Full wwPDB X-ray Structure Validation Report (i)

Feb 2, 2017 – 06:11 PM EST

PDB ID	:	5J5U
Title	:	Fjoh_4561 chitin-binding protein
Authors	:	Koropatkin, N.M.
Deposited on	:	2016-04-03
Resolution	:	2.30 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:

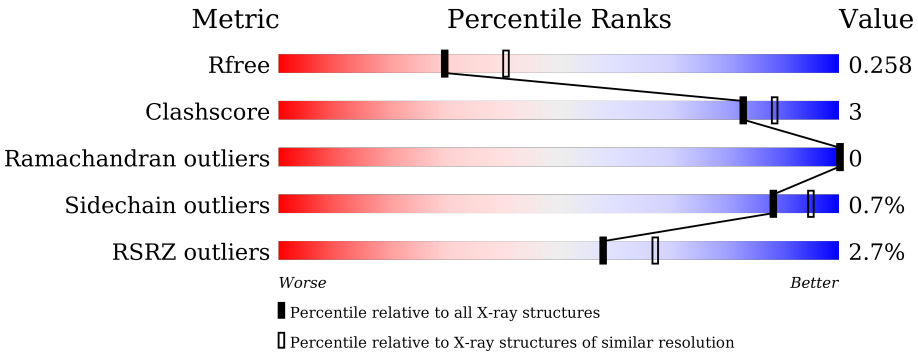
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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. 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	484	2% 86% 7% 7%
1	B	484	2% 86% 7% 7%
1	C	484	4% 87% 6% 7%
1	D	484	2% 86% 6% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14777 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 RagB/SusD domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	0	0	0
			3536	2240	603	680	13			
1	B	452	Total	C	N	O	S	0	0	0
			3544	2246	604	681	13			
1	C	451	Total	C	N	O	S	0	0	0
			3533	2237	603	680	13			
1	D	452	Total	C	N	O	S	0	0	0
			3544	2246	604	681	13			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	HIS	-	expression tag	UNP A5FB55
A	23	HIS	-	expression tag	UNP A5FB55
A	24	HIS	-	expression tag	UNP A5FB55
A	25	HIS	-	expression tag	UNP A5FB55
A	26	HIS	-	expression tag	UNP A5FB55
A	27	HIS	-	expression tag	UNP A5FB55
A	28	GLU	-	expression tag	UNP A5FB55
A	29	ASN	-	expression tag	UNP A5FB55
A	30	LEU	-	expression tag	UNP A5FB55
A	31	TYR	-	expression tag	UNP A5FB55
A	32	PHE	-	expression tag	UNP A5FB55
A	33	GLN	-	expression tag	UNP A5FB55
A	34	GLY	-	expression tag	UNP A5FB55
B	22	HIS	-	expression tag	UNP A5FB55
B	23	HIS	-	expression tag	UNP A5FB55
B	24	HIS	-	expression tag	UNP A5FB55
B	25	HIS	-	expression tag	UNP A5FB55
B	26	HIS	-	expression tag	UNP A5FB55
B	27	HIS	-	expression tag	UNP A5FB55
B	28	GLU	-	expression tag	UNP A5FB55
B	29	ASN	-	expression tag	UNP A5FB55

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Chain	Residue	Modelled	Actual	Comment	Reference
B	30	LEU	-	expression tag	UNP A5FB55
B	31	TYR	-	expression tag	UNP A5FB55
B	32	PHE	-	expression tag	UNP A5FB55
B	33	GLN	-	expression tag	UNP A5FB55
B	34	GLY	-	expression tag	UNP A5FB55
C	22	HIS	-	expression tag	UNP A5FB55
C	23	HIS	-	expression tag	UNP A5FB55
C	24	HIS	-	expression tag	UNP A5FB55
C	25	HIS	-	expression tag	UNP A5FB55
C	26	HIS	-	expression tag	UNP A5FB55
C	27	HIS	-	expression tag	UNP A5FB55
C	28	GLU	-	expression tag	UNP A5FB55
C	29	ASN	-	expression tag	UNP A5FB55
C	30	LEU	-	expression tag	UNP A5FB55
C	31	TYR	-	expression tag	UNP A5FB55
C	32	PHE	-	expression tag	UNP A5FB55
C	33	GLN	-	expression tag	UNP A5FB55
C	34	GLY	-	expression tag	UNP A5FB55
D	22	HIS	-	expression tag	UNP A5FB55
D	23	HIS	-	expression tag	UNP A5FB55
D	24	HIS	-	expression tag	UNP A5FB55
D	25	HIS	-	expression tag	UNP A5FB55
D	26	HIS	-	expression tag	UNP A5FB55
D	27	HIS	-	expression tag	UNP A5FB55
D	28	GLU	-	expression tag	UNP A5FB55
D	29	ASN	-	expression tag	UNP A5FB55
D	30	LEU	-	expression tag	UNP A5FB55
D	31	TYR	-	expression tag	UNP A5FB55
D	32	PHE	-	expression tag	UNP A5FB55
D	33	GLN	-	expression tag	UNP A5FB55
D	34	GLY	-	expression tag	UNP A5FB55

- Molecule 2 is water.

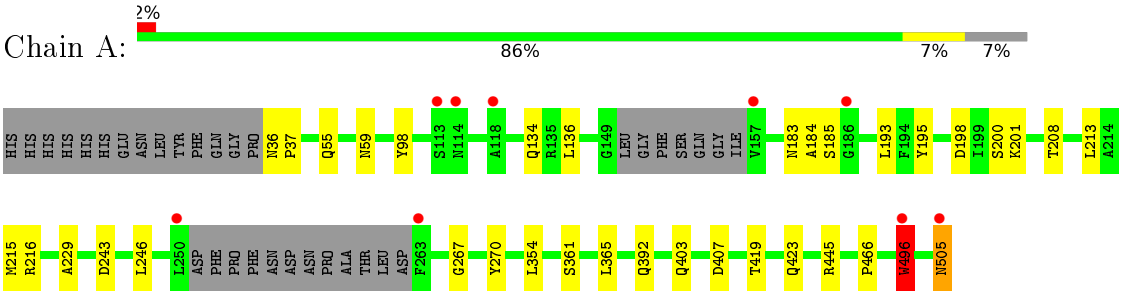
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	163	Total 163	O 163	0	0
2	B	184	Total 184	O 184	0	0
2	C	134	Total 134	O 134	0	0
2	D	139	Total 139	O 139	0	0

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.

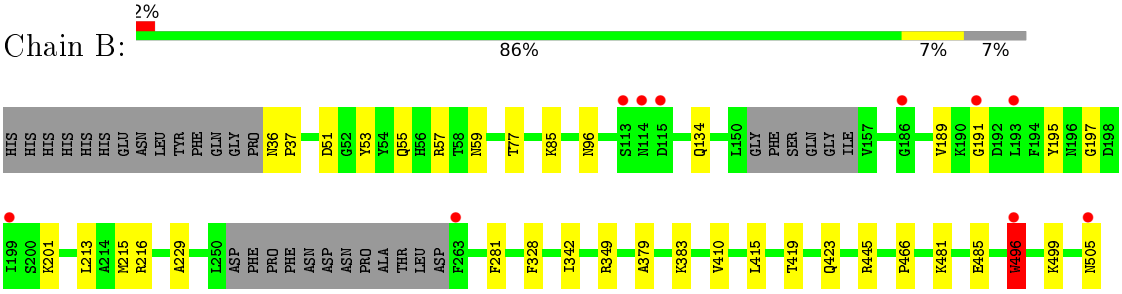
- Molecule 1: RagB/SusD domain protein

Chain A:



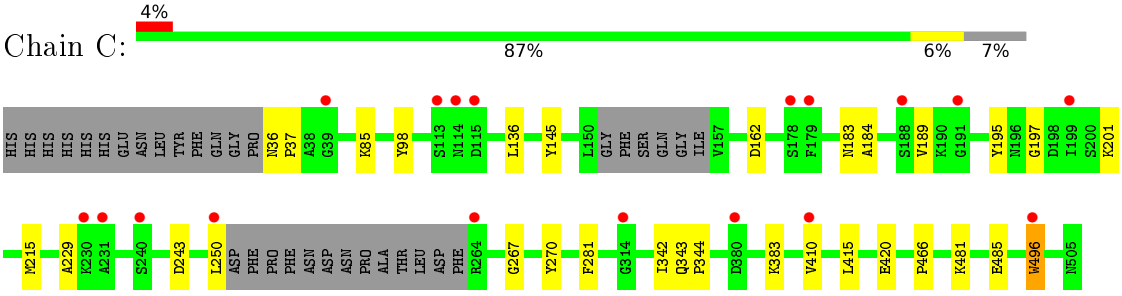
- Molecule 1: RagB/SusD domain protein

Chain B:



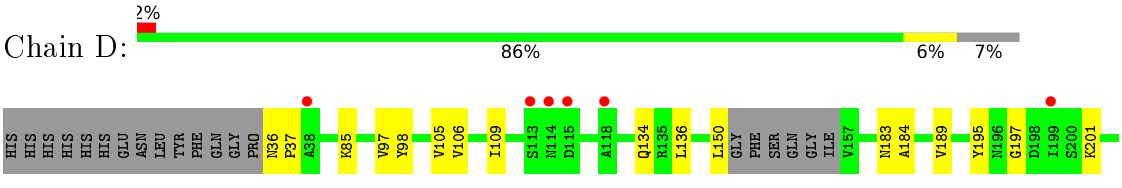
- Molecule 1: RagB/SusD domain protein

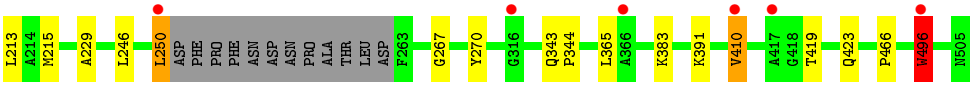
Chain C:



- Molecule 1: RagB/SusD domain protein

Chain D:




L213
A214
M215
A229
L246
L250
ASP
PHE
PRO
PHE
ASN
ASP
ASN
PRO
ALA
THR
LEU
ASP
F263
G267
Y270
G316
Q343
P344
L365
A366
K383
K391
V410
A417
G418
T419
Q423
P466
W496
N505

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	82.71Å 82.89Å 93.91Å 66.44° 78.33° 67.56°	Depositor
Resolution (Å)	44.49 – 2.30 85.93 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.8 (44.49-2.30) 82.7 (85.93-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.28 (at 2.29Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.214 , 0.263 0.211 , 0.258	Depositor DCC
R_{free} test set	1979 reflections (2.20%)	DCC
Wilson B-factor (Å^2)	21.2	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	14777	wwPDB-VP
Average B, all atoms (Å^2)	26.0	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 22.30 % 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 5.8599e-03. 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.49	0/3622	0.58	1/4909 (0.0%)
1	B	0.48	0/3630	0.58	1/4920 (0.0%)
1	C	0.47	0/3618	0.57	0/4904
1	D	0.47	0/3630	0.59	2/4920 (0.0%)
All	All	0.48	0/14500	0.58	4/19653 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	496	TRP	CA-CB-CG	6.42	125.90	113.70
1	A	496	TRP	CA-CB-CG	6.25	125.58	113.70
1	D	496	TRP	CA-CB-CG	5.81	124.73	113.70
1	D	246	LEU	CA-CB-CG	5.20	127.25	115.30

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	3536	0	3397	24	0
1	B	3544	0	3408	24	0
1	C	3533	0	3399	20	0
1	D	3544	0	3408	20	0
2	A	163	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	184	0	0	1	0
2	C	134	0	0	0	0
2	D	139	0	0	0	0
All	All	14777	0	13612	86	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 (86) 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:505:ASN:HD22	1:A:505:ASN:H	1.21	0.88
1:A:505:ASN:N	1:A:505:ASN:HD22	1.78	0.81
1:B:383:LYS:NZ	1:B:415:LEU:H	1.86	0.72
1:B:383:LYS:HG3	1:B:410:VAL:HG13	1.72	0.71
1:C:466:PRO:HB3	1:C:496:TRP:HD1	1.59	0.67
1:A:505:ASN:N	1:A:505:ASN:ND2	2.46	0.63
1:D:383:LYS:HE3	1:D:410:VAL:HG13	1.80	0.63
1:D:183:ASN:OD1	1:D:184:ALA:N	2.31	0.62
1:C:466:PRO:HB3	1:C:496:TRP:CD1	2.34	0.61
1:A:201:LYS:NZ	1:A:243:ASP:OD1	2.35	0.59
1:C:195:TYR:CD2	1:C:201:LYS:HD3	2.36	0.59
1:B:134:GLN:HG3	1:B:213:LEU:HD21	1.85	0.59
1:C:189:VAL:HB	1:C:197:GLY:HA2	1.84	0.59
1:C:85:LYS:HD3	1:C:496:TRP:CE3	2.38	0.59
1:D:419:THR:OG1	1:D:423:GLN:OE1	2.19	0.58
1:A:183:ASN:OD1	1:A:184:ALA:N	2.36	0.58
1:B:379:ALA:O	1:B:383:LYS:HD3	2.04	0.57
1:A:419:THR:OG1	1:A:423:GLN:OE1	2.22	0.57
1:B:383:LYS:HZ2	1:B:415:LEU:H	1.52	0.57
1:C:201:LYS:NZ	1:C:243:ASP:OD1	2.38	0.56
1:A:195:TYR:CD2	1:A:201:LYS:HD3	2.41	0.55
1:D:466:PRO:HB3	1:D:496:TRP:CD1	2.41	0.55
1:B:195:TYR:CD2	1:B:201:LYS:HD3	2.41	0.55
1:B:419:THR:OG1	1:B:423:GLN:OE1	2.23	0.54
1:A:98:TYR:CZ	1:A:136:LEU:HD21	2.42	0.54
1:D:383:LYS:HG3	1:D:410:VAL:HG13	1.90	0.54
1:D:195:TYR:CD2	1:D:201:LYS:HD3	2.42	0.54
1:A:134:GLN:HG3	1:A:213:LEU:HD21	1.90	0.53
1:C:183:ASN:OD1	1:C:184:ALA:N	2.43	0.51
1:A:215:MET:CE	1:A:229:ALA:HB2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:MET:CE	1:B:229:ALA:HB2	2.41	0.51
1:D:466:PRO:HB3	1:D:496:TRP:HD1	1.75	0.50
1:A:215:MET:HE1	1:A:229:ALA:HB2	1.93	0.50
1:D:134:GLN:HG3	1:D:213:LEU:HD21	1.94	0.50
1:B:191:GLY:HA2	1:D:250:LEU:HD11	1.93	0.50
1:C:98:TYR:CZ	1:C:136:LEU:HD21	2.48	0.49
1:B:215:MET:HE1	1:B:229:ALA:HB2	1.95	0.49
1:B:466:PRO:HB3	1:B:496:TRP:CD1	2.47	0.48
1:C:267:GLY:O	1:C:270:TYR:HB3	2.13	0.48
1:C:383:LYS:HG2	1:C:410:VAL:HG13	1.95	0.48
1:B:36:ASN:HB2	1:B:37:PRO:HD3	1.95	0.48
1:B:481:LYS:NZ	1:B:485:GLU:OE2	2.44	0.48
1:C:481:LYS:NZ	1:C:485:GLU:OE2	2.47	0.48
1:D:85:LYS:HD3	1:D:496:TRP:CE3	2.48	0.48
1:B:383:LYS:HZ1	1:B:415:LEU:H	1.61	0.47
1:C:281:PHE:CE2	1:C:342:ILE:HG12	2.49	0.46
1:D:215:MET:CE	1:D:229:ALA:HB2	2.45	0.46
1:B:189:VAL:HB	1:B:197:GLY:HA2	1.96	0.46
1:C:215:MET:CE	1:C:229:ALA:HB2	2.45	0.46
1:A:198:ASP:OD1	1:A:200:SER:OG	2.32	0.46
1:D:189:VAL:HB	1:D:197:GLY:HA2	1.96	0.46
1:D:106:VAL:HG11	1:D:150:LEU:HD23	1.97	0.46
1:B:216:ARG:HA	1:B:445:ARG:HD3	1.98	0.46
1:C:145:TYR:HB3	1:C:162:ASP:OD2	2.15	0.46
1:D:36:ASN:HB2	1:D:37:PRO:HD3	1.97	0.45
1:B:499:LYS:NZ	1:B:505:ASN:HD22	2.14	0.45
1:B:85:LYS:HD3	1:B:496:TRP:CE3	2.52	0.45
1:D:98:TYR:CZ	1:D:136:LEU:HD21	2.50	0.45
1:A:403:GLN:NE2	1:A:407:ASP:OD1	2.47	0.45
1:A:466:PRO:HB3	1:A:496:TRP:CD1	2.52	0.45
1:D:267:GLY:O	1:D:270:TYR:HB3	2.17	0.44
1:C:343:GLN:HA	1:C:344:PRO:HD3	1.81	0.44
1:D:343:GLN:HA	1:D:344:PRO:HD3	1.86	0.44
1:D:365:LEU:HD23	1:D:365:LEU:HA	1.86	0.44
1:D:97:VAL:HG11	1:D:136:LEU:HD22	1.99	0.44
1:C:36:ASN:HB2	1:C:37:PRO:HD3	1.99	0.43
1:A:55:GLN:O	1:A:59:ASN:HB3	2.19	0.43
1:B:51:ASP:OD2	1:B:96:ASN:ND2	2.41	0.43
1:A:208:THR:HG23	1:A:361:SER:HB3	2.00	0.43
1:B:53:TYR:O	1:B:57:ARG:HD2	2.19	0.43
1:B:77:THR:HB	1:B:328:PHE:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:LYS:HZ2	1:A:243:ASP:HA	1.83	0.43
1:B:55:GLN:O	1:B:59:ASN:HB3	2.18	0.42
1:A:193:LEU:HD21	1:C:250:LEU:HD22	2.01	0.42
1:A:267:GLY:O	1:A:270:TYR:HB3	2.18	0.42
1:A:36:ASN:HB2	1:A:37:PRO:HD3	1.99	0.42
1:A:216:ARG:HA	1:A:445:ARG:HD3	2.00	0.42
1:A:246:LEU:HD13	1:A:354:LEU:HA	2.00	0.42
1:C:415:LEU:HG	1:C:420:GLU:HG3	2.02	0.42
1:A:365:LEU:HD23	1:A:365:LEU:HA	1.89	0.42
1:B:191:GLY:N	2:B:626:HOH:O	2.52	0.41
1:C:215:MET:HE1	1:C:229:ALA:HB2	2.01	0.41
1:B:281:PHE:CE2	1:B:342:ILE:HG12	2.55	0.41
1:C:85:LYS:HD3	1:C:496:TRP:CD2	2.55	0.41
1:A:392:GLN:NE2	2:A:609:HOH:O	2.36	0.40
1:D:105:VAL:O	1:D:109:ILE:HG13	2.22	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	445/484 (92%)	431 (97%)	14 (3%)	0	100	100
1	B	446/484 (92%)	433 (97%)	13 (3%)	0	100	100
1	C	445/484 (92%)	431 (97%)	14 (3%)	0	100	100
1	D	446/484 (92%)	433 (97%)	13 (3%)	0	100	100
All	All	1782/1936 (92%)	1728 (97%)	54 (3%)	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	370/399 (93%)	367 (99%)	3 (1%)	86	94
1	B	371/399 (93%)	369 (100%)	2 (0%)	92	97
1	C	370/399 (93%)	369 (100%)	1 (0%)	94	98
1	D	371/399 (93%)	367 (99%)	4 (1%)	80	90
All	All	1482/1596 (93%)	1472 (99%)	10 (1%)	88	95

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	SER
1	A	496	TRP
1	A	505	ASN
1	B	349	ARG
1	B	496	TRP
1	C	496	TRP
1	D	250	LEU
1	D	391	LYS
1	D	410	VAL
1	D	496	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	505	ASN
1	B	505	ASN

5.3.3 RNA (i)

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

There are no ligands in this entry.

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	451/484 (93%)	0.14	9 (1%) 68 75	9, 23, 40, 59	0
1	B	452/484 (93%)	0.23	10 (2%) 65 73	9, 23, 43, 57	0
1	C	451/484 (93%)	0.36	18 (3%) 42 51	9, 28, 51, 63	0
1	D	452/484 (93%)	0.29	12 (2%) 58 67	9, 26, 48, 60	0
All	All	1806/1936 (93%)	0.25	49 (2%) 58 67	9, 24, 47, 63	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	186	GLY	4.4
1	C	496	TRP	4.0
1	A	113	SER	3.9
1	D	496	TRP	3.6
1	C	115	ASP	3.5
1	D	114	ASN	3.4
1	B	496	TRP	3.2
1	C	264	ARG	3.2
1	A	496	TRP	3.2
1	C	114	ASN	3.2
1	A	114	ASN	3.0
1	C	39	GLY	3.0
1	D	410	VAL	3.0
1	A	157	VAL	2.9
1	C	231	ALA	2.9
1	A	186	GLY	2.9
1	C	199	ILE	2.9
1	D	250	LEU	2.8
1	C	188	SER	2.8
1	D	113	SER	2.8
1	C	380	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	178	SER	2.7
1	D	38	ALA	2.7
1	C	314	GLY	2.7
1	D	118	ALA	2.6
1	B	114	ASN	2.5
1	D	366	ALA	2.5
1	D	316	GLY	2.5
1	A	118	ALA	2.5
1	C	240	SER	2.5
1	D	199	ILE	2.5
1	B	263	PHE	2.4
1	C	191	GLY	2.4
1	C	179	PHE	2.3
1	A	263	PHE	2.3
1	D	115	ASP	2.3
1	A	505	ASN	2.2
1	B	191	GLY	2.2
1	D	417	ALA	2.2
1	C	250	LEU	2.1
1	C	113	SER	2.1
1	C	230	LYS	2.1
1	A	250	LEU	2.1
1	B	113	SER	2.1
1	C	410	VAL	2.1
1	B	199	ILE	2.1
1	B	505	ASN	2.1
1	B	115	ASP	2.0
1	B	193	LEU	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.