Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2024 – 02:34 PM EST

PDB ID	:	3QI4
Title	:	Crystal structure of PDE9A(Q453E) in complex with IBMX
Authors	:	Hou, J.; Xu, J.; Liu, M.; Zhao, R.; Lou, H.; Ke, H.
Deposited on	:	2011-01-26
Resolution	:	2.50 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 (i) 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 (1)) were used in the production of this report:

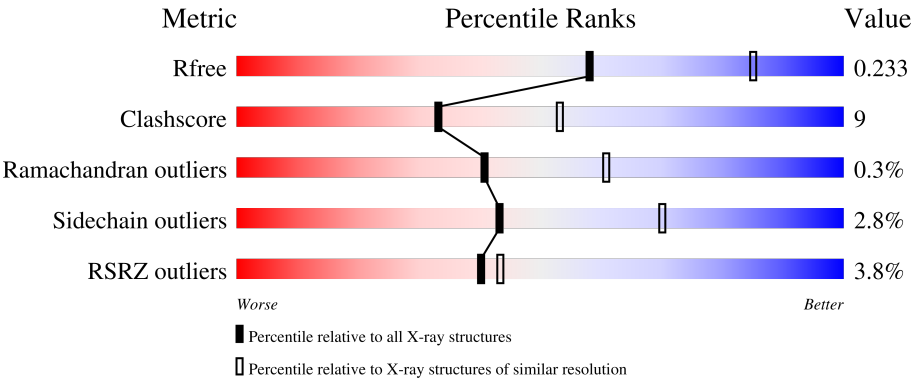
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	533	2% 49% 11% · 39%
1	B	533	3% 51% 9% · 39%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5435 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.

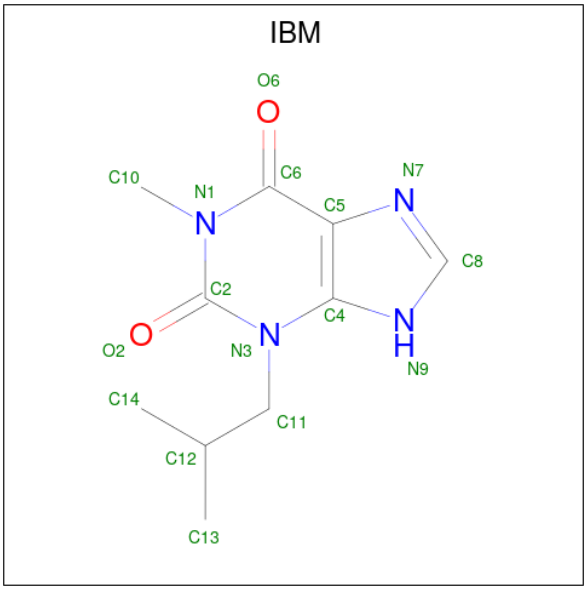
- Molecule 1 is a protein called High affinity cGMP-specific 3',5'-cyclic phosphodiesterase 9A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	0	0
			2685	1721	443	491	30			
1	B	325	Total	C	N	O	S	0	0	0
			2685	1721	443	491	30			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	453	GLU	GLN	engineered mutation	UNP O76083
B	453	GLU	GLN	engineered mutation	UNP O76083

- Molecule 2 is 3-ISOBUTYL-1-METHYLXANTHINE (three-letter code: IBM) (formula: $C_{10}H_{14}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	10	4	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C N O 16 10 4 2	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

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

- Molecule 5 is water.

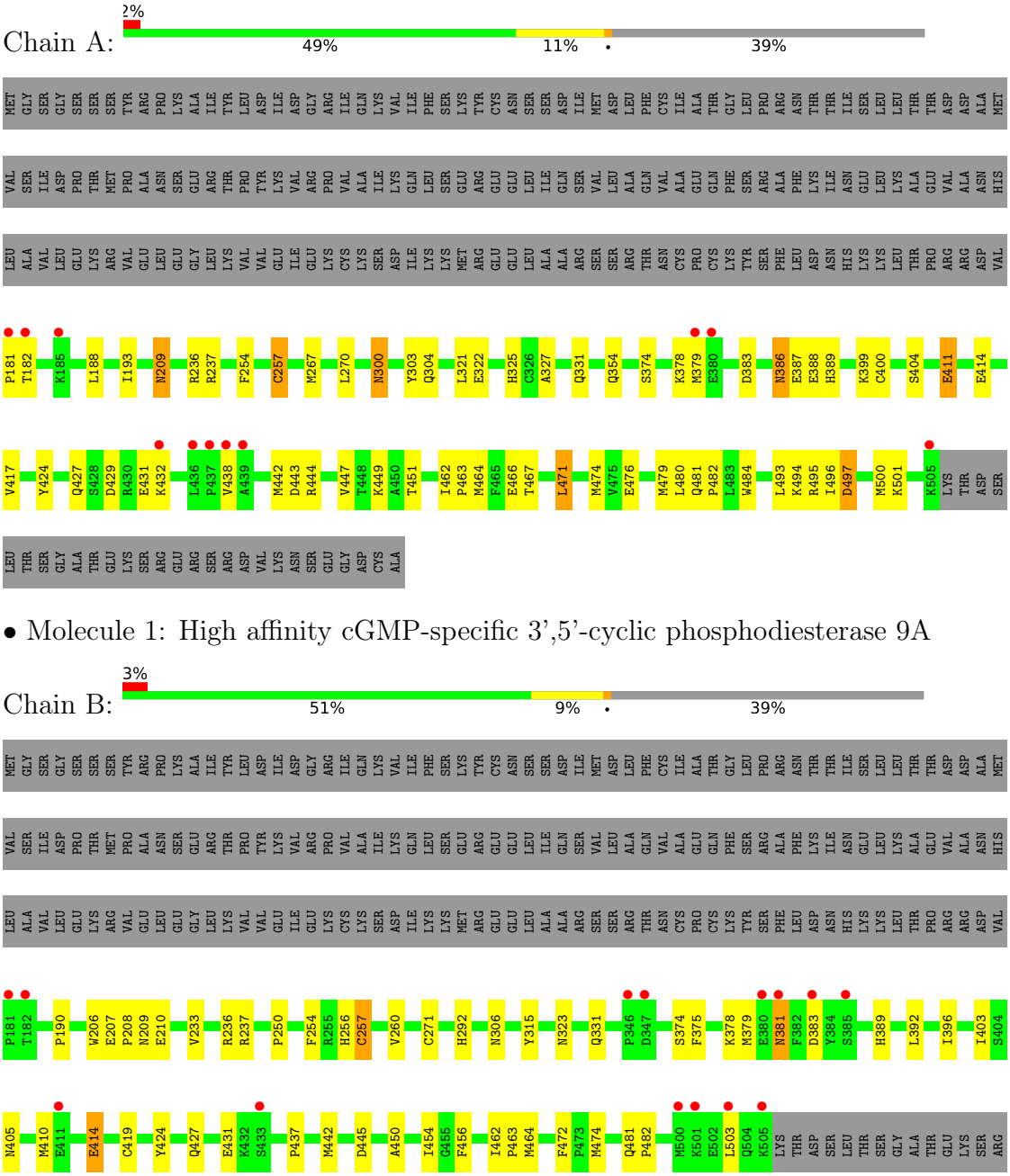
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	15	Total O 15 15	0	0
5	B	14	Total O 14 14	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: High affinity cGMP-specific 3',5'-cyclic phosphodiesterase 9A

Chain A:



• Molecule 1: High affinity cGMP-specific 3',5'-cyclic phosphodiesterase 9A

Chain B:

GLU
ARG
SER
ARG
ASP
VAL
LYS
ASN
SER
GLU
GLY
ASP
CYS
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	103.41Å 103.41Å 269.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 41.13 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.50) 94.8 (41.13-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.52 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.213 , 0.239 0.208 , 0.233	Depositor DCC
R_{free} test set	5064 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å^2)	35.4	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 34.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5435	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: IBM, ZN, MG

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	0.38	0/2755	0.56	0/3732
1	B	0.37	0/2755	0.56	0/3732
All	All	0.38	0/5510	0.56	0/7464

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	2685	0	2625	60	0
1	B	2685	0	2625	40	0
2	A	16	0	14	4	0
2	B	16	0	14	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	15	0	0	1	0
5	B	14	0	0	1	0
All	All	5435	0	5278	92	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.

All (92) 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:A:534:IBM:HN9	2:A:534:IBM:H143	1.17	1.07
1:A:451:THR:HG22	1:A:494:LYS:HE2	1.51	0.91
1:A:236:ARG:HE	1:B:236:ARG:NH2	1.72	0.86
2:A:534:IBM:H143	2:A:534:IBM:N9	1.99	0.75
2:A:534:IBM:HN9	2:A:534:IBM:C14	1.96	0.74
1:A:495:ARG:HH11	1:A:495:ARG:HG3	1.53	0.72
1:A:424:TYR:OH	2:A:534:IBM:H112	1.89	0.71
1:A:300:ASN:C	1:A:300:ASN:HD22	1.93	0.70
1:B:378:LYS:HG3	1:B:392:LEU:HD12	1.75	0.69
1:B:450:ALA:O	1:B:454:ILE:HG13	1.94	0.68
1:A:399:LYS:HE2	5:A:547:HOH:O	1.95	0.64
1:A:386:ASN:HD22	1:A:386:ASN:C	2.01	0.63
1:A:443:ASP:O	1:A:447:VAL:HG12	2.01	0.61
1:A:427:GLN:O	1:A:431:GLU:HG3	2.00	0.61
1:A:327:ALA:O	1:A:331:GLN:HG3	2.01	0.60
1:B:383:ASP:H	1:B:389:HIS:HD2	1.48	0.60
1:A:300:ASN:C	1:A:300:ASN:ND2	2.56	0.59
1:A:386:ASN:ND2	1:A:388:GLU:H	2.00	0.59
1:A:497:ASP:O	1:A:501:LYS:HG2	2.02	0.59
1:B:427:GLN:O	1:B:431:GLU:HG3	2.03	0.59
1:A:267:MET:HA	1:A:267:MET:HE2	1.85	0.59
1:A:236:ARG:HH21	1:B:236:ARG:CZ	2.16	0.58
1:A:379:MET:SD	1:A:471:LEU:HD13	2.44	0.58
1:A:383:ASP:H	1:A:389:HIS:HD2	1.50	0.58
1:A:236:ARG:NE	1:B:236:ARG:NH2	2.47	0.58
1:A:193:ILE:HD11	1:B:233:VAL:HG11	1.84	0.57
1:B:306:ASN:ND2	1:B:437:PRO:HG2	2.20	0.57
1:A:300:ASN:ND2	1:A:303:TYR:H	2.04	0.56
1:A:429:ASP:OD2	1:A:444:ARG:NH1	2.39	0.56
1:A:462:ILE:O	1:A:466:GLU:HB2	2.06	0.56
1:A:386:ASN:HD22	1:A:388:GLU:H	1.54	0.55
1:B:424:TYR:HB3	1:B:442:MET:HG2	1.87	0.55
1:A:383:ASP:H	1:A:389:HIS:CD2	2.25	0.55
1:A:400:CYS:O	1:A:404:SER:HB3	2.07	0.54
1:A:495:ARG:HG3	1:A:495:ARG:NH1	2.22	0.54
1:B:271:CYS:HB3	1:B:472:PHE:CD2	2.43	0.54
1:A:379:MET:HA	1:A:379:MET:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:ASP:H	1:B:389:HIS:CD2	2.25	0.54
1:A:236:ARG:HH21	1:B:236:ARG:NH2	2.07	0.52
1:B:379:MET:HA	1:B:379:MET:HE2	1.92	0.52
1:A:432:LYS:HG3	1:A:438:VAL:HG21	1.90	0.52
1:A:237:ARG:NH1	1:B:190:PRO:HD3	2.25	0.52
1:A:236:ARG:HE	1:B:236:ARG:HH21	1.55	0.52
1:A:300:ASN:O	1:A:304:GLN:HG2	2.10	0.52
1:A:237:ARG:HH12	1:B:190:PRO:HD3	1.75	0.52
1:B:481:GLN:HB3	1:B:482:PRO:CD	2.41	0.50
1:B:424:TYR:CG	1:B:442:MET:HG2	2.47	0.49
1:A:188:LEU:O	1:B:237:ARG:NH1	2.47	0.48
1:A:254:PHE:O	1:A:257:CYS:HB3	2.14	0.48
1:B:410:MET:SD	1:B:414:GLU:HG3	2.54	0.48
1:A:209:ASN:HD22	1:A:209:ASN:N	2.13	0.47
1:B:375:PHE:CD2	1:B:396:ILE:HG13	2.49	0.47
1:A:463:PRO:O	1:A:467:THR:HG23	2.14	0.46
1:A:411:GLU:H	1:A:411:GLU:CD	2.19	0.46
1:A:386:ASN:HD22	1:A:387:GLU:N	2.14	0.46
1:A:481:GLN:HA	1:A:484:TRP:CE3	2.51	0.46
1:A:236:ARG:HE	1:B:236:ARG:HH22	1.60	0.46
1:A:400:CYS:HA	1:A:464:MET:HE1	1.96	0.46
1:B:254:PHE:O	1:B:257:CYS:HB3	2.15	0.46
1:A:493:LEU:O	1:A:496:ILE:HG22	2.16	0.45
1:A:495:ARG:NH1	1:A:495:ARG:CG	2.80	0.45
1:B:206:TRP:HB3	1:B:210:GLU:HB2	1.99	0.45
1:B:260:VAL:HG21	1:B:292:HIS:CE1	2.51	0.45
1:A:300:ASN:HA	1:A:321:LEU:HD11	1.98	0.45
1:A:267:MET:HE1	1:A:479:MET:SD	2.57	0.45
1:A:424:TYR:CG	1:A:442:MET:HG2	2.52	0.44
1:A:481:GLN:HB3	1:A:482:PRO:CD	2.47	0.44
1:B:250:PRO:O	1:B:419:CYS:HB3	2.17	0.44
1:B:481:GLN:HB3	1:B:482:PRO:HD3	1.99	0.44
1:B:375:PHE:CG	1:B:396:ILE:HG13	2.52	0.44
1:B:424:TYR:CB	1:B:442:MET:HG2	2.48	0.44
1:A:267:MET:CE	1:A:270:LEU:HD23	2.48	0.43
1:B:456:PHE:CD1	2:B:534:IBM:H143	2.54	0.43
1:A:417:VAL:HG11	1:A:449:LYS:HG3	2.00	0.43
1:A:496:ILE:O	1:A:500:MET:HG2	2.18	0.43
1:B:462:ILE:HB	1:B:463:PRO:HD3	2.01	0.42
1:B:315:TYR:CE1	1:B:323:ASN:HB3	2.55	0.42
1:B:374:SER:O	1:B:378:LYS:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ASN:HD22	1:A:209:ASN:H	1.66	0.42
1:B:403:ILE:HD11	1:B:464:MET:CE	2.50	0.42
1:A:236:ARG:NE	1:B:236:ARG:HH22	2.15	0.41
1:B:256:HIS:O	1:B:260:VAL:HG23	2.20	0.41
1:A:424:TYR:CD2	1:A:442:MET:HG2	2.55	0.41
1:A:476:GLU:HA	1:A:480:LEU:HB2	2.02	0.41
1:B:207:GLU:HB3	1:B:208:PRO:HD2	2.02	0.41
1:A:374:SER:O	1:A:378:LYS:HG2	2.21	0.41
1:A:181:PRO:HB2	1:A:182:THR:H	1.61	0.40
1:A:386:ASN:C	1:A:386:ASN:ND2	2.72	0.40
1:B:405:ASN:ND2	5:B:548:HOH:O	2.53	0.40
1:A:322:GLU:HA	1:A:325:HIS:CD2	2.56	0.40
1:B:206:TRP:HE3	1:B:210:GLU:OE1	2.05	0.40
1:A:493:LEU:O	1:A:497:ASP:HB2	2.22	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	323/533 (61%)	309 (96%)	14 (4%)	0	100 100
1	B	323/533 (61%)	307 (95%)	14 (4%)	2 (1%)	25 43
All	All	646/1066 (61%)	616 (95%)	28 (4%)	2 (0%)	41 61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	381	ASN
1	B	445	ASP

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	302/488 (62%)	292 (97%)	10 (3%)	38 64
1	B	302/488 (62%)	295 (98%)	7 (2%)	50 76
All	All	604/976 (62%)	587 (97%)	17 (3%)	43 70

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	209	ASN
1	A	257	CYS
1	A	300	ASN
1	A	354	GLN
1	A	386	ASN
1	A	411	GLU
1	A	414	GLU
1	A	471	LEU
1	A	474	MET
1	A	497	ASP
1	B	209	ASN
1	B	257	CYS
1	B	331	GLN
1	B	381	ASN
1	B	414	GLU
1	B	474	MET
1	B	503	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	ASN
1	A	300	ASN
1	A	304	GLN
1	A	351	GLN
1	A	381	ASN

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Mol	Chain	Res	Type
1	A	386	ASN
1	A	389	HIS
1	B	220	HIS
1	B	304	GLN
1	B	351	GLN
1	B	389	HIS
1	B	405	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
2	IBM	B	534	-	8,17,17	1.11	1 (12%)	10,25,25	2.50	3 (30%)
2	IBM	A	534	-	8,17,17	0.63	0	10,25,25	2.67	3 (30%)

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	IBM	B	534	-	-	0/4/4/4	0/2/2/2
2	IBM	A	534	-	-	4/4/4/4	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	534	IBM	C11-N3	-2.23	1.45	1.48

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	534	IBM	C4-C5-C6	-5.74	116.27	119.96
2	A	534	IBM	C11-N3-C4	5.58	123.40	118.41
2	A	534	IBM	C4-C5-C6	-5.47	116.45	119.96
2	B	534	IBM	C11-N3-C4	4.35	122.30	118.41
2	A	534	IBM	C5-C4-N9	-2.55	105.62	110.87
2	B	534	IBM	C5-C4-N9	-2.53	105.67	110.87

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	534	IBM	C12-C11-N3-C4
2	A	534	IBM	C12-C11-N3-C2
2	A	534	IBM	N3-C11-C12-C13
2	A	534	IBM	N3-C11-C12-C14

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	534	IBM	1	0
2	A	534	IBM	4	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, 95^{th} 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	325/533 (60%)	0.06	11 (3%)	45	48	20, 36, 56, 81	0
1	B	325/533 (60%)	0.10	14 (4%)	35	38	23, 38, 60, 90	0
All	All	650/1066 (60%)	0.08	25 (3%)	40	43	20, 38, 60, 90	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	505	LYS	5.5
1	B	181	PRO	3.9
1	B	503	LEU	3.5
1	A	181	PRO	3.3
1	A	380	GLU	3.3
1	A	182	THR	2.9
1	B	182	THR	2.9
1	A	438	VAL	2.6
1	B	385	SER	2.6
1	B	433	SER	2.5
1	B	411	GLU	2.5
1	A	437	PRO	2.4
1	A	185	LYS	2.4
1	A	505	LYS	2.3
1	B	347	ASP	2.3
1	B	380	GLU	2.3
1	B	383	ASP	2.3
1	B	501	LYS	2.2
1	A	436	LEU	2.1
1	B	346	PRO	2.1
1	B	500	MET	2.1
1	B	381	ASN	2.0
1	A	379	MET	2.0
1	A	439	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	432	LYS	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 monosaccharides 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, 95^{th} 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(Å^2)	Q<0.9
4	MG	B	536	1/1	0.80	0.29	43,43,43,43	0
4	MG	A	536	1/1	0.82	0.15	47,47,47,47	0
3	ZN	B	535	1/1	0.86	0.08	64,64,64,64	0
2	IBM	A	534	16/16	0.88	0.21	57,58,59,60	0
3	ZN	A	535	1/1	0.93	0.06	59,59,59,59	0
2	IBM	B	534	16/16	0.98	0.15	36,39,44,45	0

6.5 Other polymers (i)

There are no such residues in this entry.