



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2017 – 12:46 PM EDT

PDB ID : 5XZE
Title : Mouse cGAS bound to the inhibitor RU332
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Imaeda, T.; Aida, J.; Rothamel, K.; Gogakos, T.; Steinberg, J.; Reasoner, S.;
Aso, K.; Tuschl, T.; Patel, D.J.; Glickman, J.F.; Ascano, M.
Deposited on : unknown
Resolution : 2.18 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
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-20030345

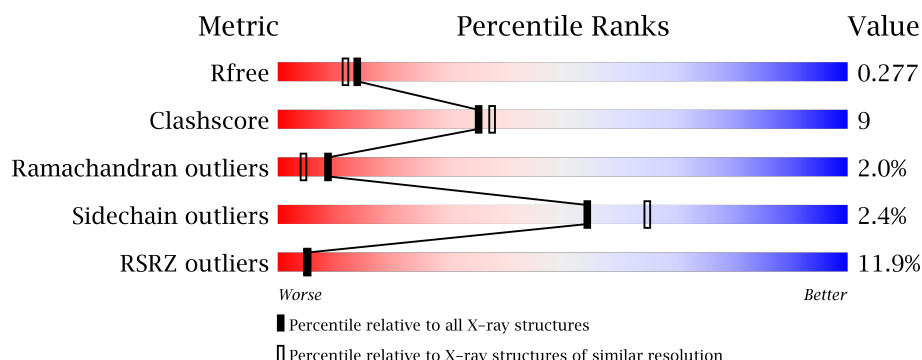
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	5526 (2.20-2.16)
Clashscore	112137	6386 (2.20-2.16)
Ramachandran outliers	110173	6282 (2.20-2.16)
Sidechain outliers	110143	6282 (2.20-2.16)
RSRZ outliers	101464	5562 (2.20-2.16)

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>12%</div> <div>76%</div> <div>20%</div> <div>..</div> </div>
2	E	15	<div> <div>13%</div> <div>80%</div> <div>20%</div> </div>
3	F	14	<div> <div>14%</div> <div>93%</div> <div>7%</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3638 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 Cyclic GMP-AMP synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	0	0
			2937	1889	497	538	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	146	SER	-	expression tag	UNP Q8C6L5

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*AP*AP*TP*TP*GP*CP*CP*GP*AP*AP*GP*AP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	15	Total	C	N	O	P	0	0	0
			308	147	63	84	14			

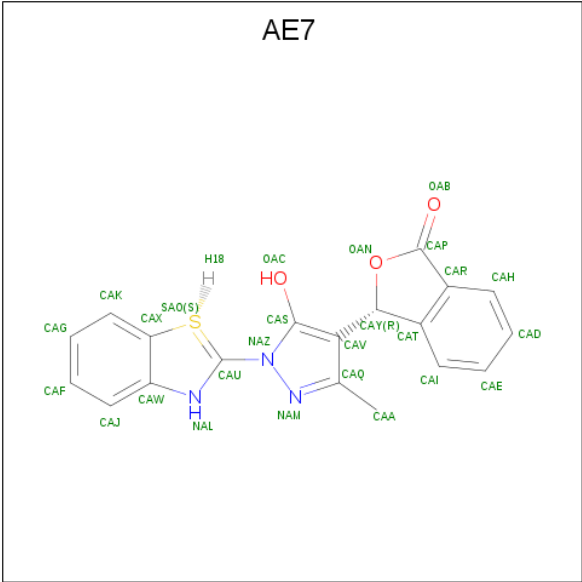
- Molecule 3 is a DNA chain called DNA (5'-D(P*CP*GP*TP*CP*TP*TP*CP*GP*GP*CP*AP*AP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	14	Total	C	N	O	P	0	0	0
			284	136	47	87	14			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

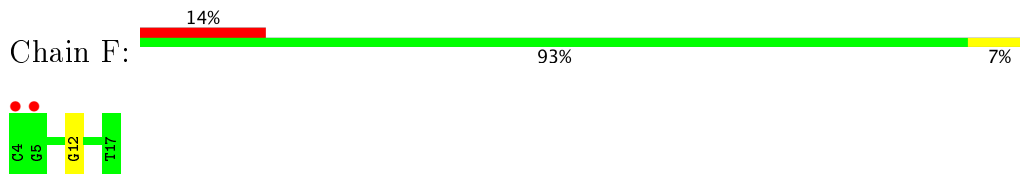
- Molecule 5 is (3R)-3-[1-(3H-lambda 4 ,3-benzothiazol-2-yl)-5-hydroxy-3-methyl-1H-pyrazol-4-yl]-2-benzofuran-1(3H)-one (three-letter code: AE7) (formula: C₁₉H₁₅N₃O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			26	19	3	3	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	63	Total	O	0	0
			63	63		
6	E	14	Total	O	0	0
			14	14		
6	F	5	Total	O	0	0
			5	5		



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	85.28 Å 98.63 Å 129.18 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.20 – 2.18 39.20 – 2.18	Depositor EDS
% Data completeness (in resolution range)	98.1 (39.20-2.18) 95.7 (39.20-2.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.18 Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.242 , 0.281 0.243 , 0.277	Depositor DCC
R_{free} test set	1393 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.966	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3638	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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, 0.333 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: ZN, AE7

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	0.45	0/3001	0.54	0/4031
2	E	0.61	0/347	0.88	0/534
3	F	0.67	0/316	1.02	0/485
All	All	0.49	0/3664	0.65	0/5050

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	243	PRO	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	2937	0	2967	61	1
2	E	308	0	169	2	0
3	F	284	0	160	2	0
4	A	1	0	0	0	0
5	A	26	0	0	1	0
6	A	63	0	0	5	0
6	E	14	0	0	1	0
6	F	5	0	0	1	0
All	All	3638	0	3296	64	1

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.

All (64) 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:315:LYS:NZ	6:A:701:HOH:O	1.90	1.01
1:A:188:GLU:N	1:A:188:GLU:OE2	1.94	1.00
1:A:356:ASN:O	1:A:356:ASN:ND2	2.03	0.90
1:A:246:ASN:HB2	1:A:247:PRO:HD2	1.68	0.76
1:A:173:LYS:NZ	1:A:279:ASP:OD2	2.17	0.74
1:A:481:ILE:O	1:A:486:LYS:NZ	2.24	0.71
1:A:184:LYS:O	1:A:184:LYS:HG3	1.91	0.71
1:A:290:GLY:HA2	1:A:350:LYS:HE2	1.75	0.69
1:A:184:LYS:N	1:A:190:LYS:HE3	2.07	0.69
1:A:354:ASP:OD1	1:A:355:GLY:N	2.26	0.69
1:A:381:GLU:OE2	6:A:703:HOH:O	2.11	0.69
1:A:190:LYS:O	1:A:192:VAL:N	2.25	0.65
1:A:222:ARG:HB3	1:A:240:LYS:HB2	1.80	0.64
1:A:248:LEU:HD22	1:A:262:MET:HE2	1.79	0.64
1:A:353:LYS:HG3	1:A:358:PHE:CE2	2.35	0.62
1:A:258:SER:OG	1:A:261:LYS:HG3	2.00	0.62
2:E:12:DG:OP1	6:E:101:HOH:O	2.16	0.61
1:A:436:GLN:HB2	1:A:439:GLN:HG3	1.84	0.60
3:F:12:DG:OP2	6:F:101:HOH:O	2.17	0.59
1:A:341:ARG:NH1	6:A:707:HOH:O	2.22	0.58
1:A:247:PRO:O	1:A:250:HIS:CD2	2.57	0.58
1:A:353:LYS:HE2	1:A:356:ASN:HA	1.87	0.55
1:A:383:THR:O	1:A:389:GLY:HA3	2.06	0.55
1:A:260:THR:OG1	1:A:360:GLY:O	2.17	0.55
1:A:249:SER:HA	1:A:252:LEU:HG	1.90	0.53
1:A:184:LYS:H	1:A:190:LYS:HE3	1.71	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:VAL:HG13	1:A:282:VAL:HG13	1.90	0.52
1:A:464:LYS:HE2	1:A:466:ASP:OD1	2.09	0.51
1:A:188:GLU:H	1:A:188:GLU:CD	2.04	0.51
1:A:483:ARG:HG2	1:A:487:GLU:OE1	2.12	0.50
1:A:183:GLN:HA	1:A:190:LYS:HD2	1.92	0.49
1:A:172:ASN:O	1:A:176:GLU:HG2	2.13	0.49
1:A:222:ARG:HH21	1:A:240:LYS:HB3	1.78	0.49
1:A:359:GLN:OE1	1:A:362:THR:HG23	2.13	0.49
1:A:184:LYS:C	1:A:185:ARG:HG3	2.34	0.48
1:A:185:ARG:O	1:A:187:SER:N	2.47	0.47
1:A:181:ARG:O	1:A:184:LYS:HG2	2.15	0.47
1:A:372:LYS:NZ	3:F:12:DG:OP1	2.39	0.47
1:A:267:ARG:NE	1:A:287:GLU:HG2	2.31	0.46
1:A:190:LYS:C	1:A:192:VAL:H	2.17	0.45
1:A:488:PHE:O	1:A:492:LYS:HG2	2.16	0.45
1:A:227:GLU:OE1	1:A:472:LYS:NZ	2.46	0.44
2:E:1:DA:H2"	2:E:2:DA:N7	2.31	0.44
1:A:351:ASN:HB3	1:A:359:GLN:O	2.18	0.44
1:A:315:LYS:NZ	6:A:704:HOH:O	2.19	0.44
1:A:179:LEU:O	1:A:183:GLN:HG2	2.18	0.44
1:A:407:GLN:HB3	1:A:503:ILE:HG12	1.99	0.44
1:A:188:GLU:OE1	1:A:265:LYS:HG2	2.19	0.43
1:A:248:LEU:HD13	1:A:262:MET:HE1	2.01	0.43
1:A:185:ARG:H	1:A:190:LYS:HZ1	1.66	0.43
1:A:220:VAL:HA	1:A:221:PRO:HD3	1.85	0.42
1:A:414:GLU:N	1:A:414:GLU:OE1	2.51	0.42
1:A:193:GLU:OE2	6:A:706:HOH:O	2.22	0.42
1:A:257:LEU:HD21	1:A:262:MET:HE1	2.00	0.42
1:A:419:CYS:SG	5:A:602:AE7:CAY	3.07	0.42
1:A:288:LYS:HA	1:A:289:PRO:HD2	1.88	0.42
1:A:354:ASP:CG	1:A:355:GLY:N	2.73	0.42
1:A:492:LYS:HA	1:A:492:LYS:HD2	1.92	0.42
1:A:185:ARG:H	1:A:190:LYS:NZ	2.18	0.42
1:A:187:SER:HA	1:A:188:GLU:OE2	2.20	0.41
1:A:170:THR:HG23	1:A:280:ILE:HD13	2.03	0.40
1:A:226:GLN:NE2	1:A:238:LYS:HE3	2.36	0.40
1:A:267:ARG:CZ	1:A:287:GLU:HG2	2.51	0.40
1:A:177:ARG:HE	1:A:177:ARG:HB3	1.68	0.40

All (1) 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)
1:A:354:ASP:OD1	1:A:354:ASP:OD1[2_895]	1.26	0.94

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	355/362 (98%)	331 (93%)	17 (5%)	7 (2%)	9 4

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	GLU
1	A	190	LYS
1	A	191	GLY
1	A	185	ARG
1	A	244	ARG
1	A	183	GLN
1	A	300	ASN

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	327/335 (98%)	319 (98%)	8 (2%)	54 65

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	LYS
1	A	185	ARG
1	A	250	HIS
1	A	353	LYS
1	A	354	ASP
1	A	356	ASN
1	A	391	LYS
1	A	479	GLU

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

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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	AE7	A	602	-	24,30,30	4.82	11 (45%)	24,45,45	3.39	6 (25%)

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	AE7	A	602	-	-	0/0/28/28	0/5/5/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	AE7	NAM-NAZ	-15.22	1.11	1.39
5	A	602	AE7	CAV-CAY	-9.03	1.41	1.53
5	A	602	AE7	CAT-CAY	-7.95	1.40	1.51
5	A	602	AE7	CAR-CAP	-5.94	1.33	1.47
5	A	602	AE7	CAK-CAX	-5.85	1.33	1.40
5	A	602	AE7	CAJ-CAW	-4.93	1.33	1.41
5	A	602	AE7	CAI-CAT	-4.51	1.33	1.39
5	A	602	AE7	OAN-CAY	-4.26	1.42	1.46
5	A	602	AE7	CAH-CAR	-3.89	1.33	1.39
5	A	602	AE7	CAR-CAT	-3.60	1.33	1.39
5	A	602	AE7	CAV-CAS	-2.80	1.32	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	602	AE7	CAY-OAN-CAP	-11.88	101.58	110.63
5	A	602	AE7	CAT-CAR-CAP	-5.09	106.29	108.50
5	A	602	AE7	CAW-CAX-SAO	-3.32	107.86	112.03
5	A	602	AE7	CAX-CAW-NAL	2.20	113.11	108.04
5	A	602	AE7	OAN-CAP-OAB	3.23	124.11	121.23
5	A	602	AE7	OAN-CAP-CAR	7.59	113.11	108.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	602	AE7	1	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	357/362 (98%)	0.98	42 (11%) 5 5	34, 59, 97, 127	0
2	E	15/15 (100%)	0.65	2 (13%) 4 4	42, 76, 143, 152	0
3	F	14/14 (100%)	0.69	2 (14%) 3 3	53, 84, 130, 139	0
All	All	386/391 (98%)	0.96	46 (11%) 5 5	34, 61, 105, 152	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	242	ILE	10.8
1	A	151	LYS	5.3
1	A	185	ARG	4.6
1	A	356	ASN	4.4
1	A	246	ASN	4.3
1	A	239	PHE	4.3
1	A	255	GLU	4.3
1	A	240	LYS	4.1
1	A	297	LEU	3.9
1	A	243	PRO	3.9
1	A	244	ARG	3.8
1	A	289	PRO	3.7
1	A	245	GLY	3.6
1	A	250	HIS	3.2
1	A	195	LEU	3.2
3	F	4	DC	3.2
1	A	248	LEU	3.1
1	A	288	LYS	3.1
2	E	15	DG	3.0
1	A	358	PHE	3.0
1	A	252	LEU	2.9
1	A	224	GLU	2.9
1	A	201	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	192	VAL	2.7
1	A	488	PHE	2.6
2	E	1	DA	2.6
1	A	222	ARG	2.6
1	A	253	GLU	2.6
1	A	223	ILE	2.6
1	A	221	PRO	2.6
1	A	226	GLN	2.5
1	A	247	PRO	2.5
1	A	405	LEU	2.4
1	A	198	GLY	2.4
1	A	310	LEU	2.4
1	A	149	LYS	2.3
1	A	214	VAL	2.3
1	A	478	GLN	2.3
1	A	421	TYR	2.2
1	A	428	PHE	2.2
1	A	354	ASP	2.2
1	A	355	GLY	2.2
1	A	440	TRP	2.2
1	A	484	LYS	2.2
3	F	5	DG	2.1
1	A	418	PHE	2.1

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	AE7	A	602	26/26	0.77	0.21	1.25	81,83,86,148	0
4	ZN	A	601	1/1	-	-	-	39,39,39,39	1

6.5 Other polymers [i](#)

There are no such residues in this entry.