Full wwPDB X-ray Structure Validation Report (i)

Jul 3, 2024 – 05:19 PM EDT

PDB ID	:	6BUU
Title	:	Crystal structure of AKT1 (aa 144-480) with a bisubstrate
Authors	:	Chu, N.; Gabelli, S.B.; Cole, P.A.
Deposited on	:	2017-12-11
Resolution	:	2.40 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 (i)) were used in the production of this report:

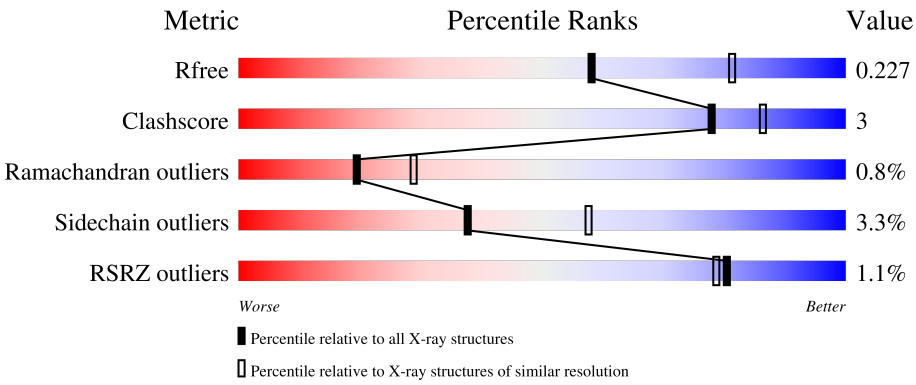
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	337	% 89% 5% • •
1	B	337	% 85% 9% • 5%
2	F	10	80% 20%
2	G	10	70% 30%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5780 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.

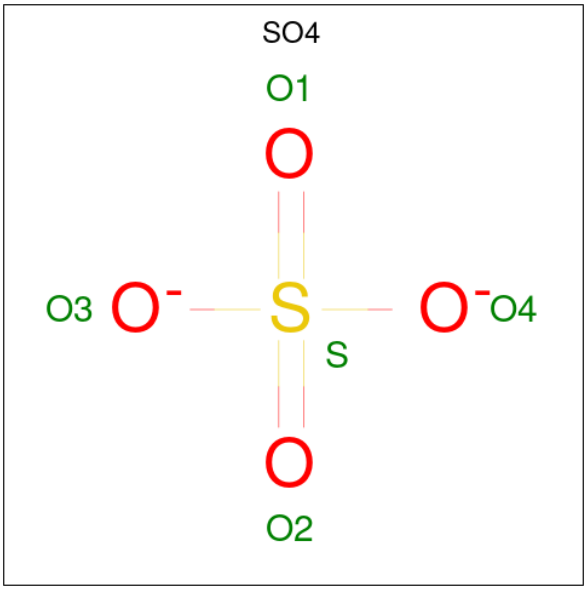
- Molecule 1 is a protein called RAC-alpha serine/threonine-protein kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	323	2666	1703	449	496	3	15	0	2	0
1	B	319	2645	1694	445	488	3	15	0	2	0

- Molecule 2 is a protein called GLY-ARG-PRO-ARG-THR-THR-ZXW-PHE-ALA-GLU.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
2	F	10	112	59	22	27	3	1	0	0	0
2	G	10	112	59	22	27	3	1	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	A	1	5	4	1	0	0

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
4	F	1	1	1	0	0
			Total	Mn		
4	G	1	1	1	0	0

- Molecule 5 is water.

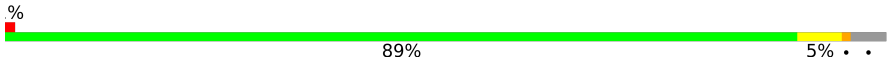
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	115	115	115	0	0
			Total	O		
5	B	113	113	113	0	0
			Total	O		
5	F	3	3	3	0	0
			Total	O		
5	G	7	7	7	0	0

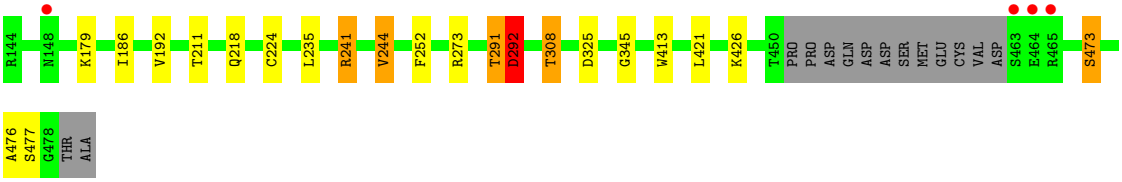
3 Residue-property plots (i)

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: RAC-alpha serine/threonine-protein kinase

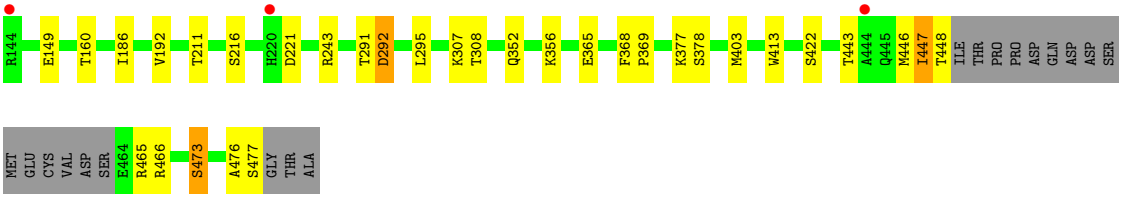
Chain A:





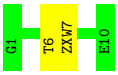
• Molecule 1: RAC-alpha serine/threonine-protein kinase

Chain B:



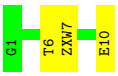
• Molecule 2: GLY-ARG-PRO-ARG-THR-THR-ZXW-PHE-ALA-GLU

Chain F:



• Molecule 2: GLY-ARG-PRO-ARG-THR-THR-ZXW-PHE-ALA-GLU

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.63Å 56.27Å 91.84Å 90.00° 105.10° 90.00°	Depositor
Resolution (Å)	47.00 – 2.40 46.69 – 2.40	Depositor EDS
% Data completeness (in resolution range)	86.9 (47.00-2.40) 86.8 (46.69-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.58 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.183 , 0.230 0.195 , 0.227	Depositor DCC
R_{free} test set	1382 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å^2)	31.7	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 39.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5780	wwPDB-VP
Average B, all atoms (Å^2)	37.0	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 48.27 % 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 8.8140e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, MN, TPO, ZXW, SO4

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	0.83	0/2694	0.89	0/3618
1	B	0.85	0/2680	0.88	0/3598
2	F	0.81	0/72	1.01	0/94
2	G	1.08	0/72	1.04	0/94
All	All	0.85	0/5518	0.89	0/7404

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	2666	0	2616	18	0
1	B	2645	0	2609	15	0
2	F	112	0	72	1	0
2	G	112	0	72	1	0
3	A	5	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
5	A	115	0	0	2	0
5	B	113	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	3	0	0	0	0
5	G	7	0	0	0	0
All	All	5780	0	5369	32	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 3.

All (32) 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:446:MET:SD	1:B:447:ILE:O	2.04	1.14
1:B:446:MET:SD	1:B:447:ILE:N	2.23	1.10
1:A:426:LYS:HB3	5:A:704:HOH:O	1.87	0.75
1:A:413:TRP:H	1:B:352:GLN:HE22	1.35	0.74
1:A:241:ARG:HG3	1:A:241:ARG:HH11	1.55	0.72
1:A:241:ARG:HH11	1:A:241:ARG:CG	2.04	0.68
1:A:476:ALA:O	1:A:477:SEP:HB3	1.91	0.68
1:B:211:THR:OG1	1:B:291:THR:HG22	1.94	0.67
1:B:221:ASP:OD1	1:B:466:ARG:NE	2.33	0.60
1:A:179:LYS:HD3	2:F:7:ZXW:O1A	2.01	0.60
1:B:291:THR:O	1:B:292:ASP:HB2	2.06	0.56
1:A:413:TRP:H	1:B:352:GLN:NE2	2.05	0.54
1:A:186:ILE:HG22	1:A:192:VAL:HG22	1.90	0.52
1:B:446:MET:CG	1:B:447:ILE:N	2.73	0.52
1:A:292:ASP:HB3	5:A:663:HOH:O	2.11	0.49
1:A:211:THR:OG1	1:A:291:THR:HG22	2.13	0.48
1:B:186:ILE:HG22	1:B:192:VAL:HG22	1.97	0.47
1:A:218:GLN:HG2	1:A:473:SEP:O3P	2.15	0.46
1:A:244:VAL:HG23	1:A:345:GLY:CA	2.47	0.45
1:B:368:PHE:CD2	1:B:377[C]:LYS:HG3	2.53	0.44
1:B:377[A]:LYS:HB2	1:B:377[A]:LYS:HE3	1.86	0.43
1:B:377[C]:LYS:CA	1:B:378:SER:N	2.80	0.43
1:A:241:ARG:CG	1:A:241:ARG:NH1	2.73	0.42
1:B:216:SER:O	1:B:473:SEP:HA	2.19	0.42
1:B:403:MET:HA	1:B:413:TRP:CZ2	2.55	0.41
1:A:252:PHE:CD1	1:A:421:LEU:HD23	2.55	0.41
1:A:273:ARG:NH1	1:A:308:TPO:O2P	2.39	0.41
1:A:186:ILE:HG22	1:A:192:VAL:CG2	2.50	0.41
1:B:446:MET:C	1:B:447:ILE:HG23	2.41	0.41
1:A:179:LYS:O	1:A:224:CYS:HA	2.21	0.41
2:G:7:ZXW:O2B	2:G:7:ZXW:S2G	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:LEU:HD23	1:A:235:LEU:HA	1.96	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	318/337 (94%)	308 (97%)	8 (2%)	2 (1%)	25	36
1	B	316/337 (94%)	300 (95%)	13 (4%)	3 (1%)	17	25
2	F	7/10 (70%)	7 (100%)	0	0	100	100
2	G	7/10 (70%)	7 (100%)	0	0	100	100
All	All	648/694 (93%)	622 (96%)	21 (3%)	5 (1%)	19	29

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	325	ASP
1	B	243	ARG
1	B	476	ALA
1	A	292	ASP
1	B	292	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	282/293 (96%)	278 (99%)	4 (1%)	67	82
1	B	280/293 (96%)	268 (96%)	12 (4%)	29	46
2	F	7/7 (100%)	6 (86%)	1 (14%)	3	4
2	G	7/7 (100%)	5 (71%)	2 (29%)	0	0
All	All	576/600 (96%)	557 (97%)	19 (3%)	38	57

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	241	ARG
1	A	244	VAL
1	A	291	THR
1	A	292	ASP
1	B	149	GLU
1	B	160	THR
1	B	295	LEU
1	B	307	LYS
1	B	356	LYS
1	B	365	GLU
1	B	369	PRO
1	B	422	SER
1	B	443	THR
1	B	447	ILE
1	B	448	THR
1	B	465	ARG
2	F	6	THR
2	G	6	THR
2	G	10	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	ASN
1	A	414	GLN
1	A	445	GLN
1	B	324	ASN
1	B	352	GLN
1	B	414	GLN
1	B	428	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)

6 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	TPO	B	308	1	8,10,11	2.50	1 (12%)	10,14,16	1.64	2 (20%)
1	SEP	B	473	1	8,9,10	0.62	0	8,12,14	3.00	4 (50%)
1	TPO	A	308	1	8,10,11	1.92	1 (12%)	10,14,16	2.60	4 (40%)
1	SEP	A	473	1	8,9,10	0.80	0	8,12,14	1.94	3 (37%)
1	SEP	A	477	1	8,9,10	0.74	0	8,12,14	1.06	0
1	SEP	B	477	1	8,9,10	0.63	0	8,12,14	2.45	1 (12%)

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
1	TPO	B	308	1	-	1/9/11/13	-
1	SEP	B	473	1	-	4/5/8/10	-
1	TPO	A	308	1	-	2/9/11/13	-
1	SEP	A	473	1	-	1/5/8/10	-
1	SEP	A	477	1	-	4/5/8/10	-
1	SEP	B	477	1	-	1/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	308	TPO	P-OG1	6.63	1.71	1.59
1	A	308	TPO	P-OG1	4.91	1.68	1.59

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	477	SEP	OG-CB-CA	6.03	114.02	108.14
1	B	473	SEP	OG-P-O1P	-6.02	89.58	106.47
1	A	308	TPO	O3P-P-OG1	4.57	126.47	105.99
1	A	308	TPO	O3P-P-O2P	-4.30	91.21	107.64
1	A	473	SEP	OG-CB-CA	3.76	111.81	108.14
1	B	308	TPO	O3P-P-OG1	3.39	121.19	105.99
1	B	473	SEP	OG-CB-CA	-3.36	104.88	108.14
1	B	473	SEP	O3P-P-O1P	3.07	122.69	110.68
1	A	308	TPO	O3P-P-O1P	3.07	122.69	110.68
1	A	308	TPO	OG1-P-O1P	-3.00	97.81	109.39
1	B	473	SEP	P-OG-CB	2.53	125.26	118.30
1	A	473	SEP	O3P-P-OG	-2.35	100.48	106.73
1	A	473	SEP	O3P-P-O2P	2.21	116.09	107.64
1	B	308	TPO	CG2-CB-CA	-2.05	109.12	113.16

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	477	SEP	N-CA-CB-OG
1	A	477	SEP	CB-OG-P-O1P
1	A	477	SEP	CB-OG-P-O2P
1	A	477	SEP	CB-OG-P-O3P
1	B	308	TPO	CB-OG1-P-O1P
1	B	473	SEP	N-CA-CB-OG
1	B	473	SEP	CB-OG-P-O1P
1	B	473	SEP	CB-OG-P-O2P
1	B	473	SEP	CB-OG-P-O3P
1	A	473	SEP	CA-CB-OG-P
1	B	477	SEP	N-CA-CB-OG
1	A	308	TPO	CB-OG1-P-O1P
1	A	308	TPO	CB-OG1-P-O2P

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	473	SEP	1	0
1	A	308	TPO	1	0
1	A	473	SEP	1	0
1	A	477	SEP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	SO4	A	501	-	4,4,4	0.44	0	6,6,6	0.91	0

There are no bond length outliers.

There are no bond angle outliers.

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 (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	320/337 (94%)	-0.32	4 (1%)	77	75	16, 32, 76, 109	0
1	B	316/337 (93%)	-0.34	3 (0%)	84	82	16, 31, 67, 109	0
2	F	9/10 (90%)	-0.19	0	100	100	27, 30, 44, 69	0
2	G	9/10 (90%)	-0.16	0	100	100	29, 37, 49, 53	0
All	All	654/694 (94%)	-0.33	7 (1%)	80	79	16, 31, 69, 109	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	465	ARG	4.2
1	A	464	GLU	4.0
1	B	444	ALA	2.9
1	B	144	ARG	2.9
1	B	220	HIS	2.3
1	A	463	SER	2.3
1	A	148	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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(Å^2)	Q<0.9
1	SEP	B	477	10/11	0.74	0.24	81,91,106,110	0
1	SEP	A	477	10/11	0.75	0.23	79,115,144,150	0
1	TPO	A	308	11/12	0.87	0.16	26,32,52,57	0
1	SEP	B	473	10/11	0.91	0.10	42,53,66,67	0
1	TPO	B	308	11/12	0.92	0.13	26,29,52,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	SEP	A	473	10/11	0.96	0.10	34,44,57,61	0

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, 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(Å^2)	Q<0.9
4	MN	F	501	1/1	0.58	0.14	90,90,90,90	0
4	MN	G	501	1/1	0.76	0.07	74,74,74,74	0
3	SO4	A	501	5/5	0.97	0.18	48,52,60,61	0

6.5 Other polymers (i)

There are no such residues in this entry.