



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:59 AM UTC

PDB ID : 4QP4 / pdb_00004qp4
Title : Crystal Structure of ERK2 in complex with N-cyclohexyl-9H-purin-6-amine
Authors : Yin, J.; Wang, W.
Deposited on : 2014-06-22
Resolution : 2.20 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

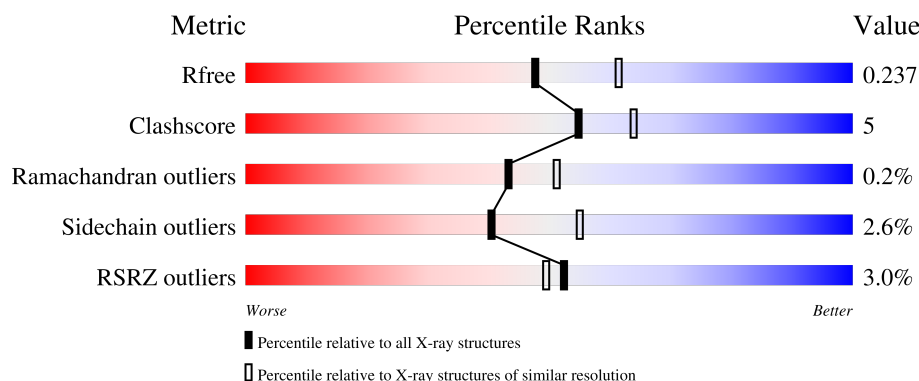
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	369	
1	B	369	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5861 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.

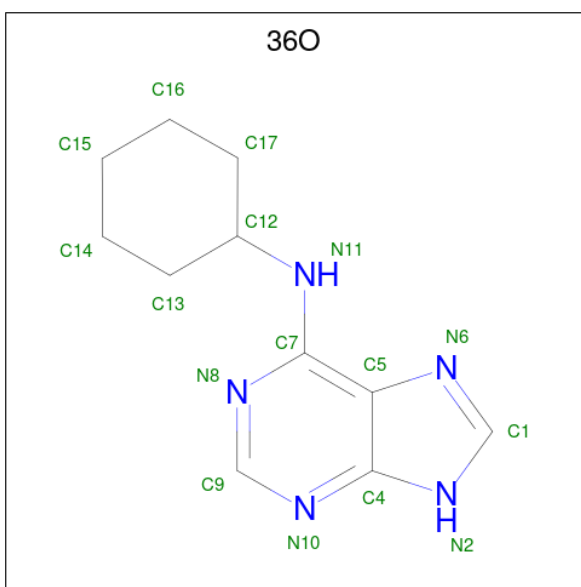
- Molecule 1 is a protein called Mitogen-activated protein kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2753	1770	470	498	15			
1	B	335	Total	C	N	O	S	0	0	0
			2739	1761	468	495	15			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	expression tag	UNP P28482
A	-7	GLY	-	expression tag	UNP P28482
A	-6	SER	-	expression tag	UNP P28482
A	-5	HIS	-	expression tag	UNP P28482
A	-4	HIS	-	expression tag	UNP P28482
A	-3	HIS	-	expression tag	UNP P28482
A	-2	HIS	-	expression tag	UNP P28482
A	-1	HIS	-	expression tag	UNP P28482
A	0	HIS	-	expression tag	UNP P28482
B	-8	MET	-	expression tag	UNP P28482
B	-7	GLY	-	expression tag	UNP P28482
B	-6	SER	-	expression tag	UNP P28482
B	-5	HIS	-	expression tag	UNP P28482
B	-4	HIS	-	expression tag	UNP P28482
B	-3	HIS	-	expression tag	UNP P28482
B	-2	HIS	-	expression tag	UNP P28482
B	-1	HIS	-	expression tag	UNP P28482
B	0	HIS	-	expression tag	UNP P28482

- Molecule 2 is N-cyclohexyl-9H-purin-6-amine (CCD ID: 36O) (formula: C₁₁H₁₅N₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	1
			32	22	10		
2	B	1	Total	C	N	0	1
			32	22	10		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	141	Total	O	0	0
			141	141		
3	B	164	Total	O	0	0
			164	164		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.43Å 67.23Å 87.00Å 90.00° 102.21° 90.00°	Depositor
Resolution (Å)	28.47 – 2.20 28.47 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.3 (28.47-2.20) 98.3 (28.47-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.187 , 0.235 0.189 , 0.237	Depositor DCC
R_{free} test set	1683 reflections (2.91%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5861	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.8639e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 36O

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	0.33	0/2816	0.70	0/3813
1	B	0.34	0/2802	0.70	0/3793
All	All	0.33	0/5618	0.70	0/7606

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	2753	0	2773	39	0
1	B	2739	0	2757	16	0
2	A	32	0	30	2	0
2	B	32	0	30	3	0
3	A	141	0	0	3	0
3	B	164	0	0	1	0
All	All	5861	0	5590	53	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 5.

All (53) 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:110:THR:HA	2:B:401[A]:36O:H3	1.77	0.67
1:A:34:GLY:HA3	1:A:36:TYR:H	1.59	0.66
1:B:62:GLN:NE2	1:B:66:GLN:OE1	2.26	0.66
1:B:80:HIS:HB3	1:B:83:ILE:HG13	1.78	0.66
1:B:106:ASP:O	2:B:401[A]:36O:H7	1.96	0.66
1:A:106:ASP:O	2:A:401[A]:36O:H7	1.97	0.64
1:A:90:ILE:HB	1:A:102:TYR:HB2	1.80	0.64
1:A:241:LEU:HD22	1:A:247:PRO:HD3	1.81	0.63
1:B:95:ILE:HD11	1:B:344:LYS:HG2	1.81	0.62
1:A:336:ASP:N	1:A:336:ASP:OD1	2.32	0.62
1:A:115:LEU:HD23	1:A:119:GLN:HB2	1.82	0.61
1:A:111:ASP:HB3	1:A:156:LEU:HD23	1.81	0.61
1:A:148:ARG:HD2	1:A:172:ARG:HG2	1.82	0.60
1:A:67:ARG:HH21	1:A:170:LEU:HD13	1.68	0.59
1:B:114:LYS:HD2	2:B:401[A]:36O:H4	1.87	0.56
1:A:126:ILE:HD13	1:A:222:LEU:HD23	1.86	0.56
1:B:338:LEU:HD12	1:B:339:PRO:HD2	1.87	0.56
1:A:19:PHE:HD2	1:A:38:MET:HE3	1.70	0.55
1:A:13:MET:N	3:A:608:HOH:O	2.40	0.54
1:A:17:GLN:HB3	1:A:38:MET:HE1	1.90	0.54
1:A:34:GLY:N	1:A:37:GLY:O	2.31	0.53
1:B:241:LEU:HD22	1:B:247:PRO:HD3	1.89	0.53
1:A:317:TYR:CZ	1:A:319:PRO:HG3	2.43	0.53
1:A:114:LYS:NZ	3:A:637:HOH:O	2.44	0.51
1:A:60:GLU:OE1	1:B:271:ASN:ND2	2.35	0.51
1:A:34:GLY:HA3	1:A:36:TYR:N	2.26	0.50
1:A:140:ILE:HD12	1:A:168:PHE:HE2	1.77	0.50
1:B:191:ARG:NH2	1:B:201:ASN:OD1	2.45	0.49
1:A:116:LEU:HD13	1:A:220:GLU:HG2	1.95	0.48
1:A:356:PRO:HA	1:A:357:GLY:HA2	1.57	0.48
1:A:155:LEU:HD11	1:A:217:ILE:HD13	1.96	0.48
1:A:232:HIS:ND1	1:B:305:GLU:OE1	2.39	0.47
1:A:288:ASP:O	1:A:292:LYS:HG2	2.15	0.47
1:A:289:LEU:O	1:A:293:MET:HG3	2.14	0.47
1:A:110:THR:HA	2:A:401[A]:36O:H3	1.96	0.47
1:A:115:LEU:HD22	1:A:121:LEU:HD11	1.97	0.46
1:A:19:PHE:CD2	1:A:38:MET:HE3	2.48	0.46
1:A:297:ASN:HB3	1:A:300:LYS:HB2	1.98	0.46
1:A:24:ARG:HG3	1:A:46:VAL:HG23	1.98	0.46
1:A:184:LEU:HB3	1:A:185:THR:H	1.61	0.45
1:A:225:ARG:NH2	3:A:612:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ILE:HD11	1:A:41:SER:HB3	2.00	0.44
1:A:146:LEU:HD22	1:A:207:LYS:HA	1.99	0.44
1:A:148:ARG:HD3	1:A:170:LEU:O	2.18	0.44
1:A:30:TYR:OH	1:A:33:GLU:HG2	2.17	0.43
1:B:59:PHE:CZ	1:B:98:MET:HE3	2.54	0.42
1:B:330:LYS:HD2	1:B:330:LYS:HA	1.83	0.42
1:A:136:GLY:O	1:A:140:ILE:HG12	2.19	0.42
1:A:59:PHE:CZ	1:A:98:MET:HE3	2.55	0.41
1:B:258:LEU:HD23	1:B:258:LEU:HA	1.92	0.41
1:B:330:LYS:NZ	3:B:536:HOH:O	2.53	0.41
1:B:241:LEU:HD11	1:B:264:LEU:HD22	2.03	0.41
1:A:140:ILE:HD12	1:A:168:PHE:CE2	2.56	0.40

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	333/369 (90%)	318 (96%)	14 (4%)	1 (0%)	36	42
1	B	331/369 (90%)	319 (96%)	12 (4%)	0	100	100
All	All	664/738 (90%)	637 (96%)	26 (4%)	1 (0%)	43	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	204	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	305/326 (94%)	296 (97%)	9 (3%)	36	49
1	B	303/326 (93%)	296 (98%)	7 (2%)	44	59
All	All	608/652 (93%)	592 (97%)	16 (3%)	40	55

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	71	GLU
1	A	76	LEU
1	A	157	LEU
1	A	170	LEU
1	A	211	ILE
1	A	330	LYS
1	A	336	ASP
1	A	338	LEU
1	B	28	LEU
1	B	56	ILE
1	B	83	ILE
1	B	191	ARG
1	B	211	ILE
1	B	303	GLU
1	B	353	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	45	ASN
1	B	45	ASN
1	B	119	GLN
1	B	238	ASN
1	B	299	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	36O	B	401[A]	-	18,18,18	0.95	1 (5%)	24,24,24	2.41	9 (37%)
2	36O	A	401[B]	-	18,18,18	1.02	1 (5%)	24,24,24	2.34	9 (37%)
2	36O	A	401[A]	-	18,18,18	0.95	1 (5%)	24,24,24	2.33	9 (37%)
2	36O	B	401[B]	-	18,18,18	1.01	1 (5%)	24,24,24	2.30	8 (33%)

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	36O	B	401[A]	-	-	2/4/12/12	0/3/3/3
2	36O	A	401[B]	-	-	0/4/12/12	0/3/3/3
2	36O	A	401[A]	-	-	0/4/12/12	0/3/3/3
2	36O	B	401[B]	-	-	0/4/12/12	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401[B]	36O	C7-N11	2.62	1.39	1.35
2	B	401[B]	36O	C7-N11	2.56	1.39	1.35
2	A	401[A]	36O	C7-N11	2.31	1.38	1.35
2	B	401[A]	36O	C7-N11	2.26	1.38	1.35

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401[A]	36O	N2-C4-N10	5.41	135.45	126.69
2	B	401[B]	36O	C5-N6-C1	5.24	109.39	103.48
2	A	401[B]	36O	C5-N6-C1	5.21	109.36	103.48
2	A	401[A]	36O	N2-C4-N10	5.17	135.06	126.69
2	B	401[A]	36O	C5-N6-C1	5.10	109.23	103.48
2	A	401[B]	36O	N2-C4-N10	5.05	134.87	126.69
2	B	401[B]	36O	N2-C4-N10	5.03	134.84	126.69
2	A	401[A]	36O	C5-N6-C1	4.86	108.97	103.48
2	B	401[A]	36O	C5-C4-N10	-4.33	118.86	126.75
2	A	401[A]	36O	C5-C4-N10	-4.26	118.98	126.75
2	B	401[B]	36O	C5-C4-N10	-4.25	119.01	126.75
2	A	401[B]	36O	C5-C4-N10	-4.21	119.07	126.75
2	A	401[A]	36O	N10-C9-N8	-4.19	122.23	128.58
2	B	401[A]	36O	N10-C9-N8	-4.10	122.38	128.58
2	A	401[B]	36O	N10-C9-N8	-4.07	122.42	128.58
2	B	401[B]	36O	N10-C9-N8	-3.93	122.64	128.58
2	B	401[A]	36O	C7-N11-C12	-3.22	118.74	124.18
2	A	401[A]	36O	C7-N11-C12	-2.67	119.67	124.18
2	B	401[B]	36O	C4-C5-N6	-2.67	106.97	110.67
2	A	401[B]	36O	C4-C5-N6	-2.57	107.10	110.67
2	A	401[B]	36O	N2-C1-N6	-2.42	110.18	113.87
2	B	401[A]	36O	N2-C1-N6	-2.40	110.22	113.87
2	A	401[A]	36O	C4-C5-N6	-2.39	107.36	110.67
2	B	401[B]	36O	N2-C1-N6	-2.38	110.25	113.87
2	B	401[A]	36O	C4-C5-N6	-2.32	107.45	110.67
2	B	401[B]	36O	C4-C5-C7	2.25	118.31	116.95
2	A	401[B]	36O	N11-C7-N8	2.21	121.14	118.00
2	A	401[A]	36O	N2-C1-N6	-2.21	110.51	113.87
2	B	401[A]	36O	N11-C7-N8	2.20	121.13	118.00
2	A	401[A]	36O	N11-C7-N8	2.20	121.12	118.00
2	A	401[A]	36O	C4-C5-C7	2.12	118.23	116.95
2	B	401[B]	36O	C7-C5-N6	2.10	134.72	132.43
2	A	401[B]	36O	C4-C5-C7	2.08	118.21	116.95
2	B	401[A]	36O	C4-C5-C7	2.08	118.20	116.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401[B]	36O	C7-C5-N6	2.08	134.69	132.43

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401[A]	36O	C5-C7-N11-C12
2	B	401[A]	36O	N8-C7-N11-C12

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401[A]	36O	3	0
2	A	401[A]	36O	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	337/369 (91%)	-0.03	8 (2%) 59 56	21, 35, 59, 110	0
1	B	335/369 (90%)	-0.01	12 (3%) 46 43	18, 35, 61, 109	0
All	All	672/738 (91%)	-0.02	20 (2%) 52 49	18, 35, 60, 110	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	205	TYR	4.7
1	B	254	CYS	3.8
1	B	203	LYS	3.8
1	A	331	PHE	3.8
1	A	184	LEU	3.6
1	A	333	MET	3.2
1	B	200	LEU	3.1
1	B	333	MET	2.9
1	A	203	LYS	2.8
1	B	331	PHE	2.8
1	B	338	LEU	2.7
1	B	256	ILE	2.6
1	B	332	ASP	2.6
1	B	159	THR	2.6
1	B	198	ILE	2.4
1	A	109	GLU	2.3
1	A	34	GLY	2.3
1	B	329	PHE	2.2
1	A	327	ALA	2.2
1	A	357	GLY	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 oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	36O	A	401[A]	16/16	0.75	0.20	39,43,45,46	16
2	36O	A	401[B]	16/16	0.75	0.20	39,40,44,44	16
2	36O	B	401[A]	16/16	0.78	0.19	46,48,50,50	16
2	36O	B	401[B]	16/16	0.78	0.19	39,47,49,49	16

6.5 Other polymers [i](#)

There are no such residues in this entry.