WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:48 PM GMT

PDB ID : 3V4J
Title : First-In-Class Small Molecule Inhibitors of the Single-strand DNA Cytosine Deaminase APOBEC3G
Authors : Shandilya, S.M.D.; Ali, A.; Schiffer, C.A.
Deposited on : 2011-12-15
Resolution : 2.04 Å(reported)

The following versions of software and data (see references (i)) 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
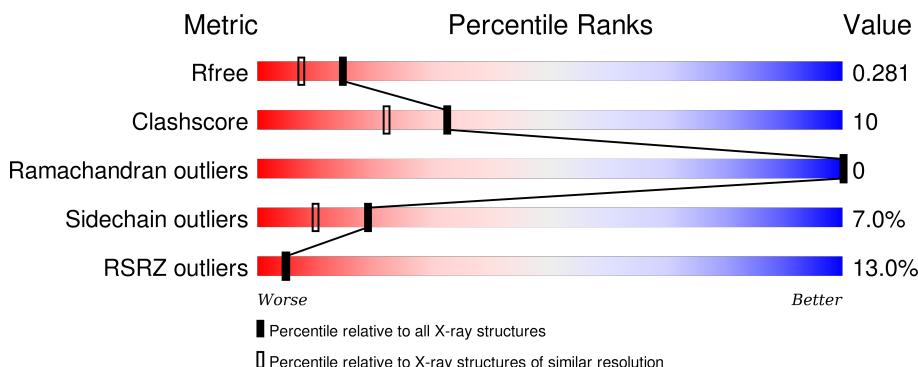
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
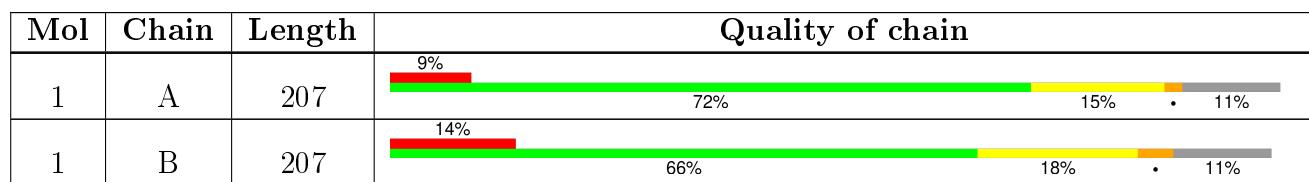
The reported resolution of this entry is 2.04 Å.

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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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 <=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	207	
1	B	207	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3085 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 DNA dC->dU-editing enzyme APOBEC-3G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	3	0
			1470	937	252	269	12			
1	B	185	Total	C	N	O	S	0	2	0
			1433	918	248	255	12			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	178	GLY	-	EXPRESSION TAG	UNP Q9HC16
A	179	PRO	-	EXPRESSION TAG	UNP Q9HC16
A	180	LEU	-	EXPRESSION TAG	UNP Q9HC16
A	181	GLY	-	EXPRESSION TAG	UNP Q9HC16
A	182	SER	-	EXPRESSION TAG	UNP Q9HC16
A	183	PRO	-	EXPRESSION TAG	UNP Q9HC16
A	184	GLU	-	EXPRESSION TAG	UNP Q9HC16
A	185	PHE	-	EXPRESSION TAG	UNP Q9HC16
A	186	GLU	-	EXPRESSION TAG	UNP Q9HC16
A	187	LEU	-	EXPRESSION TAG	UNP Q9HC16
A	188	GLY	-	EXPRESSION TAG	UNP Q9HC16
A	189	THR	-	EXPRESSION TAG	UNP Q9HC16
A	190	THR	-	EXPRESSION TAG	UNP Q9HC16
A	234	LYS	LEU	ENGINEERED MUTATION	UNP Q9HC16
A	243	ALA	CYS	ENGINEERED MUTATION	UNP Q9HC16
A	310	LYS	PHE	ENGINEERED MUTATION	UNP Q9HC16
A	321	ALA	CYS	ENGINEERED MUTATION	UNP Q9HC16
A	356	ALA	CYS	ENGINEERED MUTATION	UNP Q9HC16
B	178	GLY	-	EXPRESSION TAG	UNP Q9HC16
B	179	PRO	-	EXPRESSION TAG	UNP Q9HC16
B	180	LEU	-	EXPRESSION TAG	UNP Q9HC16
B	181	GLY	-	EXPRESSION TAG	UNP Q9HC16
B	182	SER	-	EXPRESSION TAG	UNP Q9HC16
B	183	PRO	-	EXPRESSION TAG	UNP Q9HC16
B	184	GLU	-	EXPRESSION TAG	UNP Q9HC16

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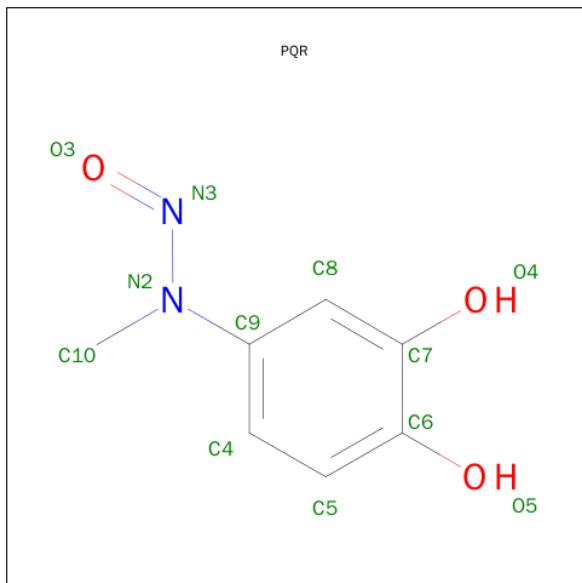
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Chain	Residue	Modelled	Actual	Comment	Reference
B	185	PHE	-	EXPRESSION TAG	UNP Q9HC16
B	186	GLU	-	EXPRESSION TAG	UNP Q9HC16
B	187	LEU	-	EXPRESSION TAG	UNP Q9HC16
B	188	GLY	-	EXPRESSION TAG	UNP Q9HC16
B	189	THR	-	EXPRESSION TAG	UNP Q9HC16
B	190	THR	-	EXPRESSION TAG	UNP Q9HC16
B	234	LYS	LEU	ENGINEERED MUTATION	UNP Q9HC16
B	243	ALA	CYS	ENGINEERED MUTATION	UNP Q9HC16
B	310	LYS	PHE	ENGINEERED MUTATION	UNP Q9HC16
B	321	ALA	CYS	ENGINEERED MUTATION	UNP Q9HC16
B	356	ALA	CYS	ENGINEERED MUTATION	UNP Q9HC16

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

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

- Molecule 3 is 4-[METHYL(NITROSO)AMINO]BENZENE-1,2-DIOL (three-letter code: PQR) (formula: $C_7H_8N_2O_3$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 12	C 7	N 2	O 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total 12	C 7	N 2	O 3	0	0
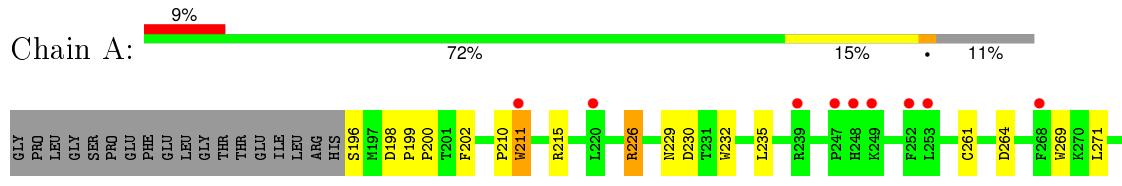
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	94	Total 94	O 94	0	0
4	B	60	Total 60	O 60	0	0
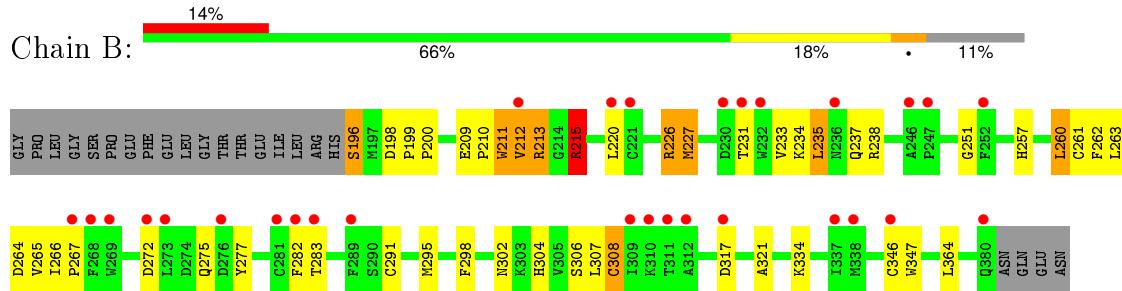
3 Residue-property plots (i)

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: DNA dC->dU-editing enzyme APOBEC-3G

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.08Å 67.76Å 64.47Å 90.00° 107.38° 90.00°	Depositor
Resolution (Å)	28.01 – 2.04 28.01 – 2.04	Depositor EDS
% Data completeness (in resolution range)	96.0 (28.01-2.04) 96.1 (28.01-2.04)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.6.0119	Depositor
R, R_{free}	0.228 , 0.276 0.233 , 0.281	Depositor DCC
R_{free} test set	1332 reflections (5.21%)	DCC
Wilson B-factor (Å^2)	39.9	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 56.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Outliers	0 of 26968 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3085	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.26% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, PQR

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	0.77	8/1526 (0.5%)	0.77	0/2079
1	B	0.78	4/1486 (0.3%)	0.75	1/2027 (0.0%)
All	All	0.77	12/3012 (0.4%)	0.76	1/4106 (0.0%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	307	LEU	C-N	10.53	1.58	1.34
1	A	308	CYS	C-N	7.76	1.51	1.34
1	B	308	CYS	C-N	7.22	1.50	1.34
1	A	347	TRP	CD2-CE2	6.25	1.48	1.41
1	B	347	TRP	CD2-CE2	5.97	1.48	1.41
1	A	307	LEU	C-N	5.70	1.47	1.34
1	B	211	TRP	CD2-CE2	5.55	1.48	1.41
1	A	269	TRP	CD2-CE2	5.50	1.48	1.41
1	A	285	TRP	CD2-CE2	5.47	1.48	1.41
1	A	232	TRP	CD2-CE2	5.42	1.47	1.41
1	A	211	TRP	CD2-CE2	5.28	1.47	1.41
1	A	361	TRP	CD2-CE2	5.26	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	215	ARG	NE-CZ-NH1	5.31	122.96	120.30

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	1470	0	1324	19	0
1	B	1433	0	1269	39	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	12	0	5	1	0
3	B	12	0	5	1	0
4	A	94	0	0	2	0
4	B	60	0	0	2	0
All	All	3085	0	2603	58	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 10.

All (58) 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:PHE:O	1:B:302:ASN:ND2	2.13	0.80
1:A:317:ASP:HB3	1:A:321:ALA:HB2	1.64	0.79
1:B:210:PRO:HD2	1:B:211:TRP:CE3	2.18	0.78
1:B:226:ARG:HB2	1:B:235:LEU:HD21	1.69	0.75
1:B:227:MET:CE	1:B:231:THR:C	2.60	0.70
1:A:334:LYS:NZ	4:A:514:HOH:O	2.30	0.65
1:A:317:ASP:CB	1:A:321:ALA:HB2	2.29	0.63
1:A:202:PHE:HE1	1:A:346[A]:CYS:HG	1.46	0.63
1:B:272:ASP:HB3	1:B:275:GLN:HG2	1.82	0.61
1:B:317:ASP:HB3	1:B:321:ALA:HB2	1.83	0.60
1:B:308:CYS:SG	3:B:403:PQR:N3	2.75	0.60
1:A:199:PRO:HB2	1:A:200:PRO:HD3	1.84	0.59
1:B:227:MET:HE2	1:B:231:THR:O	2.03	0.59
1:B:211:TRP:CD1	1:B:212:VAL:N	2.71	0.58
1:B:199:PRO:HB2	1:B:200:PRO:HD3	1.85	0.57
1:A:210:PRO:HD2	1:A:211:TRP:CE3	2.41	0.55
1:B:251:GLY:HA2	4:B:508:HOH:O	2.05	0.55
1:B:209:GLU:O	1:B:215:ARG:NH2	2.41	0.53
1:A:226:ARG:CZ	1:A:275:GLN:HG3	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:MET:HA	1:B:227:MET:HE3	1.91	0.52
1:B:272:ASP:HB3	1:B:275:GLN:CG	2.39	0.52
1:B:266:ILE:N	1:B:267:PRO:HD2	2.25	0.52
1:B:227:MET:HE1	1:B:231:THR:C	2.32	0.50
1:A:275:GLN:O	1:A:304:HIS:HB2	2.11	0.50
1:B:317:ASP:CB	1:B:321:ALA:HB2	2.41	0.49
1:B:261:CYS:O	1:B:264:ASP:HB2	2.13	0.48
1:B:235:LEU:O	1:B:237:GLN:O	2.31	0.48
1:A:226:ARG:HG3	1:A:277:TYR:CE2	2.49	0.48
1:B:227:MET:HE1	1:B:231:THR:CA	2.44	0.48
1:B:227:MET:CE	1:B:231:THR:O	2.60	0.47
1:B:262:PHE:O	1:B:265:VAL:HG22	2.14	0.47
1:B:226:ARG:HG3	1:B:277:TYR:CE1	2.50	0.47
1:B:196:SER:HB3	4:B:550:HOH:O	2.15	0.46
1:B:364:LEU:C	1:B:364:LEU:HD23	2.35	0.46
1:A:229:ASN:O	1:A:230:ASP:HB2	2.15	0.46
1:B:198:ASP:OD2	1:B:200:PRO:HD2	2.16	0.46
1:B:275:GLN:O	1:B:304:HIS:HB2	2.16	0.46
1:A:315[B]:TYR:CE2	1:A:317:ASP:HB2	2.51	0.46
1:A:308:CYS:SG	3:A:403:PQR:N3	2.89	0.45
1:A:261:CYS:O	1:A:264:ASP:HB2	2.17	0.44
1:B:227:MET:HE2	1:B:231:THR:C	2.36	0.43
1:B:291:CYS:O	1:B:295:MET:HG3	2.18	0.43
1:B:213:ARG:HD3	1:B:213:ARG:HA	1.83	0.43
1:B:257:HIS:HB2	1:B:260:LEU:HD22	2.01	0.42
1:A:291:CYS:O	1:A:295:MET:HG3	2.19	0.42
1:B:282:PHE:CG	1:B:346[B]:CYS:SG	3.13	0.42
1:B:227:MET:CE	1:B:231:THR:N	2.83	0.42
1:B:237:GLN:O	1:B:238:ARG:CB	2.68	0.42
1:B:266:ILE:HB	1:B:267:PRO:CD	2.49	0.42
1:A:198:ASP:OD1	1:A:199:PRO:HD2	2.20	0.42
1:A:226:ARG:NH2	1:A:275:GLN:HG3	2.36	0.41
1:A:371:LEU:HD21	4:A:509:HOH:O	2.19	0.41
1:B:227:MET:HA	1:B:227:MET:CE	2.51	0.41
1:A:202:PHE:HE1	1:A:346[A]:CYS:SG	2.44	0.41
1:B:235:LEU:N	1:B:235:LEU:HD13	2.36	0.41
1:B:220:LEU:HG	1:B:283:THR:HG22	2.03	0.41
1:B:302:ASN:ND2	1:B:302:ASN:N	2.69	0.40
1:A:271:LEU:HD22	1:A:277:TYR:CE2	2.57	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	185/207 (89%)	178 (96%)	7 (4%)	0	100	100
1	B	185/207 (89%)	179 (97%)	6 (3%)	0	100	100
All	All	370/414 (89%)	357 (96%)	13 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	151/182 (83%)	143 (95%)	8 (5%)	28	17
1	B	140/182 (77%)	127 (91%)	13 (9%)	11	4
All	All	291/364 (80%)	270 (93%)	21 (7%)	19	9

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	SER
1	A	215	ARG
1	A	226	ARG
1	A	235	LEU
1	A	306	SER
1	A	315[A]	TYR
1	A	315[B]	TYR
1	A	366	GLU

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Mol	Chain	Res	Type
1	B	196	SER
1	B	212	VAL
1	B	213	ARG
1	B	215	ARG
1	B	226	ARG
1	B	227	MET
1	B	233	VAL
1	B	234	LYS
1	B	235	LEU
1	B	260	LEU
1	B	263	LEU
1	B	306	SER
1	B	334	LYS

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 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
3	PQR	A	403	1	12,12,12	3.51	5 (41%)	14,16,16	1.08	1 (7%)
3	PQR	B	403	1	12,12,12	3.68	5 (41%)	14,16,16	1.30	1 (7%)

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	PQR	A	403	1	-	0/6/6/6	0/1/1/1
3	PQR	B	403	1	-	0/6/6/6	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	403	PQR	O5-C6	-5.81	1.24	1.36
3	B	403	PQR	O4-C7	-5.57	1.24	1.36
3	A	403	PQR	O5-C6	-5.41	1.25	1.36
3	A	403	PQR	O4-C7	-5.25	1.25	1.36
3	A	403	PQR	C7-C6	4.78	1.48	1.40
3	B	403	PQR	C7-C6	5.02	1.48	1.40
3	A	403	PQR	O3-N3	5.40	1.40	1.23
3	B	403	PQR	O3-N3	5.54	1.41	1.23
3	B	403	PQR	C4-C9	6.09	1.51	1.39
3	A	403	PQR	C4-C9	6.14	1.51	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	PQR	C4-C9-N2	2.23	123.52	120.62
3	B	403	PQR	O3-N3-N2	3.18	123.67	114.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	PQR	1	0
3	B	403	PQR	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	184/207 (88%)	0.47	19 (10%)	9	9	42, 55, 72, 97	2 (1%)
1	B	185/207 (89%)	0.60	29 (15%)	3	2	44, 61, 76, 87	2 (1%)
All	All	369/414 (89%)	0.54	48 (13%)	5	5	42, 57, 76, 97	4 (1%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	317	ASP	5.2
1	A	335	ILE	5.1
1	A	315[A]	TYR	4.5
1	A	252	PHE	4.2
1	A	314	ILE	3.3
1	B	252	PHE	3.3
1	B	272	ASP	3.3
1	B	312	ALA	3.2
1	B	317	ASP	3.2
1	B	267	PRO	3.2
1	B	246	ALA	3.0
1	B	380	GLN	3.0
1	A	319	GLY	3.0
1	A	253	LEU	3.0
1	B	268	PHE	3.0
1	B	232	TRP	3.0
1	B	247	PRO	2.9
1	B	231	THR	2.9
1	A	268	PHE	2.8
1	B	309	ILE	2.7
1	B	346[A]	CYS	2.7
1	B	282	PHE	2.6
1	B	230	ASP	2.6
1	B	276	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	220	LEU	2.5
1	B	311	THR	2.5
1	B	281	CYS	2.4
1	A	282	PHE	2.4
1	B	273	LEU	2.3
1	B	289	PHE	2.3
1	B	338	MET	2.3
1	A	247	PRO	2.3
1	B	283	THR	2.3
1	B	220	LEU	2.3
1	A	283	THR	2.2
1	B	221	CYS	2.2
1	A	239	ARG	2.2
1	B	269	TRP	2.2
1	B	236	ASN	2.1
1	A	281	CYS	2.1
1	A	211	TRP	2.1
1	B	337	ILE	2.1
1	A	249	LYS	2.1
1	B	310	LYS	2.1
1	B	212	VAL	2.1
1	A	289	PHE	2.0
1	A	359	GLN	2.0
1	A	248	HIS	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	PQR	B	403	12/12	0.78	0.22	1.27	70,77,83,90	0
3	PQR	A	403	12/12	0.90	0.17	0.45	63,69,75,77	0
2	ZN	A	401	1/1	0.99	0.03	-2.21	58,58,58,58	0
2	ZN	B	401	1/1	0.98	0.05	-4.28	57,57,57,57	0
2	ZN	A	402	1/1	0.97	0.05	-	57,57,57,57	0
2	ZN	B	402	1/1	0.98	0.03	-	60,60,60,60	0

6.5 Other polymers (i)

There are no such residues in this entry.