



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 11:26 AM JST

PDB ID : 7EQI
Title : ChlB3 [Acetyltransferase]
Authors : Saeed, A.U.; Zheng, J.
Deposited on : 2021-05-02
Resolution : 3.10 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

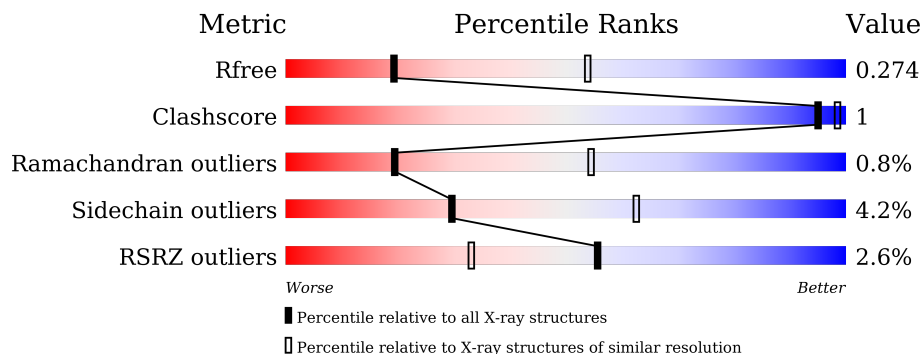
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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.



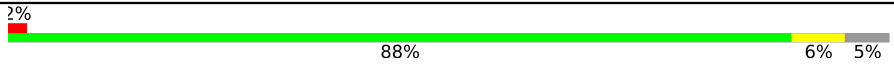
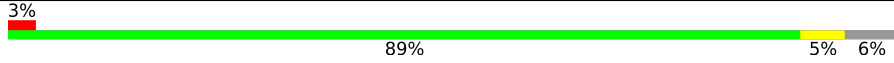
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	347	 92%
1	B	347	 90%
1	C	347	 91%
1	D	347	 87%
1	E	347	 88%
1	F	347	 88%

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Mol	Chain	Length	Quality of chain
1	G	347	 2% 88% 6% 5%
1	H	347	 3% 89% 5% 6%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 19137 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 ChlB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	Total 2371	C 1503	N 413	O 443	S 12	0	0	0
1	B	335	Total 2450	C 1550	N 429	O 458	S 13	0	0	0
1	C	333	Total 2412	C 1526	N 427	O 446	S 13	0	0	0
1	D	329	Total 2341	C 1487	N 407	O 434	S 13	0	0	0
1	E	332	Total 2324	C 1478	N 400	O 435	S 11	0	0	0
1	F	329	Total 2378	C 1508	N 415	O 443	S 12	0	0	0
1	G	328	Total 2384	C 1510	N 417	O 445	S 12	0	0	0
1	H	327	Total 2392	C 1515	N 419	O 446	S 12	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	11	Total 11	O 11	0	0
2	B	12	Total 12	O 12	0	0
2	C	14	Total 14	O 14	0	0
2	D	11	Total 11	O 11	0	0
2	E	10	Total 10	O 10	0	0
2	F	5	Total 5	O 5	0	0

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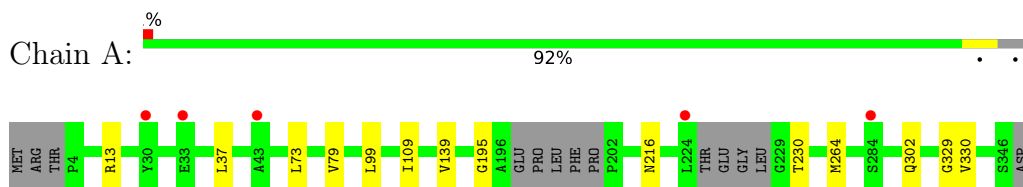
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	13	Total	O	0	0
			13	13		
2	H	9	Total	O	0	0
			9	9		

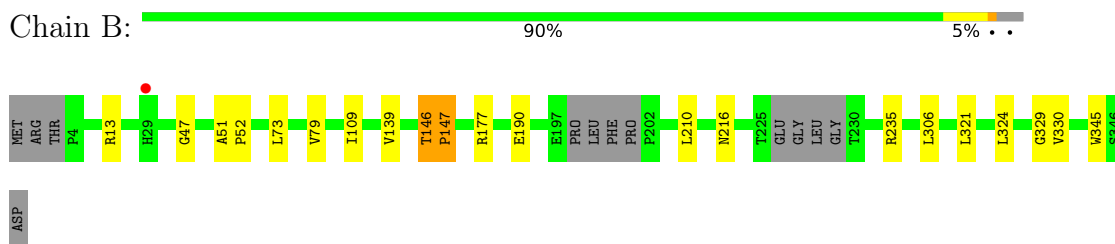
3 Residue-property plots [i](#)

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.

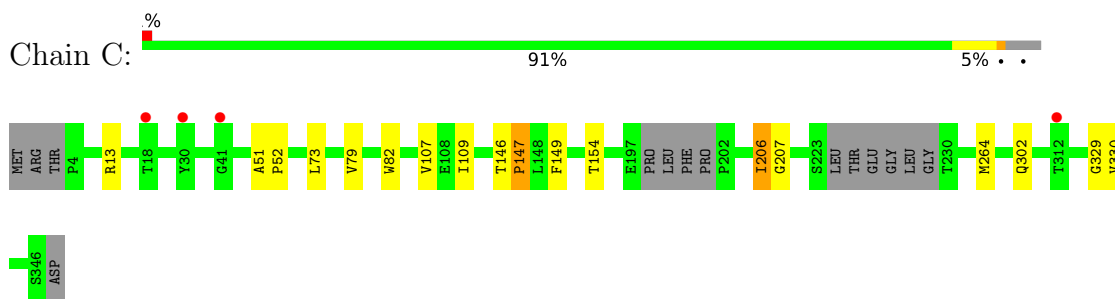
- Molecule 1: ChlB3



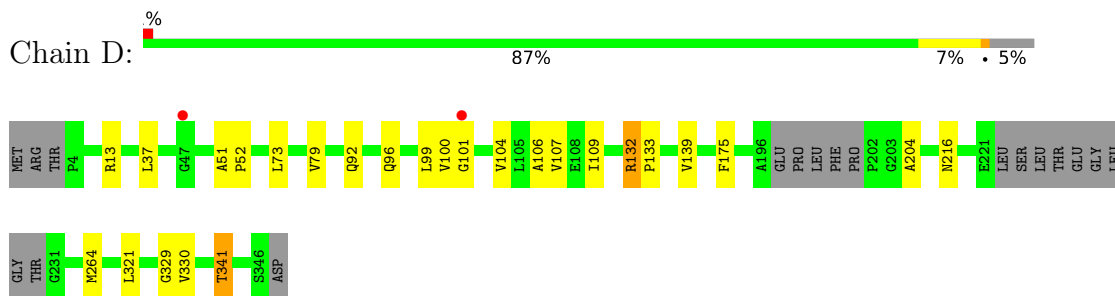
- Molecule 1: ChlB3



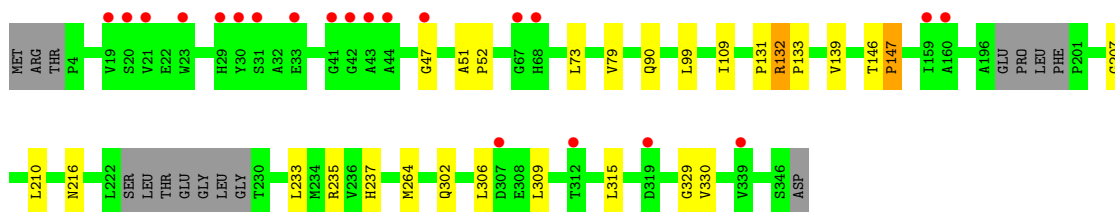
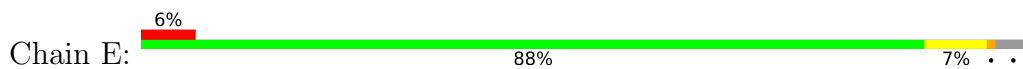
- Molecule 1: ChlB3



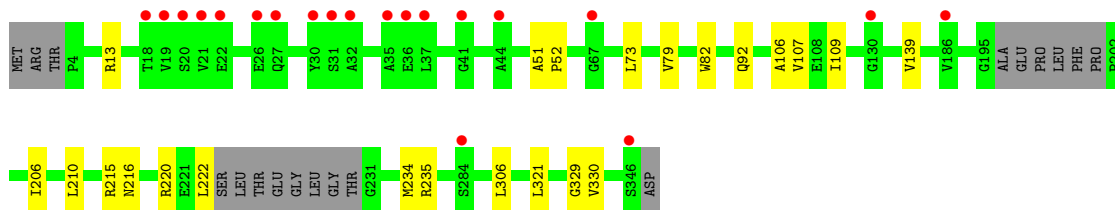
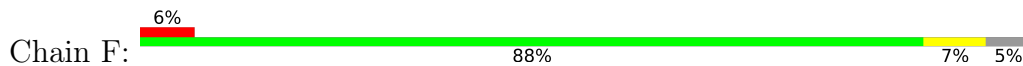
- Molecule 1: ChlB3



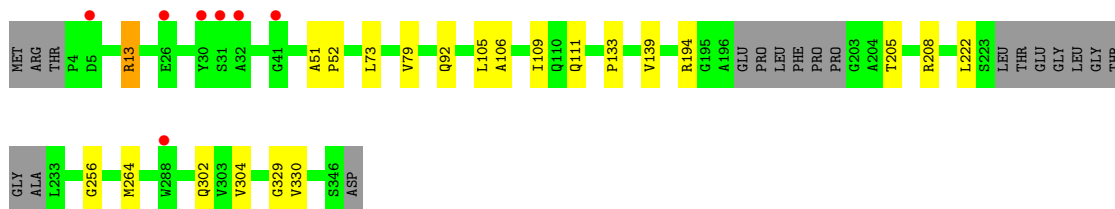
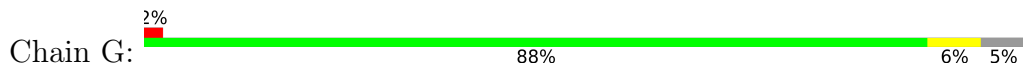
- Molecule 1: ChlB3



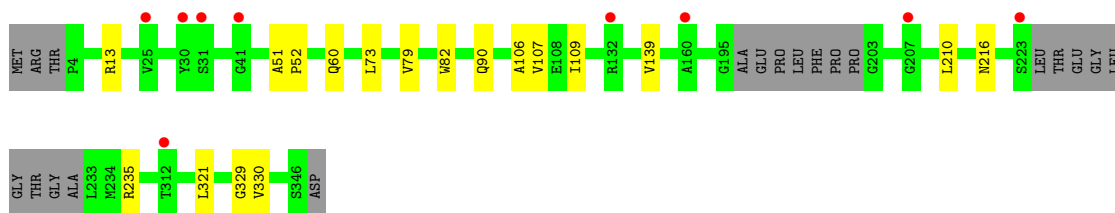
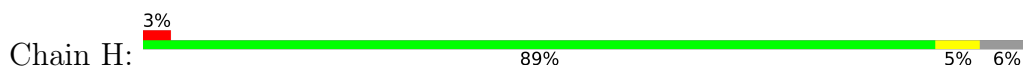
- Molecule 1: ChlB3



- Molecule 1: ChlB3



- Molecule 1: ChlB3



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.47Å 186.58Å 189.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 49.74 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-3.10) 99.4 (49.74-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.91Å)	Xtrriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.226 , 0.256 0.261 , 0.274	Depositor DCC
R_{free} test set	3931 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	70.4	Xtrriage
Anisotropy	0.086	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.007 for -h,l,k	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	19137	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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	0.25	0/2428	0.40	0/3324
1	B	0.25	0/2507	0.42	0/3420
1	C	0.25	0/2469	0.42	0/3371
1	D	0.25	0/2398	0.40	0/3282
1	E	0.25	0/2381	0.40	0/3267
1	F	0.25	0/2435	0.42	0/3328
1	G	0.25	0/2440	0.42	0/3332
1	H	0.25	0/2448	0.42	0/3341
All	All	0.25	0/19506	0.41	0/26665

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	2371	0	2215	3	0
1	B	2450	0	2361	5	0
1	C	2412	0	2299	6	0
1	D	2341	0	2201	10	0
1	E	2324	0	2157	8	0
1	F	2378	0	2257	4	0
1	G	2384	0	2274	7	0
1	H	2392	0	2293	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	11	0	0	0	0
2	B	12	0	0	0	0
2	C	14	0	0	0	0
2	D	11	0	0	0	0
2	E	10	0	0	0	0
2	F	5	0	0	0	0
2	G	13	0	0	0	0
2	H	9	0	0	0	0
All	All	19137	0	18057	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 1.

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:D:132:ARG:CB	1:D:133:PRO:CD	2.66	0.74
1:D:132:ARG:CB	1:D:133:PRO:HD2	2.26	0.66
1:B:146:THR:HB	1:B:147:PRO:HA	1.80	0.64
1:A:329:GLY:N	1:A:330:VAL:HA	2.22	0.55
1:E:132:ARG:CB	1:E:133:PRO:CD	2.86	0.53
1:C:329:GLY:N	1:C:330:VAL:HA	2.25	0.51
1:E:329:GLY:N	1:E:330:VAL:HA	2.25	0.51
1:B:329:GLY:N	1:B:330:VAL:HA	2.26	0.50
1:D:100:VAL:HG12	1:D:104:VAL:HG11	1.94	0.50
1:F:329:GLY:N	1:F:330:VAL:HA	2.26	0.50
1:D:79:VAL:HG12	1:D:109:ILE:HB	1.94	0.49
1:G:329:GLY:N	1:G:330:VAL:HA	2.27	0.49
1:D:329:GLY:N	1:D:330:VAL:HA	2.28	0.49
1:H:329:GLY:N	1:H:330:VAL:HA	2.26	0.49
1:F:79:VAL:HG12	1:F:109:ILE:HB	1.95	0.48
1:A:79:VAL:HG12	1:A:109:ILE:HB	1.94	0.48
1:G:13:ARG:HG3	1:G:304:VAL:HG23	1.96	0.48
1:C:79:VAL:HG12	1:C:109:ILE:HB	1.96	0.48
1:B:79:VAL:HG12	1:B:109:ILE:HB	1.95	0.47
1:E:233:LEU:O	1:E:237:HIS:ND1	2.46	0.47
1:H:79:VAL:HG12	1:H:109:ILE:HB	1.95	0.47
1:E:79:VAL:HG12	1:E:109:ILE:HB	1.96	0.47
1:G:79:VAL:HG12	1:G:109:ILE:HB	1.96	0.46
1:C:146:THR:N	1:C:147:PRO:HD3	2.31	0.46
1:D:96:GLN:HG2	1:D:101:GLY:HA2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:VAL:HG12	1:D:100:VAL:O	2.17	0.45
1:E:132:ARG:CB	1:E:133:PRO:HD2	2.48	0.44
1:A:230:THR:HG22	1:G:256:GLY:HA2	2.00	0.44
1:E:146:THR:N	1:E:147:PRO:HD3	2.32	0.44
1:B:146:THR:HB	1:B:147:PRO:CA	2.48	0.43
1:E:309:LEU:HB3	1:E:315:LEU:HD23	2.00	0.43
1:C:206:ILE:HA	1:C:207:GLY:HA2	1.76	0.42
1:F:92:GLN:HG3	1:F:106:ALA:HB1	2.02	0.42
1:E:51:ALA:N	1:E:52:PRO:CD	2.83	0.41
1:D:51:ALA:N	1:D:52:PRO:CD	2.84	0.41
1:C:149:PHE:CE2	1:C:154:THR:HG21	2.56	0.41
1:G:111:GLN:NE2	1:H:106:ALA:O	2.52	0.41
1:C:51:ALA:N	1:C:52:PRO:CD	2.84	0.41
1:G:51:ALA:N	1:G:52:PRO:CD	2.84	0.41
1:B:51:ALA:N	1:B:52:PRO:CD	2.84	0.41
1:D:92:GLN:HG3	1:D:106:ALA:HB1	2.03	0.41
1:F:51:ALA:N	1:F:52:PRO:CD	2.84	0.40
1:G:92:GLN:HG3	1:G:106:ALA:HB1	2.03	0.40
1:D:175:PHE:HA	1:D:341:THR:HG22	2.03	0.40
1:H:51:ALA:N	1:H:52:PRO:CD	2.84	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	328/347 (94%)	303 (92%)	23 (7%)	2 (1%)	25 59
1	B	329/347 (95%)	306 (93%)	20 (6%)	3 (1%)	17 52
1	C	327/347 (94%)	302 (92%)	24 (7%)	1 (0%)	41 73
1	D	323/347 (93%)	300 (93%)	20 (6%)	3 (1%)	17 52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	326/347 (94%)	303 (93%)	17 (5%)	6 (2%)	8	34
1	F	323/347 (93%)	301 (93%)	20 (6%)	2 (1%)	25	59
1	G	322/347 (93%)	298 (92%)	21 (6%)	3 (1%)	17	52
1	H	321/347 (92%)	308 (96%)	13 (4%)	0	100	100
All	All	2599/2776 (94%)	2421 (93%)	158 (6%)	20 (1%)	19	54

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	132	ARG
1	E	132	ARG
1	E	147	PRO
1	E	207	GLY
1	F	206	ILE
1	D	204	ALA
1	F	220	ARG
1	G	133	PRO
1	B	146	THR
1	G	205	THR
1	C	147	PRO
1	D	99	LEU
1	E	99	LEU
1	G	194	ARG
1	A	99	LEU
1	E	131	PRO
1	A	195	GLY
1	B	47	GLY
1	E	47	GLY
1	B	147	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	221/265 (83%)	214 (97%)	7 (3%)	39	69
1	B	241/265 (91%)	229 (95%)	12 (5%)	24	57
1	C	231/265 (87%)	224 (97%)	7 (3%)	41	71
1	D	220/265 (83%)	211 (96%)	9 (4%)	30	64
1	E	214/265 (81%)	205 (96%)	9 (4%)	30	62
1	F	228/265 (86%)	215 (94%)	13 (6%)	20	52
1	G	231/265 (87%)	223 (96%)	8 (4%)	36	68
1	H	234/265 (88%)	223 (95%)	11 (5%)	26	59
All	All	1820/2120 (86%)	1744 (96%)	76 (4%)	30	62

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	37	LEU
1	A	73	LEU
1	A	139	VAL
1	A	216	ASN
1	A	264	MET
1	A	302	GLN
1	B	13	ARG
1	B	73	LEU
1	B	139	VAL
1	B	177	ARG
1	B	190	GLU
1	B	210	LEU
1	B	216	ASN
1	B	235	ARG
1	B	306	LEU
1	B	321	LEU
1	B	324	LEU
1	B	345	TRP
1	C	13	ARG
1	C	73	LEU
1	C	82	TRP
1	C	107	VAL
1	C	206	ILE
1	C	264	MET
1	C	302	GLN
1	D	13	ARG

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Mol	Chain	Res	Type
1	D	37	LEU
1	D	73	LEU
1	D	107	VAL
1	D	139	VAL
1	D	216	ASN
1	D	264	MET
1	D	321	LEU
1	D	341	THR
1	E	73	LEU
1	E	90	GLN
1	E	139	VAL
1	E	210	LEU
1	E	216	ASN
1	E	235	ARG
1	E	264	MET
1	E	302	GLN
1	E	306	LEU
1	F	13	ARG
1	F	73	LEU
1	F	82	TRP
1	F	107	VAL
1	F	139	VAL
1	F	210	LEU
1	F	215	ARG
1	F	216	ASN
1	F	222	LEU
1	F	234	MET
1	F	235	ARG
1	F	306	LEU
1	F	321	LEU
1	G	13	ARG
1	G	73	LEU
1	G	105	LEU
1	G	139	VAL
1	G	208	ARG
1	G	222	LEU
1	G	264	MET
1	G	302	GLN
1	H	13	ARG
1	H	60	GLN
1	H	73	LEU
1	H	82	TRP

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Mol	Chain	Res	Type
1	H	90	GLN
1	H	107	VAL
1	H	139	VAL
1	H	210	LEU
1	H	216	ASN
1	H	235	ARG
1	H	321	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	B	191	GLN
1	C	273	GLN
1	E	90	GLN
1	E	191	GLN
1	G	191	GLN
1	H	90	GLN
1	H	216	ASN

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 monosaccharides 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

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	334/347 (96%)	0.04	5 (1%) 73 54	44, 63, 94, 129	0
1	B	335/347 (96%)	0.01	1 (0%) 94 88	40, 55, 83, 106	0
1	C	333/347 (95%)	-0.06	4 (1%) 79 61	40, 56, 84, 109	0
1	D	329/347 (94%)	-0.07	2 (0%) 89 78	40, 54, 82, 102	0
1	E	332/347 (95%)	0.39	21 (6%) 20 8	50, 76, 100, 138	0
1	F	329/347 (94%)	0.27	20 (6%) 21 9	49, 72, 100, 129	0
1	G	328/347 (94%)	0.13	7 (2%) 63 43	45, 69, 103, 133	0
1	H	327/347 (94%)	0.17	9 (2%) 53 30	42, 65, 92, 136	0
All	All	2647/2776 (95%)	0.11	69 (2%) 56 33	40, 64, 95, 138	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	41	GLY	8.9
1	F	31	SER	5.1
1	E	43	ALA	4.9
1	E	42	GLY	4.5
1	E	30	TYR	4.4
1	H	223	SER	4.4
1	A	224	LEU	3.8
1	E	31	SER	3.5
1	F	30	TYR	3.4
1	F	32	ALA	3.3
1	E	29	HIS	3.2
1	F	36	GLU	3.1
1	C	312	THR	3.1
1	F	35	ALA	3.0
1	H	30	TYR	3.0
1	E	68	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	20	SER	3.0
1	G	31	SER	2.9
1	G	26	GLU	2.9
1	D	101	GLY	2.9
1	G	41	GLY	2.9
1	E	19	VAL	2.9
1	G	30	TYR	2.8
1	E	319	ASP	2.7
1	G	5	ASP	2.7
1	H	41	GLY	2.7
1	H	160	ALA	2.7
1	H	312	THR	2.6
1	E	67	GLY	2.6
1	G	288	TRP	2.6
1	F	186	VAL	2.6
1	H	207	GLY	2.6
1	E	23	TRP	2.5
1	B	29	HIS	2.5
1	F	22	GLU	2.5
1	C	18	THR	2.5
1	F	27	GLN	2.5
1	F	44	ALA	2.5
1	E	160	ALA	2.4
1	A	284	SER	2.3
1	E	307	ASP	2.3
1	F	41	GLY	2.3
1	F	18	THR	2.3
1	F	37	LEU	2.3
1	F	346	SER	2.3
1	F	19	VAL	2.3
1	G	32	ALA	2.3
1	E	47	GLY	2.2
1	E	44	ALA	2.2
1	E	21	VAL	2.2
1	E	20	SER	2.2
1	A	33	GLU	2.2
1	H	31	SER	2.2
1	F	130	GLY	2.1
1	C	30	TYR	2.1
1	E	159	ILE	2.1
1	H	132	ARG	2.1
1	F	26	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	33	GLU	2.1
1	E	312	THR	2.1
1	F	21	VAL	2.1
1	D	47	GLY	2.1
1	A	30	TYR	2.0
1	E	339	VAL	2.0
1	F	284	SER	2.0
1	H	25	VAL	2.0
1	F	67	GLY	2.0
1	A	43	ALA	2.0
1	C	41	GLY	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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.