



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:06 PM EDT

PDB ID : 3CNC / pdb_00003cnc
Title : Crystal Structure of Ad16 fiber knob
Authors : Pache, L.; Venkataraman, S.; Nemerow, G.R.; Reddy, V.S.
Deposited on : 2008-03-25
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

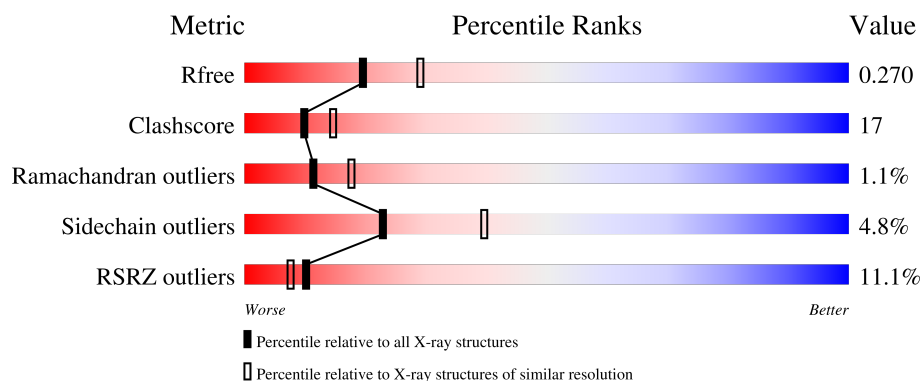
1 Overall quality at a glance

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	220	
1	B	220	
1	C	220	
1	D	220	
1	E	220	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	220	16% 58% 27% 5% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9268 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	196	Total	C	N	O	S	0	0	0
			1528	971	239	309	9			
1	B	196	Total	C	N	O	S	0	0	0
			1528	971	239	309	9			
1	C	196	Total	C	N	O	S	0	0	0
			1528	971	239	309	9			
1	D	196	Total	C	N	O	S	0	0	0
			1528	971	239	309	9			
1	E	196	Total	C	N	O	S	0	0	0
			1528	971	239	309	9			
1	F	196	Total	C	N	O	S	0	0	0
			1528	971	239	309	9			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	134	GLY	-	expression tag	UNP Q67711
A	135	SER	-	expression tag	UNP Q67711
A	136	HIS	-	expression tag	UNP Q67711
A	137	MET	-	expression tag	UNP Q67711
A	138	ALA	-	expression tag	UNP Q67711
A	139	SER	-	expression tag	UNP Q67711
A	140	MET	-	expression tag	UNP Q67711
A	141	THR	-	expression tag	UNP Q67711
A	142	GLY	-	expression tag	UNP Q67711
A	143	GLY	-	expression tag	UNP Q67711
A	144	GLN	-	expression tag	UNP Q67711
A	145	GLN	-	expression tag	UNP Q67711
A	146	MET	-	expression tag	UNP Q67711
A	147	GLY	-	expression tag	UNP Q67711
A	148	ARG	-	expression tag	UNP Q67711
A	149	GLY	-	expression tag	UNP Q67711
A	150	SER	-	expression tag	UNP Q67711

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	134	GLY	-	expression tag	UNP Q67711
B	135	SER	-	expression tag	UNP Q67711
B	136	HIS	-	expression tag	UNP Q67711
B	137	MET	-	expression tag	UNP Q67711
B	138	ALA	-	expression tag	UNP Q67711
B	139	SER	-	expression tag	UNP Q67711
B	140	MET	-	expression tag	UNP Q67711
B	141	THR	-	expression tag	UNP Q67711
B	142	GLY	-	expression tag	UNP Q67711
B	143	GLY	-	expression tag	UNP Q67711
B	144	GLN	-	expression tag	UNP Q67711
B	145	GLN	-	expression tag	UNP Q67711
B	146	MET	-	expression tag	UNP Q67711
B	147	GLY	-	expression tag	UNP Q67711
B	148	ARG	-	expression tag	UNP Q67711
B	149	GLY	-	expression tag	UNP Q67711
B	150	SER	-	expression tag	UNP Q67711
C	134	GLY	-	expression tag	UNP Q67711
C	135	SER	-	expression tag	UNP Q67711
C	136	HIS	-	expression tag	UNP Q67711
C	137	MET	-	expression tag	UNP Q67711
C	138	ALA	-	expression tag	UNP Q67711
C	139	SER	-	expression tag	UNP Q67711
C	140	MET	-	expression tag	UNP Q67711
C	141	THR	-	expression tag	UNP Q67711
C	142	GLY	-	expression tag	UNP Q67711
C	143	GLY	-	expression tag	UNP Q67711
C	144	GLN	-	expression tag	UNP Q67711
C	145	GLN	-	expression tag	UNP Q67711
C	146	MET	-	expression tag	UNP Q67711
C	147	GLY	-	expression tag	UNP Q67711
C	148	ARG	-	expression tag	UNP Q67711
C	149	GLY	-	expression tag	UNP Q67711
C	150	SER	-	expression tag	UNP Q67711
D	134	GLY	-	expression tag	UNP Q67711
D	135	SER	-	expression tag	UNP Q67711
D	136	HIS	-	expression tag	UNP Q67711
D	137	MET	-	expression tag	UNP Q67711
D	138	ALA	-	expression tag	UNP Q67711
D	139	SER	-	expression tag	UNP Q67711
D	140	MET	-	expression tag	UNP Q67711
D	141	THR	-	expression tag	UNP Q67711

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	142	GLY	-	expression tag	UNP Q67711
D	143	GLY	-	expression tag	UNP Q67711
D	144	GLN	-	expression tag	UNP Q67711
D	145	GLN	-	expression tag	UNP Q67711
D	146	MET	-	expression tag	UNP Q67711
D	147	GLY	-	expression tag	UNP Q67711
D	148	ARG	-	expression tag	UNP Q67711
D	149	GLY	-	expression tag	UNP Q67711
D	150	SER	-	expression tag	UNP Q67711
E	134	GLY	-	expression tag	UNP Q67711
E	135	SER	-	expression tag	UNP Q67711
E	136	HIS	-	expression tag	UNP Q67711
E	137	MET	-	expression tag	UNP Q67711
E	138	ALA	-	expression tag	UNP Q67711
E	139	SER	-	expression tag	UNP Q67711
E	140	MET	-	expression tag	UNP Q67711
E	141	THR	-	expression tag	UNP Q67711
E	142	GLY	-	expression tag	UNP Q67711
E	143	GLY	-	expression tag	UNP Q67711
E	144	GLN	-	expression tag	UNP Q67711
E	145	GLN	-	expression tag	UNP Q67711
E	146	MET	-	expression tag	UNP Q67711
E	147	GLY	-	expression tag	UNP Q67711
E	148	ARG	-	expression tag	UNP Q67711
E	149	GLY	-	expression tag	UNP Q67711
E	150	SER	-	expression tag	UNP Q67711
F	134	GLY	-	expression tag	UNP Q67711
F	135	SER	-	expression tag	UNP Q67711
F	136	HIS	-	expression tag	UNP Q67711
F	137	MET	-	expression tag	UNP Q67711
F	138	ALA	-	expression tag	UNP Q67711
F	139	SER	-	expression tag	UNP Q67711
F	140	MET	-	expression tag	UNP Q67711
F	141	THR	-	expression tag	UNP Q67711
F	142	GLY	-	expression tag	UNP Q67711
F	143	GLY	-	expression tag	UNP Q67711
F	144	GLN	-	expression tag	UNP Q67711
F	145	GLN	-	expression tag	UNP Q67711
F	146	MET	-	expression tag	UNP Q67711
F	147	GLY	-	expression tag	UNP Q67711
F	148	ARG	-	expression tag	UNP Q67711
F	149	GLY	-	expression tag	UNP Q67711

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	150	SER	-	expression tag	UNP Q67711

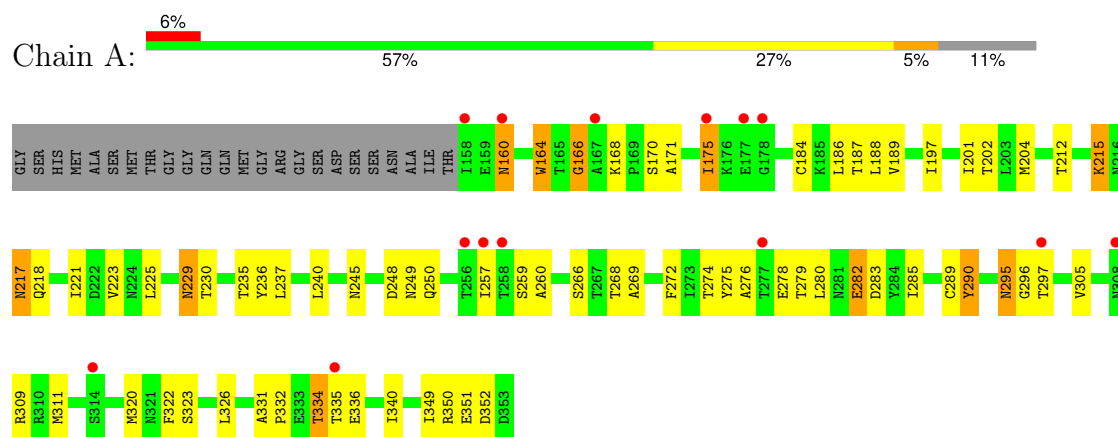
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	27	Total O 27 27	0	0
2	B	10	Total O 10 10	0	0
2	C	13	Total O 13 13	0	0
2	D	26	Total O 26 26	0	0
2	E	12	Total O 12 12	0	0
2	F	12	Total O 12 12	0	0

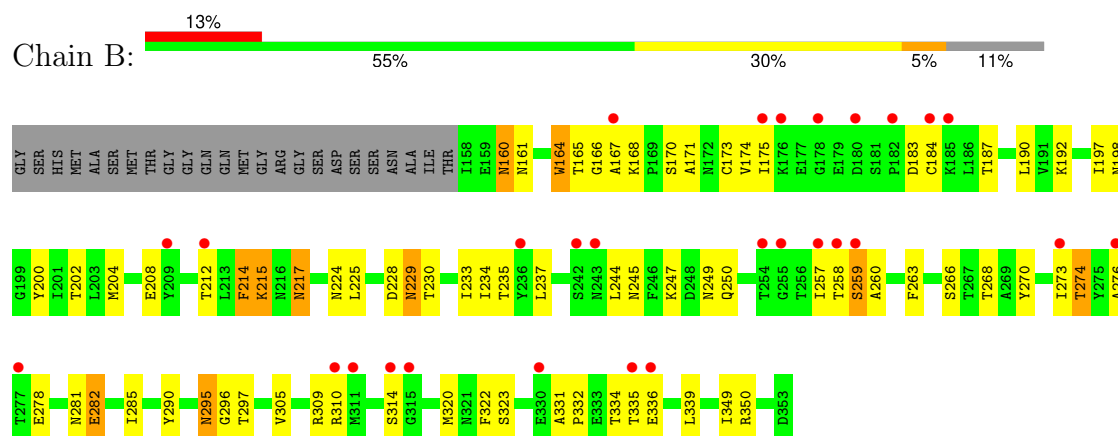
3 Residue-property plots [i](#)

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.

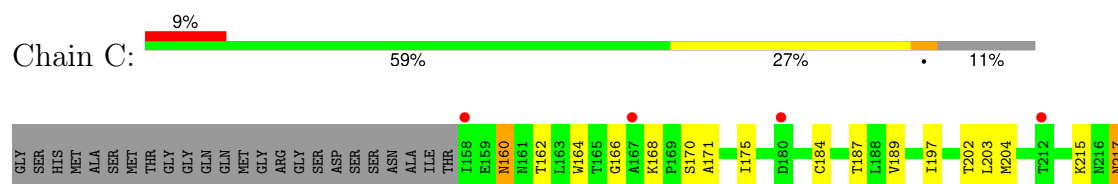
• Molecule 1: Fiber protein



• Molecule 1: Fiber protein



• Molecule 1: Fiber protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	167.83Å 167.83Å 262.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.32 – 2.40 49.32 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.32-2.40) 99.8 (49.32-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.39Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.245 , 0.272 0.241 , 0.270	Depositor DCC
R_{free} test set	4323 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	60.2	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9268	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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	0.47	0/1559	1.07	8/2121 (0.4%)
1	B	0.44	0/1559	0.98	12/2121 (0.6%)
1	C	0.44	0/1559	1.05	14/2121 (0.7%)
1	D	0.49	0/1559	1.11	9/2121 (0.4%)
1	E	0.43	0/1559	1.00	8/2121 (0.4%)
1	F	0.44	0/1559	1.02	6/2121 (0.3%)
All	All	0.45	0/9354	1.04	57/12726 (0.4%)

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	308	ASN	N-CA-C	13.34	130.94	108.67
1	C	260	ALA	N-CA-C	-7.90	101.12	111.71
1	C	215	LYS	N-CA-C	-7.75	103.41	113.17
1	C	235	THR	N-CA-C	7.50	120.41	111.33
1	E	276	ALA	N-CA-C	7.43	120.09	111.02
1	F	215	LYS	N-CA-C	-7.21	103.64	113.30
1	A	235	THR	N-CA-C	7.20	119.75	111.11
1	D	307	LEU	N-CA-C	-7.19	97.88	109.96
1	A	215	LYS	N-CA-C	-7.13	104.19	113.17
1	F	260	ALA	N-CA-C	-6.99	101.91	111.56
1	D	164	TRP	N-CA-C	6.84	118.19	108.74
1	D	260	ALA	N-CA-C	-6.74	102.25	111.56
1	C	276	ALA	N-CA-C	6.70	118.47	111.03
1	E	215	LYS	N-CA-C	-6.66	104.90	113.16
1	D	215	LYS	N-CA-C	-6.63	104.81	113.17
1	B	215	LYS	N-CA-C	-6.59	104.81	112.92
1	A	290	TYR	N-CA-C	6.52	119.08	109.24
1	A	260	ALA	N-CA-C	-6.46	102.64	111.56
1	E	260	ALA	N-CA-C	-6.45	103.52	112.30
1	E	290	TYR	N-CA-C	6.38	118.87	109.24
1	B	235	THR	N-CA-C	6.36	119.03	111.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	166	GLY	N-CA-C	-6.28	104.77	112.68
1	C	264	MET	CA-C-N	6.20	126.41	119.90
1	C	264	MET	C-N-CA	6.20	126.41	119.90
1	D	161	ASN	N-CA-C	-6.16	105.41	113.17
1	A	334	THR	N-CA-C	-6.13	107.02	114.75
1	A	166	GLY	N-CA-C	-6.13	104.96	112.68
1	C	251	ASN	N-CA-C	6.09	118.72	109.95
1	B	260	ALA	N-CA-C	-6.07	104.05	112.30
1	B	161	ASN	N-CA-C	-6.05	105.66	113.16
1	F	308	ASN	CB-CA-C	-6.04	109.59	116.54
1	C	164	TRP	N-CA-C	5.92	117.78	108.96
1	C	239	SER	N-CA-C	-5.85	104.86	112.23
1	C	308	ASN	CB-CA-C	-5.76	109.39	117.23
1	E	331	ALA	CA-C-N	5.72	125.40	119.05
1	E	331	ALA	C-N-CA	5.72	125.40	119.05
1	F	161	ASN	N-CA-C	-5.70	105.66	113.30
1	B	164	TRP	N-CA-C	5.66	116.55	108.74
1	A	164	TRP	N-CA-C	5.63	116.51	108.74
1	B	166	GLY	N-CA-C	-5.58	105.65	112.68
1	F	235	THR	N-CA-C	5.56	118.86	111.75
1	D	290	TYR	N-CA-C	5.54	117.83	109.41
1	B	290	TYR	N-CA-C	5.41	117.41	109.24
1	E	164	TRP	N-CA-C	5.34	116.11	108.74
1	E	334	THR	N-CA-C	-5.30	106.71	114.39
1	F	329	GLU	N-CA-C	-5.29	105.60	111.36
1	B	270	TYR	CA-C-N	5.20	125.18	120.03
1	B	270	TYR	C-N-CA	5.20	125.18	120.03
1	D	308	ASN	CB-CA-C	-5.15	110.22	117.23
1	C	334	THR	N-CA-C	-5.15	106.92	114.39
1	C	252	MET	N-CA-C	-5.14	101.33	109.96
1	B	334	THR	N-CA-C	-5.13	108.04	114.56
1	A	276	ALA	N-CA-C	5.13	119.83	111.37
1	C	290	TYR	N-CA-C	5.09	116.93	109.24
1	B	314	SER	N-CA-C	5.09	117.56	111.71
1	D	310	ARG	N-CA-C	5.07	117.00	108.73
1	B	165	THR	N-CA-C	-5.05	107.12	113.28

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	1528	0	1485	53	0
1	B	1528	0	1485	67	0
1	C	1528	0	1485	54	0
1	D	1528	0	1485	53	0
1	E	1528	0	1485	62	0
1	F	1528	0	1485	58	0
2	A	27	0	0	0	0
2	B	10	0	0	1	0
2	C	13	0	0	1	0
2	D	26	0	0	0	0
2	E	12	0	0	0	0
2	F	12	0	0	0	0
All	All	9268	0	8910	316	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 17.

All (316) 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:F:295:ASN:HD21	1:F:297:THR:HG23	1.18	1.04
1:C:187:THR:HB	1:C:202:THR:HG22	1.39	0.99
1:F:295:ASN:ND2	1:F:297:THR:HG23	1.81	0.95
1:A:187:THR:HB	1:A:202:THR:HG22	1.49	0.94
1:F:174:VAL:HA	1:F:183:ASP:OD1	1.68	0.93
1:F:335:THR:HG22	1:F:336:GLU:H	1.35	0.92
1:B:212:THR:HG23	1:B:215:LYS:HE2	1.53	0.91
1:B:187:THR:HB	1:B:202:THR:HG22	1.51	0.90
1:D:175:ILE:HD13	1:D:184:CYS:SG	2.14	0.87
1:D:295:ASN:HD22	1:D:296:GLY:N	1.73	0.85
1:E:187:THR:HB	1:E:202:THR:HG22	1.59	0.85
1:E:217:ASN:HD22	1:E:217:ASN:H	1.24	0.84
1:D:295:ASN:ND2	1:D:297:THR:H	1.77	0.83
1:E:245:ASN:HA	1:E:257:ILE:HD11	1.62	0.82
1:C:217:ASN:HD22	1:C:217:ASN:H	1.28	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:184:CYS:HB2	1:F:205:GLY:HA2	1.61	0.80
1:B:160:ASN:H	1:B:160:ASN:HD22	1.28	0.80
1:E:197:ILE:HG12	1:E:350:ARG:HB3	1.65	0.79
1:C:295:ASN:C	1:C:295:ASN:HD22	1.90	0.78
1:B:160:ASN:HD22	1:B:160:ASN:N	1.81	0.78
1:E:295:ASN:C	1:E:295:ASN:HD22	1.89	0.77
1:B:295:ASN:ND2	1:B:297:THR:H	1.84	0.77
1:C:232:GLN:HE22	1:C:257:ILE:HB	1.51	0.76
1:C:175:ILE:HD13	1:C:184:CYS:SG	2.26	0.76
1:B:273:ILE:HD11	1:B:309:ARG:HH12	1.50	0.76
1:F:273:ILE:HA	1:F:278:GLU:OE1	1.85	0.76
1:D:232:GLN:HE22	1:D:257:ILE:HB	1.54	0.73
1:E:160:ASN:HA	1:E:246:PHE:CD2	2.24	0.72
1:B:273:ILE:HD11	1:B:309:ARG:NH1	2.03	0.72
1:B:320:MET:HE3	1:B:322:PHE:HZ	1.52	0.72
1:C:335:THR:HG22	1:C:336:GLU:H	1.54	0.72
1:B:160:ASN:H	1:B:160:ASN:ND2	1.88	0.71
1:C:274:THR:HG23	1:C:275:TYR:HD1	1.55	0.71
1:B:175:ILE:HD13	1:B:184:CYS:SG	2.31	0.71
1:F:335:THR:HG22	1:F:336:GLU:N	2.04	0.71
1:F:295:ASN:C	1:F:295:ASN:HD22	1.98	0.71
1:B:295:ASN:C	1:B:295:ASN:HD22	2.00	0.70
1:A:295:ASN:C	1:A:295:ASN:HD22	1.99	0.70
1:A:295:ASN:HD22	1:A:296:GLY:N	1.91	0.69
1:F:228:ASP:OD2	1:F:232:GLN:HB2	1.94	0.68
1:D:208:GLU:HG3	1:D:336:GLU:OE2	1.94	0.67
1:F:245:ASN:HA	1:F:257:ILE:HD11	1.74	0.67
1:D:295:ASN:HD22	1:D:295:ASN:C	1.99	0.67
1:F:311:MET:HA	1:F:316:MET:HE2	1.77	0.66
1:B:217:ASN:H	1:B:217:ASN:HD22	1.43	0.66
1:D:295:ASN:HD21	1:D:297:THR:H	1.42	0.66
1:D:335:THR:HG22	1:D:336:GLU:H	1.59	0.66
1:A:245:ASN:HA	1:A:257:ILE:HD11	1.78	0.66
1:D:217:ASN:H	1:D:217:ASN:HD22	1.42	0.66
1:E:335:THR:HG22	1:E:336:GLU:H	1.60	0.66
1:B:229:ASN:N	1:B:229:ASN:HD22	1.93	0.66
1:B:320:MET:HE3	1:B:322:PHE:CZ	2.31	0.65
1:E:175:ILE:HG12	1:E:221:ILE:HG23	1.78	0.65
1:A:274:THR:HG23	1:A:275:TYR:HD1	1.61	0.65
1:F:245:ASN:CG	1:F:257:ILE:HD11	2.22	0.65
1:A:217:ASN:HD22	1:A:217:ASN:H	1.44	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:MET:HA	1:B:339:LEU:O	1.98	0.64
1:C:335:THR:HG22	1:C:336:GLU:N	2.13	0.63
1:C:316:MET:HE3	1:C:319:ALA:HB2	1.79	0.63
1:A:295:ASN:C	1:A:295:ASN:ND2	2.57	0.62
1:F:278:GLU:HG2	1:F:280:LEU:HG	1.82	0.62
1:D:316:MET:HE2	1:D:319:ALA:HB2	1.81	0.62
1:A:295:ASN:ND2	1:A:297:THR:H	1.97	0.62
1:D:217:ASN:HD22	1:D:217:ASN:N	1.97	0.62
1:E:279:THR:O	1:E:309:ARG:NH1	2.33	0.61
1:B:187:THR:HB	1:B:202:THR:CG2	2.27	0.61
1:B:217:ASN:HD22	1:B:217:ASN:N	1.95	0.61
1:E:304:THR:HB	1:E:323:SER:OG	2.01	0.61
1:C:197:ILE:HG12	1:C:350:ARG:HB3	1.83	0.61
1:B:160:ASN:N	1:B:160:ASN:ND2	2.49	0.60
1:B:335:THR:HG22	1:B:336:GLU:N	2.17	0.60
1:D:269:ALA:HA	1:F:168:LYS:HG2	1.84	0.60
1:D:187:THR:HB	1:D:202:THR:HG22	1.84	0.60
1:E:217:ASN:HD22	1:E:217:ASN:N	1.97	0.59
1:B:217:ASN:H	1:B:217:ASN:ND2	2.00	0.59
1:C:295:ASN:C	1:C:295:ASN:ND2	2.55	0.59
1:B:295:ASN:ND2	1:B:295:ASN:C	2.59	0.59
1:D:293:SER:OG	1:D:295:ASN:ND2	2.36	0.59
1:A:212:THR:HG23	1:A:215:LYS:HE2	1.84	0.59
1:B:197:ILE:HG12	1:B:350:ARG:HB3	1.83	0.59
1:F:160:ASN:N	1:F:160:ASN:HD22	1.99	0.59
1:A:175:ILE:HD13	1:A:184:CYS:SG	2.43	0.58
1:C:222:ASP:OD1	1:C:323:SER:HB3	2.03	0.58
1:B:190:LEU:HD21	1:B:320:MET:HE1	1.85	0.58
1:F:212:THR:HG23	1:F:215:LYS:HE2	1.86	0.58
1:C:274:THR:HG23	1:C:275:TYR:CD1	2.38	0.58
1:B:234:ILE:HG21	1:B:237:LEU:HD12	1.86	0.58
1:E:230:THR:HB	1:E:259:SER:HA	1.85	0.58
1:D:217:ASN:H	1:D:217:ASN:ND2	2.02	0.57
1:F:245:ASN:OD1	1:F:257:ILE:HD11	2.04	0.57
1:B:214:PHE:O	1:B:332:PRO:HD2	2.04	0.57
1:D:295:ASN:ND2	1:D:297:THR:HG23	2.19	0.57
1:D:320:MET:HE3	1:D:322:PHE:HZ	1.68	0.57
1:F:229:ASN:N	1:F:229:ASN:HD22	2.02	0.57
1:B:202:THR:HG21	2:B:79:HOH:O	2.04	0.57
1:B:192:LYS:HE3	1:B:263:PHE:CE1	2.39	0.57
1:E:175:ILE:CG1	1:E:221:ILE:HG23	2.34	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:GLN:NE2	1:B:266:SER:OG	2.37	0.57
1:C:221:ILE:O	1:C:323:SER:HA	2.04	0.57
1:A:175:ILE:HD11	1:A:223:VAL:HG22	1.86	0.56
1:A:320:MET:HE3	1:A:322:PHE:CZ	2.41	0.56
1:E:174:VAL:HA	1:E:183:ASP:OD1	2.04	0.56
1:E:295:ASN:C	1:E:295:ASN:ND2	2.60	0.56
1:E:204:MET:HE2	1:E:340:ILE:HD11	1.87	0.56
1:B:249:ASN:HA	1:C:352:ASP:OD2	2.05	0.56
1:C:295:ASN:HD22	1:C:296:GLY:N	2.04	0.56
1:A:204:MET:HE3	1:B:282:GLU:HG2	1.88	0.55
1:C:320:MET:HE3	1:C:322:PHE:CZ	2.41	0.55
1:F:197:ILE:HG12	1:F:350:ARG:HB3	1.87	0.55
1:E:304:THR:HB	1:E:323:SER:HG	1.71	0.55
1:F:335:THR:CG2	1:F:336:GLU:H	2.13	0.55
1:C:229:ASN:HD22	1:C:229:ASN:N	2.04	0.55
1:D:204:MET:CE	1:E:282:GLU:HG2	2.37	0.55
1:F:273:ILE:HG13	1:F:309:ARG:O	2.06	0.55
1:A:221:ILE:O	1:A:323:SER:HA	2.07	0.54
1:A:189:VAL:HG21	1:B:349:ILE:CD1	2.36	0.54
1:B:229:ASN:ND2	1:B:229:ASN:H	2.06	0.54
1:A:268:THR:HB	1:C:250:GLN:HE21	1.72	0.54
1:D:311:MET:HE2	1:D:316:MET:HG2	1.90	0.54
1:D:168:LYS:HG3	1:E:268:THR:O	2.08	0.54
1:D:230:THR:HB	1:D:259:SER:HA	1.90	0.54
1:D:295:ASN:ND2	1:D:295:ASN:C	2.63	0.53
1:D:316:MET:CE	1:D:319:ALA:HB2	2.37	0.53
1:E:186:LEU:HD11	1:E:201:ILE:HD11	1.91	0.53
1:E:274:THR:HG22	1:E:275:TYR:HD1	1.73	0.53
1:F:275:TYR:HE2	1:F:277:THR:HG23	1.74	0.53
1:D:190:LEU:HD21	1:D:320:MET:HE1	1.91	0.53
1:E:204:MET:HA	1:E:339:LEU:O	2.09	0.53
1:F:295:ASN:ND2	1:F:295:ASN:C	2.65	0.52
1:E:168:LYS:HG2	1:F:269:ALA:HA	1.91	0.52
1:C:245:ASN:HA	1:C:257:ILE:HD11	1.90	0.52
1:C:295:ASN:ND2	1:C:297:THR:H	2.06	0.52
1:B:229:ASN:N	1:B:229:ASN:ND2	2.56	0.52
1:C:285:ILE:HB	1:C:305:VAL:HB	1.92	0.52
1:E:339:LEU:HD12	1:E:340:ILE:N	2.25	0.52
1:E:160:ASN:HA	1:E:246:PHE:HD2	1.74	0.51
1:A:186:LEU:HD23	1:A:240:LEU:HD13	1.92	0.51
1:C:232:GLN:HE22	1:C:257:ILE:CB	2.19	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:VAL:HG11	1:E:179:GLU:O	2.10	0.51
1:F:217:ASN:N	1:F:217:ASN:HD22	2.07	0.51
1:E:204:MET:CE	1:F:282:GLU:HG2	2.41	0.51
1:E:164:TRP:CE2	1:E:166:GLY:HA2	2.46	0.51
1:B:208:GLU:HG3	1:B:336:GLU:OE2	2.11	0.51
1:D:311:MET:HE2	1:D:316:MET:CG	2.41	0.50
1:C:217:ASN:H	1:C:217:ASN:ND2	2.05	0.50
1:A:266:SER:OG	1:C:250:GLN:NE2	2.44	0.50
1:E:229:ASN:HD22	1:E:230:THR:N	2.10	0.50
1:A:229:ASN:HD22	1:A:230:THR:N	2.09	0.50
1:C:273:ILE:HG23	1:C:278:GLU:HB3	1.93	0.50
1:F:175:ILE:HD13	1:F:184:CYS:SG	2.52	0.50
1:C:162:THR:O	1:C:246:PHE:HA	2.12	0.49
1:C:320:MET:HE3	1:C:322:PHE:HZ	1.76	0.49
1:F:295:ASN:HD21	1:F:297:THR:CG2	2.07	0.49
1:A:197:ILE:HG12	1:A:350:ARG:HB3	1.94	0.49
1:C:270:TYR:OH	1:C:349:ILE:HG12	2.12	0.49
1:E:334:THR:HG22	1:E:334:THR:O	2.13	0.49
1:A:282:GLU:HG2	1:C:204:MET:CE	2.42	0.49
1:B:244:LEU:O	1:B:257:ILE:HD11	2.12	0.49
1:B:167:ALA:O	1:B:168:LYS:C	2.55	0.49
1:B:295:ASN:HD22	1:B:296:GLY:N	2.11	0.49
1:E:224:ASN:C	1:E:225:LEU:HD12	2.38	0.48
1:B:258:THR:O	1:B:259:SER:HB3	2.14	0.48
1:A:335:THR:HG22	1:A:336:GLU:H	1.79	0.48
1:D:160:ASN:N	1:D:160:ASN:HD22	2.10	0.48
1:E:212:THR:HG23	1:E:215:LYS:HE2	1.95	0.48
1:E:283:ASP:OD2	1:E:309:ARG:HG3	2.14	0.48
1:E:335:THR:HG22	1:E:336:GLU:N	2.26	0.48
1:A:250:GLN:HE21	1:B:268:THR:HB	1.78	0.48
1:C:299:PHE:CE2	1:C:332:PRO:HG3	2.49	0.48
1:D:282:GLU:HG2	1:F:204:MET:CE	2.44	0.48
1:F:245:ASN:HA	1:F:257:ILE:CD1	2.40	0.48
1:C:187:THR:HB	1:C:202:THR:CG2	2.27	0.48
1:F:222:ASP:OD1	1:F:323:SER:HB3	2.14	0.48
1:B:245:ASN:HA	1:B:257:ILE:HD11	1.95	0.47
1:C:299:PHE:CD2	1:C:332:PRO:HG3	2.49	0.47
1:D:304:THR:HB	1:D:323:SER:OG	2.14	0.47
1:E:308:ASN:HA	1:E:319:ALA:HB3	1.96	0.47
1:B:250:GLN:HE21	1:C:268:THR:HB	1.79	0.47
1:F:285:ILE:HB	1:F:305:VAL:HB	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:ASN:HD22	1:E:160:ASN:C	2.22	0.47
1:E:246:PHE:CE1	1:E:257:ILE:HG23	2.50	0.47
1:A:160:ASN:N	1:A:160:ASN:HD22	2.12	0.47
1:A:278:GLU:HG2	1:A:280:LEU:HG	1.96	0.47
1:B:285:ILE:HB	1:B:305:VAL:HB	1.97	0.47
1:F:164:TRP:CE2	1:F:166:GLY:HA2	2.50	0.47
1:B:170:SER:O	1:B:171:ALA:C	2.58	0.47
1:A:164:TRP:CE2	1:A:166:GLY:HA2	2.50	0.46
1:B:173:CYS:HB3	1:B:184:CYS:SG	2.55	0.46
1:D:320:MET:HE3	1:D:322:PHE:CZ	2.49	0.46
1:E:224:ASN:HA	1:E:321:ASN:OD1	2.15	0.46
1:F:175:ILE:CD1	1:F:184:CYS:SG	3.03	0.46
1:E:273:ILE:HD12	1:E:310:ARG:HG2	1.96	0.46
1:B:192:LYS:HA	1:B:197:ILE:HD13	1.98	0.46
1:B:164:TRP:CZ2	1:B:247:LYS:HG3	2.51	0.46
1:F:237:LEU:HD11	1:F:313:ALA:HB3	1.97	0.46
1:B:228:ASP:OD1	1:B:228:ASP:C	2.58	0.46
1:F:225:LEU:HB2	1:F:320:MET:O	2.16	0.46
1:B:274:THR:HG22	1:B:278:GLU:OE1	2.16	0.46
1:F:262:GLY:O	1:F:350:ARG:HD2	2.16	0.46
1:B:258:THR:O	1:B:259:SER:CB	2.64	0.46
1:F:162:THR:O	1:F:246:PHE:HA	2.15	0.46
1:B:175:ILE:O	1:B:175:ILE:CG2	2.63	0.46
1:A:217:ASN:HD22	1:A:217:ASN:N	2.07	0.45
1:A:349:ILE:CD1	1:C:189:VAL:HG21	2.47	0.45
1:F:273:ILE:HG23	1:F:278:GLU:HB3	1.97	0.45
1:A:248:ASP:O	1:A:249:ASN:HB2	2.17	0.45
1:C:217:ASN:HD22	1:C:217:ASN:N	1.97	0.45
1:D:221:ILE:O	1:D:323:SER:HA	2.17	0.45
1:E:289:CYS:C	1:E:290:TYR:CD1	2.94	0.45
1:A:335:THR:HG22	1:A:336:GLU:N	2.31	0.45
1:C:202:THR:HG21	2:C:93:HOH:O	2.15	0.45
1:D:351:GLU:HG3	1:D:352:ASP:N	2.30	0.45
1:E:204:MET:HE1	1:F:282:GLU:HG2	1.98	0.45
1:F:308:ASN:HA	1:F:319:ALA:HB3	1.98	0.45
1:B:250:GLN:NE2	1:C:266:SER:OG	2.50	0.45
1:C:272:PHE:CE2	1:C:311:MET:HE3	2.51	0.45
1:D:250:GLN:NE2	1:E:266:SER:OG	2.50	0.45
1:E:331:ALA:HA	1:E:332:PRO:HD3	1.81	0.45
1:F:320:MET:HE3	1:F:322:PHE:CZ	2.51	0.45
1:A:282:GLU:HG2	1:C:204:MET:HE3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:THR:HG22	1:B:336:GLU:H	1.81	0.45
1:C:232:GLN:HE22	1:C:257:ILE:CG2	2.30	0.45
1:D:168:LYS:HG2	1:E:269:ALA:HA	1.99	0.45
1:E:192:LYS:HE3	1:E:263:PHE:CE1	2.51	0.45
1:E:217:ASN:H	1:E:217:ASN:ND2	2.03	0.45
1:A:285:ILE:HB	1:A:305:VAL:HB	1.98	0.44
1:A:229:ASN:HD22	1:A:229:ASN:C	2.24	0.44
1:A:320:MET:HE3	1:A:322:PHE:HZ	1.81	0.44
1:C:160:ASN:N	1:C:160:ASN:HD22	2.16	0.44
1:D:248:ASP:O	1:D:249:ASN:HB2	2.16	0.44
1:A:269:ALA:HA	1:C:168:LYS:HG2	1.99	0.44
1:A:289:CYS:C	1:A:290:TYR:CD1	2.96	0.44
1:B:229:ASN:HD22	1:B:229:ASN:H	1.59	0.44
1:E:295:ASN:ND2	1:E:297:THR:H	2.14	0.44
1:A:351:GLU:HG3	1:A:352:ASP:N	2.31	0.44
1:F:160:ASN:HD22	1:F:160:ASN:H	1.65	0.44
1:A:272:PHE:CE2	1:A:311:MET:HG3	2.52	0.44
1:B:212:THR:O	1:B:215:LYS:HG3	2.18	0.44
1:D:299:PHE:CE2	1:D:332:PRO:HG3	2.53	0.44
1:D:196:LEU:CD2	1:D:349:ILE:HD13	2.48	0.44
1:B:200:TYR:C	1:B:200:TYR:CD2	2.96	0.44
1:C:274:THR:HG22	1:C:278:GLU:OE1	2.18	0.43
1:D:217:ASN:N	1:D:217:ASN:ND2	2.62	0.43
1:E:192:LYS:HA	1:E:197:ILE:HD13	2.00	0.43
1:A:188:LEU:HD13	1:A:201:ILE:HD12	1.99	0.43
1:E:168:LYS:HG3	1:F:268:THR:O	2.18	0.43
1:A:189:VAL:HG21	1:B:349:ILE:HD11	2.00	0.43
1:B:224:ASN:C	1:B:225:LEU:HD12	2.42	0.43
1:A:279:THR:O	1:A:309:ARG:NH1	2.51	0.43
1:D:229:ASN:C	1:D:229:ASN:HD22	2.27	0.43
1:B:309:ARG:NH2	1:B:310:ARG:NE	2.66	0.43
1:B:331:ALA:HA	1:B:332:PRO:HD3	1.86	0.43
1:D:208:GLU:O	1:D:212:THR:HB	2.19	0.43
1:E:258:THR:O	1:E:259:SER:HB3	2.19	0.43
1:E:316:MET:HE3	1:E:319:ALA:HB2	2.00	0.43
1:D:161:ASN:HD21	1:E:194:GLY:HA2	1.83	0.43
1:D:264:MET:HE2	1:D:264:MET:HA	2.00	0.43
1:E:290:TYR:CD1	1:E:290:TYR:N	2.87	0.42
1:F:316:MET:HE3	1:F:319:ALA:HB2	2.00	0.42
1:F:236:TYR:CE1	1:F:237:LEU:HG	2.54	0.42
1:D:227:PHE:CD1	1:D:227:PHE:N	2.87	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:ASN:HD22	1:D:230:THR:N	2.17	0.42
1:A:170:SER:O	1:A:171:ALA:C	2.61	0.42
1:B:230:THR:HB	1:B:259:SER:HA	2.00	0.42
1:D:189:VAL:HG21	1:E:349:ILE:CD1	2.50	0.42
1:E:181:SER:HA	1:E:182:PRO:HD3	1.93	0.42
1:A:320:MET:HE3	1:A:322:PHE:CE1	2.55	0.42
1:D:160:ASN:HD22	1:D:160:ASN:H	1.65	0.42
1:D:274:THR:HG23	1:D:275:TYR:HD1	1.84	0.42
1:D:164:TRP:CE2	1:D:166:GLY:HA2	2.55	0.42
1:F:289:CYS:C	1:F:290:TYR:CD1	2.98	0.42
1:A:340:ILE:HD12	1:B:281:ASN:HB2	2.02	0.42
1:C:229:ASN:N	1:C:229:ASN:ND2	2.67	0.42
1:C:289:CYS:C	1:C:290:TYR:CD1	2.98	0.42
1:D:299:PHE:CD2	1:D:332:PRO:HG3	2.54	0.42
1:F:308:ASN:O	1:F:309:ARG:HB3	2.19	0.42
1:A:218:GLN:HA	1:A:326:LEU:O	2.20	0.41
1:A:274:THR:HG23	1:A:275:TYR:CD1	2.49	0.41
1:D:290:TYR:N	1:D:290:TYR:CD1	2.87	0.41
1:E:158:ILE:HA	1:E:247:LYS:O	2.20	0.41
1:F:275:TYR:CE2	1:F:277:THR:HG23	2.53	0.41
1:C:295:ASN:ND2	1:C:297:THR:HG23	2.34	0.41
1:D:209:TYR:CD1	1:D:209:TYR:C	2.99	0.41
1:E:164:TRP:C	1:E:164:TRP:CD1	2.97	0.41
1:E:316:MET:CE	1:E:319:ALA:HB2	2.51	0.41
1:A:236:TYR:CE1	1:A:237:LEU:HG	2.55	0.41
1:C:170:SER:O	1:C:171:ALA:C	2.63	0.41
1:D:204:MET:HE1	1:E:282:GLU:HG2	2.01	0.41
1:C:217:ASN:ND2	1:C:217:ASN:N	2.68	0.41
1:C:335:THR:CG2	1:C:336:GLU:N	2.82	0.41
1:D:331:ALA:HA	1:D:332:PRO:HD3	1.90	0.41
1:F:181:SER:HA	1:F:182:PRO:HD3	1.87	0.41
1:A:331:ALA:HA	1:A:332:PRO:HD3	1.85	0.41
1:C:160:ASN:H	1:C:160:ASN:ND2	2.19	0.41
1:C:264:MET:HG3	1:C:318:TYR:CD1	2.56	0.41
1:F:204:MET:HA	1:F:339:LEU:O	2.21	0.41
1:A:168:LYS:HG3	1:B:268:THR:O	2.21	0.41
1:A:225:LEU:HB2	1:A:320:MET:O	2.20	0.41
1:F:158:ILE:HA	1:F:247:LYS:O	2.19	0.41
1:F:273:ILE:HD12	1:F:310:ARG:HG2	2.02	0.41
1:A:283:ASP:OD2	1:A:309:ARG:HG3	2.21	0.41
1:B:198:ASN:HD22	1:B:198:ASN:HA	1.62	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:ASN:HD21	1:C:297:THR:HG23	1.86	0.41
1:F:160:ASN:N	1:F:160:ASN:ND2	2.66	0.41
1:B:174:VAL:HA	1:B:183:ASP:OD1	2.21	0.41
1:A:204:MET:CE	1:B:282:GLU:HG2	2.49	0.40
1:F:229:ASN:ND2	1:F:230:THR:HG23	2.35	0.40
1:B:335:THR:CG2	1:B:336:GLU:N	2.83	0.40
1:B:233:ILE:CG2	1:B:234:ILE:N	2.84	0.40
1:E:204:MET:HE2	1:E:340:ILE:CD1	2.51	0.40
1:F:170:SER:O	1:F:171:ALA:C	2.64	0.40
1:F:229:ASN:N	1:F:229:ASN:ND2	2.64	0.40
1:C:160:ASN:N	1:C:160:ASN:ND2	2.69	0.40
1:D:170:SER:O	1:D:171:ALA:C	2.64	0.40
1:E:160:ASN:C	1:E:160:ASN:ND2	2.80	0.40
1:E:189:VAL:HG21	1:F:349:ILE:HD13	2.02	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	194/220 (88%)	184 (95%)	9 (5%)	1 (0%)	24	37
1	B	194/220 (88%)	176 (91%)	15 (8%)	3 (2%)	8	12
1	C	194/220 (88%)	178 (92%)	14 (7%)	2 (1%)	12	20
1	D	194/220 (88%)	178 (92%)	13 (7%)	3 (2%)	8	12
1	E	194/220 (88%)	181 (93%)	12 (6%)	1 (0%)	24	37
1	F	194/220 (88%)	175 (90%)	16 (8%)	3 (2%)	8	12
All	All	1164/1320 (88%)	1072 (92%)	79 (7%)	13 (1%)	11	18

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	309	ARG
1	B	276	ALA
1	D	259	SER
1	F	259	SER
1	B	259	SER
1	C	259	SER
1	D	276	ALA
1	F	277	THR
1	A	259	SER
1	B	214	PHE
1	C	309	ARG
1	E	259	SER
1	F	178	GLY

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	171/188 (91%)	164 (96%)	7 (4%)	27	46
1	B	171/188 (91%)	164 (96%)	7 (4%)	27	46
1	C	171/188 (91%)	163 (95%)	8 (5%)	23	41
1	D	171/188 (91%)	159 (93%)	12 (7%)	14	24
1	E	171/188 (91%)	164 (96%)	7 (4%)	27	46
1	F	171/188 (91%)	163 (95%)	8 (5%)	23	41
All	All	1026/1128 (91%)	977 (95%)	49 (5%)	23	40

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	A	175	ILE
1	A	217	ASN
1	A	229	ASN
1	A	282	GLU
1	A	295	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	334	THR
1	B	160	ASN
1	B	217	ASN
1	B	229	ASN
1	B	274	THR
1	B	282	GLU
1	B	295	ASN
1	B	323	SER
1	C	160	ASN
1	C	203	LEU
1	C	217	ASN
1	C	229	ASN
1	C	282	GLU
1	C	295	ASN
1	C	309	ARG
1	C	314	SER
1	D	160	ASN
1	D	202	THR
1	D	203	LEU
1	D	212	THR
1	D	217	ASN
1	D	227	PHE
1	D	229	ASN
1	D	282	GLU
1	D	295	ASN
1	D	311	MET
1	D	314	SER
1	D	335	THR
1	E	160	ASN
1	E	217	ASN
1	E	229	ASN
1	E	274	THR
1	E	282	GLU
1	E	295	ASN
1	E	309	ARG
1	F	160	ASN
1	F	184	CYS
1	F	202	THR
1	F	217	ASN
1	F	229	ASN
1	F	282	GLU
1	F	295	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	349	ILE

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	160	ASN
1	A	193	ASN
1	A	217	ASN
1	A	224	ASN
1	A	229	ASN
1	A	249	ASN
1	A	250	GLN
1	A	295	ASN
1	B	160	ASN
1	B	217	ASN
1	B	224	ASN
1	B	229	ASN
1	B	250	GLN
1	B	295	ASN
1	C	160	ASN
1	C	198	ASN
1	C	217	ASN
1	C	224	ASN
1	C	229	ASN
1	C	232	GLN
1	C	249	ASN
1	C	250	GLN
1	C	295	ASN
1	D	160	ASN
1	D	217	ASN
1	D	224	ASN
1	D	229	ASN
1	D	232	GLN
1	D	249	ASN
1	D	250	GLN
1	D	295	ASN
1	E	160	ASN
1	E	198	ASN
1	E	217	ASN
1	E	224	ASN
1	E	229	ASN
1	E	250	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	295	ASN
1	F	160	ASN
1	F	193	ASN
1	F	217	ASN
1	F	224	ASN
1	F	229	ASN
1	F	232	GLN
1	F	250	GLN
1	F	295	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	196/220 (89%)	0.41	14 (7%) 22 18	37, 56, 91, 112	0
1	B	196/220 (89%)	0.98	28 (14%) 6 5	44, 68, 109, 130	0
1	C	196/220 (89%)	0.65	19 (9%) 13 10	43, 61, 96, 138	0
1	D	196/220 (89%)	0.68	18 (9%) 14 12	39, 55, 85, 120	0
1	E	196/220 (89%)	0.75	16 (8%) 17 14	43, 65, 99, 115	0
1	F	196/220 (89%)	1.14	36 (18%) 3 3	43, 64, 105, 161	0
All	All	1176/1320 (89%)	0.77	131 (11%) 10 7	37, 61, 102, 161	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	277	THR	6.4
1	B	277	THR	6.3
1	B	276	ALA	6.2
1	C	277	THR	5.9
1	F	277	THR	5.1
1	C	167	ALA	4.8
1	F	276	ALA	4.8
1	D	158	ILE	4.5
1	A	258	THR	4.5
1	B	258	THR	4.4
1	D	335	THR	4.2
1	E	335	THR	4.1
1	F	314	SER	4.1
1	F	275	TYR	4.0
1	E	277	THR	4.0
1	B	310	ARG	3.8
1	C	275	TYR	3.8
1	C	310	ARG	3.7
1	C	276	ALA	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	274	THR	3.7
1	F	177	GLU	3.7
1	C	158	ILE	3.6
1	D	254	THR	3.6
1	F	313	ALA	3.6
1	F	312	LEU	3.6
1	E	158	ILE	3.6
1	A	335	THR	3.6
1	A	167	ALA	3.6
1	B	335	THR	3.5
1	C	274	THR	3.4
1	D	167	ALA	3.4
1	F	242	SER	3.4
1	F	178	GLY	3.3
1	A	277	THR	3.3
1	F	254	THR	3.3
1	B	273	ILE	3.3
1	F	167	ALA	3.3
1	B	209	TYR	3.2
1	C	254	THR	3.2
1	E	255	GLY	3.2
1	F	158	ILE	3.2
1	C	258	THR	3.2
1	D	180	ASP	3.1
1	B	257	ILE	3.1
1	F	310	ARG	3.1
1	C	180	ASP	3.1
1	B	243	ASN	3.1
1	F	279	THR	3.0
1	A	297	THR	3.0
1	E	256	THR	3.0
1	F	315	GLY	2.9
1	A	158	ILE	2.9
1	F	278	GLU	2.9
1	C	242	SER	2.9
1	B	236	TYR	2.9
1	D	310	ARG	2.8
1	F	176	LYS	2.8
1	E	254	THR	2.8
1	B	184	CYS	2.8
1	F	311	MET	2.8
1	B	175	ILE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	274	THR	2.8
1	D	177	GLU	2.8
1	B	180	ASP	2.8
1	B	314	SER	2.7
1	D	330	GLU	2.7
1	F	208	GLU	2.7
1	D	258	THR	2.7
1	F	256	THR	2.7
1	A	308	ASN	2.6
1	E	258	THR	2.6
1	A	178	GLY	2.6
1	A	175	ILE	2.6
1	E	249	ASN	2.6
1	A	314	SER	2.6
1	B	167	ALA	2.6
1	F	330	GLU	2.6
1	C	321	ASN	2.6
1	C	314	SER	2.6
1	D	236	TYR	2.5
1	B	185	LYS	2.5
1	F	229	ASN	2.5
1	F	258	THR	2.5
1	C	212	THR	2.5
1	A	257	ILE	2.4
1	C	222	ASP	2.4
1	B	212	THR	2.4
1	F	181	SER	2.4
1	A	160	ASN	2.4
1	F	335	THR	2.3
1	B	315	GLY	2.3
1	E	310	ARG	2.3
1	F	257	ILE	2.3
1	B	336	GLU	2.3
1	C	335	THR	2.3
1	D	249	ASN	2.3
1	D	175	ILE	2.3
1	F	206	ALA	2.3
1	C	334	THR	2.3
1	F	232	GLN	2.3
1	B	242	SER	2.3
1	B	330	GLU	2.3
1	E	243	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	182	PRO	2.2
1	F	302	LYS	2.2
1	A	256	THR	2.2
1	C	311	MET	2.2
1	B	311	MET	2.2
1	F	334	THR	2.2
1	E	232	GLN	2.1
1	E	276	ALA	2.1
1	A	177	GLU	2.1
1	D	329	GLU	2.1
1	F	224	ASN	2.1
1	E	257	ILE	2.1
1	D	242	SER	2.1
1	D	198	ASN	2.1
1	F	245	ASN	2.1
1	E	274	THR	2.1
1	F	296	GLY	2.1
1	B	176	LYS	2.1
1	D	308	ASN	2.1
1	B	178	GLY	2.1
1	B	255	GLY	2.1
1	E	297	THR	2.1
1	F	220	THR	2.1
1	E	167	ALA	2.0
1	C	288	GLU	2.0
1	B	254	THR	2.0
1	F	273	ILE	2.0
1	B	259	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.