



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 07:54 am BST

PDB ID : 5O85
Title : p34-p44 complex
Authors : Radu, L.; Poterszman, A.
Deposited on : 2017-06-12
Resolution : 3.40 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

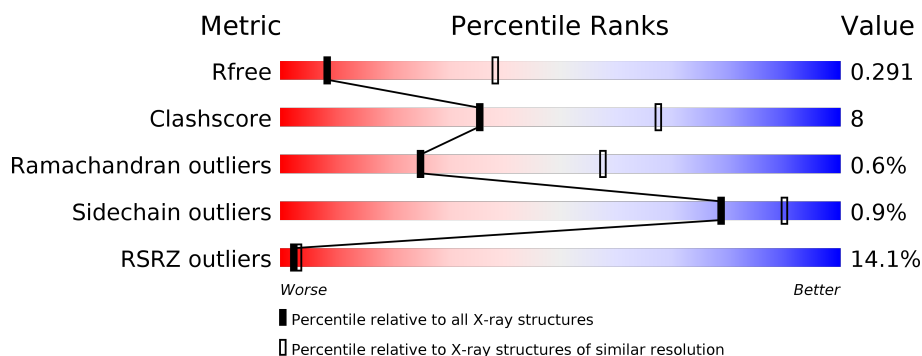
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 $\leq 5\%$. 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	308	<div> <div>11%</div> <div>47%</div> <div>15%</div> <div>38%</div> </div>
1	C	308	<div> <div>2%</div> <div>53%</div> <div>12%</div> <div>36%</div> </div>
2	B	395	<div> <div>3%</div> <div>9%</div> <div>88%</div> </div>
2	D	395	<div> <div>4%</div> <div>11%</div> <div>87%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3849 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 General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	1	0	0
			1491	961	247	271	12			
1	C	198	Total	C	N	O	S	1	0	0
			1567	1008	257	290	12			

- Molecule 2 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	49	Total	C	N	O	S	0	0	0
			372	233	59	72	8			
2	D	53	Total	C	N	O	S	0	0	0
			415	264	66	77	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	381	SER	CYS	engineered mutation	UNP Q13888
D	381	SER	CYS	engineered mutation	UNP Q13888

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Zn	0	0
			2	2		
3	D	2	Total	Zn	0	0
			2	2		

- Molecule 1: General transcription factor IIH subunit 3



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.41Å 120.39Å 128.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.70 – 3.40 45.30 – 3.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.70-3.40) 100.0 (45.30-3.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.240 , 0.290 0.240 , 0.291	Depositor DCC
R_{free} test set	445 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	133.0	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 106.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3849	wwPDB-VP
Average B, all atoms (Å ²)	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.51% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.25	0/1514	0.43	0/2045
1	C	0.27	0/1589	0.51	0/2144
2	B	0.29	0/379	0.45	0/512
2	D	0.27	0/425	0.44	0/575
All	All	0.27	0/3907	0.47	0/5276

There are no bond length outliers.

There are no bond angle outliers.

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	1491	0	1541	27	0
1	C	1567	0	1612	24	17
2	B	372	0	319	8	0
2	D	415	0	365	5	2
3	B	2	0	0	0	0
3	D	2	0	0	0	0
All	All	3849	0	3837	62	17

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 8.

All (62) 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:165:LYS:HE2	1:A:200:SER:HB3	1.58	0.85
1:C:152:LYS:O	1:C:152:LYS:HG2	1.77	0.84
1:C:151:VAL:HG13	1:C:151:VAL:O	1.89	0.71
1:C:153:ASP:O	1:C:154:ASN:HB3	2.00	0.61
1:C:184:ALA:HA	1:C:189:ILE:HD12	1.84	0.59
1:C:155:GLN:OE1	1:C:155:GLN:HA	2.04	0.58
1:A:177:PHE:CE2	1:A:181:ILE:HD11	2.39	0.58
1:A:61:ALA:HB2	1:A:70:LEU:HD11	1.85	0.58
1:A:219:GLN:HG2	1:A:221:PRO:HD2	1.87	0.56
1:C:152:LYS:CG	1:C:152:LYS:O	2.50	0.56
2:B:343:ARG:O	2:B:344:PHE:C	2.46	0.53
1:C:151:VAL:CG1	1:C:151:VAL:O	2.57	0.53
1:A:39:ASP:HA	1:A:42:MET:HE2	1.90	0.53
2:D:331:PHE:HB2	2:D:358:TYR:HB3	1.91	0.53
1:A:105:THR:HG22	1:A:107:ALA:H	1.74	0.52
1:A:44:LEU:HD22	1:A:227:LEU:HG	1.90	0.52
1:A:144:ILE:O	1:A:148:ASN:HB2	2.11	0.51
1:C:151:VAL:HG21	1:C:155:GLN:HG3	1.93	0.51
1:A:115:ILE:HG13	1:A:116:LYS:N	2.27	0.50
1:A:108:ASN:O	1:A:112:VAL:HG23	2.12	0.49
1:A:176:ASN:O	1:A:179:ASN:HB2	2.13	0.49
1:C:220:MET:N	1:C:221:PRO:HD2	2.28	0.49
2:D:328:LEU:HD23	2:D:329:ASP:N	2.27	0.49
1:A:19:PRO:HD2	1:A:64:ILE:HG23	1.94	0.49
1:A:143:TYR:O	1:A:146:ARG:HG3	2.13	0.49
1:C:219:GLN:HG2	1:C:221:PRO:HD2	1.94	0.49
2:D:336:LEU:H	2:D:336:LEU:HD22	1.79	0.48
1:C:140:ALA:O	1:C:144:ILE:HG23	2.13	0.48
1:A:177:PHE:O	1:A:180:VAL:HG22	2.14	0.47
1:A:177:PHE:CE2	1:A:202:LEU:HB3	2.49	0.47
1:A:21:TRP:HB2	1:A:167:ALA:HB2	1.97	0.47
1:C:223:LEU:HD11	1:C:227:LEU:HD13	1.98	0.46
1:A:107:ALA:O	1:A:110:VAL:HG12	2.16	0.46
1:C:38:ILE:HG13	1:C:115:ILE:HD13	1.98	0.45
1:C:19:PRO:HD2	1:C:64:ILE:HG23	1.99	0.45
1:A:191:ILE:O	1:A:212:GLY:HA3	2.16	0.45
1:C:160:ARG:HG3	1:C:190:LEU:HB3	1.98	0.45
1:C:152:LYS:O	1:C:153:ASP:CG	2.56	0.45
1:A:146:ARG:HD3	2:B:348:CYS:HB2	1.99	0.44
2:B:330:ALA:HA	2:B:376:HIS:CE1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:PHE:CE2	1:C:202:LEU:HB3	2.52	0.44
1:C:71:TYR:CD1	1:C:72:PRO:HA	2.53	0.44
1:A:169:ASP:N	1:A:169:ASP:OD1	2.42	0.44
2:B:365:ASN:HD22	2:B:384:GLY:HA3	1.82	0.43
1:A:116:LYS:O	1:A:120:THR:HG23	2.19	0.43
1:C:165:LYS:HD2	1:C:169:ASP:OD1	2.18	0.43
1:A:164:ILE:HA	1:A:194:CYS:O	2.19	0.42
1:A:121:LYS:HD2	1:A:121:LYS:HA	1.85	0.42
1:C:152:LYS:O	1:C:153:ASP:OD1	2.37	0.42
1:C:23:GLY:O	1:C:27:LEU:HG	2.19	0.42
2:B:345:CYS:SG	2:B:347:GLY:N	2.85	0.42
1:A:132:LEU:HD22	2:B:387:HIS:HA	2.01	0.42
1:C:106:SER:O	1:C:109:GLU:HB2	2.20	0.42
1:A:200:SER:OG	1:A:203:LEU:HB3	2.19	0.41
2:D:328:LEU:HD22	2:D:376:HIS:CD2	2.55	0.41
1:C:186:LYS:HD2	1:C:186:LYS:HA	1.78	0.41
2:B:332:GLN:O	2:B:359:VAL:N	2.54	0.41
2:B:331:PHE:HD1	2:B:360:CYS:HA	1.86	0.41
2:D:326:PHE:N	2:D:327:PRO:HD3	2.36	0.40
1:A:12:VAL:HG22	1:A:58:ALA:HB3	2.03	0.40
1:A:59:VAL:HG12	1:A:70:LEU:HD12	2.04	0.40
1:C:165:LYS:NZ	1:C:200:SER:HB2	2.36	0.40

All (17) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:GLU:CD	1:C:151:VAL:N[7_555]	0.57	1.63
1:C:150:GLU:C	1:C:150:GLU:CD[7_555]	0.78	1.42
1:C:150:GLU:O	1:C:150:GLU:CG[7_555]	0.85	1.35
1:C:150:GLU:O	1:C:150:GLU:CB[7_555]	0.96	1.24
1:C:150:GLU:OE2	1:C:151:VAL:N[7_555]	0.97	1.23
1:C:150:GLU:C	1:C:150:GLU:CG[7_555]	1.14	1.06
1:C:150:GLU:C	1:C:150:GLU:OE1[7_555]	1.32	0.88
1:C:150:GLU:OE1	1:C:151:VAL:N[7_555]	1.39	0.81
1:C:153:ASP:OD1	2:D:351:GLU:OE1[7_555]	1.72	0.48
1:C:149:LYS:NZ	2:D:370:ASP:OD1[7_555]	1.81	0.39
1:C:150:GLU:C	1:C:150:GLU:CB[7_555]	1.81	0.39
1:C:150:GLU:N	1:C:150:GLU:OE1[7_555]	1.82	0.38
1:C:150:GLU:O	1:C:150:GLU:CD[7_555]	1.83	0.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:GLU:CA	1:C:150:GLU:OE1[7_555]	1.84	0.36
1:C:150:GLU:CA	1:C:150:GLU:CA[7_555]	1.85	0.35
1:C:150:GLU:CA	1:C:150:GLU:CD[7_555]	1.94	0.26
1:C:150:GLU:C	1:C:150:GLU:OE2[7_555]	1.98	0.22

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	184/308 (60%)	178 (97%)	5 (3%)	1 (0%)	29	61
1	C	190/308 (62%)	180 (95%)	9 (5%)	1 (0%)	29	61
2	B	43/395 (11%)	38 (88%)	5 (12%)	0	100	100
2	D	47/395 (12%)	44 (94%)	2 (4%)	1 (2%)	7	30
All	All	464/1406 (33%)	440 (95%)	21 (4%)	3 (1%)	25	57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	218	PRO
1	A	218	PRO
2	D	327	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	167/272 (61%)	166 (99%)	1 (1%)	86	94
1	C	176/272 (65%)	175 (99%)	1 (1%)	86	94
2	B	43/352 (12%)	41 (95%)	2 (5%)	26	57
2	D	48/352 (14%)	48 (100%)	0	100	100
All	All	434/1248 (35%)	430 (99%)	4 (1%)	78	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
2	B	337	GLU
2	B	344	PHE
1	C	229	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	376	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	190/308 (61%)	0.90	35 (18%) 1 1	113, 156, 193, 212	1 (0%)
1	C	198/308 (64%)	0.35	7 (3%) 44 43	69, 113, 164, 202	1 (0%)
2	B	49/395 (12%)	0.89	11 (22%) 0 1	150, 186, 209, 228	0
2	D	53/395 (13%)	0.92	16 (30%) 0 0	119, 154, 190, 207	0
All	All	490/1406 (34%)	0.68	69 (14%) 2 3	69, 147, 194, 228	2 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	346	TYR	6.9
2	D	359	VAL	5.4
1	A	199	ASP	5.2
1	A	168	GLU	5.2
1	A	67	SER	5.1
1	A	169	ASP	5.0
1	A	151	VAL	4.4
2	B	367	PHE	4.2
2	D	358	TYR	4.1
1	A	144	ILE	4.1
1	A	149	LYS	4.0
2	B	372	ASP	4.0
1	A	143	TYR	3.9
1	A	170	SER	3.8
2	D	332	GLN	3.8
2	D	334	ILE	3.8
1	A	61	ALA	3.7
2	D	367	PHE	3.7
1	A	200	SER	3.5
2	B	375	VAL	3.5
1	A	59	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	378	SER	3.3
2	B	374	PHE	3.3
2	D	351	GLU	3.3
1	C	65	GLN	3.2
1	C	233	PRO	2.9
1	A	186	LYS	2.9
1	A	69	PHE	2.9
2	D	333	GLU	2.9
2	D	331	PHE	2.9
1	A	145	HIS	2.9
2	B	359	VAL	2.8
1	A	58	ALA	2.8
1	A	160	ARG	2.8
2	D	366	VAL	2.8
1	A	15	VAL	2.8
2	B	387	HIS	2.7
1	A	130	GLU	2.7
1	A	16	ASP	2.7
1	A	140	ALA	2.7
2	D	336	LEU	2.7
1	A	115	ILE	2.7
1	A	70	LEU	2.7
1	A	131	THR	2.7
1	A	204	GLN	2.7
1	C	182	PHE	2.7
1	A	150	GLU	2.6
1	A	171	ALA	2.5
1	C	199	ASP	2.5
2	B	351	GLU	2.5
2	D	346	TYR	2.5
2	D	357	VAL	2.4
2	B	379	LEU	2.4
1	A	201	GLY	2.4
1	A	12	VAL	2.4
1	A	139	LYS	2.4
1	C	204	GLN	2.3
2	D	387	HIS	2.3
1	C	101	TYR	2.3
1	A	147	MET	2.2
1	A	13	ILE	2.2
1	A	111	ILE	2.2
2	B	366	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	344	PHE	2.1
2	D	379	LEU	2.1
1	A	60	ILE	2.1
1	A	51	MET	2.0
1	C	222	SER	2.0
2	D	361	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ZN	D	402	1/1	0.87	0.04	170,170,170,170	0
3	ZN	B	401	1/1	0.93	0.02	220,220,220,220	0
3	ZN	D	401	1/1	0.94	0.05	163,163,163,163	0
3	ZN	B	402	1/1	0.98	0.04	199,199,199,199	0

6.5 Other polymers [i](#)

There are no such residues in this entry.