



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:24 AM UTC

PDB ID : 2Z9K / pdb_00002z9k
Title : Complex structure of SARS-CoV 3C-like protease with JMF1600
Authors : Lee, C.C.; Wang, A.H.
Deposited on : 2007-09-20
Resolution : 1.85 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

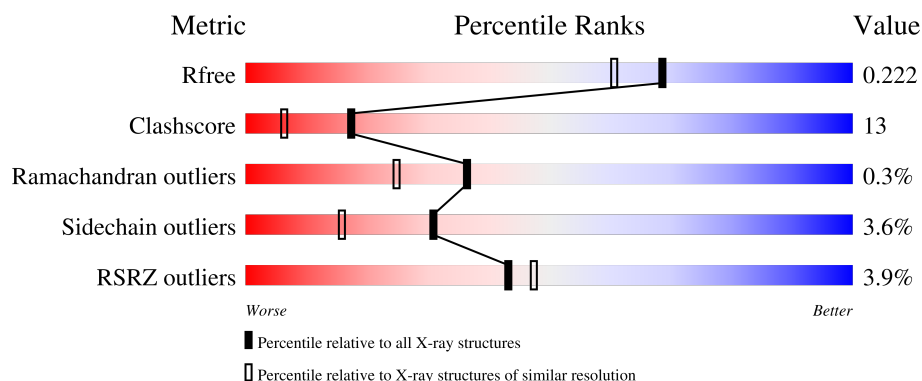
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	306	5% 75% 21% .
1	B	306	3% 76% 23% .

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	DMS	A	803	-	X	-	-
2	DMS	A	813	-	X	-	-
2	DMS	B	802	-	X	-	-
2	DMS	B	812	-	X	-	-

2 Entry composition [i](#)

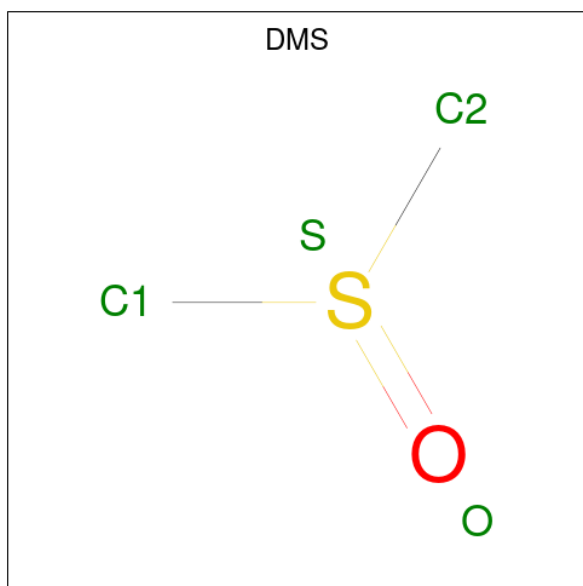
There are 4 unique types of molecules in this entry. The entry contains 5533 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3C-like proteinase.

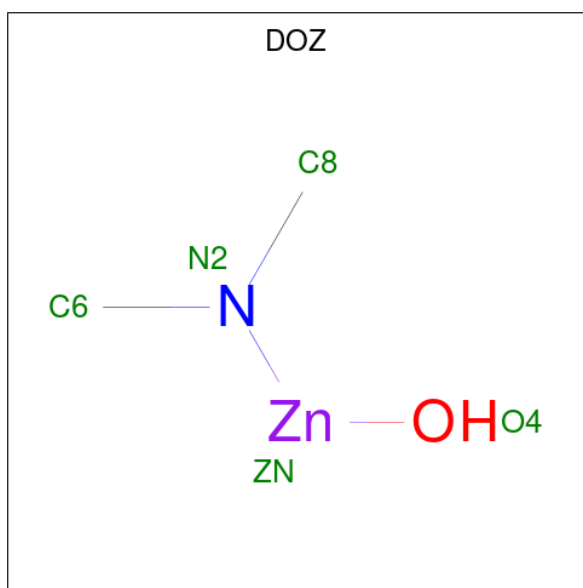
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2361	1494	403	442	22			
1	B	306	Total	C	N	O	S	0	0	0
			2371	1499	405	445	22			

- Molecule 2 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



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

- Molecule 3 is (dimethylamino)(hydroxy)zinc' (CCD ID: DOZ) (formula: C_2H_7NOZn).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	Zn	0	0
			5	2	1	1	1		
3	B	1	Total	C	N	O	Zn	0	0
			5	2	1	1	1		

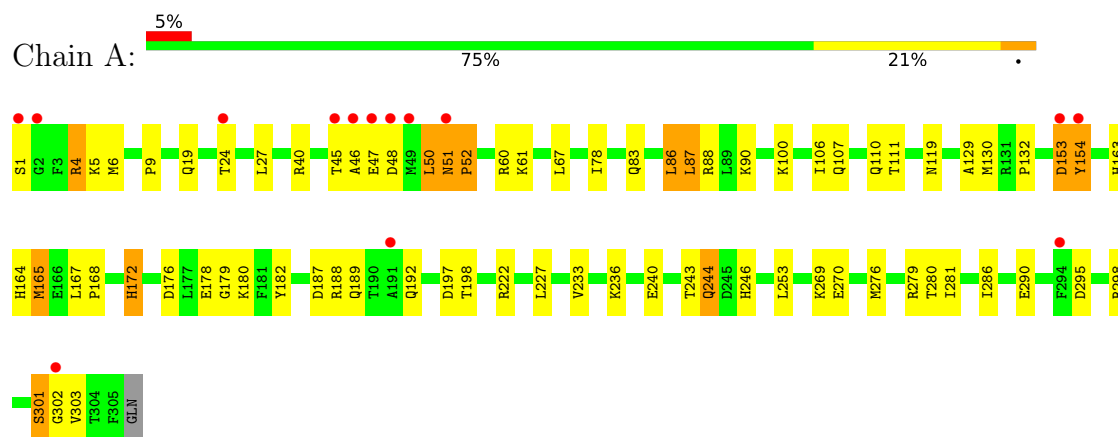
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	369	Total	O	0	0
			369	369		
4	B	406	Total	O	0	0
			406	406		

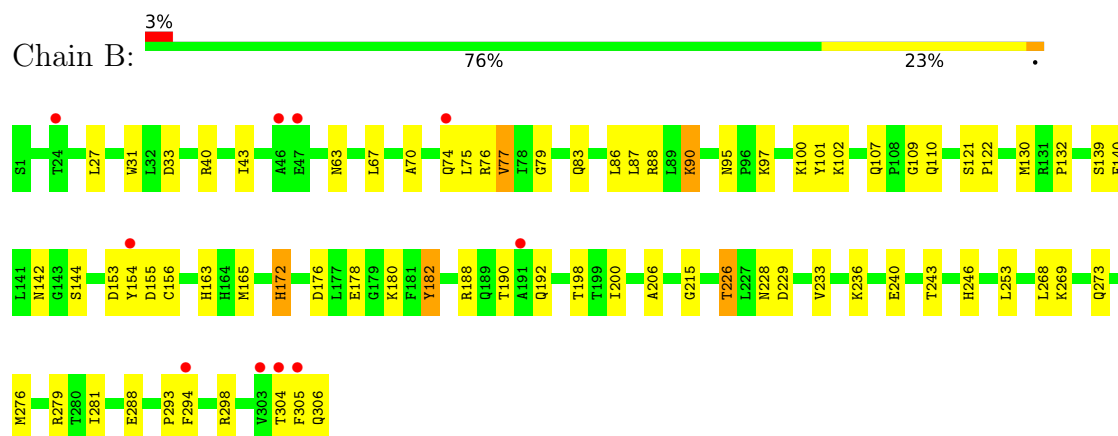
3 Residue-property plots

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: 3C-like proteinase



• Molecule 1: 3C-like proteinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.10Å 95.77Å 67.74Å 90.00° 103.24° 90.00°	Depositor
Resolution (Å)	30.00 – 1.85 30.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.85) 89.3 (30.00-1.85)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 1.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.187 , 0.224 0.184 , 0.222	Depositor DCC
R_{free} test set	2624 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.8	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	0.96	EDS
Total number of atoms	5533	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% 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: DOZ, DMS

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	0.35	0/2414	0.91	11/3280 (0.3%)
1	B	0.36	0/2424	0.89	6/3292 (0.2%)
All	All	0.35	0/4838	0.90	17/6572 (0.3%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	SER	N-CA-C	-8.26	98.29	110.52
1	A	52	PRO	N-CA-C	7.17	122.61	111.21
1	A	176	ASP	N-CA-C	-6.65	101.17	110.35
1	A	100	LYS	N-CA-C	-6.65	100.44	110.28
1	B	178	GLU	N-CA-C	-6.36	104.77	113.30
1	A	178	GLU	N-CA-C	-5.97	105.30	113.30
1	A	182	TYR	N-CA-C	-5.94	99.60	109.46
1	B	100	LYS	N-CA-C	-5.93	101.06	109.96
1	B	182	TYR	N-CA-C	-5.90	99.11	108.73
1	B	165	MET	N-CA-C	5.77	117.02	108.60
1	A	172	HIS	N-CA-C	5.64	118.75	109.72
1	A	165	MET	N-CA-C	5.59	116.76	108.60
1	A	130	MET	N-CA-C	-5.55	100.75	109.25
1	B	172	HIS	N-CA-C	5.54	118.58	109.72
1	A	9	PRO	N-CA-C	-5.12	103.15	111.03
1	B	176	ASP	N-CA-C	-5.09	101.97	109.86
1	A	5	LYS	N-CA-C	-5.07	100.82	108.67

There are no chirality outliers.

There are no planarity outliers.

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	2361	0	2313	64	0
1	B	2371	0	2321	56	1
2	A	8	0	12	1	0
2	B	8	0	12	0	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
4	A	369	0	0	16	1
4	B	406	0	0	13	0
All	All	5533	0	4658	118	1

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 13.

All (118) 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:90:LYS:HE2	4:A:1256:HOH:O	1.55	1.06
1:A:45:THR:H	1:A:48:ASP:HB2	1.22	1.03
1:B:107:GLN:H	1:B:110:GLN:HE21	1.19	0.90
1:B:305:PHE:HB3	4:B:1473:HOH:O	1.79	0.81
1:A:50:LEU:HA	1:A:189:GLN:HB2	1.64	0.80
1:A:106:ILE:HG13	1:A:110:GLN:HE21	1.47	0.78
1:A:244:GLN:HE21	1:A:244:GLN:HA	1.50	0.77
1:B:110:GLN:HG2	4:B:1306:HOH:O	1.84	0.76
1:A:276:MET:HE3	1:A:281:ILE:HG13	1.67	0.75
1:B:155:ASP:HB2	4:B:1479:HOH:O	1.89	0.73
1:B:215:GLY:HA2	4:B:1473:HOH:O	1.89	0.72
1:A:165:MET:HE1	1:A:192:GLN:NE2	2.07	0.70
1:A:45:THR:HG22	1:A:46:ALA:H	1.57	0.69
1:B:190:THR:OG1	1:B:192:GLN:HG3	1.91	0.69
1:A:270:GLU:HG3	4:A:1173:HOH:O	1.94	0.68
1:B:226:THR:HG22	1:B:229:ASP:H	1.57	0.68
1:B:198:THR:HG21	1:B:240:GLU:OE1	1.94	0.68
1:B:188:ARG:HG3	1:B:190:THR:HG23	1.76	0.67
1:A:180:LYS:HD2	4:A:1094:HOH:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:PHE:O	1:B:306:GLN:HB2	1.96	0.64
1:A:50:LEU:H	1:A:50:LEU:HD12	1.64	0.62
1:A:107:GLN:H	1:A:110:GLN:NE2	1.97	0.62
1:B:101:TYR:OH	4:B:1333:HOH:O	2.16	0.62
1:B:97:LYS:HE3	4:B:1514:HOH:O	2.00	0.62
1:B:226:THR:HG23	4:B:1227:HOH:O	1.99	0.61
1:B:74:GLN:HG2	4:B:1478:HOH:O	2.01	0.61
1:A:27:LEU:HD23	3:A:901:DOZ:C6	2.30	0.61
1:A:83:GLN:HE21	1:A:88:ARG:HD2	1.66	0.61
1:A:45:THR:HG22	1:A:46:ALA:N	2.17	0.60
1:B:67:LEU:HD11	1:B:74:GLN:OE1	2.00	0.60
1:A:51:ASN:H	1:A:52:PRO:CD	2.15	0.60
1:B:40:ARG:HA	1:B:87:LEU:HG	1.84	0.59
1:B:77:VAL:HG12	4:B:1260:HOH:O	2.01	0.59
1:A:48:ASP:O	1:A:52:PRO:HD3	2.02	0.59
1:B:33:ASP:OD2	4:B:1333:HOH:O	2.17	0.59
1:A:51:ASN:HA	4:A:1267:HOH:O	2.03	0.58
1:B:107:GLN:H	1:B:110:GLN:NE2	1.97	0.58
1:A:276:MET:CE	1:A:281:ILE:HG13	2.34	0.57
1:A:154:TYR:HA	4:A:1181:HOH:O	2.05	0.57
1:A:50:LEU:HD12	1:A:50:LEU:N	2.21	0.56
1:A:88:ARG:NH1	4:A:1257:HOH:O	2.39	0.55
1:B:132:PRO:HG2	1:B:198:THR:HG23	1.88	0.55
1:A:24:THR:HG22	4:A:1263:HOH:O	2.07	0.55
1:A:164:HIS:ND1	4:A:1268:HOH:O	2.33	0.55
1:A:78:ILE:HD11	1:A:90:LYS:HE3	1.89	0.54
1:A:153:ASP:HB2	4:A:1008:HOH:O	2.07	0.54
1:A:45:THR:N	1:A:48:ASP:HB2	2.06	0.54
1:A:154:TYR:HB3	4:A:1241:HOH:O	2.08	0.53
1:A:236:LYS:O	1:A:236:LYS:HD3	2.07	0.53
1:A:83:GLN:NE2	1:A:88:ARG:HD2	2.25	0.53
1:A:86:LEU:HD13	1:A:179:GLY:HA2	1.91	0.53
1:A:47:GLU:HA	1:A:50:LEU:HD13	1.91	0.52
1:B:294:PHE:CE2	1:B:298:ARG:NH2	2.79	0.51
1:A:60:ARG:HG2	1:A:60:ARG:HH11	1.75	0.51
1:B:79:GLY:HA3	1:B:90:LYS:HZ3	1.75	0.51
1:A:50:LEU:HG	1:A:189:GLN:HG3	1.93	0.50
1:B:180:LYS:NZ	1:B:180:LYS:HB3	2.26	0.50
1:A:50:LEU:HA	1:A:189:GLN:CB	2.40	0.50
1:B:31:TRP:CE2	1:B:95:ASN:HB2	2.47	0.49
1:A:51:ASN:N	1:A:52:PRO:CD	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:PHE:HE2	1:B:298:ARG:HH21	1.61	0.49
1:A:61:LYS:NZ	4:A:1262:HOH:O	2.46	0.49
1:A:40:ARG:HA	1:A:87:LEU:HD23	1.94	0.49
1:A:51:ASN:H	1:A:52:PRO:HD3	1.78	0.48
1:B:75:LEU:HD12	1:B:75:LEU:N	2.27	0.48
1:A:243:THR:H	1:A:246:HIS:CD2	2.30	0.48
1:B:163:HIS:CE1	1:B:172:HIS:HB3	2.49	0.48
1:B:288:GLU:HG3	4:B:1475:HOH:O	2.13	0.48
1:A:290:GLU:HB2	4:A:1004:HOH:O	2.13	0.48
1:B:243:THR:H	1:B:246:HIS:CD2	2.32	0.47
1:A:286:ILE:C	1:A:286:ILE:HD12	2.40	0.47
1:A:233:VAL:HG11	1:A:269:LYS:HG3	1.97	0.47
1:B:102:LYS:HE3	1:B:156:CYS:SG	2.54	0.47
1:B:226:THR:HG22	1:B:228:ASN:N	2.29	0.47
1:A:88:ARG:NE	4:A:1246:HOH:O	2.47	0.47
1:A:19:GLN:HE21	1:A:119:ASN:HA	1.80	0.46
1:A:4:ARG:HB2	1:B:139:SER:HB2	1.97	0.46
1:A:187:ASP:HB3	4:A:1268:HOH:O	2.15	0.46
1:B:269:LYS:O	1:B:273:GLN:HG3	2.16	0.46
1:A:302:GLY:HA3	4:A:994:HOH:O	2.14	0.46
1:A:132:PRO:HD2	1:A:197:ASP:OD2	2.15	0.45
1:B:140:PHE:HB3	1:B:144:SER:OG	2.16	0.45
1:B:153:ASP:O	1:B:154:TYR:HB2	2.17	0.45
1:B:31:TRP:CD2	1:B:95:ASN:HB2	2.51	0.45
1:B:109:GLY:HA2	1:B:200:ILE:HD13	1.99	0.45
1:B:90:LYS:HB3	1:B:90:LYS:NZ	2.31	0.44
1:B:276:MET:HE3	1:B:281:ILE:HG13	1.99	0.44
1:B:306:GLN:N	4:B:1473:HOH:O	2.37	0.44
1:A:244:GLN:HA	1:A:244:GLN:NE2	2.27	0.44
1:A:6:MET:HG3	2:A:813:DMS:H23	1.99	0.44
1:A:301:SER:OG	1:A:303:VAL:HG23	2.18	0.44
1:B:63:ASN:O	1:B:77:VAL:CG1	2.66	0.44
1:A:295:ASP:OD1	1:A:298:ARG:NH2	2.46	0.43
1:B:76:ARG:CZ	1:B:76:ARG:HB3	2.48	0.43
1:A:1:SER:HB3	1:B:140:PHE:O	2.18	0.43
1:B:163:HIS:HE1	1:B:172:HIS:HB3	1.82	0.43
1:B:40:ARG:O	1:B:43:ILE:HG12	2.19	0.43
1:B:70:ALA:CB	1:B:75:LEU:HD11	2.49	0.43
1:B:294:PHE:HE2	1:B:298:ARG:NH2	2.15	0.43
1:A:276:MET:HE1	1:A:280:THR:HA	2.01	0.42
1:B:121:SER:HA	1:B:122:PRO:HD3	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:THR:OG1	1:A:240:GLU:HG2	2.20	0.42
1:A:187:ASP:CB	4:A:1268:HOH:O	2.68	0.42
1:A:244:GLN:HE21	1:A:244:GLN:CA	2.23	0.42
1:B:279:ARG:HG2	1:B:279:ARG:HH11	1.84	0.42
1:B:83:GLN:NE2	1:B:88:ARG:HD2	2.35	0.41
1:B:206:ALA:HB2	1:B:293:PRO:HG3	2.03	0.41
1:A:167:LEU:HB3	1:A:168:PRO:HD2	2.01	0.41
1:B:79:GLY:HA3	1:B:90:LYS:NZ	2.36	0.41
1:A:188:ARG:HG2	1:A:189:GLN:N	2.34	0.41
1:B:130:MET:HE1	1:B:182:TYR:CG	2.55	0.41
1:A:50:LEU:H	1:A:50:LEU:CD1	2.31	0.41
1:A:111:THR:HG22	1:A:129:ALA:HB2	2.03	0.41
1:A:163:HIS:HE1	1:A:172:HIS:HB3	1.85	0.41
1:B:63:ASN:O	1:B:77:VAL:HG11	2.21	0.40
1:B:233:VAL:O	1:B:236:LYS:HB3	2.21	0.40
1:B:180:LYS:HD3	4:B:1438:HOH:O	2.21	0.40
1:A:78:ILE:CD1	1:A:90:LYS:HE3	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ASN:OD1	4:A:1256:HOH:O[2_644]	2.07	0.13

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	303/306 (99%)	292 (96%)	9 (3%)	2 (1%)	18	8
1	B	304/306 (99%)	293 (96%)	11 (4%)	0	100	100
All	All	607/612 (99%)	585 (96%)	20 (3%)	2 (0%)	36	25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	154	TYR

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	262/263 (100%)	251 (96%)	11 (4%)	26	12
1	B	263/263 (100%)	255 (97%)	8 (3%)	36	21
All	All	525/526 (100%)	506 (96%)	19 (4%)	31	16

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	50	LEU
1	A	67	LEU
1	A	86	LEU
1	A	87	LEU
1	A	153	ASP
1	A	222	ARG
1	A	227	LEU
1	A	244	GLN
1	A	253	LEU
1	A	279	ARG
1	B	27	LEU
1	B	77	VAL
1	B	86	LEU
1	B	90	LYS
1	B	226	THR
1	B	253	LEU
1	B	268	LEU
1	B	304	THR

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	19	GLN
1	A	64	HIS
1	A	69	GLN
1	A	83	GLN
1	A	110	GLN
1	A	119	ASN
1	A	127	GLN
1	A	142	ASN
1	A	164	HIS
1	A	244	GLN
1	A	246	HIS
1	A	274	ASN
1	B	69	GLN
1	B	83	GLN
1	B	110	GLN
1	B	119	ASN
1	B	127	GLN
1	B	214	ASN
1	B	246	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](#)

6 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	$\# Z > 2$
3	DOZ	B	902	1	2,4,4	0.54	0	0,4,4	-	-
3	DOZ	A	901	1	2,4,4	0.17	0	0,4,4	-	-
2	DMS	A	803	-	3,3,3	0.31	0	3,3,3	3.29	3 (100%)
2	DMS	B	802	-	3,3,3	0.27	0	3,3,3	3.28	3 (100%)
2	DMS	A	813	-	3,3,3	0.29	0	3,3,3	3.28	3 (100%)
2	DMS	B	812	-	3,3,3	0.29	0	3,3,3	3.27	3 (100%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	803	DMS	C2-S-C1	4.25	120.19	98.42
2	A	813	DMS	C2-S-C1	4.21	119.99	98.42
2	B	802	DMS	C2-S-C1	4.17	119.79	98.42
2	B	812	DMS	C2-S-C1	4.16	119.76	98.42
2	A	803	DMS	O-S-C2	2.75	120.25	106.49
2	B	802	DMS	O-S-C2	2.73	120.15	106.49
2	B	812	DMS	O-S-C2	2.73	120.14	106.49
2	B	812	DMS	O-S-C1	2.72	120.10	106.49
2	B	802	DMS	O-S-C1	2.71	120.05	106.49
2	A	813	DMS	O-S-C2	2.71	120.05	106.49
2	A	813	DMS	O-S-C1	2.69	119.96	106.49
2	A	803	DMS	O-S-C1	2.61	119.56	106.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	DOZ	1	0
2	A	813	DMS	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, 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	305/306 (99%)	0.13	14 (4%)	37 40	14, 23, 45, 59	0
1	B	306/306 (100%)	0.04	10 (3%)	49 53	15, 25, 42, 54	0
All	All	611/612 (99%)	0.08	24 (3%)	43 47	14, 24, 44, 59	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	46	ALA	6.4
1	A	51	ASN	4.6
1	A	47	GLU	4.0
1	B	305	PHE	3.7
1	A	48	ASP	3.5
1	A	302	GLY	3.4
1	A	191	ALA	3.3
1	A	1	SER	2.8
1	A	294	PHE	2.8
1	A	45	THR	2.7
1	B	304	THR	2.7
1	A	153	ASP	2.5
1	B	154	TYR	2.5
1	B	294	PHE	2.5
1	B	303	VAL	2.5
1	B	74	GLN	2.4
1	A	49	MET	2.3
1	A	154	TYR	2.3
1	B	24	THR	2.3
1	B	47	GLU	2.2
1	A	2	GLY	2.2
1	B	191	ALA	2.1
1	B	46	ALA	2.1
1	A	24	THR	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	DMS	B	802	4/4	0.85	0.18	54,54,55,56	0
2	DMS	A	813	4/4	0.94	0.13	43,43,44,45	0
2	DMS	A	803	4/4	0.94	0.13	41,41,42,43	0
2	DMS	B	812	4/4	0.96	0.10	38,38,38,41	0
3	DOZ	A	901	5/5	0.98	0.13	36,39,40,40	0
3	DOZ	B	902	5/5	0.98	0.12	32,33,33,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.