



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:00 pm BST

PDB ID : 3E0Q
Title : Crystal structure of Schistosoma mansoni purine nucleoside phosphorylase complexed with a novel monocyclic inhibitor
Authors : Pereira, H.M.; Berdini, V.; Ferri, M.R.; Cleasby, A.; Garratt, R.C.
Deposited on : 2008-07-31
Resolution : 1.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

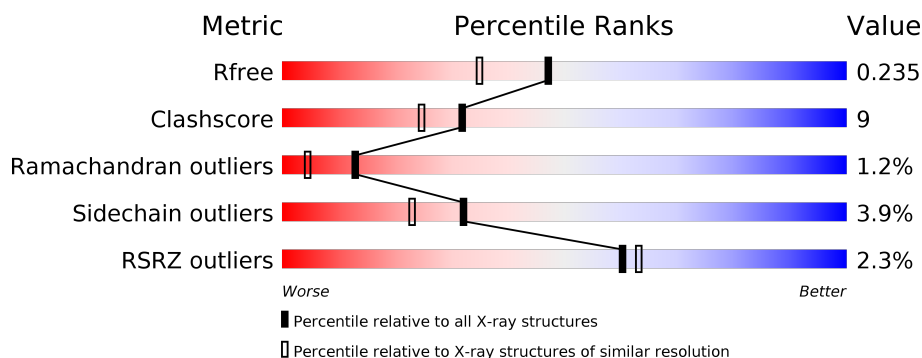
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	287	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>••</div> </div> </div>
1	B	287	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>16%</div> <div>•• 7%</div> </div> </div>
1	C	287	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>16%</div> <div>•</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	JFD	B	401	-	X	-	-
3	JFD	C	402	-	X	-	-

2 Entry composition [i](#)

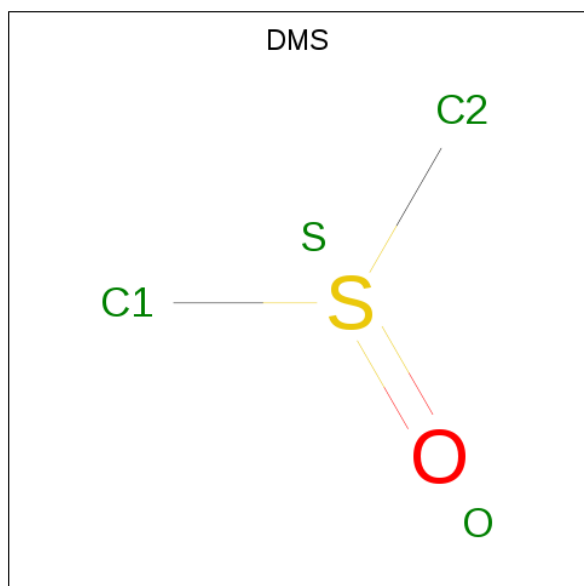
There are 4 unique types of molecules in this entry. The entry contains 6940 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Purine-nucleoside phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2128	1357	365	392	14			
1	B	266	Total	C	N	O	S	27	1	0
			2025	1294	347	369	15			
1	C	285	Total	C	N	O	S	0	0	0
			2157	1374	372	397	14			

- Molecule 2 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



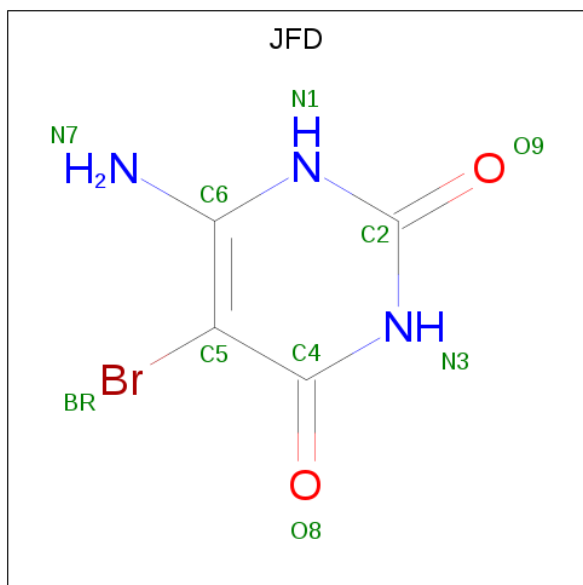
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is 6-amino-5-bromo-1,2,3,4-tetrahydropyrimidine-2,4-dione (three-letter code: JFD) (formula: C₄H₄BrN₃O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	Br	C	N	O	0	0
			10	1	4	3	2		
3	B	1	Total	Br	C	N	O	0	0
			10	1	4	3	2		
3	C	1	Total	Br	C	N	O	0	0
			10	1	4	3	2		

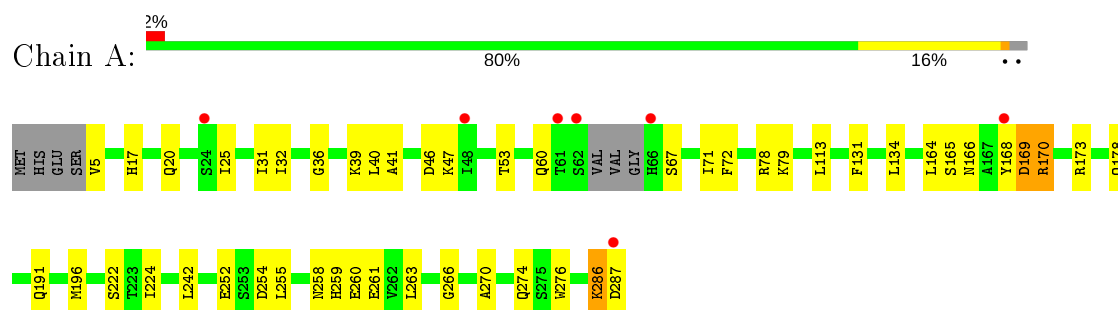
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	196	Total	O	0	0
			196	196		
4	B	180	Total	O	0	0
			180	180		
4	C	208	Total	O	0	0
			208	208		

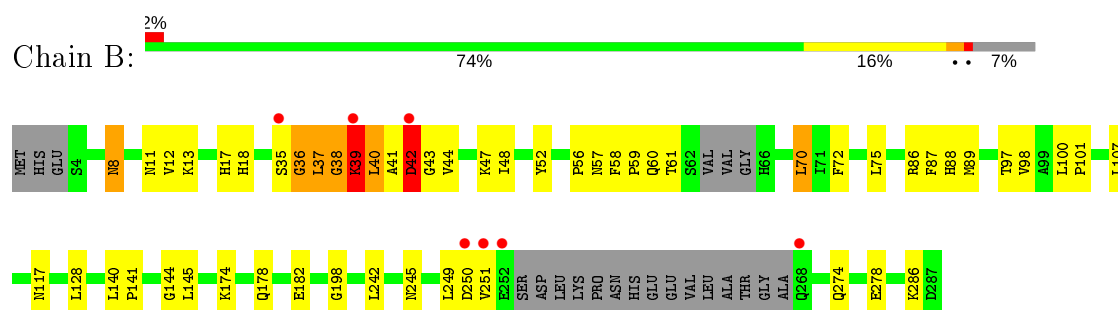
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

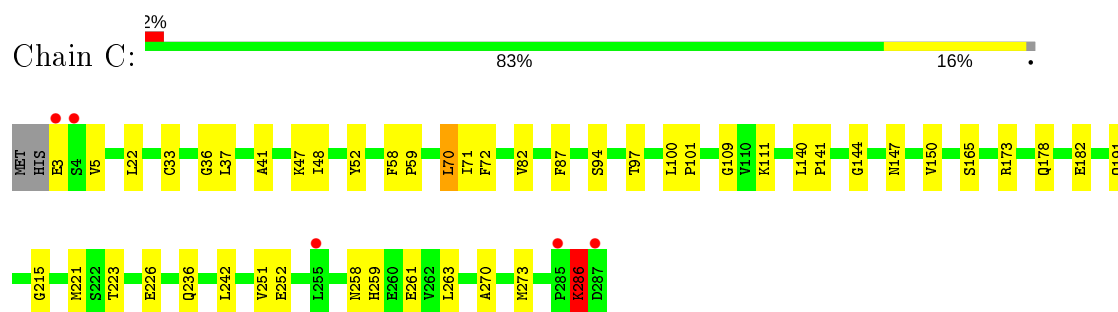
• Molecule 1: Purine-nucleoside phosphorylase



• Molecule 1: Purine-nucleoside phosphorylase



• Molecule 1: Purine-nucleoside phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.85Å 120.02Å 131.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.32 – 1.90 44.31 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.9 (44.32-1.90) 93.9 (44.31-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 1.89Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.179 , 0.236 0.179 , 0.235	Depositor DCC
R_{free} test set	2853 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6940	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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: DMS, JFD

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	0.42	0/2164	0.56	0/2929
1	B	0.37	0/2061	0.57	0/2786
1	C	0.40	0/2195	0.56	0/2973
All	All	0.40	0/6420	0.57	0/8688

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	1	6

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	37	LEU	CA

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	36	GLY	Peptide
1	B	37	LEU	Peptide
1	B	38	GLY	Peptide
1	B	39	LYS	Peptide
1	B	40	LEU	Peptide
1	B	42	ASP	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	2128	0	2181	36	1
1	B	2025	0	2077	43	1
1	C	2157	0	2207	34	0
2	A	8	0	12	1	0
2	B	4	0	6	0	0
2	C	4	0	6	0	0
3	A	10	0	4	1	0
3	B	10	0	4	1	0
3	C	10	0	4	1	0
4	A	196	0	0	8	0
4	B	180	0	0	3	0
4	C	208	0	0	4	0
All	All	6940	0	6501	114	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 9.

All (114) 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:C:59:PRO:HB3	1:C:97:THR:HG23	1.60	0.83
1:B:12:VAL:HG12	1:B:107:LEU:HD22	1.63	0.80
1:A:173:ARG:HH11	1:A:191:GLN:HE22	1.29	0.79
1:B:13:LYS:NZ	1:B:17:HIS:HE1	1.82	0.77
3:B:401:JFD:O9	4:B:474:HOH:O	2.03	0.76
1:A:134:LEU:HD23	1:A:168:TYR:OH	1.88	0.73
1:A:53:THR:HA	1:A:60:GLN:HE22	1.55	0.72
1:C:48:ILE:HA	4:C:552:HOH:O	1.92	0.70
1:B:42:ASP:OD2	1:B:42:ASP:C	2.30	0.69
1:C:173:ARG:HH11	1:C:191:GLN:HE22	1.40	0.69
1:C:236:GLN:HG3	4:C:474:HOH:O	1.94	0.67
1:A:258:ASN:HD22	1:A:261:GLU:H	1.41	0.66
1:A:173:ARG:HH11	1:A:191:GLN:NE2	1.94	0.66
1:B:52:TYR:HE1	1:B:70:LEU:HD13	1.60	0.66
1:A:196:MET:HB2	1:A:224:ILE:HD12	1.76	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ILE:HG23	1:A:79:LYS:HD2	1.79	0.65
1:B:8:ASN:ND2	1:B:11:ASN:H	1.95	0.64
1:A:168:TYR:O	1:A:169:ASP:C	2.34	0.64
1:C:3:GLU:HA	1:C:94:SER:CB	2.27	0.64
1:C:59:PRO:HB2	1:C:87:PHE:CE1	2.32	0.63
1:A:32:ILE:HG13	1:A:113:LEU:HD11	1.82	0.62
1:B:35:SER:HB3	1:B:117:ASN:C	2.21	0.61
1:C:173:ARG:HH11	1:C:191:GLN:NE2	1.99	0.60
1:C:37:LEU:HD23	1:C:273:MET:HG2	1.84	0.60
1:A:41:ALA:HB1	1:A:71:ILE:HD13	1.85	0.59
1:C:258:ASN:HD21	1:C:261:GLU:HG3	1.68	0.58
1:B:13:LYS:HZ1	1:B:17:HIS:HE1	1.51	0.58
1:B:39:LYS:CA	1:B:42:ASP:HB2	2.32	0.58
1:B:128:LEU:HD21	1:B:245:ASN:HA	1.86	0.58
1:A:165:SER:HB3	4:A:474:HOH:O	2.05	0.57
1:A:166:ASN:HD21	1:A:170:ARG:H	1.53	0.57
1:B:13:LYS:HZ2	1:B:17:HIS:HE1	1.53	0.56
1:C:178:GLN:OE1	1:C:182:GLU:HG3	2.05	0.56
1:A:78:ARG:HD3	1:A:286:LYS:NZ	2.21	0.56
1:A:78:ARG:CD	1:A:286:LYS:NZ	2.70	0.55
1:A:78:ARG:CD	1:A:286:LYS:HZ3	2.20	0.55
1:A:78:ARG:HD3	4:A:471:HOH:O	2.07	0.54
1:C:221:MET:HE2	3:C:402:JFD:BR	2.63	0.54
1:B:8:ASN:C	1:B:8:ASN:HD22	2.12	0.53
1:C:173:ARG:HD2	1:C:191:GLN:NE2	2.24	0.53
1:A:274:GLN:HB2	4:A:542:HOH:O	2.08	0.53
1:C:47:LYS:HA	1:C:72:PHE:O	2.09	0.53
2:A:301:DMS:O	1:B:144:GLY:HA3	2.09	0.52
1:C:33:CYS:SG	1:C:41:ALA:HB2	2.49	0.52
1:A:173:ARG:HD2	1:A:191:GLN:NE2	2.25	0.52
1:B:39:LYS:HA	1:B:42:ASP:HB2	1.91	0.52
1:C:3:GLU:HA	1:C:94:SER:HB3	1.90	0.51
1:B:48:ILE:HG13	4:B:521:HOH:O	2.10	0.51
1:B:52:TYR:CE1	1:B:70:LEU:HD13	2.43	0.51
1:C:58:PHE:CD2	1:C:59:PRO:HD2	2.46	0.51
1:A:178:GLN:HG3	4:A:539:HOH:O	2.11	0.50
4:A:413:HOH:O	1:B:145:LEU:HA	2.12	0.50
1:C:37:LEU:CD2	1:C:273:MET:HG2	2.41	0.50
1:A:168:TYR:O	1:A:169:ASP:O	2.30	0.50
1:B:42:ASP:O	1:B:42:ASP:OD2	2.30	0.49
1:B:86:ARG:HD3	1:B:88:HIS:CE1	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:PHE:CG	1:B:59:PRO:HD2	2.47	0.49
1:B:59:PRO:HB2	1:B:87:PHE:CE1	2.47	0.49
1:C:59:PRO:HD3	1:C:100:LEU:HD22	1.95	0.48
1:B:274:GLN:O	1:B:278:GLU:HG3	2.13	0.48
1:A:134:LEU:HD23	1:A:168:TYR:CZ	2.48	0.48
1:A:39:LYS:HB2	4:A:542:HOH:O	2.14	0.48
1:B:140:LEU:HB2	1:B:141:PRO:HD3	1.96	0.47
1:B:47:LYS:O	1:B:48:ILE:HD13	2.14	0.47
1:B:59:PRO:HB2	1:B:87:PHE:CZ	2.49	0.47
1:C:259:HIS:CD2	1:C:263:LEU:HD11	2.49	0.47
1:C:59:PRO:HB2	1:C:87:PHE:CZ	2.50	0.47
1:B:39:LYS:HA	1:B:42:ASP:CA	2.45	0.47
1:B:18:HIS:CE1	1:B:56:PRO:HD3	2.50	0.47
1:C:215:GLY:HA2	4:C:579:HOH:O	2.14	0.47
1:C:36:GLY:O	1:C:270:ALA:HA	2.15	0.46
1:A:258:ASN:HD21	1:A:260:GLU:HB2	1.80	0.46
1:C:147:ASN:HB3	1:C:150:VAL:HG23	1.96	0.46
1:A:78:ARG:HD2	1:A:286:LYS:NZ	2.30	0.46
1:B:39:LYS:HB3	1:B:274:GLN:HE22	1.80	0.45
1:B:13:LYS:HA	1:B:107:LEU:HD23	1.98	0.45
1:A:131:PHE:CD2	1:A:276:TRP:CZ3	3.04	0.45
1:A:17:HIS:HD2	1:A:20:GLN:HE22	1.64	0.45
1:B:13:LYS:HZ2	1:B:17:HIS:CE1	2.33	0.44
1:C:100:LEU:HB3	1:C:101:PRO:HD3	1.99	0.44
1:A:41:ALA:CB	1:A:71:ILE:HD13	2.47	0.44
1:B:42:ASP:HB3	1:B:274:GLN:OE1	2.17	0.44
1:B:198:GLY:HA3	1:C:144:GLY:O	2.19	0.43
1:B:39:LYS:CB	1:B:42:ASP:HB2	2.48	0.43
1:A:222:SER:HB2	4:A:536:HOH:O	2.17	0.43
1:A:259:HIS:O	1:A:263:LEU:HG	2.19	0.43
1:A:242:LEU:CD2	1:A:266:GLY:HA2	2.49	0.43
3:A:400:JFD:O9	4:A:455:HOH:O	2.21	0.43
1:A:78:ARG:HD3	1:A:286:LYS:HZ3	1.80	0.43
1:A:36:GLY:O	1:A:270:ALA:HA	2.18	0.42
1:A:47:LYS:HA	1:A:72:PHE:O	2.19	0.42
1:B:128:LEU:CD2	1:B:245:ASN:HA	2.48	0.42
1:B:286:LYS:HE3	4:B:493:HOH:O	2.19	0.42
1:B:39:LYS:HB3	1:B:42:ASP:HB2	2.01	0.42
1:C:109:GLY:O	1:C:111:LYS:HE2	2.20	0.42
1:B:59:PRO:HB3	1:B:97:THR:HG23	2.00	0.42
1:C:140:LEU:HB2	1:C:141:PRO:HD3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:ASN:HB2	4:C:476:HOH:O	2.18	0.42
1:B:39:LYS:HA	1:B:42:ASP:CB	2.49	0.42
1:C:223:THR:HA	1:C:226:GLU:OE2	2.19	0.42
1:C:52:TYR:HE1	1:C:70:LEU:HD13	1.85	0.42
1:C:286:LYS:HA	1:C:286:LYS:HE3	2.01	0.41
1:A:78:ARG:HD2	1:A:286:LYS:HZ3	1.84	0.41
1:B:47:LYS:HA	1:B:72:PHE:O	2.20	0.41
1:B:89:MET:SD	1:B:98:VAL:HG21	2.61	0.41
1:C:252:GLU:OE1	1:C:252:GLU:HA	2.21	0.41
1:B:39:LYS:HA	1:B:42:ASP:HA	2.03	0.41
1:A:131:PHE:CE1	1:A:242:LEU:HD13	2.55	0.41
1:B:100:LEU:N	1:B:101:PRO:CD	2.84	0.41
1:C:140:LEU:HA	1:C:140:LEU:HD23	1.92	0.41
1:C:71:ILE:HB	1:C:82:VAL:HB	2.03	0.41
1:A:31:ILE:HG21	1:A:40:LEU:CD2	2.52	0.40
1:B:100:LEU:HB3	1:B:101:PRO:HD3	2.04	0.40
1:B:178:GLN:O	1:B:182:GLU:HG3	2.21	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:A:287:ASP:OD1	1:B:174:LYS:NZ[2_554]	1.93	0.27

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	276/287 (96%)	270 (98%)	4 (1%)	2 (1%)	22	12
1	B	261/287 (91%)	248 (95%)	6 (2%)	7 (3%)	5	1
1	C	283/287 (99%)	272 (96%)	10 (4%)	1 (0%)	34	24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	820/861 (95%)	790 (96%)	20 (2%)	10 (1%)	13	4

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	36	GLY
1	B	39	LYS
1	B	40	LEU
1	B	41	ALA
1	A	67	SER
1	A	169	ASP
1	C	286	LYS
1	B	43	GLY
1	B	37	LEU
1	B	38	GLY

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	234/242 (97%)	226 (97%)	8 (3%)	37	28
1	B	222/242 (92%)	210 (95%)	12 (5%)	22	13
1	C	237/242 (98%)	230 (97%)	7 (3%)	41	33
All	All	693/726 (96%)	666 (96%)	27 (4%)	32	23

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	46	ASP
1	A	164	LEU
1	A	170	ARG
1	A	252	GLU
1	A	254	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	255	LEU
1	A	286	LYS
1	B	8	ASN
1	B	42	ASP
1	B	44	VAL
1	B	57	ASN
1	B	60	GLN
1	B	61	THR
1	B	70	LEU
1	B	75	LEU
1	B	242	LEU
1	B	249	LEU
1	B	250	ASP
1	B	251	VAL
1	C	5	VAL
1	C	22	LEU
1	C	70	LEU
1	C	165	SER
1	C	242	LEU
1	C	251	VAL
1	C	286	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	18	HIS
1	A	20	GLN
1	A	60	GLN
1	A	166	ASN
1	A	191	GLN
1	A	236	GLN
1	A	258	ASN
1	A	259	HIS
1	A	268	GLN
1	B	8	ASN
1	B	17	HIS
1	B	20	GLN
1	B	88	HIS
1	B	183	ASN
1	C	20	GLN
1	C	146	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	183	ASN
1	C	191	GLN
1	C	258	ASN
1	C	274	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

7 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	JFD	A	400	-	8,10,10	6.00	8 (100%)	5,14,14	3.12	1 (20%)
2	DMS	B	302	-	3,3,3	2.38	1 (33%)	3,3,3	0.30	0
2	DMS	C	303	-	3,3,3	2.43	1 (33%)	3,3,3	0.38	0
3	JFD	B	401	-	8,10,10	5.90	7 (87%)	5,14,14	4.73	3 (60%)
2	DMS	A	300	-	3,3,3	2.46	1 (33%)	3,3,3	0.26	0
3	JFD	C	402	-	8,10,10	6.21	8 (100%)	5,14,14	2.60	3 (60%)
2	DMS	A	301	-	3,3,3	2.59	1 (33%)	3,3,3	0.48	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
3	JFD	A	400	-	-	-	0/1/1/1
3	JFD	B	401	-	-	-	0/1/1/1
3	JFD	C	402	-	-	-	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	JFD	C4-C5	10.79	1.52	1.38
3	A	400	JFD	C4-C5	10.57	1.52	1.38
3	C	402	JFD	C6-N1	8.46	1.47	1.35
3	B	401	JFD	C6-N1	8.37	1.47	1.35
3	A	400	JFD	C6-N1	8.36	1.47	1.35
3	B	401	JFD	C4-C5	8.10	1.48	1.38
3	C	402	JFD	C4-N3	6.80	1.44	1.33
3	B	401	JFD	C2-N1	6.08	1.50	1.38
3	B	401	JFD	C2-N3	5.87	1.49	1.38
3	B	401	JFD	C4-N3	5.83	1.43	1.33
3	A	400	JFD	C2-N3	5.62	1.49	1.38
3	A	400	JFD	C2-N1	5.47	1.49	1.38
3	C	402	JFD	C2-N1	5.20	1.48	1.38
3	B	401	JFD	O8-C4	4.95	1.37	1.24
3	A	400	JFD	C4-N3	4.58	1.41	1.33
3	C	402	JFD	C2-N3	4.56	1.47	1.38
2	A	301	DMS	O-S	4.36	1.79	1.50
2	A	300	DMS	O-S	4.11	1.78	1.50
2	C	303	DMS	O-S	4.02	1.77	1.50
2	B	302	DMS	O-S	3.93	1.76	1.50
3	B	401	JFD	C6-N7	3.36	1.42	1.34
3	C	402	JFD	C6-N7	3.24	1.42	1.34
3	C	402	JFD	O8-C4	3.10	1.32	1.24
3	A	400	JFD	C6-N7	3.06	1.41	1.34
3	A	400	JFD	O8-C4	3.04	1.32	1.24
3	C	402	JFD	BR-C5	2.52	1.95	1.89
3	A	400	JFD	BR-C5	2.34	1.95	1.89

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	JFD	C4-N3-C2	8.55	122.36	115.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	400	JFD	C4-N3-C2	6.27	120.43	115.14
3	B	401	JFD	C5-C4-N3	-4.67	118.29	123.72
3	B	401	JFD	BR-C5-C4	-4.11	115.12	121.48
3	C	402	JFD	N7-C6-N1	3.50	121.98	117.03
3	C	402	JFD	C2-N1-C6	3.47	120.20	116.02
3	C	402	JFD	C4-N3-C2	2.73	117.45	115.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	400	JFD	1	0
3	B	401	JFD	1	0
3	C	402	JFD	1	0
2	A	301	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	280/287 (97%)	-0.15	7 (2%) 57 60	8, 16, 37, 58	0
1	B	261/287 (90%)	-0.05	7 (2%) 54 57	8, 18, 41, 59	1 (0%)
1	C	285/287 (99%)	-0.23	5 (1%) 68 71	8, 16, 37, 54	0
All	All	826/861 (95%)	-0.15	19 (2%) 60 63	8, 16, 40, 59	1 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	39	LYS	8.5
1	A	62	SER	5.9
1	B	42	ASP	5.6
1	C	287	ASP	4.7
1	B	35	SER	4.4
1	A	168	TYR	4.4
1	C	255	LEU	3.8
1	C	4	SER	3.4
1	B	268	GLN	3.3
1	A	66	HIS	3.3
1	C	3	GLU	3.1
1	A	61	THR	3.1
1	C	285	PRO	3.1
1	A	287	ASP	2.9
1	B	252	GLU	2.7
1	B	250	ASP	2.4
1	A	48	ILE	2.2
1	A	24	SER	2.1
1	B	251	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	JFD	C	402	10/10	0.89	0.20	9,14,21,32	10
3	JFD	B	401	10/10	0.90	0.17	10,19,26,34	10
2	DMS	A	301	4/4	0.92	0.14	18,18,36,47	0
3	JFD	A	400	10/10	0.93	0.16	11,14,20,36	10
2	DMS	C	303	4/4	0.98	0.10	10,12,13,13	0
2	DMS	B	302	4/4	0.98	0.09	8,12,12,15	0
2	DMS	A	300	4/4	0.99	0.10	9,10,11,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.