



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:51 PM GMT

PDB ID : 5BW8
Title : 2.8 Å crystal structure of a Get3-Get4-Get5 intermediate complex from *S.cerevisiae*
Authors : Gristick, H.B.; Chartron, J.W.; Clemons, W.M.
Deposited on : 2015-06-06
Resolution : 2.80 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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-20026982

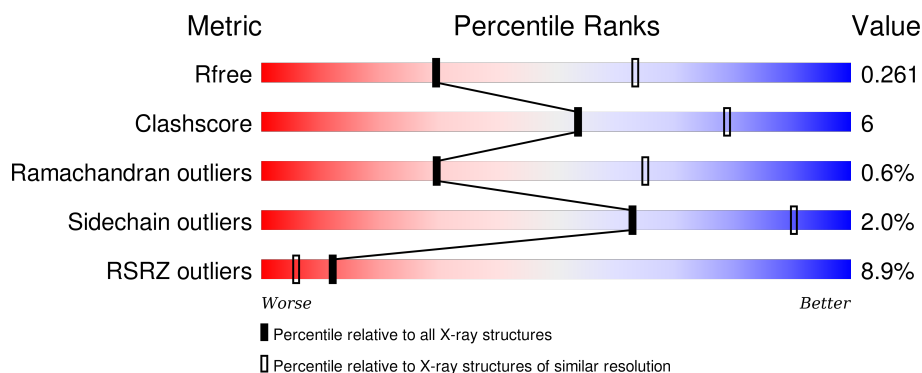
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 $\leq 5\%$. 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	373	<div> <div>6%</div> <div> <div></div> <div>72%</div> <div>12%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	373	<div> <div>4%</div> <div> <div></div> <div>68%</div> <div>12%</div> <div>•</div> <div>18%</div> </div> </div>
2	C	305	<div> <div>9%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>•</div> <div>7%</div> </div> </div>
3	D	54	<div> <div>37%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>6%</div> </div> </div>
4	Z	13	<div> <div></div> <div> <div></div> <div>77%</div> <div>23%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7742 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 ATPase GET3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2515	1589	417	491	18			
1	B	304	Total	C	N	O	S	0	0	0
			2412	1524	400	471	17			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP B3LGZ3
A	-17	GLY	-	expression tag	UNP B3LGZ3
A	-16	GLY	-	expression tag	UNP B3LGZ3
A	-15	SER	-	expression tag	UNP B3LGZ3
A	-14	HIS	-	expression tag	UNP B3LGZ3
A	-13	HIS	-	expression tag	UNP B3LGZ3
A	-12	HIS	-	expression tag	UNP B3LGZ3
A	-11	HIS	-	expression tag	UNP B3LGZ3
A	-10	HIS	-	expression tag	UNP B3LGZ3
A	-9	HIS	-	expression tag	UNP B3LGZ3
A	-8	GLY	-	expression tag	UNP B3LGZ3
A	-7	GLU	-	expression tag	UNP B3LGZ3
A	-6	ASN	-	expression tag	UNP B3LGZ3
A	-5	LEU	-	expression tag	UNP B3LGZ3
A	-4	TYR	-	expression tag	UNP B3LGZ3
A	-3	PHE	-	expression tag	UNP B3LGZ3
A	-2	GLN	-	expression tag	UNP B3LGZ3
A	-1	SER	-	expression tag	UNP B3LGZ3
A	0	VAL	-	expression tag	UNP B3LGZ3
A	1	ASP	-	expression tag	UNP B3LGZ3
B	-18	MET	-	initiating methionine	UNP B3LGZ3
B	-17	GLY	-	expression tag	UNP B3LGZ3
B	-16	GLY	-	expression tag	UNP B3LGZ3
B	-15	SER	-	expression tag	UNP B3LGZ3
B	-14	HIS	-	expression tag	UNP B3LGZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	HIS	-	expression tag	UNP B3LGZ3
B	-12	HIS	-	expression tag	UNP B3LGZ3
B	-11	HIS	-	expression tag	UNP B3LGZ3
B	-10	HIS	-	expression tag	UNP B3LGZ3
B	-9	HIS	-	expression tag	UNP B3LGZ3
B	-8	GLY	-	expression tag	UNP B3LGZ3
B	-7	GLU	-	expression tag	UNP B3LGZ3
B	-6	ASN	-	expression tag	UNP B3LGZ3
B	-5	LEU	-	expression tag	UNP B3LGZ3
B	-4	TYR	-	expression tag	UNP B3LGZ3
B	-3	PHE	-	expression tag	UNP B3LGZ3
B	-2	GLN	-	expression tag	UNP B3LGZ3
B	-1	SER	-	expression tag	UNP B3LGZ3
B	0	VAL	-	expression tag	UNP B3LGZ3
B	1	ASP	-	expression tag	UNP B3LGZ3

- Molecule 2 is a protein called Golgi to ER traffic protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	283	Total	C	N	O	S	0	0	0
			2348	1528	370	445	5			

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	258	ALA	LYS	engineered mutation	UNP Q12125
C	260	ALA	LYS	engineered mutation	UNP Q12125
C	291	GLU	-	expression tag	UNP Q12125
C	292	ASN	-	expression tag	UNP Q12125
C	293	LEU	-	expression tag	UNP Q12125
C	294	TYR	-	expression tag	UNP Q12125
C	295	PHE	-	expression tag	UNP Q12125
C	296	GLN	-	expression tag	UNP Q12125
C	297	SER	-	expression tag	UNP Q12125
C	298	LEU	-	expression tag	UNP Q12125
C	299	GLU	-	expression tag	UNP Q12125
C	300	HIS	-	expression tag	UNP Q12125
C	301	HIS	-	expression tag	UNP Q12125
C	302	HIS	-	expression tag	UNP Q12125
C	303	HIS	-	expression tag	UNP Q12125
C	304	HIS	-	expression tag	UNP Q12125
C	305	HIS	-	expression tag	UNP Q12125

- Molecule 3 is a protein called Ubiquitin-like protein MDY2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	51	Total	C	N	O	0	0	0
			401	265	62	74			

- Molecule 4 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	Z	13	Total	C	N	O	0	0	0
			65	39	13	13			

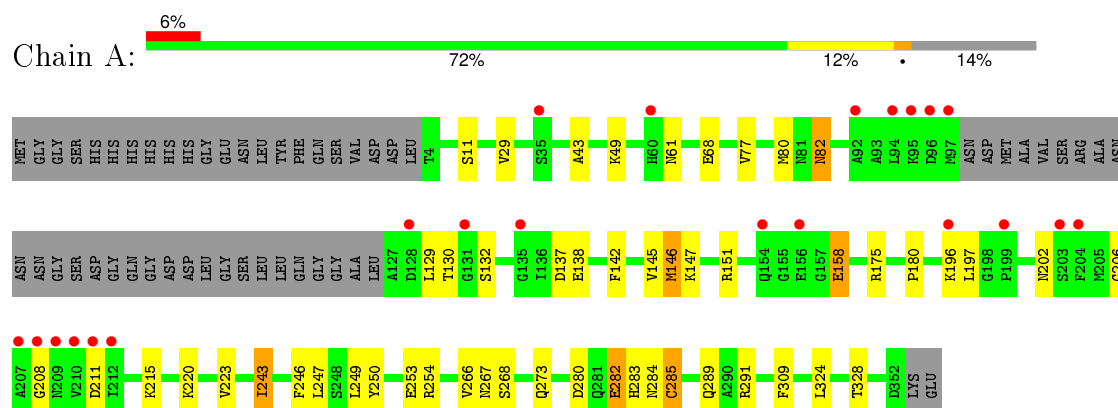
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		

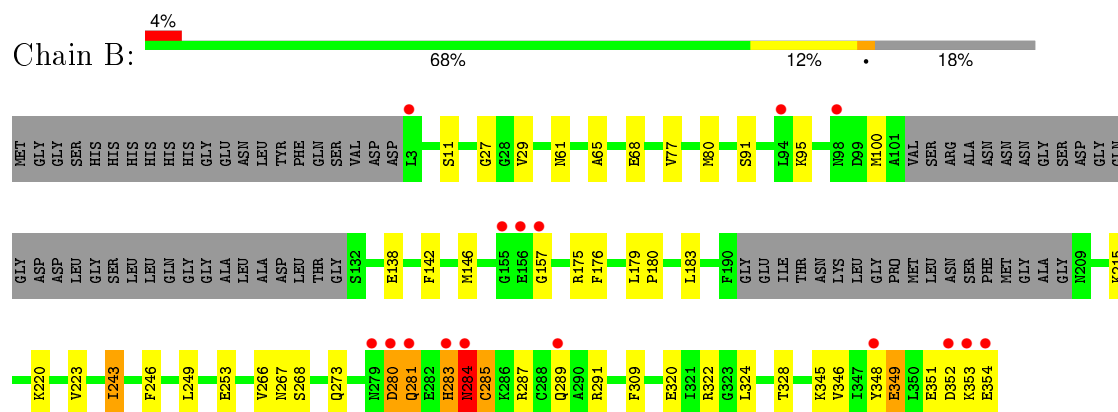
3 Residue-property plots [i](#)

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.

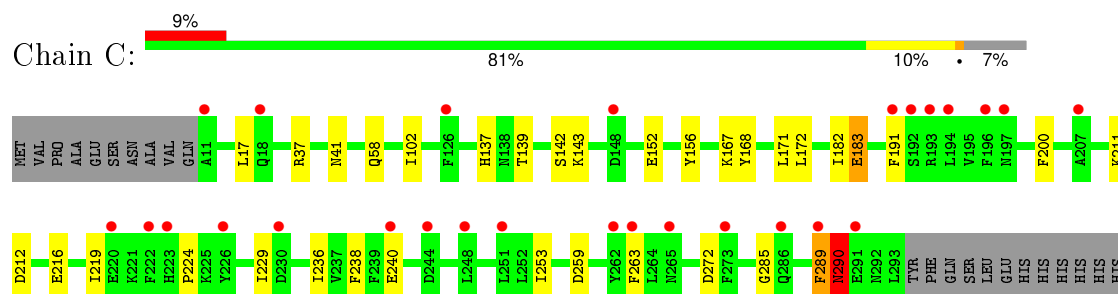
• Molecule 1: ATPase GET3



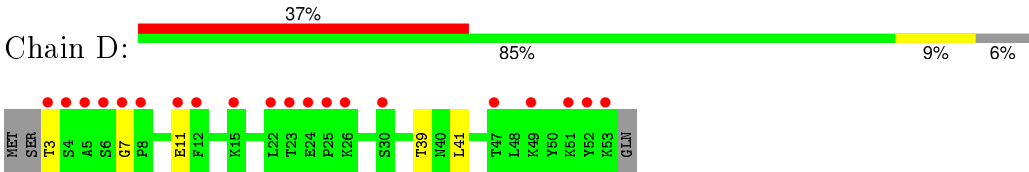
• Molecule 1: ATPase GET3



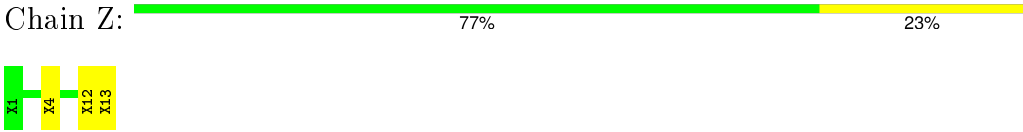
• Molecule 2: Golgi to ER traffic protein 4



• Molecule 3: Ubiquitin-like protein MDY2



● Molecule 4: Unknown Protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	111.96 Å 238.05 Å 52.19 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.80 – 2.80 29.76 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.2 (29.80-2.80) 96.3 (29.76-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.80 Å)	Xtriage
Refinement program	REFMAC 5.8.0043	Depositor
R, R_{free}	0.224 , 0.262 0.225 , 0.261	Depositor DCC
R_{free} test set	1710 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	73.2	Xtriage
Anisotropy	0.806	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 81.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 34043 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7742	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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, 0.375 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: 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	0.83	1/2558 (0.0%)	0.92	3/3451 (0.1%)
1	B	0.86	2/2452 (0.1%)	0.98	4/3306 (0.1%)
2	C	0.55	0/2405	0.74	3/3249 (0.1%)
3	D	0.50	0/412	0.67	0/560
All	All	0.75	3/7827 (0.0%)	0.88	10/10566 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	253	GLU	CG-CD	5.73	1.60	1.51
1	B	68	GLU	C-O	-5.38	1.13	1.23
1	A	253	GLU	CG-CD	5.24	1.59	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	CYS	CA-CB-SG	-7.74	100.08	114.00
2	C	289	PHE	CB-CA-C	6.66	123.72	110.40
2	C	290	ASN	N-CA-CB	5.92	121.26	110.60
1	B	287	ARG	NE-CZ-NH2	-5.89	117.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	266	VAL	CB-CA-C	-5.67	100.63	111.40
1	B	27	GLY	N-CA-C	5.62	127.16	113.10
1	A	146	MET	CG-SD-CE	5.59	109.15	100.20
1	A	82	ASN	N-CA-CB	-5.54	100.63	110.60
2	C	290	ASN	N-CA-C	-5.39	96.44	111.00
1	A	266	VAL	CB-CA-C	-5.31	101.32	111.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	LYS	Peptide
1	A	206	GLY	Peptide
1	A	68	GLU	Mainchain
1	B	100	MET	Peptide
1	B	283	HIS	Peptide

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	2515	0	2494	38	0
1	B	2412	0	2390	33	0
2	C	2348	0	2275	27	0
3	D	401	0	425	3	0
4	Z	65	0	16	2	0
5	A	1	0	0	0	0
All	All	7742	0	7600	99	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 6.

All (99) 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:B:345:LYS:O	1:B:349:GLU:HG2	1.59	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:LYS:HE2	4:Z:4:UNK:O	1.64	0.96
1:B:324:LEU:O	1:B:328:THR:HG23	1.69	0.93
1:A:324:LEU:O	1:A:328:THR:HG23	1.69	0.93
1:A:142:PHE:HE2	1:A:146:MET:HE2	1.37	0.90
2:C:212:ASP:O	2:C:216:GLU:HG2	1.72	0.88
1:B:345:LYS:O	1:B:349:GLU:CG	2.23	0.86
1:B:351:GLU:O	1:B:354:GLU:HG3	1.77	0.85
1:A:142:PHE:HE2	1:A:146:MET:CE	1.91	0.83
1:A:280:ASP:OD1	1:A:283:HIS:CD2	2.31	0.83
1:A:280:ASP:OD1	1:A:283:HIS:HD2	1.62	0.81
1:B:285:CYS:O	1:B:289:GLN:HG2	1.81	0.81
2:C:171:LEU:HD12	2:C:172:LEU:N	2.02	0.75
1:B:283:HIS:O	1:B:284:ASN:O	2.08	0.72
1:A:49:LYS:O	1:A:82:ASN:OD1	2.09	0.71
2:C:37:ARG:NH2	2:C:41:ASN:HD21	1.90	0.70
1:B:283:HIS:O	1:B:284:ASN:C	2.30	0.69
1:B:283:HIS:C	1:B:284:ASN:O	2.30	0.69
1:B:348:TYR:CD2	1:B:352:ASP:OD2	2.47	0.68
3:D:7:GLY:O	3:D:11:GLU:HG2	1.95	0.66
1:B:348:TYR:CE2	1:B:352:ASP:OD1	2.48	0.66
2:C:17:LEU:HD13	2:C:58:GLN:HG2	1.77	0.66
2:C:259:ASP:C	2:C:289:PHE:HE1	1.99	0.65
2:C:142:SER:OG	2:C:167:LYS:HE3	1.96	0.65
1:A:291:ARG:NH1	1:B:291:ARG:HD2	2.11	0.65
1:A:43:ALA:O	1:A:82:ASN:ND2	2.31	0.64
1:B:346:VAL:HA	1:B:349:GLU:HG3	1.80	0.64
1:A:142:PHE:CE2	1:A:146:MET:CE	2.78	0.62
1:A:285:CYS:O	1:A:289:GLN:HG2	1.99	0.61
1:B:91:SER:O	1:B:95:LYS:HG3	2.04	0.58
4:Z:12:UNK:O	4:Z:13:UNK:CB	2.52	0.57
2:C:236:ILE:HD11	2:C:253:ILE:HD12	1.85	0.57
1:A:129:LEU:HD12	1:A:130:THR:N	2.20	0.57
1:A:77:VAL:HG22	1:A:80:MET:CG	2.37	0.55
2:C:263:PHE:HB2	2:C:289:PHE:CZ	2.42	0.55
2:C:212:ASP:O	2:C:216:GLU:CG	2.53	0.53
1:B:346:VAL:CA	1:B:349:GLU:HG3	2.39	0.52
2:C:102:ILE:HG21	2:C:139:THR:HG22	1.92	0.52
2:C:289:PHE:O	2:C:290:ASN:HB2	2.10	0.52
2:C:200:PHE:HB3	3:D:41:LEU:O	2.09	0.52
1:B:77:VAL:HG22	1:B:80:MET:CG	2.39	0.51
1:B:138:GLU:OE2	1:B:175:ARG:NH1	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:VAL:HA	1:B:243:ILE:HD13	1.91	0.51
1:A:138:GLU:OE2	1:A:175:ARG:NH1	2.41	0.51
1:A:142:PHE:CE2	1:A:146:MET:HE2	2.30	0.50
2:C:171:LEU:C	2:C:171:LEU:HD12	2.32	0.50
2:C:259:ASP:C	2:C:289:PHE:CE1	2.84	0.49
1:B:142:PHE:O	1:B:146:MET:HG3	2.12	0.49
1:B:176:PHE:O	1:B:179:LEU:HB2	2.12	0.49
1:A:280:ASP:OD2	1:A:282:GLU:OE2	2.30	0.49
1:B:180:PRO:HD3	1:B:223:VAL:HG11	1.94	0.49
2:C:259:ASP:O	2:C:289:PHE:HE1	1.96	0.49
1:A:180:PRO:HD3	1:A:223:VAL:HG11	1.95	0.48
2:C:263:PHE:CD1	2:C:289:PHE:CE2	3.00	0.48
1:B:345:LYS:O	1:B:349:GLU:HG3	2.12	0.48
1:A:129:LEU:HA	1:A:132:SER:HB3	1.96	0.48
1:B:349:GLU:O	1:B:353:LYS:HG3	2.14	0.47
1:B:243:ILE:HD11	1:B:273:GLN:CD	2.34	0.47
2:C:152:GLU:OE1	2:C:152:GLU:N	2.44	0.47
1:B:348:TYR:HD2	1:B:352:ASP:OD2	1.96	0.47
1:B:179:LEU:HD22	1:B:183:LEU:HG	1.95	0.47
1:B:65:ALA:HA	1:B:322:ARG:HD3	1.96	0.47
1:A:142:PHE:CE2	1:A:146:MET:HE3	2.48	0.46
1:A:246:PHE:C	1:A:246:PHE:CD1	2.89	0.46
1:A:29:VAL:HA	1:A:243:ILE:HD13	1.97	0.46
2:C:168:TYR:O	2:C:171:LEU:HG	2.16	0.46
2:C:285:GLY:O	2:C:289:PHE:HB2	2.16	0.46
2:C:102:ILE:HG23	2:C:143:LYS:HG3	1.97	0.46
1:A:267:ASN:HA	1:A:309:PHE:CD2	2.51	0.45
1:A:197:LEU:HB2	1:A:202:ASN:OD1	2.17	0.45
1:A:129:LEU:HD12	1:A:129:LEU:C	2.37	0.45
1:A:208:GLY:O	1:A:211:ASP:HB3	2.16	0.45
1:B:267:ASN:HA	1:B:309:PHE:CD2	2.52	0.45
1:A:61:ASN:N	1:A:61:ASN:OD1	2.50	0.45
2:C:137:HIS:CD2	2:C:156:TYR:HD1	2.36	0.44
1:A:280:ASP:O	1:A:284:ASN:N	2.51	0.44
1:A:211:ASP:O	1:A:215:LYS:HG3	2.17	0.44
1:A:147:LYS:HE2	1:A:151:ARG:HH21	1.82	0.44
2:C:229:ILE:CD1	2:C:238:PHE:HB2	2.47	0.44
1:A:130:THR:HB	1:A:137:ASP:OD1	2.17	0.43
1:A:280:ASP:O	1:A:284:ASN:HB2	2.18	0.43
1:B:61:ASN:OD1	1:B:61:ASN:N	2.50	0.43
1:A:197:LEU:O	1:A:202:ASN:ND2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ASP:O	1:B:281:GLN:CB	2.67	0.43
1:B:246:PHE:C	1:B:246:PHE:CD1	2.92	0.43
1:A:77:VAL:HG22	1:A:80:MET:HG3	2.00	0.42
1:B:348:TYR:CD2	1:B:352:ASP:CG	2.93	0.42
2:C:143:LYS:HA	2:C:143:LYS:HD2	1.83	0.42
2:C:182:ILE:HG22	2:C:183:GLU:N	2.35	0.42
1:B:180:PRO:HA	1:B:220:LYS:HG3	2.01	0.41
1:A:250:TYR:CZ	1:A:254:ARG:HD2	2.55	0.41
1:A:142:PHE:O	1:A:146:MET:HG3	2.21	0.41
2:C:191:PHE:HE1	2:C:211:LYS:HA	1.85	0.41
1:A:247:LEU:HD23	1:A:247:LEU:HA	1.91	0.41
2:C:219:ILE:HA	2:C:224:PRO:HD2	2.03	0.40
1:A:142:PHE:O	1:A:145:VAL:HG22	2.21	0.40
1:A:243:ILE:HD11	1:A:273:GLN:CD	2.42	0.40
2:C:240:GLU:OE2	3:D:3:THR:HB	2.21	0.40
1:A:180:PRO:HA	1:A:220:LYS:HG3	2.03	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	316/373 (85%)	306 (97%)	8 (2%)	2 (1%)	30	65
1	B	298/373 (80%)	286 (96%)	9 (3%)	3 (1%)	19	52
2	C	281/305 (92%)	271 (96%)	9 (3%)	1 (0%)	39	74
3	D	49/54 (91%)	47 (96%)	2 (4%)	0	100	100
All	All	944/1105 (85%)	910 (96%)	28 (3%)	6 (1%)	30	65

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	284	ASN
2	C	290	ASN
1	A	158	GLU
1	B	157	GLY
1	B	281	GLN
1	A	285	CYS

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	284/325 (87%)	278 (98%)	6 (2%)	61	90
1	B	274/325 (84%)	266 (97%)	8 (3%)	50	83
2	C	254/274 (93%)	252 (99%)	2 (1%)	86	97
3	D	47/50 (94%)	46 (98%)	1 (2%)	61	90
All	All	859/974 (88%)	842 (98%)	17 (2%)	63	90

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	158	GLU
1	A	243	ILE
1	A	249	LEU
1	A	268	SER
1	A	282	GLU
1	B	11	SER
1	B	243	ILE
1	B	249	LEU
1	B	268	SER
1	B	280	ASP
1	B	284	ASN
1	B	320	GLU
1	B	349	GLU
2	C	183	GLU
2	C	272	ASP

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Mol	Chain	Res	Type
3	D	39	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	148	HIS
1	A	283	HIS
1	A	289	GLN
1	A	332	GLN
1	B	289	GLN
1	B	332	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 1 ligands modelled in this entry, 1 is 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	320/373 (85%)	0.28	22 (6%)	20 11	56, 94, 210, 324	0
1	B	304/373 (81%)	0.15	16 (5%)	30 20	55, 80, 159, 198	0
2	C	283/305 (92%)	0.40	27 (9%)	10 5	67, 122, 201, 222	0
3	D	51/54 (94%)	1.65	20 (39%)	0 0	122, 170, 225, 240	0
4	Z	0/13	-	-	-	-	-
All	All	958/1118 (85%)	0.35	85 (8%)	12 6	55, 97, 198, 324	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	11	ALA	10.5
1	B	284	ASN	7.3
1	B	280	ASP	7.2
3	D	3	THR	7.1
3	D	4	SER	6.7
1	A	208	GLY	6.2
1	A	209	ASN	5.6
1	B	156	GLU	5.3
1	A	203	SER	5.2
2	C	240	GLU	5.2
2	C	223	HIS	5.0
3	D	15	LYS	4.9
3	D	30	SER	4.6
1	A	128	ASP	4.6
1	A	95	LYS	4.6
3	D	25	PRO	4.5
1	A	92	ALA	4.5
3	D	23	THR	4.4
1	A	154	GLN	4.3
1	A	210	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	199	PRO	4.2
3	D	22	LEU	4.2
3	D	6	SER	4.1
3	D	53	LYS	3.9
1	B	279	ASN	3.9
1	B	354	GLU	3.8
1	B	281	GLN	3.8
1	B	353	LYS	3.8
2	C	226	TYR	3.7
1	A	96	ASP	3.6
3	D	5	ALA	3.6
1	B	352	ASP	3.5
1	A	207	ALA	3.5
1	B	155	GLY	3.4
2	C	248	LEU	3.4
3	D	26	LYS	3.4
2	C	191	PHE	3.3
2	C	251	LEU	3.3
2	C	244	ASP	3.3
1	A	196	LYS	3.2
2	C	18	GLN	3.2
1	A	131	GLY	3.1
1	A	204	PHE	3.0
1	A	97	MET	3.0
3	D	12	PHE	3.0
3	D	51	LYS	3.0
2	C	289	PHE	3.0
1	B	348	TYR	3.0
2	C	197	ASN	2.9
2	C	207	ALA	2.9
1	B	3	LEU	2.9
2	C	262	TYR	2.9
2	C	265	ASN	2.8
3	D	24	GLU	2.8
2	C	273	PHE	2.8
2	C	230	ASP	2.7
3	D	11	GLU	2.6
2	C	192	SER	2.6
1	A	94	LEU	2.6
1	B	157	GLY	2.6
1	A	35	SER	2.5
2	C	148	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
3	D	49	LYS	2.5
1	A	156	GLU	2.5
2	C	286	GLN	2.4
1	A	135	GLY	2.4
1	B	94	LEU	2.4
2	C	220	GLU	2.3
1	A	211	ASP	2.3
2	C	222	PHE	2.3
3	D	47	THR	2.3
2	C	291	GLU	2.3
3	D	52	TYR	2.2
1	B	289	GLN	2.2
3	D	8	PRO	2.2
2	C	126	PHE	2.2
2	C	196	PHE	2.2
2	C	194	LEU	2.2
2	C	193	ARG	2.1
1	A	60	HIS	2.1
1	B	98	ASN	2.1
1	A	212	ILE	2.1
2	C	263	PHE	2.1
1	B	283	HIS	2.0
3	D	7	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 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, 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	LLDF	B-factors(\AA^2)	Q<0.9
5	ZN	A	401	1/1	0.98	0.11	-1.38	111,111,111,111	0

6.5 Other polymers [i](#)

There are no such residues in this entry.