Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:43 AM 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 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

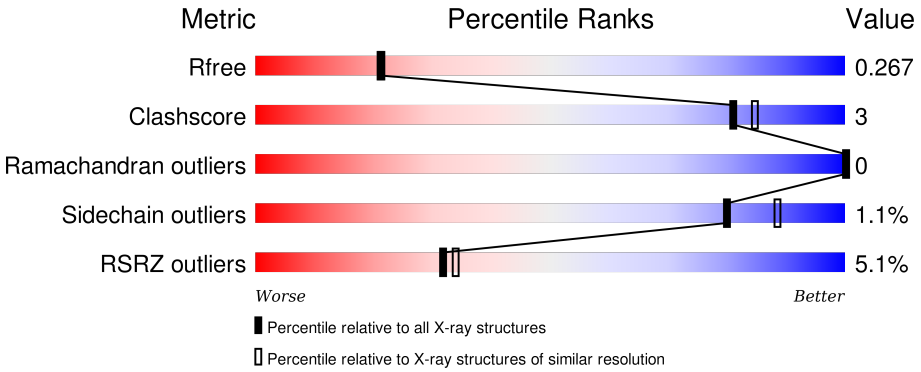
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.17 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}	91344	5130 (2.20-2.16)
Clashscore	102246	5965 (2.20-2.16)
Ramachandran outliers	100387	5863 (2.20-2.16)
Sidechain outliers	100360	5864 (2.20-2.16)
RSRZ outliers	91569	5142 (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 >=3, 2, 1 and 0 types of geometric quality criteria. 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	156	88% 7%
1	B	156	13% 90% 7%
1	C	156	3% 87% 7% 6%
1	D	156	8% 86% 7% 6%
1	E	156	85% 9% 5%

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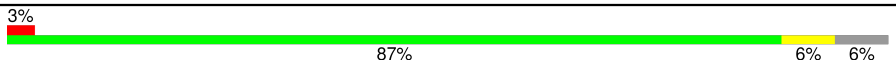
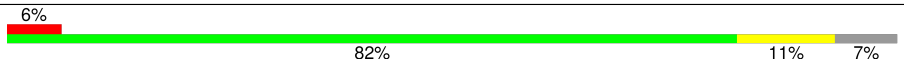
Mol	Chain	Length	Quality of chain
1	F	156	
1	G	156	
1	H	156	

2 Entry composition

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

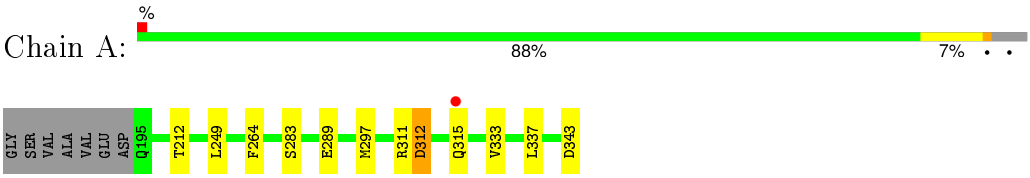
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	67	Total O 67 67	0	0
3	B	37	Total O 37 37	0	0
3	C	102	Total O 102 102	0	0
3	D	54	Total O 54 54	0	0
3	E	95	Total O 95 95	0	0
3	F	68	Total O 68 68	0	0
3	G	45	Total O 45 45	0	0
3	H	53	Total O 53 53	0	0

3 Residue-property plots (i)

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.

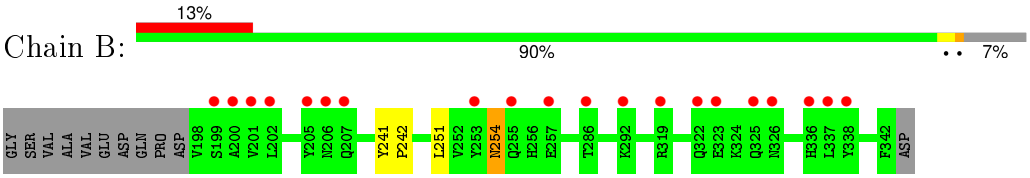
- Molecule 1: Transcription initiation factor TFIID subunit 5

Chain A:



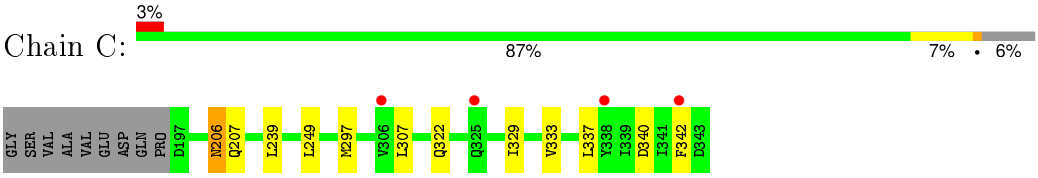
- Molecule 1: Transcription initiation factor TFIID subunit 5

Chain B:



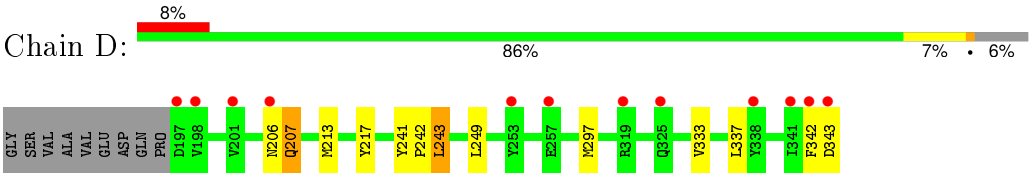
- Molecule 1: Transcription initiation factor TFIID subunit 5

Chain C:



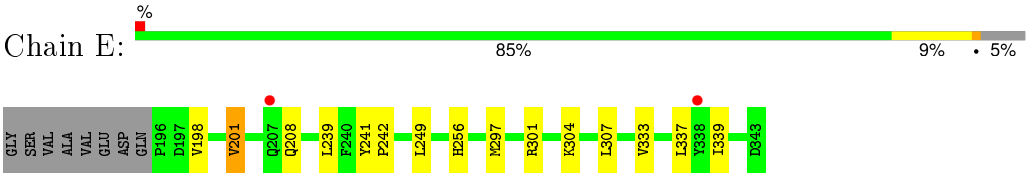
- Molecule 1: Transcription initiation factor TFIID subunit 5

Chain D:



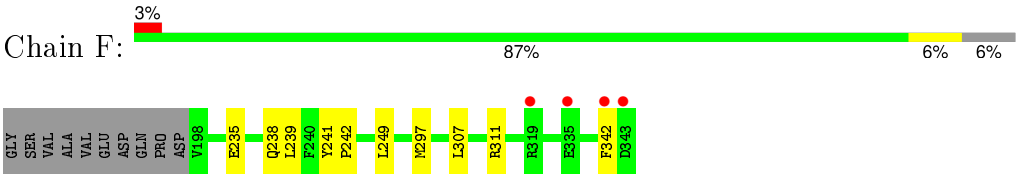
- Molecule 1: Transcription initiation factor TFIID subunit 5

Chain E:



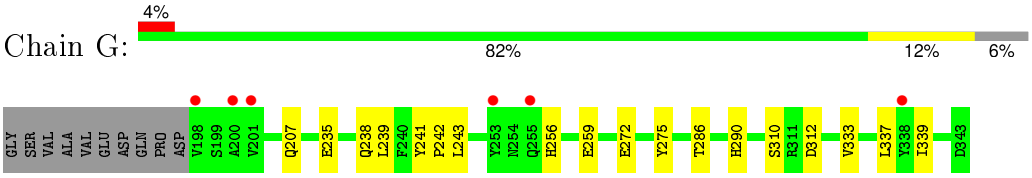
- Molecule 1: Transcription initiation factor TFIID subunit 5

Chain F:



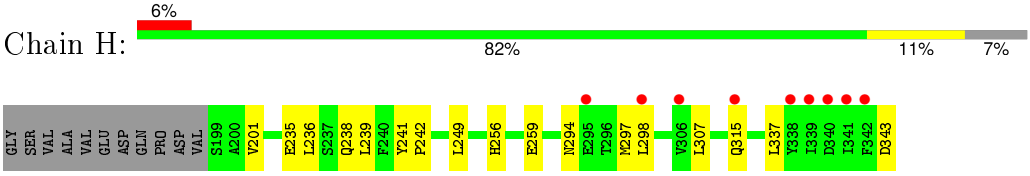
- Molecule 1: Transcription initiation factor TFIID subunit 5

Chain G:



- Molecule 1: Transcription initiation factor TFIID subunit 5

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	2.44 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.213 , 0.263 0.221 , 0.267	Depositor DCC
R_{free} test set	3837 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	27.2	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 76749 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10515	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1] Intensities estimated from amplitudes.

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

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 Too-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 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	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
1	E	1258	0	1192	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 3.

All (65) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:239:LEU:O	1:G:243:LEU:HB2	2.05	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 (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	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 (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	141/142 (99%)	139 (99%)	2 (1%)	74 84
1	B	137/142 (96%)	136 (99%)	1 (1%)	88 94
1	C	139/142 (98%)	137 (99%)	2 (1%)	74 84
1	D	139/142 (98%)	136 (98%)	3 (2%)	60 70
1	E	140/142 (99%)	138 (99%)	2 (1%)	74 84
1	F	138/142 (97%)	138 (100%)	0	100 100
1	G	138/142 (97%)	137 (99%)	1 (1%)	88 94
1	H	137/142 (96%)	136 (99%)	1 (1%)	88 94
All	All	1109/1136 (98%)	1097 (99%)	12 (1%)	80 88

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

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Mol	Chain	Res	Type
1	B	208	GLN
1	B	254	ASN
1	B	325	GLN
1	C	206	ASN
1	C	238	GLN
1	C	322	GLN
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 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 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.

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, 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	145/156 (92%)	0.23	1 (0%) 89 89	21, 36, 59, 77	0
1	B	141/156 (90%)	0.89	20 (14%) 4 4	26, 45, 68, 78	0
1	C	143/156 (91%)	0.35	4 (2%) 56 58	18, 30, 58, 69	0
1	D	143/156 (91%)	0.56	12 (8%) 14 15	21, 40, 69, 94	0
1	E	144/156 (92%)	0.28	2 (1%) 78 78	19, 30, 53, 74	0
1	F	142/156 (91%)	0.28	4 (2%) 56 58	22, 33, 54, 72	0
1	G	142/156 (91%)	0.57	6 (4%) 40 42	23, 41, 64, 73	0
1	H	141/156 (90%)	0.36	9 (6%) 23 25	21, 37, 61, 71	0
All	All	1141/1248 (91%)	0.44	58 (5%) 32 34	18, 37, 63, 94	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	306	VAL	5.6
1	D	342	PHE	5.1
1	B	253	TYR	4.9
1	G	338	TYR	4.7
1	C	338	TYR	4.6
1	B	292	LYS	4.5
1	F	342	PHE	4.4
1	B	319	ARG	4.2
1	G	253	TYR	4.1
1	D	338	TYR	4.0
1	D	343	ASP	3.7
1	B	202	LEU	3.7
1	B	338	TYR	3.5
1	B	205	TYR	3.4
1	B	255	GLN	3.3
1	B	207	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	200	ALA	3.3
1	B	201	VAL	3.2
1	B	286	THR	3.2
1	G	198	VAL	3.1
1	D	325	GLN	3.1
1	B	206	ASN	3.1
1	H	342	PHE	3.0
1	E	338	TYR	2.9
1	H	339	ILE	2.8
1	H	298	LEU	2.7
1	B	337	LEU	2.7
1	D	197	ASP	2.6
1	H	306	VAL	2.6
1	H	338	TYR	2.5
1	B	326	ASN	2.5
1	D	341	ILE	2.5
1	G	201	VAL	2.4
1	A	315[A]	GLN	2.3
1	H	315	GLN	2.3
1	B	200	ALA	2.3
1	C	342	PHE	2.3
1	B	323	GLU	2.3
1	H	295	GLU	2.3
1	D	319	ARG	2.2
1	B	336	HIS	2.2
1	D	206	ASN	2.2
1	F	319	ARG	2.1
1	G	255	GLN	2.1
1	H	341	ILE	2.1
1	B	199	SER	2.1
1	F	335	GLU	2.1
1	B	257	GLU	2.1
1	F	343	ASP	2.1
1	D	201	VAL	2.1
1	B	325	GLN	2.1
1	H	340	ASP	2.1
1	E	207	GLN	2.1
1	D	257	GLU	2.1
1	D	198	VAL	2.1
1	B	322	GLN	2.0
1	C	325	GLN	2.0
1	D	253	TYR	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. 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^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	CA	H	607	1/1	0.97	0.12	-0.26	38,38,38,38	0
2	CA	D	603	1/1	1.00	0.11	-0.42	24,24,24,24	0
2	CA	A	600	1/1	0.99	0.10	-0.55	38,38,38,38	0
2	CA	F	605	1/1	0.99	0.11	-0.74	30,30,30,30	0
2	CA	C	602	1/1	0.99	0.12	-	27,27,27,27	0
2	CA	E	604	1/1	0.99	0.14	-	26,26,26,26	0
2	CA	G	606	1/1	0.98	0.06	-	33,33,33,33	0
2	CA	B	601	1/1	1.00	0.08	-	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.