Full wwPDB X-ray Structure Validation Report (i)

Mar 23, 2023 – 12:25 pm GMT

PDB ID	:	5BXO
Title	:	Human Tankyrase-2 in Complex with Macrocyclised Extended Peptide cp4n2m3
Authors	:	Xu, W.; Fischer, G.; Hyvonen, M.; Itzhaki, L.
Deposited on	:	2015-06-09
Resolution	:	1.33 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:

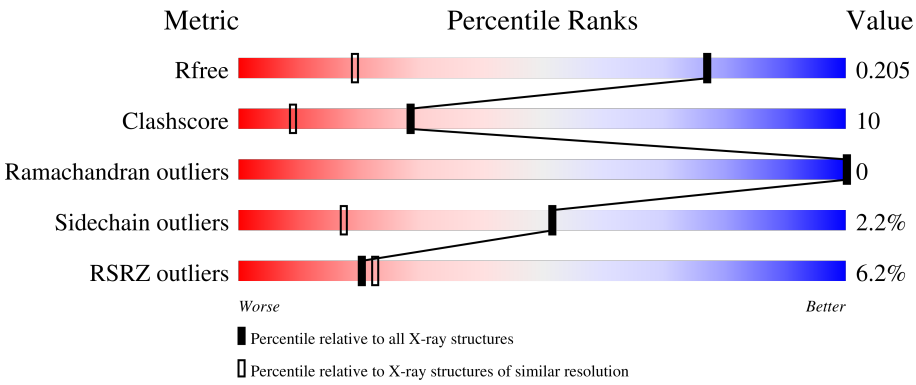
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 1.33 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	1385 (1.36-1.32)
Clashscore	141614	1417 (1.36-1.32)
Ramachandran outliers	138981	1397 (1.36-1.32)
Sidechain outliers	138945	1397 (1.36-1.32)
RSRZ outliers	127900	1369 (1.36-1.32)

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	164	6% 76% 21% • •
1	B	164	7% 79% 18% • •
2	C	10	100%
2	D	10	90% 10%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3203 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 Tankyrase-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	160	1331	831	245	251	4	13	13	0
1	B	163	1384	858	255	266	5	9	17	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	486	GLY	-	expression tag	UNP Q9H2K2
A	487	SER	-	expression tag	UNP Q9H2K2
B	486	GLY	-	expression tag	UNP Q9H2K2
B	487	SER	-	expression tag	UNP Q9H2K2

- Molecule 2 is a protein called Tankyrase-2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	10	68	37	13	18	3	1	1
2	D	10	68	37	13	18	3	1	1

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	ACE	-	expression tag	UNP Q9H2K2
C	2	GLU	CYS	conflict	UNP Q9H2K2
C	5	ASP	GLY	conflict	UNP Q9H2K2
C	8	GLU	ALA	conflict	UNP Q9H2K2
C	9	NH2	-	expression tag	UNP Q9H2K2
D	0	ACE	-	expression tag	UNP Q9H2K2
D	2	GLU	CYS	conflict	UNP Q9H2K2
D	5	ASP	GLY	conflict	UNP Q9H2K2

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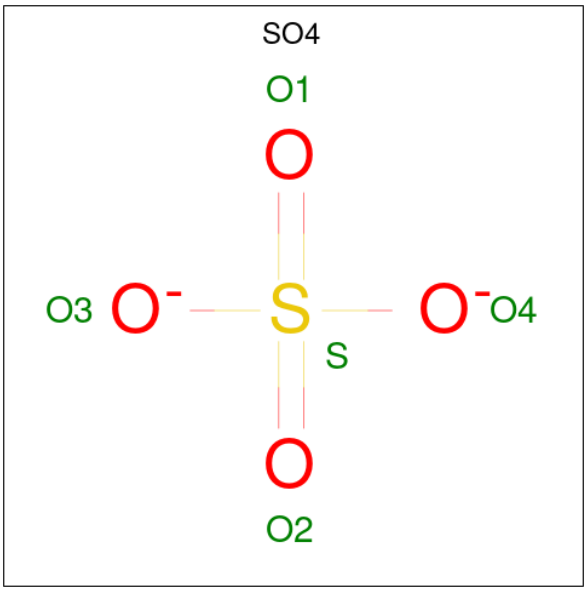
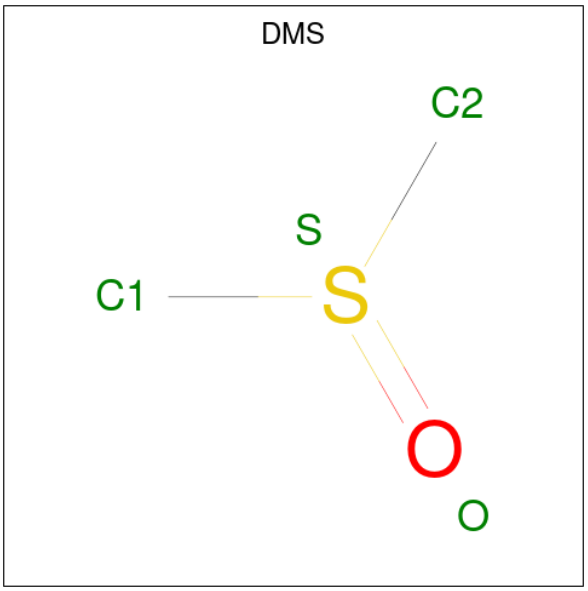
Chain	Residue	Modelled	Actual	Comment	Reference
D	8	GLU	ALA	conflict	UNP Q9H2K2
D	9	NH2	-	expression tag	UNP Q9H2K2

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



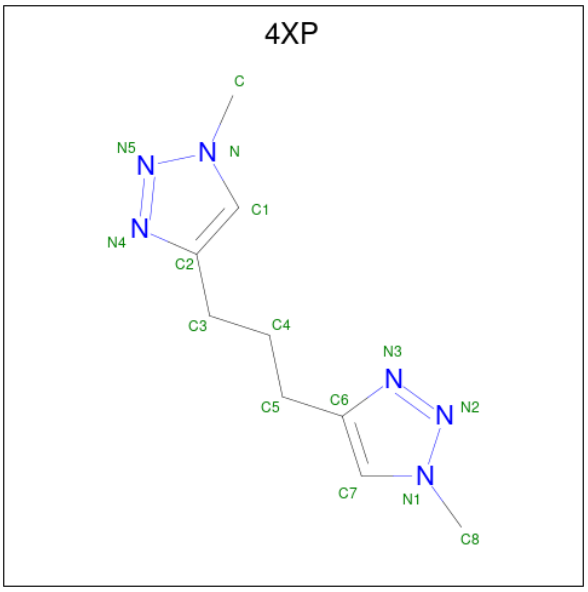
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
3	A	1	5	4	1		0	0
3	A	1	5	4	1		0	0
3	A	1	5	4	1		0	0
3	B	1	5	4	1		0	0
3	B	1	5	4	1		0	0
3	B	1	5	4	1		0	0

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
4	A	1	4	2	1	1	0	0
			Total	C	O	S		
4	B	1	4	2	1	1	0	0
			Total	C	O	S		
4	B	1	4	2	1	1	0	0

- Molecule 5 is 4,4'-propane-1,3-diylbis(1-methyl-1H-1,2,3-triazole) (three-letter code: 4XP) (formula: $C_9H_{14}N_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
5	C	1	15	9	6	0	0
			Total	C	N		
5	D	1	15	9	6	0	0

- Molecule 6 is water.

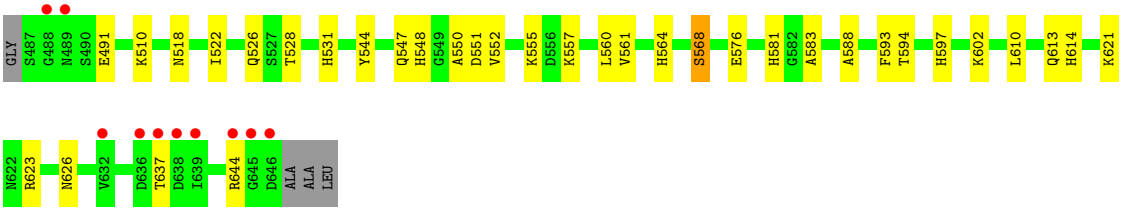
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	123	123	123	0	0
			Total	O		
6	B	127	129	129	0	1
			Total	O		
6	C	11	11	11	0	0
			Total	O		
6	D	16	17	17	0	1

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.

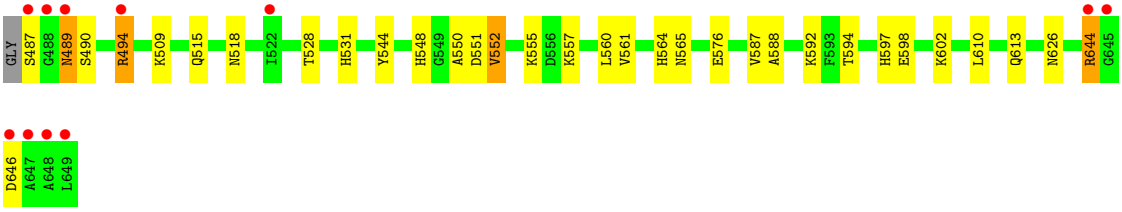
• Molecule 1: Tankyrase-2

Chain A:



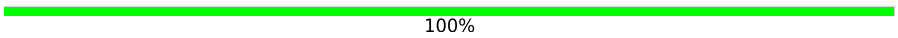
• Molecule 1: Tankyrase-2

Chain B:



• Molecule 2: Tankyrase-2

Chain C:



There are no outlier residues recorded for this chain.

• Molecule 2: Tankyrase-2

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	29.82Å 46.01Å 54.47Å 78.45° 88.99° 72.35°	Depositor
Resolution (Å)	53.31 – 1.33 42.92 – 1.33	Depositor EDS
% Data completeness (in resolution range)	95.8 (53.31-1.33) 95.7 (42.92-1.33)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	50.00 (at 1.33Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.175 , 0.203 0.177 , 0.205	Depositor DCC
R_{free} test set	2934 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	12.0	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 59.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.059 for h,h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3203	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.16% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NH2, DMS, 4XP, ACE

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	1.13	6/1359 (0.4%)	0.86	3/1833 (0.2%)
1	B	0.67	1/1409 (0.1%)	0.82	1/1900 (0.1%)
2	C	0.66	0/63	0.71	0/81
2	D	0.62	0/63	0.65	0/81
All	All	0.91	7/2894 (0.2%)	0.83	4/3895 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	491	GLU	CD-OE2	-27.20	0.95	1.25
1	A	491	GLU	CD-OE1	14.22	1.41	1.25
1	A	547	GLN	CD-OE1	10.27	1.46	1.24
1	B	489	ASN	CB-CG	-9.05	1.30	1.51
1	A	547	GLN	CD-NE2	-8.78	1.10	1.32
1	A	510	LYS	CD-CE	-6.58	1.34	1.51
1	A	568	SER	CB-OG	-5.05	1.35	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	509	LYS	CD-CE-NZ	6.16	125.87	111.70
1	A	621[A]	LYS	CD-CE-NZ	5.20	123.67	111.70
1	A	621[B]	LYS	CD-CE-NZ	5.20	123.67	111.70
1	A	491	GLU	CG-CD-OE1	-5.17	107.96	118.30

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	1331	0	1335	27	1
1	B	1384	0	1368	29	0
2	C	68	0	54	0	0
2	D	68	0	54	1	0
3	A	15	0	0	1	0
3	B	15	0	0	0	0
4	A	4	0	6	0	0
4	B	8	0	12	0	0
5	C	15	0	0	0	0
5	D	15	0	0	0	0
6	A	123	0	0	3	0
6	B	129	0	0	3	0
6	C	11	0	0	0	0
6	D	17	0	0	0	0
All	All	3203	0	2829	56	1

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 (56) 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:613[B]:GLN:HG3	6:B:866:HOH:O	1.80	0.81
1:B:644[A]:ARG:NH2	1:B:646:ASP:OD2	2.19	0.74
1:A:594:THR:H	1:A:597:HIS:HD2	1.38	0.70
1:A:552[B]:VAL:HG13	6:A:867:HOH:O	2.00	0.59
1:B:594:THR:H	1:B:597:HIS:HD2	1.48	0.59
1:A:594:THR:H	1:A:597:HIS:CD2	2.18	0.59
1:B:598:GLU:OE2	2:D:1:ARG:NH2	2.30	0.58
1:A:518:ASN:HD21	1:A:550:ALA:HA	1.68	0.57
1:B:594:THR:H	1:B:597:HIS:CD2	2.23	0.57
1:B:528:THR:H	1:B:531:HIS:CD2	2.24	0.56
1:A:528:THR:H	1:A:531:HIS:CD2	2.25	0.54
1:B:490[A]:SER:O	1:B:494[A]:ARG:HD3	2.07	0.54
1:B:531:HIS:HE1	1:B:560[A]:LEU:O	1.91	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:HIS:HE1	1:A:560[A]:LEU:O	1.91	0.54
1:A:531:HIS:HE1	1:A:560[B]:LEU:O	1.91	0.53
1:B:552[A]:VAL:HG13	6:B:896:HOH:O	2.08	0.53
1:B:528:THR:H	1:B:531:HIS:HD2	1.58	0.51
1:A:568:SER:O	1:A:602[B]:LYS:HE2	2.11	0.50
1:A:528:THR:OG1	1:A:531:HIS:HD2	1.95	0.50
1:B:518:ASN:HD21	1:B:551:ASP:H	1.59	0.50
1:A:555[A]:LYS:NZ	1:A:588:ALA:O	2.42	0.49
1:B:561:VAL:HG22	1:B:564:HIS:CD2	2.47	0.49
1:A:614:HIS:HE1	3:A:702:SO4:O2	1.96	0.49
1:B:518:ASN:HD21	1:B:550:ALA:HA	1.77	0.49
1:A:576:GLU:OE2	1:A:610:LEU:HD13	2.13	0.48
1:B:487:SER:HB2	1:B:489:ASN:N	2.30	0.47
1:B:576:GLU:OE2	1:B:610:LEU:HD13	2.14	0.47
1:A:518:ASN:HD21	1:A:551:ASP:H	1.63	0.47
1:B:555[A]:LYS:NZ	1:B:588:ALA:O	2.47	0.46
1:B:515[B]:GLN:NE2	1:B:515[B]:GLN:H	2.14	0.45
1:B:518:ASN:ND2	1:B:551:ASP:H	2.14	0.45
1:B:528:THR:OG1	1:B:531:HIS:HD2	1.99	0.45
1:A:597:HIS:HE1	1:A:626:ASN:O	1.99	0.45
1:B:602[B]:LYS:HG2	6:B:807:HOH:O	2.16	0.45
1:B:552[B]:VAL:O	1:B:552[B]:VAL:HG12	2.17	0.45
1:B:597:HIS:HE1	1:B:626:ASN:O	2.01	0.44
1:B:544:TYR:O	1:B:548:HIS:HD2	2.01	0.44
1:A:560[B]:LEU:HD11	6:A:843:HOH:O	2.17	0.44
1:A:561:VAL:HG22	1:A:564:HIS:CD2	2.53	0.43
1:A:544:TYR:O	1:A:548:HIS:HD2	2.02	0.43
1:A:560[B]:LEU:HD12	1:A:560[B]:LEU:N	2.34	0.43
1:B:557[B]:LYS:C	1:B:557[B]:LYS:HD2	2.39	0.43
1:A:552[A]:VAL:HG11	1:A:583:ALA:HB2	2.01	0.43
1:A:522:ILE:HA	1:A:526[B]:GLN:HE21	1.83	0.43
1:A:518:ASN:ND2	1:A:551:ASP:H	2.17	0.42
1:B:592[B]:LYS:HE3	1:B:592[B]:LYS:HB3	1.75	0.42
1:B:561:VAL:HG21	1:B:587:VAL:HG11	2.01	0.42
1:A:581[B]:HIS:CD2	6:A:847:HOH:O	2.73	0.41
1:A:564:HIS:HE1	1:A:593:PHE:O	2.04	0.40
1:B:531:HIS:HE1	1:B:560[B]:LEU:O	2.05	0.40
1:A:528:THR:H	1:A:531:HIS:HD2	1.66	0.40
1:A:557[B]:LYS:C	1:A:557[B]:LYS:HD2	2.42	0.40

All (1) 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:A:613:GLN:OE1	1:A:623[B]:ARG:NH2[1_455]	2.16	0.04

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	171/164 (104%)	171 (100%)	0	0	100	100
1	B	178/164 (108%)	178 (100%)	0	0	100	100
2	C	9/10 (90%)	9 (100%)	0	0	100	100
2	D	9/10 (90%)	9 (100%)	0	0	100	100
All	All	367/348 (106%)	367 (100%)	0	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	143/131 (109%)	140 (98%)	3 (2%)	53	18
1	B	148/131 (113%)	140 (95%)	8 (5%)	22	2
2	C	5/4 (125%)	5 (100%)	0	100	100
2	D	5/4 (125%)	5 (100%)	0	100	100
All	All	301/270 (112%)	290 (96%)	11 (4%)	52	5

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	637[A]	THR
1	A	637[B]	THR
1	A	644	ARG
1	B	494[A]	ARG
1	B	494[B]	ARG
1	B	552[A]	VAL
1	B	552[B]	VAL
1	B	565[A]	ASN
1	B	565[B]	ASN
1	B	644[A]	ARG
1	B	644[B]	ARG

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	515	GLN
1	A	518	ASN
1	A	531	HIS
1	A	548	HIS
1	A	564	HIS
1	A	597	HIS
1	A	614	HIS
1	B	518	ASN
1	B	531	HIS
1	B	548	HIS
1	B	564	HIS
1	B	597	HIS

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)

11 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	$\#\|Z\| > 2$
4	DMS	A	704	-	3,3,3	0.51	0	3,3,3	0.54	0
3	SO4	A	703	-	4,4,4	0.32	0	6,6,6	0.65	0
3	SO4	A	701	-	4,4,4	0.40	0	6,6,6	0.14	0
4	DMS	B	705	-	3,3,3	0.52	0	3,3,3	0.49	0
5	4XP	C	100	2	14,16,16	1.54	2 (14%)	7,21,21	3.61	3 (42%)
4	DMS	B	704	-	3,3,3	0.47	0	3,3,3	0.55	0
3	SO4	B	703	-	4,4,4	0.41	0	6,6,6	0.21	0
5	4XP	D	100	2	14,16,16	2.55	6 (42%)	7,21,21	3.98	4 (57%)
3	SO4	B	702	-	4,4,4	0.37	0	6,6,6	0.51	0
3	SO4	A	702	-	4,4,4	0.43	0	6,6,6	0.35	0
3	SO4	B	701	-	4,4,4	0.45	0	6,6,6	0.43	0

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
5	4XP	C	100	2	-	2/6/6/6	0/2/2/2
5	4XP	D	100	2	-	2/6/6/6	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	100	4XP	C2-N4	5.23	1.41	1.34
5	D	100	4XP	C6-N3	4.55	1.40	1.34
5	C	100	4XP	C6-N3	3.81	1.39	1.34
5	D	100	4XP	N4-N5	-3.28	1.28	1.34
5	D	100	4XP	C5-C6	-3.08	1.44	1.51
5	D	100	4XP	N3-N2	-2.53	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	100	4XP	C1-N	2.50	1.38	1.35
5	D	100	4XP	N5-N	2.16	1.38	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	100	4XP	C-N-N5	-8.50	104.84	117.82
5	D	100	4XP	C-N-N5	-7.09	106.99	117.82
5	D	100	4XP	C8-N1-N2	6.33	127.49	117.82
5	D	100	4XP	C1-C2-N4	-3.85	105.62	111.34
5	C	100	4XP	C1-C2-N4	-2.83	107.14	111.34
5	C	100	4XP	C7-C6-N3	-2.60	107.48	111.34
5	D	100	4XP	C7-C6-N3	-2.01	108.35	111.34

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	100	4XP	C4-C5-C6-N3
5	C	100	4XP	N4-C2-C3-C4
5	D	100	4XP	C4-C5-C6-N3
5	D	100	4XP	N4-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	SO4	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	160/164 (97%)	0.40	10 (6%)	20	22	7, 13, 33, 72	5 (3%)
1	B	163/164 (99%)	0.38	11 (6%)	17	20	8, 14, 28, 58	4 (2%)
2	C	8/10 (80%)	0.06	0	100	100	10, 11, 16, 29	1 (12%)
2	D	8/10 (80%)	0.45	0	100	100	10, 13, 26, 35	1 (12%)
All	All	339/348 (97%)	0.38	21 (6%)	20	22	7, 13, 33, 72	11 (3%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	646	ASP	8.7
1	B	646	ASP	4.9
1	B	649	LEU	4.9
1	A	489	ASN	4.8
1	B	488	GLY	4.8
1	B	645	GLY	4.0
1	A	637[A]	THR	3.5
1	A	645	GLY	3.4
1	B	648	ALA	3.4
1	B	487	SER	3.3
1	A	638	ASP	2.9
1	A	644	ARG	2.9
1	A	488	GLY	2.8
1	B	522	ILE	2.7
1	A	639	ILE	2.7
1	B	647	ALA	2.6
1	A	636	ASP	2.5
1	B	489	ASN	2.4
1	B	644[A]	ARG	2.3
1	B	494[A]	ARG	2.3
1	A	632	VAL	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, 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	DMS	A	704	4/4	0.82	0.16	63,65,66,67	0
4	DMS	B	705	4/4	0.87	0.17	60,61,62,63	0
3	SO4	A	701	5/5	0.88	0.17	51,57,58,58	0
3	SO4	A	703	5/5	0.88	0.19	28,29,31,32	0
5	4XP	D	100	15/15	0.88	0.12	15,19,25,26	0
4	DMS	B	704	4/4	0.90	0.23	33,41,43,43	0
5	4XP	C	100	15/15	0.91	0.12	13,17,21,21	0
3	SO4	B	703	5/5	0.94	0.19	33,34,36,37	0
3	SO4	A	702	5/5	0.95	0.14	30,34,35,35	0
3	SO4	B	702	5/5	0.95	0.14	30,32,32,35	0
3	SO4	B	701	5/5	0.97	0.13	18,19,20,25	0

6.5 Other polymers (i)

There are no such residues in this entry.