



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 08:00 pm GMT

PDB ID : 2PW3
Title : Structure of the PDE4D-cAMP complex
Authors : Wang, H.; Robinson, H.; Ke, H.
Deposited on : 2007-05-10
Resolution : 1.56 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 : trunk28620
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) : recalc28949

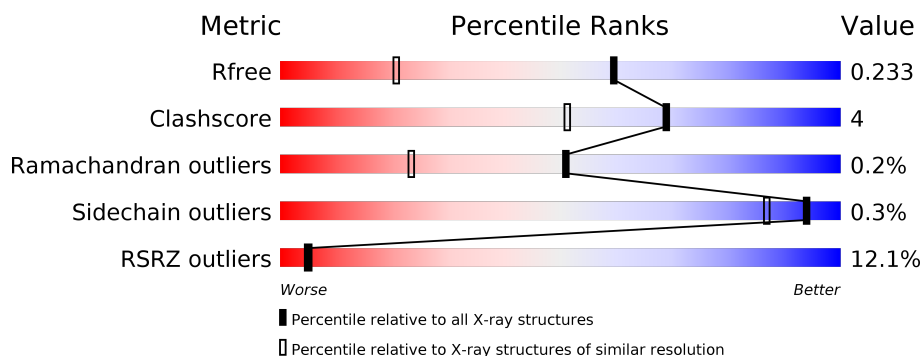
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.56 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	1088 (1.56-1.56)
Clashscore	112137	1132 (1.56-1.56)
Ramachandran outliers	110173	1110 (1.56-1.56)
Sidechain outliers	110143	1108 (1.56-1.56)
RSRZ outliers	101464	1089 (1.56-1.56)

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	327	 6% 92% 8%
1	B	327	 18% 88% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5854 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 cAMP-specific 3',5'-cyclic phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2648	1673	453	508	14			
1	B	325	Total	C	N	O	S	0	0	0
			2632	1664	451	503	14			

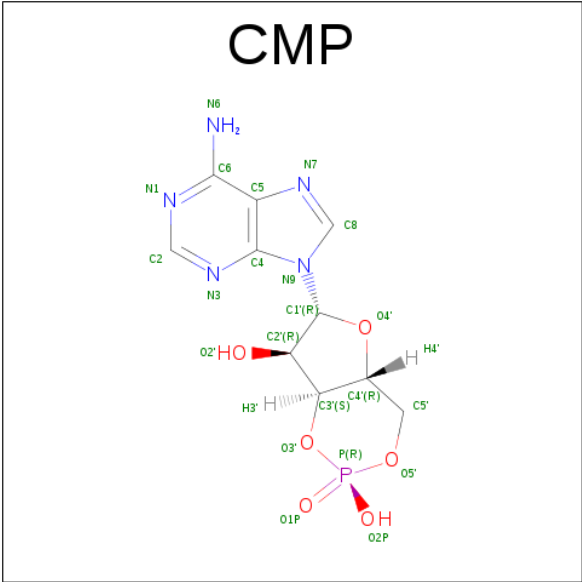
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	ASN	ASP	ENGINEERED	UNP Q08499
B	201	ASN	ASP	ENGINEERED	UNP Q08499

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (three-letter code: CMP) (formula: C₁₀H₁₂N₅O₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
3	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

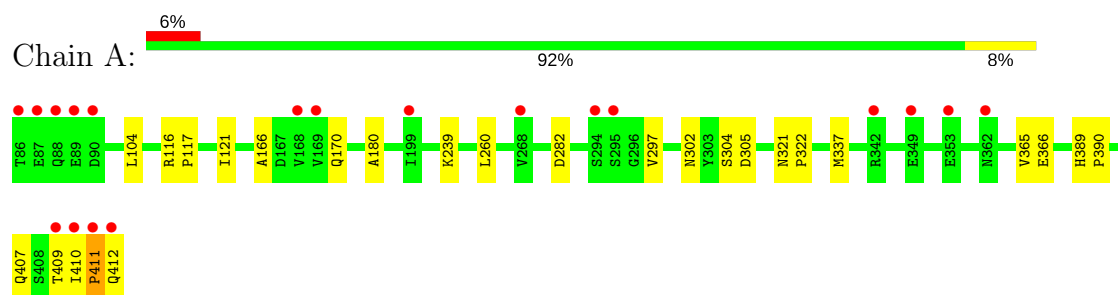
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	323	Total	O	0	0
			323	323		
4	B	205	Total	O	0	0
			205	205		

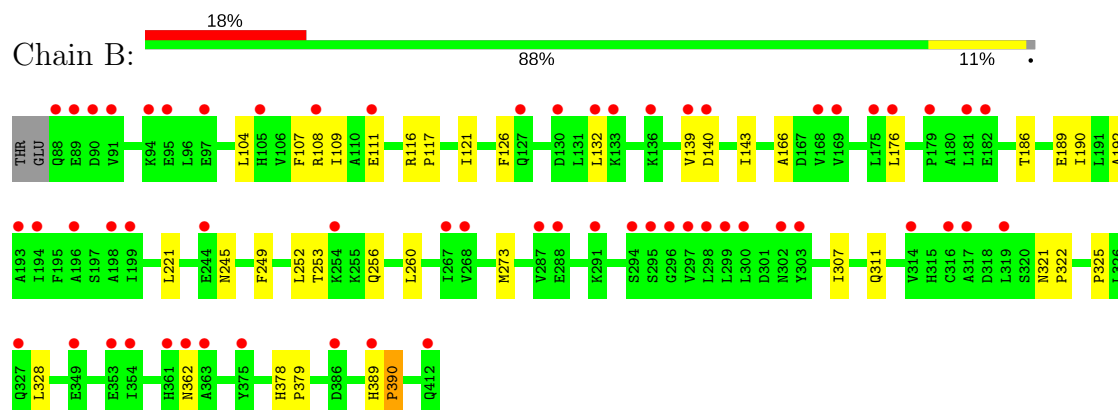
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.85Å 81.00Å 163.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.56 28.92 – 1.56	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.56) 94.8 (28.92-1.56)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 1.56Å)	Xtriage
Refinement program	CNS1.2	Depositor
R, R_{free}	0.212 , 0.231 0.215 , 0.233	Depositor DCC
R_{free} test set	10420 reflections (10.00%)	DCC
Wilson B-factor (Å ²)	17.5	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5854	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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

5.1 Standard geometry

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

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	0.28	0/2702	0.53	0/3670
1	B	0.27	0/2686	0.50	0/3648
All	All	0.27	0/5388	0.52	0/7318

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

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	2648	0	2601	18	0
1	B	2632	0	2588	26	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	22	0	11	1	0
3	B	22	0	11	2	0
4	A	323	0	0	1	0
4	B	205	0	0	1	0
All	All	5854	0	5211	45	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 4.

All (45) 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)
3:A:1:CMP:H2	3:A:1:CMP:C2	0.97	1.48
3:B:1:CMP:H2	3:B:1:CMP:C2	0.97	1.48
1:B:321:ASN:HB2	1:B:322:PRO:HD3	1.75	0.69
1:A:407:GLN:O	1:A:411:PRO:HD3	1.95	0.66
1:A:302:ASN:ND2	1:A:305:ASP:H	1.95	0.64
1:B:192:ALA:HB2	1:B:260:LEU:HD12	1.82	0.59
1:B:249:PHE:HA	1:B:252:LEU:HD13	1.84	0.59
1:A:321:ASN:HB2	1:A:322:PRO:HD3	1.84	0.58
1:B:253:THR:OG1	1:B:256:GLN:HG3	2.04	0.58
1:B:362:ASN:HB2	4:B:674:HOH:O	2.06	0.55
1:B:121:ILE:HD12	1:B:166:ALA:HB1	1.90	0.54
1:B:126:PHE:HB3	1:B:132:LEU:HD11	1.91	0.52
1:A:410:ILE:O	1:A:412:GLN:HG3	2.10	0.52
1:A:180:ALA:O	1:A:297:VAL:HG13	2.09	0.51
1:B:325:PRO:HD2	1:B:328:LEU:HD12	1.93	0.50
1:B:249:PHE:CE1	1:B:260:LEU:HD21	2.47	0.49
1:A:337:MET:CE	1:A:365:VAL:HG22	2.42	0.49
1:B:132:LEU:HD12	1:B:132:LEU:H	1.78	0.48
1:A:389:HIS:CE1	1:A:390:PRO:HB3	2.49	0.48
1:B:107:PHE:O	1:B:111:GLU:HG3	2.15	0.46
1:B:132:LEU:HD12	1:B:132:LEU:N	2.31	0.45
1:A:104:LEU:HD22	1:A:170:GLN:HG3	1.98	0.45
1:A:116:ARG:N	1:A:117:PRO:CD	2.79	0.45
1:B:139:VAL:O	1:B:143:ILE:HG12	2.16	0.45
1:B:126:PHE:HB3	1:B:132:LEU:CD1	2.46	0.45
1:B:307:ILE:O	1:B:311:GLN:HG3	2.17	0.44
1:B:249:PHE:CZ	1:B:260:LEU:HD21	2.52	0.44
1:B:186:THR:OG1	1:B:189:GLU:HG3	2.18	0.44
1:A:282:ASP:HB2	4:A:665:HOH:O	2.18	0.44
1:A:410:ILE:O	1:A:412:GLN:N	2.51	0.44
1:A:366:GLU:HG2	1:A:409:THR:OG1	2.18	0.43
1:B:139:VAL:HG13	1:B:140:ASP:N	2.32	0.43
1:B:104:LEU:HD11	1:B:109:ILE:HD11	2.00	0.43
1:B:116:ARG:N	1:B:117:PRO:CD	2.82	0.43
1:B:378:HIS:HB3	1:B:379:PRO:HD3	2.00	0.43
1:A:121:ILE:HD12	1:A:166:ALA:HB1	2.01	0.42
1:A:239:LYS:HD3	1:B:221:LEU:HD21	1.99	0.42
1:A:302:ASN:ND2	1:A:304:SER:HB3	2.34	0.42
1:A:337:MET:HE2	1:A:365:VAL:HG22	2.00	0.42
1:B:273:MET:HG3	3:B:1:CMP:H4'	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LEU:HD13	1:A:260:LEU:C	2.41	0.41
1:B:108:ARG:HG2	1:B:108:ARG:HH11	1.85	0.41
1:B:176:LEU:HD13	1:B:190:ILE:HG23	2.04	0.40
1:A:410:ILE:HB	1:A:411:PRO:HD3	2.03	0.40
1:B:389:HIS:CE1	1:B:390:PRO: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	325/327 (99%)	316 (97%)	8 (2%)	1 (0%)	44	19
1	B	323/327 (99%)	312 (97%)	11 (3%)	0	100	100
All	All	648/654 (99%)	628 (97%)	19 (3%)	1 (0%)	51	23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	411	PRO

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	299/299 (100%)	299 (100%)	0	100	100
1	B	297/299 (99%)	295 (99%)	2 (1%)	87	74
All	All	596/598 (100%)	594 (100%)	2 (0%)	94	87

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	245	ASN
1	B	390	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	242	GLN
1	A	245	ASN
1	A	302	ASN
1	A	389	HIS
1	B	88	GLN
1	B	127	GLN
1	B	242	GLN
1	B	245	ASN
1	B	278	ASN
1	B	362	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	CMP	A	1	-	21,25,25	0.97	1 (4%)	22,39,39	1.99	3 (13%)
3	CMP	B	1	-	21,25,25	0.95	1 (4%)	22,39,39	2.01	3 (13%)

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	CMP	A	1	-	-	0/0/31/31	0/4/4/4
3	CMP	B	1	-	-	0/0/31/31	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	CMP	O3'-C3'	-2.20	1.41	1.44
3	A	1	CMP	O3'-C3'	-2.17	1.41	1.44

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	CMP	O3'-C3'-C4'	-7.41	104.98	110.69
3	B	1	CMP	O3'-C3'-C4'	-7.36	105.01	110.69
3	A	1	CMP	O3'-C3'-C2'	2.55	118.22	115.67
3	B	1	CMP	O3'-C3'-C2'	3.12	118.79	115.67
3	B	1	CMP	O2P-P-O1P	3.39	119.63	108.63
3	A	1	CMP	O2P-P-O1P	3.41	119.71	108.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	CMP	1	0
3	B	1	CMP	2	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	327/327 (100%)	0.37	19 (5%) 24 27	11, 17, 31, 52	0
1	B	325/327 (99%)	1.00	60 (18%) 1 2	12, 24, 42, 57	0
All	All	652/654 (99%)	0.68	79 (12%) 5 5	11, 20, 41, 57	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	86	THR	15.3
1	A	295	SER	7.9
1	B	91	VAL	7.5
1	B	412	GLN	6.0
1	A	412	GLN	5.8
1	B	130	ASP	5.5
1	A	87	GLU	5.2
1	B	362	ASN	5.1
1	B	108	ARG	4.7
1	B	88	GLN	4.7
1	B	90	ASP	4.7
1	B	287	VAL	4.7
1	B	133	LYS	4.4
1	B	89	GLU	4.3
1	B	303	TYR	4.3
1	B	139	VAL	4.1
1	A	411	PRO	4.1
1	B	375	TYR	4.0
1	B	294	SER	4.0
1	A	410	ILE	3.9
1	B	94	LYS	3.8
1	A	89	GLU	3.7
1	A	294	SER	3.7
1	B	168	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	136	LYS	3.5
1	B	295	SER	3.5
1	A	90	ASP	3.4
1	B	140	ASP	3.4
1	B	254	LYS	3.3
1	B	132	LEU	3.2
1	B	298	LEU	3.2
1	B	300	LEU	3.1
1	B	302	ASN	3.1
1	B	319	LEU	3.0
1	B	105	HIS	3.0
1	B	182	GLU	2.9
1	A	362	ASN	2.9
1	B	193	ALA	2.9
1	B	297	VAL	2.9
1	B	314	VAL	2.8
1	A	169	VAL	2.8
1	B	175	LEU	2.7
1	B	176	LEU	2.7
1	B	181	LEU	2.7
1	B	291	LYS	2.7
1	B	361	HIS	2.7
1	B	386	ASP	2.7
1	B	363	ALA	2.7
1	B	288	GLU	2.6
1	B	199	ILE	2.6
1	B	327	GLN	2.6
1	A	342	ARG	2.6
1	A	88	GLN	2.6
1	A	353	GLU	2.5
1	A	168	VAL	2.5
1	A	199	ILE	2.5
1	A	349	GLU	2.5
1	B	179	PRO	2.5
1	B	127	GLN	2.4
1	B	198	ALA	2.4
1	B	111	GLU	2.3
1	B	194	ILE	2.3
1	B	389	HIS	2.3
1	B	244	GLU	2.3
1	B	296	GLY	2.3
1	B	354	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	268	VAL	2.3
1	B	349	GLU	2.3
1	B	299	LEU	2.2
1	B	353	GLU	2.2
1	B	317	ALA	2.2
1	A	409	THR	2.2
1	B	97	GLU	2.2
1	B	267	ILE	2.1
1	B	169	VAL	2.1
1	B	268	VAL	2.1
1	B	95	GLU	2.1
1	B	316	CYS	2.1
1	B	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
3	CMP	B	1	22/22	0.95	0.08	-0.76	20,23,26,27	0
3	CMP	A	1	22/22	0.95	0.08	-0.79	19,22,24,27	0
2	ZN	B	501	1/1	0.99	0.08	-2.05	22,22,22,22	0
2	ZN	A	501	1/1	0.99	0.06	-4.21	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.