



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:48 PM UTC

PDB ID : 6TRS / pdb_00006trs
Title : Crystal structure of TFIIH subunit p52 in complex with p8
Authors : Koelmel, W.; Kuper, J.; Schoenwetter, E.; Kisker, C.
Deposited on : 2019-12-19
Resolution : 2.68 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

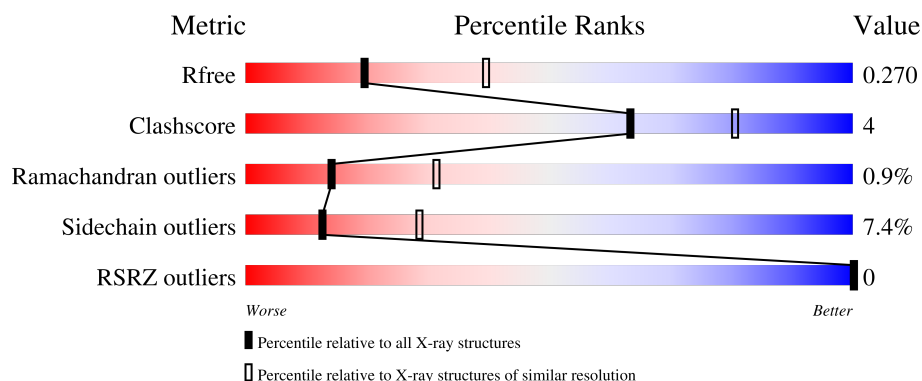
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

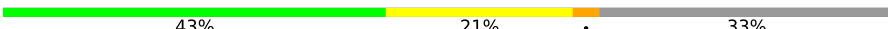
The reported resolution of this entry is 2.68 Å.

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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	420	
1	B	420	
2	D	98	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5606 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	A	292	Total	C	N	O	S	0	0	0
			2281	1461	396	418	6			
1	B	350	Total	C	N	O	S	0	0	0
			2784	1784	481	510	9			

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	95	MET	-	initiating methionine	UNP G0S965
A	96	LYS	-	expression tag	UNP G0S965
A	97	HIS	-	expression tag	UNP G0S965
A	98	HIS	-	expression tag	UNP G0S965
A	99	HIS	-	expression tag	UNP G0S965
A	100	HIS	-	expression tag	UNP G0S965
A	101	HIS	-	expression tag	UNP G0S965
A	102	HIS	-	expression tag	UNP G0S965
A	103	PRO	-	expression tag	UNP G0S965
A	104	MET	-	expression tag	UNP G0S965
A	105	SER	-	expression tag	UNP G0S965
A	106	ASP	-	expression tag	UNP G0S965
A	107	TYR	-	expression tag	UNP G0S965
A	108	ASP	-	expression tag	UNP G0S965
A	109	ILE	-	expression tag	UNP G0S965
A	110	PRO	-	expression tag	UNP G0S965
A	111	THR	-	expression tag	UNP G0S965
A	112	THR	-	expression tag	UNP G0S965
A	113	GLU	-	expression tag	UNP G0S965
A	114	ASN	-	expression tag	UNP G0S965
A	115	LEU	-	expression tag	UNP G0S965
A	116	TYR	-	expression tag	UNP G0S965
A	117	PHE	-	expression tag	UNP G0S965
A	118	GLN	-	expression tag	UNP G0S965
A	119	GLY	-	expression tag	UNP G0S965

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Chain	Residue	Modelled	Actual	Comment	Reference
A	120	ALA	-	expression tag	UNP G0S965
A	320T	SER	ASP	conflict	UNP G0S965
A	320U	ASN	ALA	conflict	UNP G0S965
A	320V	GLY	SER	conflict	UNP G0S965
A	320W	ASN	SER	conflict	UNP G0S965
A	320X	GLY	LEU	conflict	UNP G0S965
B	95	MET	-	initiating methionine	UNP G0S965
B	96	LYS	-	expression tag	UNP G0S965
B	97	HIS	-	expression tag	UNP G0S965
B	98	HIS	-	expression tag	UNP G0S965
B	99	HIS	-	expression tag	UNP G0S965
B	100	HIS	-	expression tag	UNP G0S965
B	101	HIS	-	expression tag	UNP G0S965
B	102	HIS	-	expression tag	UNP G0S965
B	103	PRO	-	expression tag	UNP G0S965
B	104	MET	-	expression tag	UNP G0S965
B	105	SER	-	expression tag	UNP G0S965
B	106	ASP	-	expression tag	UNP G0S965
B	107	TYR	-	expression tag	UNP G0S965
B	108	ASP	-	expression tag	UNP G0S965
B	109	ILE	-	expression tag	UNP G0S965
B	110	PRO	-	expression tag	UNP G0S965
B	111	THR	-	expression tag	UNP G0S965
B	112	THR	-	expression tag	UNP G0S965
B	113	GLU	-	expression tag	UNP G0S965
B	114	ASN	-	expression tag	UNP G0S965
B	115	LEU	-	expression tag	UNP G0S965
B	116	TYR	-	expression tag	UNP G0S965
B	117	PHE	-	expression tag	UNP G0S965
B	118	GLN	-	expression tag	UNP G0S965
B	119	GLY	-	expression tag	UNP G0S965
B	120	ALA	-	expression tag	UNP G0S965
B	321S	SER	ASP	conflict	UNP G0S965
B	321T	ASN	ALA	conflict	UNP G0S965
B	321U	GLY	SER	conflict	UNP G0S965
B	321V	ASN	SER	conflict	UNP G0S965
B	321W	GLY	LEU	conflict	UNP G0S965

- Molecule 2 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	66	Total	C	N	O	S	0	0	0
			541	343	94	102	2			

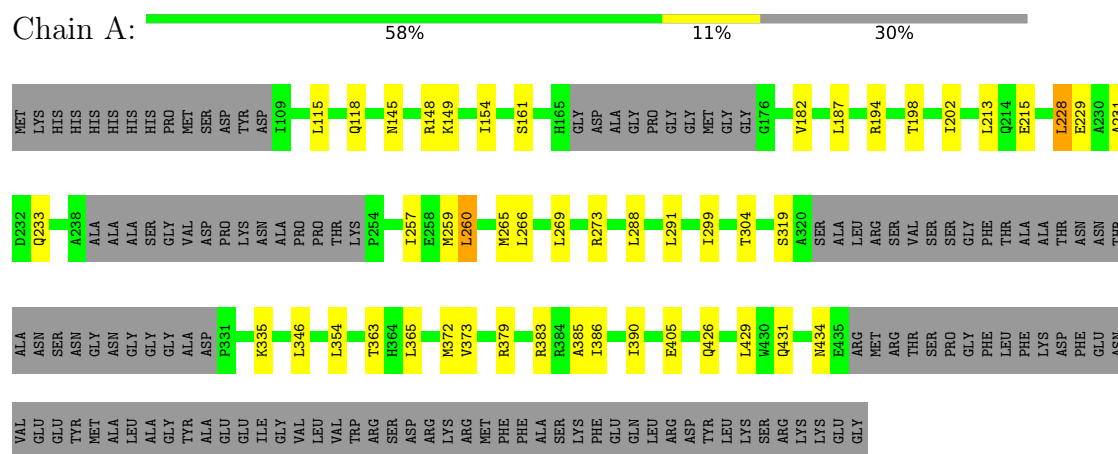
There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-25	MET	-	initiating methionine	UNP G0SDQ1
D	-24	LYS	-	expression tag	UNP G0SDQ1
D	-23	HIS	-	expression tag	UNP G0SDQ1
D	-22	HIS	-	expression tag	UNP G0SDQ1
D	-21	HIS	-	expression tag	UNP G0SDQ1
D	-20	HIS	-	expression tag	UNP G0SDQ1
D	-19	HIS	-	expression tag	UNP G0SDQ1
D	-18	HIS	-	expression tag	UNP G0SDQ1
D	-17	PRO	-	expression tag	UNP G0SDQ1
D	-16	MET	-	expression tag	UNP G0SDQ1
D	-15	SER	-	expression tag	UNP G0SDQ1
D	-14	ASP	-	expression tag	UNP G0SDQ1
D	-13	TYR	-	expression tag	UNP G0SDQ1
D	-12	ASP	-	expression tag	UNP G0SDQ1
D	-11	ILE	-	expression tag	UNP G0SDQ1
D	-10	PRO	-	expression tag	UNP G0SDQ1
D	-9	THR	-	expression tag	UNP G0SDQ1
D	-8	THR	-	expression tag	UNP G0SDQ1
D	-7	GLU	-	expression tag	UNP G0SDQ1
D	-6	ASN	-	expression tag	UNP G0SDQ1
D	-5	LEU	-	expression tag	UNP G0SDQ1
D	-4	TYR	-	expression tag	UNP G0SDQ1
D	-3	PHE	-	expression tag	UNP G0SDQ1
D	-2	GLN	-	expression tag	UNP G0SDQ1
D	-1	GLY	-	expression tag	UNP G0SDQ1
D	0	ALA	-	expression tag	UNP G0SDQ1

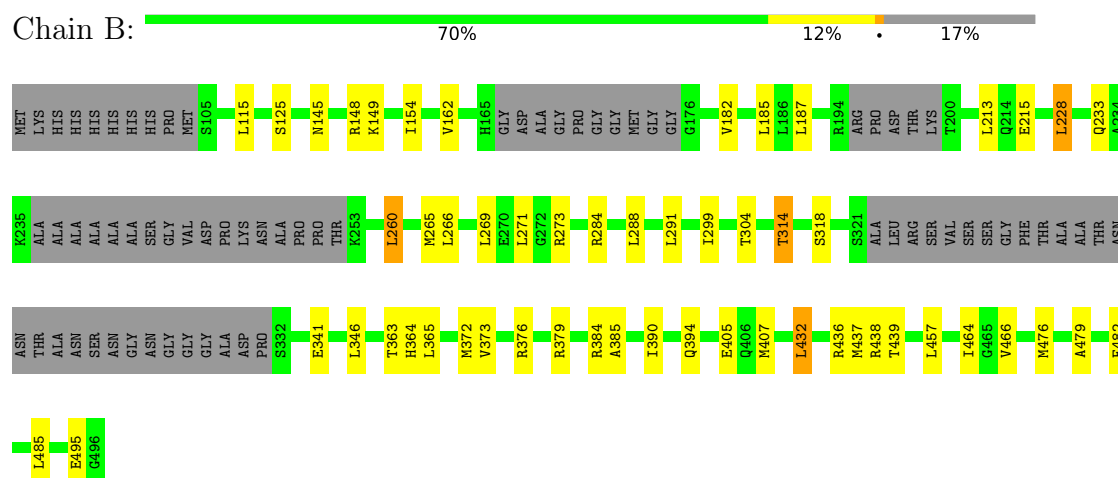
3 Residue-property plots

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.

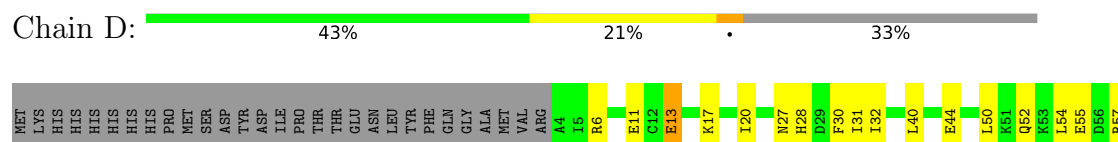
- Molecule 1: RNA polymerase II transcription factor B subunit 2



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



- Molecule 2: Uncharacterized protein



L58	
T61	
Y62	
R63	
P64	
E65	
E66	
P67	
L68	
A69	
ASP	
SER	
ASP	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.22Å 85.95Å 92.17Å 90.00° 94.93° 90.00°	Depositor
Resolution (Å)	19.92 – 2.68 19.92 – 2.68	Depositor EDS
% Data completeness (in resolution range)	52.7 (19.92-2.68) 52.7 (19.92-2.68)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.67Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.216 , 0.240 0.238 , 0.270	Depositor DCC
R_{free} test set	1091 reflections (3.35%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 1.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5606	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.39% 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	0.74	0/2330	1.37	4/3168 (0.1%)
1	B	0.73	0/2843	1.37	8/3848 (0.2%)
2	D	0.86	0/549	1.38	1/742 (0.1%)
All	All	0.75	0/5722	1.37	13/7758 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	341	GLU	CA-C-N	5.64	128.61	120.38
1	B	341	GLU	C-N-CA	5.64	128.61	120.38
1	B	228	LEU	CA-C-N	5.36	127.46	120.28
1	B	228	LEU	C-N-CA	5.36	127.46	120.28
1	B	482	PHE	CA-C-N	5.31	127.39	120.28
1	B	482	PHE	C-N-CA	5.31	127.39	120.28
1	A	228	LEU	CA-C-N	5.30	127.39	120.28
1	A	228	LEU	C-N-CA	5.30	127.39	120.28
1	A	379	ARG	CA-C-N	5.07	127.03	120.44
1	A	379	ARG	C-N-CA	5.07	127.03	120.44
2	D	68	LEU	N-CA-C	-5.07	107.76	114.04
1	B	379	ARG	CA-C-N	5.06	127.02	120.44
1	B	379	ARG	C-N-CA	5.06	127.02	120.44

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	2281	0	2299	21	0
1	B	2784	0	2784	25	0
2	D	541	0	551	7	0
All	All	5606	0	5634	45	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 4.

All (45) 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:346:LEU:HD13	1:B:363:THR:HG21	1.80	0.64
1:A:346:LEU:HD13	1:A:363:THR:HG21	1.79	0.63
1:B:145:ASN:HD22	1:B:148:ARG:HH21	1.47	0.62
1:A:145:ASN:HD22	1:A:148:ARG:HH21	1.47	0.61
1:A:383:ARG:HA	1:A:386:ILE:HD12	1.85	0.57
1:B:125:SER:HB2	1:B:284:ARG:HH12	1.68	0.57
1:A:257:ILE:HG13	1:B:384:ARG:HG3	1.87	0.56
1:B:438:ARG:HB2	2:D:11:GLU:HB3	1.86	0.56
1:B:154:ILE:HG12	1:B:182:VAL:HG11	1.88	0.56
1:A:154:ILE:HG12	1:A:182:VAL:HG11	1.88	0.55
1:B:436:ARG:HA	1:B:436:ARG:HH11	1.73	0.54
1:A:118:GLN:HE22	1:B:394:GLN:HE22	1.54	0.54
1:A:229:GLU:HG3	1:B:364:HIS:HE1	1.73	0.53
2:D:20:ILE:HG22	2:D:31:ILE:HD11	1.90	0.53
1:A:228:LEU:HD21	1:A:260:LEU:HG	1.92	0.51
1:B:228:LEU:HD21	1:B:260:LEU:HG	1.93	0.51
1:B:148:ARG:HH22	1:B:149:LYS:HE2	1.76	0.50
2:D:20:ILE:HG23	2:D:50:LEU:HD21	1.92	0.50
1:A:148:ARG:HH22	1:A:149:LYS:HE2	1.76	0.50
1:A:354:LEU:HD13	1:B:318:SER:HB2	1.94	0.49
1:A:385:ALA:HB1	1:A:390:ILE:HB	1.95	0.48
1:A:386:ILE:HD11	1:A:431:GLN:HA	1.95	0.47
1:B:385:ALA:HB1	1:B:390:ILE:HB	1.96	0.47
1:A:266:LEU:HA	1:A:269:LEU:HG	1.97	0.46
1:A:229:GLU:HG3	1:B:364:HIS:CE1	2.51	0.46
1:B:266:LEU:HA	1:B:269:LEU:HG	1.98	0.46
1:A:265:MET:HE3	1:A:269:LEU:HD21	1.97	0.45
1:B:265:MET:HE3	1:B:269:LEU:HD21	1.98	0.45
1:B:271:LEU:HB2	1:B:314:THR:HG21	1.99	0.45
2:D:63:ARG:O	2:D:64:PRO:C	2.60	0.45
1:A:161:SER:HB3	1:A:202:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:LEU:HD22	1:A:299:ILE:HD11	2.00	0.44
1:B:125:SER:HB2	1:B:284:ARG:NH1	2.33	0.44
1:A:365:LEU:HD22	1:A:373:VAL:HB	2.00	0.43
1:B:288:LEU:HD22	1:B:299:ILE:HD11	2.00	0.43
1:B:466:VAL:HG12	1:B:479:ALA:HB1	2.01	0.43
1:B:365:LEU:HD22	1:B:373:VAL:HB	2.00	0.42
1:B:436:ARG:HD2	2:D:13:GLU:HB2	2.01	0.42
1:A:426:GLN:HE22	1:A:429:LEU:HD23	1.85	0.42
1:A:231:ALA:HB3	1:A:259:MET:HE1	2.02	0.41
1:A:213:LEU:HD12	1:A:372:MET:HE3	2.03	0.41
2:D:17:LYS:HG3	2:D:40:LEU:HD22	2.02	0.41
1:B:213:LEU:HD12	1:B:372:MET:HE3	2.02	0.41
1:B:432:LEU:HD13	2:D:55:GLU:HG2	2.03	0.40
1:B:162:VAL:HG11	1:B:407:MET:HE1	2.02	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	284/420 (68%)	277 (98%)	7 (2%)	0	100	100
1	B	340/420 (81%)	326 (96%)	14 (4%)	0	100	100
2	D	64/98 (65%)	52 (81%)	6 (9%)	6 (9%)	0	0
All	All	688/938 (73%)	655 (95%)	27 (4%)	6 (1%)	14	31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	6	ARG
2	D	30	PHE
2	D	64	PRO

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Mol	Chain	Res	Type
2	D	65	GLU
2	D	44	GLU
2	D	67	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	241/339 (71%)	227 (94%)	14 (6%)	18	39
1	B	294/339 (87%)	274 (93%)	20 (7%)	14	32
2	D	62/92 (67%)	52 (84%)	10 (16%)	2	5
All	All	597/770 (78%)	553 (93%)	44 (7%)	13	28

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	LEU
1	A	187	LEU
1	A	194	ARG
1	A	198	THR
1	A	215	GLU
1	A	233	GLN
1	A	260	LEU
1	A	273	ARG
1	A	291	LEU
1	A	304	THR
1	A	319	SER
1	A	335	LYS
1	A	405	GLU
1	A	434	ASN
1	B	115	LEU
1	B	185	LEU
1	B	187	LEU
1	B	215	GLU
1	B	233	GLN

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Mol	Chain	Res	Type
1	B	260	LEU
1	B	273	ARG
1	B	291	LEU
1	B	304	THR
1	B	314	THR
1	B	376	ARG
1	B	405	GLU
1	B	432	LEU
1	B	437	MET
1	B	439	THR
1	B	457	LEU
1	B	464	ILE
1	B	476	MET
1	B	485	LEU
1	B	495	GLU
2	D	13	GLU
2	D	27	ASN
2	D	28	HIS
2	D	32	ILE
2	D	52	GLN
2	D	54	LEU
2	D	57	ARG
2	D	58	LEU
2	D	61	THR
2	D	68	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	145	ASN
1	A	206	GLN
1	A	286	ASN
1	A	343	ASN
1	A	434	ASN
1	B	145	ASN
1	B	206	GLN
1	B	219	GLN
1	B	286	ASN
1	B	343	ASN
1	B	364	HIS
1	B	394	GLN

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	292/420 (69%)	-1.84	0 100 100	22, 41, 74, 111	0
1	B	350/420 (83%)	-1.79	0 100 100	26, 47, 109, 124	0
2	D	66/98 (67%)	-1.81	0 100 100	46, 69, 107, 115	0
All	All	708/938 (75%)	-1.81	0 100 100	22, 46, 102, 124	0

There are no RSRZ outliers to report.

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.