



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:47 PM UTC

PDB ID : 1NOV / pdb_00001nov
Title : NODAMURA VIRUS
Authors : Natarajan, P.; Johnson, J.E.
Deposited on : 1997-09-16
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
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

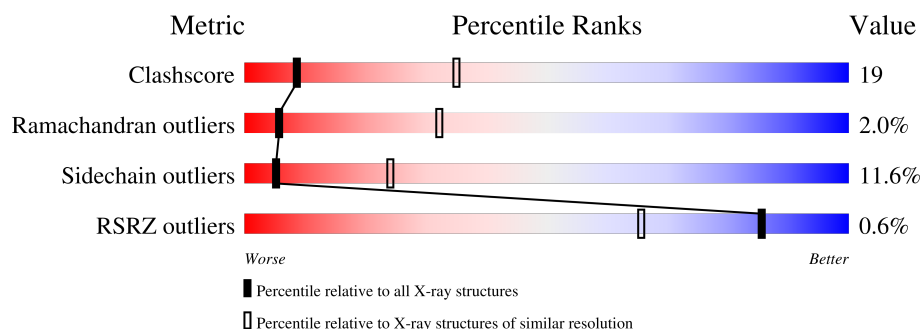
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	355	% 50% 30% 5% • 13%
1	B	355	54% 29% • • 13%
1	C	355	% 52% 32% 6% • 9%
2	D	44	25% 16% 5% 55%
2	E	44	2% 30% 9% 61%
2	F	44	18% 16% 5% 61%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7451 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 NODAMURA VIRUS COAT PROTEINS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2300	1468	373	445	14			
1	B	309	Total	C	N	O	S	0	0	0
			2297	1465	373	445	14			
1	C	324	Total	C	N	O	S	0	0	0
			2434	1541	412	467	14			

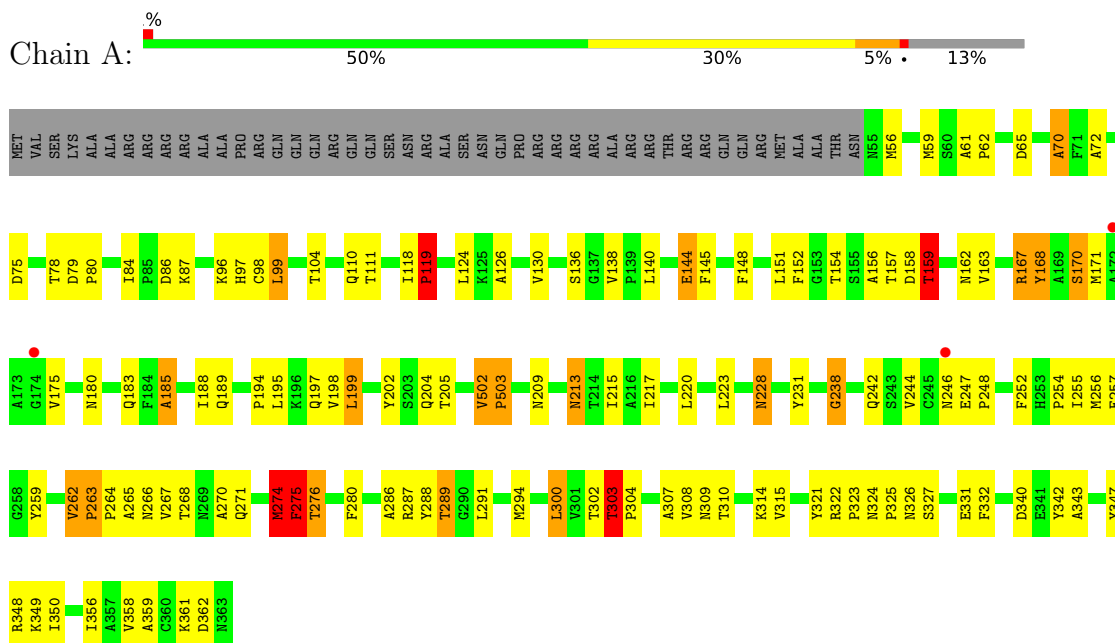
- Molecule 2 is a protein called NODAMURA VIRUS COAT PROTEINS.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	20	Total	C	N	O	0	0	0
			149	96	28	25			
2	E	17	Total	C	N	O	0	0	0
			134	87	25	22			
2	F	17	Total	C	N	O	0	0	0
			137	88	26	23			

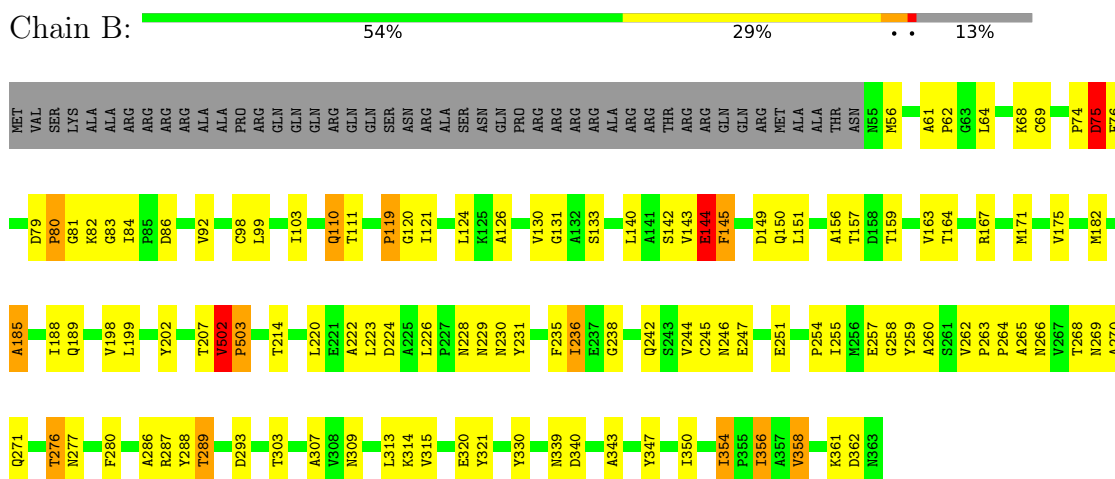
3 Residue-property plots

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.

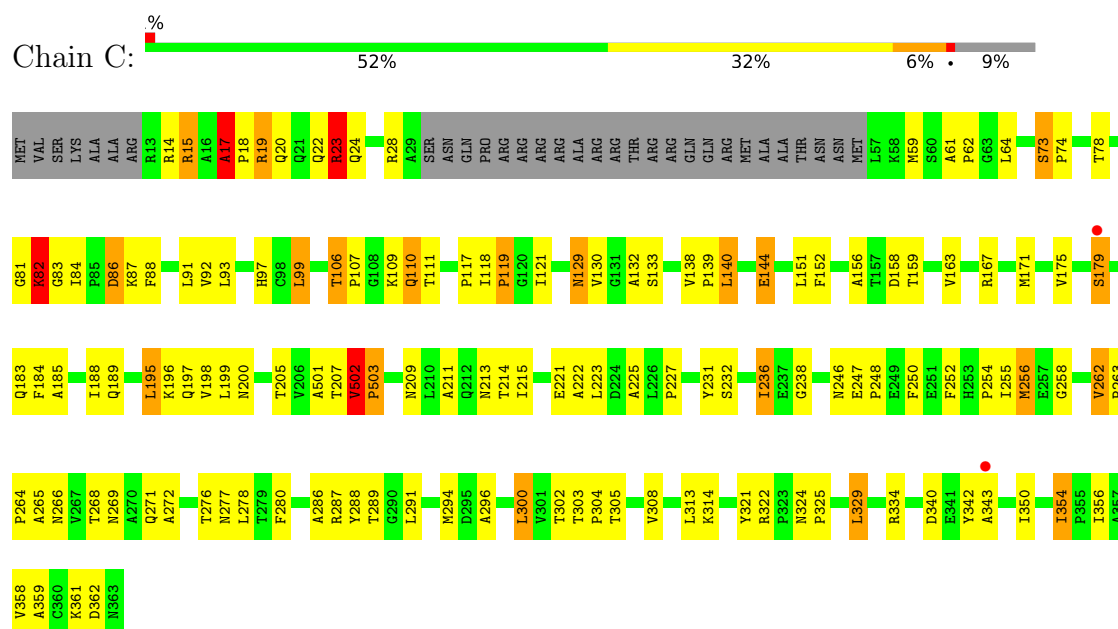
• Molecule 1: NODAMURA VIRUS COAT PROTEINS



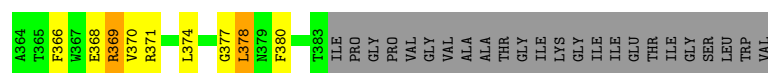
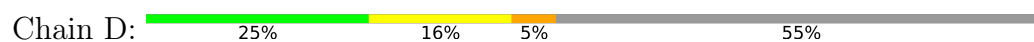
• Molecule 1: NODAMURA VIRUS COAT PROTEINS



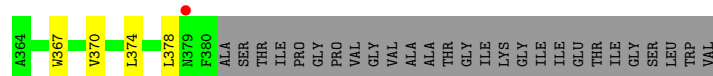
• Molecule 1: NODAMURA VIRUS COAT PROTEINS



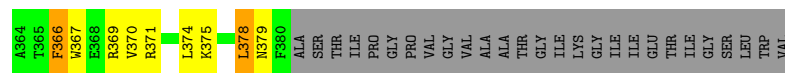
• Molecule 2: NODAMURA VIRUS COAT PROTEINS



- Molecule 2: NODAMURA VIRUS COAT PROTEINS



- Molecule 2: NODAMURA VIRUS COAT PROTEINS



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	562.09Å 354.13Å 612.77Å 90.00° 110.89° 90.00°	Depositor
Resolution (Å)	8.00 – 3.50 8.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	48.1 (8.00-3.50) 49.1 (8.00-3.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.10 (at 3.29Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.296 , (Not available) 0.322 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.05	EDS
Total number of atoms	7451	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.65% 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 (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	0.55	1/2356 (0.0%)	1.13	20/3221 (0.6%)
1	B	0.53	0/2353	1.15	14/3217 (0.4%)
1	C	0.53	0/2490	1.17	19/3396 (0.6%)
2	D	0.52	0/151	0.99	0/203
2	E	0.51	0/136	1.02	0/182
2	F	0.57	0/139	1.14	0/186
All	All	0.54	1/7625 (0.0%)	1.15	53/10405 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	274	MET	SD-CE	-5.91	1.64	1.79

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	15	ARG	N-CA-C	12.09	128.40	113.17
1	B	502	VAL	CA-C-N	-11.32	108.72	120.38
1	B	502	VAL	C-N-CA	-11.32	108.72	120.38
1	B	263	PRO	N-CA-C	-10.86	97.45	110.70
1	C	263	PRO	N-CA-C	-10.64	97.72	110.70
1	A	503	PRO	N-CA-C	-10.54	97.84	110.70
1	C	503	PRO	N-CA-C	-10.48	97.92	110.70
1	A	263	PRO	N-CA-C	-10.24	98.20	110.70
1	C	23	ARG	N-CA-C	10.00	124.73	110.23
1	B	503	PRO	N-CA-C	-9.56	99.04	110.70
1	B	262	VAL	CA-C-N	-8.78	111.34	120.38
1	B	262	VAL	C-N-CA	-8.78	111.34	120.38
1	C	262	VAL	CA-C-N	-8.66	111.46	120.38
1	C	262	VAL	C-N-CA	-8.66	111.46	120.38
1	C	502	VAL	CA-C-N	-8.58	111.54	120.38
1	C	502	VAL	C-N-CA	-8.58	111.54	120.38
1	A	262	VAL	CA-C-N	-8.17	111.97	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	VAL	C-N-CA	-8.17	111.97	120.38
1	A	157	THR	N-CA-C	-8.12	101.51	114.09
1	B	75	ASP	N-CA-C	7.73	121.59	112.93
1	C	132	ALA	N-CA-C	7.15	119.21	110.41
1	B	145	PHE	N-CA-C	-6.95	100.10	110.24
1	C	22	GLN	N-CA-C	-6.90	97.16	108.41
1	B	56	MET	N-CA-C	6.64	119.38	110.88
1	A	145	PHE	N-CA-C	-6.48	101.14	110.08
1	A	303	THR	CA-C-N	6.41	126.36	120.21
1	A	303	THR	C-N-CA	6.41	126.36	120.21
1	A	332	PHE	N-CA-C	-6.34	105.47	113.72
1	A	158	ASP	N-CA-C	-6.22	106.01	113.97
1	B	74	PRO	N-CA-C	6.19	121.64	114.03
1	A	144	GLU	N-CA-C	6.08	119.27	110.28
1	C	20	GLN	N-CA-C	6.07	119.78	112.38
1	A	70	ALA	N-CA-C	5.77	117.25	111.07
1	A	275	PHE	N-CA-C	5.66	120.32	112.90
1	A	324	ASN	N-CA-C	-5.51	102.70	109.65
1	C	106	THR	CA-C-N	5.50	125.43	119.76
1	C	106	THR	C-N-CA	5.50	125.43	119.76
1	C	78	THR	N-CA-C	5.43	117.09	110.41
1	A	118	ILE	CA-C-N	5.38	126.56	119.84
1	A	118	ILE	C-N-CA	5.38	126.56	119.84
1	A	502	VAL	CA-C-N	-5.29	114.94	120.38
1	A	502	VAL	C-N-CA	-5.29	114.94	120.38
1	C	17	ALA	CA-C-N	-5.26	113.27	119.84
1	C	17	ALA	C-N-CA	-5.26	113.27	119.84
1	A	168	TYR	N-CA-C	5.24	118.10	109.76
1	C	256	MET	N-CA-C	5.23	117.80	109.96
1	B	144	GLU	N-CA-C	5.16	117.77	110.50
1	C	118	ILE	CA-C-N	5.16	126.29	119.84
1	C	118	ILE	C-N-CA	5.16	126.29	119.84
1	B	143	VAL	N-CA-C	-5.14	99.54	106.85
1	A	276	THR	N-CA-C	-5.14	101.48	109.14
1	B	82	LYS	N-CA-C	-5.12	100.35	109.06
1	B	110	GLN	N-CA-C	-5.08	101.43	109.76

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	2300	0	2250	97	0
1	B	2297	0	2241	82	0
1	C	2434	0	2387	109	0
2	D	149	0	143	8	0
2	E	134	0	134	3	0
2	F	137	0	138	10	0
All	All	7451	0	7293	276	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 19.

All (276) 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:C:502:VAL:HB	1:C:503:PRO:HD3	1.35	1.05
1:A:180:ASN:HB3	1:A:183:GLN:HB2	1.40	1.03
1:A:502:VAL:HB	1:A:503:PRO:HD3	1.40	1.00
1:A:156:ALA:HB3	1:A:287:ARG:HD2	1.42	0.98
1:A:168:TYR:HB3	1:A:294:MET:HE2	1.50	0.93
1:C:84:ILE:HD12	1:C:167:ARG:HD3	1.52	0.92
1:B:198:VAL:HG22	1:C:254:PRO:HB2	1.57	0.86
1:A:254:PRO:HB2	1:C:198:VAL:HG22	1.59	0.83
1:A:217:ILE:H	1:A:274:MET:HE1	1.44	0.82
1:C:199:LEU:HD21	1:C:213:ASN:HB3	1.63	0.81
1:C:156:ALA:H	1:C:287:ARG:NH1	1.78	0.80
1:C:156:ALA:HA	1:C:159:THR:HG23	1.62	0.80
1:C:268:THR:OG1	1:C:271:GLN:HG3	1.84	0.78
1:A:303:THR:HB	1:A:309:ASN:HD22	1.48	0.78
1:B:502:VAL:HB	1:B:503:PRO:CD	2.12	0.77
1:A:198:VAL:HG22	1:B:254:PRO:HB2	1.67	0.76
1:B:246:ASN:HB2	1:B:293:ASP:O	1.87	0.75
1:C:152:PHE:O	1:C:159:THR:HA	1.87	0.75
1:C:502:VAL:HB	1:C:503:PRO:CD	2.15	0.74
1:A:268:THR:HB	1:A:271:GLN:HG3	1.71	0.73
1:C:189:GLN:HA	1:C:231:TYR:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:THR:HG21	1:C:272:ALA:HA	1.71	0.73
1:B:350:ILE:HD13	2:E:370:VAL:HG13	1.70	0.73
1:C:358:VAL:HG21	2:F:366:PHE:HE2	1.53	0.72
1:C:188:ILE:HD12	1:C:238:GLY:HA2	1.69	0.72
1:C:156:ALA:H	1:C:287:ARG:HH11	1.37	0.71
1:B:350:ILE:HD11	2:E:374:LEU:HD21	1.73	0.70
1:A:124:LEU:HB3	1:A:140:LEU:HB3	1.74	0.70
1:A:325:PRO:HB3	1:C:227:PRO:HG3	1.72	0.70
1:C:156:ALA:N	1:C:287:ARG:HD3	2.08	0.69
1:A:65:ASP:HB3	1:A:80:PRO:O	1.92	0.69
1:B:86:ASP:HA	1:B:339:ASN:HD22	1.57	0.69
1:C:15:ARG:O	1:C:19:ARG:HB2	1.91	0.69
1:A:356:ILE:HD12	1:A:356:ILE:H	1.58	0.68
1:A:156:ALA:HB3	1:A:287:ARG:CD	2.20	0.68
1:C:167:ARG:HB2	1:C:252:PHE:CD1	2.28	0.68
1:B:255:ILE:HG23	1:B:289:THR:HG22	1.76	0.68
1:A:257:GLU:H	1:C:200:ASN:ND2	1.93	0.66
1:C:88:PHE:HB3	1:C:167:ARG:HH22	1.60	0.66
1:A:163:VAL:HG11	1:A:321:TYR:CD1	2.31	0.66
1:B:133:SER:HB2	1:B:224:ASP:OD2	1.95	0.66
1:A:189:GLN:HA	1:A:231:TYR:O	1.96	0.66
1:C:205:THR:HG22	1:C:209:ASN:OD1	1.97	0.65
1:B:156:ALA:HB2	1:B:287:ARG:CG	2.25	0.65
1:A:59:MET:HE3	1:A:343:ALA:HA	1.79	0.64
1:A:199:LEU:HD22	1:A:213:ASN:HB2	1.79	0.64
1:A:358:VAL:HG11	1:A:362:ASP:HB2	1.79	0.64
1:B:83:GLY:HA3	1:B:320:GLU:OE2	1.98	0.64
1:C:110:GLN:HG2	1:C:130:VAL:HA	1.79	0.64
1:A:248:PRO:HD2	1:B:251:GLU:HG2	1.80	0.64
1:A:217:ILE:H	1:A:274:MET:CE	2.11	0.63
1:B:207:THR:HG22	1:B:502:VAL:H	1.62	0.63
1:A:159:THR:HG23	1:A:257:GLU:HG2	1.79	0.63
1:C:23:ARG:HD3	1:C:24:GLN:H	1.62	0.63
1:A:263:PRO:HG3	1:A:274:MET:SD	2.39	0.63
1:A:136:SER:O	1:A:276:THR:HG22	1.99	0.62
1:B:268:THR:HB	1:B:271:GLN:HG3	1.81	0.62
1:B:156:ALA:HB2	1:B:287:ARG:HG3	1.79	0.62
1:A:188:ILE:HD12	1:A:238:GLY:HA2	1.81	0.62
1:A:350:ILE:HD13	2:D:370:VAL:HG13	1.81	0.61
1:C:59:MET:HG2	1:C:342:TYR:HD1	1.66	0.61
1:A:86:ASP:OD2	1:C:248:PRO:HB3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:THR:HG22	1:B:270:ALA:H	1.65	0.61
1:B:350:ILE:O	1:B:354:ILE:HG12	2.01	0.61
1:C:81:GLY:O	1:C:83:GLY:N	2.34	0.61
1:B:159:THR:HB	1:B:257:GLU:HG2	1.81	0.60
1:A:349:LYS:CD	2:D:378:LEU:HD23	2.32	0.60
1:B:265:ALA:O	1:B:266:ASN:HB2	2.00	0.60
1:C:167:ARG:HB2	1:C:252:PHE:HD1	1.66	0.60
1:B:163:VAL:HG11	1:B:321:TYR:CD1	2.37	0.59
1:A:152:PHE:O	1:A:159:THR:HA	2.02	0.59
1:A:349:LYS:HD2	2:D:378:LEU:HD23	1.84	0.59
1:C:354:ILE:HD11	2:F:366:PHE:HE1	1.68	0.59
1:C:262:VAL:HG21	1:C:278:LEU:HD12	1.84	0.59
1:A:194:PRO:O	1:B:164:THR:HG21	2.03	0.59
1:C:163:VAL:HG11	1:C:321:TYR:CD1	2.38	0.58
1:C:175:VAL:O	1:C:238:GLY:HA3	2.03	0.58
1:A:180:ASN:HB3	1:A:183:GLN:CB	2.26	0.58
1:B:175:VAL:O	1:B:238:GLY:HA3	2.03	0.58
1:A:110:GLN:HB3	1:A:300:LEU:HD21	1.86	0.58
1:A:265:ALA:O	1:A:266:ASN:HB2	2.03	0.57
1:B:244:VAL:HG13	1:B:347:TYR:CZ	2.38	0.57
1:B:156:ALA:HB3	1:B:287:ARG:NH1	2.20	0.57
1:A:502:VAL:HB	1:A:503:PRO:CD	2.25	0.57
1:A:259:TYR:O	1:A:287:ARG:HB3	2.04	0.56
2:D:368:GLU:HG2	2:D:371:ARG:HH21	1.69	0.56
1:A:213:ASN:HD22	1:C:213:ASN:ND2	2.02	0.56
1:B:220:LEU:O	1:B:223:LEU:HB2	2.05	0.56
1:A:303:THR:CB	1:A:309:ASN:HD22	2.17	0.56
1:A:140:LEU:HD11	1:A:223:LEU:HD11	1.88	0.55
1:C:350:ILE:HD13	2:F:370:VAL:HG13	1.89	0.55
1:B:124:LEU:HB3	1:B:140:LEU:HB3	1.88	0.55
1:C:247:GLU:HG3	1:C:248:PRO:HD2	1.88	0.55
1:A:244:VAL:HG13	1:A:347:TYR:CZ	2.42	0.55
1:A:202:TYR:HE1	1:A:204:GLN:HG3	1.71	0.55
1:B:244:VAL:HG12	1:B:245:CYS:N	2.22	0.54
1:C:73:SER:N	1:C:74:PRO:HD2	2.22	0.54
1:B:149:ASP:HB2	1:B:150:GLN:NE2	2.21	0.54
1:C:156:ALA:H	1:C:287:ARG:HD3	1.72	0.54
1:A:268:THR:HG22	1:A:270:ALA:H	1.73	0.54
1:B:84:ILE:HD12	1:B:84:ILE:H	1.71	0.54
1:A:340:ASP:OD2	1:A:343:ALA:HB2	2.08	0.54
1:C:156:ALA:HB2	1:C:287:ARG:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:VAL:HG11	1:C:362:ASP:HB2	1.90	0.54
1:A:72:ALA:HB1	1:A:75:ASP:OD2	2.08	0.53
1:B:214:THR:HG23	1:B:264:PRO:HD2	1.90	0.53
1:C:358:VAL:HG21	2:F:366:PHE:CE2	2.40	0.53
1:A:167:ARG:HD2	1:A:252:PHE:CZ	2.45	0.52
1:C:144:GLU:HG2	1:C:286:ALA:HB2	1.90	0.52
1:A:138:VAL:O	1:A:276:THR:HB	2.10	0.52
1:C:19:ARG:HH12	1:C:24:GLN:HA	1.74	0.52
1:A:175:VAL:O	1:A:238:GLY:HA3	2.10	0.52
1:B:358:VAL:HG11	1:B:362:ASP:HB2	1.91	0.52
1:A:267:VAL:HG23	1:C:211:ALA:CB	2.40	0.52
1:C:171:MET:HB2	1:C:294:MET:HE2	1.92	0.52
1:C:156:ALA:CB	1:C:287:ARG:HH11	2.23	0.52
1:A:167:ARG:HD2	1:A:252:PHE:CE1	2.45	0.51
1:A:326:ASN:HD22	1:C:221:GLU:HB3	1.76	0.51
1:C:88:PHE:HZ	1:C:322:ARG:NH1	2.08	0.51
1:A:61:ALA:N	1:A:62:PRO:HD2	2.25	0.51
1:C:199:LEU:CD2	1:C:213:ASN:HB3	2.38	0.51
1:B:189:GLN:OE1	1:B:226:LEU:HD11	2.10	0.51
1:C:156:ALA:HA	1:C:159:THR:CG2	2.36	0.51
1:C:156:ALA:HB2	1:C:287:ARG:CG	2.41	0.51
1:B:502:VAL:HB	1:B:503:PRO:HD2	1.93	0.50
1:C:340:ASP:OD2	1:C:343:ALA:HB2	2.11	0.50
1:C:99:LEU:O	1:C:314:LYS:HA	2.12	0.50
1:A:257:GLU:H	1:C:200:ASN:HD22	1.60	0.50
1:B:188:ILE:HD12	1:B:238:GLY:HA2	1.93	0.50
1:C:167:ARG:HB2	1:C:252:PHE:CE1	2.47	0.50
1:B:99:LEU:O	1:B:314:LYS:HA	2.11	0.50
1:A:358:VAL:CG1	1:A:362:ASP:HB2	2.42	0.49
1:A:99:LEU:O	1:A:314:LYS:HA	2.11	0.49
1:A:183:GLN:HG2	1:A:308:VAL:HB	1.93	0.49
1:B:156:ALA:HB2	1:B:287:ARG:CD	2.42	0.49
1:C:197:GLN:HE22	1:C:256:MET:HE1	1.77	0.49
2:F:378:LEU:HD22	2:F:378:LEU:O	2.12	0.49
1:A:275:PHE:CD1	1:A:276:THR:HG23	2.47	0.49
1:C:82:LYS:NZ	1:C:334:ARG:HD2	2.27	0.49
1:A:70:ALA:HA	1:A:170:SER:HB3	1.93	0.49
1:A:148:PHE:CE2	1:A:286:ALA:HB1	2.48	0.49
1:B:214:THR:HG23	1:B:264:PRO:CD	2.42	0.49
1:A:502:VAL:CB	1:A:503:PRO:HD3	2.29	0.49
1:A:59:MET:CG	1:A:342:TYR:HD2	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ASN:O	1:B:247:GLU:HG3	2.13	0.48
1:A:59:MET:HE3	1:A:343:ALA:CA	2.43	0.48
1:B:121:ILE:HG12	1:B:142:SER:HB2	1.95	0.48
1:A:228:ASN:ND2	1:A:228:ASN:H	2.11	0.48
2:D:369:ARG:HH11	2:D:369:ARG:HB2	1.78	0.48
1:C:19:ARG:HH11	1:C:24:GLN:HG2	1.78	0.48
1:B:198:VAL:HG12	1:B:199:LEU:N	2.29	0.48
1:C:61:ALA:N	1:C:62:PRO:HD2	2.28	0.48
1:C:354:ILE:HD11	2:F:366:PHE:CE1	2.48	0.48
1:B:182:MET:O	1:B:182:MET:HG2	2.14	0.48
1:B:189:GLN:HA	1:B:231:TYR:O	2.14	0.48
1:A:110:GLN:HG3	1:A:130:VAL:HA	1.96	0.47
1:B:276:THR:CG2	1:B:277:ASN:N	2.77	0.47
1:B:260:ALA:HA	1:B:287:ARG:HD3	1.96	0.47
1:C:358:VAL:CG1	1:C:362:ASP:HB2	2.44	0.47
1:B:61:ALA:N	1:B:62:PRO:HD2	2.29	0.47
1:C:59:MET:CG	1:C:342:TYR:HD1	2.26	0.47
1:A:98:CYS:HA	1:A:315:VAL:O	2.14	0.47
1:B:229:ASN:O	1:B:356:ILE:HD12	2.14	0.47
1:B:303:THR:HB	1:B:309:ASN:HD22	1.80	0.47
1:A:59:MET:HE3	1:A:343:ALA:CB	2.45	0.47
1:B:502:VAL:HB	1:B:503:PRO:HD3	1.91	0.47
1:B:110:GLN:CG	1:B:130:VAL:HA	2.45	0.47
1:C:262:VAL:O	1:C:264:PRO:HD3	2.15	0.47
1:C:358:VAL:CG2	2:F:366:PHE:HE2	2.25	0.47
1:A:213:ASN:ND2	1:C:213:ASN:ND2	2.63	0.46
1:C:97:HIS:HE1	1:C:321:TYR:OH	1.99	0.46
1:C:198:VAL:HG12	1:C:199:LEU:N	2.30	0.46
1:A:171:MET:HB2	1:A:294:MET:CE	2.44	0.46
1:B:110:GLN:NE2	1:B:131:GLY:H	2.13	0.46
2:F:366:PHE:O	2:F:370:VAL:HG23	2.15	0.46
1:A:188:ILE:CD1	1:A:238:GLY:HA2	2.46	0.46
1:B:163:VAL:HG12	1:B:255:ILE:HD12	1.98	0.46
1:C:152:PHE:HE1	1:C:255:ILE:HD13	1.81	0.46
1:A:348:ARG:HG2	1:A:348:ARG:HH11	1.81	0.46
1:C:117:PRO:HB3	1:C:171:MET:HE2	1.97	0.46
1:C:265:ALA:O	1:C:266:ASN:HB2	2.15	0.46
1:B:68:LYS:HD2	1:B:80:PRO:HG2	1.98	0.46
1:C:15:ARG:HA	1:C:15:ARG:HD3	1.38	0.46
1:C:84:ILE:HG22	1:C:86:ASP:HB3	1.98	0.46
1:C:110:GLN:HB2	1:C:300:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:GLN:HG2	1:C:232:SER:OG	2.16	0.46
1:A:359:ALA:C	1:A:361:LYS:H	2.24	0.46
1:B:75:ASP:OD1	1:B:75:ASP:N	2.49	0.45
1:B:156:ALA:HB3	1:B:287:ARG:HH11	1.81	0.45
1:A:244:VAL:HG13	1:A:347:TYR:CE2	2.51	0.45
1:A:247:GLU:O	1:A:348:ARG:NH2	2.49	0.45
1:B:188:ILE:HG13	1:B:235:PHE:HA	1.99	0.45
1:B:120:GLY:O	1:B:145:PHE:HB2	2.16	0.45
1:C:358:VAL:HG12	1:C:359:ALA:N	2.32	0.45
1:A:198:VAL:HG12	1:A:199:LEU:N	2.32	0.45
1:A:119:PRO:HB2	1:A:289:THR:OG1	2.16	0.45
1:B:144:GLU:HG2	1:B:286:ALA:HB2	1.98	0.45
1:A:97:HIS:HE1	1:A:321:TYR:OH	1.99	0.45
1:C:358:VAL:HG12	1:C:359:ALA:H	1.82	0.45
1:A:197:GLN:HE22	1:A:256:MET:HE1	1.82	0.44
1:A:326:ASN:HA	1:C:225:ALA:HB2	1.99	0.44
1:C:156:ALA:N	1:C:287:ARG:NH1	2.57	0.44
1:C:236:ILE:HD13	1:C:236:ILE:HA	1.84	0.44
1:A:228:ASN:HD21	1:B:330:TYR:HD2	1.65	0.44
1:A:325:PRO:HD2	1:C:222:ALA:HB2	1.99	0.44
1:A:280:PHE:CE2	1:A:288:TYR:HB2	2.53	0.44
1:B:159:THR:HG22	1:B:255:ILE:CG2	2.47	0.44
1:B:207:THR:HG23	1:C:501:ALA:O	2.18	0.44
1:B:202:TYR:HE2	1:B:214:THR:OG1	2.01	0.44
1:B:84:ILE:HD12	1:B:84:ILE:N	2.33	0.44
1:B:222:ALA:HB2	1:C:324:ASN:OD1	2.18	0.44
1:C:156:ALA:C	1:C:158:ASP:H	2.26	0.44
1:A:185:ALA:HB3	1:A:307:ALA:HB2	2.00	0.43
1:B:358:VAL:CG1	1:B:362:ASP:HB2	2.48	0.43
1:C:184:PHE:CG	1:C:236:ILE:HG12	2.53	0.43
1:A:126:ALA:HB2	1:A:140:LEU:HD23	2.00	0.43
1:B:69:CYS:HA	1:B:79:ASP:OD1	2.18	0.43
1:B:103:ILE:HD11	1:B:313:LEU:HD22	1.99	0.43
1:C:156:ALA:HB3	1:C:287:ARG:HH11	1.82	0.43
1:A:262:VAL:O	1:A:264:PRO:HD3	2.18	0.43
1:C:214:THR:CG2	1:C:272:ALA:HA	2.45	0.43
1:C:156:ALA:HB1	1:C:258:GLY:H	1.84	0.43
1:C:152:PHE:HB3	1:C:159:THR:HG22	2.01	0.43
1:B:110:GLN:HG3	1:B:130:VAL:HA	2.01	0.43
1:B:340:ASP:OD2	1:B:343:ALA:HB2	2.19	0.43
1:C:140:LEU:HD11	1:C:223:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:SER:OG	1:C:308:VAL:O	2.36	0.43
1:A:148:PHE:CE1	1:A:152:PHE:HB2	2.53	0.43
1:B:98:CYS:HA	1:B:315:VAL:O	2.19	0.43
1:A:220:LEU:HD23	1:A:220:LEU:HA	1.92	0.42
1:B:244:VAL:HG13	1:B:347:TYR:CE2	2.54	0.42
1:B:226:LEU:HD13	1:B:230:ASN:ND2	2.35	0.42
1:C:15:ARG:CZ	1:C:18:PRO:HG2	2.50	0.42
1:C:93:LEU:HD11	1:C:329:LEU:HB2	2.02	0.42
2:F:367:TRP:CE3	2:F:367:TRP:HA	2.55	0.42
1:A:162:ASN:HA	1:A:327:SER:HB2	2.00	0.42
1:B:185:ALA:HB3	1:B:307:ALA:HB2	2.01	0.42
1:C:107:PRO:HA	1:C:303:THR:HG22	2.01	0.42
1:C:84:ILE:HD13	1:C:250:PHE:CD2	2.54	0.42
1:A:59:MET:HG3	1:A:342:TYR:HD2	1.84	0.42
1:B:126:ALA:HB2	1:B:140:LEU:HD23	2.01	0.42
2:D:371:ARG:O	2:D:374:LEU:HD23	2.19	0.42
1:B:244:VAL:CG1	1:B:245:CYS:N	2.83	0.42
1:A:171:MET:HB2	1:A:294:MET:HE3	2.02	0.42
1:B:68:LYS:HB3	1:B:76:PHE:CE2	2.54	0.42
2:E:367:TRP:CZ3	2:E:370:VAL:HG11	2.54	0.42
1:B:156:ALA:HB1	1:B:258:GLY:H	1.84	0.41
1:C:106:THR:HA	1:C:107:PRO:HD3	1.80	0.41
1:A:205:THR:HA	1:A:209:ASN:HA	2.02	0.41
1:A:322:ARG:NH1	1:C:246:ASN:HB2	2.34	0.41
1:C:502:VAL:CB	1:C:503:PRO:HD3	2.26	0.41
1:C:121:ILE:N	1:C:121:ILE:HD12	2.35	0.41
1:C:269:ASN:OD1	1:C:277:ASN:HB3	2.21	0.41
1:A:79:ASP:HB3	1:A:96:LYS:HD3	2.02	0.41
1:C:156:ALA:CB	1:C:258:GLY:H	2.33	0.41
1:C:17:ALA:CB	1:C:18:PRO:CD	2.99	0.41
1:B:246:ASN:HB2	1:B:293:ASP:C	2.43	0.41
1:A:322:ARG:HA	1:A:323:PRO:HD2	1.94	0.41
1:C:138:VAL:HA	1:C:139:PRO:HD3	1.87	0.41
1:C:195:LEU:HD11	1:C:296:ALA:HB2	2.03	0.41
1:B:222:ALA:HB2	1:C:325:PRO:HD2	2.02	0.41
1:A:213:ASN:HD22	1:C:213:ASN:HD21	1.68	0.40
1:A:303:THR:HA	1:A:304:PRO:HD3	1.79	0.40
1:B:142:SER:HB3	1:B:280:PHE:CD1	2.57	0.40
1:C:185:ALA:O	1:C:304:PRO:HD2	2.21	0.40
1:C:109:LYS:HE2	1:C:129:ASN:ND2	2.36	0.40
1:A:86:ASP:OD2	1:A:167:ARG:NH2	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:378:LEU:HD13	2:D:378:LEU:O	2.21	0.40
1:B:185:ALA:HB3	1:B:307:ALA:CB	2.51	0.40
1:B:198:VAL:CG2	1:C:254:PRO:HB2	2.41	0.40
1:C:156:ALA:C	1:C:158:ASP:N	2.79	0.40
2:D:366:PHE:O	2:D:370:VAL:HG23	2.22	0.40
1:B:259:TYR:HB3	1:B:288:TYR:HB3	2.03	0.40
1:C:280:PHE:CE2	1:C:288:TYR:HB2	2.56	0.40
1:A:84:ILE:HG22	1:A:86:ASP:HB2	2.04	0.40
2:F:371:ARG:O	2:F:375:LYS:N	2.49	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	307/355 (86%)	280 (91%)	20 (6%)	7 (2%)	5	30
1	B	307/355 (86%)	282 (92%)	19 (6%)	6 (2%)	6	32
1	C	320/355 (90%)	291 (91%)	24 (8%)	5 (2%)	7	36
2	D	18/44 (41%)	14 (78%)	2 (11%)	2 (11%)	0	5
2	E	15/44 (34%)	15 (100%)	0	0	100	100
2	F	15/44 (34%)	14 (93%)	1 (7%)	0	100	100
All	All	982/1197 (82%)	896 (91%)	66 (7%)	20 (2%)	6	32

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	THR
2	D	380	PHE
1	C	17	ALA

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Mol	Chain	Res	Type
1	C	82	LYS
1	A	56	MET
1	A	87	LYS
1	A	119	PRO
1	A	331	GLU
2	D	377	GLY
1	B	119	PRO
1	C	87	LYS
1	A	238	GLY
1	B	185	ALA
1	B	502	VAL
1	C	119	PRO
1	A	185	ALA
1	B	361	LYS
1	C	502	VAL
1	B	236	ILE
1	B	81	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	246/287 (86%)	219 (89%)	27 (11%)	6	26
1	B	245/287 (85%)	225 (92%)	20 (8%)	10	34
1	C	259/287 (90%)	222 (86%)	37 (14%)	3	18
2	D	13/34 (38%)	11 (85%)	2 (15%)	2	16
2	E	13/34 (38%)	12 (92%)	1 (8%)	12	37
2	F	14/34 (41%)	9 (64%)	5 (36%)	0	1
All	All	790/963 (82%)	698 (88%)	92 (12%)	5	24

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	THR

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Mol	Chain	Res	Type
1	A	99	LEU
1	A	104	THR
1	A	111	THR
1	A	119	PRO
1	A	144	GLU
1	A	151	LEU
1	A	154	THR
1	A	159	THR
1	A	167	ARG
1	A	170	SER
1	A	195	LEU
1	A	199	LEU
1	A	213	ASN
1	A	215	ILE
1	A	228	ASN
1	A	242	GLN
1	A	246	ASN
1	A	255	ILE
1	A	274	MET
1	A	275	PHE
1	A	289	THR
1	A	291	LEU
1	A	300	LEU
1	A	302	THR
1	A	303	THR
1	A	310	THR
2	D	369	ARG
2	D	378	LEU
1	B	64	LEU
1	B	75	ASP
1	B	80	PRO
1	B	92	VAL
1	B	111	THR
1	B	119	PRO
1	B	144	GLU
1	B	151	LEU
1	B	157	THR
1	B	167	ARG
1	B	171	MET
1	B	228	ASN
1	B	236	ILE
1	B	242	GLN

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Mol	Chain	Res	Type
1	B	269	ASN
1	B	276	THR
1	B	289	THR
1	B	354	ILE
1	B	356	ILE
1	B	358	VAL
2	E	378	LEU
1	C	14	ARG
1	C	19	ARG
1	C	23	ARG
1	C	28	ARG
1	C	64	LEU
1	C	73	SER
1	C	82	LYS
1	C	86	ASP
1	C	91	LEU
1	C	92	VAL
1	C	99	LEU
1	C	110	GLN
1	C	111	THR
1	C	119	PRO
1	C	129	ASN
1	C	133	SER
1	C	140	LEU
1	C	144	GLU
1	C	151	LEU
1	C	179	SER
1	C	183	GLN
1	C	195	LEU
1	C	196	LYS
1	C	207	THR
1	C	215	ILE
1	C	236	ILE
1	C	276	THR
1	C	289	THR
1	C	291	LEU
1	C	300	LEU
1	C	302	THR
1	C	305	THR
1	C	313	LEU
1	C	329	LEU
1	C	354	ILE

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Mol	Chain	Res	Type
1	C	356	ILE
1	C	361	LYS
2	F	366	PHE
2	F	369	ARG
2	F	374	LEU
2	F	378	LEU
2	F	379	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
1	A	101	GLN
1	A	110	GLN
1	A	189	GLN
1	A	197	GLN
1	A	213	ASN
1	A	228	ASN
1	A	229	ASN
1	A	246	ASN
1	A	253	HIS
1	A	309	ASN
1	A	326	ASN
1	B	97	HIS
1	B	110	GLN
1	B	183	GLN
1	B	213	ASN
1	B	246	ASN
1	B	309	ASN
1	B	326	ASN
1	B	339	ASN
1	C	97	HIS
1	C	110	GLN
1	C	129	ASN
1	C	197	GLN
1	C	200	ASN
1	C	213	ASN
1	C	253	HIS

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 [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	309/355 (87%)	0.15	3 (0%) 79 56	20, 20, 20, 20	0
1	B	309/355 (87%)	0.09	0 100 100	20, 20, 20, 20	0
1	C	324/355 (91%)	0.06	2 (0%) 85 65	20, 20, 20, 20	0
2	D	20/44 (45%)	0.08	0 100 100	20, 20, 20, 20	0
2	E	17/44 (38%)	0.22	1 (5%) 28 16	20, 20, 20, 20	0
2	F	17/44 (38%)	0.08	0 100 100	20, 20, 20, 20	0
All	All	996/1197 (83%)	0.10	6 (0%) 85 65	20, 20, 20, 20	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	246	ASN	2.6
2	E	379	ASN	2.5
1	C	343	ALA	2.4
1	A	174	GLY	2.3
1	A	172	ALA	2.1
1	C	179	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.