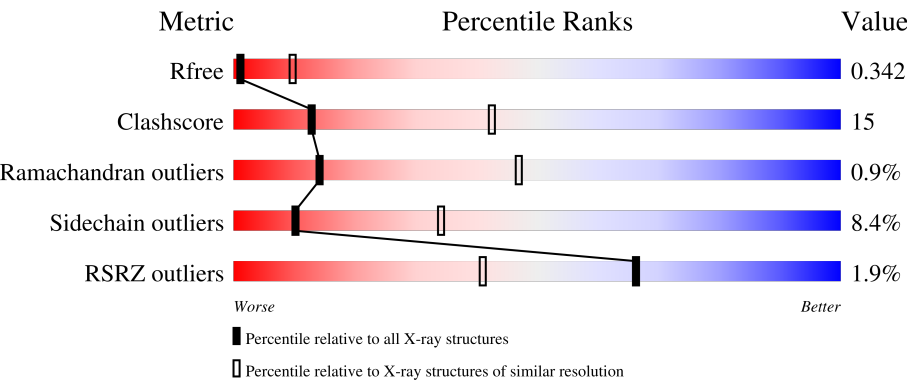
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	810	% 63%27%6%
1	F	810	2% 63%27%6%
2	C	344	% 60%28%8%
2	G	344	16%8%75%
3	D	245	% 63%24%11%

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Mol	Chain	Length	Quality of chain
3	H	245	4% 62% 24% • 11%
4	E	123	2% 37% 25% 7% • 29%
4	I	123	4% 33% 28% 11% 29%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19905 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 Outer membrane protein assembly factor BamA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	762	Total	C	N	O	S	Se	0	0	0
			6006	3786	1009	1195	2	14			
1	F	761	Total	C	N	O	S	Se	0	1	0
			5998	3781	1008	1193	2	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP P0A940
F	1	MSE	-	initiating methionine	UNP P0A940

- Molecule 2 is a protein called Outer membrane protein assembly factor BamC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	316	Total	C	N	O	S	Se	0	0	0
			2386	1478	421	479	1	7			
2	G	86	Total	C	N	O	Se		0	0	0
			623	386	107	126	4				

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MSE	-	initiating methionine	UNP P0A903
G	1	MSE	-	initiating methionine	UNP P0A903

- Molecule 3 is a protein called Outer membrane protein assembly factor BamD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	218	Total	C	N	O	Se	0	0	0
			1761	1109	309	336	7			
3	H	218	Total	C	N	O	Se	0	0	0
			1761	1109	309	336	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MSE	-	initiating methionine	UNP P0AC02
H	1	MSE	-	initiating methionine	UNP P0AC02

- Molecule 4 is a protein called Outer membrane protein assembly factor BamE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	87	Total	C	N	O	Se	0	0	0
			685	432	119	132	2			
4	I	87	Total	C	N	O	Se	0	0	0
			685	432	119	132	2			

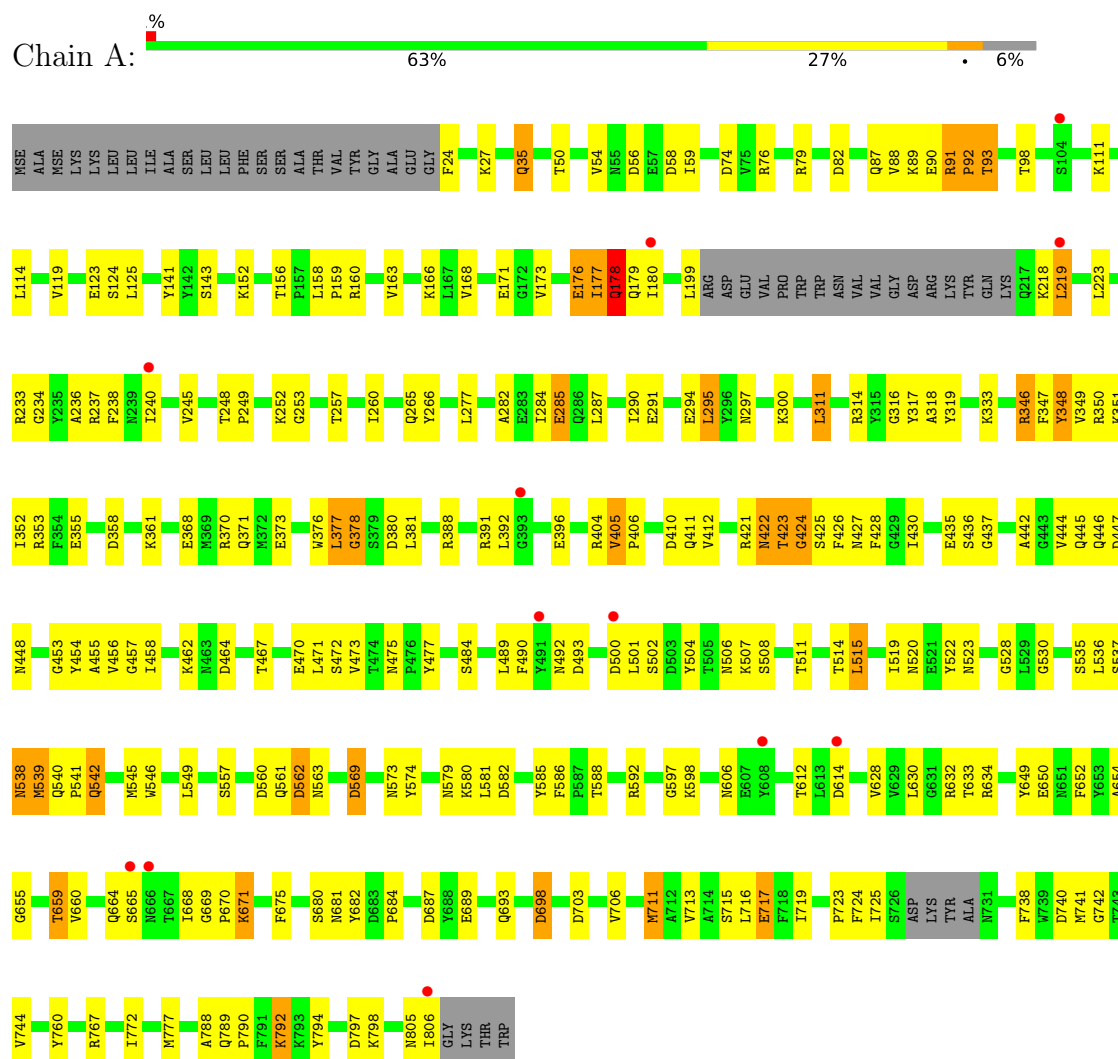
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	MSE	-	initiating methionine	UNP P0A937
E	114	GLY	-	expression tag	UNP P0A937
E	115	GLY	-	expression tag	UNP P0A937
E	116	HIS	-	expression tag	UNP P0A937
E	117	HIS	-	expression tag	UNP P0A937
E	118	HIS	-	expression tag	UNP P0A937
E	119	HIS	-	expression tag	UNP P0A937
E	120	HIS	-	expression tag	UNP P0A937
E	121	HIS	-	expression tag	UNP P0A937
E	122	HIS	-	expression tag	UNP P0A937
E	123	HIS	-	expression tag	UNP P0A937
I	1	MSE	-	initiating methionine	UNP P0A937
I	114	GLY	-	expression tag	UNP P0A937
I	115	GLY	-	expression tag	UNP P0A937
I	116	HIS	-	expression tag	UNP P0A937
I	117	HIS	-	expression tag	UNP P0A937
I	118	HIS	-	expression tag	UNP P0A937
I	119	HIS	-	expression tag	UNP P0A937
I	120	HIS	-	expression tag	UNP P0A937
I	121	HIS	-	expression tag	UNP P0A937
I	122	HIS	-	expression tag	UNP P0A937
I	123	HIS	-	expression tag	UNP P0A937

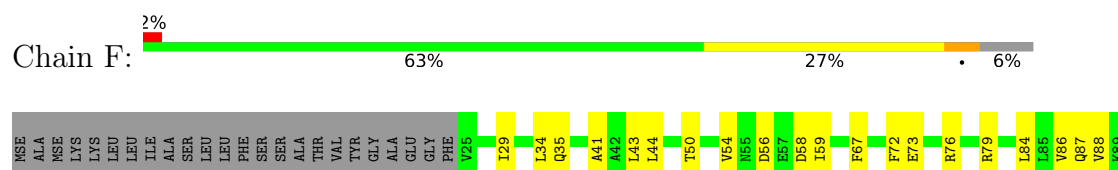
3 Residue-property plots

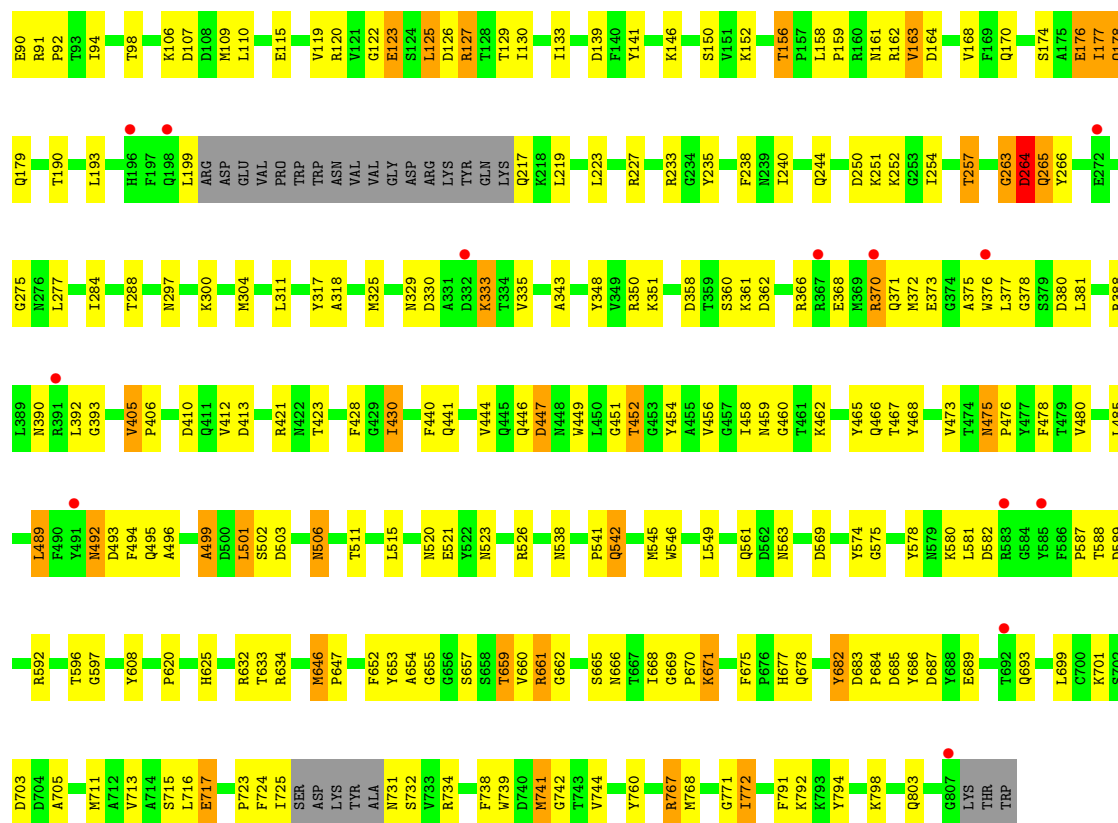
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Outer membrane protein assembly factor BamA

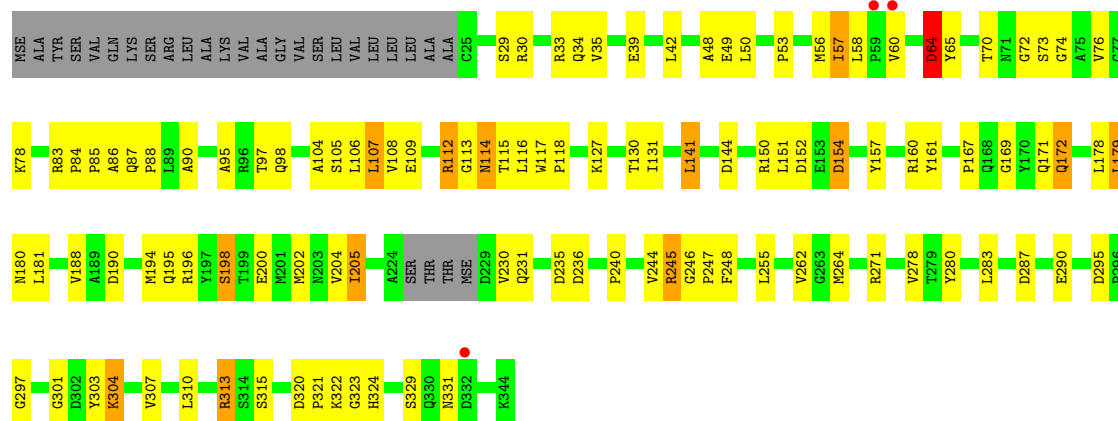


- Molecule 1: Outer membrane protein assembly factor BamA





• Molecule 2: Outer membrane protein assembly factor BamC

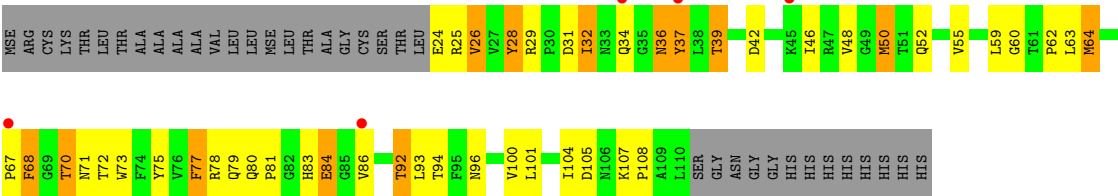
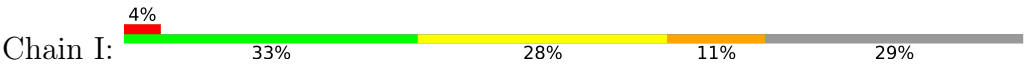


• Molecule 2: Outer membrane protein assembly factor BamC





● Molecule 4: Outer membrane protein assembly factor BamE



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	254.16Å 254.16Å 179.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 3.50 29.94 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.94-3.50) 99.8 (29.94-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.47Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.314 , 0.340 0.321 , 0.342	Depositor DCC
R_{free} test set	3727 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	128.8	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	19905	wwPDB-VP
Average B, all atoms (Å ²)	152.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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

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	0.42	0/6126	0.95	20/8285 (0.2%)
1	F	0.43	0/6120	0.94	12/8277 (0.1%)
2	C	0.38	0/2420	0.87	1/3281 (0.0%)
2	G	0.38	0/629	0.92	1/846 (0.1%)
3	D	0.41	0/1794	0.96	2/2426 (0.1%)
3	H	0.42	0/1794	0.96	4/2426 (0.2%)
4	E	0.45	0/698	1.11	4/949 (0.4%)
4	I	0.53	0/698	1.08	1/949 (0.1%)
All	All	0.42	0/20279	0.95	45/27439 (0.2%)

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	435	GLU	N-CA-C	-9.27	101.87	113.55
1	F	263	GLY	N-CA-C	-8.78	100.08	112.37
3	H	30	ASN	CA-C-N	-8.66	113.43	119.66
3	H	30	ASN	C-N-CA	-8.66	113.43	119.66
1	A	411	GLN	N-CA-C	7.51	121.60	110.48
1	A	561	GLN	N-CA-C	-7.27	100.05	110.59
1	A	346	ARG	N-CA-C	7.22	122.53	113.43
1	F	771	GLY	N-CA-C	6.89	119.88	110.58
1	A	377	LEU	N-CA-C	-6.72	99.88	109.96
1	A	475	ASN	CA-C-N	6.55	126.17	119.56
1	A	475	ASN	C-N-CA	6.55	126.17	119.56
1	F	475	ASN	CA-C-N	6.43	126.06	119.56
1	F	475	ASN	C-N-CA	6.43	126.06	119.56
1	A	378	GLY	N-CA-C	-6.38	98.05	113.18
1	A	424	GLY	N-CA-C	6.32	123.30	111.80
4	E	77	PHE	N-CA-C	-6.29	98.48	108.73
3	D	30	ASN	CA-C-N	-6.25	115.16	119.66
3	D	30	ASN	C-N-CA	-6.25	115.16	119.66
2	C	301	GLY	N-CA-C	6.09	118.37	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	68	PHE	N-CA-C	5.93	121.95	114.31
1	A	349	VAL	N-CA-C	5.87	116.84	107.98
4	I	39	THR	N-CA-C	-5.78	99.81	109.24
1	F	176	GLU	N-CA-C	5.73	118.88	109.76
1	A	219	LEU	N-CA-C	5.56	117.78	111.11
4	E	66	ASP	CA-C-N	-5.54	113.32	119.19
4	E	66	ASP	C-N-CA	-5.54	113.32	119.19
1	A	348	TYR	N-CA-C	5.54	122.59	110.80
1	F	264	ASP	N-CA-C	5.48	117.11	111.03
1	A	245	VAL	N-CA-C	5.47	115.42	106.72
1	F	499	ALA	N-CA-C	-5.39	106.48	113.16
1	A	91	ARG	CA-C-N	5.27	126.42	119.84
1	A	91	ARG	C-N-CA	5.27	126.42	119.84
1	F	661	ARG	NE-CZ-NH1	-5.26	116.24	121.50
3	H	154	TYR	CA-C-N	5.21	124.72	119.19
3	H	154	TYR	C-N-CA	5.21	124.72	119.19
1	F	430	ILE	N-CA-C	5.18	117.00	108.97
1	A	396	GLU	N-CA-C	-5.16	105.34	111.69
2	G	199	THR	N-CA-C	-5.13	107.19	113.50
1	A	405	VAL	CA-C-N	5.09	125.01	119.76
1	A	405	VAL	C-N-CA	5.09	125.01	119.76
1	F	139	ASP	N-CA-C	5.07	119.18	112.89
1	F	405	VAL	CA-C-N	5.05	124.97	119.76
1	F	405	VAL	C-N-CA	5.05	124.97	119.76
1	A	319	TYR	CA-C-N	5.00	126.11	120.66
1	A	319	TYR	C-N-CA	5.00	126.11	120.66

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6006	0	5728	171	0
1	F	5998	0	5728	172	0
2	C	2386	0	2336	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	623	0	612	20	0
3	D	1761	0	1699	51	0
3	H	1761	0	1699	58	0
4	E	685	0	666	47	0
4	I	685	0	666	49	0
All	All	19905	0	19134	589	0

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

All (589) 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:240:ILE:HA	1:A:260:ILE:HG22	1.53	0.90
1:A:632:ARG:HB2	1:A:715:SER:HB3	1.58	0.86
1:F:91:ARG:HD3	1:F:127:ARG:H	1.41	0.85
2:C:116:LEU:HB3	2:C:172:GLN:HE22	1.42	0.84
1:F:561:GLN:HB3	1:F:677:HIS:HE1	1.44	0.82
1:F:652:PHE:HB3	1:F:711:MSE:HE3	1.62	0.81
2:C:88:PRO:HB2	2:C:97:THR:HB	1.61	0.81
4:E:46:ILE:HG21	4:E:59:LEU:HD11	1.63	0.80
1:A:376:TRP:HD1	4:E:33:ASN:HD21	1.30	0.80
2:G:59:PRO:HB2	3:H:203:ARG:HG3	1.64	0.80
3:H:132:ARG:HG2	3:H:135:ARG:HD3	1.64	0.79
1:F:678:GLN:HA	1:F:693:GLN:HG2	1.63	0.79
1:F:659:THR:OG1	1:F:660:VAL:N	2.14	0.79
1:A:652:PHE:HB3	1:A:711:MSE:HE3	1.62	0.78
1:F:632:ARG:HB2	1:F:715:SER:HB3	1.64	0.78
1:A:467:THR:OG1	1:A:493:ASP:O	2.01	0.78
4:E:60:GLY:O	4:E:75:TYR:OH	2.00	0.78
1:F:739:TRP:HE1	1:F:791:PHE:HZ	1.32	0.77
1:A:348:TYR:HB3	1:A:412:VAL:HG22	1.64	0.77
1:F:446:GLN:HG2	1:F:449:TRP:HD1	1.49	0.77
1:F:94:ILE:HD11	1:F:125:LEU:HD23	1.66	0.76
1:F:370:ARG:NH2	4:I:31:ASP:OD2	2.17	0.76
1:A:361:LYS:HG2	3:D:135:ARG:NH2	2.01	0.76
1:A:668:ILE:HG23	1:A:767:ARG:HD3	1.68	0.75
1:F:277:LEU:HD23	1:F:284:ILE:HD12	1.68	0.74
1:F:264:ASP:OD1	1:F:264:ASP:N	2.21	0.74
1:F:377:LEU:HD12	1:F:412:VAL:HG21	1.68	0.73
4:E:24:GLU:OE2	4:E:24:GLU:N	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:86:ALA:O	2:C:195:GLN:NE2	2.23	0.72
1:F:423:THR:OG1	1:F:446:GLN:O	2.08	0.72
2:C:53:PRO:HD2	2:C:58:LEU:HD11	1.70	0.72
1:A:456:VAL:HG12	1:A:473:VAL:HA	1.70	0.72
4:I:24:GLU:N	4:I:24:GLU:OE2	2.23	0.71
1:A:277:LEU:HD23	1:A:284:ILE:HD13	1.72	0.71
2:C:150:ARG:NH1	2:C:200:GLU:OE2	2.23	0.71
3:H:125:GLN:O	3:H:129:GLY:N	2.24	0.71
1:A:376:TRP:HD1	4:E:33:ASN:ND2	1.89	0.70
1:F:92:PRO:HB2	1:F:163:VAL:HB	1.72	0.70
1:A:371:GLN:OE1	1:A:378:GLY:N	2.22	0.70
2:C:39:GLU:HB3	2:C:42:LEU:HD12	1.71	0.70
3:D:132:ARG:HG2	3:D:135:ARG:HD3	1.72	0.70
2:C:90:ALA:HB2	2:C:97:THR:HG23	1.73	0.70
4:I:77:PHE:HE2	4:I:79:GLN:HB2	1.57	0.70
1:A:173:VAL:HG12	1:A:252:LYS:HD2	1.72	0.70
1:A:428:PHE:HE1	1:A:430:ILE:HB	1.57	0.70
1:F:122:GLY:HA2	3:H:64:PHE:HE2	1.58	0.69
1:F:480:VAL:HG11	3:H:187:GLU:HB3	1.75	0.69
1:F:682:TYR:HD2	1:F:683:ASP:N	1.90	0.69
1:A:504:TYR:H	1:A:538:ASN:HB2	1.57	0.68
2:C:303:TYR:CZ	2:C:321:PRO:HD3	2.28	0.68
1:F:119:VAL:HG11	1:F:133:ILE:HG12	1.75	0.68
4:I:55:VAL:HG13	4:I:59:LEU:HD22	1.76	0.68
2:C:48:ALA:O	3:D:212:ARG:NH1	2.26	0.68
1:A:266:TYR:O	1:A:295:LEU:HD23	1.93	0.68
1:A:316:GLY:HA2	1:A:377:LEU:O	1.94	0.68
1:F:468:TYR:HD1	1:F:492:ASN:HB2	1.58	0.68
2:G:57:ILE:O	4:I:68:PHE:HB3	1.93	0.68
4:I:64:MSE:HE1	3:H:225:MSE:SE	2.44	0.67
4:I:26:VAL:HG11	4:I:83:HIS:NE2	2.10	0.67
1:F:462:LYS:HD2	1:F:467:THR:HG22	1.77	0.67
3:H:132:ARG:O	3:H:133:SER:OG	2.11	0.67
1:A:506:ASN:HA	1:A:536:LEU:HD23	1.77	0.67
1:A:297:ASN:HB3	1:A:300:LYS:HB2	1.78	0.66
2:G:34:GLN:HB3	2:G:78:LYS:HD2	1.75	0.66
3:D:120:ASP:OD2	3:D:173:ARG:NH1	2.28	0.66
1:A:423:THR:HB	1:A:446:GLN:O	1.96	0.66
1:F:682:TYR:HD2	1:F:683:ASP:H	1.44	0.66
1:A:462:LYS:HD2	1:A:467:THR:HG22	1.78	0.65
2:C:64:ASP:OD1	2:C:64:ASP:N	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:LYS:HG2	3:D:135:ARG:HH21	1.62	0.65
1:F:465:TYR:HB2	1:F:496:ALA:O	1.95	0.65
3:H:36:TYR:OH	3:H:70:GLN:NE2	2.29	0.64
1:A:492:ASN:OD1	1:A:508:SER:OG	2.14	0.64
1:F:449:TRP:O	1:F:452:THR:OG1	2.12	0.64
4:I:96:ASN:N	4:I:100:VAL:O	2.23	0.64
4:E:62:PRO:HG3	4:E:73:TRP:CD1	2.33	0.64
1:F:190:THR:HA	1:F:193:LEU:HD12	1.79	0.63
2:C:160:ARG:NH2	2:C:180:ASN:OD1	2.32	0.63
3:H:111:MSE:O	3:H:115:THR:OG1	2.17	0.63
1:F:235:TYR:HD1	1:F:263:GLY:O	1.81	0.63
1:F:677:HIS:O	1:F:693:GLN:NE2	2.30	0.63
1:F:125:LEU:HD11	1:F:130:ILE:HD11	1.80	0.63
3:D:125:GLN:O	3:D:129:GLY:N	2.29	0.63
3:D:135:ARG:H	3:D:135:ARG:HD2	1.63	0.63
1:A:234:GLY:HA3	1:A:295:LEU:HD22	1.81	0.63
1:A:792:LYS:NZ	1:A:794:TYR:OH	2.25	0.63
4:E:37:TYR:HA	4:E:77:PHE:CD1	2.34	0.63
4:E:96:ASN:N	4:E:100:VAL:O	2.25	0.63
2:C:30:ARG:HG2	2:C:34:GLN:NE2	2.14	0.62
1:F:360:SER:HA	1:F:451:GLY:HA3	1.81	0.62
3:H:84:ASP:HB3	3:H:87:LEU:HD13	1.80	0.62
3:D:111:MSE:O	3:D:115:THR:OG1	2.16	0.62
1:A:689:GLU:N	1:A:689:GLU:OE1	2.32	0.62
1:A:698:ASP:OD1	1:A:698:ASP:N	2.32	0.62
1:A:347:PHE:HB2	1:A:376:TRP:CZ3	2.35	0.62
1:F:371:GLN:NE2	1:F:376:TRP:O	2.30	0.62
3:H:162:ASP:OD1	3:H:166:ARG:NE	2.29	0.62
4:E:55:VAL:HG13	4:E:59:LEU:HD22	1.81	0.62
2:G:49:GLU:HA	3:H:207:ASP:HB3	1.81	0.62
1:A:410:ASP:OD1	4:E:61:THR:N	2.25	0.62
1:A:74:ASP:HB3	1:A:89:LYS:HB2	1.82	0.61
1:F:646:MSE:HG2	1:F:647:PRO:HD2	1.82	0.61
1:F:362:ASP:OD2	1:F:366:ARG:NH2	2.32	0.61
3:H:230:GLN:HA	3:H:233:LYS:HG3	1.82	0.61
4:E:32:ILE:HG12	4:E:33:ASN:N	2.13	0.61
4:E:77:PHE:HE2	4:E:79:GLN:HB2	1.63	0.61
3:D:233:LYS:HB3	4:E:68:PHE:HE2	1.66	0.61
1:F:669:GLY:HA3	1:F:744:VAL:HB	1.83	0.61
2:G:29:SER:O	2:G:33:ARG:NH2	2.34	0.61
3:D:230:GLN:HA	3:D:233:LYS:HG3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:110:TYR:OH	3:H:162:ASP:OD1	2.13	0.60
1:A:437:GLY:N	1:A:464:ASP:OD2	2.34	0.60
2:C:57:ILE:O	4:E:68:PHE:HB3	2.01	0.60
1:F:159:PRO:HG2	1:F:162:ARG:HH12	1.67	0.60
2:C:113:GLY:HA2	2:C:172:GLN:CD	2.27	0.60
1:F:654:ALA:HB3	1:F:668:ILE:HB	1.84	0.60
1:A:669:GLY:HA3	1:A:744:VAL:HB	1.85	0.59
4:I:46:ILE:HG21	4:I:59:LEU:HD11	1.84	0.59
1:A:91:ARG:N	1:A:92:PRO:HD3	2.17	0.59
1:A:723:PRO:HA	1:A:724:PHE:HB3	1.85	0.59
1:A:669:GLY:H	1:A:767:ARG:NH1	1.99	0.59
1:F:767:ARG:HG3	1:F:794:TYR:HD1	1.67	0.59
1:F:501:LEU:O	1:F:503:ASP:N	2.35	0.59
2:C:178:LEU:HD21	2:C:181:LEU:HD13	1.85	0.58
2:C:65:TYR:HE2	3:D:174:LEU:HD13	1.69	0.58
1:A:703:ASP:HB3	1:A:798:LYS:HE3	1.86	0.58
2:C:167:PRO:HA	2:C:172:GLN:HA	1.86	0.57
3:D:132:ARG:O	3:D:133:SER:OG	2.12	0.57
3:D:148:SER:HB3	3:D:152:ARG:NH1	2.19	0.57
1:F:456:VAL:HB	1:F:458:ILE:HD13	1.87	0.57
1:F:428:PHE:HE1	1:F:430:ILE:HB	1.69	0.57
3:D:89:GLN:HA	3:D:92:ILE:HD12	1.86	0.57
1:F:56:ASP:HA	1:F:59:ILE:HD12	1.87	0.57
1:A:541:PRO:HB2	1:A:675:PHE:HB2	1.87	0.57
2:C:35:VAL:HG21	3:D:166:ARG:HH22	1.68	0.57
1:F:423:THR:OG1	1:F:447:ASP:HB2	2.05	0.57
3:H:119:LEU:HD12	3:H:139:HIS:CD2	2.40	0.57
1:F:41:ALA:N	3:H:101:THR:HG21	2.19	0.57
1:F:368:GLU:HB3	1:F:388:ARG:HB3	1.87	0.57
1:F:657:SER:HA	1:F:661:ARG:HG2	1.87	0.57
4:I:62:PRO:HG3	4:I:73:TRP:CD1	2.39	0.57
2:C:70:THR:HG23	2:C:72:GLY:H	1.70	0.56
1:A:318:ALA:HB2	1:A:377:LEU:HD13	1.88	0.56
1:A:348:TYR:HA	1:A:410:ASP:O	2.06	0.56
1:F:126:ASP:HB2	1:F:129:THR:OG1	2.04	0.56
1:F:371:GLN:HB2	1:F:381:LEU:HB2	1.86	0.56
1:A:489:LEU:HG	1:A:511:THR:HG22	1.87	0.56
1:F:489:LEU:HG	1:F:511:THR:HG22	1.87	0.56
2:C:264:MSE:HG2	2:C:280:TYR:HB2	1.88	0.56
1:F:264:ASP:HB2	1:F:265:GLN:NE2	2.21	0.56
2:C:131:ILE:HG23	2:C:141:LEU:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:440:PHE:HB3	1:F:462:LYS:O	2.06	0.56
3:D:107:TYR:O	3:D:111:MSE:HG2	2.06	0.55
1:A:664:GLN:OE1	1:A:798:LYS:HD3	2.06	0.55
2:C:90:ALA:HB1	2:C:95:ALA:HB3	1.88	0.55
4:E:96:ASN:HB3	4:E:100:VAL:HB	1.88	0.55
1:F:317:TYR:CD2	1:F:343:ALA:HB1	2.41	0.55
4:I:93:LEU:HD21	4:I:104:ILE:HG23	1.87	0.55
2:C:283:LEU:HB3	2:C:287:ASP:CB	2.36	0.55
4:E:67:PRO:HB2	4:E:68:PHE:CD1	2.40	0.55
2:C:130:THR:HB	2:C:144:ASP:HB3	1.88	0.55
2:C:320:ASP:CG	2:C:321:PRO:HD2	2.32	0.55
1:F:266:TYR:HB3	1:F:335:VAL:HG23	1.88	0.55
1:F:468:TYR:CD1	1:F:492:ASN:HB2	2.39	0.55
1:A:348:TYR:O	1:A:412:VAL:N	2.28	0.55
1:A:767:ARG:NH1	1:A:797:ASP:OD1	2.40	0.55
3:H:81:LYS:HE2	3:H:81:LYS:HA	1.89	0.55
3:D:237:ILE:HD11	4:E:68:PHE:CZ	2.43	0.54
1:F:376:TRP:NE1	4:I:37:TYR:HB2	2.22	0.54
1:A:520:ASN:ND2	1:A:523:ASN:HB2	2.21	0.54
1:F:297:ASN:HB3	1:F:300:LYS:HB2	1.89	0.54
1:A:458:ILE:HG13	1:A:471:LEU:HD12	1.90	0.54
2:C:108:VAL:O	2:C:171:GLN:HB2	2.06	0.54
1:A:446:GLN:C	1:A:448:ASN:H	2.15	0.54
1:A:445:GLN:HG3	1:A:457:GLY:HA2	1.90	0.54
3:D:228:ASN:HA	3:D:231:ALA:HB3	1.89	0.54
1:F:581:LEU:HD11	1:F:592:ARG:HB2	1.89	0.54
1:A:35:GLN:HB2	1:A:90:GLU:OE1	2.09	0.53
1:A:767:ARG:H	1:A:767:ARG:HD2	1.73	0.53
1:F:669:GLY:O	1:F:671:LYS:NZ	2.40	0.53
1:F:446:GLN:HG3	1:F:449:TRP:HA	1.90	0.53
1:F:499:ALA:HB1	1:F:682:TYR:HE1	1.72	0.53
1:F:72:PHE:C	1:F:91:ARG:HG3	2.33	0.53
1:F:361:LYS:HA	3:H:135:ARG:HH21	1.74	0.53
1:A:376:TRP:HZ2	4:E:37:TYR:CB	2.21	0.53
1:A:376:TRP:CD1	4:E:33:ASN:HD21	2.18	0.53
2:C:30:ARG:HG2	2:C:34:GLN:HE21	1.73	0.53
2:C:160:ARG:HG2	2:C:179:LEU:HD12	1.90	0.53
1:A:511:THR:O	1:A:530:GLY:HA2	2.08	0.53
1:A:569:ASP:OD1	1:A:606:ASN:HB2	2.07	0.53
2:C:154:ASP:OD1	2:C:154:ASP:N	2.41	0.53
1:F:152:LYS:HB3	1:F:168:VAL:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:119:LEU:HD12	3:D:139:HIS:CD2	2.44	0.53
1:A:376:TRP:CZ2	4:E:37:TYR:CB	2.92	0.53
1:A:404:ARG:HA	1:A:412:VAL:HG12	1.91	0.53
1:A:502:SER:HA	1:A:538:ASN:CG	2.33	0.53
2:C:157:TYR:HE2	2:C:188:VAL:HG21	1.74	0.53
2:C:303:TYR:CE1	2:C:321:PRO:HD3	2.44	0.53
4:E:52:GLN:HG2	4:E:73:TRP:CH2	2.44	0.53
4:I:70:THR:OG1	4:I:71:ASN:N	2.42	0.53
4:I:81:PRO:HG2	4:I:84:GLU:CB	2.39	0.53
3:H:214:ALA:HA	3:H:217:LEU:HD13	1.91	0.53
1:A:427:ASN:ND2	1:A:806:ILE:O	2.43	0.52
1:A:428:PHE:CE1	1:A:430:ILE:HB	2.42	0.52
1:A:654:ALA:HB3	1:A:668:ILE:HB	1.91	0.52
1:F:115:GLU:HG2	1:F:120:ARG:HD2	1.92	0.52
1:A:91:ARG:HG3	1:A:92:PRO:HD3	1.92	0.52
2:C:53:PRO:HG3	3:D:237:ILE:HG12	1.91	0.52
4:I:52:GLN:HG2	4:I:73:TRP:CH2	2.45	0.52
1:A:248:THR:OG1	1:A:249:PRO:HD2	2.09	0.52
2:C:295:ASP:OD1	2:C:297:GLY:N	2.42	0.52
4:I:64:MSE:SE	3:H:192:VAL:HG13	2.59	0.52
1:F:366:ARG:HD2	3:H:184:TYR:CD2	2.44	0.52
1:F:368:GLU:HA	1:F:388:ARG:HH11	1.75	0.52
1:A:56:ASP:HA	1:A:59:ILE:HD12	1.91	0.52
4:I:77:PHE:C	4:I:77:PHE:CD2	2.87	0.52
1:A:91:ARG:HD2	1:A:124:SER:HB2	1.91	0.52
1:A:317:TYR:CD1	1:A:346:ARG:HB3	2.45	0.52
3:D:125:GLN:HE21	3:D:132:ARG:NH2	2.07	0.52
1:F:541:PRO:HB2	1:F:675:PHE:HB2	1.92	0.52
3:H:132:ARG:NH1	3:H:135:ARG:HG2	2.25	0.52
1:F:655:GLY:H	1:F:659:THR:HG1	1.55	0.51
1:A:424:GLY:HA3	1:A:446:GLN:HA	1.93	0.51
1:F:91:ARG:HH11	1:F:126:ASP:HA	1.76	0.51
1:F:362:ASP:H	3:H:134:ASP:HB3	1.75	0.51
1:A:659:THR:OG1	1:A:660:VAL:N	2.42	0.51
1:A:767:ARG:HG3	1:A:794:TYR:HD1	1.75	0.51
4:I:72:THR:C	4:I:73:TRP:HE3	2.18	0.51
1:A:24:PHE:HE1	1:A:82:ASP:HA	1.76	0.51
1:A:520:ASN:HD21	1:A:523:ASN:HB2	1.76	0.51
1:F:725:ILE:HG22	1:F:731:ASN:HD21	1.75	0.51
2:G:64:ASP:OD1	2:G:64:ASP:N	2.43	0.51
3:H:194:VAL:O	3:H:198:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:PHE:CE1	1:A:82:ASP:HA	2.45	0.51
1:A:579:ASN:HD22	1:A:592:ARG:HG3	1.75	0.51
1:F:94:ILE:HG13	1:F:125:LEU:HB2	1.93	0.51
1:F:107:ASP:HA	1:F:110:LEU:HD12	1.92	0.51
3:H:106:ASP:HB2	3:H:157:SER:OG	2.11	0.51
1:A:176:GLU:N	1:A:177:ILE:HA	2.26	0.51
4:I:26:VAL:HG11	4:I:83:HIS:CE1	2.46	0.51
1:A:428:PHE:HB3	1:A:442:ALA:HA	1.93	0.50
2:C:53:PRO:HG2	2:C:56:MSE:HB2	1.93	0.50
3:D:70:GLN:HA	3:D:73:LEU:HD12	1.93	0.50
1:F:670:PRO:HA	1:F:760:TYR:CD1	2.46	0.50
1:F:106:LYS:HB2	1:F:109:MSE:HG3	1.93	0.50
1:F:561:GLN:HB3	1:F:677:HIS:CE1	2.34	0.50
1:F:368:GLU:HG3	1:F:392:LEU:HD11	1.92	0.50
1:F:454:TYR:HB3	1:F:475:ASN:HA	1.92	0.50
1:A:655:GLY:O	1:A:665:SER:HA	2.11	0.50
1:A:358:ASP:O	3:D:132:ARG:NH1	2.44	0.50
1:F:520:ASN:ND2	1:F:523:ASN:HB2	2.27	0.50
1:F:538:ASN:HA	1:F:561:GLN:O	2.12	0.50
1:F:682:TYR:CD2	1:F:683:ASP:N	2.72	0.50
1:A:376:TRP:HZ2	4:E:37:TYR:HB2	1.77	0.50
2:C:287:ASP:HA	2:C:290:GLU:OE2	2.11	0.50
1:A:376:TRP:CZ2	4:E:37:TYR:HB2	2.47	0.50
1:A:579:ASN:HD21	1:A:581:LEU:HD12	1.76	0.50
2:C:113:GLY:HA2	2:C:172:GLN:NE2	2.27	0.50
4:E:79:GLN:HA	4:E:79:GLN:HE21	1.76	0.50
1:F:717:GLU:HA	1:F:738:PHE:HA	1.94	0.50
2:C:112:ARG:HE	2:C:115:THR:HG21	1.76	0.49
1:F:29:ILE:HD12	1:F:84:LEU:O	2.12	0.49
1:F:661:ARG:NH1	1:F:738:PHE:CE2	2.77	0.49
1:A:573:ASN:ND2	1:A:598:LYS:HE2	2.27	0.49
2:C:161:TYR:CE2	2:C:178:LEU:HD13	2.47	0.49
1:F:91:ARG:HG2	1:F:127:ARG:HB2	1.93	0.49
4:E:71:ASN:CB	4:E:95:PHE:HB2	2.42	0.49
4:I:81:PRO:HG2	4:I:84:GLU:HB3	1.94	0.49
2:C:231:GLN:OE1	2:C:245:ARG:NH2	2.45	0.49
1:A:717:GLU:HA	1:A:738:PHE:HA	1.95	0.49
3:D:84:ASP:HB3	3:D:87:LEU:HD13	1.94	0.49
1:F:158:LEU:HB3	1:F:159:PRO:HD2	1.93	0.49
1:F:454:TYR:HB3	1:F:475:ASN:HB3	1.94	0.49
1:F:456:VAL:HG12	1:F:473:VAL:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:70:GLN:HA	3:H:73:LEU:HD12	1.93	0.49
3:H:135:ARG:H	3:H:135:ARG:CD	2.26	0.49
1:A:114:LEU:HB3	1:A:119:VAL:O	2.13	0.49
1:F:587:PRO:HD2	1:F:734:ARG:HH22	1.78	0.49
1:F:589:ASP:HB2	1:F:620:PRO:HG3	1.94	0.49
1:A:314:ARG:HG3	1:A:380:ASP:CG	2.38	0.49
4:E:59:LEU:HB3	4:E:75:TYR:CZ	2.48	0.49
4:E:67:PRO:HB2	4:E:68:PHE:HD1	1.78	0.49
1:F:288:THR:HA	1:F:304:MSE:SE	2.62	0.49
2:G:74:GLY:H	3:H:161:THR:CB	2.26	0.49
4:I:77:PHE:C	4:I:77:PHE:HD2	2.20	0.49
1:A:158:LEU:HB3	1:A:159:PRO:HD2	1.95	0.49
1:A:371:GLN:NE2	1:A:376:TRP:O	2.46	0.49
1:A:348:TYR:HB3	1:A:412:VAL:CG2	2.38	0.48
2:C:196:ARG:O	2:C:200:GLU:HG2	2.12	0.48
1:F:329:ASN:O	1:F:333:LYS:HA	2.13	0.48
3:H:119:LEU:HD12	3:H:139:HIS:CG	2.48	0.48
3:D:79:TYR:HB3	3:D:88:ALA:HB2	1.94	0.48
1:F:767:ARG:HG3	1:F:794:TYR:CD1	2.47	0.48
2:C:58:LEU:O	2:C:60:VAL:N	2.47	0.48
1:F:122:GLY:HA2	3:H:64:PHE:CE2	2.42	0.48
1:F:661:ARG:NH1	1:F:738:PHE:CZ	2.81	0.48
4:I:101:LEU:HD21	4:I:104:ILE:HG12	1.94	0.48
1:A:370:ARG:C	1:A:381:LEU:HB3	2.39	0.48
1:A:581:LEU:HD11	1:A:592:ARG:HB2	1.94	0.48
1:A:660:VAL:HG23	1:A:740:ASP:HB3	1.96	0.48
3:D:81:LYS:HE2	3:D:81:LYS:HA	1.94	0.48
3:D:191:TRP:HE1	4:E:78:ARG:HH12	1.61	0.48
4:I:29:ARG:NH1	4:I:80:GLN:HE21	2.11	0.48
1:A:352:ILE:HG13	1:A:373:GLU:HG3	1.96	0.48
1:A:368:GLU:HB3	1:A:388:ARG:HB3	1.96	0.48
4:E:71:ASN:HB3	4:E:95:PHE:HB2	1.96	0.48
1:F:376:TRP:HE1	4:I:37:TYR:HB2	1.78	0.48
1:A:507:LYS:HB2	1:A:535:SER:OG	2.13	0.48
1:A:537:SER:OG	1:A:538:ASN:OD1	2.29	0.48
2:C:57:ILE:HG22	4:E:68:PHE:HB3	1.94	0.48
2:C:283:LEU:HB3	2:C:287:ASP:HB3	1.95	0.48
2:G:84:PRO:HD3	3:H:77:TYR:CG	2.49	0.48
4:I:93:LEU:CD2	4:I:104:ILE:HG23	2.43	0.48
1:A:223:LEU:HD11	1:A:240:ILE:HG21	1.96	0.48
1:F:250:ASP:OD1	1:F:252:LYS:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:80:GLN:OE1	4:I:86:VAL:HB	2.14	0.48
2:G:65:TYR:OH	3:H:141:ARG:NE	2.46	0.48
2:C:230:VAL:HG22	2:C:244:VAL:HG22	1.95	0.47
1:A:282:ALA:O	1:A:285:GLU:HG2	2.15	0.47
2:G:61:THR:HG21	2:G:66:ALA:HB2	1.95	0.47
2:G:194:MSE:O	2:G:198:SER:HB2	2.14	0.47
4:I:29:ARG:HH12	4:I:80:GLN:HE21	1.62	0.47
1:A:173:VAL:H	1:A:252:LYS:HD2	1.79	0.47
2:C:33:ARG:HG2	2:C:83:ARG:HG3	1.95	0.47
1:F:376:TRP:HZ2	4:I:36:ASN:C	2.22	0.47
4:I:77:PHE:CE2	4:I:79:GLN:HB2	2.44	0.47
1:A:54:VAL:HG13	1:A:58:ASP:HB2	1.97	0.47
1:A:573:ASN:HD21	1:A:598:LYS:HE2	1.80	0.47
2:C:151:LEU:HB2	3:D:44:GLN:HB3	1.97	0.47
1:F:669:GLY:H	1:F:767:ARG:NH1	2.12	0.47
1:A:453:GLY:O	1:A:455:ALA:N	2.47	0.47
4:E:77:PHE:C	4:E:77:PHE:CD2	2.93	0.47
1:F:494:PHE:HB3	1:F:506:ASN:HB3	1.96	0.47
2:G:82:ILE:HD11	3:H:81:LYS:HD2	1.97	0.47
2:C:116:LEU:HD23	2:C:172:GLN:NE2	2.30	0.47
1:F:467:THR:OG1	1:F:493:ASP:HB2	2.14	0.47
1:F:542:GLN:HG3	1:F:545:MSE:HB2	1.96	0.47
1:F:739:TRP:NE1	1:F:791:PHE:HZ	2.08	0.47
4:I:96:ASN:HB3	4:I:100:VAL:HB	1.96	0.47
2:C:114:ASN:OD1	2:C:114:ASN:N	2.39	0.47
4:I:67:PRO:HB2	4:I:68:PHE:CD1	2.50	0.47
1:A:76:ARG:HB3	1:A:87:GLN:HB2	1.97	0.47
1:A:445:GLN:HG3	1:A:457:GLY:CA	2.45	0.47
1:F:741:MSE:HB3	1:F:768:MSE:HG2	1.97	0.47
2:G:71:ASN:O	2:G:73:SER:OG	2.28	0.47
4:I:28:TYR:CG	4:I:29:ARG:N	2.82	0.47
1:F:478:PHE:CE1	1:F:485:LEU:HD13	2.50	0.47
1:F:526:ARG:HB2	1:F:575:GLY:HA3	1.97	0.47
1:F:668:ILE:HG23	1:F:767:ARG:HD3	1.97	0.47
1:F:703:ASP:HB3	1:F:798:LYS:HE3	1.97	0.47
3:D:106:ASP:HB2	3:D:157:SER:OG	2.14	0.46
1:F:177:ILE:O	1:F:178:GLN:HB2	2.15	0.46
1:F:506:ASN:O	1:F:506:ASN:ND2	2.40	0.46
1:F:713:VAL:HG12	1:F:742:GLY:HA3	1.96	0.46
3:H:79:TYR:HB3	3:H:88:ALA:HB2	1.97	0.46
1:F:723:PRO:HA	1:F:724:PHE:HA	1.75	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:76:VAL:HG12	3:H:162:ASP:HA	1.97	0.46
1:A:436:SER:HB2	1:A:464:ASP:OD2	2.16	0.46
1:F:123:GLU:CD	3:H:97:ARG:HH12	2.24	0.46
1:F:701:LYS:HE2	1:F:760:TYR:OH	2.15	0.46
1:A:248:THR:HG22	1:A:253:GLY:H	1.81	0.46
2:C:95:ALA:HB1	2:C:106:LEU:HD11	1.98	0.46
3:D:116:ASN:HB2	3:D:143:ALA:HB2	1.96	0.46
1:A:24:PHE:HB3	1:A:54:VAL:O	2.16	0.46
4:E:77:PHE:CE2	4:E:79:GLN:HB2	2.47	0.46
1:F:588:THR:OG1	1:F:625:HIS:HB3	2.15	0.46
3:H:28:PRO:HB2	3:H:30:ASN:OD1	2.15	0.46
1:A:350:ARG:HG2	1:A:351:LYS:HG2	1.97	0.46
1:A:574:TYR:CZ	1:A:597:GLY:HA3	2.51	0.46
3:H:132:ARG:HB2	3:H:173:ARG:NH2	2.31	0.46
4:E:68:PHE:CD1	4:E:68:PHE:N	2.84	0.46
4:I:37:TYR:HD1	4:I:77:PHE:CE1	2.33	0.46
1:F:107:ASP:O	1:F:110:LEU:HB2	2.16	0.46
1:F:499:ALA:HB1	1:F:682:TYR:CE1	2.51	0.46
1:A:361:LYS:HD3	3:D:134:ASP:OD2	2.16	0.45
1:A:522:TYR:CD1	1:A:580:LYS:HG3	2.51	0.45
1:F:360:SER:HA	1:F:451:GLY:CA	2.46	0.45
3:H:200:GLY:HA2	3:H:203:ARG:NH2	2.31	0.45
1:F:465:TYR:CG	1:F:466:GLN:N	2.83	0.45
2:G:47:LEU:HG	3:H:168:VAL:HG13	1.99	0.45
2:C:194:MSE:O	2:C:198:SER:HB3	2.16	0.45
2:C:150:ARG:HB3	2:C:152:ASP:OD1	2.17	0.45
1:F:390:ASN:ND2	1:F:582:ASP:O	2.49	0.45
1:A:470:GLU:HA	1:A:490:PHE:HA	1.98	0.45
2:C:76:VAL:HA	3:D:162:ASP:HB2	1.98	0.45
1:F:662:GLY:H	1:F:803:GLN:CD	2.24	0.45
1:A:484:SER:O	1:A:515:LEU:HA	2.17	0.45
2:C:310:LEU:HD12	2:C:313:ARG:HB2	1.99	0.45
3:D:198:VAL:HG11	3:D:218:MSE:HB2	1.97	0.45
1:A:457:GLY:N	1:A:472:SER:OG	2.50	0.45
2:C:235:ASP:O	2:C:236:ASP:HB2	2.15	0.45
1:F:92:PRO:HB3	1:F:161:ASN:O	2.17	0.45
1:F:655:GLY:O	1:F:665:SER:HA	2.16	0.45
1:A:376:TRP:CZ2	4:E:37:TYR:HB3	2.52	0.45
3:D:90:ALA:O	3:D:94:ARG:HG3	2.17	0.45
1:F:410:ASP:OD2	1:F:410:ASP:N	2.48	0.45
2:G:82:ILE:O	3:H:107:TYR:OH	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ARG:NH2	1:A:355:GLU:OE2	2.50	0.45
1:A:612:THR:HG22	1:A:652:PHE:HE1	1.81	0.45
2:C:117:TRP:HB3	2:C:118:PRO:HD3	1.98	0.45
1:F:682:TYR:CD2	1:F:684:PRO:HD3	2.52	0.45
3:H:117:MSE:HG3	3:H:170:LEU:HD21	1.98	0.45
1:A:445:GLN:HG2	1:A:447:ASP:OD1	2.17	0.45
2:C:169:GLY:C	2:C:171:GLN:H	2.25	0.45
2:C:283:LEU:HB3	2:C:287:ASP:HB2	1.98	0.45
1:F:405:VAL:HA	1:F:406:PRO:HD3	1.80	0.45
1:A:91:ARG:H	1:A:92:PRO:HD3	1.81	0.44
1:A:348:TYR:CB	1:A:412:VAL:HG22	2.41	0.44
1:A:670:PRO:HA	1:A:760:TYR:CD1	2.51	0.44
1:A:805:ASN:HB3	1:A:806:ILE:HD12	1.99	0.44
2:C:262:VAL:HG23	2:C:264:MSE:HG3	1.99	0.44
1:F:731:ASN:OD1	1:F:732:SER:N	2.45	0.44
1:F:738:PHE:HE2	1:F:772:ILE:C	2.25	0.44
3:H:133:SER:O	3:H:177:TYR:HD2	2.00	0.44
1:A:287:LEU:HD11	1:A:311:LEU:HD13	1.99	0.44
4:E:29:ARG:HH12	4:E:80:GLN:NE2	2.14	0.44
1:F:475:ASN:HA	1:F:476:PRO:HD3	1.66	0.44
1:F:685:ASP:HA	1:F:686:TYR:HA	1.62	0.44
3:H:135:ARG:H	3:H:135:ARG:HD2	1.82	0.44
1:A:166:LYS:HE3	2:C:304:LYS:HZ2	1.80	0.44
1:A:166:LYS:HE3	2:C:304:LYS:NZ	2.32	0.44
1:A:542:GLN:HG2	1:A:545:MSE:HE3	1.98	0.44
1:F:176:GLU:OE1	1:F:178:GLN:HG2	2.17	0.44
1:F:351:LYS:HE3	3:H:197:ARG:HH21	1.82	0.44
3:H:48:TRP:HB2	3:H:82:ASN:HD22	1.82	0.44
1:A:351:LYS:HA	1:A:373:GLU:HG2	2.00	0.44
1:A:368:GLU:HG3	1:A:392:LEU:HD11	2.00	0.44
1:A:557:SER:HB3	1:A:560:ASP:HB2	1.99	0.44
4:E:28:TYR:CG	4:E:29:ARG:N	2.85	0.44
4:E:81:PRO:HG2	4:E:84:GLU:HB3	2.00	0.44
1:F:350:ARG:O	1:F:351:LYS:HD2	2.18	0.44
3:H:105:ILE:HG12	3:H:109:MSE:HE3	1.98	0.44
2:C:85:PRO:HD3	3:D:107:TYR:CD1	2.53	0.44
4:E:59:LEU:HD12	4:E:59:LEU:N	2.32	0.44
1:F:380:ASP:N	1:F:380:ASP:OD1	2.50	0.44
2:G:72:GLY:HA3	2:G:73:SER:HA	1.52	0.44
2:C:320:ASP:HB3	2:C:324:HIS:H	1.83	0.44
4:I:60:GLY:O	4:I:75:TYR:OH	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:198:VAL:HG11	3:H:218:MSE:HB2	2.00	0.44
1:A:574:TYR:CE2	1:A:597:GLY:HA3	2.53	0.44
2:C:172:GLN:H	2:C:172:GLN:HG3	1.67	0.44
3:D:214:ALA:HA	3:D:217:LEU:HD13	2.00	0.44
1:F:446:GLN:HG2	1:F:449:TRP:CD1	2.39	0.44
1:F:446:GLN:CG	1:F:449:TRP:HA	2.48	0.44
4:I:78:ARG:HH12	3:H:191:TRP:HE1	1.64	0.44
1:A:682:TYR:HD2	1:A:684:PRO:HD3	1.82	0.44
2:C:72:GLY:HA3	2:C:73:SER:HA	1.54	0.44
2:G:201:MSE:H	2:G:201:MSE:HG3	1.62	0.44
1:A:317:TYR:CZ	1:A:346:ARG:HD3	2.53	0.43
2:C:240:PRO:HB2	2:C:331:ASN:CG	2.42	0.43
1:F:541:PRO:HA	1:F:546:TRP:CZ3	2.53	0.43
1:F:669:GLY:CA	1:F:744:VAL:HB	2.46	0.43
4:I:37:TYR:CD1	4:I:77:PHE:HE1	2.37	0.43
3:H:207:ASP:OD1	3:H:207:ASP:N	2.48	0.43
1:A:348:TYR:CD2	1:A:412:VAL:HG13	2.53	0.43
2:C:115:THR:O	2:C:118:PRO:HD2	2.18	0.43
3:D:233:LYS:O	3:D:237:ILE:HG13	2.19	0.43
4:I:92:THR:HB	4:I:105:ASP:HB3	1.99	0.43
1:A:421:ARG:O	1:A:421:ARG:HG2	2.16	0.43
1:A:540:GLN:HG3	1:A:541:PRO:HD2	2.01	0.43
1:F:459:ASN:OD1	1:F:460:GLY:N	2.51	0.43
1:F:671:LYS:HE2	1:F:705:ALA:HB2	2.01	0.43
2:C:84:PRO:HD3	3:D:77:TYR:CG	2.53	0.43
2:C:98:GLN:NE2	2:C:107:LEU:HD21	2.33	0.43
1:A:628:VAL:HB	1:A:719:ILE:HB	2.00	0.43
2:C:57:ILE:HD12	2:C:57:ILE:HA	1.85	0.43
4:E:110:LEU:HD23	4:E:110:LEU:HA	1.90	0.43
3:D:109:MSE:HB2	3:D:150:LEU:HD13	1.99	0.43
1:F:358:ASP:O	3:H:132:ARG:NH1	2.51	0.43
1:F:465:TYR:O	1:F:495:GLN:HB2	2.18	0.43
1:A:152:LYS:HB3	1:A:168:VAL:HB	2.00	0.43
1:A:318:ALA:CB	1:A:377:LEU:HD13	2.48	0.43
4:I:50:MSE:H	4:I:101:LEU:HB3	1.83	0.43
1:A:380:ASP:OD1	1:A:380:ASP:N	2.51	0.43
1:F:156:THR:HB	1:F:164:ASP:OD2	2.19	0.43
3:H:230:GLN:O	3:H:234:VAL:HG23	2.18	0.43
1:A:291:GLU:HB2	1:A:294:GLU:HB2	2.00	0.43
1:F:275:GLY:O	1:F:277:LEU:HD12	2.19	0.43
4:I:62:PRO:HG3	4:I:73:TRP:CG	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:TYR:CG	1:A:586:PHE:N	2.87	0.42
1:A:723:PRO:HA	1:A:724:PHE:CB	2.47	0.42
2:C:240:PRO:HB2	2:C:331:ASN:CB	2.49	0.42
4:E:29:ARG:HH12	4:E:80:GLN:HE21	1.67	0.42
4:E:70:THR:OG1	4:E:71:ASN:N	2.40	0.42
1:F:348:TYR:HB2	1:F:375:ALA:O	2.19	0.42
1:F:608:TYR:HB2	1:F:646:MSE:HG3	2.01	0.42
3:D:197:ARG:O	3:D:201:MSE:HG3	2.20	0.42
4:E:72:THR:C	4:E:73:TRP:HE3	2.28	0.42
1:F:634:ARG:HB3	1:F:713:VAL:HG22	2.01	0.42
4:I:39:THR:O	4:I:42:ASP:N	2.52	0.42
4:I:81:PRO:HG2	4:I:84:GLU:HB2	2.01	0.42
4:E:37:TYR:CD1	4:E:77:PHE:HE1	2.37	0.42
1:F:393:GLY:O	1:F:421:ARG:NH2	2.52	0.42
1:F:521:GLU:OE1	4:I:28:TYR:OH	2.37	0.42
4:E:77:PHE:C	4:E:77:PHE:HD2	2.27	0.42
1:F:90:GLU:HB2	1:F:161:ASN:HD21	1.84	0.42
1:F:150:SER:O	1:F:170:GLN:HB2	2.19	0.42
1:F:227:ARG:HA	1:F:238:PHE:CE2	2.54	0.42
1:A:159:PRO:HD3	2:C:248:PHE:CD1	2.54	0.42
2:C:190:ASP:O	2:C:194:MSE:HG2	2.19	0.42
1:F:388:ARG:O	1:F:392:LEU:HG	2.19	0.42
4:I:63:LEU:HD23	3:H:192:VAL:HG11	2.01	0.42
3:H:27:VAL:HA	3:H:28:PRO:HD3	1.90	0.42
1:A:143:SER:HB2	1:A:218:LYS:HD2	2.00	0.42
1:A:388:ARG:O	1:A:392:LEU:HG	2.20	0.42
3:D:148:SER:HB3	3:D:152:ARG:HH12	1.85	0.42
3:D:205:TYR:O	3:D:211:THR:OG1	2.30	0.42
1:F:72:PHE:HA	1:F:90:GLU:HA	2.00	0.42
1:A:27:LYS:HG2	1:A:82:ASP:HB3	2.02	0.42
1:A:669:GLY:O	1:A:671:LYS:NZ	2.37	0.42
3:D:145:SER:O	3:D:149:LYS:HG3	2.20	0.42
1:A:541:PRO:HA	1:A:546:TRP:CZ3	2.54	0.42
1:A:630:LEU:HB3	1:A:717:GLU:HG3	2.00	0.42
2:C:307:VAL:HA	2:C:315:SER:O	2.19	0.42
1:A:316:GLY:O	1:A:318:ALA:N	2.52	0.42
1:F:350:ARG:O	1:F:373:GLU:HG2	2.20	0.42
1:A:713:VAL:HG12	1:A:742:GLY:HA3	2.02	0.41
1:F:223:LEU:HD11	1:F:240:ILE:HG21	2.01	0.41
3:H:147:PHE:HB2	3:H:167:LEU:HD21	2.01	0.41
1:A:789:GLN:HA	1:A:790:PRO:HD3	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:371:GLN:OE1	1:F:378:GLY:N	2.36	0.41
1:F:520:ASN:HD21	1:F:523:ASN:HB2	1.84	0.41
1:F:646:MSE:HE2	1:F:646:MSE:HB3	1.85	0.41
1:F:653:TYR:HB3	1:F:666:ASN:HA	2.01	0.41
4:I:25:ARG:HA	4:I:25:ARG:HD3	1.83	0.41
1:A:538:ASN:OD1	1:A:562:ASP:HA	2.20	0.41
1:A:680:SER:O	1:A:681:ASN:HB2	2.20	0.41
2:C:74:GLY:N	3:D:161:THR:OG1	2.50	0.41
1:F:73:GLU:OE1	1:F:127:ARG:NH1	2.53	0.41
4:I:36:ASN:O	4:I:37:TYR:C	2.62	0.41
1:A:634:ARG:HB3	1:A:713:VAL:HG22	2.01	0.41
2:C:29:SER:O	2:C:30:ARG:HB3	2.20	0.41
2:C:179:LEU:H	2:C:179:LEU:HG	1.59	0.41
4:E:48:VAL:HG22	4:E:104:ILE:HD12	2.03	0.41
4:E:75:TYR:HB2	4:E:91:LEU:HB3	2.02	0.41
1:F:574:TYR:CE2	1:F:597:GLY:HA3	2.55	0.41
3:D:132:ARG:NH1	3:D:135:ARG:HG2	2.36	0.41
1:F:76:ARG:HB3	1:F:87:GLN:HB2	2.03	0.41
2:G:65:TYR:HA	3:H:144:PHE:CE1	2.55	0.41
1:A:92:PRO:HB2	1:A:93:THR:OG1	2.21	0.41
2:C:112:ARG:HG3	2:C:112:ARG:HH11	1.85	0.41
2:C:56:MSE:HE1	3:D:233:LYS:HA	2.02	0.41
1:F:54:VAL:HG13	1:F:58:ASP:HB2	2.01	0.41
1:F:578:TYR:OH	1:F:580:LYS:HD2	2.20	0.41
4:I:46:ILE:CG2	4:I:59:LEU:HD11	2.51	0.41
1:A:539:MSE:CE	1:A:545:MSE:HB3	2.51	0.41
1:A:738:PHE:CZ	1:A:788:ALA:HB2	2.56	0.41
2:C:65:TYR:CE2	3:D:174:LEU:HD13	2.52	0.41
2:C:271:ARG:H	3:D:29:ASP:CG	2.28	0.41
3:D:147:PHE:HB2	3:D:167:LEU:HD21	2.03	0.41
1:F:372:MSE:HE3	4:I:32:ILE:HA	2.03	0.41
2:G:41:TYR:HB2	3:H:169:PHE:CG	2.56	0.41
1:A:178:GLN:HG3	1:A:179:GLN:CB	2.50	0.41
1:A:236:ALA:C	1:A:238:PHE:H	2.28	0.41
1:A:368:GLU:HA	1:A:388:ARG:HH11	1.85	0.41
1:A:368:GLU:OE2	1:A:477:TYR:OH	2.36	0.41
1:A:514:THR:HA	1:A:528:GLY:HA3	2.03	0.41
2:C:34:GLN:HB3	2:C:78:LYS:HD2	2.03	0.41
2:C:49:GLU:HB3	3:D:207:ASP:HB3	2.03	0.41
2:C:262:VAL:HG21	2:C:264:MSE:HE3	2.02	0.41
1:F:29:ILE:HD11	1:F:86:VAL:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:235:TYR:CD1	1:F:263:GLY:O	2.68	0.41
4:I:26:VAL:HG21	4:I:83:HIS:CE1	2.56	0.41
2:C:127:LYS:HE3	2:C:204:VAL:HG13	2.03	0.41
2:C:246:GLY:HA2	2:C:247:PRO:HD3	1.87	0.41
4:E:59:LEU:HD12	4:E:59:LEU:H	1.86	0.41
1:F:362:ASP:CG	1:F:366:ARG:HH21	2.26	0.41
1:F:687:ASP:O	1:F:689:GLU:HG3	2.21	0.41
3:H:233:LYS:O	3:H:237:ILE:HG13	2.20	0.41
1:A:176:GLU:H	1:A:177:ILE:HA	1.86	0.40
1:A:649:TYR:CE1	1:A:650:GLU:HG2	2.55	0.40
1:F:318:ALA:HB2	1:F:377:LEU:HD13	2.03	0.40
1:A:92:PRO:CB	1:A:93:THR:HA	2.51	0.40
1:A:405:VAL:HA	1:A:406:PRO:HD3	1.79	0.40
1:F:244:GLN:HB2	1:F:257:THR:HG23	2.03	0.40
1:A:91:ARG:N	1:A:92:PRO:CD	2.85	0.40
1:A:316:GLY:O	1:A:346:ARG:O	2.39	0.40
1:F:141:TYR:HD2	1:F:146:LYS:HB2	1.87	0.40
1:A:446:GLN:O	1:A:448:ASN:N	2.54	0.40
1:A:582:ASP:CG	1:A:588:THR:HG22	2.47	0.40
2:C:65:TYR:OH	3:D:141:ARG:NE	2.54	0.40
2:C:104:ALA:C	2:C:202:MSE:HE2	2.47	0.40
1:F:454:TYR:HB3	1:F:475:ASN:CA	2.52	0.40
1:A:91:ARG:HG3	1:A:92:PRO:CD	2.50	0.40
1:A:141:TYR:OH	1:A:171:GLU:OE1	2.29	0.40
1:A:178:GLN:HG3	1:A:179:GLN:HB2	2.04	0.40
1:A:542:GLN:HE21	1:A:706:VAL:HG11	1.86	0.40
2:C:205:ILE:H	2:C:205:ILE:HG13	1.70	0.40
4:I:34:GLN:HG2	4:I:78:ARG:HB3	2.02	0.40

There are no symmetry-related clashes.

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	756/810 (93%)	688 (91%)	62 (8%)	6 (1%)	16	49
1	F	756/810 (93%)	696 (92%)	57 (8%)	3 (0%)	30	62
2	C	312/344 (91%)	288 (92%)	21 (7%)	3 (1%)	12	44
2	G	82/344 (24%)	70 (85%)	10 (12%)	2 (2%)	4	29
3	D	216/245 (88%)	209 (97%)	7 (3%)	0	100	100
3	H	216/245 (88%)	209 (97%)	7 (3%)	0	100	100
4	E	85/123 (69%)	78 (92%)	4 (5%)	3 (4%)	3	23
4	I	85/123 (69%)	76 (89%)	4 (5%)	5 (6%)	1	12
All	All	2508/3044 (82%)	2314 (92%)	172 (7%)	22 (1%)	14	47

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	36	ASN
4	E	70	THR
2	C	329	SER
1	F	178	GLN
1	F	502	SER
4	I	28	TYR
4	I	37	TYR
4	I	70	THR
1	A	454	TYR
2	C	64	ASP
2	G	61	THR
4	I	36	ASN
1	A	178	GLN
4	E	28	TYR
1	F	447	ASP
1	A	35	GLN
1	A	92	PRO
1	A	422	ASN
1	A	562	ASP
2	G	87	GLN
2	C	323	GLY
4	I	108	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	649/672 (97%)	592 (91%)	57 (9%)	9	32
1	F	648/672 (96%)	591 (91%)	57 (9%)	9	32
2	C	254/267 (95%)	233 (92%)	21 (8%)	10	34
2	G	63/267 (24%)	54 (86%)	9 (14%)	3	18
3	D	183/195 (94%)	178 (97%)	5 (3%)	39	62
3	H	183/195 (94%)	177 (97%)	6 (3%)	33	58
4	E	76/99 (77%)	62 (82%)	14 (18%)	1	9
4	I	76/99 (77%)	65 (86%)	11 (14%)	3	17
All	All	2132/2466 (86%)	1952 (92%)	180 (8%)	10	34

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	THR
1	A	79	ARG
1	A	88	VAL
1	A	93	THR
1	A	98	THR
1	A	111	LYS
1	A	123	GLU
1	A	125	LEU
1	A	156	THR
1	A	160	ARG
1	A	163	VAL
1	A	176	GLU
1	A	177	ILE
1	A	178	GLN
1	A	180	ILE
1	A	199	LEU
1	A	219	LEU
1	A	233	ARG
1	A	237	ARG
1	A	257	THR
1	A	265	GLN
1	A	285	GLU
1	A	290	ILE

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Mol	Chain	Res	Type
1	A	295	LEU
1	A	311	LEU
1	A	333	LYS
1	A	391	ARG
1	A	422	ASN
1	A	423	THR
1	A	425	SER
1	A	426	PHE
1	A	444	VAL
1	A	500	ASP
1	A	501	LEU
1	A	515	LEU
1	A	519	ILE
1	A	538	ASN
1	A	539	MSE
1	A	542	GLN
1	A	549	LEU
1	A	563	ASN
1	A	569	ASP
1	A	614	ASP
1	A	633	THR
1	A	659	THR
1	A	671	LYS
1	A	687	ASP
1	A	693	GLN
1	A	698	ASP
1	A	711	MSE
1	A	716	LEU
1	A	717	GLU
1	A	725	ILE
1	A	741	MSE
1	A	772	ILE
1	A	777	MSE
1	A	792	LYS
2	C	50	LEU
2	C	57	ILE
2	C	64	ASP
2	C	87	GLN
2	C	105	SER
2	C	107	LEU
2	C	109	GLU
2	C	112	ARG

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Mol	Chain	Res	Type
2	C	114	ASN
2	C	141	LEU
2	C	154	ASP
2	C	172	GLN
2	C	179	LEU
2	C	198	SER
2	C	205	ILE
2	C	245	ARG
2	C	255	LEU
2	C	278	VAL
2	C	304	LYS
2	C	313	ARG
2	C	322	LYS
3	D	115	THR
3	D	124	LEU
3	D	135	ARG
3	D	141	ARG
3	D	192	VAL
4	E	32	ILE
4	E	38	LEU
4	E	48	VAL
4	E	64	MSE
4	E	68	PHE
4	E	77	PHE
4	E	78	ARG
4	E	79	GLN
4	E	84	GLU
4	E	86	VAL
4	E	91	LEU
4	E	92	THR
4	E	94	THR
4	E	107	LYS
1	F	34	LEU
1	F	35	GLN
1	F	43	LEU
1	F	44	LEU
1	F	50	THR
1	F	67	PHE
1	F	79	ARG
1	F	88	VAL
1	F	98	THR
1	F	123	GLU

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Mol	Chain	Res	Type
1	F	125	LEU
1	F	127	ARG
1	F	156	THR
1	F	163	VAL
1	F	174	SER
1	F	177	ILE
1	F	179	GLN
1	F	199	LEU
1	F	217	GLN
1	F	219	LEU
1	F	233	ARG
1	F	251	LYS
1	F	254	ILE
1	F	257	THR
1	F	264	ASP
1	F	265	GLN
1	F	311	LEU
1	F	325	MSE
1	F	330	ASP
1	F	333	LYS
1	F	370	ARG
1	F	413	ASP
1	F	441	GLN
1	F	444	VAL
1	F	452	THR
1	F	489	LEU
1	F	492	ASN
1	F	501	LEU
1	F	506	ASN
1	F	515	LEU
1	F	542	GLN
1	F	549	LEU
1	F	563	ASN
1	F	569	ASP
1	F	596	THR
1	F	633	THR
1	F	646	MSE
1	F	659	THR
1	F	671	LYS
1	F	682	TYR
1	F	699	LEU
1	F	716	LEU

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Mol	Chain	Res	Type
1	F	717	GLU
1	F	741	MSE
1	F	767	ARG
1	F	772	ILE
1	F	792	LYS
2	G	50	LEU
2	G	58	LEU
2	G	64	ASP
2	G	193	SER
2	G	198	SER
2	G	201	MSE
2	G	204	VAL
2	G	205	ILE
2	G	209	LEU
4	I	26	VAL
4	I	32	ILE
4	I	48	VAL
4	I	50	MSE
4	I	64	MSE
4	I	68	PHE
4	I	77	PHE
4	I	84	GLU
4	I	92	THR
4	I	94	THR
4	I	107	LYS
3	H	115	THR
3	H	124	LEU
3	H	125	GLN
3	H	135	ARG
3	H	141	ARG
3	H	192	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	61	ASN
1	A	186	HIS
1	A	239	ASN
1	A	427	ASN
1	A	495	GLN
1	A	579	ASN

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Mol	Chain	Res	Type
1	A	606	ASN
1	A	625	HIS
1	A	693	GLN
1	A	801	GLN
2	C	172	GLN
2	C	183	GLN
2	C	203	ASN
2	C	249	ASN
2	C	306	GLN
3	D	41	GLN
3	D	47	ASN
3	D	89	GLN
3	D	125	GLN
3	D	138	GLN
3	D	139	HIS
3	D	196	ASN
3	D	230	GLN
4	E	79	GLN
4	E	80	GLN
1	F	55	ASN
1	F	61	ASN
1	F	71	ASN
1	F	239	ASN
1	F	280	HIS
1	F	390	ASN
1	F	446	GLN
1	F	534	ASN
1	F	606	ASN
1	F	677	HIS
1	F	678	GLN
1	F	801	GLN
4	I	89	GLN
3	H	47	ASN
3	H	82	ASN
3	H	89	GLN
3	H	116	ASN
3	H	138	GLN
3	H	139	HIS
3	H	196	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](#)

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](#)

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	748/810 (92%)	-0.07	12 (1%) 70 45	100, 156, 213, 238	0
1	F	747/810 (92%)	-0.05	13 (1%) 69 43	81, 158, 215, 243	4 (0%)
2	C	309/344 (89%)	-0.15	3 (0%) 79 56	95, 137, 202, 206	0
2	G	82/344 (23%)	0.08	1 (1%) 76 52	137, 161, 271, 279	0
3	D	211/245 (86%)	-0.04	3 (1%) 73 48	87, 109, 138, 154	0
3	H	211/245 (86%)	0.24	9 (4%) 40 21	126, 147, 194, 202	0
4	E	85/123 (69%)	0.09	2 (2%) 59 35	121, 141, 168, 178	0
4	I	85/123 (69%)	0.38	5 (5%) 28 16	131, 151, 174, 196	0
All	All	2478/3044 (81%)	-0.02	48 (1%) 66 41	81, 150, 207, 279	4 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	60	VAL	5.7
3	H	121	ASP	4.5
1	F	370	ARG	4.3
1	A	491	TYR	4.2
4	I	45	LYS	4.2
1	F	807	GLY	4.2
3	H	64	PHE	4.2
1	F	585	TYR	3.9
4	I	86	VAL	3.8
4	I	67	PRO	3.5
1	F	272	GLU	3.4
2	C	59	PRO	3.4
3	H	67	TYR	3.4
1	A	104	SER	3.4
4	I	37	TYR	3.4
3	H	50	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	391	ARG	3.0
1	F	196	HIS	3.0
4	I	34	GLN	2.9
1	F	376	TRP	2.8
1	A	500	ASP	2.8
3	D	48	TRP	2.8
1	A	806	ILE	2.8
3	H	63	PRO	2.6
1	A	219	LEU	2.6
3	D	67	TYR	2.6
3	H	54	GLN	2.5
1	F	198	GLN	2.5
2	G	59	PRO	2.4
1	A	666	ASN	2.4
1	A	608	TYR	2.3
1	A	180	ILE	2.2
3	H	243	SER	2.2
1	A	614	ASP	2.2
1	F	332	ASP	2.2
3	D	158	GLN	2.2
1	A	665	SER	2.2
4	E	63	LEU	2.2
3	H	202	LEU	2.2
1	A	393	GLY	2.2
1	F	367	ARG	2.1
4	E	34	GLN	2.1
2	C	332	ASP	2.1
1	A	240	ILE	2.1
3	H	239	ALA	2.1
1	F	583	ARG	2.1
1	F	491	TYR	2.0
1	F	692	THR	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.