Full wwPDB X-ray Structure Validation Report (i)

Sep 14, 2017 – 05:33 PM EDT

PDB ID	:	4XTR
Title	:	Structure of Get3 bound to the transmembrane domain of Pep12
Authors	:	Mateja, A.; Paduch, M.; Chang, H.-Y.; Szydlowska, A.; Kossiakoff, A.A.; Hegde, R.S.; Keenan, R.J.
Deposited on	:	unknown
Resolution	:	2.05 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 (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20029824

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 2.05 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.
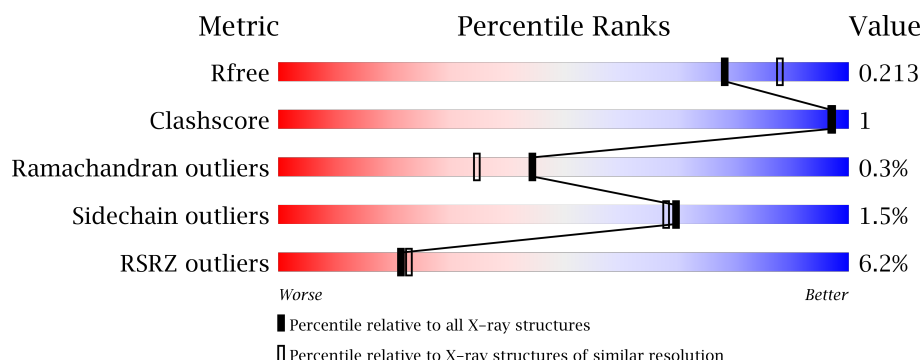
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1316 (2.04-2.04)
Clashscore	112137	1394 (2.04-2.04)
Ramachandran outliers	110173	1383 (2.04-2.04)
Sidechain outliers	110143	1383 (2.04-2.04)
RSRZ outliers	101464	1319 (2.04-2.04)

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	354	
1	B	354	
2	C	230	
2	E	230	
3	D	217	

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Mol	Chain	Length	Quality of chain
3	F	217	
4	G	37	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 24293 atoms, of which 11564 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	305	Total 4815	C 1530	H 2400	N 401	O 466	S 18	0	2	0
1	B	311	Total 4873	C 1543	H 2432	N 404	O 476	S 18	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	ASN	ASP	engineered mutation	UNP Q12154
B	57	ASN	ASP	engineered mutation	UNP Q12154

- Molecule 2 is a protein called Antibody Heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	217	Total 3241	C 1037	H 1600	N 278	O 320	S 6	0	1	0
2	E	222	Total 3306	C 1055	H 1633	N 284	O 328	S 6	0	1	0

- Molecule 3 is a protein called Antibody Light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	216	Total 3269	C 1038	H 1611	N 276	O 338	S 6	0	0	0
3	F	216	Total 3269	C 1038	H 1611	N 276	O 338	S 6	0	0	0

- Molecule 4 is a protein called Pep12p.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	G	22	Total 427	C 141	H 231	N 30	O 23	S 2	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	252	MET	-	initiating methionine	UNP E7M086
G	253	GLY	-	expression tag	UNP E7M086
G	254	SER	-	expression tag	UNP E7M086
G	255	HIS	-	expression tag	UNP E7M086
G	256	HIS	-	expression tag	UNP E7M086
G	257	HIS	-	expression tag	UNP E7M086
G	258	HIS	-	expression tag	UNP E7M086
G	259	HIS	-	expression tag	UNP E7M086
G	260	HIS	-	expression tag	UNP E7M086
G	261	SER	-	expression tag	UNP E7M086

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
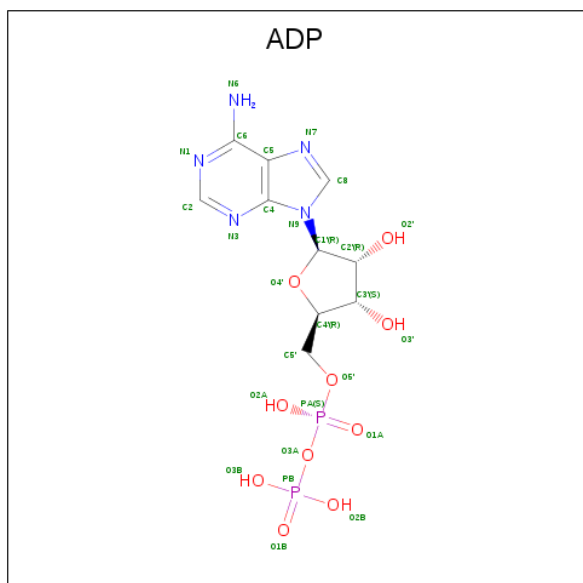
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	P	0	1
			38	10	11	5	10	2		
5	B	1	Total	C	H	N	O	P	0	1
			39	10	12	5	10	2		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	Mg 1	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).
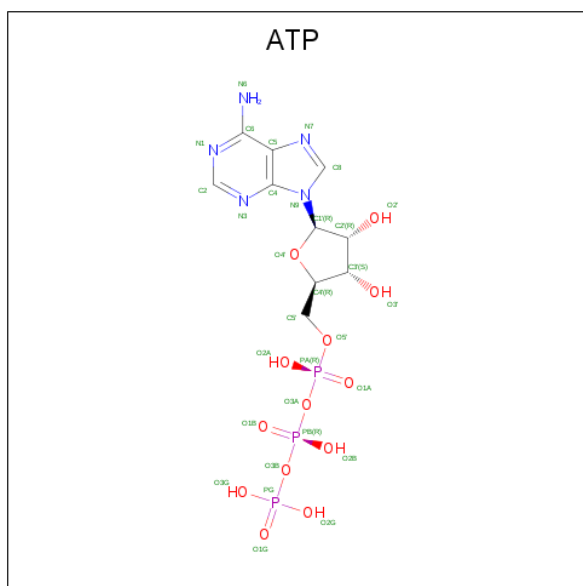
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	A	1	Total 42	C 10	H 11	N 5	O 13	P 3	0	1
8	B	1	Total 43	C 10	H 12	N 5	O 13	P 3	0	1

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	104	Total 104	O 104	0	0
9	B	149	Total 149	O 149	0	0

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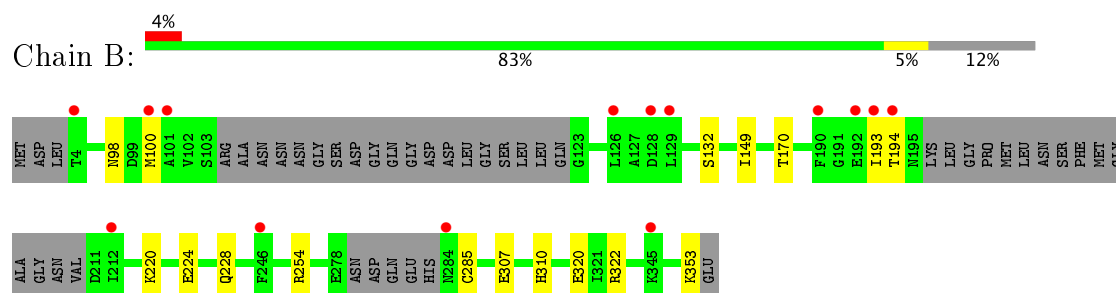| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	162	Total 162	O 162	0	0
9	D	164	Total 164	O 164	0	0
9	E	211	Total 211	O 211	0	0
9	F	137	Total 137	O 137	0	0
9	G	1	Total 1	O 1	0	0

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 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: ATPase GET3
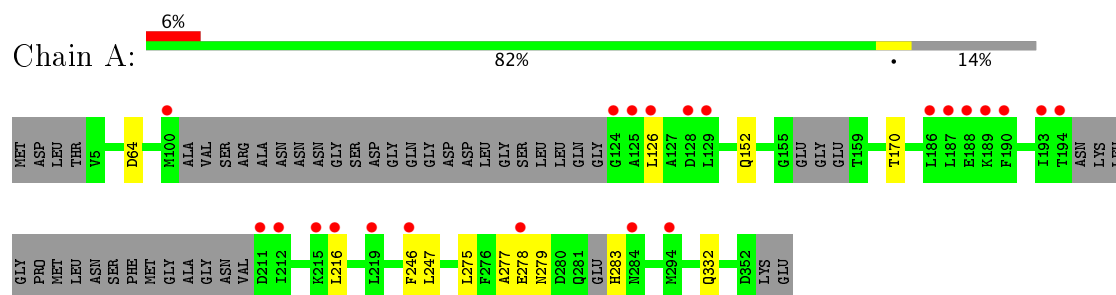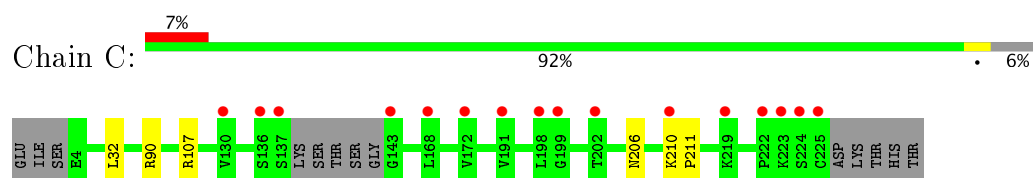
Chain A:

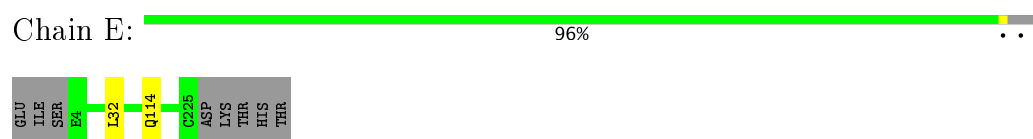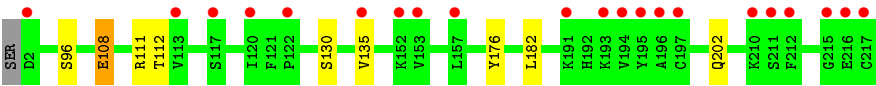- Molecule 1: ATPase GET3

Chain B:

- Molecule 2: Antibody Heavy chain

Chain C:

- Molecule 2: Antibody Heavy chain

Chain E:

- Molecule 3: Antibody Light chain

Chain D:

• Molecule 3: Antibody Light chain

Chain F:

• Molecule 4: Pep12p

Chain G:
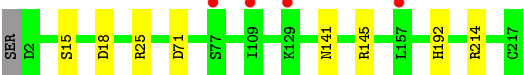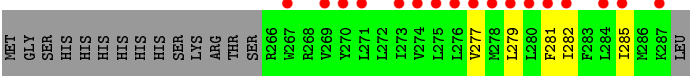
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	102.87Å 112.03Å 153.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.95 – 2.05 61.56 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.8 (53.95-2.05) 92.1 (61.56-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 2.05Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, R_{free}	0.187 , 0.216 0.185 , 0.213	Depositor DCC
R_{free} test set	5177 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	35.4	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 48.4	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	24293	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, ZN, 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	0.23	0/2457	0.40	0/3310
1	B	0.24	0/2482	0.41	0/3345
2	C	0.23	0/1682	0.43	0/2293
2	E	0.23	0/1715	0.44	0/2338
3	D	0.23	0/1694	0.41	0/2299
3	F	0.23	0/1694	0.41	0/2299
4	G	0.24	0/200	0.47	0/269
All	All	0.23	0/11924	0.42	0/16153

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	2415	2400	2397	6	0
1	B	2441	2432	2431	6	0
2	C	1641	1600	1598	4	0
2	E	1673	1633	1632	0	0
3	D	1658	1611	1611	4	0
3	F	1658	1611	1611	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	196	231	230	3	0
5	A	27	11	12	0	0
5	B	27	12	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	1	0	0	0	0
8	A	31	11	12	0	0
8	B	31	12	12	0	0
9	A	104	0	0	0	0
9	B	149	0	0	2	0
9	C	162	0	0	2	0
9	D	164	0	0	0	0
9	E	211	0	0	0	0
9	F	137	0	0	2	0
9	G	1	0	0	0	0
All	All	12729	11564	11558	25	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 (25) 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:320:GLU:OE1	1:B:322:ARG:NH1	2.01	0.93
3:D:111:ARG:NH1	3:D:112:THR:O	2.10	0.83
1:A:277:ALA:O	1:A:279:ASN:N	2.17	0.77
3:F:192:HIS:O	3:F:214:ARG:NH1	2.24	0.70
1:B:310:HIS:NE2	9:B:577:HOH:O	2.30	0.63
1:B:307:GLU:OE2	9:B:599:HOH:O	2.15	0.63
3:F:141:ASN:ND2	9:F:412:HOH:O	2.31	0.63
3:D:108:GLU:OE2	3:D:176:TYR:OH	2.17	0.56
2:C:107:ARG:NH1	9:C:439:HOH:O	2.37	0.56
1:B:220:LYS:NZ	1:B:224:GLU:OE2	2.44	0.51
1:A:275:LEU:O	1:A:277:ALA:N	2.42	0.50
3:F:25:ARG:NE	3:F:71:ASP:OD2	2.37	0.47
4:G:281:PHE:CZ	4:G:285:ILE:HD11	2.50	0.47
4:G:277:VAL:O	4:G:281:PHE:N	2.49	0.46
3:F:145:ARG:NH1	9:F:413:HOH:O	2.49	0.45
4:G:279:LEU:HA	4:G:282:ILE:HD12	1.99	0.45
1:A:64:ASP:OD1	1:B:254:ARG:NH1	2.48	0.45
3:F:15:SER:N	3:F:18:ASP:OD2	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246[B]:PHE:CG	1:A:247:LEU:N	2.83	0.43
2:C:210:LYS:N	2:C:211:PRO:HD2	2.33	0.43
2:C:90:ARG:NH1	9:C:357:HOH:O	2.43	0.43
1:A:277:ALA:O	1:A:279:ASN:ND2	2.52	0.42
3:D:135:VAL:HG13	3:D:182:LEU:HB3	2.01	0.42
2:C:107:ARG:NH2	3:D:96:SER:O	2.53	0.41
1:A:246[B]:PHE:CZ	1:B:322:ARG:HB3	2.56	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	297/354 (84%)	285 (96%)	10 (3%)	2 (1%)	25	14
1	B	304/354 (86%)	297 (98%)	5 (2%)	2 (1%)	25	14
2	C	214/230 (93%)	208 (97%)	6 (3%)	0	100	100
2	E	221/230 (96%)	218 (99%)	3 (1%)	0	100	100
3	D	214/217 (99%)	209 (98%)	5 (2%)	0	100	100
3	F	214/217 (99%)	210 (98%)	4 (2%)	0	100	100
4	G	20/37 (54%)	19 (95%)	1 (5%)	0	100	100
All	All	1484/1639 (90%)	1446 (97%)	34 (2%)	4 (0%)	44	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	170	THR
1	A	170	THR
1	A	278	GLU
1	B	285	CYS

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	273/309 (88%)	268 (98%)	5 (2%)	64	60
1	B	276/309 (89%)	268 (97%)	8 (3%)	48	40
2	C	182/193 (94%)	180 (99%)	2 (1%)	78	77
2	E	186/193 (96%)	183 (98%)	3 (2%)	68	65
3	D	191/192 (100%)	188 (98%)	3 (2%)	68	65
3	F	191/192 (100%)	191 (100%)	0	100	100
4	G	22/36 (61%)	22 (100%)	0	100	100
All	All	1321/1424 (93%)	1300 (98%)	21 (2%)	70	65

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	LEU
1	A	152	GLN
1	A	216	LEU
1	A	283	HIS
1	A	332	GLN
1	B	98	ASN
1	B	100	MET
1	B	132	SER
1	B	149	ILE
1	B	193	ILE
1	B	194	THR
1	B	228	GLN
1	B	353	LYS
2	C	32	LEU
2	C	206	ASN
3	D	108	GLU
3	D	130	SER
3	D	202	GLN
2	E	32	LEU
2	E	114[A]	GLN

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Mol	Chain	Res	Type
2	E	114[B]	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

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	#$|Z| > 2$
5	ADP	A	401[B]	6	25,29,29	4.56	10 (40%)	24,45,45	3.05	3 (12%)
8	ATP	A	404[A]	6	27,33,33	2.22	9 (33%)	25,52,52	2.02	4 (16%)
5	ADP	B	401[B]	6	25,29,29	4.56	11 (44%)	24,45,45	3.06	3 (12%)
8	ATP	B	403[A]	6	27,33,33	2.21	9 (33%)	25,52,52	2.04	4 (16%)

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
5	ADP	A	401[B]	6	-	0/12/32/32	0/3/3/3
8	ATP	A	404[A]	6	-	0/18/38/38	0/3/3/3
5	ADP	B	401[B]	6	-	0/12/32/32	0/3/3/3
8	ATP	B	403[A]	6	-	0/18/38/38	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	401[B]	ADP	C2'-C1'	-13.83	1.31	1.53
5	B	401[B]	ADP	C2'-C1'	-13.76	1.31	1.53
5	B	401[B]	ADP	O4'-C4'	-5.64	1.32	1.45
5	A	401[B]	ADP	O4'-C4'	-5.61	1.32	1.45
8	B	403[A]	ATP	C2-N1	-5.16	1.24	1.33
8	A	404[A]	ATP	C2-N1	-5.15	1.24	1.33
8	A	404[A]	ATP	C2'-C1'	-3.47	1.48	1.53
8	B	403[A]	ATP	C2'-C1'	-3.46	1.48	1.53
8	A	404[A]	ATP	C6-N1	-2.66	1.25	1.37
8	B	403[A]	ATP	C6-N1	-2.65	1.25	1.37
5	B	401[B]	ADP	C5-C4	-2.41	1.35	1.40
5	A	401[B]	ADP	C5-C4	-2.38	1.35	1.40
8	B	403[A]	ATP	C2'-C3'	-2.31	1.47	1.53
8	A	404[A]	ATP	C2'-C3'	-2.25	1.47	1.53
5	A	401[B]	ADP	O3'-C3'	-2.10	1.38	1.43
5	B	401[B]	ADP	O3'-C3'	-2.05	1.38	1.43
5	B	401[B]	ADP	PA-O5'	2.01	1.67	1.59
5	B	401[B]	ADP	C2-N3	2.03	1.35	1.32
5	A	401[B]	ADP	C2-N1	2.04	1.37	1.33
5	A	401[B]	ADP	C2-N3	2.05	1.35	1.32
5	B	401[B]	ADP	C2-N1	2.11	1.37	1.33
8	A	404[A]	ATP	C6-N6	2.36	1.43	1.34
8	B	403[A]	ATP	C6-N6	2.36	1.43	1.34
5	B	401[B]	ADP	O2'-C2'	3.35	1.50	1.43
5	A	401[B]	ADP	O2'-C2'	3.37	1.50	1.43
5	B	401[B]	ADP	PB-O3A	3.44	1.65	1.60
8	B	403[A]	ATP	C5-C4	3.48	1.48	1.40
8	A	404[A]	ATP	C5-C4	3.48	1.48	1.40
5	A	401[B]	ADP	PB-O3A	3.52	1.65	1.60
8	B	403[A]	ATP	C8-N7	3.76	1.41	1.34
8	A	404[A]	ATP	C8-N7	3.77	1.41	1.34
8	B	403[A]	ATP	O4'-C1'	3.86	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	404[A]	ATP	C4-N3	3.96	1.41	1.35
8	B	403[A]	ATP	C4-N3	3.96	1.41	1.35
8	A	404[A]	ATP	O4'-C1'	3.98	1.46	1.41
5	A	401[B]	ADP	C6-N6	4.00	1.50	1.34
5	B	401[B]	ADP	C6-N6	4.01	1.50	1.34
5	A	401[B]	ADP	O4'-C1'	14.92	1.61	1.41
5	B	401[B]	ADP	O4'-C1'	14.97	1.62	1.41

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	401[B]	ADP	N3-C2-N1	-10.37	119.83	128.86
5	A	401[B]	ADP	N3-C2-N1	-10.26	119.92	128.86
5	A	401[B]	ADP	N6-C6-N1	-7.25	104.39	118.77
5	B	401[B]	ADP	N6-C6-N1	-7.20	104.49	118.77
8	B	403[A]	ATP	N3-C2-N1	-7.12	122.66	128.86
8	A	404[A]	ATP	N3-C2-N1	-7.03	122.73	128.86
8	A	404[A]	ATP	O2B-PB-O1B	-2.12	101.33	112.28
8	A	404[A]	ATP	O2A-PA-O1A	-2.07	101.58	112.28
8	B	403[A]	ATP	O2B-PB-O1B	-2.04	101.73	112.28
8	B	403[A]	ATP	O2A-PA-O1A	-2.01	101.90	112.28
8	A	404[A]	ATP	C2-N1-C6	5.23	127.92	118.77
8	B	403[A]	ATP	C2-N1-C6	5.32	128.08	118.77
5	B	401[B]	ADP	C5-C6-N6	7.51	135.79	120.47
5	A	401[B]	ADP	C5-C6-N6	7.52	135.80	120.47

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 (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 (i)

6.1 Protein, DNA and RNA chains (i)

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	305/354 (86%)	0.57	22 (7%)	16	18	32, 50, 122, 138	0
1	B	311/354 (87%)	0.44	14 (4%)	34	37	25, 40, 97, 134	0
2	C	217/230 (94%)	0.52	16 (7%)	15	17	24, 42, 97, 131	0
2	E	222/230 (96%)	0.13	0	100	100	22, 35, 58, 102	0
3	D	216/217 (99%)	0.49	21 (9%)	8	9	26, 46, 90, 135	0
3	F	216/217 (99%)	0.22	4 (1%)	67	72	28, 49, 71, 111	0
4	G	22/37 (59%)	3.95	17 (77%)	0	0	90, 112, 124, 143	0
All	All	1509/1639 (92%)	0.46	94 (6%)	21	23	22, 44, 103, 143	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	212	ILE	10.1
4	G	275	LEU	8.6
1	A	126	LEU	8.1
1	A	190	PHE	7.7
4	G	270	TYR	7.6
4	G	281	PHE	7.2
1	B	190	PHE	6.5
4	G	279	LEU	6.2
4	G	274	VAL	6.2
4	G	271	LEU	6.0
3	D	157	LEU	6.0
3	D	217	CYS	5.9
2	C	225	CYS	5.9
2	C	223	LYS	5.8
4	G	267	TRP	5.6
1	A	193	ILE	5.4
3	D	153	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
4	G	280	LEU	5.1
1	A	125	ALA	5.0
2	C	224	SER	4.9
1	A	186	LEU	4.8
1	B	193	ILE	4.7
1	A	100	MET	4.7
2	C	137	SER	4.6
1	A	189	LYS	4.5
2	C	168	LEU	4.4
4	G	277	VAL	4.4
3	D	212	PHE	4.4
4	G	276	LEU	4.3
4	G	278	MET	3.7
3	D	216	GLU	3.7
1	A	246[A]	PHE	3.6
1	A	129	LEU	3.6
3	D	152	LYS	3.6
1	B	129	LEU	3.6
1	A	216	LEU	3.5
2	C	198	LEU	3.4
1	A	219	LEU	3.4
1	A	215	LYS	3.3
1	B	284	ASN	3.3
1	A	187	LEU	3.3
1	A	124	GLY	3.2
4	G	285	ILE	3.2
1	B	100	MET	3.2
2	C	143	GLY	3.1
1	B	128	ASP	3.1
3	D	215	GLY	3.1
2	C	210	LYS	3.0
3	D	197	CYS	3.0
3	D	210	LYS	2.9
3	F	77	SER	2.8
2	C	222	PRO	2.8
1	A	211	ASP	2.8
1	B	246	PHE	2.8
1	A	128	ASP	2.7
3	D	193	LYS	2.7
1	B	212	ILE	2.7
4	G	284	LEU	2.7
1	B	192	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
3	D	117	SER	2.6
1	B	126	LEU	2.6
3	D	211	SER	2.6
1	B	345	LYS	2.5
4	G	282	ILE	2.5
3	F	157	LEU	2.4
3	D	194	VAL	2.4
4	G	287	LYS	2.4
2	C	136	SER	2.4
3	D	195	TYR	2.4
1	A	278	GLU	2.3
3	D	191	LYS	2.3
4	G	273	ILE	2.3
2	C	191	VAL	2.3
3	D	135	VAL	2.2
4	G	269	VAL	2.2
1	A	188	GLU	2.2
1	A	284	ASN	2.2
1	B	101	ALA	2.2
1	B	194	THR	2.2
2	C	130	VAL	2.2
3	D	113	VAL	2.2
3	F	129	LYS	2.2
2	C	172	VAL	2.2
1	B	4	THR	2.2
1	A	194	THR	2.1
1	A	294	MET	2.1
2	C	219	LYS	2.1
3	D	2	ASP	2.1
3	F	109	ILE	2.1
3	D	122	PRO	2.1
3	D	120	ILE	2.1
2	C	202	THR	2.1
2	C	199	GLY	2.1
3	D	196	ALA	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(Å^2)	Q<0.9
8	ATP	A	404[A]	31/31	0.96	0.14	0.33	30,36,45,48	42
5	ADP	A	401[B]	27/27	0.97	0.14	0.17	30,36,46,48	38
8	ATP	B	403[A]	31/31	0.96	0.15	0.07	25,34,45,52	43
5	ADP	B	401[B]	27/27	0.95	0.15	-0.10	30,36,45,50	39
7	ZN	A	403	1/1	0.94	0.09	-2.01	68,68,68,68	0
6	MG	A	402	1/1	0.94	0.05	-3.54	41,41,41,41	0
6	MG	B	402	1/1	0.94	0.08	-4.22	35,35,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.