



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:23 PM GMT

PDB ID : 3ZBR
Title : Catalytic domain of mouse 2',3'-cyclic nucleotide 3'- phosphodiesterase, with mutation H230S, crystallized with NADP
Authors : Myllykoski, M.; Raasakka, A.; Lehtimäki, M.; Han, H.; Kursula, P.
Deposited on : 2012-11-13
Resolution : 2.30 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 (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

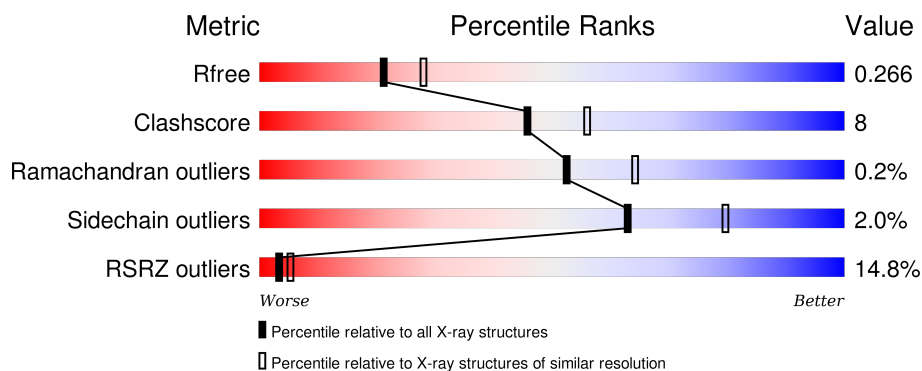
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	221	<div> <div>8%</div> <div>79%</div> <div>17%</div> <div>• •</div> </div>
1	B	221	<div> <div>20%</div> <div>76%</div> <div>19%</div> <div>• 5%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6890 atoms, of which 3403 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.

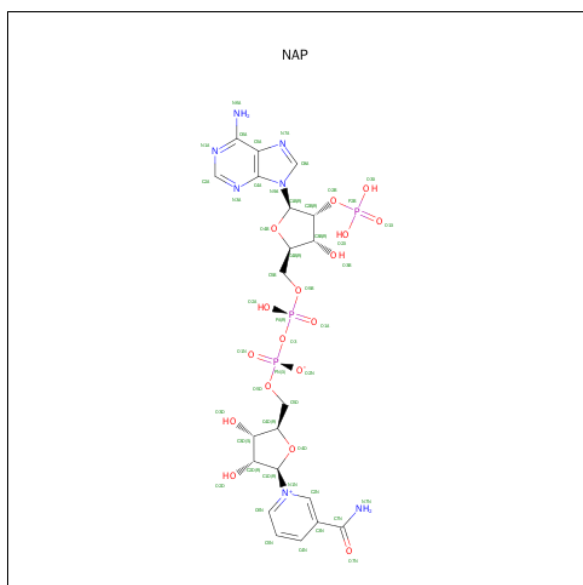
- Molecule 1 is a protein called 2', 3'-CYCLIC-NUCLEOTIDE 3'-PHOSPHODIESTERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	215	Total	C	H	N	O	S	0	0	0
			3359	1074	1691	279	310	5			
1	B	211	Total	C	H	N	O	S	0	0	0
			3297	1054	1662	274	302	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	158	GLY	-	EXPRESSION TAG	UNP P16330
A	230	SER	HIS	ENGINEERED MUTATION	UNP P16330
B	158	GLY	-	EXPRESSION TAG	UNP P16330
B	230	SER	HIS	ENGINEERED MUTATION	UNP P16330

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
2	B	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		

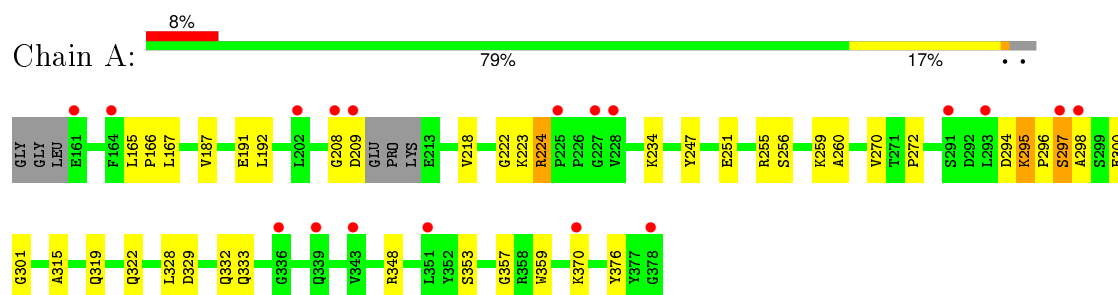
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	51	Total	O	0	0
			51	51		
3	B	37	Total	O	0	0
			37	37		

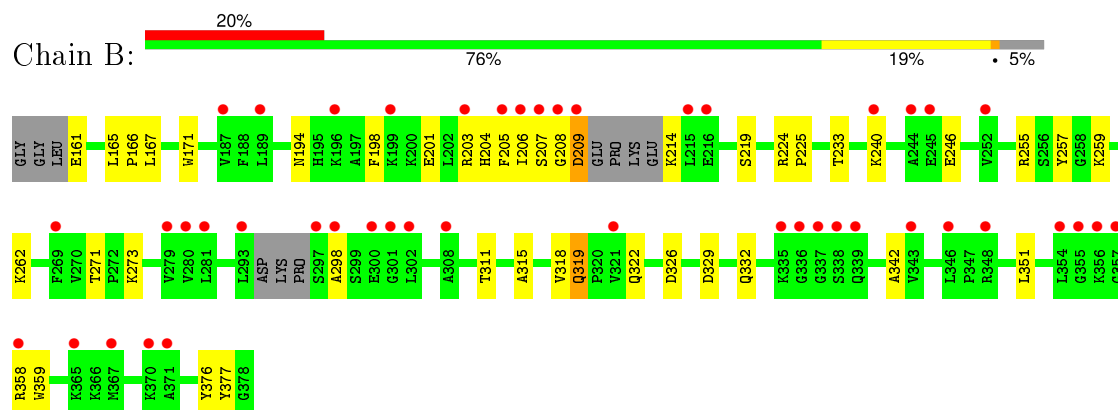
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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: 2', 3'-CYCLIC-NUCLEOTIDE 3'-PHOSPHODIESTERASE



• Molecule 1: 2', 3'-CYCLIC-NUCLEOTIDE 3'-PHOSPHODIESTERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.10 Å 47.10 Å 111.17 Å 90.00° 90.26° 90.00°	Depositor
Resolution (Å)	29.12 – 2.30 29.12 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.12-2.30) 97.4 (29.12-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.31 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.220 , 0.261 0.222 , 0.266	Depositor DCC
R_{free} test set	966 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.662	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 24.1	EDS
Estimated twinning fraction	0.460 for H,-K,-L 0.397 for h,-k,-l	Xtriage
Reported twinning fraction	0.460 for H,-K,-L	Depositor
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 19304 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6890	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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: NAP

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	0/1704	0.48	0/2292
1	B	0.24	0/1669	0.46	0/2243
All	All	0.25	0/3373	0.47	0/4535

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	1668	1691	1688	29	0
1	B	1635	1662	1657	23	3
2	A	48	25	25	0	0
2	B	48	25	25	0	0
3	A	51	0	0	4	0
3	B	37	0	0	2	0
All	All	3487	3403	3395	52	3

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 8.

All (52) 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:298:ALA:O	1:B:332:GLN:NE2	2.21	0.72
1:A:348:ARG:NH1	3:A:2046:HOH:O	2.24	0.69
1:A:322:GLN:OE1	3:A:2041:HOH:O	2.11	0.69
1:B:194:ASN:ND2	3:B:2006:HOH:O	2.24	0.68
1:B:271:THR:OG1	1:B:326:ASP:OD2	2.12	0.66
1:A:297:SER:O	3:A:2037:HOH:O	2.16	0.61
1:A:300:GLU:O	1:A:332:GLN:NE2	2.33	0.60
1:B:262:LYS:NZ	3:B:2023:HOH:O	2.28	0.58
1:B:198:PHE:HA	1:B:359:TRP:CZ2	2.39	0.58
1:A:218:VAL:O	1:A:224:ARG:NH2	2.38	0.56
1:B:342:ALA:HA	1:B:351:LEU:O	2.06	0.56
1:B:201:GLU:O	1:B:205:PHE:N	2.41	0.53
1:B:225:PRO:HG2	1:B:311:THR:O	2.09	0.53
1:A:192:LEU:HD21	1:A:270:VAL:HG21	1.92	0.51
1:B:246:GLU:OE1	1:B:246:GLU:N	2.43	0.51
1:B:201:GLU:HB3	1:B:204:HIS:HB2	1.93	0.50
1:A:251:GLU:O	1:A:255:ARG:HG3	2.12	0.50
1:B:167:LEU:N	1:B:376:TYR:O	2.44	0.50
1:B:165:LEU:HB3	1:B:166:PRO:CD	2.42	0.50
1:A:295:LYS:NZ	1:A:300:GLU:HB2	2.26	0.49
1:B:208:GLY:O	1:B:209:ASP:HB2	2.12	0.48
1:B:171:TRP:CZ3	1:B:233:THR:CG2	2.97	0.48
1:B:259:LYS:HD3	1:B:259:LYS:N	2.29	0.48
1:A:348:ARG:NH2	3:A:2047:HOH:O	2.48	0.47
1:A:298:ALA:HB1	1:A:328:LEU:HB3	1.97	0.47
1:A:300:GLU:HG2	1:A:301:GLY:N	2.29	0.47
1:B:329:ASP:OD1	1:B:358:ARG:NH1	2.48	0.47
1:A:192:LEU:CD2	1:A:270:VAL:HG21	2.45	0.46
1:A:165:LEU:HB3	1:A:166:PRO:CD	2.46	0.46
1:A:167:LEU:N	1:A:376:TYR:O	2.50	0.45
1:A:294:ASP:O	1:A:296:PRO:HD3	2.17	0.45
1:B:273:LYS:HD3	1:B:322:GLN:HG2	1.99	0.44
1:A:295:LYS:HZ2	1:A:300:GLU:HB2	1.81	0.44
1:A:223:LYS:HE2	1:A:315:ALA:O	2.18	0.44
1:A:295:LYS:HD2	1:A:295:LYS:C	2.37	0.44
1:B:315:ALA:HB3	1:B:318:VAL:CG2	2.48	0.44
1:A:260:ALA:HB1	1:A:370:LYS:HE2	2.00	0.43
1:B:319:GLN:H	1:B:319:GLN:CD	2.22	0.42
1:A:234:LYS:HB3	1:A:247:TYR:CE2	2.54	0.42
1:A:187:VAL:O	1:A:191:GLU:HG3	2.20	0.42
1:A:222:GLY:O	1:A:224:ARG:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ASP:O	1:A:333:GLN:HG2	2.21	0.41
1:B:208:GLY:O	1:B:209:ASP:CB	2.68	0.41
1:B:208:GLY:C	1:B:209:ASP:OD1	2.59	0.41
1:A:296:PRO:O	1:A:298:ALA:N	2.53	0.41
1:A:294:ASP:CG	1:A:294:ASP:O	2.58	0.41
1:B:166:PRO:HA	1:B:377:TYR:CD2	2.55	0.40
1:A:256:SER:HA	1:A:259:LYS:HG2	2.02	0.40
1:A:208:GLY:O	1:A:209:ASP:CB	2.69	0.40
1:A:272:PRO:HD3	1:A:357:GLY:O	2.22	0.40
1:B:203:ARG:O	1:B:206:ILE:O	2.39	0.40
1:A:353:SER:HB2	1:A:359:TRP:CZ3	2.57	0.40

All (3) 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:B:219:SER:O	1:B:257:TYR:OH[2_745]	1.97	0.23
1:B:240:LYS:O	1:B:255:ARG:NH1[2_645]	2.15	0.05
1:B:161:GLU:OE2	1:B:214:LYS:N[2_755]	2.15	0.05

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	211/221 (96%)	198 (94%)	12 (6%)	1 (0%)	34	41
1	B	205/221 (93%)	193 (94%)	12 (6%)	0	100	100
All	All	416/442 (94%)	391 (94%)	24 (6%)	1 (0%)	52	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	297	SER

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	176/180 (98%)	173 (98%)	3 (2%)	68	83
1	B	172/180 (96%)	168 (98%)	4 (2%)	58	75
All	All	348/360 (97%)	341 (98%)	7 (2%)	63	79

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	224	ARG
1	A	295	LYS
1	A	319	GLN
1	B	207	SER
1	B	209	ASP
1	B	224	ARG
1	B	319	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	319	GLN

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](#)

2 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	$\# Z > 2$
2	NAP	A	1379	-	42,52,52	0.82	1 (2%)	54,80,80	1.62	6 (11%)
2	NAP	B	1379	-	42,52,52	0.85	1 (2%)	54,80,80	1.50	3 (5%)

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
2	NAP	A	1379	-	-	0/27/67/67	0/5/5/5
2	NAP	B	1379	-	-	0/27/67/67	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1379	NAP	C5A-C4A	3.09	1.47	1.40
2	B	1379	NAP	C5A-C4A	3.19	1.47	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1379	NAP	N3A-C2A-N1A	-7.99	122.77	128.89
2	B	1379	NAP	N3A-C2A-N1A	-7.55	123.11	128.89
2	A	1379	NAP	PN-O3-PA	-4.62	119.77	132.73
2	B	1379	NAP	PN-O3-PA	-3.85	121.91	132.73
2	A	1379	NAP	C4A-C5A-N7A	-3.33	106.42	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1379	NAP	C4A-C5A-N7A	-3.01	106.71	109.48
2	A	1379	NAP	O3-PA-O5B	-2.01	97.59	102.94
2	A	1379	NAP	C2A-N1A-C6A	2.09	122.50	118.77
2	A	1379	NAP	O4D-C1D-N1N	2.69	111.08	108.13

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

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	215/221 (97%)	0.76	18 (8%) 14 19	18, 34, 61, 112	0
1	B	211/221 (95%)	1.20	45 (21%) 1 2	28, 45, 78, 142	0
All	All	426/442 (96%)	0.98	63 (14%) 3 5	18, 40, 71, 142	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	355	GLY	7.8
1	B	208	GLY	7.6
1	B	356	LYS	5.5
1	B	189	LEU	4.9
1	B	205	PHE	4.7
1	A	227	GLY	4.7
1	B	293	LEU	4.4
1	A	293	LEU	4.3
1	B	298	ALA	4.3
1	A	298	ALA	4.0
1	B	343	VAL	3.8
1	B	206	ILE	3.6
1	B	302	LEU	3.6
1	B	301	GLY	3.5
1	B	244	ALA	3.4
1	B	203	ARG	3.3
1	B	321	VAL	3.3
1	A	336	GLY	3.3
1	B	339	GLN	3.0
1	B	199	LYS	2.9
1	B	354	LEU	2.9
1	B	281	LEU	2.8
1	A	161	GLU	2.8
1	B	371	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	207	SER	2.7
1	B	209	ASP	2.7
1	B	337	GLY	2.6
1	B	338	SER	2.6
1	B	308	ALA	2.6
1	B	365	LYS	2.5
1	B	187	VAL	2.5
1	A	202	LEU	2.5
1	B	346	LEU	2.5
1	A	209	ASP	2.5
1	A	208	GLY	2.4
1	B	336	GLY	2.4
1	A	291	SER	2.4
1	A	297	SER	2.4
1	B	245	GLU	2.4
1	B	215	LEU	2.4
1	B	358	ARG	2.3
1	A	164	PHE	2.3
1	B	196	LYS	2.3
1	B	252	VAL	2.3
1	A	228	VAL	2.2
1	B	279	VAL	2.2
1	B	335	LYS	2.2
1	B	216	GLU	2.2
1	B	370	LYS	2.1
1	B	280	VAL	2.1
1	A	339	GLN	2.1
1	B	240	LYS	2.1
1	B	367	MET	2.1
1	A	343	VAL	2.1
1	B	300	GLU	2.0
1	A	370	LYS	2.0
1	A	351	LEU	2.0
1	B	269	PHE	2.0
1	B	297	SER	2.0
1	A	378	GLY	2.0
1	B	357	GLY	2.0
1	A	225	PRO	2.0
1	B	348	ARG	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(\AA^2)	Q<0.9
2	NAP	A	1379	48/48	0.89	0.21	0.33	23,57,92,105	0
2	NAP	B	1379	48/48	0.88	0.17	-0.22	25,57,79,209	0

6.5 Other polymers [i](#)

There are no such residues in this entry.