



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:53 PM UTC

PDB ID : 1QIU / pdb_00001qiu
Title : A triple beta-spiral in the adenovirus fibre shaft reveals a new structural motif for biological fibres
Authors : van Raaij, M.J.; Lavigne, G.; Mitraki, A.; Cusack, S.
Deposited on : 1999-06-16
Resolution : 2.40 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

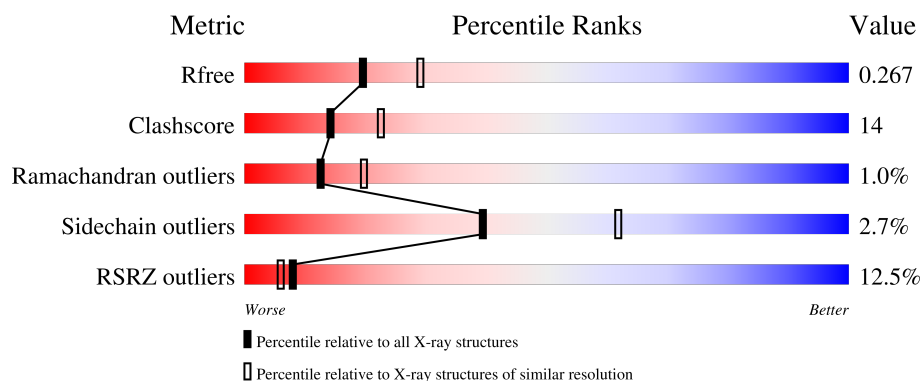
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	264	9% 70% 28% .
1	B	264	12% 68% 30% .
1	C	264	18% 75% 22% .
1	D	264	10% 73% 23% .
1	E	264	14% 67% 30% .

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Mol	Chain	Length	Quality of chain
1	F	264	12% 72% 25%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12621 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 ADENOVIRUS FIBRE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total 2007	C 1254	N 331	O 413	S 9	0	0	0
1	B	264	Total 2007	C 1254	N 331	O 413	S 9	0	0	0
1	C	264	Total 2007	C 1254	N 331	O 413	S 9	0	0	0
1	D	264	Total 2007	C 1254	N 331	O 413	S 9	0	0	0
1	E	264	Total 2007	C 1254	N 331	O 413	S 9	0	0	0
1	F	264	Total 2007	C 1254	N 331	O 413	S 9	0	0	0

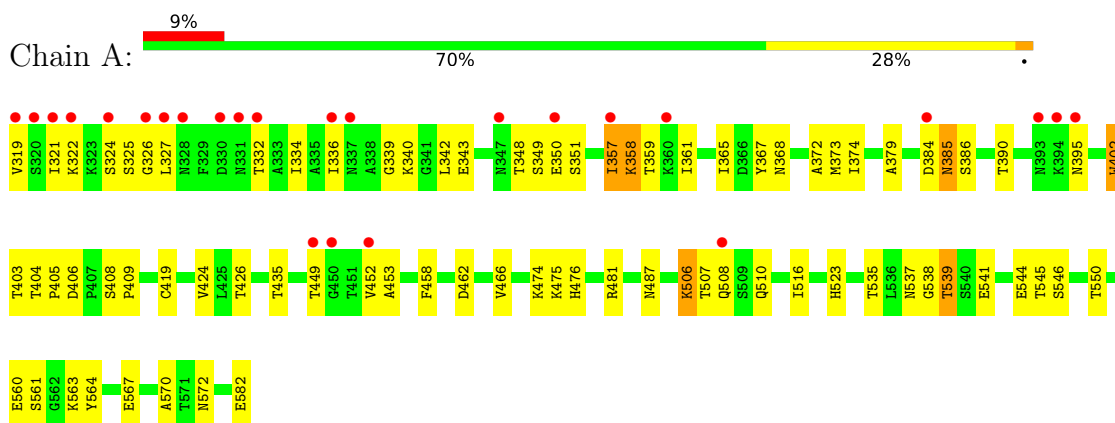
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	99	Total 99	O 99	0	0
2	B	96	Total 96	O 96	0	0
2	C	85	Total 85	O 85	0	0
2	D	95	Total 95	O 95	0	0
2	E	92	Total 92	O 92	0	0
2	F	112	Total 112	O 112	0	0

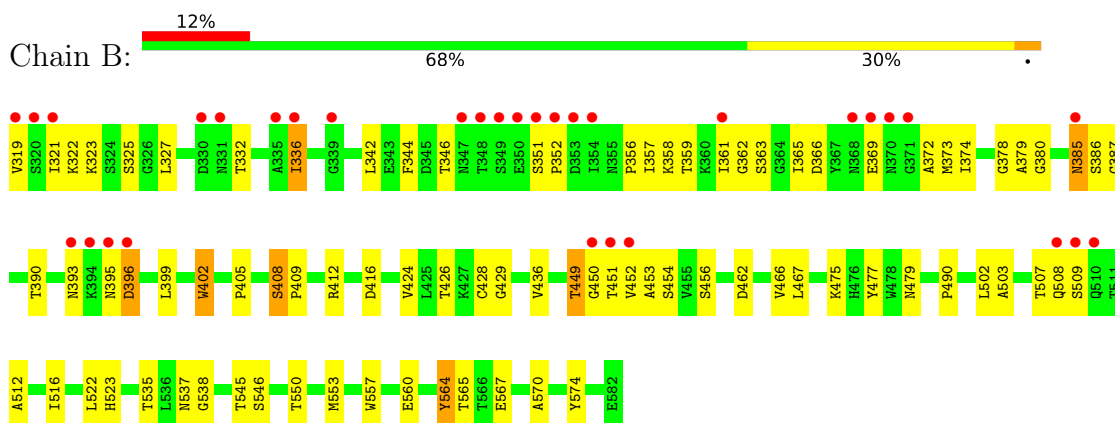
3 Residue-property plots

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

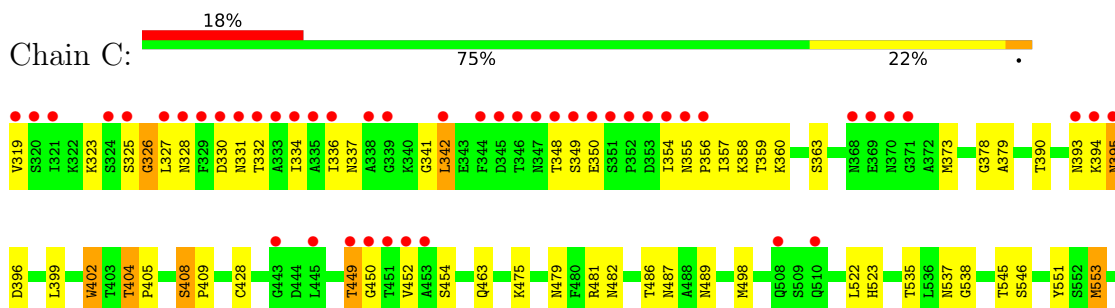
• Molecule 1: ADENOVIRUS FIBRE



• Molecule 1: ADENOVIRUS FIBRE

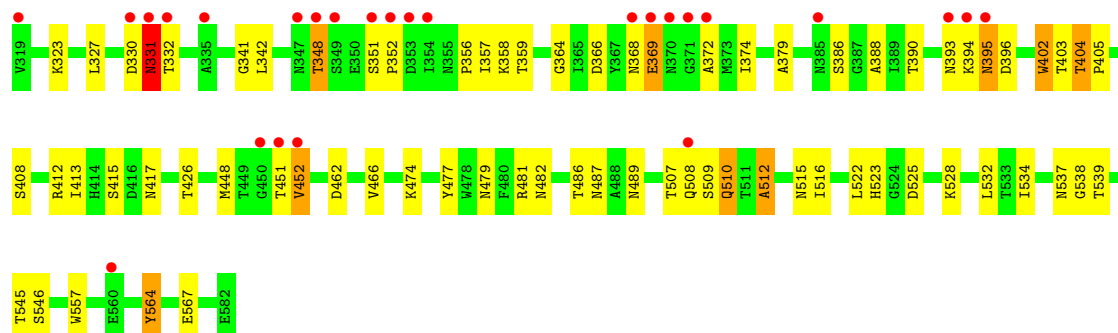
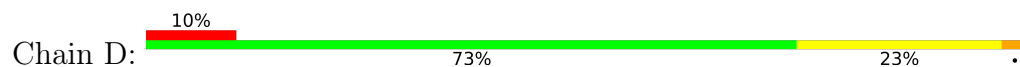


• Molecule 1: ADENOVIRUS FIBRE

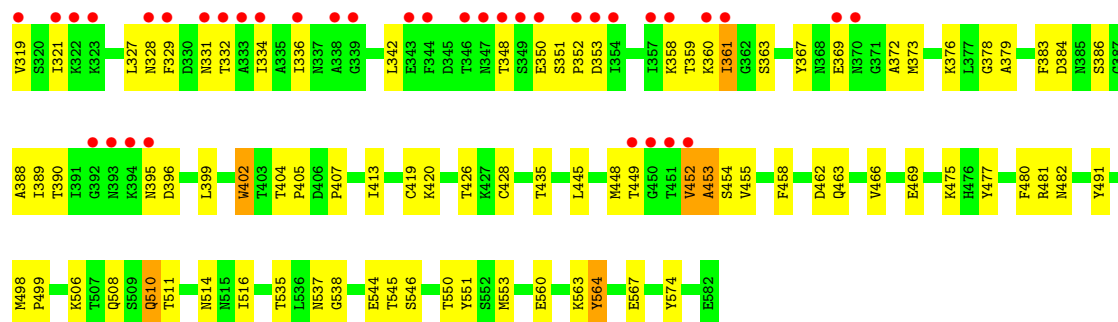




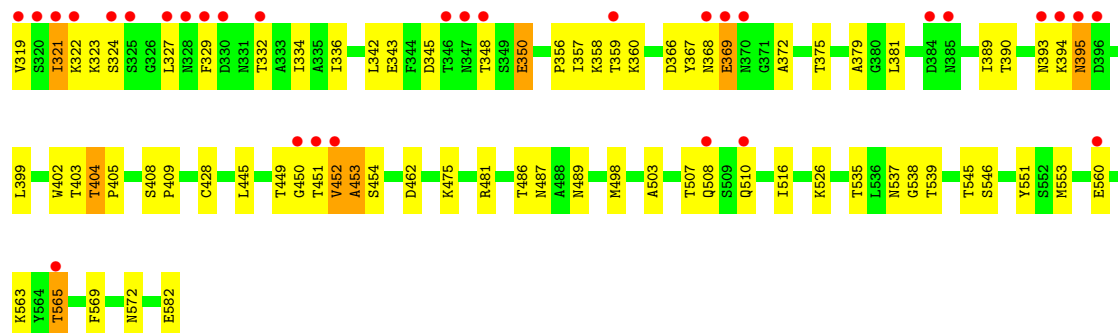
● Molecule 1: ADENOVIRUS FIBRE



● Molecule 1: ADENOVIRUS FIBRE



● Molecule 1: ADENOVIRUS FIBRE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	165.51Å 95.87Å 211.77Å 90.00° 106.83° 90.00°	Depositor
Resolution (Å)	25.00 – 2.40 25.00 – 2.41	Depositor EDS
% Data completeness (in resolution range)	84.0 (25.00-2.40) 84.0 (25.00-2.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.232 , 0.265 0.232 , 0.267	Depositor DCC
R_{free} test set	827 reflections (0.80%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 59.2	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12621	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.43	0/2046	0.96	8/2780 (0.3%)
1	B	0.44	0/2046	0.97	9/2780 (0.3%)
1	C	0.42	0/2046	0.95	8/2780 (0.3%)
1	D	0.44	0/2046	0.97	10/2780 (0.4%)
1	E	0.44	0/2046	0.97	8/2780 (0.3%)
1	F	0.42	0/2046	0.94	6/2780 (0.2%)
All	All	0.43	0/12276	0.96	49/16680 (0.3%)

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	475	LYS	N-CA-C	9.02	121.19	111.36
1	E	402	TRP	N-CA-C	7.05	117.34	108.45
1	B	449	THR	N-CA-C	7.00	119.22	108.30
1	C	475	LYS	N-CA-C	6.75	118.64	111.28
1	D	516	ILE	N-CA-C	-6.39	98.31	107.77
1	F	369	GLU	N-CA-C	-6.27	105.11	112.89
1	D	408	SER	N-CA-C	-6.18	99.96	109.41
1	D	369	GLU	N-CA-C	-6.14	104.70	111.82
1	C	402	TRP	N-CA-C	6.10	116.61	108.38
1	B	369	GLU	N-CA-C	-6.02	104.84	111.82
1	A	508	GLN	N-CA-C	-6.00	105.96	113.28
1	E	458	PHE	N-CA-C	5.95	119.09	109.40
1	F	451	THR	N-CA-C	-5.92	106.41	113.21
1	B	516	ILE	N-CA-C	-5.80	99.19	107.77
1	D	402	TRP	N-CA-C	5.79	116.20	108.38
1	B	408	SER	N-CA-C	-5.76	100.59	109.41
1	F	475	LYS	N-CA-C	5.75	117.54	111.28
1	A	476	HIS	N-CA-C	5.72	118.00	111.02
1	C	399	LEU	N-CA-C	-5.68	105.66	112.59
1	E	477	TYR	N-CA-C	5.65	118.95	112.57
1	F	516	ILE	N-CA-C	-5.63	99.39	107.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	ILE	N-CA-C	-5.62	99.45	107.77
1	C	489	ASN	CA-C-N	5.61	125.54	119.76
1	C	489	ASN	C-N-CA	5.61	125.54	119.76
1	E	516	ILE	N-CA-C	-5.57	100.09	108.12
1	D	477	TYR	N-CA-C	5.54	118.83	112.57
1	A	475	LYS	N-CA-C	5.50	119.15	112.23
1	F	399	LEU	N-CA-C	-5.48	105.90	112.59
1	D	512	ALA	N-CA-C	5.45	117.93	111.33
1	F	565	THR	N-CA-C	5.40	117.92	111.71
1	E	506	LYS	N-CA-C	-5.39	101.19	109.76
1	C	449	THR	N-CA-C	5.35	119.29	112.12
1	B	550	THR	N-CA-C	-5.34	106.45	113.12
1	D	489	ASN	CA-C-N	5.29	125.20	119.76
1	D	489	ASN	C-N-CA	5.29	125.20	119.76
1	B	402	TRP	N-CA-C	5.28	115.26	108.34
1	B	508	GLN	N-CA-C	-5.27	106.80	113.18
1	D	451	THR	N-CA-C	-5.23	106.76	112.72
1	E	369	GLU	N-CA-C	-5.21	105.78	111.82
1	E	550	THR	N-CA-C	-5.16	106.67	113.12
1	C	408	SER	N-CA-C	-5.12	101.58	109.41
1	A	550	THR	N-CA-C	-5.11	106.73	113.12
1	A	458	PHE	N-CA-C	5.08	117.53	109.50
1	B	399	LEU	N-CA-C	-5.08	106.39	112.59
1	D	508	GLN	N-CA-C	-5.02	107.12	113.20
1	A	402	TRP	N-CA-C	5.01	114.76	108.45
1	A	506	LYS	N-CA-C	-5.01	101.79	109.76
1	B	477	TYR	N-CA-C	5.01	119.07	112.25
1	C	326	GLY	N-CA-C	5.01	122.61	114.90

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	2007	0	1949	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2007	0	1949	76	0
1	C	2007	0	1949	63	0
1	D	2007	0	1949	60	0
1	E	2007	0	1949	74	0
1	F	2007	0	1949	72	0
2	A	99	0	0	4	0
2	B	96	0	0	3	0
2	C	85	0	0	0	0
2	D	95	0	0	2	0
2	E	92	0	0	1	0
2	F	112	0	0	7	0
All	All	12621	0	11694	336	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 14.

All (336) 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:321:ILE:HD11	1:B:327:LEU:HB3	1.45	0.98
1:A:321:ILE:HD11	1:A:334:ILE:HG12	1.51	0.92
1:B:336:ILE:HD11	1:C:326:GLY:HA3	1.47	0.92
1:A:336:ILE:HD11	1:B:336:ILE:HG22	1.51	0.91
1:A:560:GLU:HB2	1:A:563:LYS:HD2	1.56	0.88
1:C:350:GLU:HB2	1:C:354:ILE:HB	1.56	0.86
1:A:510:GLN:HE22	1:A:539:THR:HG21	1.41	0.84
1:F:560:GLU:HB2	1:F:563:LYS:HD2	1.62	0.81
1:A:326:GLY:HA3	1:C:336:ILE:HD11	1.63	0.80
1:D:417:ASN:HD21	1:D:474:LYS:HD2	1.52	0.74
1:E:462:ASP:OD2	1:E:466:VAL:HB	1.87	0.74
1:C:452:VAL:HG12	1:C:454:SER:H	1.51	0.74
1:B:452:VAL:HA	2:B:2031:HOH:O	1.88	0.73
1:A:368:ASN:HD21	1:A:372:ALA:HB3	1.54	0.73
1:F:449:THR:HB	1:F:452:VAL:HB	1.72	0.72
1:C:319:VAL:HG11	1:C:334:ILE:HD11	1.73	0.71
1:A:321:ILE:HD11	1:A:334:ILE:CG1	2.21	0.70
1:D:510:GLN:HA	1:D:510:GLN:HE21	1.57	0.70
1:B:359:THR:HG23	1:C:342:LEU:HD13	1.73	0.69
1:F:445:LEU:HD21	1:F:569:PHE:HB2	1.74	0.68
1:D:379:ALA:N	1:F:390:THR:HG22	2.08	0.68
1:F:342:LEU:O	1:F:343:GLU:HG3	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:390:THR:HG22	1:F:379:ALA:N	2.10	0.67
1:A:402:TRP:CZ2	1:A:481:ARG:HG3	2.31	0.66
1:F:322:LYS:HE3	1:F:324:SER:OG	1.95	0.66
1:F:321:ILE:HD11	1:F:334:ILE:HG23	1.77	0.66
1:B:356:PRO:HB3	1:C:337:ASN:ND2	2.10	0.66
1:E:402:TRP:CZ2	1:E:481:ARG:HG3	2.30	0.66
1:A:379:ALA:N	1:C:390:THR:HG22	2.12	0.65
1:A:545:THR:O	1:A:546:SER:HB2	1.95	0.65
1:C:348:THR:HG22	1:C:350:GLU:H	1.60	0.65
1:D:413:ILE:HD12	1:D:448:MET:HE1	1.78	0.65
1:E:449:THR:HB	1:E:452:VAL:HB	1.78	0.64
1:D:393:ASN:HB2	2:D:2015:HOH:O	1.96	0.64
1:E:321:ILE:HD11	1:E:334:ILE:HG12	1.78	0.64
1:E:564:TYR:HB3	1:E:567:GLU:HG3	1.78	0.64
1:E:361:ILE:HD12	1:E:367:TYR:CZ	2.33	0.64
1:D:394:LYS:O	1:D:395:ASN:HB2	1.97	0.64
1:B:374:ILE:HG22	1:C:363:SER:N	2.14	0.62
1:F:332:THR:O	1:F:332:THR:HG22	2.00	0.61
1:B:361:ILE:HD11	1:B:373:MET:SD	2.40	0.61
1:D:390:THR:HG22	1:E:379:ALA:N	2.14	0.61
1:D:402:TRP:CH2	1:D:405:PRO:HD3	2.35	0.61
1:D:404:THR:HG22	1:D:486:THR:HG23	1.82	0.61
1:A:449:THR:HB	1:A:452:VAL:O	2.00	0.61
1:F:368:ASN:ND2	1:F:369:GLU:H	1.97	0.61
1:E:348:THR:HG22	1:E:350:GLU:H	1.66	0.61
1:F:452:VAL:HG12	1:F:454:SER:H	1.64	0.61
1:E:560:GLU:HB3	1:E:563:LYS:HD2	1.83	0.61
1:B:449:THR:HB	1:B:452:VAL:HB	1.83	0.60
1:C:332:THR:O	1:C:332:THR:HG22	2.01	0.60
1:F:368:ASN:HD22	1:F:369:GLU:H	1.48	0.60
1:B:358:LYS:HD2	1:B:359:THR:O	2.02	0.60
1:D:357:ILE:O	1:E:342:LEU:HD12	2.02	0.60
1:F:452:VAL:HG12	1:F:454:SER:N	2.15	0.60
1:F:452:VAL:HA	2:F:2045:HOH:O	1.99	0.60
1:B:336:ILE:HG12	1:C:325:SER:O	2.01	0.60
1:A:342:LEU:HD12	1:C:358:LYS:HA	1.82	0.60
1:E:508:GLN:CD	1:E:508:GLN:H	2.09	0.59
1:D:368:ASN:OD1	1:D:369:GLU:N	2.35	0.59
1:E:510:GLN:HA	1:E:510:GLN:HE21	1.67	0.59
1:A:332:THR:O	1:A:332:THR:HG22	2.02	0.59
1:B:361:ILE:HG23	1:B:365:ILE:HB	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:GLN:HE22	1:A:539:THR:CG2	2.15	0.59
1:A:319:VAL:HG13	1:A:334:ILE:HD11	1.84	0.58
1:A:507:THR:H	1:A:538:GLY:HA2	1.68	0.58
1:C:393:ASN:HB3	1:C:396:ASP:O	2.03	0.58
1:C:449:THR:HB	1:C:452:VAL:O	2.03	0.58
1:F:359:THR:HG23	1:F:367:TYR:OH	2.03	0.58
1:A:390:THR:HG22	1:B:378:GLY:HA3	1.85	0.58
1:A:426:THR:HG21	1:B:428:CYS:O	2.04	0.58
1:A:324:SER:HA	1:C:355:ASN:HB2	1.85	0.57
1:A:336:ILE:HD11	1:B:336:ILE:CG2	2.29	0.57
1:F:452:VAL:O	1:F:453:ALA:HB3	2.04	0.57
1:B:336:ILE:HG23	1:C:327:LEU:HD11	1.86	0.57
1:F:375:THR:HG21	1:F:389:ILE:HD11	1.86	0.57
1:A:510:GLN:NE2	1:A:539:THR:OG1	2.38	0.57
1:E:545:THR:O	1:E:546:SER:HB2	2.05	0.57
1:E:327:LEU:HD23	1:E:336:ILE:HA	1.86	0.56
1:E:342:LEU:HD23	1:E:359:THR:HA	1.87	0.56
1:A:523:HIS:CD2	1:A:570:ALA:HB3	2.40	0.56
1:B:545:THR:O	1:B:546:SER:HB2	2.06	0.56
1:E:510:GLN:HE21	1:E:510:GLN:CA	2.16	0.56
1:A:358:LYS:HD3	1:A:359:THR:O	2.06	0.56
1:D:372:ALA:HA	1:E:360:LYS:HG3	1.88	0.56
1:D:379:ALA:H	1:F:390:THR:HG22	1.71	0.55
1:C:450:GLY:C	1:C:452:VAL:H	2.14	0.55
1:D:510:GLN:HE21	1:D:510:GLN:CA	2.19	0.55
1:A:357:ILE:O	1:B:342:LEU:HD12	2.06	0.55
1:E:452:VAL:O	1:E:453:ALA:HB3	2.05	0.55
1:B:462:ASP:OD2	1:B:466:VAL:HB	2.07	0.55
1:A:359:THR:CG2	1:C:373:MET:HE2	2.36	0.55
1:C:402:TRP:CH2	1:C:405:PRO:HD3	2.41	0.55
1:D:374:ILE:HG22	1:E:363:SER:N	2.21	0.54
1:E:361:ILE:HD11	1:E:373:MET:HG2	1.90	0.54
1:D:510:GLN:HG2	1:D:539:THR:HG21	1.89	0.54
1:D:374:ILE:HG22	1:E:363:SER:H	1.71	0.54
1:A:321:ILE:CD1	1:A:334:ILE:HG12	2.33	0.54
1:A:506:LYS:HG3	1:A:541:GLU:HG3	1.90	0.54
1:D:390:THR:HG22	1:E:379:ALA:H	1.72	0.54
1:A:340:LYS:O	1:C:358:LYS:HB2	2.08	0.54
1:F:319:VAL:HA	2:F:2002:HOH:O	2.08	0.54
1:C:545:THR:O	1:C:546:SER:HB2	2.09	0.53
1:A:405:PRO:HB2	1:B:503:ALA:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:LEU:O	1:B:475:LYS:HE3	2.08	0.53
1:A:385:ASN:HD22	1:A:386:SER:N	2.07	0.53
1:C:522:LEU:HG	1:C:523:HIS:CD2	2.44	0.53
1:C:349:SER:HB3	1:C:350:GLU:OE2	2.08	0.53
1:E:358:LYS:HA	1:F:342:LEU:HD12	1.90	0.53
1:B:323:LYS:HA	1:B:327:LEU:O	2.09	0.52
1:A:325:SER:O	1:C:336:ILE:HG12	2.09	0.52
1:A:384:ASP:OD2	1:A:386:SER:HB3	2.08	0.52
1:B:390:THR:HG22	1:C:379:ALA:N	2.25	0.52
1:D:388:ALA:HB2	1:E:376:LYS:HG2	1.92	0.52
1:A:343:GLU:OE2	1:A:358:LYS:HD2	2.09	0.52
1:B:452:VAL:O	1:B:453:ALA:HB3	2.09	0.52
1:E:321:ILE:HD11	1:E:334:ILE:CG1	2.39	0.52
1:D:452:VAL:HG13	2:D:2025:HOH:O	2.09	0.52
1:D:357:ILE:O	1:D:357:ILE:HG23	2.09	0.51
1:F:560:GLU:HB2	1:F:563:LYS:CD	2.35	0.51
1:B:327:LEU:HD23	1:B:336:ILE:HG22	1.92	0.51
1:C:330:ASP:O	1:C:331:ASN:HB3	2.10	0.51
1:F:366:ASP:OD1	1:F:367:TYR:N	2.44	0.51
1:A:535:THR:HG21	1:A:539:THR:HG22	1.90	0.51
1:F:327:LEU:HD23	1:F:336:ILE:HA	1.93	0.51
1:A:368:ASN:ND2	1:A:372:ALA:HB3	2.22	0.51
1:A:453:ALA:HB2	1:A:561:SER:HA	1.92	0.51
1:A:462:ASP:OD2	1:A:466:VAL:HB	2.11	0.51
1:C:498:MET:HG3	1:C:551:TYR:CD2	2.46	0.51
1:A:406:ASP:HB2	1:B:502:LEU:HB3	1.92	0.51
1:C:408:SER:O	1:C:409:PRO:C	2.53	0.51
1:B:402:TRP:CH2	1:B:405:PRO:HD3	2.46	0.51
1:D:479:ASN:ND2	1:D:487:ASN:HB3	2.26	0.51
1:B:408:SER:O	1:B:409:PRO:C	2.52	0.51
1:A:359:THR:HG21	1:A:373:MET:SD	2.50	0.50
1:E:449:THR:O	1:E:452:VAL:HG23	2.11	0.50
1:E:560:GLU:O	1:E:563:LYS:HB2	2.11	0.50
1:F:404:THR:HG22	1:F:486:THR:HG23	1.93	0.50
1:A:582:GLU:HB3	2:A:2097:HOH:O	2.10	0.50
1:D:358:LYS:HD2	1:D:359:THR:O	2.10	0.50
1:A:390:THR:HG22	1:B:379:ALA:N	2.26	0.50
1:A:564:TYR:HB3	1:A:567:GLU:HG3	1.92	0.50
1:B:436:VAL:HG12	1:B:574:TYR:HB3	1.93	0.50
1:C:402:TRP:CZ2	1:C:481:ARG:HG3	2.46	0.50
1:D:342:LEU:HD12	1:F:357:ILE:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:SER:HB2	1:B:352:PRO:HA	1.94	0.49
1:D:417:ASN:ND2	1:D:474:LYS:HD2	2.25	0.49
1:D:512:ALA:O	1:F:572:ASN:HA	2.12	0.49
1:F:408:SER:O	1:F:409:PRO:C	2.55	0.49
1:F:445:LEU:CD2	1:F:569:PHE:HB2	2.41	0.49
1:A:327:LEU:HD21	1:C:336:ILE:HG23	1.94	0.49
1:B:450:GLY:O	1:B:452:VAL:HG23	2.12	0.49
1:C:404:THR:HG22	1:C:486:THR:HG23	1.93	0.49
1:D:402:TRP:CZ2	1:D:481:ARG:HG3	2.48	0.49
1:D:545:THR:O	1:D:546:SER:HB2	2.13	0.49
1:E:445:LEU:HD12	1:E:564:TYR:O	2.12	0.49
1:B:321:ILE:HG22	1:F:489:ASN:OD1	2.11	0.49
1:B:380:GLY:H	1:B:393:ASN:ND2	2.11	0.49
1:D:394:LYS:O	1:D:395:ASN:CB	2.58	0.49
1:E:328:ASN:OD1	1:E:329:PHE:N	2.39	0.49
1:D:532:LEU:HD13	1:D:557:TRP:CE2	2.48	0.49
1:D:364:GLY:HA3	1:F:375:THR:HG22	1.93	0.48
1:E:481:ARG:HG2	1:E:482:ASN:N	2.27	0.48
1:F:450:GLY:C	1:F:452:VAL:H	2.21	0.48
1:A:408:SER:O	1:A:409:PRO:C	2.56	0.48
1:C:537:ASN:O	1:C:538:GLY:C	2.55	0.48
1:D:323:LYS:HA	1:D:327:LEU:O	2.14	0.48
1:F:348:THR:HG22	1:F:350:GLU:H	1.78	0.48
1:B:535:THR:O	1:B:553:MET:HA	2.13	0.48
1:C:463:GLN:CD	1:C:463:GLN:H	2.22	0.48
1:D:341:GLY:HA3	1:F:359:THR:HG22	1.95	0.48
1:D:372:ALA:CB	1:E:360:LYS:HG3	2.43	0.48
1:D:348:THR:HG21	1:D:356:PRO:CD	2.43	0.47
1:D:426:THR:HG21	1:E:428:CYS:O	2.13	0.47
1:A:507:THR:N	1:A:538:GLY:HA2	2.28	0.47
1:D:330:ASP:O	1:D:331:ASN:CB	2.61	0.47
1:A:374:ILE:HG22	1:B:363:SER:N	2.29	0.47
1:A:403:THR:O	1:A:404:THR:OG1	2.26	0.47
1:D:341:GLY:HA3	1:F:359:THR:CG2	2.45	0.47
1:F:323:LYS:HA	1:F:327:LEU:O	2.13	0.47
1:F:453:ALA:HB3	2:F:2044:HOH:O	2.14	0.47
1:A:395:ASN:HB2	2:A:2015:HOH:O	2.14	0.47
1:E:413:ILE:HD12	1:E:448:MET:HE1	1.97	0.47
1:E:537:ASN:O	1:E:538:GLY:C	2.57	0.47
1:F:358:LYS:HD2	1:F:358:LYS:C	2.40	0.47
1:F:402:TRP:CZ2	1:F:481:ARG:HG3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:THR:HG22	1:B:332:THR:O	2.14	0.47
1:E:402:TRP:CH2	1:E:405:PRO:HD3	2.50	0.47
1:F:394:LYS:HB3	2:F:2060:HOH:O	2.14	0.47
1:D:386:SER:HB3	1:E:376:LYS:NZ	2.30	0.46
1:B:319:VAL:HG21	1:C:319:VAL:HG22	1.97	0.46
1:B:372:ALA:HA	1:C:360:LYS:HG2	1.97	0.46
1:C:479:ASN:HB3	1:C:486:THR:HB	1.98	0.46
1:D:462:ASP:OD2	1:D:466:VAL:HB	2.16	0.46
1:B:385:ASN:C	1:B:387:GLY:H	2.24	0.46
1:B:564:TYR:HB3	1:B:567:GLU:HG3	1.97	0.46
1:A:334:ILE:HG22	1:B:327:LEU:CD1	2.45	0.46
1:B:322:LYS:HD3	2:B:2001:HOH:O	2.15	0.46
1:B:537:ASN:O	1:B:538:GLY:C	2.57	0.46
1:B:374:ILE:HG22	1:C:363:SER:H	1.81	0.46
1:C:323:LYS:HA	1:C:327:LEU:O	2.14	0.46
1:D:537:ASN:O	1:D:538:GLY:C	2.59	0.46
1:F:403:THR:O	1:F:404:THR:OG1	2.29	0.46
1:F:510:GLN:HG2	1:F:539:THR:HG21	1.98	0.46
1:B:359:THR:HG23	1:C:342:LEU:CD1	2.42	0.45
1:D:390:THR:HG22	1:E:378:GLY:HA3	1.98	0.45
1:D:510:GLN:HA	1:D:510:GLN:NE2	2.28	0.45
1:F:545:THR:O	1:F:546:SER:HB2	2.16	0.45
1:B:323:LYS:C	1:B:325:SER:H	2.24	0.45
1:D:507:THR:HG23	1:D:509:SER:O	2.17	0.45
1:D:393:ASN:HB3	1:D:396:ASP:O	2.16	0.45
1:E:452:VAL:O	1:E:453:ALA:CB	2.64	0.45
1:F:394:LYS:O	1:F:395:ASN:O	2.35	0.45
1:A:334:ILE:O	1:B:327:LEU:HD12	2.17	0.45
1:D:327:LEU:HG	1:F:336:ILE:HG13	1.98	0.45
1:E:463:GLN:CD	1:E:463:GLN:H	2.25	0.45
1:F:402:TRP:CH2	1:F:405:PRO:HD3	2.51	0.45
1:A:374:ILE:HG22	1:B:363:SER:H	1.81	0.45
1:D:403:THR:O	1:D:404:THR:OG1	2.33	0.45
1:E:480:PHE:CE2	1:E:491:TYR:HB2	2.52	0.45
1:A:321:ILE:HD11	1:A:334:ILE:CD1	2.47	0.45
1:F:357:ILE:O	1:F:357:ILE:HG23	2.17	0.45
1:A:339:GLY:N	1:C:357:ILE:O	2.46	0.44
1:A:474:LYS:HE2	2:A:2043:HOH:O	2.17	0.44
1:E:384:ASP:OD2	1:E:388:ALA:HB3	2.17	0.44
1:F:321:ILE:HB	1:F:329:PHE:CZ	2.52	0.44
1:F:452:VAL:O	1:F:453:ALA:CB	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:TRP:CD1	1:A:402:TRP:C	2.96	0.44
1:E:361:ILE:HD12	1:E:367:TYR:CE1	2.52	0.44
1:E:351:SER:HB3	1:E:352:PRO:HA	1.99	0.44
1:B:522:LEU:O	1:B:523:HIS:HB2	2.18	0.44
1:E:390:THR:HG22	1:F:379:ALA:H	1.81	0.44
1:A:348:THR:O	1:A:349:SER:C	2.61	0.44
1:E:348:THR:HG21	2:E:2008:HOH:O	2.18	0.44
1:F:498:MET:HG3	1:F:551:TYR:CD2	2.53	0.44
1:A:322:LYS:HG3	1:C:330:ASP:OD2	2.18	0.44
1:B:523:HIS:CE1	1:B:570:ALA:HB3	2.53	0.44
1:D:372:ALA:CA	1:E:360:LYS:HG3	2.48	0.44
1:F:582:GLU:OXT	1:F:582:GLU:HG3	2.17	0.44
1:E:321:ILE:HD12	1:E:329:PHE:CZ	2.52	0.44
1:E:404:THR:O	1:E:407:PRO:HD3	2.18	0.44
1:E:498:MET:HG3	1:E:551:TYR:CD2	2.53	0.43
1:B:321:ILE:HG22	1:F:489:ASN:CG	2.44	0.43
1:B:412:ARG:HD2	1:B:416:ASP:OD1	2.18	0.43
1:D:481:ARG:HG2	1:D:482:ASN:N	2.33	0.43
1:E:510:GLN:HA	1:E:510:GLN:NE2	2.30	0.43
1:D:330:ASP:O	1:D:331:ASN:HB2	2.18	0.43
1:D:522:LEU:HG	1:D:523:HIS:CD2	2.54	0.43
1:E:407:PRO:O	1:E:420:LYS:HD3	2.18	0.43
1:F:321:ILE:HD12	1:F:334:ILE:HG12	1.99	0.43
1:A:572:ASN:HA	1:B:512:ALA:O	2.19	0.43
1:C:482:ASN:HB2	1:C:487:ASN:HD22	1.82	0.43
1:C:358:LYS:HD2	1:C:359:THR:O	2.18	0.43
1:D:545:THR:O	1:D:546:SER:CB	2.66	0.43
1:A:321:ILE:CG2	1:A:327:LEU:HB2	2.49	0.43
1:B:560:GLU:HB3	2:B:2089:HOH:O	2.19	0.43
1:E:399:LEU:HD23	1:E:399:LEU:HA	1.84	0.43
1:E:426:THR:HG21	1:F:428:CYS:O	2.18	0.43
1:E:511:THR:O	1:E:514:ASN:HB2	2.18	0.43
1:F:507:THR:HG22	1:F:538:GLY:HA2	2.00	0.43
1:C:394:LYS:O	1:C:395:ASN:HB2	2.19	0.43
1:D:412:ARG:HG3	1:D:415:SER:O	2.18	0.43
1:E:498:MET:HA	1:E:499:PRO:HD3	1.88	0.43
1:F:345:ASP:HB3	1:F:356:PRO:HD2	2.01	0.43
1:A:357:ILE:H	1:A:357:ILE:HG13	1.65	0.43
1:C:564:TYR:HB3	1:C:567:GLU:HG3	2.00	0.43
1:E:405:PRO:HB2	1:F:503:ALA:HB2	2.01	0.43
1:A:385:ASN:HD22	1:A:385:ASN:C	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:THR:HG21	1:C:428:CYS:O	2.19	0.42
1:F:535:THR:O	1:F:553:MET:HA	2.19	0.42
1:F:537:ASN:O	1:F:538:GLY:C	2.62	0.42
1:B:450:GLY:C	1:B:452:VAL:N	2.76	0.42
1:E:319:VAL:HG21	1:F:319:VAL:HG22	2.01	0.42
1:E:359:THR:HG23	1:F:342:LEU:HG	2.01	0.42
1:E:372:ALA:HA	1:F:360:LYS:HG3	2.01	0.42
1:D:390:THR:CG2	1:E:378:GLY:HA3	2.49	0.42
1:A:322:LYS:HD3	1:A:322:LYS:HA	1.84	0.42
1:A:424:VAL:HB	1:A:435:THR:HG22	2.01	0.42
1:C:450:GLY:C	1:C:452:VAL:N	2.74	0.42
1:F:449:THR:O	1:F:452:VAL:HG23	2.19	0.42
1:F:462:ASP:HB2	2:F:2049:HOH:O	2.19	0.42
2:A:2018:HOH:O	1:B:429:GLY:HA3	2.19	0.42
1:C:341:GLY:O	1:C:342:LEU:HD12	2.19	0.42
1:E:351:SER:HA	1:E:353:ASP:N	2.34	0.42
1:E:389:ILE:O	1:F:381:LEU:HD12	2.19	0.42
1:B:319:VAL:CG2	1:C:319:VAL:HG22	2.50	0.42
1:B:424:VAL:HG21	1:C:579:ILE:CD1	2.50	0.42
1:F:368:ASN:N	1:F:372:ALA:O	2.51	0.42
1:A:334:ILE:HG22	1:B:327:LEU:HD11	2.01	0.42
1:F:368:ASN:ND2	1:F:369:GLU:N	2.65	0.42
1:B:507:THR:OG1	1:B:509:SER:HB3	2.20	0.42
1:C:402:TRP:CD1	1:C:402:TRP:C	2.98	0.42
1:E:402:TRP:CD1	1:E:402:TRP:C	2.98	0.42
1:E:435:THR:HA	1:E:574:TYR:O	2.19	0.42
1:B:454:SER:HA	1:B:557:TRP:O	2.19	0.42
1:D:525:ASP:OD2	1:D:528:LYS:HE2	2.19	0.42
1:D:564:TYR:HB3	1:D:567:GLU:HG3	2.01	0.42
1:F:350:GLU:HB3	2:F:2013:HOH:O	2.19	0.42
1:A:537:ASN:O	1:A:538:GLY:C	2.62	0.42
1:B:344:PHE:O	1:B:346:THR:HG23	2.19	0.42
1:B:390:THR:HG22	1:C:378:GLY:HA3	2.02	0.42
1:B:395:ASN:O	1:B:396:ASP:HB2	2.20	0.42
1:D:372:ALA:HB2	1:E:360:LYS:HG3	2.02	0.41
1:F:368:ASN:HD22	1:F:369:GLU:N	2.14	0.41
1:B:336:ILE:HG23	1:C:327:LEU:CD1	2.50	0.41
1:B:424:VAL:HG21	1:C:579:ILE:HD11	2.01	0.41
1:D:515:ASN:HA	1:D:534:ILE:O	2.20	0.41
1:E:383:PHE:HA	1:E:388:ALA:O	2.20	0.41
1:B:450:GLY:C	1:B:452:VAL:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:SER:HB3	1:D:352:PRO:HA	2.02	0.41
1:F:560:GLU:HG2	1:F:563:LYS:HZ1	1.85	0.41
1:C:394:LYS:H	1:C:394:LYS:HG2	1.46	0.41
1:D:332:THR:O	1:D:332:THR:HG22	2.20	0.41
1:C:326:GLY:O	1:C:327:LEU:HD12	2.20	0.41
1:C:535:THR:O	1:C:553:MET:HA	2.20	0.41
1:A:379:ALA:H	1:C:390:THR:HG22	1.85	0.41
1:A:361:ILE:HD11	1:A:367:TYR:CE2	2.56	0.41
1:B:321:ILE:CD1	1:B:327:LEU:HB3	2.33	0.41
1:B:336:ILE:HD12	1:B:357:ILE:HD12	2.03	0.41
1:B:452:VAL:HG12	1:B:454:SER:N	2.35	0.41
1:B:545:THR:O	1:B:546:SER:CB	2.67	0.41
1:E:321:ILE:HD11	1:E:334:ILE:CD1	2.51	0.41
1:E:402:TRP:CD1	1:E:404:THR:H	2.39	0.41
1:E:452:VAL:HG12	1:E:454:SER:N	2.35	0.41
1:F:526:LYS:HG2	2:F:2095:HOH:O	2.20	0.41
1:C:354:ILE:HG22	1:C:356:PRO:HD3	2.02	0.41
1:A:384:ASP:C	1:A:386:SER:H	2.29	0.40
1:A:365:ILE:HD12	1:C:373:MET:O	2.21	0.40
1:B:361:ILE:HG22	1:B:362:GLY:N	2.36	0.40
1:B:479:ASN:HD21	1:B:490:PRO:HA	1.86	0.40
1:C:560:GLU:CD	1:C:563:LYS:HZ3	2.24	0.40
1:A:351:SER:O	1:E:386:SER:CB	2.70	0.40
1:E:331:ASN:O	1:E:332:THR:HB	2.21	0.40
1:E:372:ALA:HA	1:F:360:LYS:CG	2.52	0.40
1:E:535:THR:O	1:E:553:MET:HA	2.21	0.40
1:B:336:ILE:CG1	1:C:325:SER:O	2.67	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	262/264 (99%)	241 (92%)	21 (8%)	0	100	100
1	B	262/264 (99%)	230 (88%)	30 (12%)	2 (1%)	16	25
1	C	262/264 (99%)	234 (89%)	26 (10%)	2 (1%)	16	25
1	D	262/264 (99%)	235 (90%)	23 (9%)	4 (2%)	8	12
1	E	262/264 (99%)	238 (91%)	21 (8%)	3 (1%)	11	18
1	F	262/264 (99%)	242 (92%)	16 (6%)	4 (2%)	8	12
All	All	1572/1584 (99%)	1420 (90%)	137 (9%)	15 (1%)	12	20

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	395	ASN
1	E	452	VAL
1	F	395	ASN
1	D	331	ASN
1	D	395	ASN
1	E	453	ALA
1	F	452	VAL
1	B	396	ASP
1	F	453	ALA
1	B	386	SER
1	C	395	ASN
1	D	348	THR
1	D	404	THR
1	C	404	THR
1	F	404	THR

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	228/228 (100%)	220 (96%)	8 (4%)	32	53
1	B	228/228 (100%)	221 (97%)	7 (3%)	35	57
1	C	228/228 (100%)	225 (99%)	3 (1%)	61	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	228/228 (100%)	223 (98%)	5 (2%)	45	67
1	E	228/228 (100%)	220 (96%)	8 (4%)	32	53
1	F	228/228 (100%)	222 (97%)	6 (3%)	40	63
All	All	1368/1368 (100%)	1331 (97%)	37 (3%)	39	62

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	350	GLU
1	A	357	ILE
1	A	358	LYS
1	A	385	ASN
1	A	419	CYS
1	A	487	ASN
1	A	539	THR
1	A	544	GLU
1	B	336	ILE
1	B	366	ASP
1	B	385	ASN
1	B	451	THR
1	B	456	SER
1	B	564	TYR
1	B	565	THR
1	C	328	ASN
1	C	342	LEU
1	C	553	MET
1	D	331	ASN
1	D	366	ASP
1	D	452	VAL
1	D	510	GLN
1	D	564	TYR
1	E	361	ILE
1	E	396	ASP
1	E	419	CYS
1	E	455	VAL
1	E	469	GLU
1	E	510	GLN
1	E	544	GLU
1	E	564	TYR
1	F	321	ILE
1	F	350	GLU

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Mol	Chain	Res	Type
1	F	393	ASN
1	F	487	ASN
1	F	508	GLN
1	F	565	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	385	ASN
1	A	393	ASN
1	A	417	ASN
1	A	482	ASN
1	A	510	GLN
1	A	515	ASN
1	A	523	HIS
1	B	331	ASN
1	B	337	ASN
1	B	370	ASN
1	B	393	ASN
1	B	464	ASN
1	B	482	ASN
1	C	328	ASN
1	C	337	ASN
1	C	355	ASN
1	C	370	ASN
1	C	464	ASN
1	C	476	HIS
1	C	487	ASN
1	C	515	ASN
1	C	519	GLN
1	D	337	ASN
1	D	370	ASN
1	D	393	ASN
1	D	417	ASN
1	D	476	HIS
1	D	482	ASN
1	D	508	GLN
1	D	510	GLN
1	D	515	ASN
1	E	370	ASN
1	E	395	ASN
1	E	417	ASN

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Mol	Chain	Res	Type
1	E	464	ASN
1	E	476	HIS
1	E	487	ASN
1	E	510	GLN
1	E	515	ASN
1	E	519	GLN
1	F	337	ASN
1	F	347	ASN
1	F	368	ASN
1	F	370	ASN
1	F	385	ASN
1	F	464	ASN
1	F	482	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	264/264 (100%)	0.29	25 (9%) 14 11	7, 29, 68, 89	0
1	B	264/264 (100%)	0.34	32 (12%) 8 6	10, 31, 68, 87	0
1	C	264/264 (100%)	0.49	47 (17%) 4 3	11, 30, 75, 89	0
1	D	264/264 (100%)	0.30	26 (9%) 13 10	9, 31, 68, 90	0
1	E	264/264 (100%)	0.46	37 (14%) 6 5	10, 31, 75, 89	0
1	F	264/264 (100%)	0.30	31 (11%) 9 7	10, 30, 66, 76	0
All	All	1584/1584 (100%)	0.36	198 (12%) 8 6	7, 30, 72, 90	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	354	ILE	5.7
1	E	332	THR	5.7
1	D	508	GLN	5.5
1	A	321	ILE	5.4
1	E	354	ILE	5.3
1	C	352	PRO	5.3
1	A	452	VAL	5.1
1	B	395	ASN	4.8
1	D	452	VAL	4.7
1	D	394	LYS	4.7
1	B	508	GLN	4.7
1	C	452	VAL	4.6
1	E	395	ASN	4.6
1	A	322	LYS	4.4
1	D	352	PRO	4.4
1	E	331	ASN	4.3
1	F	450	GLY	4.3
1	C	333	ALA	4.3
1	C	351	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	319	VAL	4.2
1	E	338	ALA	4.2
1	E	394	LYS	4.0
1	A	320	SER	3.9
1	E	353	ASP	3.8
1	E	352	PRO	3.8
1	B	394	LYS	3.7
1	B	348	THR	3.6
1	D	353	ASP	3.6
1	B	320	SER	3.6
1	B	451	THR	3.5
1	E	449	THR	3.5
1	D	370	ASN	3.5
1	E	361	ILE	3.5
1	F	451	THR	3.5
1	C	331	ASN	3.5
1	C	368	ASN	3.4
1	E	357	ILE	3.4
1	B	335	ALA	3.4
1	B	370	ASN	3.4
1	D	395	ASN	3.4
1	C	394	LYS	3.4
1	B	321	ILE	3.4
1	C	451	THR	3.3
1	B	393	ASN	3.3
1	E	452	VAL	3.3
1	A	350	GLU	3.3
1	F	384	ASP	3.3
1	C	319	VAL	3.3
1	F	395	ASN	3.2
1	B	352	PRO	3.2
1	D	385	ASN	3.2
1	C	332	THR	3.2
1	C	355	ASN	3.2
1	D	371	GLY	3.2
1	C	508	GLN	3.2
1	E	346	THR	3.2
1	F	321	ILE	3.2
1	E	333	ALA	3.1
1	C	356	PRO	3.1
1	B	452	VAL	3.1
1	E	450	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	328	ASN	3.1
1	D	393	ASN	3.1
1	E	349	SER	3.1
1	B	349	SER	3.1
1	C	349	SER	3.0
1	D	450	GLY	3.0
1	F	319	VAL	3.0
1	F	348	THR	3.0
1	C	327	LEU	3.0
1	D	368	ASN	3.0
1	C	346	THR	3.0
1	A	384	ASP	3.0
1	D	351	SER	3.0
1	C	450	GLY	3.0
1	E	369	GLU	2.9
1	E	451	THR	2.9
1	C	330	ASP	2.9
1	F	452	VAL	2.9
1	F	327	LEU	2.9
1	B	353	ASP	2.9
1	F	330	ASP	2.9
1	C	329	PHE	2.9
1	D	348	THR	2.9
1	D	349	SER	2.8
1	E	393	ASN	2.8
1	B	319	VAL	2.8
1	F	510	GLN	2.8
1	C	334	ILE	2.8
1	D	354	ILE	2.8
1	E	344	PHE	2.8
1	E	348	THR	2.8
1	F	369	GLU	2.8
1	C	339	GLY	2.7
1	C	342	LEU	2.7
1	D	451	THR	2.7
1	D	347	ASN	2.7
1	F	508	GLN	2.7
1	F	385	ASN	2.7
1	B	450	GLY	2.7
1	E	347	ASN	2.7
1	E	358	LYS	2.7
1	F	393	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	350	GLU	2.7
1	B	361	ILE	2.6
1	B	368	ASN	2.6
1	B	369	GLU	2.6
1	D	335	ALA	2.6
1	E	322	LYS	2.6
1	C	336	ILE	2.6
1	A	327	LEU	2.6
1	A	324	SER	2.6
1	C	353	ASP	2.6
1	E	370	ASN	2.6
1	F	370	ASN	2.6
1	F	322	LYS	2.6
1	A	450	GLY	2.6
1	C	371	GLY	2.6
1	E	334	ILE	2.6
1	C	395	ASN	2.6
1	D	332	THR	2.6
1	F	332	THR	2.6
1	A	360	LYS	2.6
1	F	329	PHE	2.5
1	A	332	THR	2.5
1	B	510	GLN	2.5
1	A	393	ASN	2.5
1	E	323	LYS	2.5
1	C	338	ALA	2.5
1	B	354	ILE	2.5
1	B	331	ASN	2.5
1	C	348	THR	2.5
1	A	508	GLN	2.5
1	E	339	GLY	2.4
1	C	393	ASN	2.4
1	F	328	ASN	2.4
1	D	560	GLU	2.4
1	D	330	ASP	2.4
1	C	328	ASN	2.4
1	C	320	SER	2.4
1	B	330	ASP	2.4
1	A	337	ASN	2.4
1	A	357	ILE	2.3
1	D	319	VAL	2.3
1	C	370	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	369	GLU	2.3
1	C	453	ALA	2.3
1	A	330	ASP	2.3
1	E	328	ASN	2.3
1	F	320	SER	2.3
1	B	385	ASN	2.3
1	D	331	ASN	2.3
1	E	321	ILE	2.3
1	D	372	ALA	2.2
1	C	321	ILE	2.2
1	C	324	SER	2.2
1	C	345	ASP	2.2
1	E	329	PHE	2.2
1	E	319	VAL	2.2
1	A	395	ASN	2.2
1	F	565	THR	2.2
1	A	394	LYS	2.2
1	C	325	SER	2.2
1	F	324	SER	2.2
1	B	396	ASP	2.2
1	E	360	LYS	2.2
1	B	339	GLY	2.2
1	F	396	ASP	2.2
1	C	510	GLN	2.2
1	A	449	THR	2.2
1	F	347	ASN	2.1
1	E	392	GLY	2.1
1	D	369	GLU	2.1
1	E	343	GLU	2.1
1	B	351	SER	2.1
1	A	331	ASN	2.1
1	C	347	ASN	2.1
1	C	443	GLY	2.1
1	C	445	LEU	2.1
1	F	346	THR	2.1
1	C	350	GLU	2.1
1	B	347	ASN	2.1
1	A	336	ILE	2.1
1	E	336	ILE	2.1
1	F	325	SER	2.1
1	F	368	ASN	2.1
1	B	336	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	344	PHE	2.0
1	C	335	ALA	2.0
1	A	347	ASN	2.0
1	A	326	GLY	2.0
1	B	350	GLU	2.0
1	B	371	GLY	2.0
1	B	509	SER	2.0
1	F	394	LYS	2.0
1	F	560	GLU	2.0
1	C	449	THR	2.0
1	F	359	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.