



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:30 AM GMT

PDB ID : 3B2E
Title : Crystal structure of *S. cerevisiae* Get3 in the open conformation in complex with Get1 cytosolic domain
Authors : Kubota, K.; Yamagata, A.; Fukai, S.
Deposited on : 2011-07-30
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 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

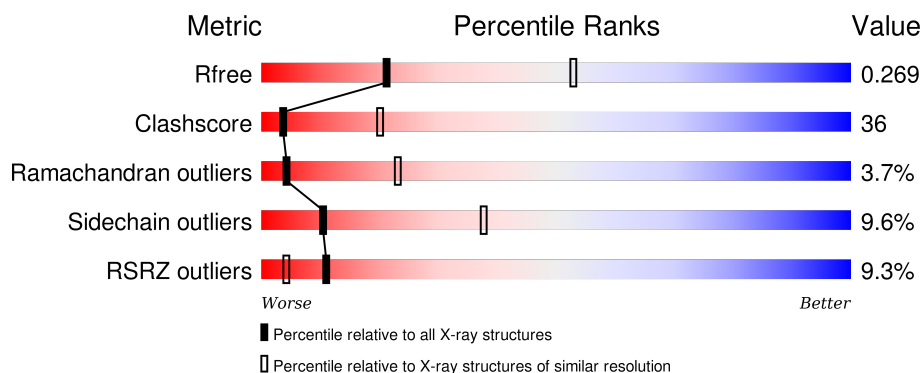
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	362	<div> <div>3%</div> <div> <div>44%</div> <div>34%</div> <div>6%</div> <div>15%</div> </div> </div>
1	B	362	<div> <div>5%</div> <div> <div>42%</div> <div>41%</div> <div>7%</div> <div>10%</div> </div> </div>
1	C	362	<div> <div>8%</div> <div> <div>39%</div> <div>45%</div> <div>8%</div> <div>7%</div> </div> </div>
1	D	362	<div> <div>8%</div> <div> <div>38%</div> <div>41%</div> <div>6%</div> <div>15%</div> </div> </div>
2	E	84	<div> <div>8%</div> <div> <div>42%</div> <div>30%</div> <div>8%</div> <div>20%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	84	<div><div></div><div>11%</div><div>36%</div><div>31%</div><div>7%</div><div>26%</div></div>
2	G	84	<div><div></div><div>32%</div><div>38%</div><div>35%</div><div>7%</div><div>20%</div></div>
2	H	84	<div><div></div><div>17%</div><div>40%</div><div>30%</div><div>6%</div><div>24%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12146 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.

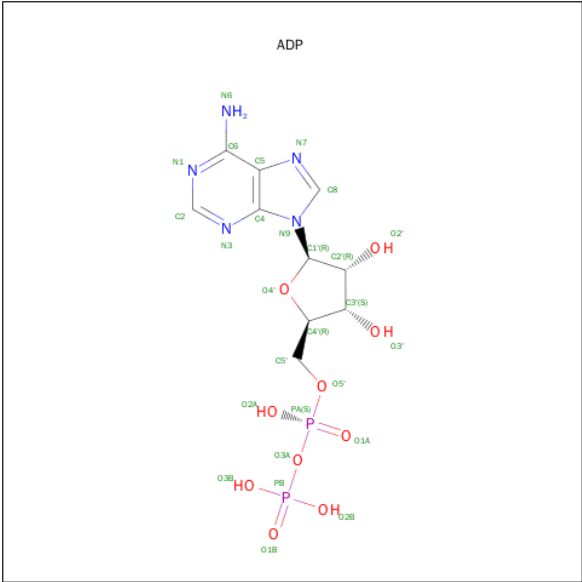
- Molecule 1 is a protein called ATPase GET3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2416	1525	401	474	16			
1	B	325	Total	C	N	O	S	0	0	0
			2495	1575	414	487	19			
1	C	335	Total	C	N	O	S	0	0	0
			2592	1632	436	505	19			
1	D	307	Total	C	N	O	S	0	0	0
			2385	1507	395	466	17			

- Molecule 2 is a protein called Golgi to ER traffic protein 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	67	Total	C	N	O	0	0	0
			555	345	101	109			
2	F	62	Total	C	N	O	0	0	0
			512	316	93	103			
2	G	67	Total	C	N	O	0	0	0
			551	343	99	109			
2	H	64	Total	C	N	O	0	0	0
			532	330	96	106			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

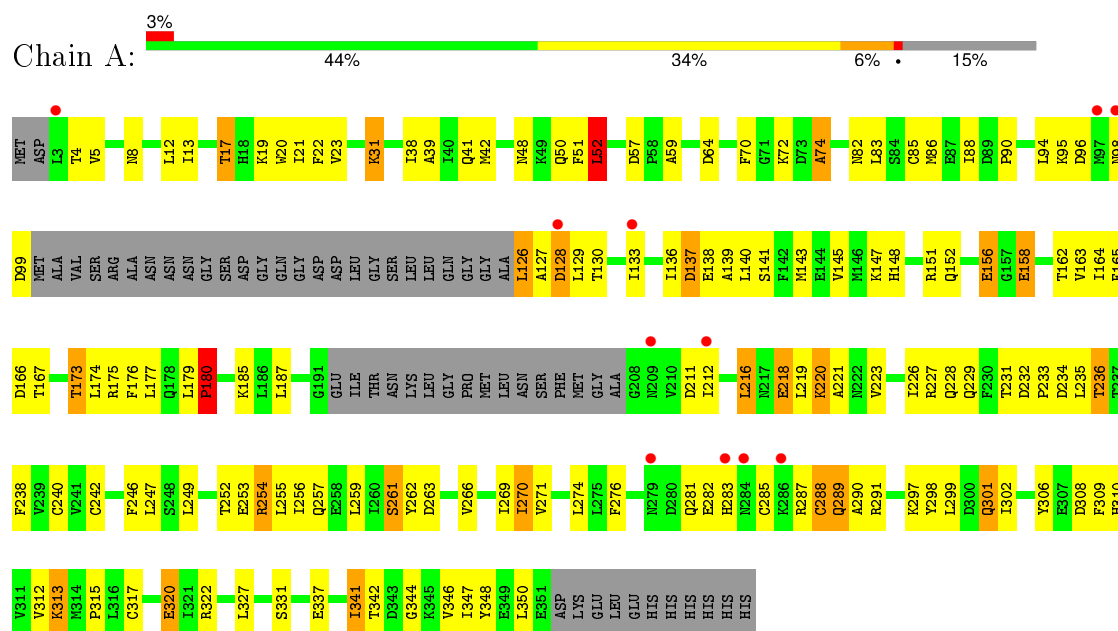


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

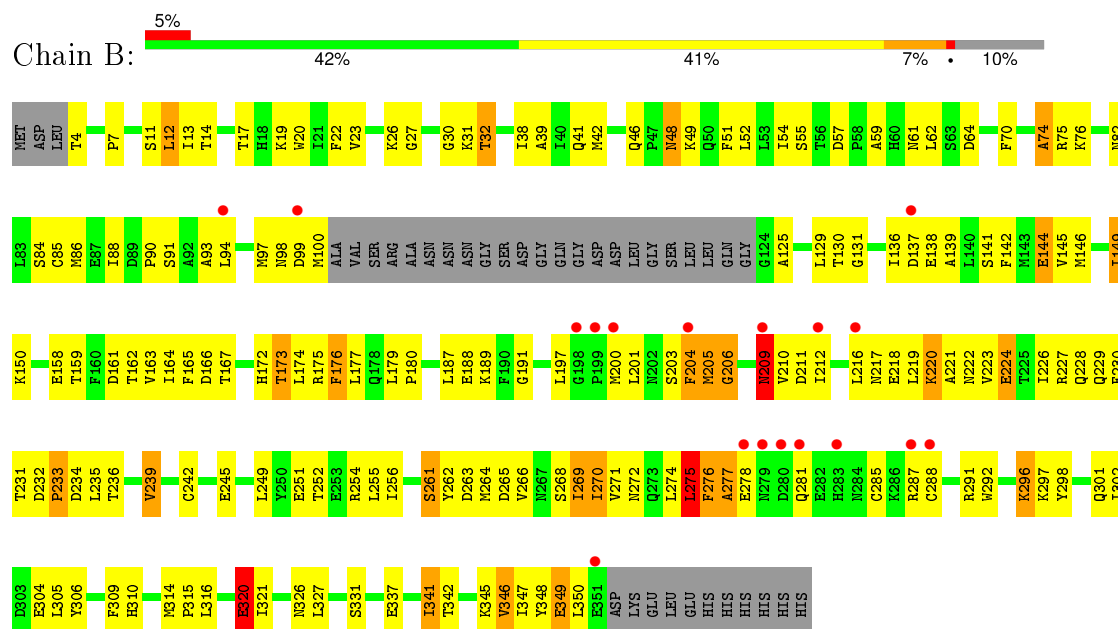
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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

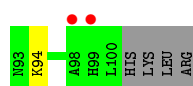


Chain C: 8% 39% 45% 8% 7%

Residue	Amino Acid	Residue	Amino Acid	Residue	Amino Acid	Residue	Amino Acid	Residue	Amino Acid
1	MET	384	ASP	758	ASP	1136	ASP	1436	ASP
2	ASP	385	LEU	759	LEU	1137	LEU	1437	LEU
3	LEU	386	THR	760	THR	1138	THR	1438	THR
4	THR	387	VAL	761	VAL	1139	VAL	1439	VAL
5	VAL	388	ASP	762	ASP	1140	ASP	1440	ASP
6	ASP	389	LEU	763	LEU	1141	LEU	1441	LEU
7	LEU	390	THR	764	THR	1142	THR	1442	THR
8	THR	391	VAL	765	VAL	1143	VAL	1443	VAL
9	VAL	392	ASP	766	ASP	1144	ASP	1444	ASP
10	ASP	393	LEU	767	LEU	1145	LEU	1445	LEU
11	ASP	394	LEU	768	LEU	1146	LEU	1446	LEU
12	ASP	395	THR	769	THR	1147	THR	1447	THR
13	THR	396	VAL	770	VAL	1148	VAL	1448	VAL
14	THR	397	ASP	771	ASP	1149	ASP	1449	ASP
15	THR	398	LEU	772	LEU	1150	LEU	1450	LEU
16	THR	399	THR	773	THR	1151	THR	1451	THR
17	THR	400	VAL	774	VAL	1152	VAL	1452	VAL
18	THR	401	ASP	775	ASP	1153	ASP	1453	ASP
19	THR	402	LEU	776	LEU	1154	LEU	1454	LEU
20	THR	403	THR	777	THR	1155	THR	1455	THR
21	THR	404	VAL	778	VAL	1156	VAL	1456	VAL
22	THR	405	ASP	779	ASP	1157	ASP	1457	ASP
23	THR	406	LEU	780	LEU	1158	LEU	1458	LEU
24	THR	407	THR	781	THR	1159	THR	1459	THR
25	THR	408	VAL	782	VAL	1160	VAL	1460	VAL
26	THR	409	ASP	783	ASP	1161	ASP	1461	ASP
27	THR	410	LEU	784	LEU	1162	LEU	1462	LEU
28	THR	411	THR	785	THR	1163	THR	1463	THR
29	THR	412	VAL	786	VAL	1164	VAL	1464	VAL
30	THR	413	ASP	787	ASP	1165	ASP	1465	ASP
31	THR	414	LEU	788	LEU	1166	LEU	1466	LEU
32	THR	415	THR	789	THR	1167	THR	1467	THR
33	THR	416	VAL	790	VAL	1168	VAL	1468	VAL
34	THR	417	ASP	791	ASP	1169	ASP	1469	ASP
35	THR	418	LEU	792	LEU	1170	LEU	1470	LEU
36	THR	419	THR	793	THR	1171	THR	1471	THR
37	THR	420	VAL	794	VAL	1172	VAL	1472	VAL
38	THR	421	ASP	795	ASP	1173	ASP	1473	ASP
39	THR	422	LEU	796	LEU	1174	LEU	1474	LEU
40	THR	423	THR	797	THR	1175	THR	1475	THR
41	THR	424	VAL	798	VAL	1176	VAL	1476	VAL
42	THR	425	ASP	799	ASP	1177	ASP	1477	ASP
43	THR	426	LEU	800	LEU	1178	LEU	1478	LEU
44	THR	427	THR	801	THR	1179	THR	1479	THR
45	THR	428	VAL	802	VAL	1180	VAL	1480	VAL
46	THR	429	ASP	803	ASP	1181	ASP	1481	ASP
47	THR	430	LEU	804	LEU	1182	LEU	1482	LEU
48	THR	431	THR	805	THR	1183	THR	1483	THR
49	THR	432	VAL	806	VAL	1184	VAL	1484	VAL
50	THR	433	ASP	807					

[illegible]

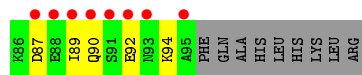
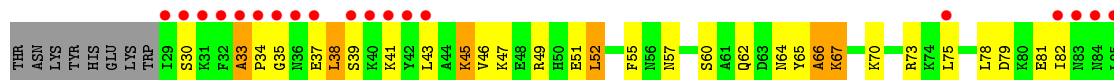
Chain E:



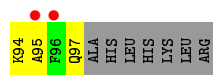
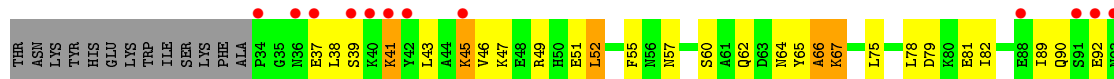
- Molecule 2: Golgi to ER traffic protein 1



- Molecule 2: Golgi to ER traffic protein 1



- Molecule 2: Golgi to ER traffic protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	114.34Å 167.66Å 244.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 42.25 – 3.01	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.00) 94.5 (42.25-3.01)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.274 , 0.306 0.276 , 0.269	Depositor DCC
R_{free} test set	2243 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	73.4	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 38.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 44437 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12146	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.59	1/2455 (0.0%)	0.74	2/3313 (0.1%)
1	B	0.61	2/2536 (0.1%)	0.74	2/3426 (0.1%)
1	C	0.53	3/2634 (0.1%)	0.72	1/3556 (0.0%)
1	D	0.42	0/2423	0.69	1/3270 (0.0%)
2	E	0.37	0/563	0.54	0/751
2	F	0.37	0/518	0.55	0/690
2	G	0.35	0/558	0.54	0/744
2	H	0.34	0/539	0.54	0/718
All	All	0.51	6/12226 (0.0%)	0.70	6/16468 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	204	PHE	CE2-CZ	10.18	1.56	1.37
1	B	204	PHE	CG-CD2	8.05	1.50	1.38
1	C	204	PHE	CG-CD1	7.62	1.50	1.38
1	B	204	PHE	CE2-CZ	6.40	1.49	1.37
1	C	204	PHE	CD2-CE2	-5.98	1.27	1.39

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	275	LEU	CA-CB-CG	6.70	130.72	115.30
1	A	269	ILE	CB-CA-C	-5.75	100.09	111.60
1	D	341	ILE	CB-CA-C	-5.47	100.66	111.60
1	C	204	PHE	CG-CD2-CE2	-5.42	114.84	120.80
1	B	269	ILE	CB-CA-C	-5.10	101.39	111.60

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	2416	0	2392	160	0
1	B	2495	0	2433	174	1
1	C	2592	0	2549	200	1
1	D	2385	0	2349	191	0
2	E	555	0	551	35	0
2	F	512	0	511	42	0
2	G	551	0	553	45	0
2	H	532	0	528	31	1
3	A	27	0	12	3	0
3	B	27	0	12	5	0
3	C	27	0	12	3	0
3	D	27	0	12	3	0
All	All	12146	0	11914	855	2

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 36.

The worst 5 of 855 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:48:ASN:N	1:B:48:ASN:HD22	1.46	1.11
1:A:257:GLN:HA	1:A:257:GLN:HE21	1.15	1.10
1:B:48:ASN:ND2	1:B:48:ASN:H	1.42	1.09
1:B:200:MET:O	1:B:204:PHE:HB2	1.59	1.00
2:E:38:LEU:HD13	2:E:89:ILE:HG13	1.41	1.00

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:95:ALA:CB	2:H:95:ALA:CB[3_554]	1.74	0.46
1:B:125:ALA:CB	1:C:204:PHE:CE2[3_654]	1.96	0.24

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	301/362 (83%)	248 (82%)	43 (14%)	10 (3%)	5	26
1	B	321/362 (89%)	258 (80%)	50 (16%)	13 (4%)	4	21
1	C	331/362 (91%)	259 (78%)	59 (18%)	13 (4%)	4	21
1	D	301/362 (83%)	246 (82%)	42 (14%)	13 (4%)	3	19
2	E	65/84 (77%)	52 (80%)	12 (18%)	1 (2%)	13	50
2	F	60/84 (71%)	48 (80%)	11 (18%)	1 (2%)	11	46
2	G	65/84 (77%)	49 (75%)	13 (20%)	3 (5%)	3	18
2	H	62/84 (74%)	50 (81%)	11 (18%)	1 (2%)	12	48
All	All	1506/1784 (84%)	1210 (80%)	241 (16%)	55 (4%)	4	23

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	LYS
1	A	320	GLU
1	B	277	ALA
1	D	129	LEU
1	A	74	ALA

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	273/318 (86%)	247 (90%)	26 (10%)	11	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	272/318 (86%)	242 (89%)	30 (11%)	8	30
1	C	286/318 (90%)	254 (89%)	32 (11%)	7	29
1	D	264/318 (83%)	244 (92%)	20 (8%)	16	51
2	E	61/77 (79%)	55 (90%)	6 (10%)	10	36
2	F	57/77 (74%)	52 (91%)	5 (9%)	12	42
2	G	61/77 (79%)	56 (92%)	5 (8%)	14	46
2	H	59/77 (77%)	55 (93%)	4 (7%)	20	56
All	All	1333/1580 (84%)	1205 (90%)	128 (10%)	10	38

5 of 128 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	296	LYS
1	C	85	CYS
1	D	270	ILE
1	B	316	LEU
2	F	52	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	178	GLN
1	C	228	GLN
1	D	335	ASN
1	C	181	ASN
1	C	217	ASN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	ADP	A	401	-	22,29,29	2.41	4 (18%)	27,45,45	2.67	6 (22%)
3	ADP	B	401	-	22,29,29	2.37	3 (13%)	27,45,45	2.48	6 (22%)
3	ADP	C	401	-	22,29,29	2.27	3 (13%)	27,45,45	2.62	5 (18%)
3	ADP	D	401	-	22,29,29	2.40	3 (13%)	27,45,45	2.56	6 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	401	-	-	0/12/32/32	0/3/3/3
3	ADP	B	401	-	-	0/12/32/32	0/3/3/3
3	ADP	C	401	-	-	0/12/32/32	0/3/3/3
3	ADP	D	401	-	-	0/12/32/32	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	ADP	O4'-C4'	-9.89	1.22	1.45
3	A	401	ADP	O4'-C4'	-9.28	1.23	1.45
3	C	401	ADP	O4'-C4'	-9.07	1.24	1.45
3	B	401	ADP	O4'-C4'	-8.48	1.25	1.45
3	D	401	ADP	C8-N7	-2.56	1.29	1.34

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	401	ADP	N3-C2-N1	-10.28	121.02	128.89
3	C	401	ADP	N3-C2-N1	-9.97	121.26	128.89
3	D	401	ADP	N3-C2-N1	-9.86	121.34	128.89
3	B	401	ADP	N3-C2-N1	-9.37	121.72	128.89
3	D	401	ADP	PA-O3A-PB	-6.50	110.88	132.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	ADP	3	0
3	B	401	ADP	5	0
3	C	401	ADP	3	0
3	D	401	ADP	3	0

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	307/362 (84%)	0.11	11 (3%)	46 20	43, 86, 147, 169	0
1	B	325/362 (89%)	0.12	18 (5%)	29 11	43, 89, 169, 192	0
1	C	335/362 (92%)	0.33	28 (8%)	14 5	66, 113, 185, 193	0
1	D	307/362 (84%)	0.42	29 (9%)	11 4	80, 133, 181, 188	0
2	E	67/84 (79%)	0.23	7 (10%)	8 3	61, 111, 159, 167	0
2	F	62/84 (73%)	0.59	9 (14%)	3 1	66, 121, 164, 167	0
2	G	67/84 (79%)	1.64	27 (40%)	0 0	112, 165, 195, 197	0
2	H	64/84 (76%)	0.94	14 (21%)	1 1	105, 145, 174, 179	0
All	All	1534/1784 (85%)	0.35	143 (9%)	11 4	43, 115, 178, 197	0

The worst 5 of 143 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	95	ALA	9.8
1	C	99	ASP	7.2
2	F	95	ALA	7.0
2	G	88	GLU	6.6
1	C	121	LEU	6.2

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 [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
3	ADP	C	401	27/27	0.88	0.30	1.12	91,99,102,106	0
3	ADP	A	401	27/27	0.92	0.28	0.74	65,72,77,85	0
3	ADP	B	401	27/27	0.93	0.25	0.42	64,73,78,85	0
3	ADP	D	401	27/27	0.84	0.33	0.41	104,107,110,113	0

6.5 Other polymers [i](#)

There are no such residues in this entry.