



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:32 PM UTC

PDB ID : 6QPM / pdb_00006qpm
Title : Adenovirus serotype 10 Fiber-Knob
Authors : Baker, A.T.; Rizkallah, P.J.
Deposited on : 2019-02-14
Resolution : 3.39 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:

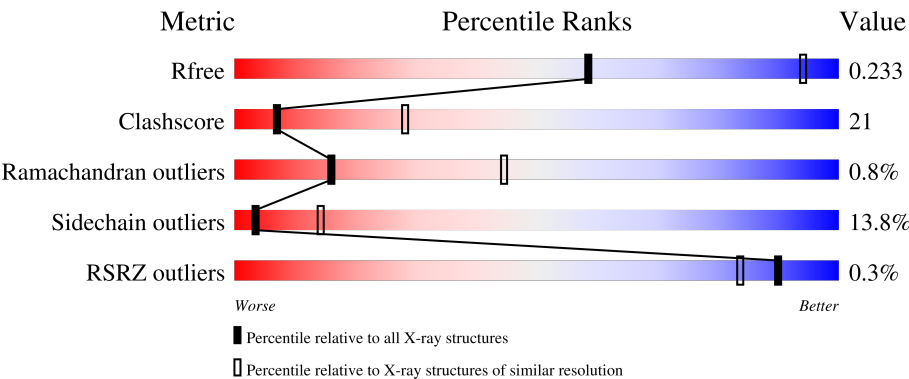
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.39 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	205	58%25%6%11%
1	B	205	% 60%21%7%11%
1	C	205	60%24%5%11%
1	D	205	60%20%.15%
1	E	205	52%28%9%11%

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Mol	Chain	Length	Quality of chain
1	F	205	59% 23% 8% 11%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8631 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 Fiber protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	0	0	0
			1449	929	233	283	4			
1	B	183	Total	C	N	O	S	0	0	0
			1449	929	233	283	4			
1	C	183	Total	C	N	O	S	0	0	0
			1449	929	233	283	4			
1	D	175	Total	C	N	O	S	0	0	0
			1386	890	223	269	4			
1	E	183	Total	C	N	O	S	0	0	0
			1449	929	233	283	4			
1	F	183	Total	C	N	O	S	0	0	0
			1449	929	233	283	4			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	165	MET	-	initiating methionine	UNP B5BQ05
A	166	ARG	-	expression tag	UNP B5BQ05
A	167	GLY	-	expression tag	UNP B5BQ05
A	168	HIS	-	expression tag	UNP B5BQ05
A	169	HIS	-	expression tag	UNP B5BQ05
A	170	HIS	-	expression tag	UNP B5BQ05
A	171	HIS	-	expression tag	UNP B5BQ05
A	172	HIS	-	expression tag	UNP B5BQ05
A	173	HIS	-	expression tag	UNP B5BQ05
A	174	GLY	-	expression tag	UNP B5BQ05
A	175	SER	-	expression tag	UNP B5BQ05
B	165	MET	-	initiating methionine	UNP B5BQ05
B	166	ARG	-	expression tag	UNP B5BQ05
B	167	GLY	-	expression tag	UNP B5BQ05
B	168	HIS	-	expression tag	UNP B5BQ05
B	169	HIS	-	expression tag	UNP B5BQ05
B	170	HIS	-	expression tag	UNP B5BQ05

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Chain	Residue	Modelled	Actual	Comment	Reference
B	171	HIS	-	expression tag	UNP B5BQ05
B	172	HIS	-	expression tag	UNP B5BQ05
B	173	HIS	-	expression tag	UNP B5BQ05
B	174	GLY	-	expression tag	UNP B5BQ05
B	175	SER	-	expression tag	UNP B5BQ05
C	165	MET	-	initiating methionine	UNP B5BQ05
C	166	ARG	-	expression tag	UNP B5BQ05
C	167	GLY	-	expression tag	UNP B5BQ05
C	168	HIS	-	expression tag	UNP B5BQ05
C	169	HIS	-	expression tag	UNP B5BQ05
C	170	HIS	-	expression tag	UNP B5BQ05
C	171	HIS	-	expression tag	UNP B5BQ05
C	172	HIS	-	expression tag	UNP B5BQ05
C	173	HIS	-	expression tag	UNP B5BQ05
C	174	GLY	-	expression tag	UNP B5BQ05
C	175	SER	-	expression tag	UNP B5BQ05
D	165	MET	-	initiating methionine	UNP B5BQ05
D	166	ARG	-	expression tag	UNP B5BQ05
D	167	GLY	-	expression tag	UNP B5BQ05
D	168	HIS	-	expression tag	UNP B5BQ05
D	169	HIS	-	expression tag	UNP B5BQ05
D	170	HIS	-	expression tag	UNP B5BQ05
D	171	HIS	-	expression tag	UNP B5BQ05
D	172	HIS	-	expression tag	UNP B5BQ05
D	173	HIS	-	expression tag	UNP B5BQ05
D	174	GLY	-	expression tag	UNP B5BQ05
D	175	SER	-	expression tag	UNP B5BQ05
E	165	MET	-	initiating methionine	UNP B5BQ05
E	166	ARG	-	expression tag	UNP B5BQ05
E	167	GLY	-	expression tag	UNP B5BQ05
E	168	HIS	-	expression tag	UNP B5BQ05
E	169	HIS	-	expression tag	UNP B5BQ05
E	170	HIS	-	expression tag	UNP B5BQ05
E	171	HIS	-	expression tag	UNP B5BQ05
E	172	HIS	-	expression tag	UNP B5BQ05
E	173	HIS	-	expression tag	UNP B5BQ05
E	174	GLY	-	expression tag	UNP B5BQ05
E	175	SER	-	expression tag	UNP B5BQ05
F	165	MET	-	initiating methionine	UNP B5BQ05
F	166	ARG	-	expression tag	UNP B5BQ05
F	167	GLY	-	expression tag	UNP B5BQ05
F	168	HIS	-	expression tag	UNP B5BQ05

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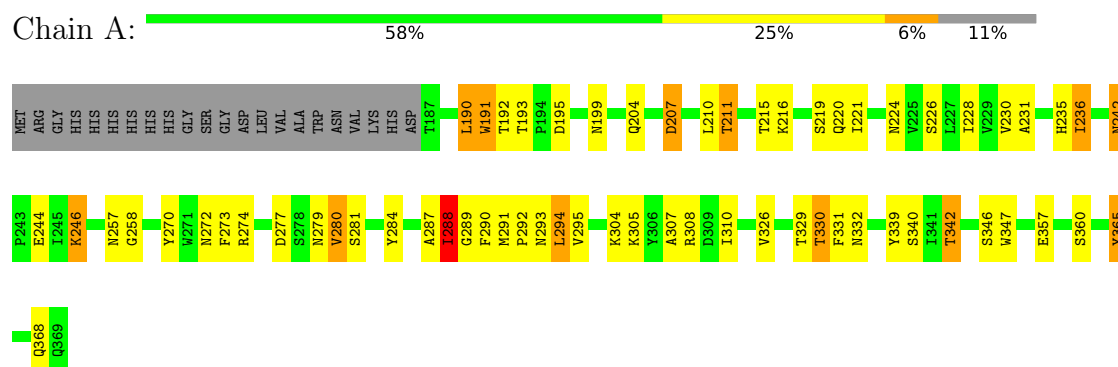
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Chain	Residue	Modelled	Actual	Comment	Reference
F	169	HIS	-	expression tag	UNP B5BQ05
F	170	HIS	-	expression tag	UNP B5BQ05
F	171	HIS	-	expression tag	UNP B5BQ05
F	172	HIS	-	expression tag	UNP B5BQ05
F	173	HIS	-	expression tag	UNP B5BQ05
F	174	GLY	-	expression tag	UNP B5BQ05
F	175	SER	-	expression tag	UNP B5BQ05

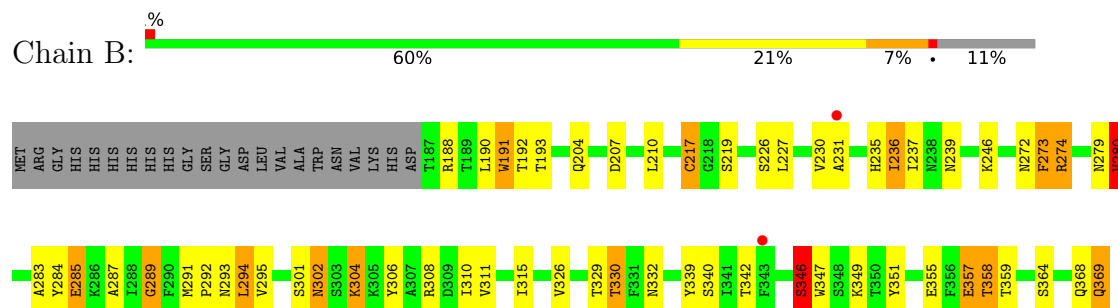
3 Residue-property plots [i](#)

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

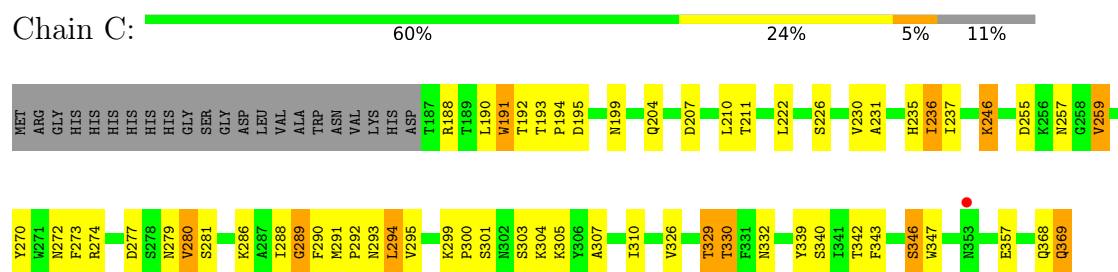
• Molecule 1: Fiber protein



• Molecule 1: Fiber protein

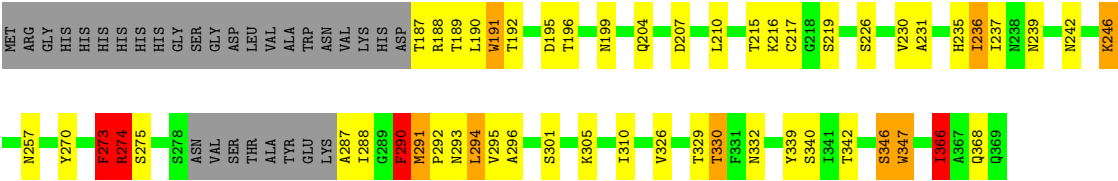


• Molecule 1: Fiber protein

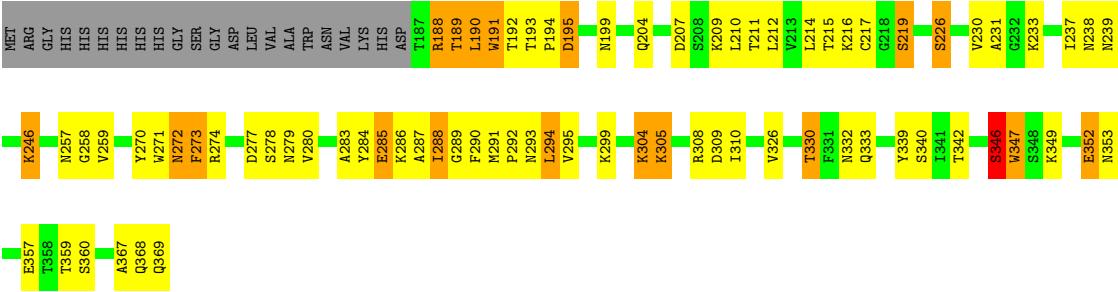


• Molecule 1: Fiber protein

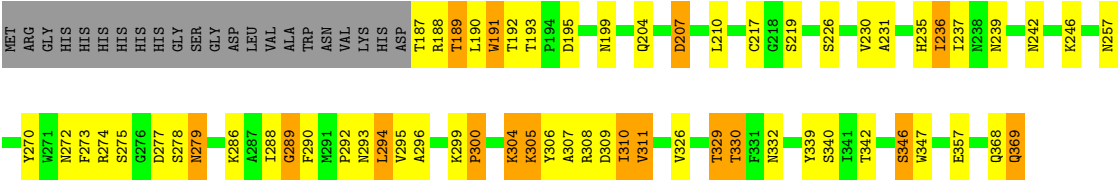




● Molecule 1: Fiber protein



● Molecule 1: Fiber protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	183.57Å 183.57Å 94.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	79.49 – 3.39 79.49 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.9 (79.49-3.39) 98.9 (79.49-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 3.41Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.199 , 0.232 0.200 , 0.233	Depositor DCC
R_{free} test set	1235 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	153.6	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 180.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.097 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8631	wwPDB-VP
Average B, all atoms (Å ²)	186.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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	1.01	0/1483	1.44	6/2014 (0.3%)
1	B	1.02	1/1483 (0.1%)	1.46	5/2014 (0.2%)
1	C	0.99	0/1483	1.42	3/2014 (0.1%)
1	D	0.99	0/1418	1.42	5/1924 (0.3%)
1	E	1.02	0/1483	1.48	6/2014 (0.3%)
1	F	1.00	0/1483	1.47	6/2014 (0.3%)
All	All	1.01	1/8833 (0.0%)	1.45	31/11994 (0.3%)

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	B	0	1
1	C	0	1
1	F	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	364	SER	C-O	5.42	1.30	1.23

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	302	ASN	CA-CB-CG	9.15	121.75	112.60
1	D	273	PHE	CA-CB-CG	7.52	121.32	113.80
1	A	288	ILE	CA-C-O	-7.46	114.06	121.67
1	F	273	PHE	CA-CB-CG	7.03	120.83	113.80
1	A	273	PHE	CA-CB-CG	7.01	120.81	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	273	PHE	CA-CB-CG	6.69	120.49	113.80
1	A	288	ILE	N-CA-C	-6.18	99.78	108.80
1	F	309	ASP	CA-CB-CG	6.11	118.71	112.60
1	B	346	SER	CA-C-O	-6.07	114.77	121.33
1	B	302	ASN	CB-CA-C	6.06	122.30	110.67
1	F	187	THR	CA-CB-OG1	-5.84	100.84	109.60
1	E	352	GLU	CB-CG-CD	5.67	122.23	112.60
1	C	288	ILE	N-CA-C	-5.63	103.84	110.21
1	E	195	ASP	CA-CB-CG	5.59	118.19	112.60
1	C	195	ASP	CA-CB-CG	5.54	118.14	112.60
1	E	273	PHE	CA-C-O	-5.53	114.45	120.81
1	E	346	SER	CA-C-O	-5.46	114.87	120.99
1	F	207	ASP	CA-CB-CG	5.31	117.91	112.60
1	D	195	ASP	CA-CB-CG	5.29	117.89	112.60
1	B	273	PHE	CA-CB-CG	5.24	119.04	113.80
1	C	290	PHE	N-CA-C	-5.21	106.93	113.28
1	A	195	ASP	CA-CB-CG	5.19	117.79	112.60
1	A	207	ASP	CA-CB-CG	5.18	117.78	112.60
1	F	195	ASP	CA-CB-CG	5.14	117.74	112.60
1	D	366	ILE	CB-CA-C	5.13	117.27	110.91
1	E	233	LYS	CA-C-O	-5.10	115.06	121.02
1	A	342	THR	CB-CA-C	5.09	117.98	110.14
1	D	275	SER	N-CA-C	-5.08	107.22	113.41
1	F	290	PHE	N-CA-C	-5.07	106.95	113.23
1	D	274	ARG	CG-CD-NE	5.05	123.11	112.00
1	B	358	THR	CA-CB-OG1	-5.01	102.09	109.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	289	GLY	Peptide
1	B	289	GLY	Peptide
1	C	289	GLY	Peptide
1	F	289	GLY	Peptide

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1449	0	1429	72	0
1	B	1449	0	1429	76	0
1	C	1449	0	1429	54	0
1	D	1386	0	1368	52	0
1	E	1449	0	1424	97	0
1	F	1449	0	1429	42	0
All	All	8631	0	8508	360	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 21.

All (360) 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:B:272:ASN:C	1:B:279:ASN:HD21	1.20	1.45
1:E:272:ASN:ND2	1:E:279:ASN:OD1	1.58	1.33
1:B:272:ASN:O	1:B:279:ASN:ND2	1.66	1.24
1:B:273:PHE:C	1:B:279:ASN:OD1	1.83	1.21
1:B:272:ASN:C	1:B:279:ASN:ND2	1.99	1.19
1:E:258:GLY:N	1:E:286:LYS:CE	2.03	1.19
1:E:258:GLY:N	1:E:286:LYS:HE3	1.57	1.18
1:B:284:TYR:OH	1:B:287:ALA:HB3	1.43	1.17
1:E:359:THR:HG22	1:F:310:ILE:HD11	1.18	1.14
1:E:305:LYS:HE3	1:E:309:ASP:OD2	1.54	1.08
1:B:349:LYS:HB3	1:B:351:TYR:CE1	1.88	1.08
1:E:359:THR:HG22	1:F:310:ILE:CD1	1.83	1.07
1:A:293:ASN:HA	1:A:368:GLN:OE1	1.52	1.07
1:A:272:ASN:HB3	1:A:279:ASN:HD22	1.09	1.07
1:A:221:ILE:HB	1:A:365:TYR:CE1	1.89	1.06
1:B:349:LYS:HB3	1:B:351:TYR:HE1	1.26	1.00
1:D:291:MET:HG3	1:D:292:PRO:HD2	1.46	0.95
1:A:272:ASN:CB	1:A:279:ASN:HD22	1.79	0.94
1:E:258:GLY:H	1:E:286:LYS:HE3	1.28	0.94
1:E:259:VAL:HG23	1:E:286:LYS:HD3	1.50	0.94
1:B:227:LEU:H	1:B:358:THR:HG22	1.32	0.94
1:E:272:ASN:ND2	1:E:279:ASN:CG	2.26	0.92
1:A:221:ILE:CG1	1:A:365:TYR:HE1	1.84	0.91
1:B:274:ARG:N	1:B:279:ASN:OD1	2.04	0.90
1:E:274:ARG:HG3	1:E:279:ASN:HA	1.52	0.90
1:B:272:ASN:CA	1:B:279:ASN:HD21	1.82	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:259:VAL:HG23	1:E:286:LYS:CD	2.03	0.89
1:C:272:ASN:HB3	1:C:279:ASN:HD22	1.38	0.89
1:C:272:ASN:C	1:C:279:ASN:HD21	1.81	0.88
1:C:257:ASN:O	1:C:286:LYS:HA	1.75	0.87
1:A:272:ASN:O	1:A:279:ASN:ND2	2.07	0.87
1:B:273:PHE:O	1:B:279:ASN:OD1	1.94	0.86
1:E:359:THR:CG2	1:F:310:ILE:HD11	2.05	0.86
1:E:305:LYS:CE	1:E:309:ASP:OD2	2.25	0.85
1:B:272:ASN:O	1:B:279:ASN:CG	2.21	0.83
1:B:272:ASN:CA	1:B:279:ASN:ND2	2.41	0.83
1:D:296:ALA:HB2	1:D:366:ILE:HD11	1.61	0.82
1:F:272:ASN:HB3	1:F:279:ASN:OD1	1.78	0.82
1:A:216:LYS:HB2	1:A:290:PHE:CE1	2.14	0.82
1:C:272:ASN:HB3	1:C:279:ASN:ND2	1.94	0.82
1:A:272:ASN:HB3	1:A:279:ASN:ND2	1.94	0.81
1:E:257:ASN:CA	1:E:286:LYS:HE3	2.08	0.81
1:E:257:ASN:HB2	1:E:286:LYS:CE	2.10	0.81
1:C:272:ASN:O	1:C:279:ASN:ND2	2.13	0.81
1:D:290:PHE:HD1	1:D:290:PHE:O	1.65	0.80
1:A:272:ASN:C	1:A:279:ASN:ND2	2.39	0.79
1:E:304:LYS:HE2	1:E:304:LYS:HA	1.65	0.78
1:A:221:ILE:CB	1:A:365:TYR:CE1	2.65	0.77
1:B:272:ASN:HB3	1:B:279:ASN:HD22	1.49	0.77
1:A:216:LYS:HB2	1:A:290:PHE:HE1	1.47	0.76
1:A:294:LEU:N	1:A:368:GLN:OE1	2.17	0.76
1:C:272:ASN:C	1:C:279:ASN:ND2	2.43	0.76
1:F:310:ILE:HG22	1:F:330:THR:HG23	1.67	0.76
1:D:191:TRP:CE2	1:D:274:ARG:HD2	2.20	0.75
1:E:272:ASN:ND2	1:E:272:ASN:C	2.43	0.75
1:B:227:LEU:H	1:B:358:THR:CG2	2.00	0.75
1:E:258:GLY:H	1:E:286:LYS:CE	1.85	0.75
1:E:272:ASN:HD22	1:E:279:ASN:ND2	1.85	0.75
1:A:191:TRP:CE2	1:A:274:ARG:HG3	2.22	0.74
1:A:295:VAL:HG21	1:C:277:ASP:OD2	1.87	0.74
1:D:291:MET:CG	1:D:292:PRO:HD2	2.17	0.74
1:B:272:ASN:HB3	1:B:279:ASN:ND2	2.02	0.74
1:C:191:TRP:CE2	1:C:274:ARG:HG3	2.23	0.74
1:E:258:GLY:N	1:E:286:LYS:NZ	2.36	0.73
1:B:274:ARG:HA	1:B:279:ASN:HA	1.69	0.73
1:E:195:ASP:OD1	1:E:209:LYS:NZ	2.21	0.73
1:E:272:ASN:HD22	1:E:279:ASN:HD21	1.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:PRO:HG2	1:C:332:ASN:HD21	1.54	0.72
1:B:274:ARG:CA	1:B:279:ASN:OD1	2.37	0.71
1:F:191:TRP:CE2	1:F:274:ARG:HG3	2.25	0.71
1:D:274:ARG:HH11	1:D:274:ARG:HG3	1.53	0.71
1:D:291:MET:HG2	1:D:339:TYR:CB	2.20	0.71
1:D:291:MET:HG2	1:D:339:TYR:CG	2.27	0.70
1:A:292:PRO:HG2	1:A:332:ASN:HD21	1.57	0.70
1:B:284:TYR:OH	1:B:287:ALA:CB	2.32	0.70
1:D:191:TRP:NE1	1:D:274:ARG:HD2	2.05	0.70
1:A:221:ILE:HB	1:A:365:TYR:HE1	1.56	0.70
1:B:272:ASN:CB	1:B:279:ASN:ND2	2.54	0.70
1:B:292:PRO:HG2	1:B:332:ASN:HD21	1.57	0.70
1:D:292:PRO:HG2	1:D:332:ASN:HD21	1.57	0.70
1:E:258:GLY:C	1:E:286:LYS:HD2	2.11	0.70
1:B:332:ASN:HD22	1:B:340:SER:H	1.39	0.70
1:E:257:ASN:CB	1:E:286:LYS:CD	2.66	0.69
1:A:221:ILE:CB	1:A:365:TYR:HE1	2.03	0.69
1:E:190:LEU:HA	1:E:273:PHE:HA	1.73	0.69
1:C:272:ASN:CB	1:C:279:ASN:ND2	2.56	0.69
1:C:332:ASN:HD22	1:C:340:SER:H	1.40	0.69
1:A:332:ASN:HD22	1:A:340:SER:H	1.41	0.69
1:E:259:VAL:CG2	1:E:286:LYS:HD3	2.21	0.69
1:E:292:PRO:HG2	1:E:332:ASN:HD21	1.58	0.69
1:B:191:TRP:CE2	1:B:274:ARG:HG3	2.28	0.69
1:A:257:ASN:O	1:A:287:ALA:O	2.11	0.69
1:A:272:ASN:CB	1:A:279:ASN:ND2	2.55	0.69
1:A:272:ASN:CA	1:A:279:ASN:ND2	2.55	0.68
1:F:332:ASN:HD22	1:F:340:SER:H	1.41	0.68
1:E:332:ASN:HD22	1:E:340:SER:H	1.41	0.68
1:E:289:GLY:CA	1:E:369:GLN:OXT	2.41	0.68
1:E:287:ALA:CB	1:E:291:MET:HE3	2.23	0.68
1:F:292:PRO:HG2	1:F:332:ASN:HD21	1.59	0.68
1:A:331:PHE:CE1	1:A:365:TYR:HD2	2.12	0.67
1:D:332:ASN:HD22	1:D:340:SER:H	1.41	0.67
1:C:272:ASN:CA	1:C:279:ASN:ND2	2.57	0.67
1:E:304:LYS:HA	1:E:304:LYS:CE	2.24	0.67
1:E:272:ASN:ND2	1:E:279:ASN:ND2	2.42	0.66
1:A:246:LYS:HA	1:A:347:TRP:CZ2	2.31	0.66
1:E:257:ASN:CB	1:E:286:LYS:CE	2.73	0.66
1:A:191:TRP:CZ2	1:A:274:ARG:HG3	2.31	0.66
1:E:257:ASN:HB3	1:E:286:LYS:CB	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:TRP:CZ2	1:B:274:ARG:HG3	2.31	0.66
1:B:192:THR:HG21	1:B:210:LEU:O	1.96	0.66
1:E:189:THR:HG22	1:E:215:THR:HG23	1.77	0.65
1:A:307:ALA:N	1:C:357:GLU:OE1	2.28	0.65
1:E:192:THR:HG21	1:E:210:LEU:O	1.95	0.65
1:A:293:ASN:CA	1:A:368:GLN:OE1	2.36	0.65
1:F:294:LEU:HB2	1:F:368:GLN:HE22	1.61	0.65
1:D:191:TRP:CE2	1:D:274:ARG:CD	2.80	0.65
1:E:287:ALA:HB2	1:E:291:MET:HE3	1.77	0.65
1:A:190:LEU:HB2	1:A:290:PHE:CE2	2.31	0.65
1:B:274:ARG:HA	1:B:279:ASN:OD1	1.95	0.65
1:C:191:TRP:CZ2	1:C:274:ARG:HG3	2.32	0.65
1:B:284:TYR:CD1	1:B:285:GLU:N	2.65	0.65
1:C:272:ASN:CA	1:C:279:ASN:HD21	2.09	0.65
1:E:259:VAL:HG23	1:E:286:LYS:CE	2.26	0.65
1:E:272:ASN:C	1:E:272:ASN:HD22	2.04	0.65
1:F:192:THR:HG21	1:F:210:LEU:O	1.97	0.64
1:F:239:ASN:HD21	1:F:347:TRP:HZ3	1.46	0.64
1:C:192:THR:HG21	1:C:210:LEU:O	1.98	0.64
1:B:315:ILE:HB	1:B:358:THR:OG1	1.98	0.63
1:C:294:LEU:HB2	1:C:368:GLN:HE22	1.64	0.63
1:D:192:THR:HG21	1:D:210:LEU:O	1.97	0.63
1:A:228:ILE:HG21	1:B:306:TYR:CE2	2.34	0.63
1:E:257:ASN:HB2	1:E:286:LYS:HE2	1.80	0.63
1:E:294:LEU:HB2	1:E:368:GLN:HE22	1.63	0.63
1:B:294:LEU:HB2	1:B:368:GLN:HE22	1.64	0.62
1:A:277:ASP:OD2	1:B:295:VAL:HG21	2.00	0.62
1:E:194:PRO:O	1:F:308:ARG:NH1	2.33	0.62
1:A:192:THR:HG21	1:A:210:LEU:O	1.98	0.62
1:B:191:TRP:CH2	1:B:274:ARG:HD2	2.34	0.62
1:E:272:ASN:HD22	1:E:279:ASN:CG	2.05	0.62
1:F:296:ALA:O	1:F:308:ARG:NH2	2.32	0.62
1:B:239:ASN:HD21	1:B:347:TRP:HZ3	1.48	0.61
1:A:284:TYR:CE2	1:A:287:ALA:HB3	2.36	0.61
1:D:239:ASN:HD21	1:D:347:TRP:HZ3	1.47	0.61
1:A:211:THR:HB	1:B:308:ARG:NH1	2.16	0.61
1:D:237:ILE:HG21	1:D:347:TRP:CZ3	2.36	0.60
1:E:258:GLY:H	1:E:286:LYS:NZ	1.96	0.60
1:E:239:ASN:HD21	1:E:347:TRP:HZ3	1.50	0.60
1:A:236:ILE:HG12	1:E:353:ASN:HB3	1.84	0.60
1:D:216:LYS:HB2	1:D:290:PHE:CE2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:MET:HG2	1:D:339:TYR:HB3	1.83	0.60
1:C:237:ILE:HG21	1:C:347:TRP:CZ3	2.36	0.60
1:D:294:LEU:HB2	1:D:368:GLN:HE22	1.66	0.60
1:E:237:ILE:HG21	1:E:347:TRP:CZ3	2.37	0.60
1:E:257:ASN:HB3	1:E:286:LYS:HB2	1.83	0.60
1:B:237:ILE:HG21	1:B:347:TRP:CZ3	2.37	0.60
1:F:191:TRP:CZ2	1:F:274:ARG:HG3	2.37	0.59
1:D:187:THR:CA	1:D:273:PHE:CE2	2.85	0.59
1:B:357:GLU:OE1	1:C:307:ALA:N	2.34	0.59
1:D:187:THR:CA	1:D:273:PHE:HE2	2.16	0.58
1:B:349:LYS:CB	1:B:351:TYR:HE1	2.09	0.58
1:F:304:LYS:HE2	1:F:306:TYR:CE1	2.39	0.58
1:F:237:ILE:HG21	1:F:347:TRP:CZ3	2.38	0.58
1:A:246:LYS:HA	1:A:347:TRP:CE2	2.39	0.58
1:B:310:ILE:HG12	1:B:330:THR:HG23	1.86	0.58
1:E:259:VAL:CG2	1:E:286:LYS:CD	2.77	0.58
1:E:289:GLY:HA3	1:E:369:GLN:OXT	2.04	0.57
1:D:274:ARG:HH11	1:D:274:ARG:CG	2.17	0.57
1:E:288:ILE:CG2	1:E:369:GLN:HE22	2.18	0.57
1:E:310:ILE:HG12	1:E:330:THR:HG23	1.87	0.57
1:E:258:GLY:HA3	1:E:287:ALA:HB3	1.87	0.57
1:A:284:TYR:HE2	1:A:287:ALA:HB3	1.69	0.56
1:E:257:ASN:CB	1:E:286:LYS:HE3	2.35	0.56
1:B:273:PHE:O	1:B:279:ASN:CG	2.49	0.56
1:D:290:PHE:O	1:D:290:PHE:CD1	2.52	0.55
1:D:219:SER:HB2	1:F:189:THR:HG21	1.89	0.55
1:A:221:ILE:HG12	1:A:365:TYR:HE1	1.69	0.55
1:E:305:LYS:NZ	1:E:333:GLN:OE1	2.34	0.55
1:A:360:SER:HB2	1:B:311:VAL:HG22	1.88	0.54
1:B:188:ARG:HA	1:B:188:ARG:NE	2.21	0.54
1:D:189:THR:HG23	1:D:274:ARG:HG3	1.89	0.54
1:E:257:ASN:N	1:E:286:LYS:HE3	2.23	0.54
1:E:359:THR:HG22	1:F:310:ILE:HD13	1.83	0.54
1:E:272:ASN:CG	1:E:279:ASN:OD1	2.41	0.54
1:E:292:PRO:HG2	1:E:332:ASN:ND2	2.23	0.54
1:D:291:MET:HG3	1:D:292:PRO:CD	2.31	0.54
1:E:347:TRP:CD1	1:E:347:TRP:N	2.76	0.53
1:E:360:SER:HB2	1:F:311:VAL:HG13	1.89	0.53
1:F:299:LYS:HD2	1:F:300:PRO:HD2	1.90	0.53
1:F:347:TRP:CD1	1:F:347:TRP:N	2.76	0.53
1:A:221:ILE:HG13	1:A:365:TYR:HE1	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:PRO:HG2	1:B:332:ASN:ND2	2.24	0.53
1:F:305:LYS:NZ	1:F:305:LYS:HB3	2.24	0.53
1:B:272:ASN:O	1:B:279:ASN:OD1	2.26	0.52
1:D:216:LYS:HD2	1:D:290:PHE:CD2	2.44	0.52
1:D:347:TRP:N	1:D:347:TRP:CD1	2.76	0.52
1:E:305:LYS:HE3	1:E:333:GLN:CD	2.35	0.52
1:B:273:PHE:CZ	1:B:287:ALA:HB2	2.44	0.52
1:B:347:TRP:N	1:B:347:TRP:CD1	2.75	0.52
1:D:237:ILE:CG2	1:D:347:TRP:CZ3	2.93	0.52
1:B:346:SER:C	1:B:347:TRP:CD1	2.87	0.52
1:F:293:ASN:OD1	1:F:295:VAL:N	2.43	0.52
1:E:212:LEU:HD11	1:E:214:LEU:HG	1.92	0.52
1:B:283:ALA:O	1:B:285:GLU:OE1	2.26	0.52
1:D:189:THR:HG21	1:E:219:SER:OG	2.10	0.52
1:D:296:ALA:CB	1:D:366:ILE:HD11	2.36	0.52
1:E:293:ASN:OD1	1:E:295:VAL:N	2.43	0.52
1:F:292:PRO:HG2	1:F:332:ASN:ND2	2.23	0.52
1:F:237:ILE:CG2	1:F:347:TRP:CZ3	2.93	0.52
1:F:346:SER:C	1:F:347:TRP:CD1	2.88	0.52
1:A:211:THR:CG2	1:B:308:ARG:HH11	2.23	0.52
1:A:292:PRO:HG2	1:A:332:ASN:ND2	2.23	0.52
1:B:293:ASN:OD1	1:B:295:VAL:N	2.43	0.52
1:C:237:ILE:CG2	1:C:347:TRP:CZ3	2.93	0.52
1:C:293:ASN:OD1	1:C:295:VAL:N	2.43	0.52
1:D:292:PRO:HG2	1:D:332:ASN:ND2	2.23	0.52
1:D:310:ILE:HG12	1:D:330:THR:HG23	1.92	0.51
1:A:293:ASN:OD1	1:A:295:VAL:N	2.43	0.51
1:D:346:SER:C	1:D:347:TRP:CD1	2.88	0.51
1:E:277:ASP:OD2	1:F:295:VAL:HG21	2.10	0.51
1:E:346:SER:C	1:E:347:TRP:CD1	2.89	0.51
1:A:220:GLN:NE2	1:C:222:LEU:O	2.44	0.51
1:A:308:ARG:NH2	1:C:194:PRO:O	2.41	0.51
1:E:237:ILE:CG2	1:E:347:TRP:CZ3	2.93	0.51
1:E:238:ASN:HA	1:E:352:GLU:O	2.11	0.51
1:C:310:ILE:HG12	1:C:330:THR:HG23	1.93	0.51
1:C:346:SER:C	1:C:347:TRP:CD1	2.89	0.51
1:E:289:GLY:HA2	1:E:369:GLN:OXT	2.11	0.51
1:A:211:THR:HB	1:B:308:ARG:HH11	1.76	0.51
1:C:347:TRP:CD1	1:C:347:TRP:N	2.76	0.51
1:F:307:ALA:O	1:F:310:ILE:HD13	2.11	0.50
1:B:289:GLY:HA3	1:B:369:GLN:OXT	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:ASN:OD1	1:D:295:VAL:N	2.45	0.50
1:E:257:ASN:HB2	1:E:286:LYS:CD	2.40	0.50
1:E:289:GLY:O	1:E:367:ALA:HB1	2.11	0.50
1:B:237:ILE:CG2	1:B:347:TRP:CZ3	2.94	0.50
1:E:212:LEU:HD21	1:E:214:LEU:HD21	1.94	0.50
1:C:292:PRO:HG2	1:C:332:ASN:ND2	2.23	0.50
1:A:221:ILE:CG1	1:A:365:TYR:CE1	2.76	0.49
1:B:227:LEU:N	1:B:358:THR:CG2	2.74	0.49
1:B:227:LEU:N	1:B:358:THR:HG22	2.14	0.49
1:D:257:ASN:HB3	1:D:287:ALA:HB1	1.94	0.49
1:E:188:ARG:NH2	1:E:216:LYS:O	2.45	0.49
1:C:289:GLY:HA3	1:C:369:GLN:OXT	2.12	0.49
1:F:289:GLY:HA3	1:F:369:GLN:OXT	2.13	0.49
1:A:228:ILE:HG21	1:B:306:TYR:HE2	1.75	0.48
1:B:346:SER:C	1:B:347:TRP:HD1	2.21	0.48
1:B:272:ASN:C	1:B:279:ASN:CG	2.78	0.48
1:E:274:ARG:HD2	1:E:278:SER:O	2.13	0.48
1:E:258:GLY:HA3	1:E:287:ALA:CB	2.43	0.48
1:A:310:ILE:HG12	1:A:330:THR:HG23	1.96	0.48
1:D:191:TRP:CD2	1:D:274:ARG:HD3	2.48	0.48
1:E:207:ASP:HB2	1:E:231:ALA:HB3	1.96	0.48
1:C:301:SER:O	1:C:303:SER:N	2.46	0.48
1:A:221:ILE:HB	1:A:365:TYR:CD1	2.45	0.47
1:B:191:TRP:CZ3	1:B:274:ARG:HD2	2.49	0.47
1:E:257:ASN:HB2	1:E:286:LYS:HE3	1.91	0.47
1:A:284:TYR:CE2	1:A:287:ALA:CB	2.97	0.47
1:A:242:ASN:HB3	1:A:244:GLU:OE1	2.15	0.47
1:E:272:ASN:ND2	1:E:279:ASN:HD21	2.02	0.47
1:E:283:ALA:C	1:E:285:GLU:H	2.22	0.47
1:E:346:SER:C	1:E:347:TRP:HD1	2.23	0.47
1:B:207:ASP:HB2	1:B:231:ALA:HB3	1.97	0.47
1:A:207:ASP:HB2	1:A:231:ALA:HB3	1.97	0.47
1:F:346:SER:C	1:F:347:TRP:HD1	2.23	0.47
1:C:280:VAL:HG12	1:C:280:VAL:O	2.14	0.46
1:A:331:PHE:CZ	1:A:365:TYR:HD2	2.33	0.46
1:F:207:ASP:HB2	1:F:231:ALA:HB3	1.97	0.46
1:C:273:PHE:C	1:C:279:ASN:OD1	2.58	0.46
1:F:311:VAL:HG23	1:F:329:THR:HB	1.97	0.46
1:A:360:SER:OG	1:B:308:ARG:NH2	2.41	0.46
1:C:286:LYS:CG	1:C:286:LYS:O	2.63	0.46
1:D:207:ASP:HB2	1:D:231:ALA:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:346:SER:C	1:D:347:TRP:HD1	2.24	0.46
1:C:286:LYS:O	1:C:286:LYS:HG3	2.15	0.46
1:C:346:SER:C	1:C:347:TRP:HD1	2.23	0.46
1:D:191:TRP:CD2	1:D:274:ARG:CD	2.99	0.46
1:E:288:ILE:HG23	1:E:369:GLN:HE22	1.81	0.46
1:E:259:VAL:HG23	1:E:286:LYS:HE2	1.98	0.46
1:D:216:LYS:HD2	1:D:290:PHE:HD2	1.78	0.46
1:E:190:LEU:HD11	1:E:271:TRP:CH2	2.51	0.46
1:E:305:LYS:CE	1:E:333:GLN:CD	2.89	0.46
1:D:219:SER:CB	1:F:189:THR:HG21	2.45	0.46
1:F:275:SER:H	1:F:279:ASN:HA	1.81	0.45
1:A:284:TYR:CD2	1:A:287:ALA:HB2	2.51	0.45
1:C:294:LEU:CD2	1:C:339:TYR:CE2	3.00	0.45
1:C:272:ASN:N	1:C:279:ASN:HD21	2.13	0.45
1:F:236:ILE:N	1:F:236:ILE:HD13	2.32	0.45
1:B:355:GLU:OE1	1:C:304:LYS:NZ	2.46	0.45
1:B:236:ILE:HD13	1:B:236:ILE:N	2.32	0.45
1:E:190:LEU:HB2	1:E:290:PHE:CE2	2.52	0.45
1:D:294:LEU:HD22	1:D:368:GLN:NE2	2.32	0.44
1:A:288:ILE:C	1:A:290:PHE:H	2.26	0.44
1:D:196:THR:HG22	1:E:308:ARG:NH1	2.33	0.44
1:F:294:LEU:CD2	1:F:339:TYR:CE2	3.01	0.44
1:E:294:LEU:CD2	1:E:339:TYR:CE2	3.01	0.44
1:A:236:ILE:N	1:A:236:ILE:HD13	2.33	0.44
1:C:274:ARG:HA	1:C:279:ASN:OD1	2.18	0.44
1:C:273:PHE:O	1:C:279:ASN:OD1	2.36	0.43
1:A:258:GLY:HA3	1:A:287:ALA:O	2.17	0.43
1:B:304:LYS:O	1:B:304:LYS:HG3	2.19	0.43
1:C:279:ASN:C	1:C:281:SER:H	2.26	0.43
1:D:236:ILE:N	1:D:236:ILE:HD13	2.33	0.43
1:B:358:THR:HG23	1:B:359:THR:O	2.17	0.43
1:A:279:ASN:C	1:A:281:SER:H	2.25	0.43
1:E:286:LYS:O	1:E:288:ILE:HG13	2.18	0.43
1:C:236:ILE:HD13	1:C:236:ILE:N	2.33	0.43
1:A:294:LEU:CD2	1:A:339:TYR:CE2	3.02	0.43
1:B:294:LEU:CD2	1:B:339:TYR:CE2	3.01	0.43
1:E:190:LEU:HG	1:E:273:PHE:HB3	2.01	0.43
1:B:235:HIS:C	1:B:236:ILE:HD13	2.44	0.43
1:C:207:ASP:HB2	1:C:231:ALA:HB3	2.00	0.43
1:A:224:ASN:OD1	1:B:308:ARG:NH2	2.47	0.42
1:C:294:LEU:HD11	1:C:299:LYS:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:ASN:O	1:C:279:ASN:CG	2.62	0.42
1:D:215:THR:HG21	1:E:217:CYS:O	2.19	0.42
1:E:211:THR:OG1	1:E:226:SER:HB3	2.18	0.42
1:E:246:LYS:HB3	1:E:347:TRP:CE3	2.54	0.42
1:D:235:HIS:C	1:D:236:ILE:HD13	2.45	0.42
1:F:257:ASN:O	1:F:288:ILE:HG13	2.20	0.42
1:F:235:HIS:C	1:F:236:ILE:HD13	2.45	0.42
1:A:211:THR:CB	1:B:308:ARG:HH11	2.32	0.42
1:D:295:VAL:HG21	1:F:277:ASP:CG	2.45	0.42
1:A:291:MET:HB3	1:A:339:TYR:CD2	2.54	0.42
1:A:211:THR:CG2	1:B:308:ARG:NH1	2.83	0.42
1:A:215:THR:HG21	1:B:217:CYS:O	2.20	0.42
1:B:285:GLU:N	1:B:285:GLU:OE1	2.53	0.42
1:C:191:TRP:CD1	1:C:191:TRP:C	2.98	0.42
1:C:199:ASN:HB2	1:C:270:TYR:CD1	2.55	0.42
1:C:246:LYS:HB3	1:C:347:TRP:CE3	2.55	0.42
1:A:191:TRP:CD1	1:A:191:TRP:C	2.98	0.41
1:D:293:ASN:OD1	1:D:295:VAL:HB	2.21	0.41
1:E:192:THR:O	1:E:193:THR:C	2.64	0.41
1:A:211:THR:HG21	1:B:308:ARG:HH11	1.85	0.41
1:B:291:MET:HB3	1:B:339:TYR:CD2	2.55	0.41
1:E:199:ASN:HB2	1:E:270:TYR:CD1	2.56	0.41
1:F:191:TRP:C	1:F:191:TRP:CD1	2.99	0.41
1:B:191:TRP:CD1	1:B:191:TRP:C	2.99	0.41
1:F:192:THR:O	1:F:193:THR:C	2.64	0.41
1:A:199:ASN:HB2	1:A:270:TYR:CD1	2.56	0.41
1:A:235:HIS:C	1:A:236:ILE:HD13	2.45	0.41
1:C:235:HIS:C	1:C:236:ILE:HD13	2.45	0.41
1:C:329:THR:HG23	1:C:343:PHE:CE1	2.55	0.41
1:A:293:ASN:C	1:A:368:GLN:OE1	2.64	0.41
1:B:279:ASN:O	1:B:280:VAL:HG22	2.20	0.41
1:D:291:MET:HG2	1:D:339:TYR:CD2	2.55	0.41
1:A:284:TYR:CD2	1:A:287:ALA:CB	3.03	0.41
1:C:291:MET:HB3	1:C:339:TYR:CD2	2.55	0.41
1:A:192:THR:O	1:A:193:THR:C	2.64	0.41
1:C:192:THR:O	1:C:193:THR:C	2.64	0.40
1:D:199:ASN:HB2	1:D:270:TYR:CD1	2.56	0.40
1:E:191:TRP:CD1	1:E:191:TRP:C	2.99	0.40
1:E:294:LEU:HD11	1:E:299:LYS:HG2	2.03	0.40
1:C:191:TRP:CH2	1:C:194:PRO:HD3	2.55	0.40
1:F:199:ASN:HB2	1:F:270:TYR:CD1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:LYS:HD2	1:C:300:PRO:HD2	2.02	0.40
1:D:188:ARG:NE	1:D:188:ARG:HA	2.34	0.40
1:B:192:THR:O	1:B:193:THR:C	2.64	0.40
1:C:255:ASP:OD1	1:C:259:VAL:HG13	2.20	0.40
1:D:246:LYS:HB3	1:D:347:TRP:CE3	2.57	0.40
1:A:365:TYR:HD1	1:A:365:TYR:C	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	181/205 (88%)	162 (90%)	18 (10%)	1 (1%)	21	50
1	B	181/205 (88%)	161 (89%)	19 (10%)	1 (1%)	21	50
1	C	181/205 (88%)	159 (88%)	21 (12%)	1 (1%)	21	50
1	D	171/205 (83%)	152 (89%)	17 (10%)	2 (1%)	10	35
1	E	181/205 (88%)	156 (86%)	22 (12%)	3 (2%)	7	28
1	F	181/205 (88%)	163 (90%)	17 (9%)	1 (1%)	21	50
All	All	1076/1230 (88%)	953 (89%)	114 (11%)	9 (1%)	16	44

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	280	VAL
1	B	280	VAL
1	C	280	VAL
1	D	301	SER
1	E	284	TYR
1	E	288	ILE

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Mol	Chain	Res	Type
1	D	290	PHE
1	E	305	LYS
1	F	300	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	163/182 (90%)	141 (86%)	22 (14%)	4	15
1	B	163/182 (90%)	140 (86%)	23 (14%)	3	13
1	C	163/182 (90%)	145 (89%)	18 (11%)	6	22
1	D	156/182 (86%)	133 (85%)	23 (15%)	3	12
1	E	163/182 (90%)	142 (87%)	21 (13%)	4	16
1	F	163/182 (90%)	136 (83%)	27 (17%)	2	10
All	All	971/1092 (89%)	837 (86%)	134 (14%)	3	14

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	LEU
1	A	191	TRP
1	A	204	GLN
1	A	211	THR
1	A	219	SER
1	A	226	SER
1	A	230	VAL
1	A	236	ILE
1	A	242	ASN
1	A	246	LYS
1	A	280	VAL
1	A	288	ILE
1	A	294	LEU
1	A	304	LYS
1	A	305	LYS

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Mol	Chain	Res	Type
1	A	326	VAL
1	A	329	THR
1	A	330	THR
1	A	342	THR
1	A	346	SER
1	A	357	GLU
1	A	365	TYR
1	B	190	LEU
1	B	191	TRP
1	B	204	GLN
1	B	217	CYS
1	B	219	SER
1	B	226	SER
1	B	230	VAL
1	B	236	ILE
1	B	246	LYS
1	B	274	ARG
1	B	280	VAL
1	B	285	GLU
1	B	294	LEU
1	B	301	SER
1	B	302	ASN
1	B	304	LYS
1	B	326	VAL
1	B	329	THR
1	B	330	THR
1	B	342	THR
1	B	346	SER
1	B	357	GLU
1	B	369	GLN
1	C	188	ARG
1	C	190	LEU
1	C	191	TRP
1	C	204	GLN
1	C	211	THR
1	C	226	SER
1	C	230	VAL
1	C	236	ILE
1	C	246	LYS
1	C	259	VAL
1	C	294	LEU
1	C	305	LYS

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Mol	Chain	Res	Type
1	C	326	VAL
1	C	329	THR
1	C	330	THR
1	C	342	THR
1	C	346	SER
1	C	369	GLN
1	D	190	LEU
1	D	191	TRP
1	D	204	GLN
1	D	217	CYS
1	D	226	SER
1	D	230	VAL
1	D	236	ILE
1	D	242	ASN
1	D	246	LYS
1	D	273	PHE
1	D	274	ARG
1	D	288	ILE
1	D	290	PHE
1	D	291	MET
1	D	294	LEU
1	D	305	LYS
1	D	326	VAL
1	D	329	THR
1	D	330	THR
1	D	342	THR
1	D	346	SER
1	D	347	TRP
1	D	366	ILE
1	E	188	ARG
1	E	189	THR
1	E	190	LEU
1	E	191	TRP
1	E	204	GLN
1	E	219	SER
1	E	226	SER
1	E	230	VAL
1	E	246	LYS
1	E	272	ASN
1	E	280	VAL
1	E	285	GLU
1	E	294	LEU

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Mol	Chain	Res	Type
1	E	304	LYS
1	E	326	VAL
1	E	330	THR
1	E	342	THR
1	E	346	SER
1	E	347	TRP
1	E	349	LYS
1	E	357	GLU
1	F	188	ARG
1	F	189	THR
1	F	190	LEU
1	F	191	TRP
1	F	204	GLN
1	F	217	CYS
1	F	219	SER
1	F	226	SER
1	F	230	VAL
1	F	236	ILE
1	F	242	ASN
1	F	246	LYS
1	F	278	SER
1	F	279	ASN
1	F	286	LYS
1	F	294	LEU
1	F	304	LYS
1	F	305	LYS
1	F	310	ILE
1	F	311	VAL
1	F	326	VAL
1	F	329	THR
1	F	330	THR
1	F	342	THR
1	F	346	SER
1	F	357	GLU
1	F	369	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	ASN
1	A	279	ASN
1	A	323	GLN

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Mol	Chain	Res	Type
1	A	332	ASN
1	B	239	ASN
1	B	302	ASN
1	B	323	GLN
1	B	332	ASN
1	B	368	GLN
1	B	369	GLN
1	C	241	ASN
1	C	323	GLN
1	C	332	ASN
1	C	368	GLN
1	D	239	ASN
1	D	272	ASN
1	D	323	GLN
1	D	332	ASN
1	D	368	GLN
1	E	239	ASN
1	E	242	ASN
1	E	302	ASN
1	E	323	GLN
1	E	332	ASN
1	E	368	GLN
1	E	369	GLN
1	F	239	ASN
1	F	302	ASN
1	F	323	GLN
1	F	332	ASN
1	F	368	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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	183/205 (89%)	-0.70	0	100	100	110, 166, 232, 305	0
1	B	183/205 (89%)	-0.72	2 (1%)	78	65	119, 158, 224, 285	0
1	C	183/205 (89%)	-0.81	1 (0%)	87	78	134, 187, 246, 290	0
1	D	175/205 (85%)	-0.81	0	100	100	163, 226, 263, 309	0
1	E	183/205 (89%)	-0.73	0	100	100	138, 191, 263, 309	0
1	F	183/205 (89%)	-0.87	0	100	100	127, 165, 222, 285	0
All	All	1090/1230 (88%)	-0.78	3 (0%)	90	84	110, 181, 257, 309	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	343	PHE	3.8
1	C	353	ASN	3.1
1	B	231	ALA	2.1

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.