



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:35 AM UTC

PDB ID : 6TRU / pdb_00006tru
Title : Crystal structure of the N-terminal half of the TFIIF subunit p52
Authors : Koelmel, W.; Kuper, J.; Schoenwetter, E.; Kisker, C.
Deposited on : 2019-12-19
Resolution : 2.80 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

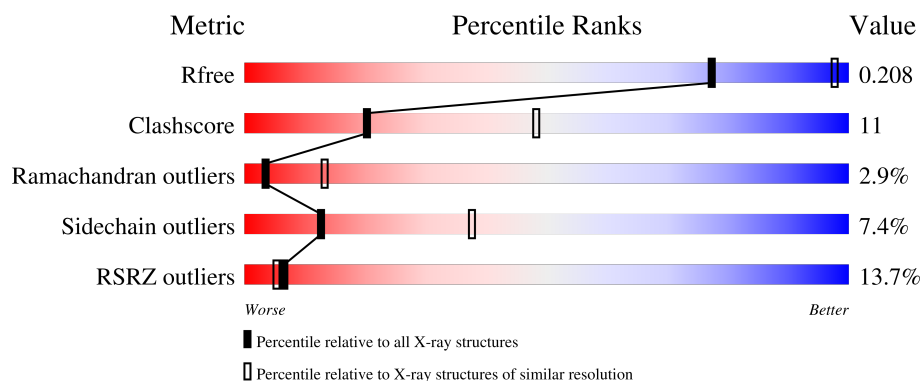
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	347	7% 54% 21% • • 21%
1	B	347	8% 60% 16% • 19%
1	C	347	12% 54% 18% • • 24%
1	D	347	16% 57% 16% • 24%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8572 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 RNA polymerase II transcription factor B subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	280	Total	C	N	O	S	0	0	0
			2214	1429	381	398	6			
1	A	275	Total	C	N	O	S	0	0	0
			2173	1403	372	392	6			
1	C	263	Total	C	N	O	S	0	0	0
			2078	1346	351	375	6			
1	D	264	Total	C	N	O	S	0	1	0
			2107	1366	358	377	6			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-25	MET	-	initiating methionine	UNP G0S965
B	-24	LYS	-	expression tag	UNP G0S965
B	-23	HIS	-	expression tag	UNP G0S965
B	-22	HIS	-	expression tag	UNP G0S965
B	-21	HIS	-	expression tag	UNP G0S965
B	-20	HIS	-	expression tag	UNP G0S965
B	-19	HIS	-	expression tag	UNP G0S965
B	-18	HIS	-	expression tag	UNP G0S965
B	-17	PRO	-	expression tag	UNP G0S965
B	-16	MET	-	expression tag	UNP G0S965
B	-15	SER	-	expression tag	UNP G0S965
B	-14	ASP	-	expression tag	UNP G0S965
B	-13	TYR	-	expression tag	UNP G0S965
B	-12	ASP	-	expression tag	UNP G0S965
B	-11	ILE	-	expression tag	UNP G0S965
B	-10	PRO	-	expression tag	UNP G0S965
B	-9	THR	-	expression tag	UNP G0S965
B	-8	THR	-	expression tag	UNP G0S965
B	-7	GLU	-	expression tag	UNP G0S965
B	-6	ASN	-	expression tag	UNP G0S965
B	-5	LEU	-	expression tag	UNP G0S965

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	TYR	-	expression tag	UNP G0S965
B	-3	PHE	-	expression tag	UNP G0S965
B	-2	GLN	-	expression tag	UNP G0S965
B	-1	GLY	-	expression tag	UNP G0S965
B	0	ALA	-	expression tag	UNP G0S965
A	-25	MET	-	initiating methionine	UNP G0S965
A	-24	LYS	-	expression tag	UNP G0S965
A	-23	HIS	-	expression tag	UNP G0S965
A	-22	HIS	-	expression tag	UNP G0S965
A	-21	HIS	-	expression tag	UNP G0S965
A	-20	HIS	-	expression tag	UNP G0S965
A	-19	HIS	-	expression tag	UNP G0S965
A	-18	HIS	-	expression tag	UNP G0S965
A	-17	PRO	-	expression tag	UNP G0S965
A	-16	MET	-	expression tag	UNP G0S965
A	-15	SER	-	expression tag	UNP G0S965
A	-14	ASP	-	expression tag	UNP G0S965
A	-13	TYR	-	expression tag	UNP G0S965
A	-12	ASP	-	expression tag	UNP G0S965
A	-11	ILE	-	expression tag	UNP G0S965
A	-10	PRO	-	expression tag	UNP G0S965
A	-9	THR	-	expression tag	UNP G0S965
A	-8	THR	-	expression tag	UNP G0S965
A	-7	GLU	-	expression tag	UNP G0S965
A	-6	ASN	-	expression tag	UNP G0S965
A	-5	LEU	-	expression tag	UNP G0S965
A	-4	TYR	-	expression tag	UNP G0S965
A	-3	PHE	-	expression tag	UNP G0S965
A	-2	GLN	-	expression tag	UNP G0S965
A	-1	GLY	-	expression tag	UNP G0S965
A	0	ALA	-	expression tag	UNP G0S965
C	-25	MET	-	initiating methionine	UNP G0S965
C	-24	LYS	-	expression tag	UNP G0S965
C	-23	HIS	-	expression tag	UNP G0S965
C	-22	HIS	-	expression tag	UNP G0S965
C	-21	HIS	-	expression tag	UNP G0S965
C	-20	HIS	-	expression tag	UNP G0S965
C	-19	HIS	-	expression tag	UNP G0S965
C	-18	HIS	-	expression tag	UNP G0S965
C	-17	PRO	-	expression tag	UNP G0S965
C	-16	MET	-	expression tag	UNP G0S965
C	-15	SER	-	expression tag	UNP G0S965

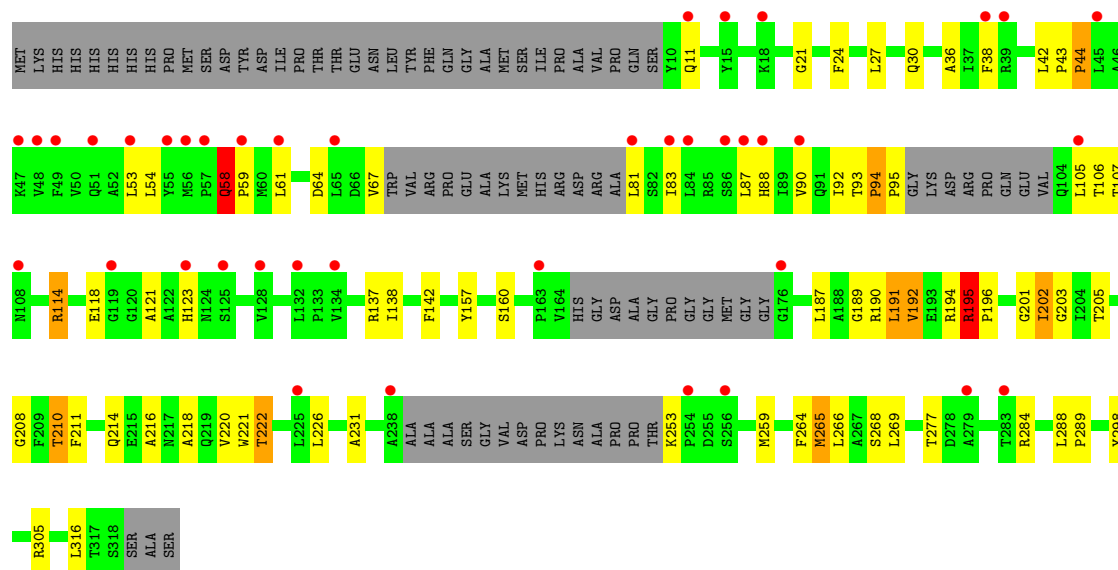
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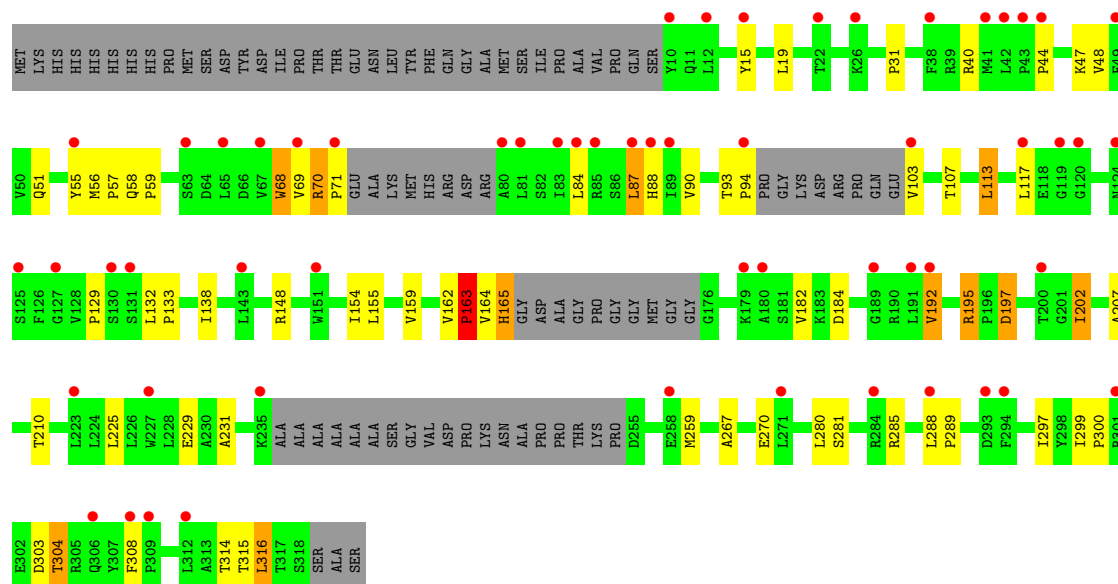
Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	ASP	-	expression tag	UNP G0S965
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C	-10	PRO	-	expression tag	UNP G0S965
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C	-6	ASN	-	expression tag	UNP G0S965
C	-5	LEU	-	expression tag	UNP G0S965
C	-4	TYR	-	expression tag	UNP G0S965
C	-3	PHE	-	expression tag	UNP G0S965
C	-2	GLN	-	expression tag	UNP G0S965
C	-1	GLY	-	expression tag	UNP G0S965
C	0	ALA	-	expression tag	UNP G0S965
D	-25	MET	-	initiating methionine	UNP G0S965
D	-24	LYS	-	expression tag	UNP G0S965
D	-23	HIS	-	expression tag	UNP G0S965
D	-22	HIS	-	expression tag	UNP G0S965
D	-21	HIS	-	expression tag	UNP G0S965
D	-20	HIS	-	expression tag	UNP G0S965
D	-19	HIS	-	expression tag	UNP G0S965
D	-18	HIS	-	expression tag	UNP G0S965
D	-17	PRO	-	expression tag	UNP G0S965
D	-16	MET	-	expression tag	UNP G0S965
D	-15	SER	-	expression tag	UNP G0S965
D	-14	ASP	-	expression tag	UNP G0S965
D	-13	TYR	-	expression tag	UNP G0S965
D	-12	ASP	-	expression tag	UNP G0S965
D	-11	ILE	-	expression tag	UNP G0S965
D	-10	PRO	-	expression tag	UNP G0S965
D	-9	THR	-	expression tag	UNP G0S965
D	-8	THR	-	expression tag	UNP G0S965
D	-7	GLU	-	expression tag	UNP G0S965
D	-6	ASN	-	expression tag	UNP G0S965
D	-5	LEU	-	expression tag	UNP G0S965
D	-4	TYR	-	expression tag	UNP G0S965
D	-3	PHE	-	expression tag	UNP G0S965
D	-2	GLN	-	expression tag	UNP G0S965
D	-1	GLY	-	expression tag	UNP G0S965
D	0	ALA	-	expression tag	UNP G0S965

- Molecule 1: RNA polymerase II transcription factor B subunit 2





- Molecule 1: RNA polymerase II transcription factor B subunit 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	104.31Å 104.31Å 164.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.97 – 2.80 46.97 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.97-2.80) 100.0 (46.97-2.80)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.186 , 0.208 0.184 , 0.208	Depositor DCC
R_{free} test set	2487 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	73.9	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 68.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.159 for -h,-k,l 0.317 for h,-h-k,-l 0.180 for -k,-h,-l	Xtriage
Reported twinning fraction	0.550 for H, K, L 0.071 for -h,-k,l 0.249 for K, H, -L 0.130 for -K, -H, -L	Depositor
Outliers	0 of 49481 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8572	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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	1.07	2/2220 (0.1%)	1.53	10/3016 (0.3%)
1	B	1.08	0/2264	1.52	5/3077 (0.2%)
1	C	1.06	2/2122 (0.1%)	1.55	12/2882 (0.4%)
1	D	1.07	1/2156 (0.0%)	1.52	3/2929 (0.1%)
All	All	1.07	5/8762 (0.1%)	1.53	30/11904 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	165	HIS	CE1-NE2	7.70	1.40	1.32
1	A	195	ARG	CZ-NH2	-6.56	1.25	1.33
1	A	195	ARG	NE-CZ	-5.58	1.26	1.33
1	C	195	ARG	CZ-NH2	-5.32	1.26	1.33
1	C	222	THR	C-O	5.10	1.30	1.24

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	ARG	CD-NE-CZ	10.72	139.41	124.40
1	B	40	ARG	NE-CZ-NH2	10.46	128.61	119.20
1	A	195	ARG	NH1-CZ-NH2	-10.42	105.76	119.30
1	C	195	ARG	NE-CZ-NH2	10.23	128.41	119.20
1	D	40	ARG	CD-NE-CZ	9.93	138.31	124.40
1	B	40	ARG	NE-CZ-NH1	-9.82	111.68	121.50
1	A	114	ARG	NE-CZ-NH2	9.72	127.95	119.20
1	C	195	ARG	NH1-CZ-NH2	-9.67	106.73	119.30
1	C	114	ARG	CD-NE-CZ	9.66	137.93	124.40
1	A	114	ARG	CD-NE-CZ	9.53	137.73	124.40
1	A	114	ARG	NE-CZ-NH1	-8.92	112.58	121.50
1	B	40	ARG	CG-CD-NE	-8.21	93.94	112.00
1	C	114	ARG	NE-CZ-NH2	-7.92	112.07	119.20
1	D	40	ARG	NE-CZ-NH2	-7.54	112.42	119.20
1	A	94	PRO	N-CA-C	7.00	119.23	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	114	ARG	NE-CZ-NH1	6.90	128.40	121.50
1	D	40	ARG	NE-CZ-NH1	6.81	128.31	121.50
1	C	94	PRO	N-CA-C	6.68	118.85	110.70
1	A	195	ARG	NE-CZ-NH2	6.28	124.85	119.20
1	A	195	ARG	NE-CZ-NH1	6.23	127.73	121.50
1	C	298	TYR	CA-C-N	6.22	128.26	122.85
1	C	298	TYR	C-N-CA	6.22	128.26	122.85
1	C	210	THR	N-CA-C	-6.19	104.45	111.07
1	A	191	LEU	N-CA-C	-6.02	105.89	113.18
1	A	195	ARG	CD-NE-CZ	-5.68	116.44	124.40
1	A	210	THR	N-CA-C	-5.59	105.09	111.07
1	C	202	ILE	CA-C-N	5.49	126.34	122.33
1	C	202	ILE	C-N-CA	5.49	126.34	122.33
1	B	165	HIS	CA-C-O	-5.43	111.57	120.80
1	C	191	LEU	N-CA-C	-5.26	106.81	113.18

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2173	0	2225	64	0
1	B	2214	0	2259	51	0
1	C	2078	0	2128	44	0
1	D	2107	0	2154	48	0
All	All	8572	0	8766	195	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 11.

All (195) 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:A:58:GLN:HB3	1:A:59:PRO:CD	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:GLN:HB3	1:C:59:PRO:CD	2.03	0.87
1:B:48:VAL:HG22	1:A:56:MET:HE2	1.58	0.84
1:B:90:VAL:O	1:B:94:PRO:HD2	1.82	0.79
1:D:70:ARG:HB3	1:D:71:PRO:CD	2.14	0.78
1:B:70:ARG:HB3	1:B:71:PRO:CD	2.13	0.78
1:D:164:VAL:O	1:D:165:HIS:C	2.21	0.78
1:B:95:PRO:HB2	1:B:106:THR:OG1	1.85	0.75
1:B:192:VAL:HG13	1:B:202:ILE:HG23	1.68	0.74
1:C:58:GLN:HB3	1:C:59:PRO:HD2	1.69	0.74
1:D:90:VAL:O	1:D:94:PRO:HD2	1.86	0.74
1:B:95:PRO:O	1:B:106:THR:OG1	2.02	0.73
1:D:192:VAL:HG13	1:D:202:ILE:HG23	1.69	0.72
1:A:58:GLN:HB3	1:A:59:PRO:HD2	1.69	0.71
1:A:317:THR:O	1:A:317:THR:OG1	2.00	0.71
1:A:137:ARG:CZ	1:D:132:LEU:HD22	2.22	0.69
1:A:214:GLN:OE1	1:A:218:ALA:HB1	1.91	0.69
1:D:159:VAL:O	1:D:162:VAL:HG23	1.92	0.69
1:B:164:VAL:O	1:B:165:HIS:C	2.37	0.66
1:A:157:TYR:O	1:A:160:SER:OG	2.09	0.65
1:B:126:PHE:CD1	1:A:119:GLY:O	2.50	0.64
1:C:123:HIS:ND1	1:D:129:PRO:HD2	2.12	0.64
1:B:159:VAL:O	1:B:162:VAL:HG23	1.98	0.64
1:B:155:LEU:O	1:B:159:VAL:HG23	1.98	0.64
1:A:231:ALA:CB	1:A:259:MET:HE1	2.28	0.63
1:B:70:ARG:HB3	1:B:71:PRO:HD3	1.80	0.63
1:D:231:ALA:CB	1:D:259:MET:HE1	2.29	0.63
1:D:70:ARG:HB3	1:D:71:PRO:HD3	1.80	0.63
1:C:231:ALA:CB	1:C:259:MET:HE1	2.30	0.61
1:C:95:PRO:O	1:C:106:THR:N	2.33	0.61
1:B:231:ALA:CB	1:B:259:MET:HE1	2.31	0.61
1:A:90:VAL:O	1:A:95:PRO:CD	2.48	0.61
1:C:90:VAL:O	1:C:95:PRO:CD	2.48	0.60
1:A:137:ARG:HH11	1:D:133:PRO:HD2	1.66	0.60
1:A:58:GLN:HB3	1:A:59:PRO:HD3	1.84	0.59
1:B:90:VAL:O	1:B:94:PRO:CD	2.50	0.59
1:D:155:LEU:O	1:D:159:VAL:HG23	2.03	0.59
1:B:70:ARG:CB	1:B:71:PRO:CD	2.81	0.58
1:A:137:ARG:NH1	1:D:132:LEU:HD22	2.19	0.58
1:D:70:ARG:CB	1:D:71:PRO:CD	2.81	0.58
1:D:162:VAL:O	1:D:163:PRO:C	2.47	0.58
1:C:58:GLN:HB3	1:C:59:PRO:HD3	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ARG:NH2	1:D:132:LEU:HD22	2.20	0.57
1:A:30:GLN:HE22	1:A:284:ARG:HH22	1.53	0.57
1:A:195:ARG:HG3	1:A:195:ARG:NH2	2.19	0.56
1:B:164:VAL:O	1:B:164:VAL:HG12	2.03	0.56
1:C:90:VAL:O	1:C:95:PRO:HD3	2.05	0.56
1:B:138:ILE:HG21	1:B:308:PHE:CE2	2.40	0.56
1:B:44:PRO:O	1:B:48:VAL:HG23	2.05	0.56
1:D:90:VAL:O	1:D:94:PRO:CD	2.53	0.56
1:A:302:GLU:H	1:A:302:GLU:CD	2.14	0.56
1:A:95:PRO:O	1:A:106:THR:N	2.39	0.56
1:D:164:VAL:O	1:D:164:VAL:HG12	2.06	0.56
1:C:214:GLN:OE1	1:C:218:ALA:HB1	2.06	0.55
1:B:275:TYR:O	1:B:306:GLN:HA	2.07	0.55
1:C:195:ARG:HG3	1:C:195:ARG:NH1	2.22	0.55
1:D:44:PRO:O	1:D:48:VAL:HG23	2.06	0.55
1:A:90:VAL:O	1:A:95:PRO:HD3	2.07	0.54
1:A:303:ASP:OD1	1:A:304:THR:N	2.40	0.54
1:A:194:ARG:O	1:A:196:PRO:HD3	2.07	0.54
1:C:30:GLN:HE22	1:C:284:ARG:HH22	1.56	0.54
1:B:70:ARG:HB3	1:B:71:PRO:HD2	1.89	0.54
1:B:95:PRO:HB2	1:B:106:THR:CB	2.38	0.54
1:D:70:ARG:HB3	1:D:71:PRO:HD2	1.90	0.53
1:A:98:ASP:HB3	1:A:103:VAL:HA	1.90	0.53
1:A:265:MET:O	1:A:266:LEU:C	2.52	0.53
1:C:231:ALA:HB2	1:C:259:MET:HE1	1.89	0.53
1:A:96:GLY:HA2	1:A:104:GLN:O	2.08	0.53
1:D:267:ALA:HA	1:D:314:THR:HA	1.89	0.53
1:C:88:HIS:O	1:C:92:ILE:HG13	2.09	0.52
1:A:231:ALA:HB2	1:A:259:MET:HE1	1.90	0.52
1:B:280:LEU:O	1:B:285:ARG:NH2	2.43	0.51
1:B:113:LEU:HD12	1:B:117:LEU:CD1	2.40	0.51
1:D:280:LEU:O	1:D:285:ARG:NH2	2.42	0.51
1:B:288:LEU:N	1:B:289:PRO:HD2	2.26	0.51
1:A:88:HIS:O	1:A:92:ILE:HG13	2.11	0.51
1:A:214:GLN:NE2	1:A:222:THR:OG1	2.44	0.51
1:A:61:LEU:HB2	1:A:64:ASP:HB2	1.94	0.50
1:A:93:THR:C	1:A:95:PRO:HD3	2.36	0.50
1:D:113:LEU:HD12	1:D:117:LEU:CD1	2.42	0.50
1:A:189:GLY:HA3	1:A:226:LEU:HD22	1.94	0.50
1:A:195:ARG:O	1:A:201:GLY:HA2	2.11	0.50
1:C:189:GLY:HA3	1:C:226:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:VAL:O	1:D:163:PRO:O	2.29	0.49
1:B:217:ASN:HD21	1:B:319:SER:C	2.21	0.49
1:D:288:LEU:N	1:D:289:PRO:HD2	2.27	0.49
1:A:79:ARG:O	1:A:83:ILE:HG23	2.12	0.49
1:A:142:PHE:C	1:A:142:PHE:CD1	2.90	0.48
1:B:70:ARG:CB	1:B:71:PRO:HD2	2.43	0.48
1:C:61:LEU:HB2	1:C:64:ASP:HB2	1.95	0.48
1:C:265:MET:O	1:C:266:LEU:C	2.56	0.48
1:A:137:ARG:HH12	1:D:132:LEU:HA	1.79	0.48
1:C:288:LEU:O	1:C:289:PRO:C	2.56	0.48
1:B:315:THR:O	1:B:316:LEU:C	2.57	0.48
1:A:98:ASP:OD2	1:A:98:ASP:N	2.46	0.48
1:C:138:ILE:HG22	1:C:138:ILE:O	2.14	0.47
1:D:315:THR:O	1:D:316:LEU:C	2.57	0.47
1:A:187:LEU:HD12	1:A:192:VAL:HG12	1.96	0.47
1:B:217:ASN:ND2	1:B:319:SER:C	2.73	0.47
1:B:55:TYR:CE2	1:B:56:MET:HE2	2.50	0.47
1:D:55:TYR:CE2	1:D:56:MET:HE2	2.49	0.47
1:A:36:ALA:O	1:A:37:ILE:C	2.58	0.47
1:D:56:MET:HE3	1:D:68:TRP:CH2	2.50	0.47
1:A:53:LEU:O	1:A:53:LEU:HD23	2.14	0.47
1:C:93:THR:C	1:C:95:PRO:HD3	2.40	0.47
1:A:43:PRO:O	1:A:44:PRO:C	2.57	0.46
1:D:70:ARG:CB	1:D:71:PRO:HD2	2.43	0.46
1:D:197:ASP:OD1	1:D:197:ASP:N	2.48	0.46
1:C:43:PRO:O	1:C:44:PRO:C	2.58	0.46
1:B:149:LYS:O	1:B:150:LYS:C	2.59	0.46
1:A:54:LEU:O	1:A:114:ARG:NH2	2.48	0.46
1:C:195:ARG:O	1:C:201:GLY:HA2	2.15	0.46
1:C:157:TYR:O	1:C:160:SER:OG	2.19	0.46
1:C:194:ARG:O	1:C:196:PRO:HD3	2.16	0.46
1:C:265:MET:O	1:C:268:SER:N	2.40	0.46
1:B:195:ARG:CG	1:B:195:ARG:HH21	2.30	0.45
1:B:195:ARG:NH2	1:B:197:ASP:OD2	2.49	0.45
1:B:98:ASP:CB	1:B:103:VAL:HA	2.46	0.45
1:B:154:ILE:HG12	1:B:182:VAL:HG11	1.98	0.45
1:A:204:ILE:HG23	1:A:204:ILE:O	2.15	0.45
1:B:15:TYR:O	1:B:19:LEU:HD23	2.17	0.45
1:B:95:PRO:O	1:B:106:THR:CB	2.65	0.45
1:B:56:MET:HE3	1:B:68:TRP:CH2	2.52	0.45
1:D:195:ARG:NH2	1:D:197:ASP:OD2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:GLU:O	1:A:202:ILE:HA	2.17	0.45
1:C:67:VAL:HG12	1:D:68:TRP:CD1	2.52	0.45
1:D:299:ILE:HG22	1:D:304:THR:HB	1.99	0.45
1:A:36:ALA:CB	1:A:264:PHE:CD1	3.00	0.45
1:C:142:PHE:C	1:C:142:PHE:CD1	2.95	0.45
1:D:303:ASP:O	1:D:304:THR:OG1	2.29	0.45
1:A:195:ARG:HG2	1:A:203:GLY:N	2.32	0.45
1:A:265:MET:O	1:A:268:SER:N	2.36	0.45
1:D:56:MET:HE3	1:D:68:TRP:HH2	1.82	0.45
1:A:304:THR:HG22	1:C:305:ARG:HH11	1.80	0.44
1:C:67:VAL:CG1	1:D:68:TRP:HA	2.46	0.44
1:C:54:LEU:O	1:C:114:ARG:NH2	2.50	0.44
1:B:113:LEU:HD12	1:B:117:LEU:HD11	1.99	0.44
1:A:120:GLY:O	1:A:124:ASN:ND2	2.34	0.44
1:A:275:TYR:O	1:A:306:GLN:HA	2.18	0.44
1:D:15:TYR:O	1:D:19:LEU:HD23	2.17	0.44
1:B:40:ARG:HG2	1:B:317:THR:O	2.17	0.44
1:B:197:ASP:N	1:B:197:ASP:OD1	2.50	0.44
1:C:216:ALA:O	1:C:220:VAL:HG23	2.18	0.44
1:B:98:ASP:HB3	1:B:103:VAL:HA	2.00	0.44
1:C:265:MET:SD	1:C:269:LEU:HD21	2.58	0.43
1:D:316:LEU:HD23	1:D:316:LEU:HA	1.87	0.43
1:B:96:GLY:HA2	1:B:105:LEU:HA	1.99	0.43
1:A:30:GLN:O	1:A:31:PRO:C	2.61	0.43
1:C:316:LEU:HD23	1:C:316:LEU:HA	1.89	0.43
1:D:154:ILE:HG12	1:D:182:VAL:HG11	2.00	0.43
1:B:162:VAL:O	1:B:163:PRO:C	2.62	0.43
1:A:21:GLY:O	1:A:24:PHE:HB2	2.19	0.43
1:A:302:GLU:CD	1:A:302:GLU:N	2.76	0.43
1:C:187:LEU:HD12	1:C:192:VAL:HG12	1.99	0.43
1:C:195:ARG:HG2	1:C:203:GLY:N	2.33	0.43
1:B:56:MET:HE3	1:B:68:TRP:HH2	1.84	0.43
1:B:126:PHE:CE1	1:A:119:GLY:O	2.72	0.43
1:D:47:LYS:O	1:D:51:GLN:HG3	2.19	0.43
1:D:84:LEU:O	1:D:87:LEU:HB2	2.19	0.43
1:D:195:ARG:HH21	1:D:195:ARG:CG	2.32	0.42
1:A:36:ALA:HB1	1:A:264:PHE:CD1	2.53	0.42
1:A:80:ALA:O	1:A:83:ILE:HG12	2.19	0.42
1:A:190:ARG:O	1:A:205:THR:HG21	2.18	0.42
1:D:225:LEU:O	1:D:229:GLU:HG3	2.19	0.42
1:B:47:LYS:O	1:B:51:GLN:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LEU:HD11	1:A:226:LEU:HD11	2.01	0.42
1:C:36:ALA:HB1	1:C:264:PHE:CD1	2.55	0.42
1:B:278:ASP:O	1:B:285:ARG:NH2	2.53	0.42
1:A:55:TYR:CE1	1:A:114:ARG:HD3	2.54	0.42
1:B:84:LEU:O	1:B:87:LEU:HB2	2.19	0.42
1:A:304:THR:OG1	1:A:305:ARG:N	2.52	0.42
1:C:38:PHE:HA	1:C:42:LEU:HD12	2.02	0.42
1:D:113:LEU:HD12	1:D:117:LEU:HD11	2.00	0.42
1:B:66:ASP:O	1:B:69:VAL:HB	2.20	0.42
1:A:288:LEU:HB2	1:A:289:PRO:HD3	2.02	0.41
1:A:288:LEU:O	1:A:289:PRO:C	2.63	0.41
1:C:195:ARG:HG3	1:C:195:ARG:HH11	1.84	0.41
1:D:138:ILE:HG21	1:D:308:PHE:CE2	2.55	0.41
1:C:190:ARG:O	1:C:205:THR:HG21	2.20	0.41
1:C:221:TRP:O	1:C:222:THR:C	2.62	0.41
1:B:318:SER:O	1:B:319:SER:OG	2.35	0.41
1:C:191:LEU:HD11	1:C:226:LEU:HD11	2.02	0.41
1:C:208:GLY:O	1:C:211:PHE:HB3	2.21	0.41
1:C:277:THR:HG23	1:C:305:ARG:O	2.21	0.41
1:D:288:LEU:HD22	1:D:297:ILE:HD13	2.02	0.41
1:A:87:LEU:HD22	1:A:87:LEU:C	2.46	0.41
1:C:21:GLY:O	1:C:24:PHE:HB2	2.20	0.41
1:C:36:ALA:CB	1:C:264:PHE:CD1	3.03	0.41
1:D:300:PRO:O	1:D:304:THR:HG22	2.20	0.41
1:B:27:LEU:HD13	1:B:257:ILE:HG23	2.02	0.41
1:A:200:THR:HG22	1:A:202:ILE:HB	2.03	0.41
1:B:106:THR:O	1:B:107:THR:C	2.63	0.40
1:A:69:VAL:HG11	1:A:79:ARG:CG	2.51	0.40
1:D:207:ALA:O	1:D:210:THR:N	2.54	0.40
1:A:274:ALA:C	1:A:275:TYR:CD1	2.99	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	267/347 (77%)	221 (83%)	38 (14%)	8 (3%)	3	12
1	B	272/347 (78%)	214 (79%)	51 (19%)	7 (3%)	4	15
1	C	253/347 (73%)	206 (81%)	40 (16%)	7 (3%)	4	14
1	D	255/347 (74%)	209 (82%)	38 (15%)	8 (3%)	3	12
All	All	1047/1388 (75%)	850 (81%)	167 (16%)	30 (3%)	3	13

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	70	ARG
1	A	58	GLN
1	A	94	PRO
1	A	195	ARG
1	C	58	GLN
1	C	94	PRO
1	D	70	ARG
1	B	95	PRO
1	A	107	THR
1	C	107	THR
1	D	163	PRO
1	B	238	ALA
1	A	95	PRO
1	A	121	ALA
1	C	121	ALA
1	D	304	THR
1	A	118	GLU
1	C	118	GLU
1	C	195	ARG
1	B	57	PRO
1	A	44	PRO
1	C	44	PRO
1	D	57	PRO
1	D	316	LEU
1	B	69	VAL
1	D	69	VAL
1	B	59	PRO
1	B	163	PRO
1	D	59	PRO
1	D	31	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	236/291 (81%)	217 (92%)	19 (8%)	11	33
1	B	239/291 (82%)	220 (92%)	19 (8%)	11	35
1	C	226/291 (78%)	212 (94%)	14 (6%)	16	45
1	D	230/291 (79%)	213 (93%)	17 (7%)	13	37
All	All	931/1164 (80%)	862 (93%)	69 (7%)	13	37

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	58	GLN
1	B	68	TRP
1	B	87	LEU
1	B	88	HIS
1	B	93	THR
1	B	103	VAL
1	B	107	THR
1	B	113	LEU
1	B	148	ARG
1	B	163	PRO
1	B	184	ASP
1	B	192	VAL
1	B	195	ARG
1	B	197	ASP
1	B	202	ILE
1	B	270	GLU
1	B	281	SER
1	B	299	ILE
1	B	317	THR
1	A	11	GLN
1	A	27	LEU
1	A	53	LEU
1	A	58	GLN
1	A	81	LEU

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Mol	Chain	Res	Type
1	A	83	ILE
1	A	87	LEU
1	A	97	LYS
1	A	102	GLU
1	A	105	LEU
1	A	114	ARG
1	A	137	ARG
1	A	192	VAL
1	A	198	THR
1	A	202	ILE
1	A	210	THR
1	A	253	LYS
1	A	265	MET
1	A	302	GLU
1	C	11	GLN
1	C	27	LEU
1	C	53	LEU
1	C	58	GLN
1	C	81	LEU
1	C	83	ILE
1	C	87	LEU
1	C	105	LEU
1	C	137	ARG
1	C	192	VAL
1	C	202	ILE
1	C	210	THR
1	C	253	LYS
1	C	265	MET
1	D	58	GLN
1	D	68	TRP
1	D	87	LEU
1	D	88	HIS
1	D	93	THR
1	D	103	VAL
1	D	107	THR
1	D	113	LEU
1	D	148	ARG
1	D	163	PRO
1	D	184	ASP
1	D	192	VAL
1	D	195	ARG
1	D	197	ASP

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Mol	Chain	Res	Type
1	D	202	ILE
1	D	270	GLU
1	D	281	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	11	GLN
1	B	91	GLN
1	B	108	ASN
1	B	145	ASN
1	B	217	ASN
1	B	306	GLN
1	A	11	GLN
1	A	30	GLN
1	A	111	ASN
1	A	145	ASN
1	C	11	GLN
1	C	30	GLN
1	C	111	ASN
1	C	306	GLN
1	D	11	GLN
1	D	91	GLN
1	D	108	ASN
1	D	145	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	275/347 (79%)	0.65	23 (8%) 17 12	33, 77, 136, 157	0
1	B	280/347 (80%)	0.67	28 (10%) 12 9	18, 78, 147, 183	0
1	C	263/347 (75%)	0.98	40 (15%) 5 4	36, 90, 147, 185	0
1	D	264/347 (76%)	1.29	57 (21%) 2 2	19, 112, 177, 200	1 (0%)
All	All	1082/1388 (77%)	0.89	148 (13%) 6 5	18, 90, 153, 200	1 (0%)

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	87	LEU	7.4
1	C	86	SER	5.9
1	C	49	PHE	5.3
1	D	80	ALA	4.8
1	D	81	LEU	4.8
1	C	119	GLY	4.7
1	D	294	PHE	4.5
1	D	71	PRO	4.5
1	A	86	SER	4.5
1	B	84	LEU	4.5
1	D	189	GLY	4.4
1	D	94	PRO	4.3
1	C	51	GLN	4.1
1	B	63	SER	4.1
1	B	62	LEU	4.0
1	D	124	ASN	3.9
1	B	83	ILE	3.9
1	C	254	PRO	3.8
1	D	179	LYS	3.8
1	D	84	LEU	3.7
1	D	127	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	123	HIS	3.5
1	C	83	ILE	3.5
1	D	83	ILE	3.5
1	B	87	LEU	3.5
1	C	84	LEU	3.5
1	D	306	GLN	3.4
1	C	225	LEU	3.4
1	D	43	PRO	3.4
1	A	57	PRO	3.4
1	D	143	LEU	3.3
1	D	192	VAL	3.3
1	D	65	LEU	3.2
1	D	10	TYR	3.2
1	C	39	ARG	3.2
1	C	105	LEU	3.1
1	D	87	LEU	3.1
1	D	309	PRO	3.1
1	B	42	LEU	3.1
1	B	49	PHE	3.1
1	A	69	VAL	3.1
1	B	89	ILE	3.1
1	B	122	ALA	3.1
1	C	279	ALA	3.0
1	A	89	ILE	3.0
1	B	184	ASP	3.0
1	A	84	LEU	3.0
1	B	98	ASP	2.9
1	B	67	VAL	2.9
1	B	90	VAL	2.9
1	C	134	VAL	2.9
1	C	238	ALA	2.9
1	A	49	PHE	2.9
1	C	45	LEU	2.9
1	C	15	TYR	2.8
1	C	81	LEU	2.8
1	D	191	LEU	2.8
1	D	44	PRO	2.8
1	D	151	TRP	2.8
1	C	90	VAL	2.8
1	D	120	GLY	2.8
1	A	11	GLN	2.7
1	D	103	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	176	GLY	2.7
1	D	288	LEU	2.7
1	D	88	HIS	2.7
1	B	70	ARG	2.7
1	A	87	LEU	2.7
1	D	42	LEU	2.7
1	D	38	PHE	2.7
1	B	96	GLY	2.7
1	C	59	PRO	2.7
1	D	63	SER	2.7
1	B	95	PRO	2.6
1	A	254	PRO	2.6
1	D	22	THR	2.6
1	D	15	TYR	2.6
1	D	85	ARG	2.6
1	D	12	LEU	2.6
1	C	11	GLN	2.6
1	D	131	SER	2.5
1	D	227	TRP	2.5
1	B	57	PRO	2.5
1	B	81	LEU	2.5
1	C	65	LEU	2.5
1	D	67	VAL	2.4
1	D	49	PHE	2.4
1	D	55	TYR	2.4
1	B	55	TYR	2.4
1	C	55	TYR	2.4
1	C	88	HIS	2.4
1	C	61	LEU	2.4
1	A	90	VAL	2.4
1	A	25	ARG	2.4
1	C	108	ASN	2.4
1	B	10	TYR	2.4
1	C	56	MET	2.3
1	C	132	LEU	2.3
1	D	308	PHE	2.3
1	D	223	LEU	2.3
1	C	283	THR	2.3
1	C	18	LYS	2.3
1	A	40	ARG	2.3
1	C	38	PHE	2.3
1	B	94	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	57	PRO	2.3
1	C	128	VAL	2.3
1	A	46	ALA	2.3
1	D	293	ASP	2.3
1	D	200	THR	2.3
1	D	271	LEU	2.2
1	D	130	SER	2.2
1	A	81	LEU	2.2
1	D	117	LEU	2.2
1	B	60	MET	2.2
1	C	256	SER	2.2
1	D	258	GLU	2.2
1	B	123	HIS	2.2
1	D	41	MET	2.2
1	A	319	SER	2.2
1	A	43	PRO	2.1
1	D	69	VAL	2.1
1	C	47	LYS	2.1
1	D	235	LYS	2.1
1	D	312	LEU	2.1
1	D	284	ARG	2.1
1	B	254	PRO	2.1
1	C	163	PRO	2.1
1	C	53	LEU	2.1
1	A	238	ALA	2.1
1	A	307	TYR	2.1
1	A	156	HIS	2.1
1	C	48	VAL	2.1
1	D	26	LYS	2.1
1	D	89	ILE	2.1
1	D	180	ALA	2.1
1	D	125	SER	2.1
1	B	38	PHE	2.1
1	B	100	PRO	2.0
1	A	100	PRO	2.0
1	D	119	GLY	2.0
1	B	88	HIS	2.0
1	A	67	VAL	2.0
1	A	88	HIS	2.0
1	C	125	SER	2.0
1	D	301	ARG	2.0
1	B	80	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	237	ALA	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.