Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2020 – 06:02 PM BST

PDB ID	:	6TRU
Title	:	Crystal structure of the N-terminal half of the TFIIH 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 following versions of software and data (see references ①) were used in the production of this report:

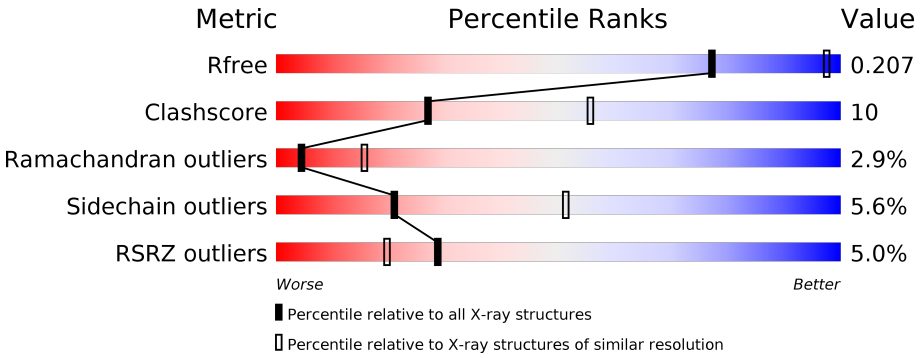
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 on 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 <=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	2% 54% 22% 21%
1	B	347	3% 62% 16% 19%
1	C	347	2% 55% 19% 24%
1	D	347	8% 59% 14% 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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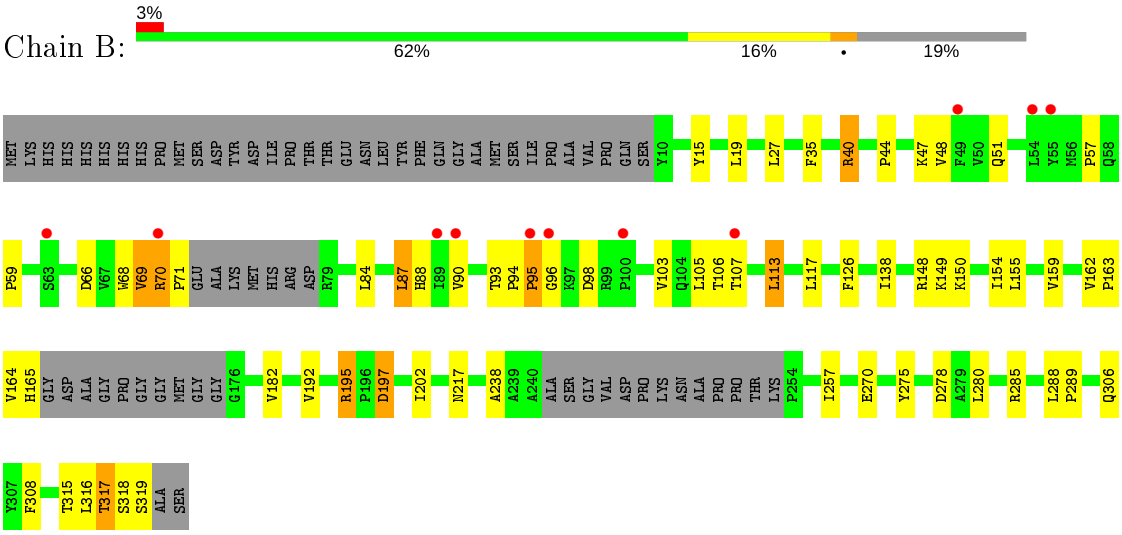
Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	ASP	-	expression tag	UNP G0S965
C	-13	TYR	-	expression tag	UNP G0S965
C	-12	ASP	-	expression tag	UNP G0S965
C	-11	ILE	-	expression tag	UNP G0S965
C	-10	PRO	-	expression tag	UNP G0S965
C	-9	THR	-	expression tag	UNP G0S965
C	-8	THR	-	expression tag	UNP G0S965
C	-7	GLU	-	expression tag	UNP G0S965
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

3 Residue-property plots (i)

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

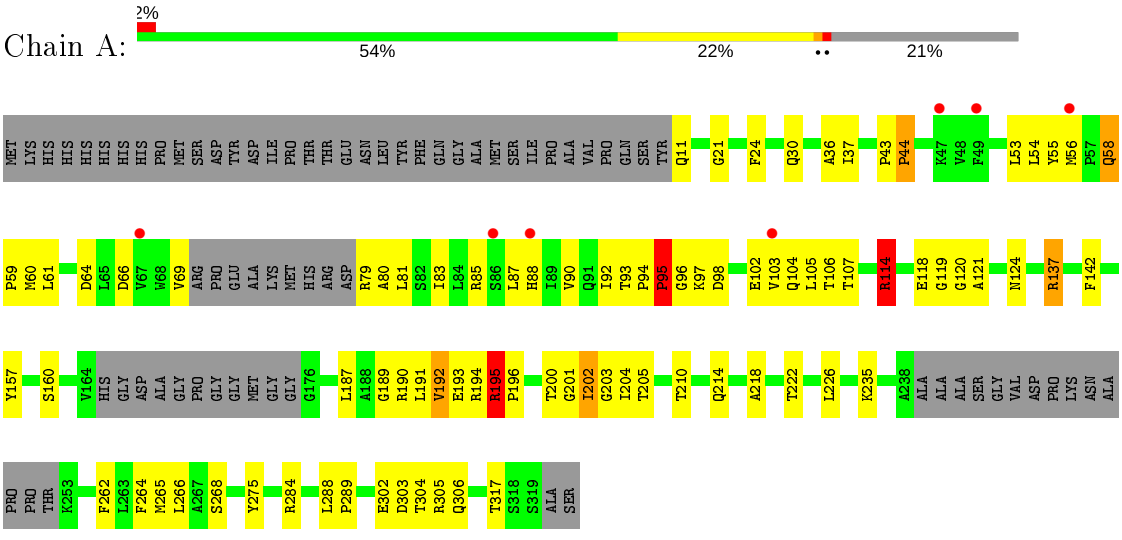
- Molecule 1: RNA polymerase II transcription factor B subunit 2

Chain B:



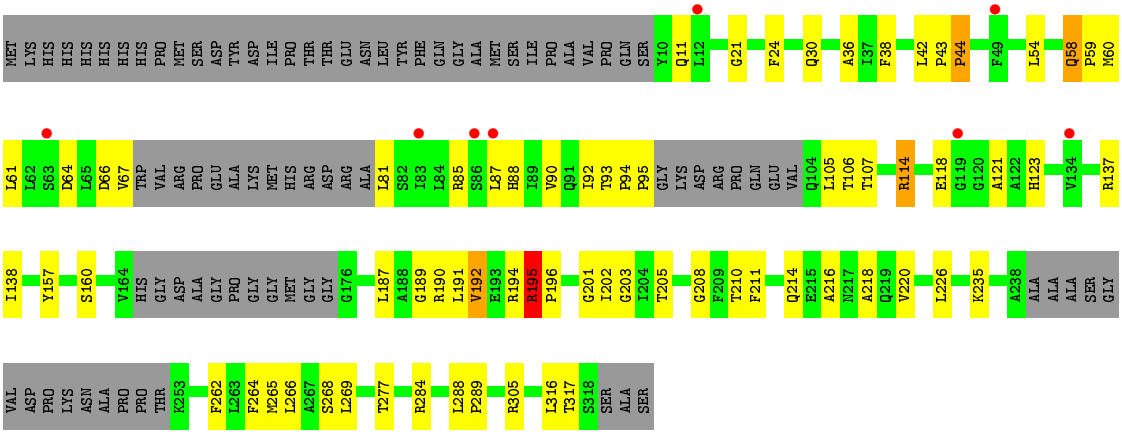
- Molecule 1: RNA polymerase II transcription factor B subunit 2

Chain A:

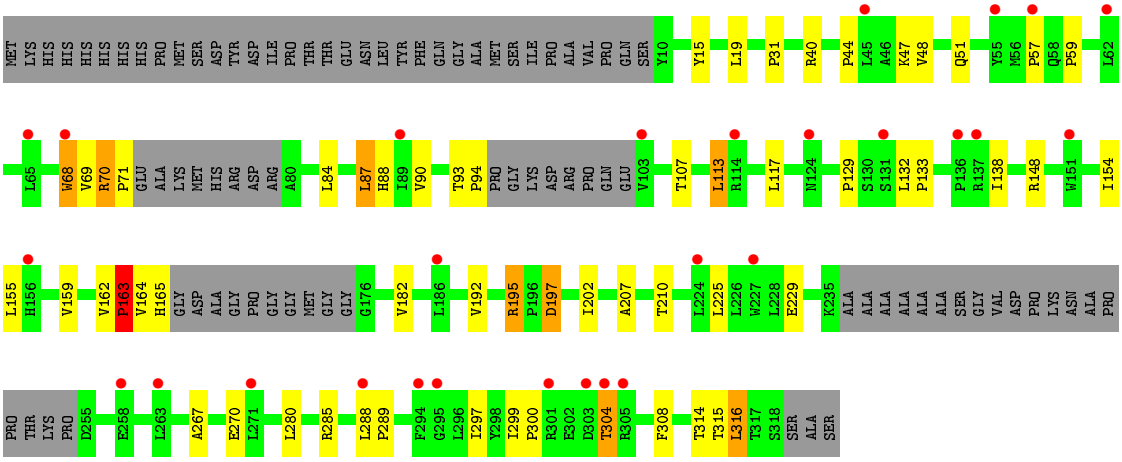


- Molecule 1: RNA polymerase II transcription factor B subunit 2

Chain C:



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



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.58 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.186 , 0.208 0.186 , 0.207	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 , 41.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.19$	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	0.95	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.73	2/2220 (0.1%)	0.99	7/3016 (0.2%)
1	B	0.71	0/2264	0.94	4/3077 (0.1%)
1	C	0.72	2/2122 (0.1%)	0.99	6/2882 (0.2%)
1	D	0.70	0/2156	0.90	4/2929 (0.1%)
All	All	0.71	4/8762 (0.0%)	0.95	21/11904 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	195	ARG	CZ-NH2	-6.25	1.25	1.33
1	C	195	ARG	CZ-NH1	-5.38	1.26	1.33
1	A	195	ARG	CZ-NH1	-5.32	1.26	1.33
1	C	195	ARG	CZ-NH2	-5.01	1.26	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	40	ARG	NE-CZ-NH1	-17.24	111.68	120.30
1	B	40	ARG	NE-CZ-NH2	16.63	128.61	120.30
1	C	114	ARG	NE-CZ-NH2	-16.46	112.07	120.30
1	C	195	ARG	NE-CZ-NH2	16.22	128.41	120.30
1	C	114	ARG	NE-CZ-NH1	16.19	128.40	120.30
1	D	40	ARG	NE-CZ-NH1	16.02	128.31	120.30
1	D	40	ARG	NE-CZ-NH2	-15.77	112.42	120.30
1	A	114	ARG	NE-CZ-NH1	-15.44	112.58	120.30
1	A	114	ARG	NE-CZ-NH2	15.30	127.95	120.30
1	A	195	ARG	NE-CZ-NH1	14.87	127.73	120.30
1	A	195	ARG	NH1-CZ-NH2	-12.40	105.76	119.40
1	C	195	ARG	NH1-CZ-NH2	-11.52	106.73	119.40
1	B	40	ARG	CD-NE-CZ	11.29	139.41	123.60
1	D	40	ARG	CD-NE-CZ	10.50	138.31	123.60
1	C	114	ARG	CD-NE-CZ	10.23	137.93	123.60
1	A	114	ARG	CD-NE-CZ	10.10	137.73	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	195	ARG	NE-CZ-NH2	9.10	124.85	120.30
1	B	40	ARG	CG-CD-NE	-8.50	93.94	111.80
1	C	195	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	D	40	ARG	CG-CD-NE	5.20	122.71	111.80
1	A	195	ARG	CD-NE-CZ	-5.11	116.44	123.60

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	59	0
1	B	2214	0	2259	47	0
1	C	2078	0	2128	41	0
1	D	2107	0	2154	43	0
All	All	8572	0	8766	176	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 10.

All (176) 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
1:C:58:GLN:HB3	1:C:59:PRO:CD	2.03	0.87
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: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:164:VAL:O	1:D:165:HIS:C	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:157:TYR:O	1:A:160:SER:OG	2.09	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:126:PHE:CD1	1:A:119:GLY:O	2.50	0.64
1:C:317:THR:O	1:C:317:THR:OG1	2.15	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:B:70:ARG:HB3	1:B:71:PRO:HD3	1.80	0.63
1:D:70:ARG:HB3	1:D:71:PRO:HD3	1.80	0.63
1:B:164:VAL:O	1:B:165:HIS:C	2.37	0.61
1:C:95:PRO:O	1:C:106:THR:N	2.33	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:B:164:VAL:HG12	1:B:164:VAL:O	2.03	0.58
1:B:48:VAL:HG22	1:A:56:MET:HE1	1.83	0.58
1:D:70:ARG:CB	1:D:71:PRO:CD	2.81	0.58
1:C:157:TYR:O	1:C:160:SER:OG	2.19	0.57
1:C:58:GLN:HB3	1:C:59:PRO:HD3	1.84	0.57
1:A:317:THR:OG1	1:A:317:THR:O	2.00	0.57
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: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: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:NH1	1:C:195:ARG:HG3	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:95:PRO:HB2	1:B:106:THR:CB	2.38	0.54
1:B:70:ARG:HB3	1:B:71:PRO:HD2	1.89	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:D:162:VAL:O	1:D:163:PRO:C	2.47	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: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:A:302:GLU:H	1:A:302:GLU:CD	2.14	0.51
1:D:280:LEU:O	1:D:285:ARG:NH2	2.42	0.51
1:A:88:HIS:O	1:A:92:ILE:HG13	2.11	0.51
1:B:288:LEU:N	1:B:289:PRO:HD2	2.26	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: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
1:D:162:VAL:O	1:D:163:PRO:O	2.29	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:265:MET:O	1:A:266:LEU:C	2.52	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:A:137:ARG:HH12	1:D:132:LEU:HA	1.79	0.48
1:C:138:ILE:O	1:C:138:ILE:HG22	2.14	0.48
1:A:98:ASP:N	1:A:98:ASP:OD2	2.46	0.48
1:A:187:LEU:HD12	1:A:192:VAL:HG12	1.96	0.47
1:A:53:LEU:HD23	1:A:53:LEU:O	2.14	0.47
1:D:70:ARG:CB	1:D:71:PRO:HD2	2.43	0.46
1:A:204:ILE:O	1:A:204:ILE:HG23	2.15	0.46
1:D:197:ASP:OD1	1:D:197:ASP:N	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:48:VAL:HG22	1:A:56:MET:CE	2.46	0.45
1:A:93:THR:C	1:A:95:PRO:HD3	2.36	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:D:195:ARG:NH2	1:D:197:ASP:OD2	2.49	0.45
1:A:193:GLU:O	1:A:202:ILE:HA	2.17	0.45
1:D:299:ILE:HG22	1:D:304:THR:HB	1.99	0.45
1:C:67:VAL:HG12	1:D:68:TRP:CD1	2.52	0.45
1:A:36:ALA:CB	1:A:264:PHE:CD1	3.00	0.45
1:B:217:ASN:HD21	1:B:319:SER:C	2.21	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: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:A:142:PHE:C	1:A:142:PHE:CD1	2.90	0.44
1:B:197:ASP:N	1:B:197:ASP:OD1	2.50	0.44
1:B:40:ARG:HG2	1:B:317:THR:O	2.17	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:HA	1:D:316:LEU:HD23	1.87	0.43
1:B:96:GLY:HA2	1:B:105:LEU:HA	1.99	0.43
1:C:265:MET:O	1:C:266:LEU:C	2.56	0.43
1:C:316:LEU:HA	1:C:316:LEU:HD23	1.89	0.43
1:A:43:PRO:O	1:A:44:PRO:C	2.57	0.43
1:C:288:LEU:O	1:C:289:PRO:C	2.56	0.43
1:D:154:ILE:HG12	1:D:182:VAL:HG11	2.00	0.43
1:A:21:GLY:O	1:A:24:PHE:HB2	2.19	0.43
1:C:187:LEU:HD12	1:C:192:VAL:HG12	1.99	0.43
1:B:315:THR:O	1:B:316:LEU:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:THR:O	1:D:316:LEU:C	2.57	0.43
1:C:195:ARG:HG2	1:C:203:GLY:N	2.33	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:B:217:ASN:ND2	1:B:319:SER:C	2.73	0.42
1:D:195:ARG:CG	1:D:195:ARG:HH21	2.32	0.42
1:A:36:ALA:HB1	1:A:264:PHE:CD1	2.53	0.42
1:A:190:ARG:O	1:A:205:THR:HG21	2.18	0.42
1:A:80:ALA:O	1:A:83:ILE:HG12	2.19	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
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:A:55:TYR:CE1	1:A:114:ARG:HD3	2.54	0.42
1:A:304:THR:OG1	1:A:305:ARG:N	2.52	0.42
1:A:36:ALA:O	1:A:37:ILE:C	2.58	0.42
1:B:278:ASP:O	1:B:285:ARG:NH2	2.53	0.42
1:C:93:THR:C	1:C:95:PRO:HD3	2.40	0.42
1:B:84:LEU:O	1:B:87:LEU:HB2	2.19	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:C:195:ARG:HH11	1:C:195:ARG:HG3	1.84	0.41
1:C:43:PRO:O	1:C:44:PRO:C	2.58	0.41
1:D:138:ILE:HG21	1:D:308:PHE:CE2	2.55	0.41
1:B:149:LYS:O	1:B:150:LYS:C	2.59	0.41
1:C:190:ARG:O	1:C:205:THR:HG21	2.20	0.41
1:B:318:SER:O	1:B:319:SER:OG	2.35	0.41
1:C:208:GLY:O	1:C:211:PHE:HB3	2.21	0.41
1:C:191:LEU:HD11	1:C:226:LEU:HD11	2.02	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: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:C:21:GLY:O	1:C:24:PHE:HB2	2.20	0.41
1:A:200:THR:HG22	1:A:202:ILE:HB	2.03	0.41
1:B:27:LEU:HD13	1:B:257:ILE:HG23	2.02	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:PHE:HZ	1:A:55:TYR:HH	1.64	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%)	4	15
1	B	272/347 (78%)	214 (79%)	51 (19%)	7 (3%)	5	18
1	C	253/347 (73%)	206 (81%)	40 (16%)	7 (3%)	5	17
1	D	255/347 (74%)	209 (82%)	38 (15%)	8 (3%)	4	14
All	All	1047/1388 (75%)	850 (81%)	167 (16%)	30 (3%)	4	15

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

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Mol	Chain	Res	Type
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 (i)

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%)	219 (93%)	17 (7%)	14	38
1	B	239/291 (82%)	228 (95%)	11 (5%)	27	60
1	C	226/291 (78%)	213 (94%)	13 (6%)	20	50
1	D	230/291 (79%)	219 (95%)	11 (5%)	25	58
All	All	931/1164 (80%)	879 (94%)	52 (6%)	21	51

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	68	TRP
1	B	87	LEU
1	B	88	HIS
1	B	93	THR
1	B	107	THR

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Mol	Chain	Res	Type
1	B	113	LEU
1	B	148	ARG
1	B	195	ARG
1	B	197	ASP
1	B	270	GLU
1	B	317	THR
1	A	11	GLN
1	A	60	MET
1	A	66	ASP
1	A	81	LEU
1	A	85	ARG
1	A	87	LEU
1	A	95	PRO
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	202	ILE
1	A	210	THR
1	A	235	LYS
1	A	262	PHE
1	C	11	GLN
1	C	60	MET
1	C	66	ASP
1	C	81	LEU
1	C	85	ARG
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	235	LYS
1	C	262	PHE
1	D	68	TRP
1	D	87	LEU
1	D	88	HIS
1	D	93	THR
1	D	107	THR
1	D	113	LEU

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Mol	Chain	Res	Type
1	D	148	ARG
1	D	163	PRO
1	D	195	ARG
1	D	197	ASP
1	D	270	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	11	GLN
1	B	214	GLN
1	B	217	ASN
1	B	306	GLN
1	A	11	GLN
1	A	30	GLN
1	A	111	ASN
1	A	306	GLN
1	C	11	GLN
1	C	30	GLN
1	C	111	ASN
1	C	286	ASN
1	C	306	GLN
1	D	11	GLN
1	D	214	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

There are no monosaccharides 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, 95^{th} 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%)	0.20	7 (2%) 57 47	33, 77, 136, 157	0
1	B	280/347 (80%)	0.20	11 (3%) 39 29	18, 78, 147, 183	0
1	C	263/347 (75%)	0.28	8 (3%) 50 40	36, 90, 147, 185	0
1	D	264/347 (76%)	0.53	28 (10%) 6 3	19, 112, 177, 200	0
All	All	1082/1388 (77%)	0.30	54 (4%) 28 19	18, 90, 153, 200	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	87	LEU	6.7
1	B	96	GLY	6.2
1	D	131	SER	6.0
1	B	49	PHE	5.0
1	D	124	ASN	4.9
1	D	303	ASP	4.3
1	D	55	TYR	4.2
1	D	89	ILE	4.1
1	A	103	VAL	4.0
1	D	294	PHE	3.8
1	D	301	ARG	3.7
1	B	95	PRO	3.7
1	D	271	LEU	3.6
1	B	55	TYR	3.4
1	D	114	ARG	3.3
1	C	86	SER	3.3
1	C	63	SER	3.3
1	C	134	VAL	3.2
1	C	83	ILE	3.1
1	B	70	ARG	3.0
1	B	63	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	47	LYS	2.9
1	D	295	GLY	2.9
1	B	100	PRO	2.9
1	D	305	ARG	2.8
1	D	136	PRO	2.8
1	D	304	THR	2.8
1	A	88	HIS	2.7
1	D	156	HIS	2.6
1	D	103	VAL	2.6
1	D	227	TRP	2.6
1	C	12	LEU	2.5
1	A	67	VAL	2.4
1	A	56	MET	2.4
1	D	258	GLU	2.4
1	D	68	TRP	2.3
1	D	62	LEU	2.3
1	C	119	GLY	2.3
1	C	49	PHE	2.3
1	A	49	PHE	2.3
1	D	137	ARG	2.3
1	D	288	LEU	2.2
1	D	57	PRO	2.2
1	D	263	LEU	2.2
1	B	90	VAL	2.2
1	B	107	THR	2.2
1	D	224	LEU	2.2
1	D	45	LEU	2.1
1	D	65	LEU	2.1
1	B	89	ILE	2.1
1	A	86	SER	2.1
1	B	54	LEU	2.0
1	D	186	LEU	2.0
1	D	151	TRP	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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.