



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 10:10 am BST

PDB ID : 5XXZ
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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

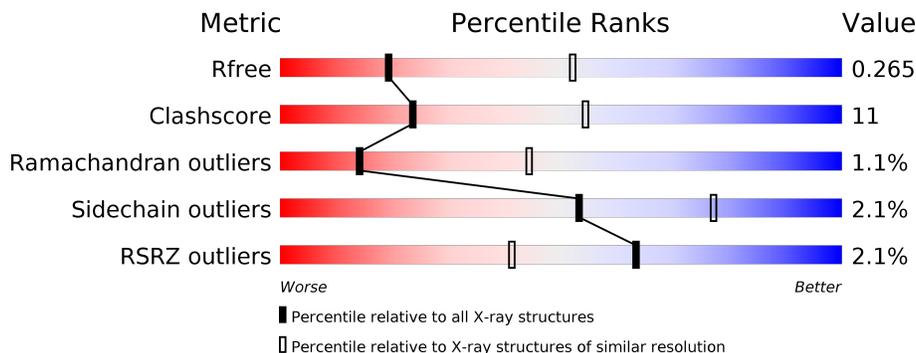
1 Overall quality at a glance

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}	130704	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (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 on 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	 2% 64% 22% • 13%
1	B	1533	 % 64% 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.

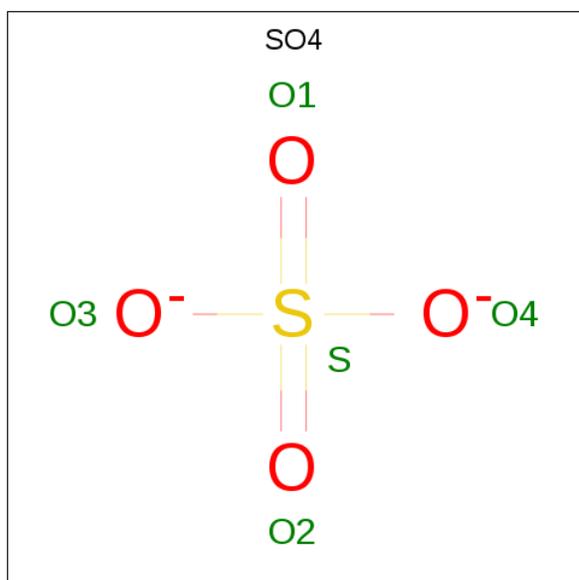
- Molecule 1 is a protein called Chemokine protease C.

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

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 (three-letter code: 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		

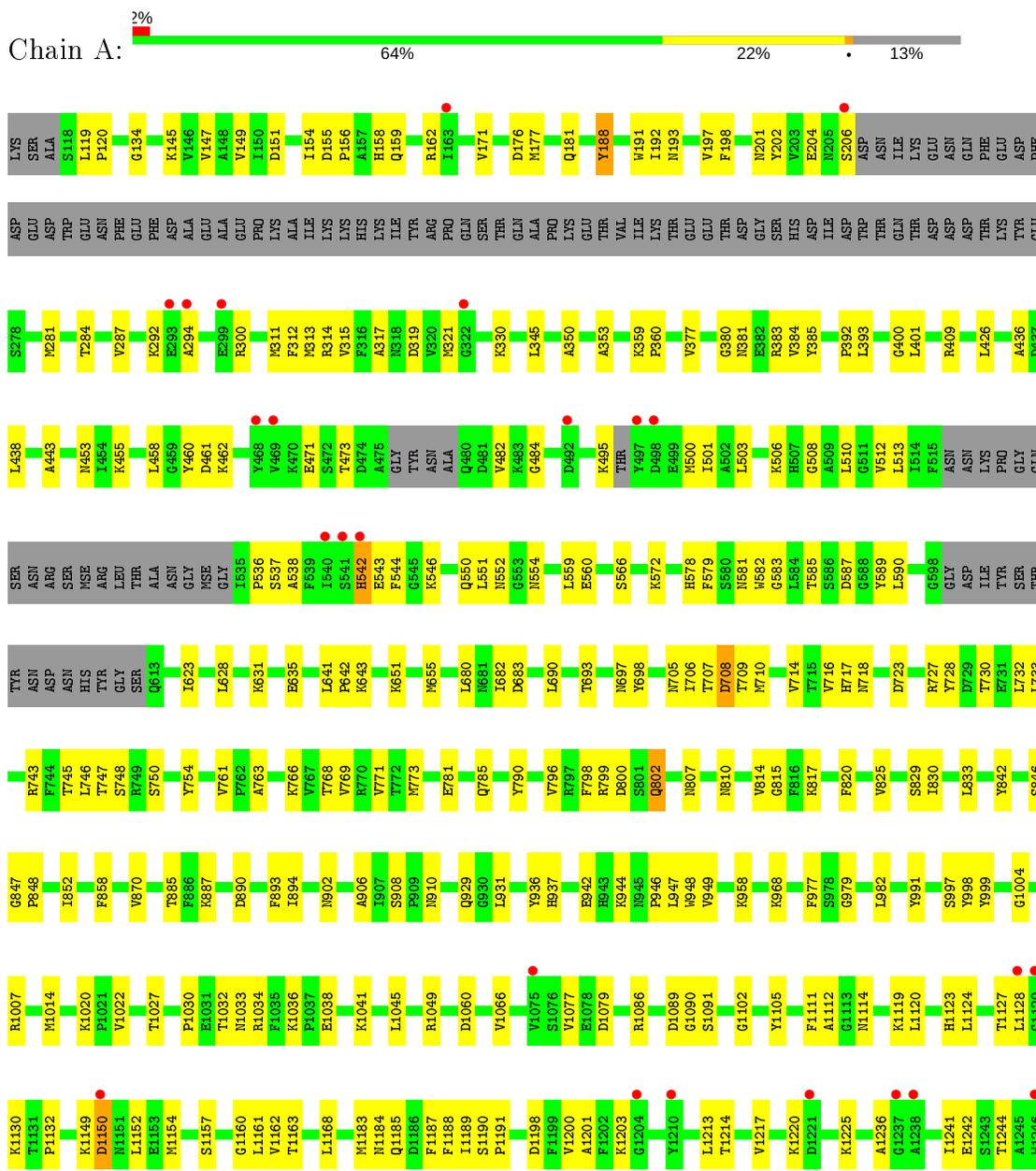
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

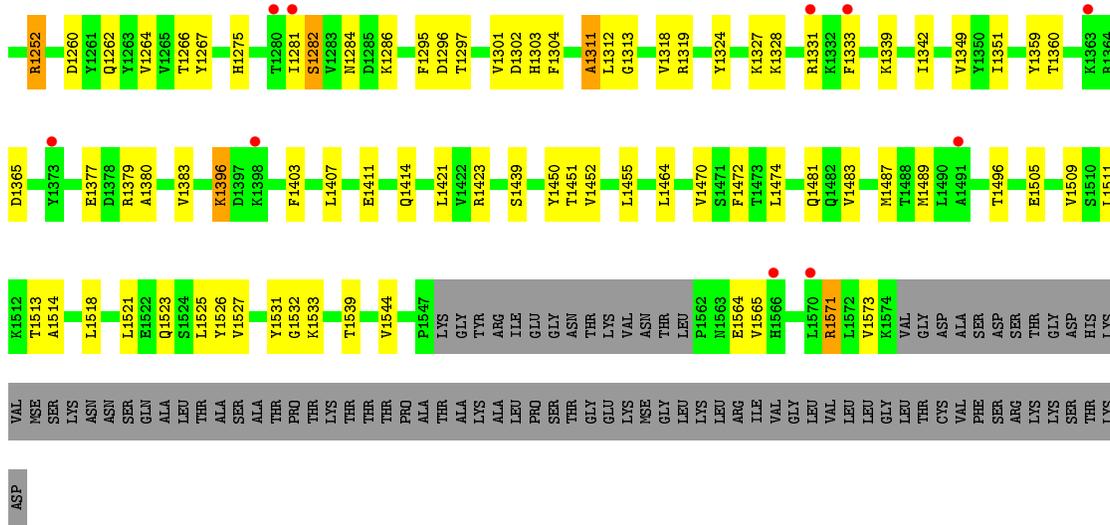
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Ca	0	0
			3	3		
3	A	4	Total	Ca	0	0
			4	4		

3 Residue-property plots [i](#)

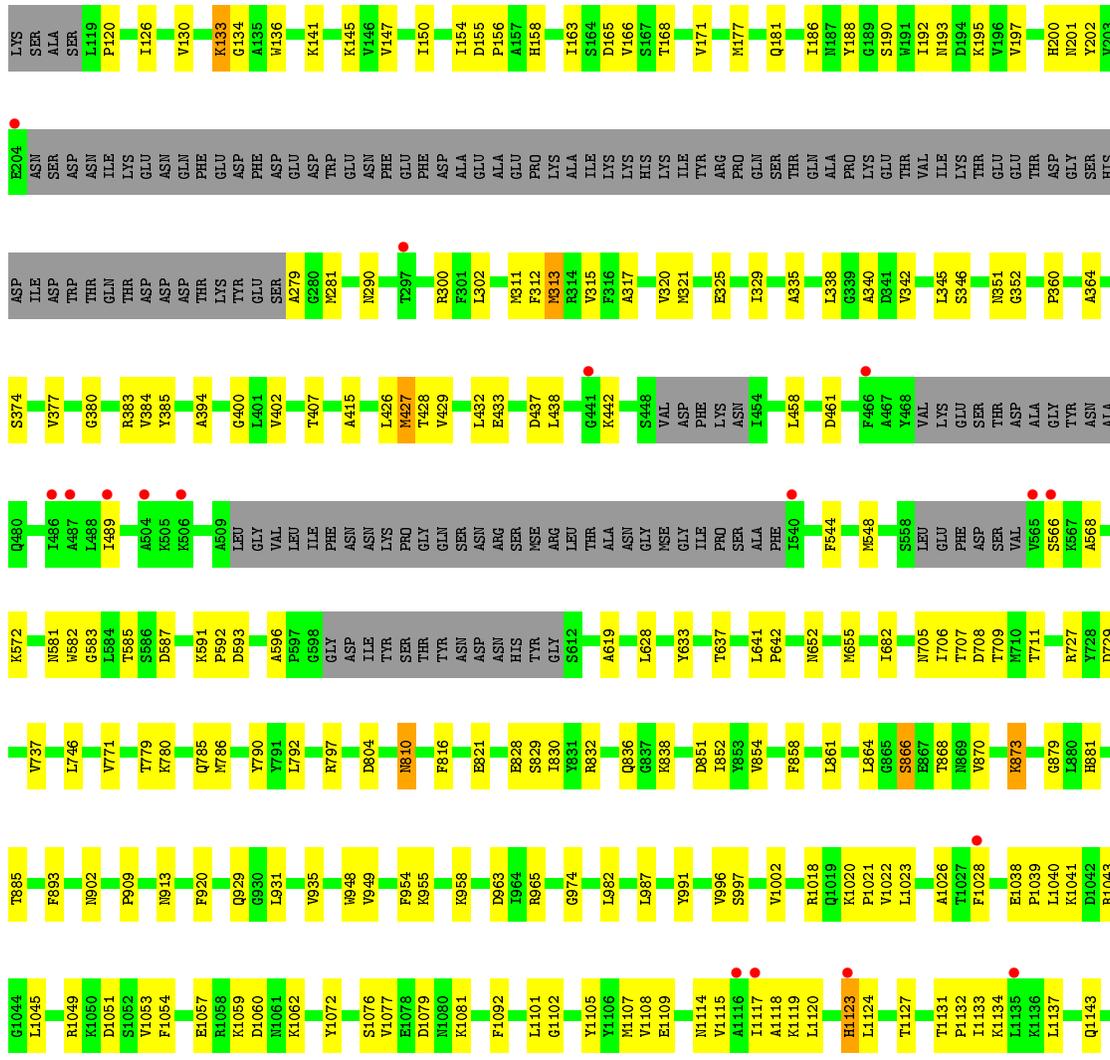
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



LEU	S1545	Y1420	T1147
PRO	L1546	F1295	L1148
SER	I1552	D1302	K1149
THR	E1553	K1308	N1151
GLY	ASN	T1309	L1152
LYS	THR	E1320	E1153
NSE	LYS	F1321	M1154
GLY	VAL	V1322	T1159
LEU	ASN	R1331	G1160
LYS	THR	A1462	L1161
LEU	ARG	E1465	V1162
ILE	L1561	S1471	T1163
VAL	E1567	F1480	L1168
GLY	L1568	K1486	A1169
LEU	LEU	M1487	V1170
VAL	R1571	I1360	R1173
LEU	L1572	I1361	L1180
LEU	V1573	R1364	T1181
GLY	K1574	V1367	K1182
LEU	VAL	I1368	M1183
THR	GLY	L1369	I1189
THR	THR	S1370	D1198
CYS	ASP	D1371	F1199
ALA	ALA	Y1372	V1200
PHE	SER	Y1373	M1211
SER	ASP	Y1374	D1212
ARG	ASP	D1378	V1215
LYS	THR	M1382	N1216
LYS	THR	V1383	V1217
LYS	GLY	S1384	Y1218
LYS	ASP	F1385	A1219
THR	HIS	L1388	I1229
LYS	LYS	Q1523	H1230
ASP	VAL	S1524	Y1247
	NSE	L1525	R1252
	SER	Y1526	V1265
	SER	V1527	R1268
	LEU	P1528	K1273
	ALA	K1529	I1281
	THR	A1530	N1284
	PRO	Y1531	T1291
	LYS	G1532	Q1292
	THR	K1533	
	THR	T1534	
	PRO	V1535	
	ALA	Q1536	
	THR	E1537	
	ALA	Y1540	
	ALA		

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 49.78 – 3.09	Depositor EDS
% Data completeness (in resolution range)	98.7 (19.98-3.08) 93.0 (49.78-3.09)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 3.07Å)	Xtrriage
Refinement program	PHENIX (dev_2733: ???)	Depositor
R, R_{free}	0.205 , 0.263 0.211 , 0.265	Depositor DCC
R_{free} test set	1980 reflections (3.07%)	wwPDB-VP
Wilson B-factor (Å ²)	51.1	Xtrriage
Anisotropy	0.458	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 25.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	19914	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage'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	0.60	0/10170	0.76	1/13731 (0.0%)
1	B	0.60	0/10051	0.75	1/13571 (0.0%)
All	All	0.60	0/20221	0.75	2/27302 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1198	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	A	1198	ASP	CB-CG-OD1	5.09	122.88	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	10007	0	9601	224	0
1	B	9890	0	9560	215	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	4	0	0	2	0
3	B	3	0	0	0	0
All	All	19914	0	19161	439	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 11.

The worst 5 of 439 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%)	9	35
1	B	1294/1533 (84%)	1165 (90%)	121 (9%)	8 (1%)	25	57
All	All	2614/3066 (85%)	2347 (90%)	238 (9%)	29 (1%)	14	44

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	537	SER
1	A	538	ALA
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%)	1015 (98%)	21 (2%)	55	78
1	B	1033/1271 (81%)	1011 (98%)	22 (2%)	53	77
All	All	2069/2542 (81%)	2026 (98%)	43 (2%)	53	77

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1439	SER
1	B	427	MSE
1	B	1389	ARG
1	A	1571	ARG
1	B	133	LYS

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

Mol	Chain	Res	Type
1	B	200	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 carbohydrates 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	0.28	0	6,6,6	0.59	0
2	SO4	A	1701	-	4,4,4	0.19	0	6,6,6	0.42	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%)	0.02	34 (2%) 56 31	32, 57, 117, 196	0
1	B	1285/1533 (83%)	-0.09	20 (1%) 72 51	30, 54, 111, 204	0
All	All	2594/3066 (84%)	-0.04	54 (2%) 63 41	30, 56, 115, 204	0

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1129	GLY	5.5
1	A	498	ASP	4.9
1	A	492	ASP	4.5
1	A	1128	LEU	4.5
1	B	506	LYS	4.1

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. 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(\AA^2)	Q<0.9
3	CA	A	1704	1/1	0.83	0.12	53,53,53,53	0
2	SO4	B	1701	5/5	0.86	0.27	98,98,99,99	0
2	SO4	A	1701	5/5	0.87	0.30	115,115,116,116	0
3	CA	A	1702	1/1	0.91	0.35	74,74,74,74	0
3	CA	B	1703	1/1	0.94	0.06	48,48,48,48	0
3	CA	B	1704	1/1	0.96	0.10	43,43,43,43	0
3	CA	B	1702	1/1	0.98	0.04	35,35,35,35	0
3	CA	A	1703	1/1	0.98	0.14	37,37,37,37	0
3	CA	A	1705	1/1	0.98	0.17	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.