



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:02 PM UTC

PDB ID : 8OFP / pdb_00008ofp
Title : Human adenovirus type 24 fiber-knob protein
Authors : Rizkallah, P.J.; Parker, A.L.; Mundy, R.M.; Baker, A.T.
Deposited on : 2023-03-16
Resolution : 3.10 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:

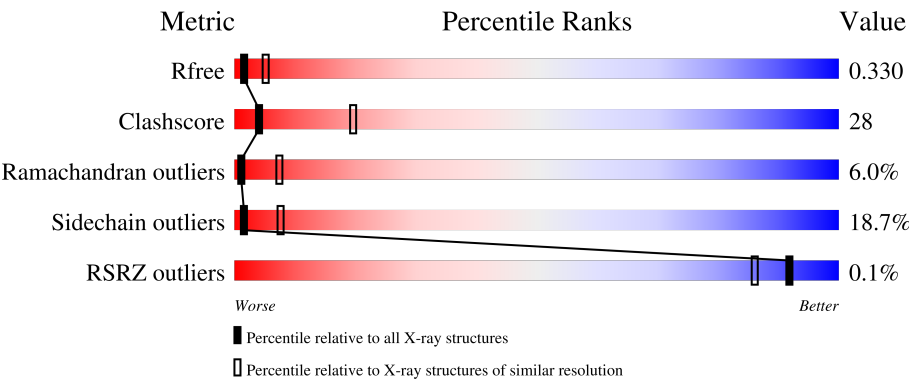
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	196	39%40%12%•8%
1	B	196	41%43%9%•6%
1	C	196	46%40%10%••
1	D	196	42%38%14%•5%
1	E	196	% 43%41%14%••

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Mol	Chain	Length	Quality of chain
1	F	196	40% 45% 12% ••

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8946 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	0	0
			1442	920	231	286	5			
1	B	185	Total	C	N	O	S	0	0	0
			1472	939	236	292	5			
1	C	190	Total	C	N	O	S	0	0	0
			1510	960	242	303	5			
1	D	187	Total	C	N	O	S	0	0	0
			1478	944	237	292	5			
1	E	193	Total	C	N	O	S	0	0	0
			1530	974	245	306	5			
1	F	191	Total	C	N	O	S	0	0	0
			1514	964	243	302	5			

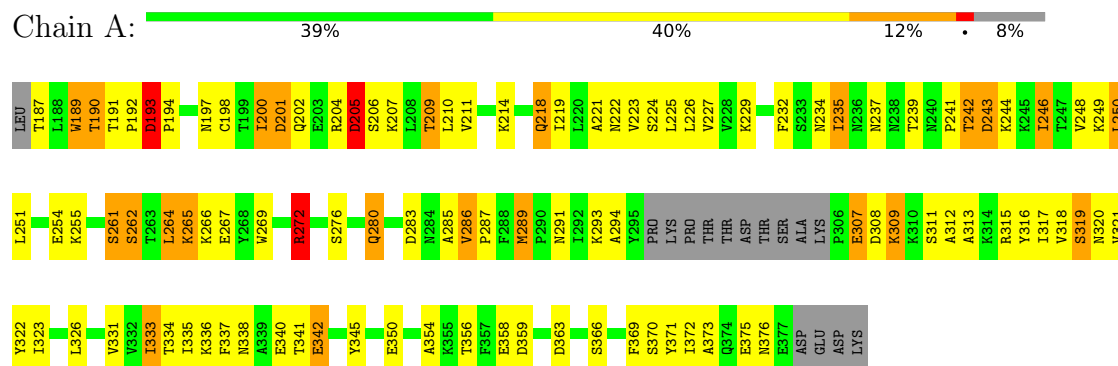
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	186	LEU	-	expression tag	UNP M0QUI2
B	186	LEU	-	expression tag	UNP M0QUI2
C	186	LEU	-	expression tag	UNP M0QUI2
D	186	LEU	-	expression tag	UNP M0QUI2
E	186	LEU	-	expression tag	UNP M0QUI2
F	186	LEU	-	expression tag	UNP M0QUI2

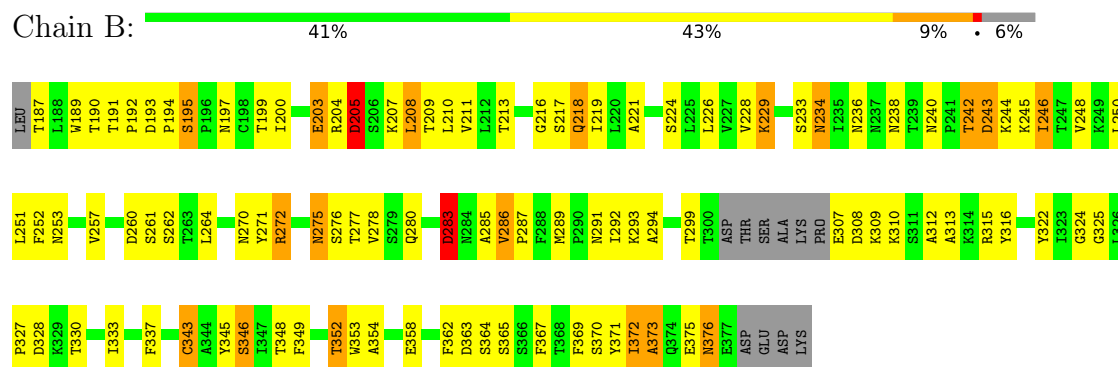
3 Residue-property plots

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.

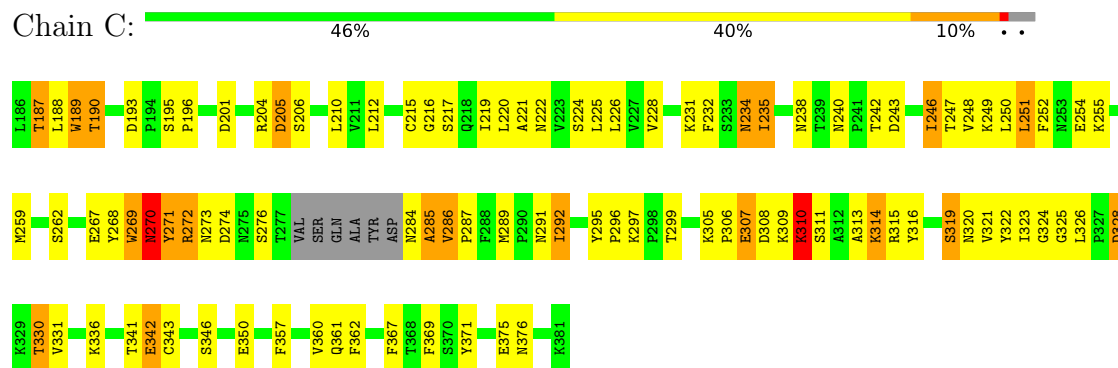
• Molecule 1: Fiber



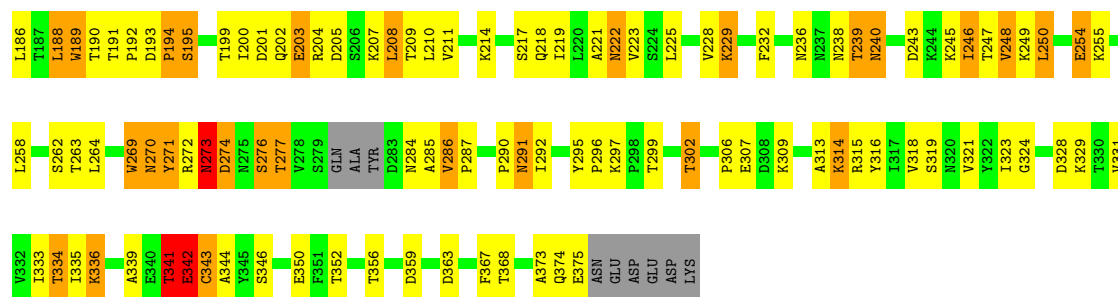
• Molecule 1: Fiber



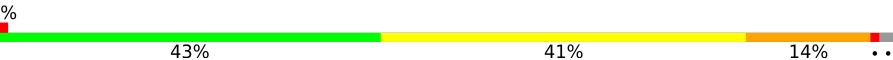
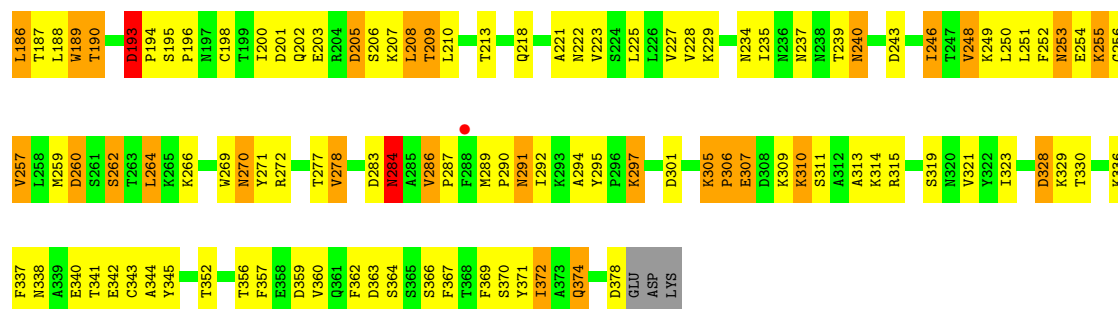
• Molecule 1: Fiber



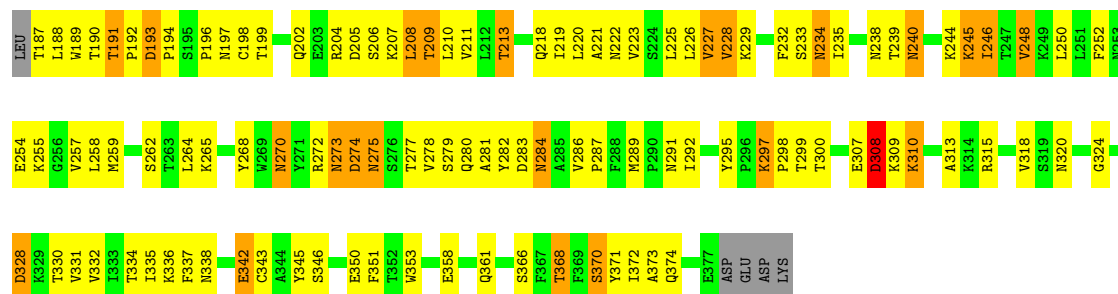
• Molecule 1: Fiber

Chain D:  42% 38% 14% • 5%

• Molecule 1: Fiber

Chain E:  43% 41% 14% ••

• Molecule 1: Fiber

Chain F:  40% 45% 12% ••

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.26Å 99.62Å 113.55Å 90.00° 100.26° 90.00°	Depositor
Resolution (Å)	55.87 – 3.10 55.87 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (55.87-3.10) 99.9 (55.87-3.10)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.234 , 0.337 0.233 , 0.330	Depositor DCC
R_{free} test set	1226 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	70.7	Xtriage
Anisotropy	0.739	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 72.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.043 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8946	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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	1.17	0/1472	1.35	0/1998
1	B	1.17	0/1503	1.35	1/2042 (0.0%)
1	C	1.15	2/1541 (0.1%)	1.33	2/2091 (0.1%)
1	D	1.12	0/1509	1.29	0/2051
1	E	1.16	0/1563	1.36	0/2126
1	F	1.17	2/1547 (0.1%)	1.33	2/2104 (0.1%)
All	All	1.16	4/9135 (0.0%)	1.34	5/12412 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	5
1	C	0	4
1	D	0	3
1	E	0	7
All	All	0	23

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	310	LYS	C-O	5.71	1.31	1.23
1	F	350	GLU	C-O	5.32	1.29	1.23
1	F	318	VAL	C-O	5.31	1.29	1.24
1	C	367	PHE	C-O	-5.00	1.18	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	308	ASP	CA-C-N	5.70	127.92	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	308	ASP	C-N-CA	5.70	127.92	120.28
1	B	283	ASP	CB-CA-C	5.42	116.47	109.80
1	F	227	VAL	CA-C-N	5.23	127.10	120.72
1	F	227	VAL	C-N-CA	5.23	127.10	120.72

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	193	ASP	Peptide
1	A	205	ASP	Peptide
1	A	266	LYS	Peptide
1	A	373	ALA	Peptide
1	B	204	ARG	Peptide
1	B	205	ASP	Peptide
1	B	253	ASN	Peptide
1	B	312	ALA	Peptide
1	B	316	TYR	Peptide
1	C	189	TRP	Peptide
1	C	205	ASP	Peptide
1	C	268	TYR	Peptide
1	C	274	ASP	Peptide
1	D	189	TRP	Peptide
1	D	274	ASP	Peptide
1	D	302	THR	Peptide
1	E	189	TRP	Peptide
1	E	194	PRO	Peptide
1	E	205	ASP	Peptide
1	E	249	LYS	Peptide
1	E	284	ASN	Peptide
1	E	307	GLU	Peptide
1	E	374	GLN	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	1442	0	1420	83	0
1	B	1472	0	1454	88	0
1	C	1510	0	1492	82	0
1	D	1478	0	1468	92	0
1	E	1530	0	1511	89	0
1	F	1514	0	1495	95	0
All	All	8946	0	8840	492	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 28.

All (492) 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:291:ASN:HD22	1:B:373:ALA:HA	1.03	1.19
1:A:363:ASP:OD1	1:C:311:SER:OG	1.65	1.13
1:F:193:ASP:O	1:F:207:LYS:NZ	1.81	1.13
1:B:289:MET:O	1:B:373:ALA:HB3	1.47	1.11
1:A:205:ASP:OD1	1:A:229:LYS:O	1.81	0.98
1:E:297:LYS:NZ	1:E:343:CYS:O	2.00	0.95
1:B:291:ASN:N	1:B:373:ALA:HB2	1.85	0.92
1:A:193:ASP:O	1:A:207:LYS:NZ	2.03	0.90
1:E:253:ASN:O	1:E:255:LYS:O	1.89	0.89
1:B:291:ASN:ND2	1:B:373:ALA:HA	1.89	0.88
1:C:187:THR:O	1:C:271:TYR:HB2	1.73	0.87
1:B:193:ASP:O	1:B:207:LYS:NZ	2.07	0.86
1:B:218:GLN:OE1	1:C:222:ASN:HB2	1.76	0.85
1:E:270:ASN:C	1:E:270:ASN:HD22	1.85	0.85
1:B:289:MET:O	1:B:373:ALA:CB	2.24	0.84
1:B:291:ASN:CA	1:B:373:ALA:HB2	2.09	0.83
1:C:251:LEU:HD23	1:C:251:LEU:N	1.94	0.83
1:E:193:ASP:O	1:E:207:LYS:NZ	2.13	0.82
1:C:324:GLY:O	1:C:326:LEU:N	2.11	0.81
1:C:252:PHE:CD2	1:C:289:MET:HE1	2.17	0.80
1:E:306:PRO:O	1:F:228:VAL:HG13	1.81	0.79
1:C:201:ASP:N	1:C:205:ASP:OD2	2.15	0.78
1:B:217:SER:O	1:B:372:ILE:HG22	1.84	0.78
1:C:235:ILE:HD11	1:C:357:PHE:HB2	1.66	0.77
1:F:239:THR:C	1:F:240:ASN:HD22	1.91	0.77
1:F:225:LEU:CD2	1:F:246:ILE:HD11	2.14	0.77
1:E:253:ASN:ND2	1:E:255:LYS:O	2.18	0.76
1:D:239:THR:O	1:D:240:ASN:ND2	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:370:SER:OG	1:F:368:THR:OG1	2.04	0.76
1:A:194:PRO:HG3	1:C:309:LYS:HA	1.67	0.74
1:F:295:TYR:CE2	1:F:372:ILE:HG22	2.23	0.73
1:B:313:ALA:HB2	1:C:324:GLY:HA2	1.70	0.72
1:C:320:ASN:ND2	1:C:330:THR:HG22	2.05	0.72
1:B:244:LYS:NZ	1:B:354:ALA:O	2.24	0.71
1:E:270:ASN:C	1:E:270:ASN:ND2	2.47	0.71
1:A:313:ALA:O	1:B:365:SER:HA	1.90	0.71
1:D:190:THR:HG21	1:D:208:LEU:O	1.89	0.70
1:A:232:PHE:HD1	1:A:235:ILE:HD11	1.57	0.70
1:A:234:ASN:OD1	1:A:234:ASN:O	2.10	0.70
1:D:193:ASP:HB3	1:D:194:PRO:HD2	1.72	0.70
1:C:270:ASN:N	1:C:270:ASN:HD22	1.89	0.69
1:A:194:PRO:HA	1:A:207:LYS:HE2	1.74	0.69
1:F:240:ASN:HD22	1:F:240:ASN:N	1.88	0.69
1:A:192:PRO:O	1:C:314:LYS:NZ	2.19	0.68
1:D:323:ILE:HA	1:D:363:ASP:O	1.93	0.68
1:E:225:LEU:HD21	1:E:246:ILE:HD11	1.75	0.68
1:B:362:PHE:CE1	1:B:364:SER:HB3	2.28	0.68
1:D:202:GLN:O	1:D:205:ASP:HB2	1.94	0.68
1:A:206:SER:HB3	1:A:227:VAL:HA	1.76	0.68
1:A:311:SER:HB2	1:B:226:LEU:HD22	1.76	0.67
1:F:223:VAL:O	1:F:223:VAL:HG13	1.94	0.67
1:C:252:PHE:CG	1:C:289:MET:HE1	2.28	0.67
1:B:293:LYS:HE3	1:B:293:LYS:HA	1.75	0.67
1:D:286:VAL:N	1:D:287:PRO:HD2	2.09	0.67
1:C:320:ASN:HD22	1:C:330:THR:HG22	1.59	0.67
1:C:249:LYS:C	1:C:250:LEU:HD12	2.20	0.67
1:C:269:TRP:C	1:C:270:ASN:ND2	2.53	0.66
1:B:234:ASN:HD22	1:B:234:ASN:C	2.03	0.66
1:A:280:GLN:HE22	1:A:285:ALA:HB2	1.60	0.66
1:E:295:TYR:OH	1:E:372:ILE:HG13	1.97	0.65
1:F:225:LEU:HD21	1:F:246:ILE:HD11	1.79	0.65
1:D:201:ASP:OD2	1:D:202:GLN:HG3	1.96	0.65
1:F:194:PRO:HA	1:F:207:LYS:HE2	1.78	0.65
1:E:253:ASN:C	1:E:253:ASN:HD22	2.04	0.64
1:D:193:ASP:HB3	1:D:194:PRO:CD	2.26	0.64
1:C:232:PHE:CE2	1:C:246:ILE:HG22	2.32	0.64
1:B:199:THR:HG22	1:B:199:THR:O	1.98	0.64
1:C:305:LYS:O	1:C:307:GLU:N	2.27	0.64
1:D:189:TRP:CZ2	1:D:271:TYR:HD2	2.16	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:TRP:C	1:D:270:ASN:HD22	2.06	0.64
1:E:314:LYS:HE3	1:F:209:THR:HG21	1.79	0.64
1:F:199:THR:HG23	1:F:202:GLN:O	1.97	0.64
1:C:297:LYS:NZ	1:C:343:CYS:SG	2.71	0.63
1:F:235:ILE:HD13	1:F:353:TRP:CZ2	2.33	0.63
1:E:370:SER:HG	1:F:368:THR:HG1	1.41	0.63
1:F:190:THR:HG21	1:F:208:LEU:O	1.96	0.63
1:A:239:THR:O	1:A:241:PRO:HD3	1.97	0.63
1:F:210:LEU:HA	1:F:222:ASN:O	1.99	0.63
1:D:239:THR:C	1:D:240:ASN:ND2	2.57	0.62
1:C:219:ILE:HG21	1:C:371:TYR:CZ	2.33	0.62
1:A:307:GLU:C	1:A:309:LYS:H	2.07	0.62
1:C:189:TRP:CG	1:C:190:THR:O	2.53	0.62
1:C:324:GLY:C	1:C:326:LEU:H	2.08	0.62
1:A:316:TYR:CD2	1:B:325:GLY:HA3	2.36	0.61
1:D:225:LEU:CD2	1:D:246:ILE:HD11	2.30	0.61
1:B:189:TRP:HZ2	1:B:272:ARG:HG3	1.65	0.61
1:B:200:ILE:HD13	1:B:246:ILE:HD12	1.83	0.60
1:A:187:THR:HG22	1:C:217:SER:OG	2.02	0.60
1:D:264:LEU:HD23	1:D:269:TRP:HE1	1.66	0.60
1:F:273:ASN:HA	1:F:277:THR:HG21	1.84	0.60
1:B:229:LYS:C	1:B:233:SER:OG	2.44	0.60
1:D:341:THR:O	1:D:343:CYS:N	2.35	0.60
1:A:286:VAL:HG13	1:A:287:PRO:HD3	1.84	0.59
1:B:322:TYR:CD2	1:B:327:PRO:HA	2.37	0.59
1:A:232:PHE:CD1	1:A:235:ILE:HD11	2.35	0.59
1:F:252:PHE:C	1:F:259:MET:SD	2.85	0.59
1:D:258:LEU:HD22	1:D:269:TRP:CD1	2.36	0.59
1:A:206:SER:CB	1:A:227:VAL:HA	2.32	0.59
1:F:191:THR:HG22	1:F:273:ASN:HD21	1.67	0.59
1:D:225:LEU:HD23	1:D:246:ILE:HD11	1.85	0.59
1:F:295:TYR:HE2	1:F:372:ILE:HG22	1.65	0.59
1:E:372:ILE:HD13	1:F:211:VAL:HG21	1.85	0.59
1:F:223:VAL:O	1:F:223:VAL:CG1	2.50	0.59
1:B:219:ILE:HG21	1:B:371:TYR:CZ	2.38	0.58
1:D:272:ARG:O	1:D:274:ASP:N	2.36	0.58
1:A:249:LYS:HD3	1:A:340:GLU:OE1	2.03	0.58
1:C:252:PHE:CE2	1:C:289:MET:HE1	2.38	0.58
1:D:318:VAL:HG22	1:D:334:THR:HG23	1.85	0.58
1:E:253:ASN:ND2	1:E:253:ASN:C	2.62	0.58
1:C:251:LEU:N	1:C:251:LEU:CD2	2.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:219:ILE:HG21	1:F:371:TYR:CZ	2.38	0.58
1:B:362:PHE:HE1	1:B:364:SER:HB3	1.67	0.58
1:A:194:PRO:HA	1:A:207:LYS:CE	2.34	0.58
1:C:286:VAL:HG22	1:C:287:PRO:HD3	1.85	0.58
1:D:240:ASN:HB3	1:D:243:ASP:CG	2.29	0.58
1:B:191:THR:O	1:B:193:ASP:N	2.37	0.57
1:E:311:SER:HB2	1:F:226:LEU:HD22	1.86	0.57
1:E:200:ILE:HD12	1:E:206:SER:OG	2.03	0.57
1:F:206:SER:HB3	1:F:227:VAL:HA	1.86	0.57
1:E:188:LEU:CD2	1:E:269:TRP:CZ2	2.86	0.57
1:B:270:ASN:HD22	1:B:278:VAL:HA	1.70	0.57
1:D:188:LEU:HD23	1:D:269:TRP:CZ3	2.39	0.57
1:E:223:VAL:O	1:E:223:VAL:HG13	2.03	0.57
1:D:189:TRP:NE1	1:D:271:TYR:HB2	2.20	0.57
1:E:201:ASP:OD2	1:E:202:GLN:HG2	2.04	0.57
1:B:218:GLN:OE1	1:C:222:ASN:CB	2.50	0.56
1:C:252:PHE:O	1:C:259:MET:SD	2.63	0.56
1:D:341:THR:O	1:D:342:GLU:C	2.49	0.56
1:E:250:LEU:HA	1:E:262:SER:HB3	1.87	0.56
1:A:341:THR:C	1:A:342:GLU:CD	2.72	0.56
1:E:201:ASP:OD2	1:E:202:GLN:CG	2.53	0.56
1:F:204:ARG:HE	1:F:265:LYS:HG3	1.70	0.56
1:B:245:LYS:HB2	1:B:352:THR:HG22	1.87	0.56
1:C:295:TYR:CD1	1:C:315:ARG:HA	2.41	0.56
1:C:269:TRP:O	1:C:270:ASN:CG	2.49	0.56
1:C:310:LYS:HG2	1:C:311:SER:O	2.05	0.56
1:C:270:ASN:N	1:C:270:ASN:ND2	2.53	0.56
1:A:200:ILE:N	1:A:200:ILE:HD13	2.21	0.56
1:F:187:THR:OG1	1:F:213:THR:HG23	2.06	0.56
1:F:219:ILE:HG21	1:F:371:TYR:OH	2.06	0.56
1:B:291:ASN:CA	1:B:373:ALA:CB	2.81	0.55
1:B:293:LYS:O	1:C:193:ASP:HB2	2.06	0.55
1:D:232:PHE:CE1	1:D:246:ILE:HG22	2.42	0.55
1:A:226:LEU:HD13	1:C:311:SER:OG	2.07	0.55
1:E:286:VAL:N	1:E:287:PRO:CD	2.70	0.55
1:B:251:LEU:HD23	1:B:346:SER:HB2	1.88	0.55
1:A:315:ARG:HD3	1:A:337:PHE:O	2.07	0.55
1:F:189:TRP:CZ2	1:F:272:ARG:HG3	2.42	0.55
1:D:264:LEU:HD23	1:D:269:TRP:NE1	2.20	0.55
1:E:190:THR:HG21	1:E:209:THR:HA	1.88	0.55
1:A:272:ARG:O	1:A:276:SER:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:VAL:HG23	1:D:331:VAL:HB	1.87	0.55
1:E:188:LEU:HD21	1:E:269:TRP:CZ2	2.42	0.55
1:E:252:PHE:HB3	1:E:256:GLY:O	2.06	0.55
1:A:225:LEU:HD21	1:A:246:ILE:HD11	1.88	0.55
1:B:252:PHE:CD2	1:B:289:MET:HE1	2.42	0.55
1:C:210:LEU:HD11	1:C:212:LEU:HD21	1.87	0.55
1:A:218:GLN:NE2	1:B:213:THR:OG1	2.37	0.54
1:C:272:ARG:O	1:C:272:ARG:HG2	2.07	0.54
1:A:319:SER:OG	1:A:320:ASN:N	2.40	0.54
1:C:187:THR:O	1:C:271:TYR:CB	2.51	0.54
1:D:319:SER:OG	1:D:367:PHE:CE1	2.60	0.54
1:D:199:THR:HG23	1:D:203:GLU:HA	1.89	0.54
1:F:257:VAL:CG2	1:F:284:ASN:HB3	2.37	0.54
1:D:205:ASP:OD1	1:D:229:LYS:O	2.25	0.54
1:A:333:ILE:CD1	1:A:335:ILE:HD11	2.37	0.54
1:A:337:PHE:CE1	1:A:371:TYR:CD2	2.96	0.54
1:B:271:TYR:CZ	1:B:285:ALA:HB2	2.42	0.54
1:C:210:LEU:HD11	1:C:212:LEU:CD2	2.38	0.54
1:C:226:LEU:HD11	1:C:361:GLN:HE21	1.71	0.54
1:C:231:LYS:HE2	1:C:232:PHE:CE1	2.43	0.54
1:D:335:ILE:N	1:D:335:ILE:HD12	2.22	0.54
1:B:291:ASN:HD22	1:B:373:ALA:CA	1.97	0.54
1:B:291:ASN:HB3	1:B:294:ALA:HB3	1.90	0.54
1:E:225:LEU:CD2	1:E:246:ILE:HD11	2.37	0.53
1:E:340:GLU:O	1:E:343:CYS:SG	2.66	0.53
1:A:227:VAL:HG11	1:A:232:PHE:HB2	1.90	0.53
1:A:187:THR:CG2	1:C:217:SER:OG	2.56	0.53
1:A:244:LYS:NZ	1:A:354:ALA:O	2.42	0.53
1:F:232:PHE:HA	1:F:235:ILE:HG13	1.89	0.53
1:A:250:LEU:HA	1:A:262:SER:HB3	1.90	0.53
1:C:319:SER:OG	1:C:320:ASN:N	2.41	0.53
1:A:200:ILE:O	1:A:202:GLN:O	2.27	0.53
1:F:190:THR:O	1:F:191:THR:C	2.50	0.53
1:C:234:ASN:HA	1:C:360:VAL:O	2.09	0.53
1:F:252:PHE:O	1:F:259:MET:SD	2.67	0.53
1:D:223:VAL:HG13	1:D:223:VAL:O	2.09	0.52
1:A:193:ASP:HB2	1:A:194:PRO:CD	2.39	0.52
1:E:323:ILE:HA	1:E:363:ASP:O	2.09	0.52
1:E:328:ASP:HB2	1:E:329:LYS:HE3	1.91	0.52
1:B:190:THR:HG21	1:B:208:LEU:O	2.10	0.52
1:D:324:GLY:HA2	1:F:313:ALA:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ASN:O	1:A:264:LEU:HA	2.10	0.52
1:C:232:PHE:HA	1:C:235:ILE:HG22	1.91	0.52
1:B:252:PHE:HA	1:B:257:VAL:O	2.10	0.52
1:B:315:ARG:HD3	1:B:337:PHE:O	2.09	0.52
1:E:306:PRO:O	1:F:228:VAL:CG1	2.54	0.52
1:B:234:ASN:C	1:B:234:ASN:ND2	2.68	0.52
1:C:235:ILE:C	1:C:235:ILE:HD12	2.34	0.52
1:F:189:TRP:CZ3	1:F:192:PRO:HD3	2.44	0.52
1:F:218:GLN:NE2	1:F:370:SER:OG	2.33	0.52
1:F:307:GLU:CD	1:F:307:GLU:O	2.53	0.52
1:F:190:THR:O	1:F:191:THR:O	2.28	0.52
1:F:274:ASP:O	1:F:275:ASN:HB2	2.10	0.52
1:B:217:SER:OG	1:C:187:THR:HB	2.10	0.51
1:C:225:LEU:CD2	1:C:246:ILE:HD11	2.40	0.51
1:E:200:ILE:HD13	1:E:246:ILE:HD12	1.92	0.51
1:E:337:PHE:CZ	1:E:371:TYR:CD2	2.99	0.51
1:D:190:THR:HB	1:D:210:LEU:H	1.74	0.51
1:C:269:TRP:C	1:C:270:ASN:HD22	2.17	0.51
1:E:206:SER:HB3	1:E:227:VAL:HA	1.92	0.51
1:B:291:ASN:CB	1:B:373:ALA:HB2	2.40	0.51
1:E:342:GLU:CG	1:E:342:GLU:O	2.57	0.51
1:A:242:THR:O	1:A:244:LYS:N	2.44	0.51
1:D:189:TRP:HD1	1:D:189:TRP:O	1.93	0.51
1:F:273:ASN:H	1:F:273:ASN:ND2	2.09	0.51
1:A:375:GLU:O	1:A:375:GLU:HG3	2.11	0.51
1:D:218:GLN:NE2	1:E:213:THR:OG1	2.44	0.51
1:D:297:LYS:NZ	1:D:343:CYS:O	2.43	0.51
1:E:259:MET:HE2	1:E:342:GLU:OE1	2.11	0.51
1:F:270:ASN:HD21	1:F:282:TYR:H	1.59	0.51
1:A:211:VAL:O	1:A:221:ALA:HA	2.10	0.51
1:C:286:VAL:N	1:C:287:PRO:CD	2.74	0.51
1:E:272:ARG:HB2	1:E:272:ARG:NH2	2.26	0.51
1:B:291:ASN:HA	1:B:373:ALA:CB	2.40	0.51
1:D:193:ASP:O	1:D:207:LYS:NZ	2.43	0.50
1:E:240:ASN:N	1:E:240:ASN:HD22	2.08	0.50
1:E:252:PHE:HA	1:E:257:VAL:O	2.11	0.50
1:A:214:LYS:HA	1:A:219:ILE:HD13	1.93	0.50
1:A:289:MET:N	1:A:289:MET:SD	2.85	0.50
1:C:219:ILE:HG21	1:C:371:TYR:OH	2.11	0.50
1:E:239:THR:C	1:E:240:ASN:HD22	2.19	0.50
1:B:286:VAL:N	1:B:287:PRO:CD	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:ILE:O	1:C:296:PRO:CA	2.59	0.50
1:F:274:ASP:O	1:F:275:ASN:CB	2.59	0.50
1:F:281:ALA:O	1:F:284:ASN:ND2	2.44	0.50
1:E:222:ASN:HD21	1:E:366:SER:HB3	1.76	0.50
1:B:276:SER:O	1:B:280:GLN:NE2	2.44	0.50
1:A:333:ILE:HD13	1:A:335:ILE:HD11	1.94	0.50
1:B:190:THR:O	1:B:191:THR:C	2.55	0.50
1:F:189:TRP:O	1:F:189:TRP:CD1	2.65	0.50
1:F:291:ASN:HB2	1:F:372:ILE:HG23	1.93	0.50
1:D:189:TRP:CE2	1:D:271:TYR:HB2	2.47	0.50
1:D:316:TYR:CE2	1:D:336:LYS:HD2	2.47	0.50
1:A:197:ASN:O	1:A:265:LYS:N	2.35	0.49
1:D:254:GLU:OE1	1:D:344:ALA:HB2	2.12	0.49
1:A:307:GLU:C	1:A:309:LYS:N	2.68	0.49
1:B:270:ASN:ND2	1:B:277:THR:O	2.45	0.49
1:E:206:SER:HA	1:E:228:VAL:HG23	1.94	0.49
1:E:188:LEU:HD21	1:E:269:TRP:CE2	2.48	0.49
1:E:342:GLU:O	1:E:342:GLU:CD	2.55	0.49
1:F:250:LEU:HD12	1:F:250:LEU:N	2.28	0.49
1:F:291:ASN:ND2	1:F:373:ALA:O	2.36	0.49
1:A:251:LEU:HD12	1:A:261:SER:HB2	1.94	0.49
1:E:259:MET:CE	1:E:342:GLU:OE1	2.60	0.49
1:F:289:MET:HB3	1:F:345:TYR:CD2	2.47	0.49
1:A:286:VAL:N	1:A:287:PRO:CD	2.75	0.49
1:B:219:ILE:HG21	1:B:371:TYR:OH	2.13	0.49
1:E:290:PRO:O	1:E:338:ASN:ND2	2.43	0.49
1:F:308:ASP:C	1:F:310:LYS:H	2.20	0.49
1:C:205:ASP:HB3	1:C:206:SER:OG	2.12	0.49
1:D:201:ASP:OD1	1:D:205:ASP:OD2	2.31	0.49
1:B:307:GLU:OE1	1:B:309:LYS:HD3	2.11	0.49
1:E:256:GLY:O	1:E:257:VAL:O	2.31	0.49
1:A:291:ASN:HB3	1:A:294:ALA:HB3	1.95	0.49
1:C:341:THR:O	1:C:342:GLU:C	2.56	0.49
1:D:236:ASN:OD1	1:D:238:ASN:N	2.36	0.49
1:A:312:ALA:N	1:B:363:ASP:OD2	2.36	0.48
1:B:193:ASP:HB3	1:B:194:PRO:CD	2.43	0.48
1:E:195:SER:O	1:E:196:PRO:C	2.55	0.48
1:F:291:ASN:CB	1:F:372:ILE:HG23	2.44	0.48
1:C:295:TYR:CE1	1:C:315:ARG:HA	2.48	0.48
1:F:307:GLU:O	1:F:307:GLU:CG	2.61	0.48
1:F:227:VAL:HG11	1:F:232:PHE:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:TYR:OH	1:B:285:ALA:HB2	2.13	0.48
1:B:271:TYR:OH	1:B:285:ALA:CB	2.61	0.48
1:C:195:SER:O	1:C:196:PRO:C	2.56	0.48
1:D:222:ASN:HB2	1:F:218:GLN:NE2	2.29	0.48
1:F:258:LEU:HD21	1:F:264:LEU:HD23	1.95	0.48
1:A:200:ILE:O	1:A:202:GLN:N	2.47	0.48
1:A:318:VAL:HG22	1:A:334:THR:HG23	1.96	0.48
1:B:293:LYS:HA	1:B:293:LYS:CE	2.40	0.48
1:F:278:VAL:O	1:F:280:GLN:HG2	2.14	0.48
1:B:193:ASP:HB3	1:B:194:PRO:HD2	1.94	0.47
1:B:376:ASN:C	1:B:376:ASN:OD1	2.57	0.47
1:E:337:PHE:CE1	1:E:371:TYR:CD2	3.02	0.47
1:A:223:VAL:HG13	1:A:223:VAL:O	2.15	0.47
1:D:272:ARG:NH1	1:D:273:ASN:HB2	2.29	0.47
1:B:189:TRP:CZ2	1:B:272:ARG:HG3	2.47	0.47
1:C:292:ILE:O	1:C:296:PRO:HA	2.14	0.47
1:F:320:ASN:HD22	1:F:332:VAL:HA	1.80	0.47
1:B:194:PRO:HA	1:B:207:LYS:HE2	1.96	0.47
1:D:239:THR:O	1:D:240:ASN:CG	2.58	0.47
1:E:208:LEU:HD22	1:E:264:LEU:HD13	1.97	0.47
1:D:313:ALA:O	1:D:315:ARG:N	2.48	0.47
1:E:287:PRO:HA	1:E:374:GLN:O	2.14	0.47
1:E:315:ARG:HD3	1:E:337:PHE:O	2.15	0.47
1:F:189:TRP:O	1:F:189:TRP:HD1	1.96	0.47
1:F:331:VAL:HG22	1:F:353:TRP:HB3	1.97	0.47
1:B:286:VAL:HG13	1:B:287:PRO:HD3	1.96	0.47
1:B:245:LYS:HB2	1:B:352:THR:CG2	2.43	0.47
1:D:313:ALA:O	1:D:314:LYS:C	2.58	0.47
1:F:308:ASP:C	1:F:310:LYS:N	2.73	0.47
1:D:324:GLY:CA	1:F:313:ALA:HB2	2.45	0.47
1:E:289:MET:HB3	1:E:345:TYR:CD2	2.50	0.47
1:B:221:ALA:CB	1:B:369:PHE:CZ	2.98	0.46
1:D:270:ASN:HD22	1:D:270:ASN:N	2.12	0.46
1:E:251:LEU:HD13	1:E:342:GLU:OE2	2.15	0.46
1:A:219:ILE:O	1:A:370:SER:HA	2.15	0.46
1:D:239:THR:C	1:D:240:ASN:HD22	2.23	0.46
1:B:291:ASN:HB2	1:B:373:ALA:HB2	1.97	0.46
1:B:333:ILE:HD13	1:B:367:PHE:CD2	2.49	0.46
1:C:247:THR:HG23	1:C:350:GLU:HG2	1.96	0.46
1:D:194:PRO:O	1:D:207:LYS:HD3	2.15	0.46
1:D:285:ALA:O	1:D:286:VAL:HB	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:TYR:O	1:D:272:ARG:HB3	2.16	0.46
1:A:237:ASN:ND2	1:A:243:ASP:O	2.49	0.46
1:A:372:ILE:HG12	1:B:211:VAL:HG21	1.97	0.46
1:A:189:TRP:CD1	1:A:189:TRP:C	2.94	0.46
1:D:193:ASP:O	1:D:207:LYS:CE	2.63	0.46
1:E:305:LYS:O	1:E:307:GLU:N	2.49	0.46
1:F:229:LYS:C	1:F:233:SER:OG	2.59	0.46
1:A:204:ARG:O	1:A:206:SER:N	2.49	0.46
1:E:277:THR:O	1:E:278:VAL:HG13	2.15	0.46
1:E:305:LYS:CE	1:E:305:LYS:HA	2.45	0.46
1:B:313:ALA:HB2	1:C:324:GLY:CA	2.42	0.46
1:C:326:LEU:HB3	1:C:328:ASP:OD1	2.15	0.46
1:E:223:VAL:O	1:E:223:VAL:CG1	2.64	0.46
1:A:194:PRO:HA	1:A:207:LYS:HG2	1.97	0.46
1:C:240:ASN:HB3	1:C:243:ASP:OD1	2.16	0.46
1:C:323:ILE:HG13	1:C:331:VAL:HG21	1.98	0.46
1:E:188:LEU:HD23	1:E:269:TRP:CZ2	2.51	0.46
1:E:237:ASN:HB2	1:E:356:THR:HA	1.98	0.46
1:F:190:THR:HG21	1:F:197:ASN:HD21	1.81	0.46
1:E:362:PHE:CE1	1:E:364:SER:HB3	2.51	0.45
1:F:286:VAL:HB	1:F:287:PRO:HD3	1.97	0.45
1:D:248:VAL:HA	1:D:263:THR:OG1	2.17	0.45
1:E:310:LYS:O	1:E:310:LYS:HD3	2.16	0.45
1:F:297:LYS:CE	1:F:297:LYS:H	2.29	0.45
1:A:286:VAL:CG1	1:A:287:PRO:HD3	2.47	0.45
1:C:221:ALA:HB3	1:C:369:PHE:CE1	2.51	0.45
1:C:357:PHE:HB3	1:C:360:VAL:HG21	1.98	0.45
1:D:249:LYS:N	1:D:263:THR:OG1	2.46	0.45
1:E:189:TRP:NE1	1:E:272:ARG:HA	2.31	0.45
1:E:314:LYS:CE	1:F:209:THR:HG21	2.47	0.45
1:F:194:PRO:HA	1:F:207:LYS:CE	2.44	0.45
1:A:190:THR:HG23	1:A:210:LEU:O	2.16	0.45
1:F:245:LYS:HA	1:F:351:PHE:O	2.17	0.45
1:B:238:ASN:HD21	1:B:358:GLU:HG2	1.81	0.45
1:D:221:ALA:O	1:D:368:THR:HA	2.16	0.45
1:E:321:VAL:CG1	1:E:367:PHE:HB2	2.46	0.45
1:D:201:ASP:CG	1:D:202:GLN:N	2.75	0.45
1:C:322:TYR:HE1	1:C:330:THR:HG23	1.81	0.45
1:D:189:TRP:C	1:D:189:TRP:CD1	2.95	0.45
1:D:190:THR:O	1:D:191:THR:C	2.60	0.45
1:D:341:THR:C	1:D:342:GLU:CD	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:189:TRP:NE1	1:F:272:ARG:HA	2.32	0.45
1:B:200:ILE:HB	1:B:205:ASP:OD2	2.17	0.44
1:D:193:ASP:O	1:D:207:LYS:HE2	2.17	0.44
1:E:221:ALA:HB1	1:E:369:PHE:CZ	2.52	0.44
1:A:200:ILE:O	1:A:201:ASP:C	2.59	0.44
1:A:311:SER:HA	1:B:363:ASP:OD2	2.17	0.44
1:D:250:LEU:HA	1:D:262:SER:HB3	1.98	0.44
1:E:313:ALA:HB2	1:F:324:GLY:HA2	1.99	0.44
1:F:273:ASN:CA	1:F:277:THR:HG21	2.47	0.44
1:F:292:ILE:HD12	1:F:292:ILE:HA	1.87	0.44
1:E:254:GLU:CD	1:E:254:GLU:H	2.25	0.44
1:E:291:ASN:HB3	1:E:294:ALA:HB3	1.98	0.44
1:F:238:ASN:HD21	1:F:358:GLU:HG2	1.82	0.44
1:C:321:VAL:O	1:C:331:VAL:HB	2.17	0.44
1:C:357:PHE:HB3	1:C:360:VAL:CG2	2.46	0.44
1:B:343:CYS:HB2	1:B:345:TYR:O	2.17	0.44
1:D:189:TRP:O	1:D:189:TRP:CD1	2.70	0.44
1:E:193:ASP:O	1:E:207:LYS:CE	2.66	0.44
1:F:225:LEU:HD23	1:F:246:ILE:HD11	1.95	0.44
1:B:197:ASN:OD1	1:B:197:ASN:C	2.61	0.44
1:B:200:ILE:HD13	1:B:246:ILE:CD1	2.47	0.44
1:E:319:SER:OG	1:E:367:PHE:CE1	2.61	0.44
1:F:259:MET:O	1:F:262:SER:OG	2.25	0.44
1:B:221:ALA:HB1	1:B:369:PHE:CZ	2.53	0.43
1:F:335:ILE:N	1:F:335:ILE:HD12	2.32	0.43
1:A:200:ILE:O	1:A:205:ASP:HB2	2.18	0.43
1:A:209:THR:O	1:A:223:VAL:HA	2.18	0.43
1:A:338:ASN:HD21	1:A:345:TYR:HD2	1.66	0.43
1:C:313:ALA:O	1:C:316:TYR:N	2.50	0.43
1:D:194:PRO:O	1:D:207:LYS:CD	2.66	0.43
1:D:306:PRO:HB3	1:E:229:LYS:HB3	2.00	0.43
1:C:324:GLY:C	1:C:326:LEU:N	2.72	0.43
1:D:194:PRO:O	1:D:195:SER:C	2.61	0.43
1:D:200:ILE:HD13	1:D:246:ILE:HD12	2.00	0.43
1:F:286:VAL:N	1:F:287:PRO:CD	2.81	0.43
1:F:343:CYS:O	1:F:343:CYS:SG	2.76	0.43
1:A:223:VAL:O	1:A:223:VAL:CG1	2.66	0.43
1:D:342:GLU:CD	1:D:342:GLU:N	2.76	0.43
1:E:252:PHE:HD2	1:E:256:GLY:O	2.01	0.43
1:D:214:LYS:HA	1:D:219:ILE:HD13	2.00	0.43
1:D:225:LEU:HD21	1:D:246:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:TYR:HD1	1:D:315:ARG:HA	1.83	0.43
1:D:341:THR:O	1:D:343:CYS:SG	2.73	0.43
1:F:240:ASN:N	1:F:240:ASN:ND2	2.61	0.43
1:A:317:ILE:HD13	1:A:369:PHE:HB2	1.99	0.43
1:E:201:ASP:OD2	1:E:202:GLN:HG3	2.18	0.43
1:E:210:LEU:HD23	1:E:269:TRP:CZ3	2.54	0.43
1:C:272:ARG:O	1:C:273:ASN:ND2	2.52	0.43
1:D:295:TYR:CD1	1:D:315:ARG:HA	2.54	0.43
1:F:292:ILE:HD11	1:F:297:LYS:HE2	2.00	0.43
1:B:203:GLU:C	1:B:205:ASP:H	2.27	0.43
1:C:232:PHE:CD2	1:C:246:ILE:HG22	2.53	0.43
1:E:186:LEU:HB3	1:E:187:THR:H	1.67	0.43
1:E:253:ASN:C	1:E:344:ALA:HB3	2.44	0.43
1:A:323:ILE:HD11	1:A:331:VAL:HG21	2.01	0.43
1:D:286:VAL:HG12	1:D:287:PRO:CD	2.49	0.43
1:E:189:TRP:HD1	1:E:189:TRP:O	2.02	0.43
1:F:219:ILE:HB	1:F:371:TYR:CE1	2.54	0.43
1:A:321:VAL:C	1:A:322:TYR:CD1	2.97	0.42
1:C:286:VAL:HA	1:C:289:MET:HG3	2.01	0.42
1:B:291:ASN:N	1:B:373:ALA:CB	2.70	0.42
1:C:204:ARG:HH12	1:C:267:GLU:CD	2.26	0.42
1:D:297:LYS:CE	1:D:343:CYS:O	2.67	0.42
1:F:221:ALA:O	1:F:368:THR:HA	2.19	0.42
1:D:285:ALA:C	1:D:287:PRO:HD2	2.43	0.42
1:D:286:VAL:CG1	1:D:287:PRO:CD	2.97	0.42
1:D:292:ILE:O	1:D:296:PRO:HA	2.19	0.42
1:E:205:ASP:OD1	1:E:229:LYS:O	2.38	0.42
1:B:236:ASN:OD1	1:B:238:ASN:N	2.40	0.42
1:C:252:PHE:CD2	1:C:289:MET:CE	2.96	0.42
1:D:286:VAL:N	1:D:287:PRO:CD	2.80	0.42
1:D:246:ILE:HG13	1:D:247:THR:N	2.34	0.42
1:E:309:LYS:HA	1:F:194:PRO:HG3	2.02	0.42
1:B:221:ALA:CB	1:B:369:PHE:CE1	3.03	0.42
1:B:240:ASN:HB3	1:B:243:ASP:OD2	2.20	0.42
1:B:260:ASP:C	1:B:262:SER:N	2.78	0.42
1:B:262:SER:C	1:B:264:LEU:H	2.26	0.42
1:C:284:ASN:O	1:C:285:ALA:HB3	2.20	0.42
1:F:286:VAL:CG1	1:F:374:GLN:NE2	2.83	0.42
1:A:191:THR:O	1:A:193:ASP:O	2.38	0.42
1:F:234:ASN:O	1:F:234:ASN:ND2	2.51	0.42
1:A:209:THR:HG21	1:C:314:LYS:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:248:VAL:HG22	1:E:248:VAL:O	2.19	0.42
1:C:313:ALA:O	1:C:314:LYS:C	2.62	0.41
1:D:191:THR:CG2	1:D:192:PRO:HD2	2.50	0.41
1:D:245:LYS:HB2	1:D:352:THR:HG22	2.02	0.41
1:F:244:LYS:HA	1:F:353:TRP:CE2	2.55	0.41
1:A:210:LEU:HA	1:A:222:ASN:O	2.20	0.41
1:B:250:LEU:HD22	1:B:264:LEU:HD22	2.01	0.41
1:F:190:THR:CG2	1:F:197:ASN:ND2	2.84	0.41
1:A:234:ASN:O	1:A:234:ASN:CG	2.62	0.41
1:C:297:LYS:NZ	1:C:343:CYS:O	2.52	0.41
1:F:239:THR:C	1:F:240:ASN:ND2	2.70	0.41
1:A:194:PRO:O	1:A:207:LYS:HD3	2.21	0.41
1:A:335:ILE:N	1:A:335:ILE:HD12	2.35	0.41
1:D:272:ARG:CZ	1:D:273:ASN:HB2	2.51	0.41
1:D:315:ARG:HD3	1:D:339:ALA:HB2	2.02	0.41
1:A:190:THR:HG23	1:A:210:LEU:H	1.86	0.41
1:B:194:PRO:O	1:B:195:SER:C	2.62	0.41
1:C:322:TYR:CE1	1:C:330:THR:HG23	2.55	0.41
1:D:217:SER:HA	1:D:373:ALA:HB3	2.02	0.41
1:E:252:PHE:CD2	1:E:289:MET:HE1	2.55	0.41
1:A:326:LEU:HD11	1:E:301:ASP:HB2	2.02	0.41
1:E:328:ASP:OD1	1:E:328:ASP:N	2.53	0.41
1:C:284:ASN:O	1:C:285:ALA:CB	2.68	0.41
1:C:324:GLY:O	1:C:326:LEU:HG	2.21	0.41
1:D:290:PRO:O	1:D:291:ASN:C	2.64	0.41
1:D:335:ILE:HD12	1:D:335:ILE:H	1.85	0.41
1:E:190:THR:O	1:E:190:THR:HG22	2.21	0.41
1:E:235:ILE:HB	1:E:360:VAL:HB	2.02	0.41
1:E:259:MET:O	1:E:262:SER:OG	2.37	0.41
1:F:270:ASN:ND2	1:F:282:TYR:HB2	2.36	0.41
1:F:308:ASP:O	1:F:310:LYS:N	2.54	0.41
1:F:315:ARG:O	1:F:337:PHE:HD2	2.03	0.41
1:A:337:PHE:CZ	1:A:371:TYR:HB3	2.56	0.41
1:B:219:ILE:O	1:B:370:SER:HA	2.21	0.41
1:E:284:ASN:OD1	1:E:284:ASN:N	2.54	0.41
1:F:208:LEU:HD13	1:F:248:VAL:HG21	2.03	0.41
1:C:252:PHE:CD1	1:C:289:MET:HE1	2.56	0.40
1:B:242:THR:O	1:B:244:LYS:N	2.54	0.40
1:D:204:ARG:O	1:D:205:ASP:C	2.64	0.40
1:D:270:ASN:O	1:D:277:THR:HB	2.22	0.40
1:F:270:ASN:HD21	1:F:282:TYR:HB2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ASN:O	1:A:235:ILE:C	2.64	0.40
1:B:244:LYS:HA	1:B:353:TRP:NE1	2.37	0.40
1:B:260:ASP:O	1:B:262:SER:N	2.55	0.40
1:F:338:ASN:HA	1:F:346:SER:OG	2.21	0.40
1:A:313:ALA:HB2	1:B:324:GLY:CA	2.51	0.40
1:D:292:ILE:O	1:D:296:PRO:CA	2.70	0.40
1:D:319:SER:OG	1:D:367:PHE:CZ	2.74	0.40
1:D:328:ASP:CG	1:D:329:LYS:HE2	2.47	0.40
1:F:226:LEU:HD11	1:F:361:GLN:NE2	2.37	0.40
1:A:190:THR:CG2	1:A:210:LEU:HB3	2.52	0.40
1:A:363:ASP:CG	1:A:363:ASP:O	2.62	0.40
1:B:210:LEU:HD22	1:B:349:PHE:CE2	2.56	0.40
1:B:283:ASP:C	1:B:283:ASP:OD1	2.65	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	177/196 (90%)	138 (78%)	31 (18%)	8 (4%)	2	12
1	B	181/196 (92%)	142 (78%)	27 (15%)	12 (7%)	1	6
1	C	186/196 (95%)	138 (74%)	33 (18%)	15 (8%)	1	4
1	D	183/196 (93%)	145 (79%)	26 (14%)	12 (7%)	1	6
1	E	191/196 (97%)	156 (82%)	29 (15%)	6 (3%)	3	18
1	F	189/196 (96%)	142 (75%)	34 (18%)	13 (7%)	1	5
All	All	1107/1176 (94%)	861 (78%)	180 (16%)	66 (6%)	1	7

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201	ASP
1	A	243	ASP
1	A	272	ARG
1	B	205	ASP
1	C	276	SER
1	C	325	GLY
1	D	273	ASN
1	D	286	VAL
1	D	291	ASN
1	D	314	LYS
1	D	342	GLU
1	F	205	ASP
1	F	274	ASP
1	F	275	ASN
1	F	308	ASP
1	A	235	ILE
1	B	216	GLY
1	B	228	VAL
1	B	243	ASP
1	B	261	SER
1	B	299	THR
1	B	343	CYS
1	B	373	ALA
1	C	190	THR
1	C	228	VAL
1	C	269	TRP
1	C	270	ASN
1	C	375	GLU
1	D	350	GLU
1	E	193	ASP
1	E	257	VAL
1	E	260	ASP
1	E	291	ASN
1	A	359	ASP
1	B	346	SER
1	C	306	PRO
1	C	314	LYS
1	D	228	VAL
1	E	271	TYR
1	F	245	LYS
1	F	309	LYS
1	F	328	ASP
1	F	342	GLU

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Mol	Chain	Res	Type
1	A	267	GLU
1	B	192	PRO
1	B	275	ASN
1	C	216	GLY
1	C	262	SER
1	C	272	ARG
1	C	342	GLU
1	C	362	PHE
1	D	276	SER
1	D	343	CYS
1	F	279	SER
1	F	366	SER
1	A	308	ASP
1	C	285	ALA
1	D	195	SER
1	D	341	THR
1	E	306	PRO
1	F	191	THR
1	F	196	PRO
1	A	205	ASP
1	B	195	SER
1	F	298	PRO
1	D	194	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	166/180 (92%)	130 (78%)	36 (22%)	1	5
1	B	170/180 (94%)	145 (85%)	25 (15%)	3	14
1	C	175/180 (97%)	147 (84%)	28 (16%)	2	12
1	D	171/180 (95%)	135 (79%)	36 (21%)	1	5
1	E	177/180 (98%)	140 (79%)	37 (21%)	1	5
1	F	175/180 (97%)	144 (82%)	31 (18%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1034/1080 (96%)	841 (81%)	193 (19%)	1 7

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	TRP
1	A	190	THR
1	A	193	ASP
1	A	198	CYS
1	A	200	ILE
1	A	209	THR
1	A	218	GLN
1	A	224	SER
1	A	242	THR
1	A	246	ILE
1	A	248	VAL
1	A	250	LEU
1	A	254	GLU
1	A	255	LYS
1	A	261	SER
1	A	262	SER
1	A	264	LEU
1	A	265	LYS
1	A	269	TRP
1	A	272	ARG
1	A	280	GLN
1	A	283	ASP
1	A	286	VAL
1	A	289	MET
1	A	293	LYS
1	A	307	GLU
1	A	309	LYS
1	A	319	SER
1	A	333	ILE
1	A	336	LYS
1	A	342	GLU
1	A	350	GLU
1	A	356	THR
1	A	358	GLU
1	A	366	SER
1	A	376	ASN
1	B	187	THR

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Mol	Chain	Res	Type
1	B	203	GLU
1	B	208	LEU
1	B	209	THR
1	B	218	GLN
1	B	224	SER
1	B	229	LYS
1	B	234	ASN
1	B	242	THR
1	B	246	ILE
1	B	248	VAL
1	B	272	ARG
1	B	275	ASN
1	B	283	ASP
1	B	286	VAL
1	B	292	ILE
1	B	308	ASP
1	B	310	LYS
1	B	328	ASP
1	B	330	THR
1	B	348	THR
1	B	352	THR
1	B	372	ILE
1	B	375	GLU
1	B	376	ASN
1	C	187	THR
1	C	188	LEU
1	C	215	CYS
1	C	220	LEU
1	C	224	SER
1	C	234	ASN
1	C	235	ILE
1	C	238	ASN
1	C	242	THR
1	C	246	ILE
1	C	248	VAL
1	C	251	LEU
1	C	254	GLU
1	C	255	LYS
1	C	270	ASN
1	C	271	TYR
1	C	286	VAL
1	C	291	ASN

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Mol	Chain	Res	Type
1	C	292	ILE
1	C	299	THR
1	C	307	GLU
1	C	310	LYS
1	C	319	SER
1	C	328	ASP
1	C	330	THR
1	C	336	LYS
1	C	346	SER
1	C	376	ASN
1	D	186	LEU
1	D	188	LEU
1	D	203	GLU
1	D	208	LEU
1	D	209	THR
1	D	211	VAL
1	D	222	ASN
1	D	229	LYS
1	D	239	THR
1	D	240	ASN
1	D	246	ILE
1	D	248	VAL
1	D	250	LEU
1	D	254	GLU
1	D	255	LYS
1	D	269	TRP
1	D	270	ASN
1	D	271	TYR
1	D	273	ASN
1	D	276	SER
1	D	277	THR
1	D	284	ASN
1	D	299	THR
1	D	302	THR
1	D	307	GLU
1	D	309	LYS
1	D	333	ILE
1	D	334	THR
1	D	336	LYS
1	D	341	THR
1	D	342	GLU
1	D	346	SER

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Mol	Chain	Res	Type
1	D	356	THR
1	D	359	ASP
1	D	374	GLN
1	D	375	GLU
1	E	186	LEU
1	E	190	THR
1	E	193	ASP
1	E	198	CYS
1	E	203	GLU
1	E	208	LEU
1	E	209	THR
1	E	218	GLN
1	E	234	ASN
1	E	240	ASN
1	E	243	ASP
1	E	246	ILE
1	E	248	VAL
1	E	253	ASN
1	E	255	LYS
1	E	260	ASP
1	E	262	SER
1	E	264	LEU
1	E	266	LYS
1	E	270	ASN
1	E	278	VAL
1	E	283	ASP
1	E	284	ASN
1	E	286	VAL
1	E	292	ILE
1	E	297	LYS
1	E	305	LYS
1	E	310	LYS
1	E	328	ASP
1	E	330	THR
1	E	336	LYS
1	E	341	THR
1	E	352	THR
1	E	357	PHE
1	E	359	ASP
1	E	372	ILE
1	E	378	ASP
1	F	188	LEU

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Mol	Chain	Res	Type
1	F	193	ASP
1	F	198	CYS
1	F	208	LEU
1	F	209	THR
1	F	213	THR
1	F	220	LEU
1	F	228	VAL
1	F	234	ASN
1	F	240	ASN
1	F	246	ILE
1	F	248	VAL
1	F	254	GLU
1	F	255	LYS
1	F	268	TYR
1	F	270	ASN
1	F	273	ASN
1	F	283	ASP
1	F	284	ASN
1	F	297	LYS
1	F	299	THR
1	F	300	THR
1	F	308	ASP
1	F	310	LYS
1	F	328	ASP
1	F	330	THR
1	F	334	THR
1	F	336	LYS
1	F	342	GLU
1	F	368	THR
1	F	370	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	GLN
1	A	218	GLN
1	A	234	ASN
1	A	240	ASN
1	A	273	ASN
1	A	280	GLN
1	A	374	GLN
1	B	222	ASN

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Mol	Chain	Res	Type
1	B	234	ASN
1	B	238	ASN
1	B	240	ASN
1	B	270	ASN
1	B	280	GLN
1	B	320	ASN
1	B	374	GLN
1	C	234	ASN
1	C	253	ASN
1	C	270	ASN
1	C	273	ASN
1	C	284	ASN
1	C	320	ASN
1	C	361	GLN
1	D	218	GLN
1	D	222	ASN
1	D	240	ASN
1	D	270	ASN
1	D	291	ASN
1	D	320	ASN
1	E	222	ASN
1	E	240	ASN
1	E	253	ASN
1	E	270	ASN
1	E	320	ASN
1	F	222	ASN
1	F	238	ASN
1	F	240	ASN
1	F	270	ASN
1	F	273	ASN
1	F	275	ASN
1	F	284	ASN
1	F	320	ASN
1	F	374	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 [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 [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	181/196 (92%)	-0.35	0	100	100	71, 115, 159, 190	0
1	B	185/196 (94%)	-0.46	0	100	100	66, 102, 143, 195	0
1	C	190/196 (96%)	-0.41	0	100	100	55, 82, 135, 196	0
1	D	187/196 (95%)	-0.51	0	100	100	64, 101, 143, 166	0
1	E	193/196 (98%)	-0.50	1 (0%)	87	73	55, 87, 148, 200	0
1	F	191/196 (97%)	-0.37	0	100	100	63, 108, 169, 187	0
All	All	1127/1176 (95%)	-0.43	1 (0%)	92	86	55, 100, 155, 200	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	288	PHE	2.7

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.