wwPDB X-ray Structure Validation Summary Report (i)

Jun 24, 2024 – 04:17 AM EDT

PDB ID	:	6QJ2
Title	:	Crystal structure of the C. thermophilum condensin Smc4 ATPase head in complex with the C-terminal domain of Brn1
Authors	:	Hassler, M.; Haering, C.H.
Deposited on	:	2019-01-22
Resolution	:	3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

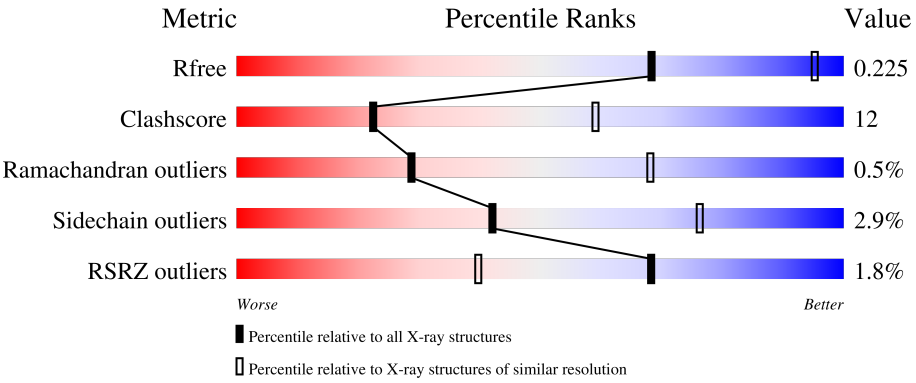
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	403	2% 67% 20% 12%
2	B	134	% 43% 19% 37%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3504 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 Smc4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	356	2793	1790	479	511	13	0	0	0

There are 199 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	261	MET	-	initiating methionine	UNP G0S2G2
A	262	ALA	-	expression tag	UNP G0S2G2
A	1360	SER	-	expression tag	UNP G0S2G2
A	1361	GLY	-	expression tag	UNP G0S2G2
A	1362	GLY	-	expression tag	UNP G0S2G2
A	1363	SER	-	expression tag	UNP G0S2G2
A	1364	GLY	-	expression tag	UNP G0S2G2
A	1365	GLY	-	expression tag	UNP G0S2G2
A	1366	SER	-	expression tag	UNP G0S2G2
A	1367	THR	-	expression tag	UNP G0S2G2
A	1368	ALA	-	expression tag	UNP G0S2G2
A	1369	VAL	-	expression tag	UNP G0S2G2
A	1370	ALA	-	expression tag	UNP G0S2G2
A	1371	GLN	-	expression tag	UNP G0S2G2
A	1372	ARG	-	expression tag	UNP G0S2G2
A	1373	ASP	-	expression tag	UNP G0S2G2
A	1374	ALA	-	expression tag	UNP G0S2G2
A	1375	ALA	-	expression tag	UNP G0S2G2
A	1376	LYS	-	expression tag	UNP G0S2G2
A	1377	LYS	-	expression tag	UNP G0S2G2
A	1378	ARG	-	expression tag	UNP G0S2G2
A	1379	CYS	-	expression tag	UNP G0S2G2
A	1380	ASP	-	expression tag	UNP G0S2G2
A	1381	GLU	-	expression tag	UNP G0S2G2
A	1382	LEU	-	expression tag	UNP G0S2G2
A	1383	ARG	-	expression tag	UNP G0S2G2
A	1384	ARG	-	expression tag	UNP G0S2G2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1385	MET	-	expression tag	UNP G0S2G2
A	1386	ARG	-	expression tag	UNP G0S2G2
A	1387	LEU	-	expression tag	UNP G0S2G2
A	1388	GLU	-	expression tag	UNP G0S2G2
A	1389	GLY	-	expression tag	UNP G0S2G2
A	1390	PHE	-	expression tag	UNP G0S2G2
A	1391	MET	-	expression tag	UNP G0S2G2
A	1392	GLU	-	expression tag	UNP G0S2G2
A	1393	GLY	-	expression tag	UNP G0S2G2
A	1394	PHE	-	expression tag	UNP G0S2G2
A	1395	SER	-	expression tag	UNP G0S2G2
A	1396	THR	-	expression tag	UNP G0S2G2
A	1397	ILE	-	expression tag	UNP G0S2G2
A	1398	SER	-	expression tag	UNP G0S2G2
A	1399	LEU	-	expression tag	UNP G0S2G2
A	1400	ARG	-	expression tag	UNP G0S2G2
A	1401	LEU	-	expression tag	UNP G0S2G2
A	1402	LYS	-	expression tag	UNP G0S2G2
A	1403	GLU	-	expression tag	UNP G0S2G2
A	1404	MET	-	expression tag	UNP G0S2G2
A	1405	TYR	-	expression tag	UNP G0S2G2
A	1406	GLN	-	expression tag	UNP G0S2G2
A	1407	MET	-	expression tag	UNP G0S2G2
A	1408	ILE	-	expression tag	UNP G0S2G2
A	1409	THR	-	expression tag	UNP G0S2G2
A	1410	MET	-	expression tag	UNP G0S2G2
A	1411	GLY	-	expression tag	UNP G0S2G2
A	1412	GLY	-	expression tag	UNP G0S2G2
A	1413	ASN	-	expression tag	UNP G0S2G2
A	1414	ALA	-	expression tag	UNP G0S2G2
A	1415	GLU	-	expression tag	UNP G0S2G2
A	1416	LEU	-	expression tag	UNP G0S2G2
A	1417	GLU	-	expression tag	UNP G0S2G2
A	1418	LEU	-	expression tag	UNP G0S2G2
A	1419	VAL	-	expression tag	UNP G0S2G2
A	1420	ASP	-	expression tag	UNP G0S2G2
A	1421	SER	-	expression tag	UNP G0S2G2
A	1422	LEU	-	expression tag	UNP G0S2G2
A	1423	ASP	-	expression tag	UNP G0S2G2
A	1424	PRO	-	expression tag	UNP G0S2G2
A	1425	PHE	-	expression tag	UNP G0S2G2
A	1426	SER	-	expression tag	UNP G0S2G2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1427	GLU	-	expression tag	UNP G0S2G2
A	1428	GLY	-	expression tag	UNP G0S2G2
A	1429	ILE	-	expression tag	UNP G0S2G2
A	1430	LEU	-	expression tag	UNP G0S2G2
A	1431	PHE	-	expression tag	UNP G0S2G2
A	1432	SER	-	expression tag	UNP G0S2G2
A	1433	VAL	-	expression tag	UNP G0S2G2
A	1434	MET	-	expression tag	UNP G0S2G2
A	1435	PRO	-	expression tag	UNP G0S2G2
A	1436	PRO	-	expression tag	UNP G0S2G2
A	1437	LYS	-	expression tag	UNP G0S2G2
A	1438	LYS	-	expression tag	UNP G0S2G2
A	1439	SER	-	expression tag	UNP G0S2G2
A	1440	TRP	-	expression tag	UNP G0S2G2
A	1441	LYS	-	expression tag	UNP G0S2G2
A	1442	ASN	-	expression tag	UNP G0S2G2
A	1443	ILE	-	expression tag	UNP G0S2G2
A	1444	SER	-	expression tag	UNP G0S2G2
A	1445	ASN	-	expression tag	UNP G0S2G2
A	1446	LEU	-	expression tag	UNP G0S2G2
A	1447	SER	-	expression tag	UNP G0S2G2
A	1448	GLY	-	expression tag	UNP G0S2G2
A	1449	GLY	-	expression tag	UNP G0S2G2
A	1450	GLU	-	expression tag	UNP G0S2G2
A	1451	LYS	-	expression tag	UNP G0S2G2
A	1452	THR	-	expression tag	UNP G0S2G2
A	1453	LEU	-	expression tag	UNP G0S2G2
A	1454	SER	-	expression tag	UNP G0S2G2
A	1455	SER	-	expression tag	UNP G0S2G2
A	1456	LEU	-	expression tag	UNP G0S2G2
A	1457	ALA	-	expression tag	UNP G0S2G2
A	1458	LEU	-	expression tag	UNP G0S2G2
A	1459	VAL	-	expression tag	UNP G0S2G2
A	1460	PHE	-	expression tag	UNP G0S2G2
A	1461	ALA	-	expression tag	UNP G0S2G2
A	1462	LEU	-	expression tag	UNP G0S2G2
A	1463	HIS	-	expression tag	UNP G0S2G2
A	1464	HIS	-	expression tag	UNP G0S2G2
A	1465	TYR	-	expression tag	UNP G0S2G2
A	1466	LYS	-	expression tag	UNP G0S2G2
A	1467	PRO	-	expression tag	UNP G0S2G2
A	1468	THR	-	expression tag	UNP G0S2G2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1469	PRO	-	expression tag	UNP G0S2G2
A	1470	LEU	-	expression tag	UNP G0S2G2
A	1471	TYR	-	expression tag	UNP G0S2G2
A	1472	VAL	-	expression tag	UNP G0S2G2
A	1473	MET	-	expression tag	UNP G0S2G2
A	1474	ASP	-	expression tag	UNP G0S2G2
A	1475	GLU	-	expression tag	UNP G0S2G2
A	1476	ILE	-	expression tag	UNP G0S2G2
A	1477	ASP	-	expression tag	UNP G0S2G2
A	1478	ALA	-	expression tag	UNP G0S2G2
A	1479	ALA	-	expression tag	UNP G0S2G2
A	1480	LEU	-	expression tag	UNP G0S2G2
A	1481	ASP	-	expression tag	UNP G0S2G2
A	1482	PHE	-	expression tag	UNP G0S2G2
A	1483	ARG	-	expression tag	UNP G0S2G2
A	1484	ASN	-	expression tag	UNP G0S2G2
A	1485	VAL	-	expression tag	UNP G0S2G2
A	1486	SER	-	expression tag	UNP G0S2G2
A	1487	ILE	-	expression tag	UNP G0S2G2
A	1488	VAL	-	expression tag	UNP G0S2G2
A	1489	ALA	-	expression tag	UNP G0S2G2
A	1490	ASN	-	expression tag	UNP G0S2G2
A	1491	TYR	-	expression tag	UNP G0S2G2
A	1492	ILE	-	expression tag	UNP G0S2G2
A	1493	LYS	-	expression tag	UNP G0S2G2
A	1494	GLU	-	expression tag	UNP G0S2G2
A	1495	ARG	-	expression tag	UNP G0S2G2
A	1496	THR	-	expression tag	UNP G0S2G2
A	1497	ARG	-	expression tag	UNP G0S2G2
A	1498	ASN	-	expression tag	UNP G0S2G2
A	1499	ALA	-	expression tag	UNP G0S2G2
A	1500	GLN	-	expression tag	UNP G0S2G2
A	1501	PHE	-	expression tag	UNP G0S2G2
A	1502	ILE	-	expression tag	UNP G0S2G2
A	1503	VAL	-	expression tag	UNP G0S2G2
A	1504	ILE	-	expression tag	UNP G0S2G2
A	1505	SER	-	expression tag	UNP G0S2G2
A	1506	LEU	-	expression tag	UNP G0S2G2
A	1507	ARG	-	expression tag	UNP G0S2G2
A	1508	ASN	-	expression tag	UNP G0S2G2
A	1509	ASN	-	expression tag	UNP G0S2G2
A	1510	MET	-	expression tag	UNP G0S2G2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1511	PHE	-	expression tag	UNP G0S2G2
A	1512	GLU	-	expression tag	UNP G0S2G2
A	1513	LEU	-	expression tag	UNP G0S2G2
A	1514	ALA	-	expression tag	UNP G0S2G2
A	1515	SER	-	expression tag	UNP G0S2G2
A	1516	ARG	-	expression tag	UNP G0S2G2
A	1517	LEU	-	expression tag	UNP G0S2G2
A	1518	VAL	-	expression tag	UNP G0S2G2
A	1519	GLY	-	expression tag	UNP G0S2G2
A	1520	VAL	-	expression tag	UNP G0S2G2
A	1521	TYR	-	expression tag	UNP G0S2G2
A	1522	LYS	-	expression tag	UNP G0S2G2
A	1523	VAL	-	expression tag	UNP G0S2G2
A	1524	ASN	-	expression tag	UNP G0S2G2
A	1525	HIS	-	expression tag	UNP G0S2G2
A	1526	MET	-	expression tag	UNP G0S2G2
A	1527	THR	-	expression tag	UNP G0S2G2
A	1528	LYS	-	expression tag	UNP G0S2G2
A	1529	SER	-	expression tag	UNP G0S2G2
A	1530	VAL	-	expression tag	UNP G0S2G2
A	1531	THR	-	expression tag	UNP G0S2G2
A	1532	ILE	-	expression tag	UNP G0S2G2
A	1533	ASP	-	expression tag	UNP G0S2G2
A	1534	ASN	-	expression tag	UNP G0S2G2
A	1535	LYS	-	expression tag	UNP G0S2G2
A	1536	ASP	-	expression tag	UNP G0S2G2
A	1537	TYR	-	expression tag	UNP G0S2G2
A	1538	VAL	-	expression tag	UNP G0S2G2
A	1539	ILE	-	expression tag	UNP G0S2G2
A	1540	GLY	-	expression tag	UNP G0S2G2
A	1541	ARG	-	expression tag	UNP G0S2G2
A	1542	ALA	-	expression tag	UNP G0S2G2
A	1543	GLY	-	expression tag	UNP G0S2G2
A	1544	ILE	-	expression tag	UNP G0S2G2
A	1545	SER	-	expression tag	UNP G0S2G2
A	1546	SER	-	expression tag	UNP G0S2G2
A	1547	ALA	-	expression tag	UNP G0S2G2
A	1548	SER	-	expression tag	UNP G0S2G2
A	1549	HIS	-	expression tag	UNP G0S2G2
A	1550	HIS	-	expression tag	UNP G0S2G2
A	1551	HIS	-	expression tag	UNP G0S2G2
A	1552	HIS	-	expression tag	UNP G0S2G2

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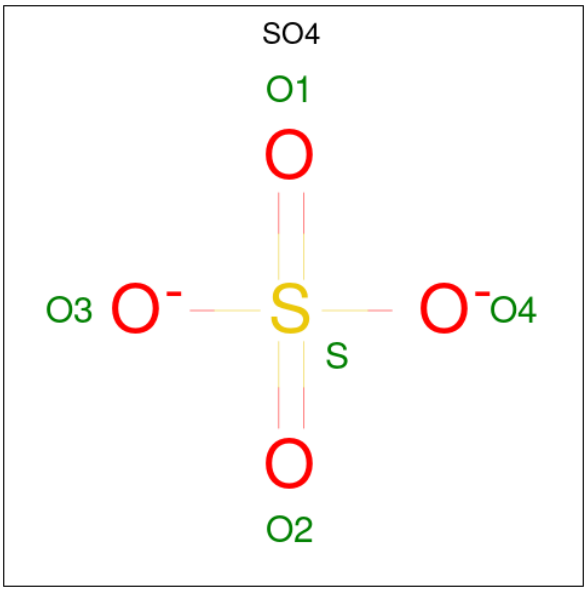
Chain	Residue	Modelled	Actual	Comment	Reference
A	1553	HIS	-	expression tag	UNP G0S2G2
A	1554	HIS	-	expression tag	UNP G0S2G2
A	1555	HIS	-	expression tag	UNP G0S2G2
A	1556	HIS	-	expression tag	UNP G0S2G2

- Molecule 2 is a protein called Condensin complex subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	85	Total	C	N	O	S	0	0	0
			681	438	113	125	5			

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



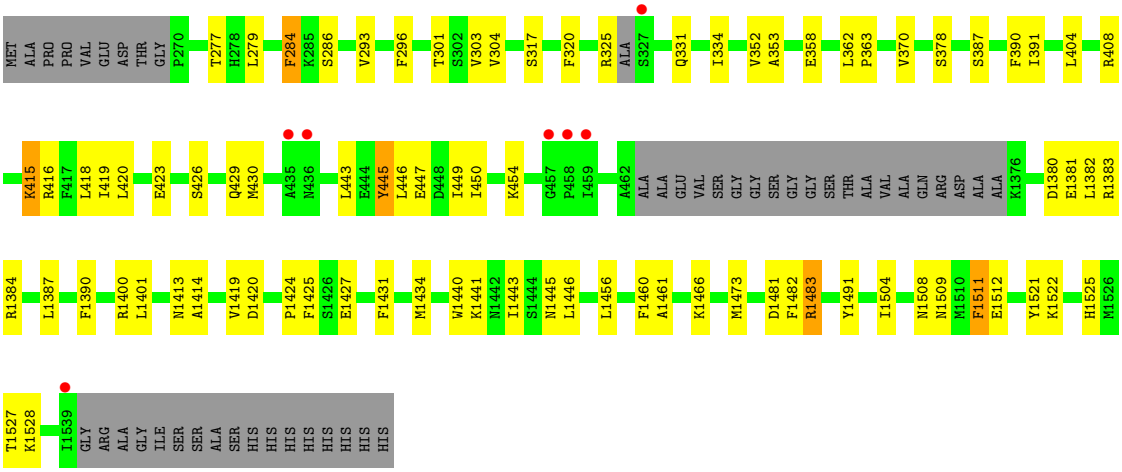
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	O	S		0	0
			5	4	1			
3	A	1	Total	O	S		0	0
			5	4	1			
3	A	1	Total	O	S		0	0
			5	4	1			
3	A	1	Total	O	S		0	0
			5	4	1			
3	A	1	Total	O	S		0	0
			5	4	1			
3	B	1	Total	O	S		0	0
			5	4	1			

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.

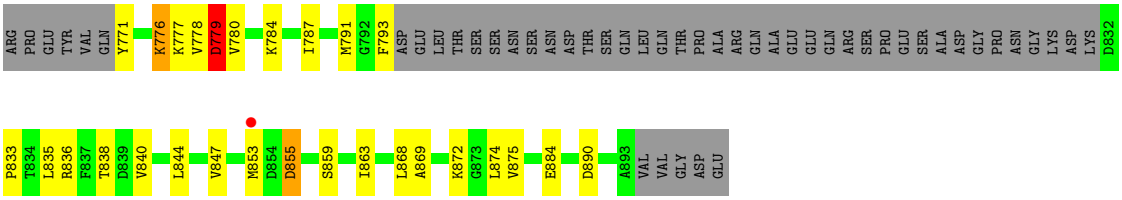
• Molecule 1: Smc4

Chain A:



• Molecule 2: Condensin complex subunit 2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α, β, γ	132.73Å 132.73Å 75.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.45 – 3.00 43.45 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.45-3.00) 99.8 (43.45-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.214 , 0.243 0.220 , 0.225	Depositor DCC
R_{free} test set	775 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	107.1	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 94.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3504	wwPDB-VP
Average B, all atoms (Å^2)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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: 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	0.28	0/2850	0.52	1/3843 (0.0%)
2	B	0.31	0/692	0.54	0/931
All	All	0.28	0/3542	0.52	1/4774 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1382	LEU	CA-CB-CG	5.24	127.35	115.30

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	2793	0	2813	64	0
2	B	681	0	684	22	0
3	A	25	0	0	1	0
3	B	5	0	0	0	0
All	All	3504	0	3497	81	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 12.

The worst 5 of 81 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:B:777:LYS:HG2	2:B:779:ASP:H	1.34	0.92
1:A:1508:ASN:HA	1:A:1511:PHE:CE1	2.10	0.87
1:A:1508:ASN:HA	1:A:1511:PHE:HE1	1.44	0.81
1:A:445:TYR:O	1:A:449:ILE:CD1	2.32	0.77
2:B:875:VAL:HG23	2:B:890:ASP:HB2	1.71	0.72

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	350/403 (87%)	327 (93%)	23 (7%)	0	100 100
2	B	81/134 (60%)	76 (94%)	3 (4%)	2 (2%)	5 28
All	All	431/537 (80%)	403 (94%)	26 (6%)	2 (0%)	29 68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	779	ASP
2	B	833	PRO

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	307/345 (89%)	300 (98%)	7 (2%)	50 80
2	B	74/121 (61%)	70 (95%)	4 (5%)	22 57
All	All	381/466 (82%)	370 (97%)	11 (3%)	42 76

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	776	LYS
2	B	779	ASP
2	B	855	ASP
2	B	793	PHE
1	A	454	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1509	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)

6 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	$\#\|Z\| > 2$
3	SO4	A	1604	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	B	901	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	A	1601	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	A	1603	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	A	1605	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	A	1602	-	4,4,4	0.23	0	6,6,6	0.08	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1605	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

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	356/403 (88%)	-0.16	7 (1%)	65	36	73, 109, 199, 279	0
2	B	85/134 (63%)	0.25	1 (1%)	79	54	94, 148, 196, 221	0
All	All	441/537 (82%)	-0.08	8 (1%)	68	40	73, 115, 199, 279	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	459	ILE	2.9
1	A	1539	ILE	2.5
2	B	853	MET	2.5
1	A	436	ASN	2.4
1	A	458	PRO	2.3

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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
3	SO4	A	1603	5/5	0.74	0.21	203,207,210,212	0
3	SO4	A	1605	5/5	0.85	0.37	228,231,234,237	0
3	SO4	B	901	5/5	0.87	0.28	193,194,202,208	0
3	SO4	A	1602	5/5	0.90	0.23	149,152,170,173	0
3	SO4	A	1604	5/5	0.96	0.17	127,129,137,163	0
3	SO4	A	1601	5/5	0.98	0.31	78,79,90,127	0

6.5 Other polymers (i)

There are no such residues in this entry.