



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 03:17 PM UTC

PDB ID : 5XXZ / pdb_00005xxz
Title : Crystal structure of a serine protease from Streptococcus species
Authors : Jobichen, C.; Sivaraman, J.
Deposited on : 2017-07-05
Resolution : 3.08 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

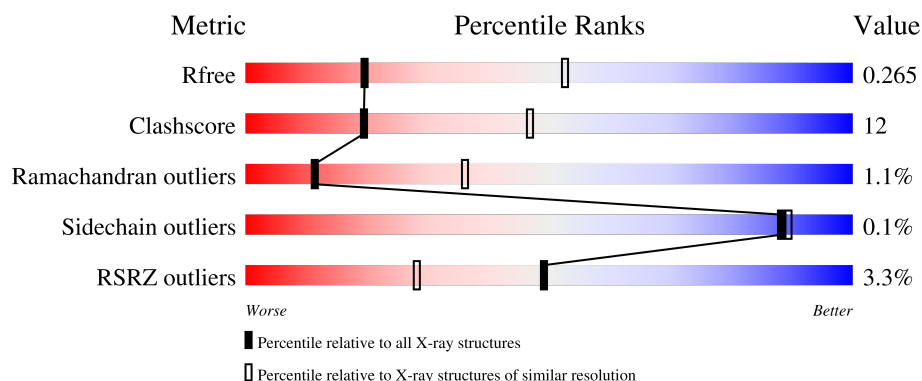
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.08 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}	180053	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

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 $\leq 5\%$. 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	1533	3% 64% 22% 13%
1	B	1533	3% 65% 20% 15%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CA	A	1705	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 19914 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.

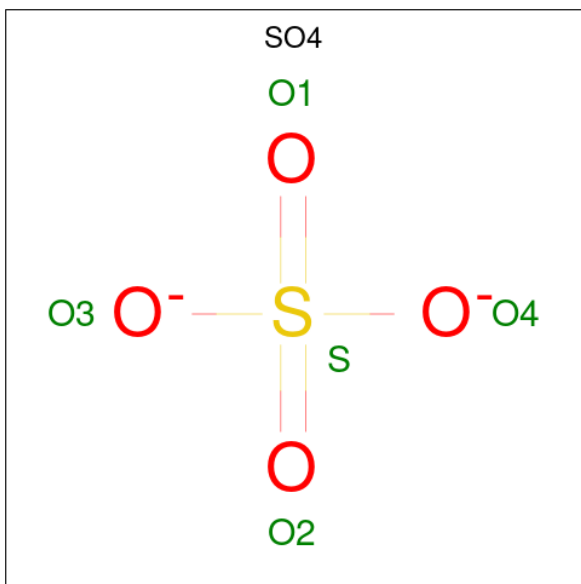
- Molecule 1 is a protein called Chemokine protease C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1334	Total	C	N	O	Se	0	0	0
			10007	6297	1722	1964	24			
1	B	1310	Total	C	N	O	Se	0	0	0
			9890	6229	1701	1936	24			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	ALA	HIS	engineered mutation	UNP Q3HV58
A	617	ALA	SER	engineered mutation	UNP Q3HV58
B	279	ALA	HIS	engineered mutation	UNP Q3HV58
B	617	ALA	SER	engineered mutation	UNP Q3HV58

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

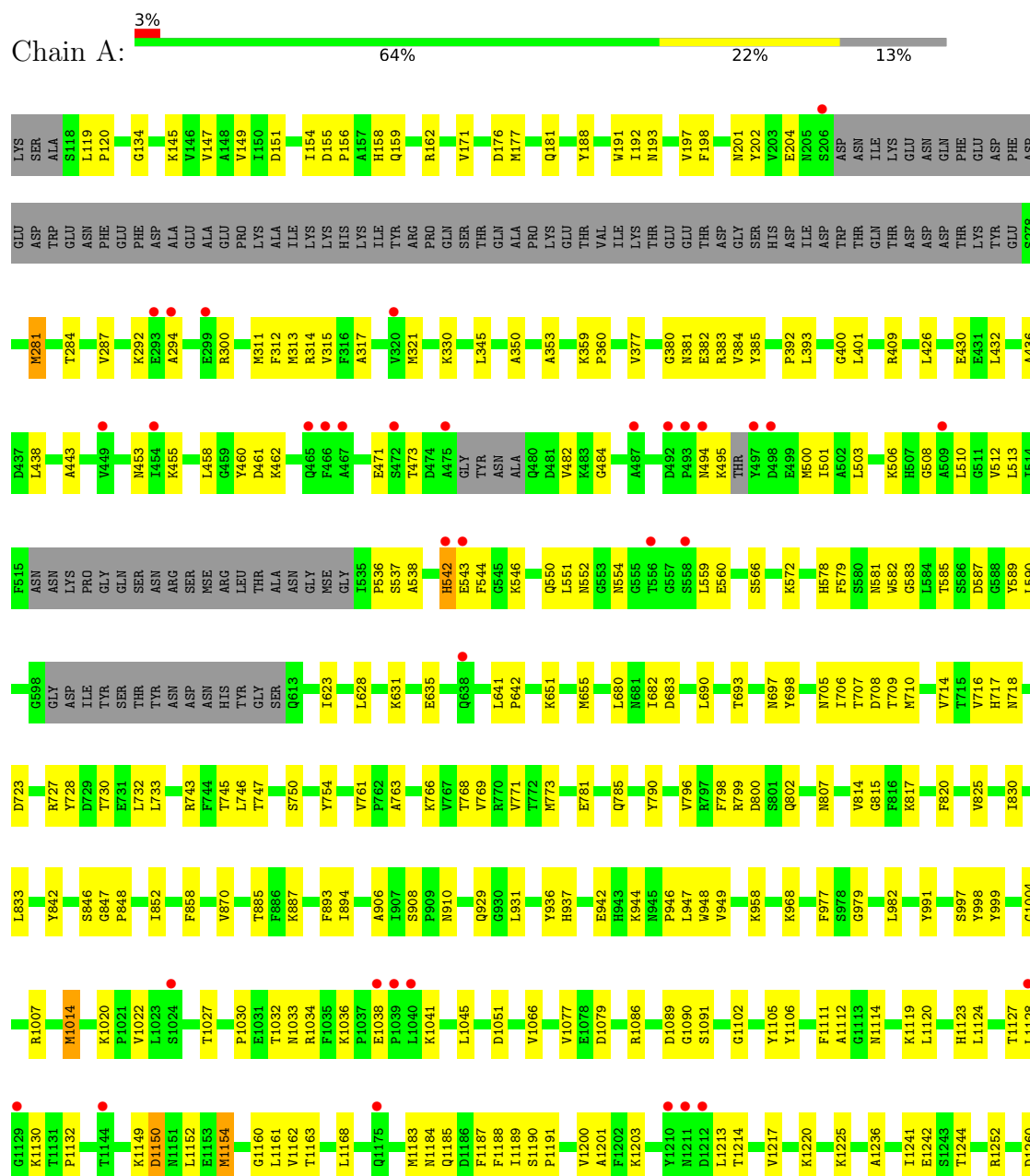
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

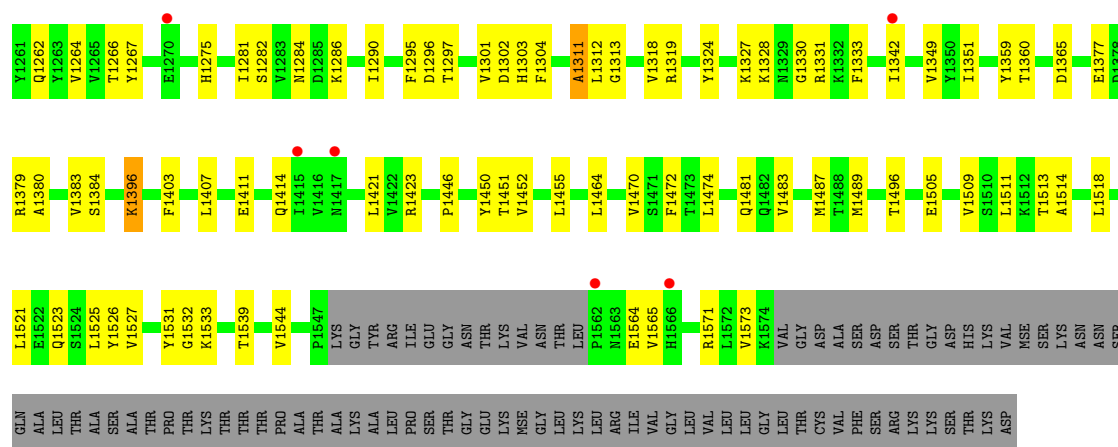
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Ca	0	0
			4	4		
3	B	3	Total	Ca	0	0
			3	3		

3 Residue-property plots

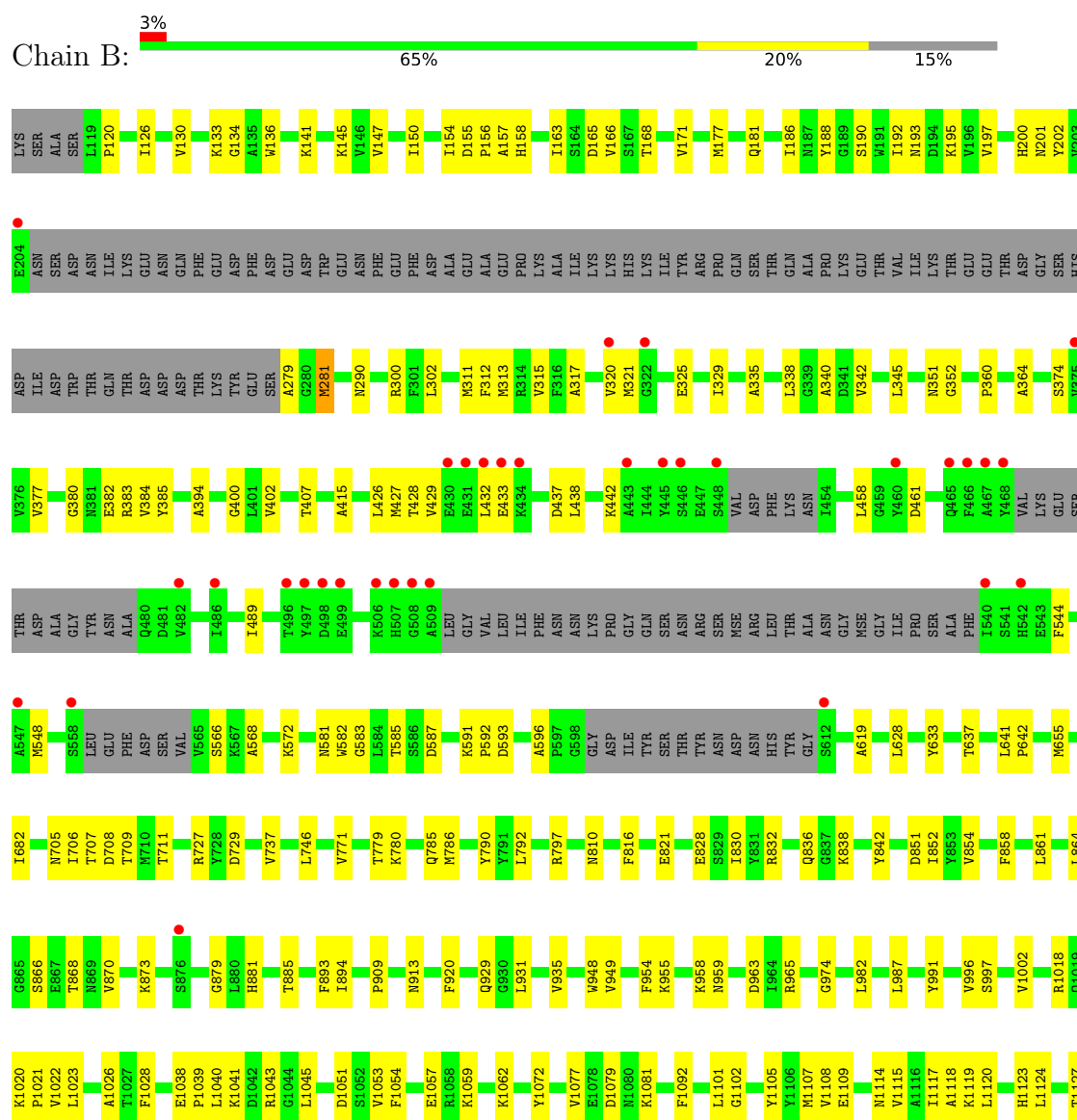
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Chemokine protease C





• Molecule 1: Chemokine protease C



THR	THR	THR	THR	PRO	ALA	THR	ALA	LYS	ALA	LEU	PRO	SER	THR	GLY	GLU	LYS	ASN	THR	LYS	VAL	ASN	THR	ARG	ILE	VAL	GLY	LEU	VAL	LEU	LEU	GLY	LEU	THR	CYS	VAL	PHE	SER	SER	ARG	LYS	LYS	SER	THR	LYS	ASP								
A1530	Y1531	G1532	K1533	T1534	V1535	Q1536	E1537	Y1540	S1545	L1546	I1552	E1553	GLY	ASN	THR	LYS	VAL	ASN	THR	L1561	E1567	L1568	R1571	L1572	V1573	K1574	VAL	GLY	THR	ASP	ALA	ALA	SER	ASP	SER	ASP	SER	THR	GLY	THR	GLY	LEU	THR	ASP									
V1400	L1405	E1411	Q1414	I1415	V1416	N1417	Y1420	D1424	A1425	D1426	I1430	Y1436	I1444	Y1450	E1453	A1462	F1480	K1486	M1487	A1491	I1495	T1496	P1504	S1507	R1508	L1511	K1512	T1513	L1518	L1521	E1522	Q1523	S1524	L1525	Y1526	V1527	P1528	K1529															
G1272	K1273	Y1279	T1280	I1281	T1291	Q1292	F1295	D1302	K1308	T1309	E1320	E1321	V1322	K1328	R1331	E1337	G1338	K1339	D1340	G1341	I1342	Y1359	T1360	I1361	R1364	V1367	T1368	L1369	S1370	D1371	Y1372	Y1373	Y1374	D1378	N1382	V1383	S1384	F1385	L1388	R1389	D1390	L1391	K1396										
T1131	P1132	I1133	K1134	L1137	Q1143	T1147	L1148	K1149	D1150	R1151	L1152	E1153	M1154	T1159	G1160	L1161	V1162	T1163	L1168	A1169	V1170	R1173	L1180	T1181	K1182	M1183	I1189	F1199	V1200	N1211	V1215	N1216	V1217	Y1218	A1219	I1229	W1230	Y1247	R1252	V1265	R1268												

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	182.13Å 132.85Å 151.99Å 90.00° 100.69° 90.00°	Depositor
Resolution (Å)	19.98 – 3.08 19.98 – 3.08	Depositor EDS
% Data completeness (in resolution range)	98.7 (19.98-3.08) 92.6 (19.98-3.08)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 3.07Å)	Xtriage
Refinement program	PHENIX (dev_2733: ???)	Depositor
R, R_{free}	0.205 , 0.263 0.208 , 0.265	Depositor DCC
R_{free} test set	2000 reflections (3.05%)	wwPDB-VP
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 25.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	19914	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: CA, 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	0.56	0/10170	0.81	6/13731 (0.0%)
1	B	0.55	0/10051	0.78	5/13571 (0.0%)
All	All	0.56	0/20221	0.80	11/27302 (0.0%)

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	494	ASN	N-CA-C	7.46	121.49	110.30
1	A	1154	MSE	N-CA-C	6.44	119.71	110.24
1	A	382	GLU	CA-C-N	6.40	133.76	121.54
1	A	382	GLU	C-N-CA	6.40	133.76	121.54
1	A	281	MSE	N-CA-C	-5.78	106.36	113.41

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	10007	0	9601	233	0
1	B	9890	0	9560	222	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	4	0	0	2	0
3	B	3	0	0	0	0
All	All	19914	0	19161	455	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 455 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:433:GLU:CA	1:B:437:ASP:CB	2.10	1.30
1:A:1496:THR:HA	1:A:1532:GLY:HA3	1.36	1.05
1:A:1190:SER:OG	3:A:1705:CA:CA	1.48	0.90
1:B:1496:THR:HA	1:B:1532:GLY:HA3	1.51	0.90
1:B:1147:THR:HG22	1:B:1148:LEU:H	1.40	0.86

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	1320/1533 (86%)	1182 (90%)	117 (9%)	21 (2%)	7	28
1	B	1294/1533 (84%)	1165 (90%)	121 (9%)	8 (1%)	21	49
All	All	2614/3066 (85%)	2347 (90%)	238 (9%)	29 (1%)	11	36

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	537	SER
1	A	538	ALA

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Mol	Chain	Res	Type
1	A	554	ASN
1	A	1038	GLU
1	A	1184	ASN

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	1036/1271 (82%)	1034 (100%)	2 (0%)	87	87
1	B	1033/1271 (81%)	1033 (100%)	0	100	100
All	All	2069/2542 (81%)	2067 (100%)	2 (0%)	88	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1123	HIS
1	A	1396	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1223	HIS
1	B	1292	GLN
1	B	1498	HIS
1	B	1402	ASN
1	B	1262	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 7 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	SO4	B	1701	-	4,4,4	0.38	0	6,6,6	0.58	0
2	SO4	A	1701	-	4,4,4	0.29	0	6,6,6	0.44	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	1309/1533 (85%)	0.19	41 (3%)	51 29	32, 57, 117, 196	0
1	B	1285/1533 (83%)	0.05	45 (3%)	47 26	30, 54, 111, 204	0
All	All	2594/3066 (84%)	0.12	86 (3%)	49 28	30, 56, 115, 204	0

The worst 5 of 86 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1128	LEU	6.4
1	B	433	GLU	5.2
1	A	1270	GLU	4.5
1	B	612	SER	4.4
1	A	1211	ASN	4.2

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	SO4	B	1701	5/5	0.83	0.26	98,98,99,99	0
2	SO4	A	1701	5/5	0.85	0.18	115,115,116,116	0
3	CA	A	1702	1/1	0.90	0.18	74,74,74,74	0
3	CA	A	1704	1/1	0.95	0.05	53,53,53,53	0
3	CA	B	1703	1/1	0.96	0.05	48,48,48,48	0
3	CA	B	1704	1/1	0.98	0.03	43,43,43,43	0
3	CA	A	1705	1/1	0.99	0.25	30,30,30,30	0
3	CA	B	1702	1/1	0.99	0.03	35,35,35,35	0
3	CA	A	1703	1/1	1.00	0.02	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.