



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:42 AM UTC

PDB ID : 5JBS / pdb_00005jbs
Title : Conformational changes during monomer-to-dimer transition of Brucella suis VirB8
Authors : Arya, T.; Sharifahmadian, M.; Sygusch, J.; Baron, B.
Deposited on : 2016-04-13
Resolution : 1.95 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

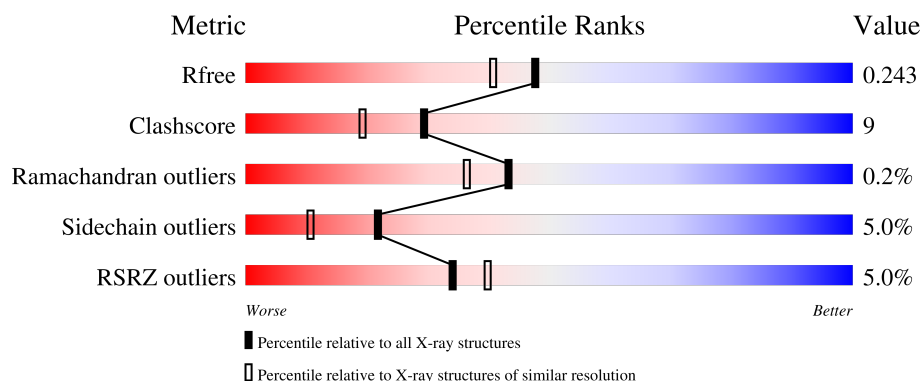
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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 $\leq 5\%$. 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	142	6% 81% 15% ..
1	B	142	5% 75% 13% 11%
1	C	142	4% 69% 16% 15%
1	D	142	4% 80% 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
2	CL	A	301	-	-	X	-
4	PEG	A	303[A]	-	-	X	-
4	PEG	A	303[B]	-	-	X	-
4	PEG	B	303	-	-	X	-
4	PEG	D	301	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4580 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 virB8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	139	Total	C	N	O	S	0	1	0
			1110	699	188	220	3			
1	B	126	Total	C	N	O	S	0	0	0
			1006	634	168	202	2			
1	C	121	Total	C	N	O	S	0	0	0
			965	612	159	192	2			
1	D	136	Total	C	N	O	S	0	0	0
			1083	681	181	218	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ARG	MET	engineered mutation	UNP Q7CEG3
B	102	ARG	MET	engineered mutation	UNP Q7CEG3
C	102	ARG	MET	engineered mutation	UNP Q7CEG3
D	102	ARG	MET	engineered mutation	UNP Q7CEG3

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



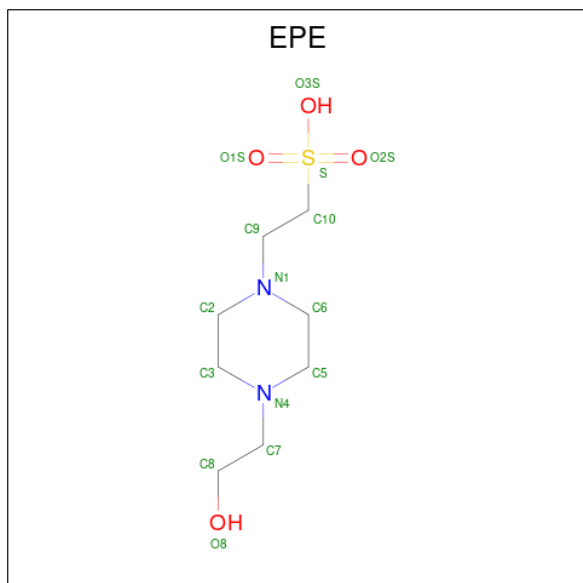
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			14	8	6		
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

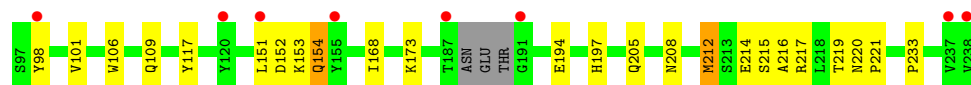
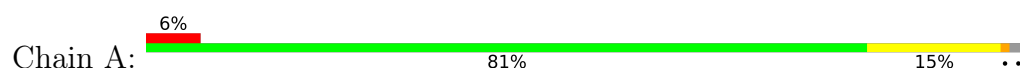
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	84	Total	O	0	0
			84	84		
6	B	86	Total	O	0	0
			86	86		
6	C	67	Total	O	0	0
			67	67		
6	D	84	Total	O	0	0
			84	84		

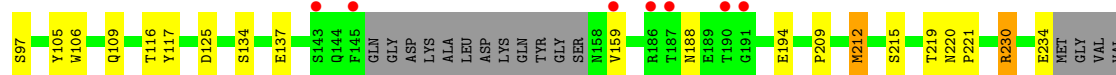
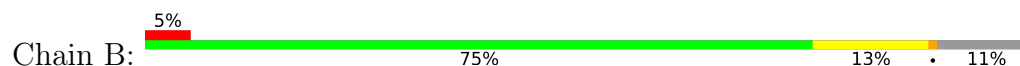
3 Residue-property plots [i](#)

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.

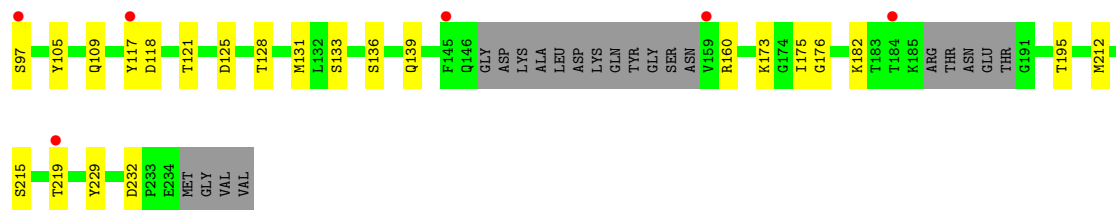
- Molecule 1: Type IV secretion system protein virB8



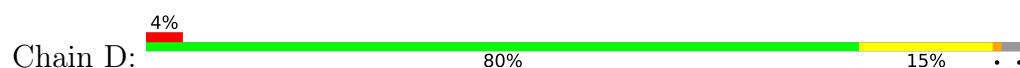
- Molecule 1: Type IV secretion system protein virB8



- Molecule 1: Type IV secretion system protein virB8



- Molecule 1: Type IV secretion system protein virB8



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.50Å 78.72Å 70.84Å 90.00° 111.56° 90.00°	Depositor
Resolution (Å)	42.20 – 1.95 42.20 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.9 (42.20-1.95) 96.9 (42.20-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.86 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.191 , 0.241 (Not available) , 0.243	Depositor DCC
R_{free} test set	2497 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4580	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 6.45% 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: CL, PEG, EPE, GOL

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	1.31	4/1134 (0.4%)	1.17	0/1539
1	B	1.20	0/1029	1.07	0/1401
1	C	1.23	3/987 (0.3%)	1.07	1/1342 (0.1%)
1	D	1.22	2/1107 (0.2%)	1.14	2/1504 (0.1%)
All	All	1.24	9/4257 (0.2%)	1.11	3/5786 (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	D	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	229	TYR	CA-C	-6.90	1.44	1.52
1	A	205	GLN	C-O	-6.01	1.16	1.23
1	A	98	TYR	CA-C	5.74	1.60	1.52
1	C	128	THR	C-O	-5.34	1.18	1.24
1	D	137	GLU	C-O	5.22	1.30	1.24
1	A	168	ILE	N-CA	-5.20	1.40	1.46
1	C	133	SER	C-O	5.15	1.30	1.23
1	D	235	MET	CA-C	5.15	1.59	1.52
1	A	197	HIS	N-CA	5.04	1.52	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	176	GLY	CA-C-O	-5.22	117.03	121.57
1	D	129	VAL	CA-C-N	5.01	125.65	119.99
1	D	129	VAL	C-N-CA	5.01	125.65	119.99

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	188	ASN	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	1110	0	1072	21	0
1	B	1006	0	963	25	0
1	C	965	0	925	11	0
1	D	1083	0	1036	13	0
2	A	1	0	0	2	0
2	B	1	0	0	1	0
3	A	6	0	8	1	0
4	A	14	0	19	21	0
4	B	7	0	10	5	0
4	C	14	0	20	2	0
4	D	7	0	10	4	0
5	B	15	0	18	4	0
5	C	30	0	36	3	0
6	A	84	0	0	3	0
6	B	86	0	0	2	0
6	C	67	0	0	2	0
6	D	84	0	0	3	0
All	All	4580	0	4117	72	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 9.

All (72) 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:217:ARG:HB2	6:A:405:HOH:O	1.71	0.90
1:C:97:SER:N	6:C:401:HOH:O	2.13	0.81
1:A:109:GLN:OE1	6:A:401:HOH:O	2.02	0.76
1:A:106:TRP:CH2	4:A:303[B]:PEG:H42	2.22	0.73
1:D:106:TRP:CH2	4:D:301:PEG:H42	2.25	0.70
1:C:131:MET:HE1	1:C:219:THR:HG21	1.76	0.67
1:C:118:ASP:HB3	1:C:121:THR:HG22	1.76	0.67
1:D:146:GLN:OE1	6:D:401:HOH:O	2.12	0.66
1:A:212:MET:HB2	1:A:216:ALA:HB3	1.82	0.61
1:A:233:PRO:HG3	3:A:302:GOL:H32	1.81	0.61
4:A:303[A]:PEG:H12	1:B:219:THR:O	1.99	0.61
4:A:303[B]:PEG:C2	1:B:106:TRP:CH2	2.84	0.60
1:B:97:SER:N	6:B:403:HOH:O	2.34	0.60
1:B:137:GLU:HB2	4:B:303:PEG:H21	1.83	0.59
4:A:303[B]:PEG:H22	1:B:106:TRP:CH2	2.38	0.58
4:A:303[B]:PEG:H32	1:B:221:PRO:HD2	1.86	0.57
1:A:219:THR:O	4:A:303[B]:PEG:O2	2.22	0.57
4:A:303[A]:PEG:O4	1:B:221:PRO:HG2	2.05	0.57
1:D:212:MET:HE2	1:D:216:ALA:HB1	1.87	0.56
1:A:101:VAL:HG13	6:B:415:HOH:O	2.05	0.56
1:A:106:TRP:CZ2	4:A:303[B]:PEG:H42	2.42	0.55
4:A:303[B]:PEG:H22	1:B:106:TRP:CZ2	2.42	0.55
1:B:230:ARG:NH1	1:C:232:ASP:OD2	2.40	0.54
4:C:302:PEG:H21	1:D:233:PRO:HG3	1.89	0.54
4:A:303[B]:PEG:H21	1:B:106:TRP:CH2	2.44	0.53
4:A:303[B]:PEG:H21	1:B:106:TRP:HH2	1.72	0.53
1:D:212:MET:HE1	1:D:220:ASN:HD22	1.74	0.53
1:A:109:GLN:HG2	6:A:401:HOH:O	2.09	0.52
1:A:106:TRP:HZ2	4:A:303[B]:PEG:C1	2.22	0.52
1:A:173:LYS:O	1:A:173:LYS:HG2	2.10	0.52
1:B:105:TYR:O	1:B:109:GLN:HG2	2.10	0.51
1:B:116:THR:HG21	5:B:301:EPE:H52	1.93	0.51
4:A:303[B]:PEG:C2	1:B:106:TRP:HH2	2.25	0.49
1:B:209:PRO:O	1:B:212:MET:HG2	2.12	0.49
1:B:134:SER:OG	4:B:303:PEG:H32	2.13	0.49
4:C:302:PEG:H11	6:C:413:HOH:O	2.13	0.48
1:D:219:THR:O	4:D:301:PEG:O2	2.31	0.48
1:D:179:ARG:NE	1:D:234:GLU:OE2	2.46	0.48
1:C:121:THR:HG21	5:C:304:EPE:C3	2.45	0.47
1:A:221:PRO:HD2	4:A:303[A]:PEG:H22	1.96	0.47
1:A:173:LYS:O	1:A:173:LYS:CG	2.63	0.46
1:B:125:ASP:OD2	5:B:301:EPE:H51	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:SER:OG	4:B:303:PEG:C3	2.64	0.46
1:D:129:VAL:HG11	1:D:141:TYR:CG	2.50	0.46
4:B:303:PEG:C4	1:C:173:LYS:HB2	2.46	0.45
1:D:98:TYR:OH	6:D:402:HOH:O	2.20	0.45
1:A:220:ASN:HA	2:A:301:CL:CL	2.54	0.45
4:A:303[B]:PEG:H41	1:B:106:TRP:HZ2	1.80	0.44
1:D:106:TRP:CZ2	4:D:301:PEG:H42	2.52	0.44
1:A:208:ASN:OD1	1:A:208:ASN:C	2.59	0.44
1:B:220:ASN:OD1	2:B:302:CL:CL	2.72	0.44
1:A:220:ASN:OD1	2:A:301:CL:CL	2.72	0.44
1:C:105:TYR:O	1:C:109:GLN:HG2	2.18	0.44
1:D:221:PRO:HD2	4:D:301:PEG:H12	2.00	0.43
1:C:117:TYR:CD1	1:C:117:TYR:C	2.95	0.43
1:B:117:TYR:CD1	1:B:117:TYR:C	2.96	0.43
1:B:137:GLU:N	4:B:303:PEG:H22	2.34	0.43
1:A:106:TRP:HZ2	4:A:303[B]:PEG:H11	1.84	0.43
5:B:301:EPE:N1	5:B:301:EPE:C7	2.80	0.42
5:B:301:EPE:N1	5:B:301:EPE:H72	2.34	0.42
4:A:303[B]:PEG:H41	1:B:106:TRP:CZ2	2.54	0.42
1:C:139:GLN:HG2	5:C:301:EPE:O3S	2.20	0.42
1:A:154:GLN:HE21	1:A:154:GLN:HB3	1.71	0.42
1:A:219:THR:O	4:A:303[A]:PEG:O2	2.38	0.41
1:A:106:TRP:HZ2	4:A:303[B]:PEG:H12	1.84	0.41
1:D:151:LEU:N	6:D:414:HOH:O	2.54	0.41
1:D:212:MET:HE1	1:D:220:ASN:ND2	2.35	0.41
4:A:303[B]:PEG:H32	1:B:221:PRO:CD	2.49	0.41
1:A:117:TYR:OH	1:A:152:ASP:HA	2.21	0.40
4:A:303[A]:PEG:C1	1:B:219:THR:O	2.67	0.40
1:C:125:ASP:OD1	5:C:304:EPE:H32	2.21	0.40
1:C:182:LYS:O	1:C:195:THR:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	136/142 (96%)	134 (98%)	2 (2%)	0	100	100
1	B	122/142 (86%)	118 (97%)	3 (2%)	1 (1%)	16	8
1	C	115/142 (81%)	115 (100%)	0	0	100	100
1	D	132/142 (93%)	128 (97%)	4 (3%)	0	100	100
All	All	505/568 (89%)	495 (98%)	9 (2%)	1 (0%)	43	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	188	ASN

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	122/124 (98%)	115 (94%)	7 (6%)	18	8
1	B	112/124 (90%)	106 (95%)	6 (5%)	20	9
1	C	107/124 (86%)	102 (95%)	5 (5%)	23	12
1	D	120/124 (97%)	115 (96%)	5 (4%)	26	16
All	All	461/496 (93%)	438 (95%)	23 (5%)	22	11

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	LEU
1	A	153	LYS
1	A	154	GLN
1	A	194	GLU
1	A	212	MET
1	A	214	GLU
1	A	215	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	159	VAL
1	B	194	GLU
1	B	212	MET
1	B	215	SER
1	B	230	ARG
1	B	234	GLU
1	C	136	SER
1	C	160	ARG
1	C	175	ILE
1	C	212	MET
1	C	215	SER
1	D	123	GLN
1	D	185	LYS
1	D	186	ARG
1	D	213	SER
1	D	214	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	GLN
1	B	123	GLN
1	B	188	ASN
1	B	197	HIS
1	C	139	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

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	$\# Z > 2$
4	PEG	C	303	-	6,6,6	1.08	0	5,5,5	1.10	0
5	EPE	C	301	-	15,15,15	2.19	1 (6%)	19,20,20	1.96	5 (26%)
4	PEG	D	301	-	6,6,6	1.14	0	5,5,5	1.36	1 (20%)
5	EPE	B	301	-	15,15,15	2.38	1 (6%)	19,20,20	2.07	6 (31%)
4	PEG	C	302	-	6,6,6	0.69	0	5,5,5	1.02	0
5	EPE	C	304	-	15,15,15	2.28	1 (6%)	19,20,20	1.23	2 (10%)
4	PEG	B	303	-	6,6,6	0.48	0	5,5,5	0.85	0
3	GOL	A	302	-	5,5,5	0.90	0	5,5,5	1.17	0
4	PEG	A	303[A]	-	6,6,6	0.57	0	5,5,5	1.22	1 (20%)
4	PEG	A	303[B]	-	6,6,6	0.68	0	5,5,5	0.52	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	C	303	-	-	2/4/4/4	-
5	EPE	C	301	-	-	5/9/19/19	0/1/1/1
4	PEG	D	301	-	-	2/4/4/4	-
5	EPE	B	301	-	-	4/9/19/19	0/1/1/1
4	PEG	C	302	-	-	0/4/4/4	-
5	EPE	C	304	-	-	4/9/19/19	0/1/1/1
4	PEG	B	303	-	-	4/4/4/4	-
3	GOL	A	302	-	-	4/4/4/4	-
4	PEG	A	303[A]	-	-	2/4/4/4	-
4	PEG	A	303[B]	-	-	3/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	301	EPE	C10-S	-8.79	1.65	1.77
5	C	304	EPE	C10-S	-8.39	1.65	1.77
5	C	301	EPE	C10-S	-7.91	1.66	1.77

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	301	EPE	C5-C6-N1	-5.49	99.57	110.65
5	C	301	EPE	O1S-S-C10	4.71	113.84	106.73
5	B	301	EPE	C9-N1-C2	3.39	120.28	111.24
5	C	301	EPE	O3S-S-O2S	-3.11	103.61	111.40
5	B	301	EPE	O1S-S-C10	3.01	111.27	106.73
5	C	301	EPE	O3S-S-C10	2.98	111.84	106.00
5	C	301	EPE	C8-C7-N4	-2.82	103.56	113.44
5	B	301	EPE	C3-C2-N1	-2.75	105.10	110.65
5	B	301	EPE	C10-C9-N1	-2.71	102.11	112.36
5	C	301	EPE	C7-N4-C3	2.48	117.83	111.24
4	D	301	PEG	O2-C2-C1	2.46	120.96	110.11
4	A	303[A]	PEG	O2-C3-C4	-2.39	99.56	110.11
5	C	304	EPE	C7-N4-C3	2.27	117.30	111.24
5	C	304	EPE	C2-C3-N4	2.14	114.96	110.65
5	B	301	EPE	O3S-S-C10	2.06	110.04	106.00

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	GOL	O1-C1-C2-C3
3	A	302	GOL	C1-C2-C3-O3
5	B	301	EPE	C9-C10-S-O2S
5	B	301	EPE	C9-C10-S-O3S
5	C	301	EPE	C9-C10-S-O1S
5	C	304	EPE	C8-C7-N4-C3
4	A	303[A]	PEG	C1-C2-O2-C3
4	A	303[B]	PEG	O1-C1-C2-O2
3	A	302	GOL	O2-C2-C3-O3
4	A	303[B]	PEG	C4-C3-O2-C2
4	B	303	PEG	O1-C1-C2-O2
4	C	303	PEG	O2-C3-C4-O4
4	D	301	PEG	O1-C1-C2-O2
5	C	304	EPE	N4-C7-C8-O8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	301	EPE	N4-C7-C8-O8
4	A	303[A]	PEG	O2-C3-C4-O4
5	C	301	EPE	C8-C7-N4-C5
3	A	302	GOL	O1-C1-C2-O2
5	C	301	EPE	C8-C7-N4-C3
5	B	301	EPE	C10-C9-N1-C2
5	B	301	EPE	C9-C10-S-O1S
5	C	301	EPE	C9-C10-S-O2S
4	A	303[B]	PEG	C1-C2-O2-C3
5	C	304	EPE	S-C10-C9-N1
4	B	303	PEG	C4-C3-O2-C2
4	D	301	PEG	O2-C3-C4-O4
4	C	303	PEG	C4-C3-O2-C2
4	B	303	PEG	C1-C2-O2-C3
5	C	304	EPE	C8-C7-N4-C5
4	B	303	PEG	O2-C3-C4-O4

There are no ring outliers.

9 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	301	EPE	1	0
4	D	301	PEG	4	0
5	B	301	EPE	4	0
4	C	302	PEG	2	0
5	C	304	EPE	2	0
4	B	303	PEG	5	0
3	A	302	GOL	1	0
4	A	303[A]	PEG	5	0
4	A	303[B]	PEG	16	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	139/142 (97%)	0.40	8 (5%)	29 33	19, 40, 86, 108	1 (0%)
1	B	126/142 (88%)	0.29	7 (5%)	30 35	28, 40, 80, 116	0
1	C	121/142 (85%)	0.33	6 (4%)	34 40	28, 39, 79, 96	0
1	D	136/142 (95%)	0.35	5 (3%)	45 52	29, 40, 86, 106	0
All	All	522/568 (91%)	0.34	26 (4%)	34 40	19, 40, 85, 116	1 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	120	TYR	5.9
1	A	238	VAL	4.4
1	B	159	VAL	3.3
1	C	159	VAL	2.9
1	A	187	THR	2.9
1	D	151	LEU	2.9
1	A	237	VAL	2.8
1	D	236	GLY	2.7
1	C	184	THR	2.7
1	D	155	TYR	2.7
1	A	151	LEU	2.6
1	D	171	ASN	2.5
1	A	155	TYR	2.5
1	A	98	TYR	2.4
1	B	191	GLY	2.4
1	C	97	SER	2.4
1	C	219	THR	2.3
1	B	143	SER	2.3
1	C	117	TYR	2.2
1	D	98	TYR	2.2
1	B	187	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	145	PHE	2.2
1	A	191	GLY	2.2
1	B	190	THR	2.1
1	B	145	PHE	2.0
1	B	186	ARG	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(Å ²)	Q<0.9
5	EPE	C	304	15/15	0.73	0.22	84,102,158,177	0
5	EPE	C	301	15/15	0.76	0.25	43,71,80,90	10
4	PEG	B	303	7/7	0.82	0.30	37,39,42,44	7
5	EPE	B	301	15/15	0.82	0.21	65,76,82,84	9
4	PEG	C	303	7/7	0.86	0.16	51,65,72,75	0
4	PEG	C	302	7/7	0.86	0.14	40,57,65,66	0
4	PEG	D	301	7/7	0.87	0.14	36,42,53,57	2
2	CL	A	301	1/1	0.89	0.21	72,72,72,72	0
4	PEG	A	303[B]	7/7	0.90	0.13	21,23,25,26	7
4	PEG	A	303[A]	7/7	0.90	0.13	21,25,28,30	7
3	GOL	A	302	6/6	0.91	0.16	23,26,28,31	6
2	CL	B	302	1/1	0.96	0.15	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.