



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:19 PM GMT

PDB ID : 4RIY  
Title : Crystal structure of an EGFR/HER3 kinase domain heterodimer containing the cancer-associated HER3-E909G mutation  
Authors : Littlefield, P.; Liu, L.; Jura, N.  
Deposited on : 2014-10-07  
Resolution : 2.98 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](mailto: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.

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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

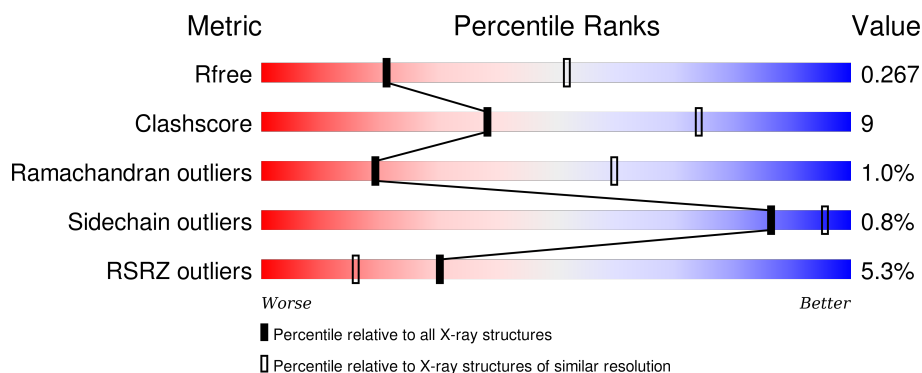
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.98 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	1992 (3.00-2.96)
Clashscore	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)
RSRZ outliers	91569	2007 (3.00-2.96)

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  $\geq 3$ , 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	326	<div> <div>7%</div> <div>73%10%17%</div> </div>
1	C	326	<div> <div>2%</div> <div>73%11%16%</div> </div>
2	B	345	<div> <div>7%</div> <div>69%14%15%</div> </div>
2	D	345	<div> <div>7%</div> <div>64%20%14%</div> </div>

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 9122 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 Receptor tyrosine-protein kinase erbB-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2118	1371	369	365	13			
1	C	275	Total	C	N	O	S	0	0	0
			2172	1407	373	379	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	676	GLY	-	EXPRESSION TAG	UNP P21860
A	677	ALA	-	EXPRESSION TAG	UNP P21860
A	678	GLY	-	EXPRESSION TAG	UNP P21860
A	909	GLY	GLU	ENGINEERED MUTATION	UNP P21860
C	676	GLY	-	EXPRESSION TAG	UNP P21860
C	677	ALA	-	EXPRESSION TAG	UNP P21860
C	678	GLY	-	EXPRESSION TAG	UNP P21860
C	909	GLY	GLU	ENGINEERED MUTATION	UNP P21860

- Molecule 2 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	293	Total	C	N	O	S	0	0	0
			2343	1510	397	421	15			
2	D	297	Total	C	N	O	S	0	0	0
			2369	1525	402	427	15			

There are 14 discrepancies between the modelled and reference sequences:

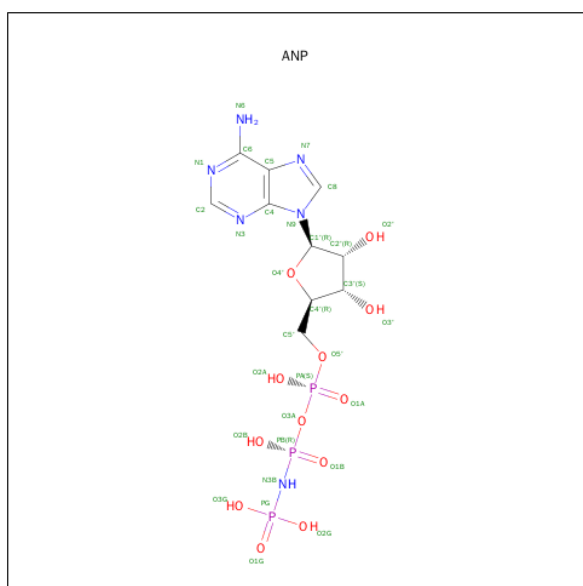
Chain	Residue	Modelled	Actual	Comment	Reference
B	654	GLY	-	EXPRESSION TAG	UNP P00533
B	655	ALA	-	EXPRESSION TAG	UNP P00533
B	656	MET	-	EXPRESSION TAG	UNP P00533
B	657	GLY	-	EXPRESSION TAG	UNP P00533

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Chain	Residue	Modelled	Actual	Comment	Reference
B	924	ARG	VAL	ENGINEERED MUTATION	UNP P00533
B	973	ALA	PHE	ENGINEERED MUTATION	UNP P00533
B	977	ALA	LEU	ENGINEERED MUTATION	UNP P00533
D	654	GLY	-	EXPRESSION TAG	UNP P00533
D	655	ALA	-	EXPRESSION TAG	UNP P00533
D	656	MET	-	EXPRESSION TAG	UNP P00533
D	657	GLY	-	EXPRESSION TAG	UNP P00533
D	924	ARG	VAL	ENGINEERED MUTATION	UNP P00533
D	973	ALA	PHE	ENGINEERED MUTATION	UNP P00533
D	977	ALA	LEU	ENGINEERED MUTATION	UNP P00533

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

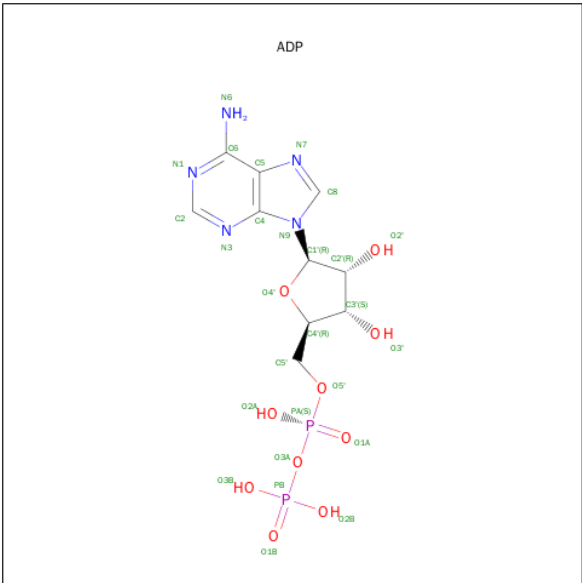
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).

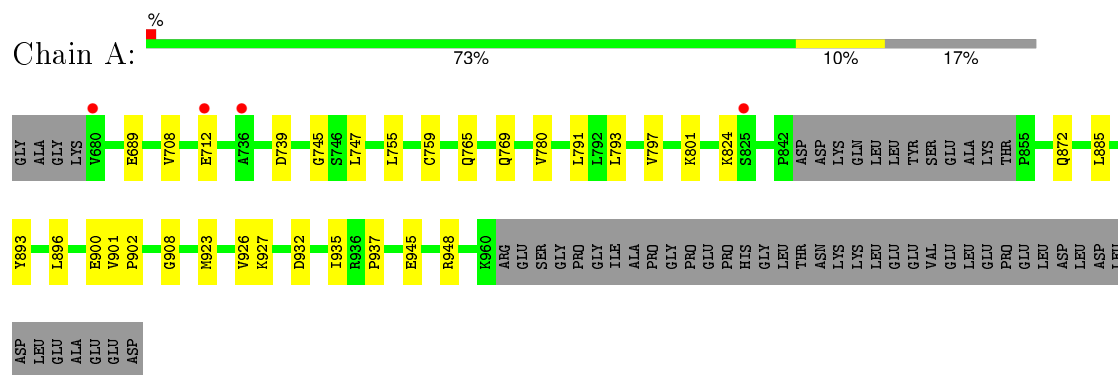


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

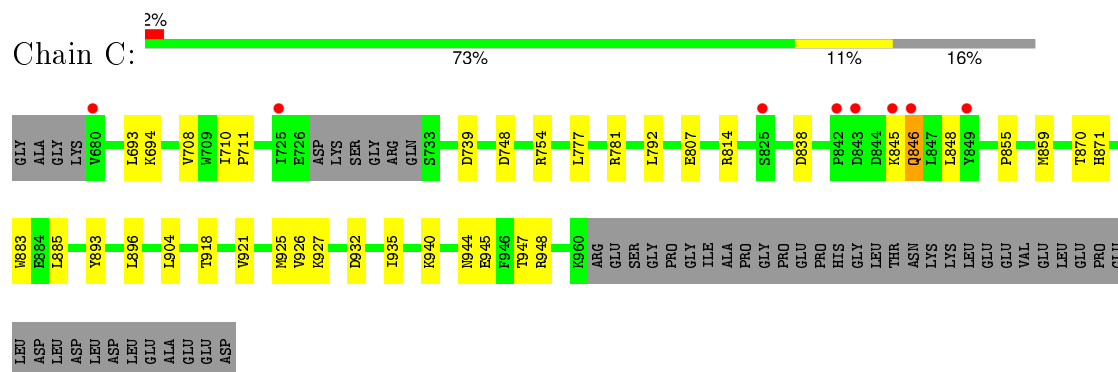
### 3 Residue-property plots [i](#)

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

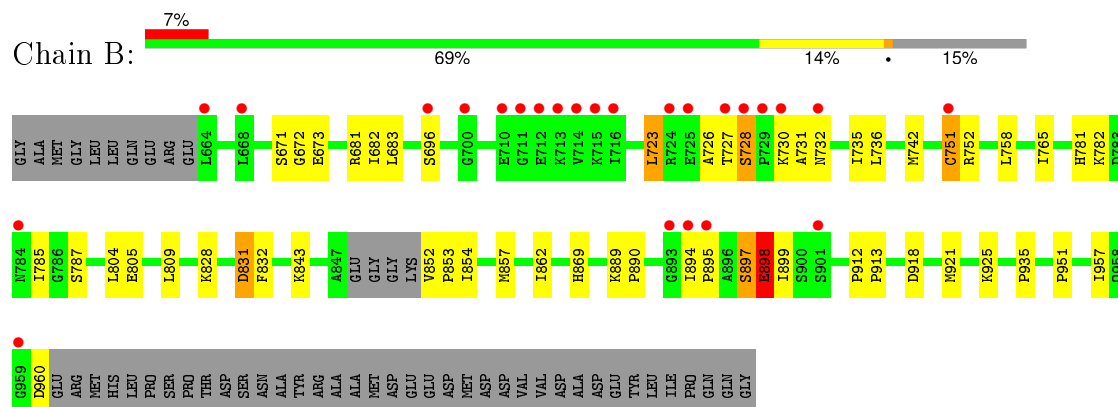
- Molecule 1: Receptor tyrosine-protein kinase erbB-3



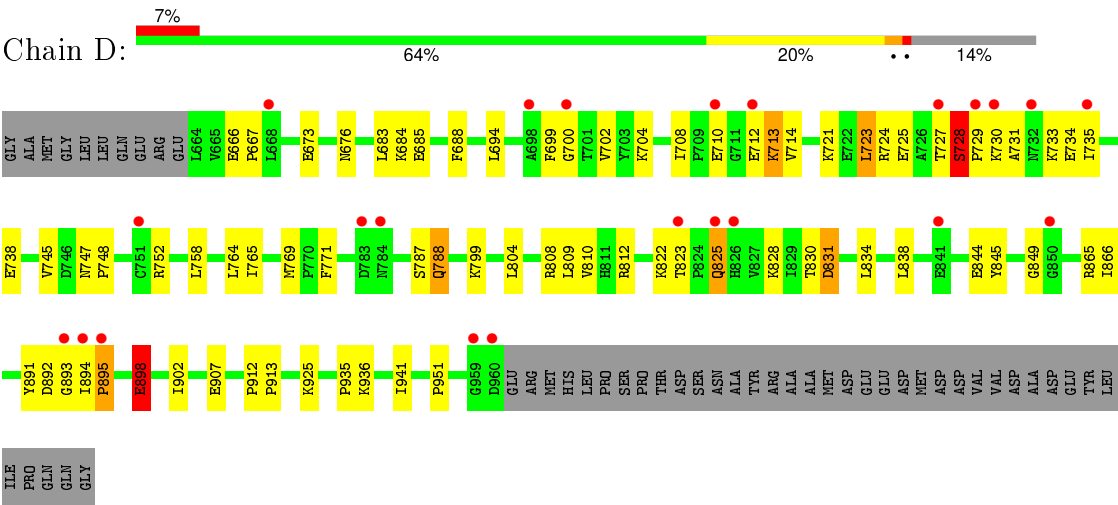
- Molecule 1: Receptor tyrosine-protein kinase erbB-3



- Molecule 2: Epidermal growth factor receptor



● Molecule 2: Epidermal growth factor receptor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.33Å 155.14Å 87.30Å 90.00° 110.93° 90.00°	Depositor
Resolution (Å)	56.20 – 2.98 56.79 – 2.98	Depositor EDS
% Data completeness (in resolution range)	97.6 (56.20-2.98) 93.2 (56.79-2.98)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.216 , 0.267 0.217 , 0.267	Depositor DCC
$R_{free}$ test set	3085 reflections (10.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.7	Xtriage
Anisotropy	0.643	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 54.9	EDS
Estimated twinning fraction	0.036 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 32359 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	9122	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.43% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, ANP, 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	0.26	0/2169	0.45	0/2940
1	C	0.24	0/2224	0.46	0/3017
2	B	0.33	1/2395 (0.0%)	0.56	0/3243
2	D	0.41	1/2422 (0.0%)	0.64	1/3279 (0.0%)
All	All	0.32	2/9210 (0.0%)	0.54	1/12479 (0.0%)

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	C	0	1
2	B	0	1
2	D	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	898	GLU	CG-CD	-8.07	1.39	1.51
2	B	898	GLU	CD-OE2	-5.26	1.19	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	723	LEU	CB-CG-CD2	-13.27	88.44	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	751	CYS	Peptide
1	C	846	GLN	Peptide
2	D	728	SER	Peptide

## 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	2118	0	2171	26	0
1	C	2172	0	2222	28	0
2	B	2343	0	2402	43	0
2	D	2369	0	2428	75	0
3	A	31	0	13	0	0
3	C	31	0	13	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	B	27	0	12	1	0
5	D	27	0	12	2	0
All	All	9122	0	9273	167	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 9.

The worst 5 of 167 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)
2:B:751:CYS:HB2	2:B:828:LYS:HD3	1.57	0.84
2:D:734:GLU:HG2	2:D:735:ILE:N	1.91	0.84
2:D:723:LEU:HD21	2:D:734:GLU:OE2	1.77	0.83
1:C:945:GLU:HG2	1:C:948:ARG:NH1	1.96	0.80
2:B:751:CYS:SG	2:B:752:ARG:N	2.56	0.78

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	265/326 (81%)	259 (98%)	5 (2%)	1 (0%)	39	79
1	C	271/326 (83%)	265 (98%)	6 (2%)	0	100	100
2	B	289/345 (84%)	271 (94%)	13 (4%)	5 (2%)	11	44
2	D	295/345 (86%)	276 (94%)	14 (5%)	5 (2%)	11	44
All	All	1120/1342 (84%)	1071 (96%)	38 (3%)	11 (1%)	19	60

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	747	LEU
2	B	897	SER
2	B	898	GLU
2	D	713	LYS
2	B	672	GLY

### 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	228/277 (82%)	227 (100%)	1 (0%)	93	98
1	C	235/277 (85%)	235 (100%)	0	100	100
2	B	258/300 (86%)	255 (99%)	3 (1%)	78	93
2	D	260/300 (87%)	256 (98%)	4 (2%)	72	91
All	All	981/1154 (85%)	973 (99%)	8 (1%)	86	95

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	843	LYS
2	D	898	GLU
2	D	788	GLN
2	B	723	LEU
2	D	728	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 8 ligands modelled in this entry, 4 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	$\# Z  > 2$
3	ANP	A	1101	4	27,33,33	1.28	4 (14%)	30,52,52	1.00	2 (6%)
5	ADP	B	1001	4	22,29,29	1.00	1 (4%)	27,45,45	1.95	4 (14%)
3	ANP	C	1101	4	27,33,33	1.32	4 (14%)	30,52,52	0.94	1 (3%)
5	ADP	D	1001	4	22,29,29	1.03	1 (4%)	27,45,45	1.95	5 (18%)

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	ANP	A	1101	4	-	0/12/38/38	0/3/3/3
5	ADP	B	1001	4	-	0/12/32/32	0/3/3/3
3	ANP	C	1101	4	-	0/12/38/38	0/3/3/3
5	ADP	D	1001	4	-	0/12/32/32	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	ANP	PB-N3B	2.11	1.68	1.63
3	C	1101	ANP	PB-N3B	2.11	1.68	1.63
3	A	1101	ANP	PG-N3B	2.57	1.70	1.63
3	C	1101	ANP	PG-N3B	2.66	1.70	1.63
5	B	1001	ADP	C5-C4	3.13	1.47	1.40

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1001	ADP	N3-C2-N1	-6.92	123.60	128.89
5	D	1001	ADP	N3-C2-N1	-6.60	123.84	128.89
5	B	1001	ADP	C2'-C1'-N9	-3.74	108.58	114.29
5	D	1001	ADP	PA-O3A-PB	-3.61	120.56	132.67
5	D	1001	ADP	C2'-C1'-N9	-3.44	109.03	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1001	ADP	1	0
3	C	1101	ANP	1	0
5	D	1001	ADP	2	0

## 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	269/326 (82%)	0.31	4 (1%) 76 56	18, 38, 67, 110	0
1	C	275/326 (84%)	0.30	8 (2%) 55 33	17, 37, 72, 107	0
2	B	293/345 (84%)	0.75	25 (8%) 13 6	20, 42, 98, 123	0
2	D	297/345 (86%)	0.71	23 (7%) 16 8	20, 44, 93, 128	0
All	All	1134/1342 (84%)	0.52	60 (5%) 30 16	17, 41, 88, 128	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	714	VAL	6.9
2	B	729	PRO	5.4
2	B	713	LYS	5.4
2	D	729	PRO	5.0
2	D	710	GLU	4.4

### 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
5	ADP	B	1001	27/27	0.73	0.32	1.98	62,74,145,146	0
5	ADP	D	1001	27/27	0.79	0.26	0.45	50,62,144,145	0
3	ANP	A	1101	31/31	0.95	0.20	-0.04	25,42,62,89	0
3	ANP	C	1101	31/31	0.96	0.16	-0.76	17,31,47,79	0
4	MG	B	1002	1/1	0.77	0.34	-	60,60,60,60	0
4	MG	A	1102	1/1	0.88	0.10	-	23,23,23,23	0
4	MG	C	1102	1/1	0.90	0.21	-	17,17,17,17	0
4	MG	D	1002	1/1	0.82	0.17	-	59,59,59,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.