Full wwPDB X-ray Structure Validation Report (i)

Dec 4, 2024 – 02:10 PM JST

PDB ID	:	8ZAF
Title	:	Crystal structure of SkABA3 from Shimazuella kribbensis
Authors	:	Li, S.Y.; Li, H.; Yang, Y.; Huang, J.-W.; Chen, C.-C.; Guo, R.-T.
Deposited on	:	2024-04-25
Resolution	:	1.96 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 (1)) were used in the production of this report:

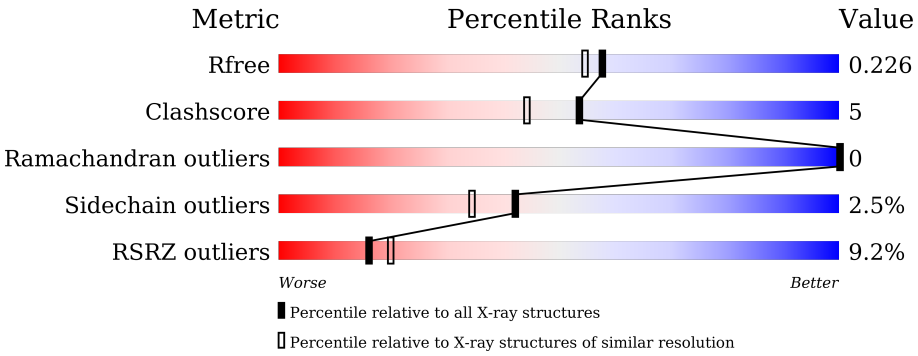
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 1.96 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}	164625	3187 (1.96-1.96)
Clashscore	180529	3412 (1.96-1.96)
Ramachandran outliers	177936	3390 (1.96-1.96)
Sidechain outliers	177891	3390 (1.96-1.96)
RSRZ outliers	164620	3186 (1.96-1.96)

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	6% 78% 8% • 12%
1	B	403	5% 77% 7% • 15%
1	C	403	12% 70% 11% • 17%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9076 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.

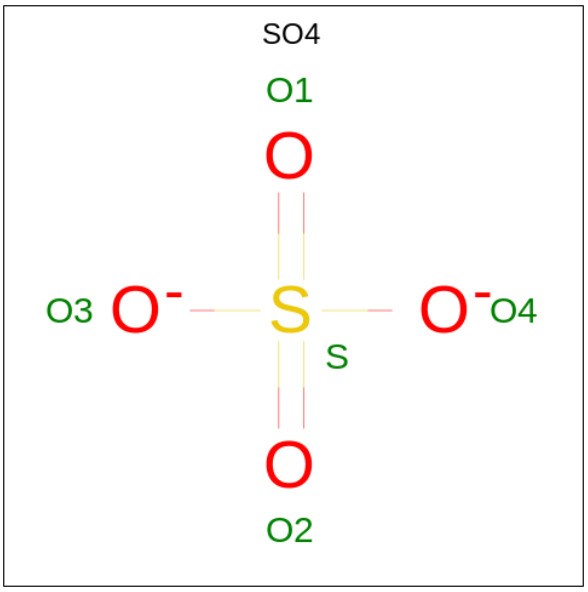
- Molecule 1 is a protein called Sesquiterpene synthases.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	S	0	0	0
			2869	1821	487	539	22			
1	B	343	Total	C	N	O	S	0	0	0
			2793	1778	468	525	22			
1	C	334	Total	C	N	O	S	0	0	0
			2731	1741	459	510	21			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

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



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

- Molecule 4 is water.

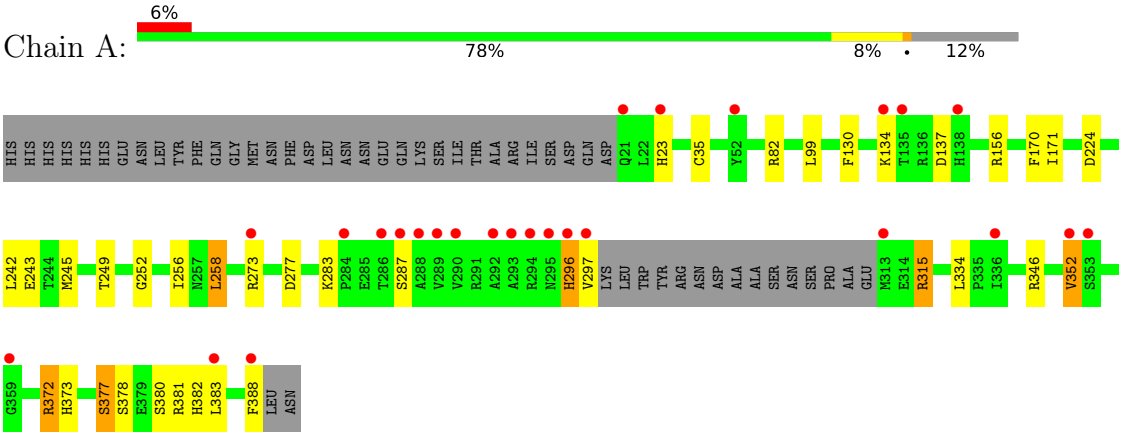
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	251	Total O 251 251	0	0
4	B	275	Total O 275 275	0	0
4	C	134	Total O 134 134	0	0

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.

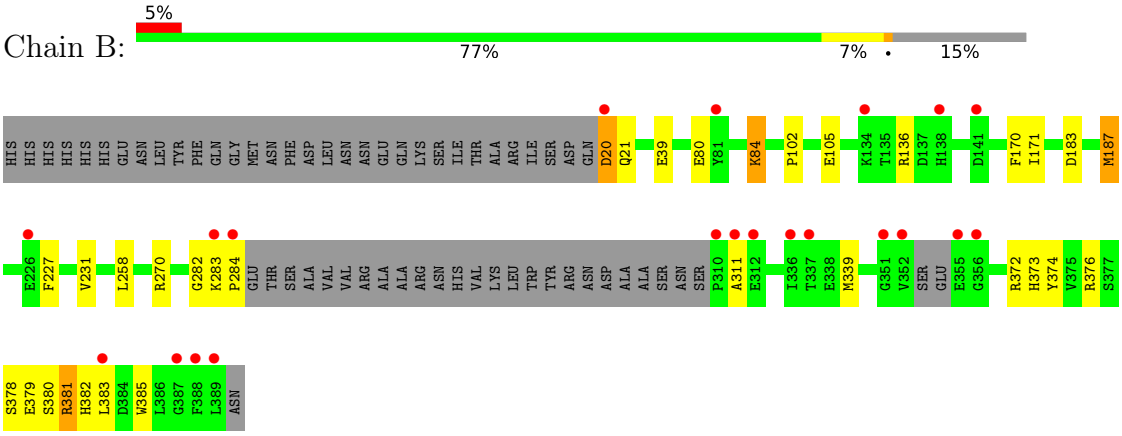
• Molecule 1: Sesquiterpene synthases

Chain A:



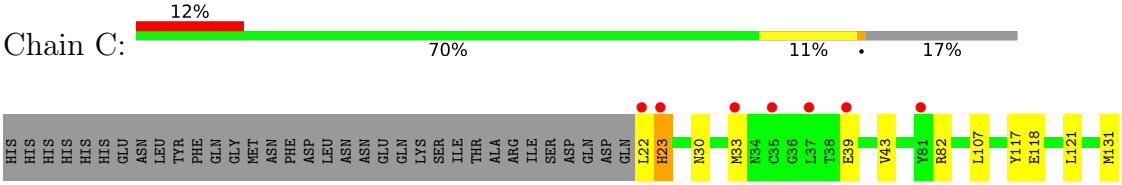
• Molecule 1: Sesquiterpene synthases

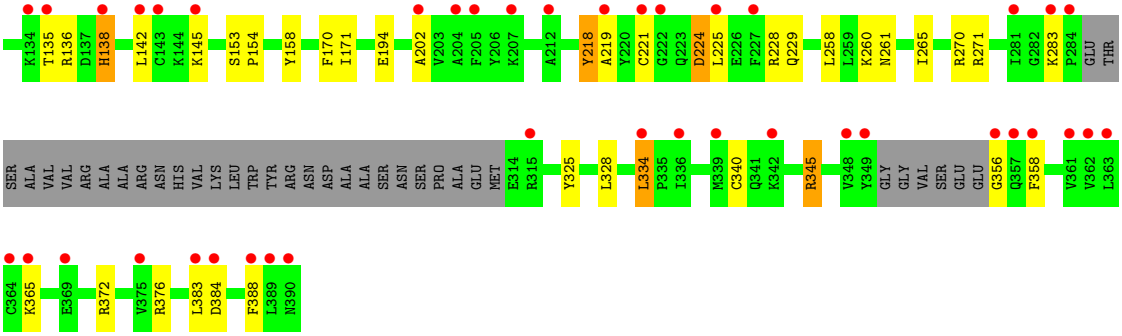
Chain B:



• Molecule 1: Sesquiterpene synthases

Chain C:




K134 T135 R136 D137 H138 L142 C143 K144 K145 S153 P154 Y158 F170 I171 E194 A202 V203 A204 F205 Y206 K207 A212 Y218 A219 Y220 C221 G222 Q223 D224 L225 E226 F227 R228 Q229 L258 L259 K260 N261 I265 R270 R271 I281 G282 K283 P284 GLU THR
SER ALA VAL VAL ARG ALA ALA ARG ASN HIS VAL LYS LEU TRP TYR ARG ASN ASP ALA ALA SER ASN SER PRO ALA GLU MET E314 R315 Y325 L328 L334 P335 I336 M339 C340 Q341 K342 R345 V348 Y349 GLY GLY VAL SER GLU GLU G356 Q357 F358 V361 V362 L363
C364 K365 E369 R372 V375 R376 L383 D384 F388 L389 N390

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	220.22Å 107.80Å 81.53Å 90.00° 103.65° 90.00°	Depositor
Resolution (Å)	24.87 – 1.96 24.87 – 1.96	Depositor EDS
% Data completeness (in resolution range)	96.9 (24.87-1.96) 97.1 (24.87-1.96)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 1.96Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.196 , 0.223 0.202 , 0.226	Depositor DCC
R_{free} test set	6639 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	32.9	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9076	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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, ZN

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	0.80	0/2930	0.92	5/3964 (0.1%)
1	B	0.81	0/2853	0.96	5/3858 (0.1%)
1	C	0.75	1/2790 (0.0%)	0.86	1/3774 (0.0%)
All	All	0.79	1/8573 (0.0%)	0.92	11/11596 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	118	GLU	CD-OE2	5.36	1.31	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	372	ARG	NE-CZ-NH2	7.88	124.24	120.30
1	B	372	ARG	NE-CZ-NH1	-7.52	116.54	120.30
1	B	381	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	A	315	ARG	NE-CZ-NH2	7.06	123.83	120.30
1	B	381	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	B	376	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	A	381	ARG	NE-CZ-NH2	5.86	123.23	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	258	LEU	CA-CB-CG	-5.30	103.10	115.30
1	A	372	ARG	CG-CD-NE	-5.16	100.96	111.80
1	C	218	TYR	CB-CA-C	5.12	120.64	110.40
1	A	372	ARG	NE-CZ-NH2	-5.08	117.76	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	296	HIS	Peptide
1	B	311	ALA	Peptide

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	2869	0	2799	32	0
1	B	2793	0	2723	18	0
1	C	2731	0	2669	33	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	10	0	0	1	0
3	B	10	0	0	0	0
4	A	251	0	0	12	0
4	B	275	0	0	5	0
4	C	134	0	0	3	0
All	All	9076	0	8191	80	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 5.

All (80) 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:A:249:THR:HG22	1:A:252:GLY:H	1.28	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:MET:CE	4:B:628:HOH:O	2.21	0.88
1:C:170:PHE:HB3	1:C:258:LEU:HD13	1.71	0.73
1:A:297:VAL:HG11	4:A:744:HOH:O	1.90	0.71
1:B:339:MET:HE2	4:B:628:HOH:O	1.85	0.69
1:A:82:ARG:NH2	4:A:503:HOH:O	2.26	0.68
1:C:23:HIS:CE1	4:C:554:HOH:O	2.46	0.67
1:B:373:HIS:ND1	4:B:501:HOH:O	2.28	0.67
1:B:374:TYR:O	1:B:381:ARG:NH2	2.22	0.65
1:A:170:PHE:HB3	1:A:258:LEU:HD13	1.80	0.64
1:C:224:ASP:OD1	1:C:224:ASP:N	2.29	0.63
1:A:245:MET:HE1	4:A:720:HOH:O	1.98	0.63
1:C:228:ARG:HH11	1:C:228:ARG:HG3	1.65	0.61
1:A:277:ASP:CG	1:A:287:SER:HA	2.23	0.59
1:A:224:ASP:OD1	1:A:372:ARG:NH2	2.35	0.59
1:A:249:THR:HG21	4:A:719:HOH:O	2.03	0.58
1:A:273:ARG:HD3	4:A:600:HOH:O	2.04	0.58
1:A:373:HIS:O	1:A:377:SER:OG	2.22	0.58
1:A:283:LYS:HZ1	1:B:283:LYS:HB2	1.69	0.57
1:C:219:ALA:HA	1:C:358:PHE:CD2	2.41	0.56
1:C:383:LEU:HA	1:C:388:PHE:HD1	1.71	0.56
1:B:170:PHE:HB3	1:B:258:LEU:HD13	1.89	0.55
1:A:296:HIS:O	1:A:297:VAL:HB	2.06	0.55
1:C:39:GLU:O	1:C:43:VAL:HG13	2.09	0.53
1:A:245:MET:HB3	4:A:725:HOH:O	2.08	0.53
1:A:130:PHE:O	1:A:134:LYS:HG3	2.10	0.52
1:B:84:LYS:HG2	4:B:663:HOH:O	2.10	0.52
1:C:202:ALA:N	1:C:218:TYR:HE1	2.07	0.52
1:C:261:ASN:O	1:C:265:ILE:HG23	2.10	0.52
1:B:136:ARG:NH1	4:B:508:HOH:O	2.42	0.51
1:C:228:ARG:HG3	1:C:228:ARG:NH1	2.25	0.51
1:A:352:VAL:HG11	1:C:33:MET:HE3	1.93	0.51
1:B:378:SER:HB2	1:B:382:HIS:CE1	2.46	0.51
1:C:225:LEU:HD21	1:C:229:GLN:NE2	2.26	0.50
1:C:22:LEU:HA	1:C:270:ARG:NH2	2.27	0.50
1:C:23:HIS:CD2	4:C:610:HOH:O	2.65	0.49
1:C:340:CYS:O	1:C:345:ARG:NH1	2.46	0.49
1:C:383:LEU:HD12	1:C:383:LEU:C	2.33	0.48
1:A:171:ILE:HG13	1:A:258:LEU:HD22	1.95	0.48
1:C:131:MET:O	1:C:135:THR:HG23	2.14	0.48
1:B:379:GLU:O	1:B:383:LEU:HG	2.14	0.48
1:B:39:GLU:OE1	1:B:39:GLU:HA	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:ARG:HG2	1:C:138:HIS:O	2.13	0.48
1:C:356:GLY:N	4:C:503:HOH:O	2.47	0.48
1:C:30:ASN:O	1:C:33:MET:HE2	2.13	0.48
1:A:156:ARG:CZ	1:A:334:LEU:HD11	2.44	0.47
1:C:171:ILE:HG13	1:C:258:LEU:HD22	1.97	0.47
1:C:325:TYR:CZ	1:C:328:LEU:HB2	2.51	0.46
1:A:297:VAL:CG1	4:A:744:HOH:O	2.57	0.46
1:A:315:ARG:NH2	3:A:403:SO4:O1	2.49	0.46
1:A:378:SER:HB2	1:A:382:HIS:CE1	2.51	0.46
1:A:258:LEU:O	1:A:258:LEU:HG	2.09	0.45
1:B:102:PRO:HB2	1:B:105:GLU:HB3	1.98	0.45
1:A:245:MET:CB	4:A:725:HOH:O	2.63	0.45
1:A:249:THR:HG23	4:A:595:HOH:O	2.17	0.45
1:B:20:ASP:OD1	1:B:270:ARG:HD2	2.16	0.45
1:C:221:CYS:O	1:C:372:ARG:HD2	2.17	0.45
1:C:372:ARG:O	1:C:376:ARG:HG3	2.17	0.45
1:A:243:GLU:HA	1:A:256:ILE:CD1	2.47	0.44
1:A:245:MET:O	4:A:501:HOH:O	2.21	0.44
1:C:158:TYR:CD2	1:C:194:GLU:HG2	2.52	0.44
1:C:107:LEU:HD13	1:C:121:LEU:HD23	1.99	0.44
1:A:383:LEU:HD22	1:A:388:PHE:CD2	2.53	0.44
1:C:30:ASN:HB3	1:C:33:MET:HE2	1.99	0.44
1:C:142:LEU:HD23	1:C:142:LEU:HA	1.86	0.44
1:B:282:GLY:O	1:B:284:PRO:HD3	2.18	0.43
1:B:227:PHE:O	1:B:231:VAL:HG22	2.18	0.43
1:A:23:HIS:HB3	4:A:733:HOH:O	2.17	0.43
1:A:242:LEU:HA	1:A:388:PHE:HZ	1.83	0.43
1:C:153:SER:HB2	1:C:154:PRO:CD	2.49	0.43
1:A:245:MET:CG	4:A:725:HOH:O	2.68	0.42
1:C:334:LEU:HD22	1:C:334:LEU:HA	1.90	0.42
1:B:187:MET:HG3	1:B:385:TRP:CD1	2.55	0.42
1:B:21:GLN:O	1:B:270:ARG:NH1	2.51	0.41
1:A:352:VAL:CG1	1:C:33:MET:HE3	2.50	0.41
1:A:35:CYS:HB3	1:A:99:LEU:HD22	2.01	0.41
1:B:171:ILE:HG13	1:B:258:LEU:HD22	2.03	0.41
1:C:117:TYR:CZ	1:C:121:LEU:HD11	2.56	0.41
1:C:383:LEU:HD12	1:C:384:ASP:N	2.36	0.41
1:A:224:ASP:CG	1:A:372:ARG:HH22	2.24	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	349/403 (87%)	343 (98%)	6 (2%)	0	100	100
1	B	337/403 (84%)	335 (99%)	2 (1%)	0	100	100
1	C	328/403 (81%)	314 (96%)	14 (4%)	0	100	100
All	All	1014/1209 (84%)	992 (98%)	22 (2%)	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	306/351 (87%)	301 (98%)	5 (2%)	58	55
1	B	298/351 (85%)	292 (98%)	6 (2%)	50	44
1	C	292/351 (83%)	281 (96%)	11 (4%)	28	18
All	All	896/1053 (85%)	874 (98%)	22 (2%)	42	34

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	ASP
1	A	346	ARG
1	A	352	VAL
1	A	377	SER
1	A	380	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	20	ASP
1	B	80	GLU
1	B	84	LYS
1	B	183	ASP
1	B	187	MET
1	B	380	SER
1	C	23	HIS
1	C	82	ARG
1	C	138	HIS
1	C	145	LYS
1	C	224	ASP
1	C	260	LYS
1	C	271	ARG
1	C	283	LYS
1	C	334	LEU
1	C	345	ARG
1	C	365	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	C	390	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	B	403	-	4,4,4	0.25	0	6,6,6	0.12	0
3	SO4	A	402	-	4,4,4	0.43	0	6,6,6	0.23	0
3	SO4	A	403	-	4,4,4	0.37	0	6,6,6	0.17	0
3	SO4	B	402	-	4,4,4	0.50	0	6,6,6	0.34	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	403	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	353/403 (87%)	0.37	26 (7%)	22	27	24, 39, 74, 122	0
1	B	343/403 (85%)	0.31	21 (6%)	28	34	26, 38, 70, 103	0
1	C	334/403 (82%)	0.97	48 (14%)	7	9	31, 51, 89, 113	0
All	All	1030/1209 (85%)	0.54	95 (9%)	16	20	24, 42, 81, 122	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	352	VAL	7.5
1	A	288	ALA	6.0
1	A	289	VAL	5.9
1	C	389	LEU	5.9
1	A	286	THR	5.9
1	A	290	VAL	5.8
1	C	22	LEU	5.6
1	A	135	THR	5.5
1	B	389	LEU	5.4
1	B	310	PRO	5.3
1	B	352	VAL	5.2
1	A	297	VAL	5.2
1	A	336	ILE	4.8
1	A	383	LEU	4.5
1	B	336	ILE	4.3
1	C	81	TYR	4.3
1	C	334	LEU	4.1
1	B	311	ALA	3.9
1	A	313	MET	3.8
1	B	388	PHE	3.6
1	C	356	GLY	3.6
1	A	388	PHE	3.6
1	A	138	HIS	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	283	LYS	3.5
1	A	287	SER	3.4
1	B	20	ASP	3.3
1	B	81	TYR	3.2
1	C	135	THR	3.2
1	C	358	PHE	3.1
1	C	225	LEU	3.1
1	A	295	ASN	3.0
1	B	284	PRO	3.0
1	B	356	GLY	3.0
1	C	362	VAL	3.0
1	B	355	GLU	3.0
1	C	212	ALA	3.0
1	B	383	LEU	3.0
1	B	351	GLY	2.9
1	A	293	ALA	2.9
1	A	284	PRO	2.9
1	C	227	PHE	2.9
1	C	348	VAL	2.8
1	A	292	ALA	2.8
1	C	342	LYS	2.8
1	C	219	ALA	2.8
1	C	383	LEU	2.7
1	C	336	ILE	2.7
1	C	388	PHE	2.7
1	C	384	ASP	2.7
1	C	35	CYS	2.6
1	C	23	HIS	2.6
1	A	294	ARG	2.6
1	C	205	PHE	2.6
1	C	39	GLU	2.6
1	C	284	PRO	2.6
1	B	134	LYS	2.5
1	C	375	VAL	2.5
1	C	369	GLU	2.5
1	A	353	SER	2.5
1	A	296	HIS	2.5
1	B	387	GLY	2.5
1	B	337	THR	2.5
1	C	221	CYS	2.4
1	A	273	ARG	2.4
1	C	365	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	361	VAL	2.4
1	A	52	TYR	2.4
1	A	134	LYS	2.4
1	C	349	TYR	2.4
1	C	142	LEU	2.3
1	C	339	MET	2.3
1	C	363	LEU	2.3
1	C	390	ASN	2.2
1	B	141	ASP	2.2
1	C	357	GLN	2.2
1	B	138	HIS	2.2
1	B	312	GLU	2.2
1	A	359	GLY	2.2
1	C	364	CYS	2.2
1	C	283	LYS	2.2
1	C	33	MET	2.2
1	A	21	GLN	2.2
1	C	281	ILE	2.2
1	C	222	GLY	2.1
1	C	138	HIS	2.1
1	C	204	ALA	2.1
1	C	207	LYS	2.1
1	C	315	ARG	2.1
1	C	134	LYS	2.1
1	C	145	LYS	2.1
1	A	23	HIS	2.1
1	C	143	CYS	2.1
1	C	202	ALA	2.0
1	C	37	LEU	2.0
1	B	226	GLU	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, 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	403	5/5	0.88	0.11	50,56,59,68	0
3	SO4	B	403	5/5	0.92	0.09	56,61,64,83	0
3	SO4	B	402	5/5	0.93	0.09	54,57,63,69	0
3	SO4	A	402	5/5	0.95	0.08	54,56,63,67	0
2	ZN	C	400	1/1	0.96	0.06	72,72,72,72	0
2	ZN	A	401	1/1	0.98	0.04	54,54,54,54	0
2	ZN	B	401	1/1	0.99	0.02	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.