



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:09 PM UTC

PDB ID : 2GZA / pdb_00002gza
Title : Crystal structure of the VirB11 ATPase from the Brucella Suis type IV secretion system in complex with sulphate
Authors : Hare, S.; Bayliss, R.; Baron, C.; Waksman, G.
Deposited on : 2006-05-11
Resolution : 2.60 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 ⓘ 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

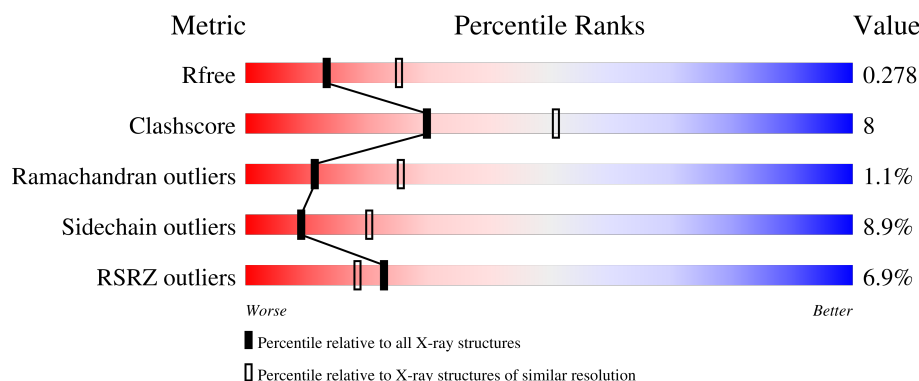
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	361	7% 73% 13% • 10%
1	B	361	3% 72% 13% • 11%
1	C	361	8% 72% 16% • 7%

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
2	SO4	A	1001	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7777 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 Type IV secretion system protein VirB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2494	1583	441	458	12			
1	B	322	Total	C	N	O	S	0	0	0
			2482	1582	432	456	12			
1	C	336	Total	C	N	O	S	0	0	0
			2593	1645	456	480	12			

- 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		
2	C	1	Total	O	S	0	0
			5	4	1		

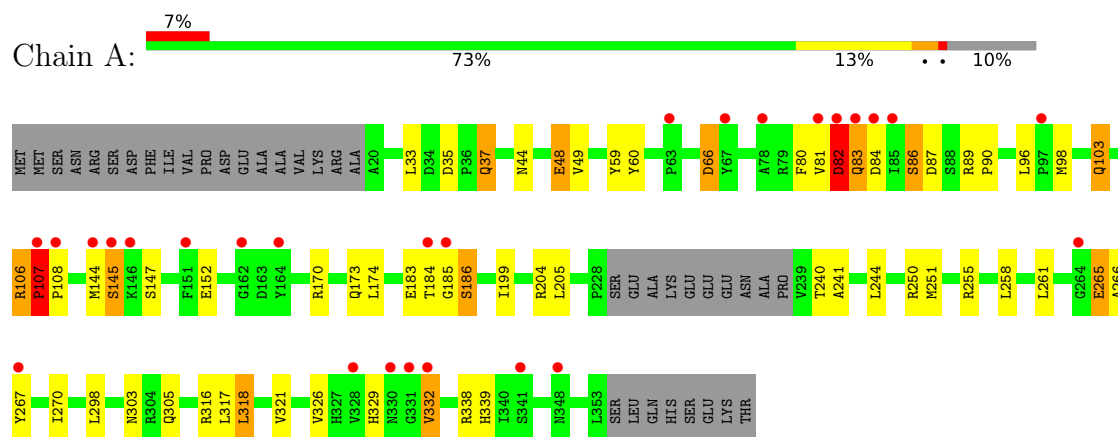
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	58	Total 58	O 58	0	0
3	B	80	Total 80	O 80	0	0
3	C	55	Total 55	O 55	0	0

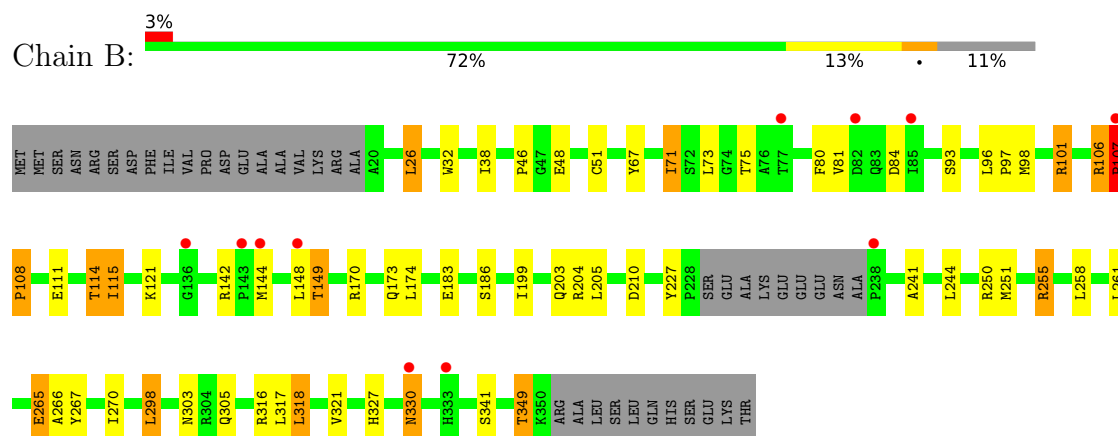
3 Residue-property plots [i](#)

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.

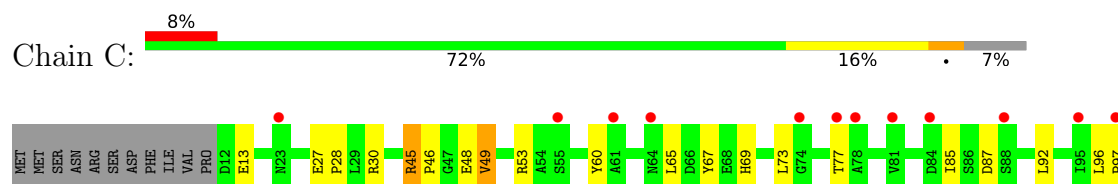
- Molecule 1: Type IV secretion system protein VirB11

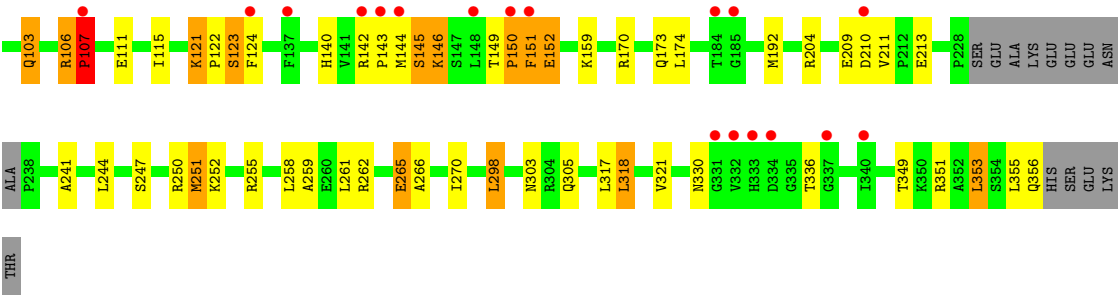


- Molecule 1: Type IV secretion system protein VirB11



- Molecule 1: Type IV secretion system protein VirB11





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	118.21Å 125.81Å 164.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.71 – 2.60 29.71 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.7 (29.71-2.60) 97.6 (29.71-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.97 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.238 , 0.279 0.236 , 0.278	Depositor DCC
R_{free} test set	3746 reflections (7.53%)	wwPDB-VP
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7777	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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 ⓘ

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	0.55	0/2552	1.01	15/3479 (0.4%)
1	B	0.53	0/2541	0.85	7/3465 (0.2%)
1	C	0.57	2/2649 (0.1%)	1.15	17/3608 (0.5%)
All	All	0.55	2/7742 (0.0%)	1.01	39/10552 (0.4%)

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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	53	ARG	C-O	-8.17	1.13	1.24
1	C	251	MET	C-O	-6.05	1.15	1.24

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	356	GLN	CA-C-O	23.71	161.11	120.80
1	C	106	ARG	CA-C-N	14.23	135.04	120.38
1	C	106	ARG	C-N-CA	14.23	135.04	120.38
1	A	106	ARG	CA-C-N	14.22	135.03	120.38
1	A	106	ARG	C-N-CA	14.22	135.03	120.38
1	C	152	GLU	N-CA-C	-12.90	97.63	113.50
1	C	107	PRO	N-CA-C	12.85	126.38	110.70
1	C	107	PRO	CA-C-N	-11.45	106.37	118.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	107	PRO	C-N-CA	-11.45	106.37	118.85
1	B	107	PRO	N-CA-C	11.31	124.50	110.70
1	A	107	PRO	N-CA-C	10.68	123.72	110.70
1	A	83	GLN	N-CA-C	8.09	121.16	108.79
1	B	142	ARG	CA-C-N	7.82	128.23	119.32
1	B	142	ARG	C-N-CA	7.82	128.23	119.32
1	C	251	MET	CA-C-N	-7.34	114.27	123.15
1	C	251	MET	C-N-CA	-7.34	114.27	123.15
1	B	349	THR	N-CA-C	-7.02	105.34	114.04
1	A	86	SER	CA-C-N	7.01	134.93	121.54
1	A	86	SER	C-N-CA	7.01	134.93	121.54
1	A	107	PRO	CA-C-N	-6.11	112.20	119.84
1	A	107	PRO	C-N-CA	-6.11	112.20	119.84
1	A	87	ASP	N-CA-C	-6.03	97.96	110.80
1	A	82	ASP	CA-C-N	-5.99	110.65	121.62
1	A	82	ASP	C-N-CA	-5.99	110.65	121.62
1	B	107	PRO	CA-C-N	-5.97	112.38	119.84
1	B	107	PRO	C-N-CA	-5.97	112.38	119.84
1	C	251	MET	N-CA-C	-5.94	100.61	109.94
1	A	80	PHE	CA-C-N	-5.86	115.06	123.03
1	A	80	PHE	C-N-CA	-5.86	115.06	123.03
1	B	148	LEU	N-CA-C	5.29	122.06	110.80
1	C	251	MET	O-C-N	-5.26	115.40	122.14
1	C	151	PHE	CA-C-N	5.22	130.96	121.92
1	C	151	PHE	C-N-CA	5.22	130.96	121.92
1	C	121	LYS	CA-C-N	5.22	125.20	120.03
1	C	121	LYS	C-N-CA	5.22	125.20	120.03
1	A	84	ASP	N-CA-C	5.21	117.97	109.59
1	A	87	ASP	N-CA-CB	5.06	119.04	110.49
1	C	144	MET	CA-C-N	5.01	131.11	121.54
1	C	144	MET	C-N-CA	5.01	131.11	121.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	107	PRO	Peptide

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	2494	0	2411	37	0
1	B	2482	0	2418	39	0
1	C	2593	0	2560	57	0
2	A	5	0	0	3	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	58	0	0	2	0
3	B	80	0	0	1	0
3	C	55	0	0	5	0
All	All	7777	0	7389	127	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 8.

All (127) 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:81:VAL:O	1:A:83:GLN:N	1.98	0.97
1:B:107:PRO:HG3	1:B:114:THR:O	1.69	0.93
1:B:204:ARG:NH1	1:B:251:MET:O	2.06	0.88
1:C:106:ARG:HB2	1:C:107:PRO:HD2	1.58	0.85
1:A:86:SER:CB	1:A:89:ARG:H	1.89	0.84
1:B:101:ARG:NH1	1:C:210:ASP:OD2	2.12	0.83
1:C:149:THR:CG2	1:C:152:GLU:HB2	2.09	0.83
1:C:107:PRO:HD3	1:C:115:ILE:HD13	1.61	0.81
1:A:103:GLN:HG3	1:A:250:ARG:CB	2.14	0.78
1:A:98:MET:HA	1:A:98:MET:HE2	1.67	0.77
1:C:149:THR:HG22	1:C:152:GLU:HB2	1.67	0.74
1:A:183:GLU:O	1:A:186:SER:HB2	1.87	0.74
1:C:204:ARG:NH1	1:C:252:LYS:H	1.87	0.72
1:A:204:ARG:NH1	1:A:251:MET:O	2.24	0.71
1:B:98:MET:HA	1:B:98:MET:HE2	1.74	0.70
1:B:111:GLU:O	1:B:114:THR:HB	1.91	0.70
1:A:103:GLN:HG3	1:A:250:ARG:HB3	1.73	0.69
1:C:303:ASN:HD22	1:C:305:GLN:H	1.41	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:TYR:OH	1:C:107:PRO:HG2	1.94	0.67
1:A:185:GLY:HA2	2:A:1001:SO4:O1	1.95	0.66
1:A:103:GLN:HG3	1:A:250:ARG:HB2	1.77	0.65
1:B:106:ARG:HB2	1:B:107:PRO:HD3	1.79	0.64
1:A:170:ARG:HH11	1:A:173:GLN:HE21	1.46	0.63
1:C:106:ARG:HB2	1:C:107:PRO:CD	2.29	0.62
1:B:241:ALA:HB3	1:B:265:GLU:HG2	1.82	0.61
1:A:185:GLY:N	2:A:1001:SO4:O2	2.34	0.60
1:B:303:ASN:HD22	1:B:305:GLN:H	1.47	0.60
1:C:96:LEU:HB3	1:C:97:PRO:HD2	1.84	0.60
1:A:241:ALA:HB3	1:A:265:GLU:HG2	1.84	0.60
1:C:330:ASN:HB2	3:C:3034:HOH:O	2.01	0.60
1:A:303:ASN:HD22	1:A:305:GLN:H	1.51	0.59
1:C:262:ARG:HG2	1:C:262:ARG:HH11	1.67	0.59
1:B:38:ILE:O	1:B:121:LYS:HE2	2.03	0.59
1:B:327:HIS:HD2	1:B:341:SER:OG	1.87	0.57
1:C:241:ALA:HB3	1:C:265:GLU:HG2	1.85	0.57
1:C:270:ILE:HD11	1:C:318:LEU:HD13	1.86	0.57
1:C:123:SER:HB2	3:C:3015:HOH:O	2.04	0.57
1:C:303:ASN:HD22	1:C:305:GLN:N	2.04	0.56
1:A:270:ILE:HD11	1:A:318:LEU:HD13	1.87	0.56
1:B:26:LEU:HD21	1:B:96:LEU:HD13	1.86	0.56
1:A:170:ARG:HH11	1:A:173:GLN:NE2	2.03	0.55
1:B:106:ARG:HB2	1:B:107:PRO:CD	2.37	0.55
1:A:267:TYR:OH	1:B:298:LEU:HG	2.06	0.55
1:B:32:TRP:CG	1:B:51:CYS:HG	2.25	0.54
1:C:123:SER:OG	1:C:124:PHE:N	2.32	0.54
1:B:170:ARG:HH11	1:B:173:GLN:NE2	2.06	0.54
1:C:209:GLU:HB2	3:C:3024:HOH:O	2.07	0.54
1:C:85:ILE:HB	1:C:92:LEU:HD12	1.88	0.54
1:C:265:GLU:HG3	3:C:3008:HOH:O	2.07	0.54
1:C:45:ARG:HB2	1:C:46:PRO:HD2	1.90	0.53
1:B:80:PHE:CZ	1:B:97:PRO:HG3	2.43	0.53
1:C:149:THR:HG23	1:C:152:GLU:OE1	2.10	0.52
1:C:204:ARG:HH11	1:C:252:LYS:H	1.56	0.52
1:B:267:TYR:OH	1:C:298:LEU:HG	2.10	0.51
1:B:303:ASN:ND2	1:B:305:GLN:H	2.09	0.51
1:C:140:HIS:C	1:C:142:ARG:H	2.18	0.51
1:B:330:ASN:ND2	1:B:330:ASN:N	2.59	0.51
1:C:303:ASN:ND2	1:C:305:GLN:H	2.06	0.50
1:B:71:ILE:HG12	1:B:115:ILE:HD11	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ARG:HH11	1:B:173:GLN:HE21	1.59	0.50
1:B:303:ASN:HD22	1:B:305:GLN:N	2.09	0.50
1:A:185:GLY:CA	2:A:1001:SO4:O1	2.60	0.50
1:C:73:LEU:O	1:C:77:THR:HG23	2.12	0.50
1:C:247:SER:OG	1:C:251:MET:CE	2.60	0.49
1:A:106:ARG:CB	1:A:107:PRO:HD2	2.41	0.49
1:B:32:TRP:CD1	1:B:51:CYS:HG	2.30	0.49
1:A:44:ASN:HD21	1:A:204:ARG:HH21	1.61	0.49
1:A:90:PRO:HB3	1:A:108:PRO:HG2	1.94	0.49
1:C:85:ILE:O	1:C:85:ILE:HG23	2.13	0.49
1:B:250:ARG:NH2	1:C:262:ARG:NH2	2.61	0.48
1:B:203:GLN:OE1	1:B:255:ARG:HD3	2.15	0.47
1:C:103:GLN:HG3	1:C:250:ARG:HB2	1.95	0.47
1:C:170:ARG:HH11	1:C:173:GLN:NE2	2.13	0.47
1:B:250:ARG:NH2	1:C:262:ARG:HH21	2.13	0.47
1:B:106:ARG:O	1:B:108:PRO:HD2	2.15	0.46
1:B:183:GLU:HG2	1:B:330:ASN:HD21	1.80	0.46
1:C:45:ARG:NH2	1:C:111:GLU:OE1	2.48	0.46
1:A:199:ILE:HG21	1:A:205:LEU:HD21	1.97	0.46
1:B:81:VAL:HG12	1:B:81:VAL:O	2.16	0.46
1:B:210:ASP:HB3	1:B:227:TYR:CE1	2.51	0.45
1:C:106:ARG:CB	1:C:107:PRO:CD	2.91	0.45
1:C:209:GLU:HG2	3:C:3017:HOH:O	2.14	0.45
1:B:67:TYR:OH	1:B:107:PRO:HG2	2.15	0.45
1:A:145:SER:C	1:A:147:SER:H	2.24	0.45
1:C:96:LEU:HB3	1:C:97:PRO:CD	2.46	0.45
1:C:262:ARG:HG2	1:C:262:ARG:NH1	2.32	0.45
1:B:186:SER:HB3	1:B:330:ASN:ND2	2.32	0.45
1:C:146:LYS:HA	1:C:146:LYS:HD2	1.58	0.45
1:C:210:ASP:OD2	1:C:211:VAL:HG23	2.16	0.45
1:C:265:GLU:H	1:C:265:GLU:CD	2.24	0.45
1:C:107:PRO:CD	1:C:115:ILE:HD13	2.42	0.45
1:C:103:GLN:HG3	1:C:250:ARG:CB	2.48	0.44
1:B:199:ILE:HG21	1:B:205:LEU:HD21	2.00	0.44
1:C:192:MET:HE1	1:C:259:ALA:O	2.18	0.44
1:B:46:PRO:HG2	3:B:2081:HOH:O	2.16	0.44
1:B:101:ARG:CZ	1:C:210:ASP:OD2	2.65	0.43
1:A:170:ARG:HD2	1:A:173:GLN:NE2	2.34	0.43
1:C:170:ARG:HH11	1:C:173:GLN:HE21	1.66	0.43
1:C:170:ARG:HD2	1:C:173:GLN:NE2	2.34	0.43
1:A:44:ASN:ND2	1:A:204:ARG:HH21	2.15	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:VAL:CG1	1:A:60:TYR:HB2	2.49	0.43
1:A:82:ASP:CG	1:A:82:ASP:O	2.60	0.43
1:A:332:VAL:HG12	3:A:1033:HOH:O	2.18	0.43
1:A:86:SER:CB	1:A:89:ARG:N	2.71	0.42
1:B:261:LEU:HD22	1:B:266:ALA:HA	2.01	0.42
1:C:28:PRO:HB2	1:C:65:LEU:HD13	2.01	0.42
1:C:261:LEU:HD22	1:C:266:ALA:HA	2.01	0.42
1:C:142:ARG:N	1:C:143:PRO:HD2	2.34	0.42
1:C:150:PRO:HB2	1:C:151:PHE:H	1.68	0.42
1:A:329:HIS:HB3	1:A:339:HIS:CE1	2.55	0.42
1:C:121:LYS:HA	1:C:122:PRO:HD2	1.92	0.42
1:C:247:SER:OG	1:C:251:MET:HE3	2.19	0.41
1:C:349:THR:O	1:C:353:LEU:HB2	2.20	0.41
1:A:329:HIS:O	1:A:338:ARG:HA	2.21	0.41
1:C:49:VAL:HG22	1:C:60:TYR:HB2	2.02	0.41
1:A:66:ASP:OD1	1:A:66:ASP:N	2.53	0.41
1:B:170:ARG:HD2	1:B:173:GLN:NE2	2.35	0.41
1:C:149:THR:HA	1:C:150:PRO:HD3	1.88	0.41
1:C:211:VAL:HG12	1:C:213:GLU:HG3	2.02	0.41
1:A:261:LEU:HD22	1:A:266:ALA:HA	2.03	0.41
1:A:240:THR:HB	3:A:1037:HOH:O	2.19	0.40
1:A:35:ASP:OD1	1:A:37:GLN:HB2	2.21	0.40
1:A:48:GLU:HB3	1:A:59:TYR:CE1	2.56	0.40
1:B:330:ASN:N	1:B:330:ASN:HD22	2.19	0.40
1:A:103:GLN:HE21	1:A:103:GLN:HB3	1.63	0.40
1:A:183:GLU:H	1:A:183:GLU:HG3	1.55	0.40
1:B:270:ILE:HD11	1:B:318:LEU:HD13	2.04	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	320/361 (89%)	299 (93%)	17 (5%)	4 (1%)	9	21
1	B	318/361 (88%)	300 (94%)	15 (5%)	3 (1%)	14	30
1	C	332/361 (92%)	313 (94%)	15 (4%)	4 (1%)	10	23
All	All	970/1083 (90%)	912 (94%)	47 (5%)	11 (1%)	11	25

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ASP
1	A	107	PRO
1	C	123	SER
1	A	144	MET
1	C	150	PRO
1	C	107	PRO
1	C	145	SER
1	B	144	MET
1	A	145	SER
1	B	108	PRO
1	B	149	THR

5.3.2 Protein sidechains ⓘ

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	261/314 (83%)	240 (92%)	21 (8%)	11	25
1	B	263/314 (84%)	239 (91%)	24 (9%)	9	19
1	C	277/314 (88%)	251 (91%)	26 (9%)	8	18
All	All	801/942 (85%)	730 (91%)	71 (9%)	9	20

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	37	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	48	GLU
1	A	66	ASP
1	A	96	LEU
1	A	103	GLN
1	A	152	GLU
1	A	174	LEU
1	A	184	THR
1	A	186	SER
1	A	244	LEU
1	A	255	ARG
1	A	258	LEU
1	A	265	GLU
1	A	298	LEU
1	A	316	ARG
1	A	317	LEU
1	A	318	LEU
1	A	321	VAL
1	A	326	VAL
1	A	332	VAL
1	B	26	LEU
1	B	48	GLU
1	B	71	ILE
1	B	73	LEU
1	B	75	THR
1	B	84	ASP
1	B	93	SER
1	B	101	ARG
1	B	106	ARG
1	B	114	THR
1	B	115	ILE
1	B	149	THR
1	B	174	LEU
1	B	244	LEU
1	B	255	ARG
1	B	258	LEU
1	B	265	GLU
1	B	298	LEU
1	B	316	ARG
1	B	317	LEU
1	B	318	LEU
1	B	321	VAL
1	B	330	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	349	THR
1	C	13	GLU
1	C	27	GLU
1	C	30	ARG
1	C	45	ARG
1	C	48	GLU
1	C	49	VAL
1	C	69	HIS
1	C	87	ASP
1	C	103	GLN
1	C	107	PRO
1	C	145	SER
1	C	146	LYS
1	C	159	LYS
1	C	174	LEU
1	C	244	LEU
1	C	255	ARG
1	C	258	LEU
1	C	265	GLU
1	C	298	LEU
1	C	317	LEU
1	C	318	LEU
1	C	321	VAL
1	C	336	THR
1	C	351	ARG
1	C	353	LEU
1	C	355	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	37	GLN
1	A	44	ASN
1	A	64	ASN
1	A	173	GLN
1	A	219	HIS
1	A	285	HIS
1	A	303	ASN
1	A	327	HIS
1	A	330	ASN
1	A	339	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	173	GLN
1	B	285	HIS
1	B	303	ASN
1	B	327	HIS
1	B	330	ASN
1	C	173	GLN
1	C	303	ASN
1	C	327	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
2	SO4	C	3001	-	4,4,4	0.21	0	6,6,6	0.12	0
2	SO4	A	1001	-	4,4,4	0.18	0	6,6,6	0.22	0
2	SO4	B	2001	-	4,4,4	0.25	0	6,6,6	0.14	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 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	SO4	3	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, 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	324/361 (89%)	0.91	27 (8%)	17 13	31, 39, 54, 59	0
1	B	322/361 (89%)	0.41	11 (3%)	48 42	31, 39, 55, 64	0
1	C	336/361 (93%)	0.84	30 (8%)	15 12	31, 39, 55, 62	0
All	All	982/1083 (90%)	0.72	68 (6%)	23 18	31, 39, 55, 64	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	107	PRO	4.5
1	C	142	ARG	4.5
1	C	331	GLY	4.4
1	C	78	ALA	4.4
1	B	144	MET	4.3
1	A	146	LYS	4.0
1	A	82	ASP	4.0
1	A	331	GLY	4.0
1	C	151	PHE	4.0
1	C	107	PRO	3.9
1	A	107	PRO	3.8
1	C	332	VAL	3.8
1	A	85	ILE	3.5
1	C	210	ASP	3.3
1	C	337	GLY	3.3
1	B	143	PRO	3.2
1	C	55	SER	3.2
1	A	264	GLY	3.2
1	B	136	GLY	3.1
1	C	143	PRO	3.1
1	C	144	MET	3.1
1	A	83	GLN	3.0
1	C	77	THR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	81	VAL	3.0
1	A	330	ASN	3.0
1	C	95	ILE	3.0
1	A	84	ASP	3.0
1	A	151	PHE	2.9
1	C	64	ASN	2.8
1	C	334	ASP	2.8
1	C	84	ASP	2.8
1	A	108	PRO	2.7
1	C	61	ALA	2.7
1	A	67	TYR	2.7
1	A	184	THR	2.7
1	A	63	PRO	2.7
1	C	148	LEU	2.6
1	B	330	ASN	2.6
1	C	333	HIS	2.5
1	C	97	PRO	2.5
1	C	150	PRO	2.5
1	B	85	ILE	2.4
1	B	148	LEU	2.4
1	C	23	ASN	2.4
1	A	144	MET	2.4
1	C	124	PHE	2.4
1	A	145	SER	2.3
1	C	185	GLY	2.3
1	A	328	VAL	2.3
1	B	82	ASP	2.3
1	C	340	ILE	2.2
1	B	238	PRO	2.2
1	A	341	SER	2.2
1	A	185	GLY	2.1
1	C	137	PHE	2.1
1	A	78	ALA	2.1
1	A	162	GLY	2.1
1	A	348	ASN	2.1
1	A	164	TYR	2.1
1	B	333	HIS	2.1
1	A	97	PRO	2.1
1	A	267	TYR	2.1
1	C	184	THR	2.0
1	A	81	VAL	2.0
1	C	88	SER	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	77	THR	2.0
1	C	74	GLY	2.0
1	A	332	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 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	A	1001	5/5	0.86	0.16	60,61,61,62	0
2	SO4	C	3001	5/5	0.95	0.08	53,54,54,54	0
2	SO4	B	2001	5/5	0.96	0.10	43,43,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.