



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 03:00 PM GMT

PDB ID : 2NXP  
Title : Structure of NTD2 domain of the human TAF5 subunit of TFIID  
Authors : Bhattacharya, S.; Takada, S.; Jacobson, R.H.  
Deposited on : 2006-11-17  
Resolution : 2.17 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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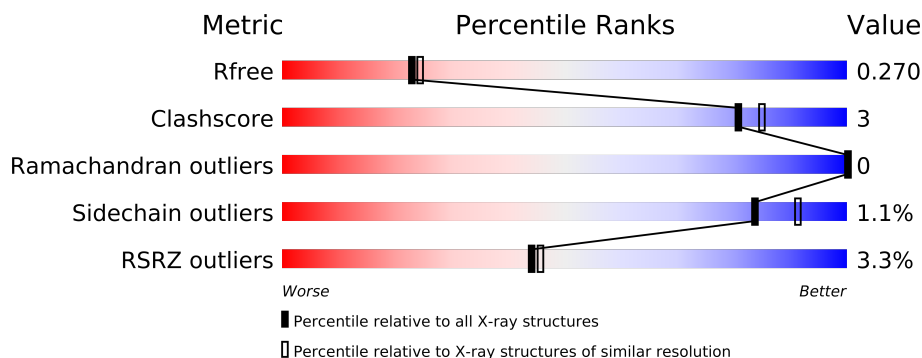
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.17 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))
$R_{free}$	66092	3841 (2.20-2.16)
Clashscore	79885	4835 (2.20-2.16)
Ramachandran outliers	78287	4740 (2.20-2.16)
Sidechain outliers	78261	4741 (2.20-2.16)
RSRZ outliers	66119	3842 (2.20-2.16)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	156	
1	B	156	
1	C	156	
1	D	156	
1	E	156	
1	F	156	
1	G	156	
1	H	156	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10515 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Transcription initiation factor TFIID subunit 5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	Se	0	1	0
			1269	810	212	240	3	4			
1	B	145	Total	C	N	O	S	Se	0	0	0
			1235	790	207	231	3	4			
1	C	147	Total	C	N	O	S	Se	0	0	0
			1251	798	209	237	3	4			
1	D	147	Total	C	N	O	S	Se	0	0	0
			1251	798	209	237	3	4			
1	E	148	Total	C	N	O	S	Se	0	0	0
			1258	803	210	238	3	4			
1	F	146	Total	C	N	O	S	Se	0	0	0
			1243	794	208	234	3	4			
1	G	146	Total	C	N	O	S	Se	0	0	0
			1243	794	208	234	3	4			
1	H	145	Total	C	N	O	S	Se	0	0	0
			1236	789	207	233	3	4			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	213	MSE	MET	MODIFIED RESIDUE	UNP Q15542
A	247	MSE	MET	MODIFIED RESIDUE	UNP Q15542
A	291	MSE	MET	MODIFIED RESIDUE	UNP Q15542
A	297	MSE	MET	MODIFIED RESIDUE	UNP Q15542
B	213	MSE	MET	MODIFIED RESIDUE	UNP Q15542
B	247	MSE	MET	MODIFIED RESIDUE	UNP Q15542
B	291	MSE	MET	MODIFIED RESIDUE	UNP Q15542
B	297	MSE	MET	MODIFIED RESIDUE	UNP Q15542
C	213	MSE	MET	MODIFIED RESIDUE	UNP Q15542
C	247	MSE	MET	MODIFIED RESIDUE	UNP Q15542
C	291	MSE	MET	MODIFIED RESIDUE	UNP Q15542
C	297	MSE	MET	MODIFIED RESIDUE	UNP Q15542
D	213	MSE	MET	MODIFIED RESIDUE	UNP Q15542

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Chain	Residue	Modelled	Actual	Comment	Reference
D	247	MSE	MET	MODIFIED RESIDUE	UNP Q15542
D	291	MSE	MET	MODIFIED RESIDUE	UNP Q15542
D	297	MSE	MET	MODIFIED RESIDUE	UNP Q15542
E	213	MSE	MET	MODIFIED RESIDUE	UNP Q15542
E	247	MSE	MET	MODIFIED RESIDUE	UNP Q15542
E	291	MSE	MET	MODIFIED RESIDUE	UNP Q15542
E	297	MSE	MET	MODIFIED RESIDUE	UNP Q15542
F	213	MSE	MET	MODIFIED RESIDUE	UNP Q15542
F	247	MSE	MET	MODIFIED RESIDUE	UNP Q15542
F	291	MSE	MET	MODIFIED RESIDUE	UNP Q15542
F	297	MSE	MET	MODIFIED RESIDUE	UNP Q15542
G	213	MSE	MET	MODIFIED RESIDUE	UNP Q15542
G	247	MSE	MET	MODIFIED RESIDUE	UNP Q15542
G	291	MSE	MET	MODIFIED RESIDUE	UNP Q15542
G	297	MSE	MET	MODIFIED RESIDUE	UNP Q15542
H	213	MSE	MET	MODIFIED RESIDUE	UNP Q15542
H	247	MSE	MET	MODIFIED RESIDUE	UNP Q15542
H	291	MSE	MET	MODIFIED RESIDUE	UNP Q15542
H	297	MSE	MET	MODIFIED RESIDUE	UNP Q15542

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	67	Total O 67 67	0	0
3	B	37	Total O 37 37	0	0
3	C	102	Total O 102 102	0	0
3	D	54	Total O 54 54	0	0
3	E	95	Total O 95 95	0	0
3	F	68	Total O 68 68	0	0
3	G	45	Total O 45 45	0	0
3	H	53	Total O 53 53	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

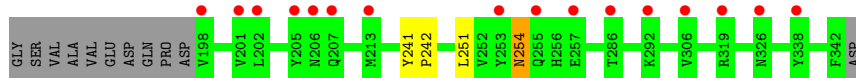
- Molecule 1: Transcription initiation factor TFIID subunit 5

Chain A: 



- Molecule 1: Transcription initiation factor TFIID subunit 5

Chain B: 



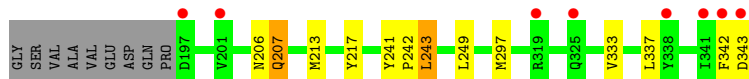
- Molecule 1: Transcription initiation factor TFIID subunit 5

Chain C: 



- Molecule 1: Transcription initiation factor TFIID subunit 5

Chain D: 



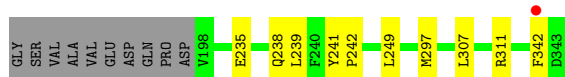
- Molecule 1: Transcription initiation factor TFIID subunit 5

Chain E: 

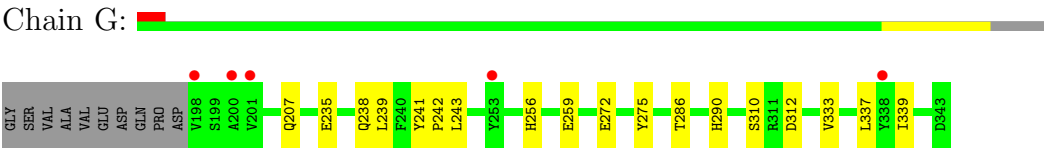


- Molecule 1: Transcription initiation factor TFIID subunit 5

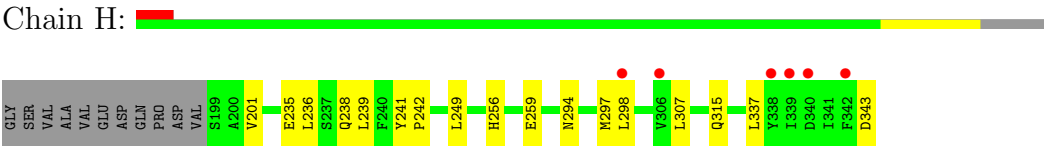
Chain F: 



● Molecule 1: Transcription initiation factor TFIID subunit 5



● Molecule 1: Transcription initiation factor TFIID subunit 5



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.62Å 61.83Å 133.36Å 90.00° 105.16° 90.00°	Depositor
Resolution (Å)	64.42 – 2.17 64.36 – 2.17	Depositor EDS
% Data completeness (in resolution range)	97.9 (64.42-2.17) 97.9 (64.36-2.17)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.213 , 0.263 0.222 , 0.270	Depositor DCC
$R_{free}$ test set	3837 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.2	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 33.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 76749 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10515	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.41 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.9596e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.



## 5 Model quality

### 5.1 Standard geometry

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

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	0.27	0/1300	0.42	0/1746
1	B	0.24	0/1262	0.37	0/1693
1	C	0.27	0/1278	0.41	0/1715
1	D	0.25	0/1278	0.39	0/1715
1	E	0.26	0/1286	0.41	0/1726
1	F	0.26	0/1270	0.40	0/1704
1	G	0.25	0/1270	0.38	0/1704
1	H	0.26	0/1263	0.40	0/1694
All	All	0.26	0/10207	0.40	0/13697

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1269	0	1201	8	0
1	B	1235	0	1176	5	0
1	C	1251	0	1184	7	0
1	D	1251	0	1184	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1258	0	1192	7	0
1	F	1243	0	1180	6	0
1	G	1243	0	1180	11	0
1	H	1236	0	1171	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	67	0	0	2	0
3	B	37	0	0	2	0
3	C	102	0	0	1	0
3	D	54	0	0	1	0
3	E	95	0	0	0	0
3	F	68	0	0	0	0
3	G	45	0	0	0	0
3	H	53	0	0	1	0
All	All	10515	0	9468	65	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (65) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:235:GLU:O	1:F:238:GLN:HG2	1.92	0.69
1:B:254:ASN:HB2	3:B:638:HOH:O	1.93	0.68
1:D:243:LEU:HD13	1:D:337:LEU:HD11	1.77	0.66
1:D:206:ASN:ND2	1:H:259:GLU:OE1	2.30	0.65
1:E:249:LEU:HD13	1:E:297:MSE:HE1	1.80	0.63
1:C:333:VAL:HG22	1:C:337:LEU:HD12	1.80	0.63
1:C:249:LEU:HD13	1:C:297:MSE:HE1	1.82	0.61
1:H:249:LEU:HD13	1:H:297:MSE:HE1	1.84	0.60
1:A:249:LEU:HD13	1:A:297:MSE:HE1	1.83	0.60
1:E:239:LEU:HD23	1:E:307:LEU:HD13	1.83	0.59
1:A:311:ARG:O	1:A:315[A]:GLN:HG3	2.02	0.59
1:B:251:LEU:HA	3:B:638:HOH:O	2.04	0.58
1:H:256:HIS:HB3	1:H:259:GLU:CG	2.34	0.57
1:G:243:LEU:HD13	1:G:337:LEU:HD11	1.87	0.56
1:G:239:LEU:O	1:G:243:LEU:HB2	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:241:TYR:HB3	1:H:242:PRO:HD3	1.88	0.56
1:H:238:GLN:HE21	1:H:307:LEU:HA	1.71	0.55
1:C:239:LEU:HD23	1:C:307:LEU:HD13	1.89	0.54
1:G:333:VAL:HG13	1:G:339:ILE:HD12	1.90	0.54
1:G:310:SER:OG	1:G:312:ASP:OD1	2.11	0.54
1:C:206:ASN:HD22	1:C:207:GLN:N	2.05	0.53
1:H:256:HIS:HB3	1:H:259:GLU:HG2	1.90	0.53
1:B:254:ASN:HD22	1:B:254:ASN:N	2.08	0.52
1:D:241:TYR:HB3	1:D:242:PRO:HD3	1.92	0.52
1:D:243:LEU:CD1	1:D:337:LEU:HD11	2.41	0.51
1:F:241:TYR:HB3	1:F:242:PRO:HD3	1.91	0.51
1:G:256:HIS:HB3	1:G:259:GLU:CG	2.41	0.51
1:B:241:TYR:HB3	1:B:242:PRO:HD3	1.94	0.49
1:D:249:LEU:HD13	1:D:297:MSE:HE1	1.93	0.49
1:C:322:GLN:NE2	3:C:623:HOH:O	2.46	0.49
1:H:235:GLU:O	1:H:238:GLN:HG2	2.12	0.49
1:G:235:GLU:O	1:G:238:GLN:HG2	2.13	0.49
1:A:311:ARG:O	1:A:315[A]:GLN:CG	2.61	0.48
1:A:312:ASP:HA	1:A:315[A]:GLN:HG3	1.95	0.48
1:D:207:GLN:HG2	3:D:632:HOH:O	2.14	0.48
1:H:315:GLN:HG2	3:H:643:HOH:O	2.14	0.47
1:A:212:THR:O	3:A:666:HOH:O	2.21	0.47
1:C:342:PHE:CZ	1:D:342:PHE:CE2	3.03	0.47
1:H:238:GLN:HG3	1:H:307:LEU:HD22	1.97	0.45
1:F:238:GLN:HG3	1:F:307:LEU:HD22	1.97	0.45
1:E:333:VAL:HG22	1:E:337:LEU:HD12	1.98	0.45
1:H:236:LEU:O	1:H:239:LEU:HB2	2.17	0.45
1:H:294:ASN:HB3	1:H:297:MSE:HG2	1.99	0.45
1:H:201:VAL:HG21	1:H:298:LEU:HD23	1.99	0.45
1:B:254:ASN:N	1:B:254:ASN:ND2	2.65	0.44
1:E:301:ARG:O	1:E:304:LYS:HG2	2.17	0.44
1:G:286:THR:H	1:G:290:HIS:HD2	1.65	0.44
1:E:241:TYR:HB3	1:E:242:PRO:HD3	1.99	0.44
1:E:198:VAL:O	1:E:201:VAL:HG22	2.17	0.44
1:F:311:ARG:N	1:F:342:PHE:O	2.50	0.44
1:E:208:GLN:OE1	1:E:256:HIS:NE2	2.48	0.44
1:A:333:VAL:HG22	1:A:337:LEU:HD12	2.00	0.44
1:D:333:VAL:HA	1:D:337:LEU:HD12	2.01	0.42
1:G:272:GLU:HB2	1:G:275:TYR:CD1	2.54	0.42
1:G:241:TYR:HB3	1:G:242:PRO:HD3	2.01	0.42
1:D:213:MSE:HB3	1:D:217:TYR:CZ	2.54	0.42
1:F:249:LEU:HD13	1:F:297:MSE:HE1	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:239:LEU:HD23	1:F:307:LEU:HD13	2.02	0.41
1:A:264:PHE:CZ	1:A:283:SER:HB3	2.56	0.41
1:C:329:ILE:O	1:C:333:VAL:HG23	2.21	0.41
1:H:238:GLN:NE2	1:H:307:LEU:HA	2.33	0.41
1:A:289:GLU:HG3	3:A:634:HOH:O	2.20	0.41
1:G:256:HIS:HB3	1:G:259:GLU:HG2	2.03	0.41
1:H:239:LEU:HD23	1:H:337:LEU:HD21	2.02	0.40
1:G:333:VAL:HG22	1:G:337:LEU:HD12	2.04	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	148/156 (95%)	147 (99%)	1 (1%)	0	100	100
1	B	143/156 (92%)	141 (99%)	2 (1%)	0	100	100
1	C	145/156 (93%)	143 (99%)	2 (1%)	0	100	100
1	D	145/156 (93%)	142 (98%)	3 (2%)	0	100	100
1	E	146/156 (94%)	145 (99%)	1 (1%)	0	100	100
1	F	144/156 (92%)	143 (99%)	1 (1%)	0	100	100
1	G	144/156 (92%)	141 (98%)	3 (2%)	0	100	100
1	H	143/156 (92%)	140 (98%)	3 (2%)	0	100	100
All	All	1158/1248 (93%)	1142 (99%)	16 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	141/142 (99%)	139 (99%)	2 (1%)	78	87
1	B	137/142 (96%)	136 (99%)	1 (1%)	91	96
1	C	139/142 (98%)	137 (99%)	2 (1%)	78	87
1	D	139/142 (98%)	136 (98%)	3 (2%)	64	75
1	E	140/142 (99%)	138 (99%)	2 (1%)	78	87
1	F	138/142 (97%)	138 (100%)	0	100	100
1	G	138/142 (97%)	137 (99%)	1 (1%)	91	96
1	H	137/142 (96%)	136 (99%)	1 (1%)	91	96
All	All	1109/1136 (98%)	1097 (99%)	12 (1%)	84	91

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	312	ASP
1	A	343	ASP
1	B	254	ASN
1	C	206	ASN
1	C	340	ASP
1	D	207	GLN
1	D	243	LEU
1	D	343	ASP
1	E	201	VAL
1	E	339	ILE
1	G	207	GLN
1	H	343	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	232	HIS
1	B	206	ASN
1	B	208	GLN
1	B	254	ASN
1	B	325	GLN
1	C	206	ASN
1	C	238	GLN
1	C	322	GLN

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Mol	Chain	Res	Type
1	D	331	ASN
1	E	258	ASN
1	E	315	GLN
1	G	206	ASN
1	G	207	GLN
1	G	255	GLN
1	G	258	ASN
1	G	290	HIS
1	H	223	HIS
1	H	238	GLN
1	H	268	HIS
1	H	334	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 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.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	149/156 (95%)	0.08	1 (0%) 84 87	21, 36, 59, 77	0
1	B	145/156 (92%)	0.72	16 (11%) 6 6	26, 45, 68, 78	0
1	C	147/156 (94%)	0.08	2 (1%) 72 73	18, 30, 58, 69	0
1	D	147/156 (94%)	0.31	8 (5%) 25 26	21, 40, 69, 94	0
1	E	148/156 (94%)	0.03	0 100 100	19, 30, 53, 74	0
1	F	146/156 (93%)	0.04	1 (0%) 84 87	22, 34, 54, 72	0
1	G	146/156 (93%)	0.38	5 (3%) 43 44	23, 41, 64, 73	0
1	H	145/156 (92%)	0.23	6 (4%) 35 37	21, 38, 62, 71	0
All	All	1173/1248 (93%)	0.23	39 (3%) 44 46	18, 37, 63, 94	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	338	TYR	4.3
1	D	342	PHE	4.1
1	B	202	LEU	4.0
1	B	292	LYS	3.9
1	B	201	VAL	3.8
1	B	253	TYR	3.8
1	C	306	VAL	3.7
1	B	319	ARG	3.5
1	G	253	TYR	3.5
1	G	200	ALA	3.4
1	B	286	THR	3.1
1	F	342	PHE	3.0
1	D	343	ASP	2.9
1	C	338	TYR	2.9
1	B	338	TYR	2.9
1	D	325	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	339	ILE	2.8
1	H	342	PHE	2.8
1	G	198	VAL	2.7
1	B	326	ASN	2.7
1	D	197	ASP	2.6
1	H	298	LEU	2.6
1	B	207	GLN	2.5
1	B	255	GLN	2.4
1	H	306	VAL	2.3
1	A	315[A]	GLN	2.3
1	B	206	ASN	2.3
1	D	338	TYR	2.3
1	H	338	TYR	2.3
1	B	306	VAL	2.2
1	B	257	GLU	2.2
1	B	205	TYR	2.2
1	B	198	VAL	2.2
1	G	201	VAL	2.2
1	D	319	ARG	2.1
1	H	340	ASP	2.1
1	D	201	VAL	2.1
1	B	213	MSE	2.1
1	D	341	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	C	602	1/1	0.11	0.12	27,27,27,27	0
2	CA	E	604	1/1	0.12	0.06	26,26,26,26	0
2	CA	D	603	1/1	0.10	-0.28	24,24,24,24	0
2	CA	H	607	1/1	0.12	-0.32	38,38,38,38	0
2	CA	F	605	1/1	0.10	-0.53	30,30,30,30	0
2	CA	A	600	1/1	0.10	-0.55	38,38,38,38	0
2	CA	B	601	1/1	0.08	-1.15	32,32,32,32	0
2	CA	G	606	1/1	0.07	-5.29	33,33,33,33	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.