



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2025 – 02:12 AM JST

PDB ID : 7VUF / pdb\_00007vuf  
Title : Crystal Structure of the core region of Thermus thermophilus MutS2.  
Authors : Fukui, K.; Yano, T.  
Deposited on : 2021-11-02  
Resolution : 3.11 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](mailto: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>.

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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) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

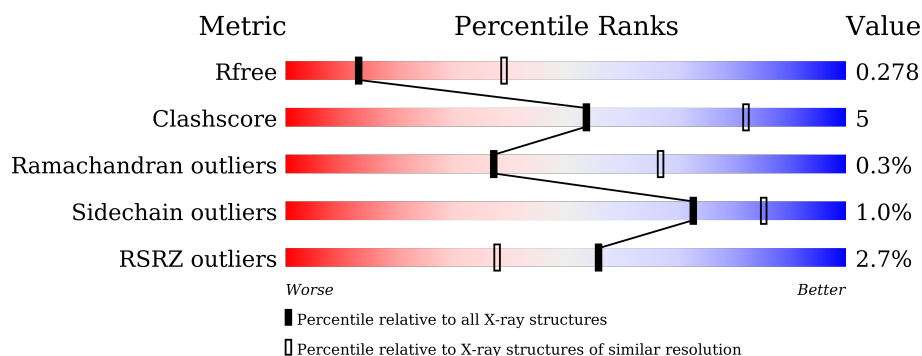
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.11 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1668 (3.14-3.10)
Clashscore	180529	1788 (3.14-3.10)
Ramachandran outliers	177936	1696 (3.14-3.10)
Sidechain outliers	177891	1696 (3.14-3.10)
RSRZ outliers	164620	1668 (3.14-3.10)

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  $\geq 3$ , 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	488	 3% 80% 14% • 5%
1	B	488	 2% 84% 11% • •
1	C	488	 2% 83% 13% • •
1	D	488	 3% 81% 13% • 5%

## 2 Entry composition [i](#)

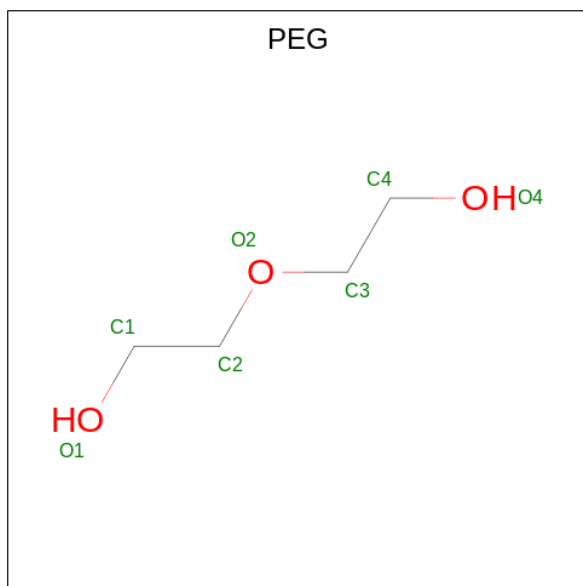
There are 4 unique types of molecules in this entry. The entry contains 14442 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Endonuclease MutS2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	471	Total	C	N	O	S	0	0	0
			3584	2269	642	665	8			
1	A	462	Total	C	N	O	S	0	0	0
			3541	2246	635	651	9			
1	C	473	Total	C	N	O	S	0	0	0
			3624	2296	646	673	9			
1	D	463	Total	C	N	O	S	0	0	0
			3536	2231	643	653	9			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total Mg 1 1	0	0

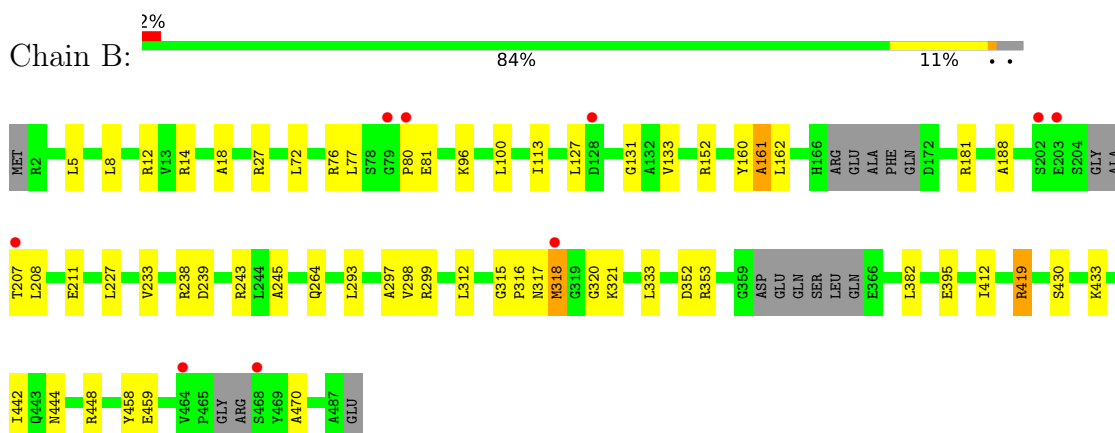
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	22	Total O 22 22	0	0
4	A	35	Total O 35 35	0	0
4	C	31	Total O 31 31	0	0
4	D	19	Total O 19 19	0	0

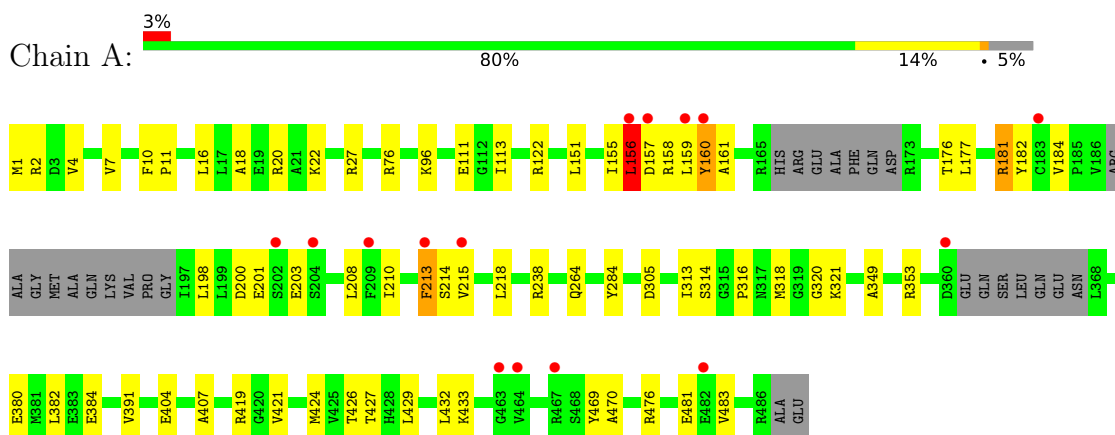
### 3 Residue-property plots [i](#)

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.

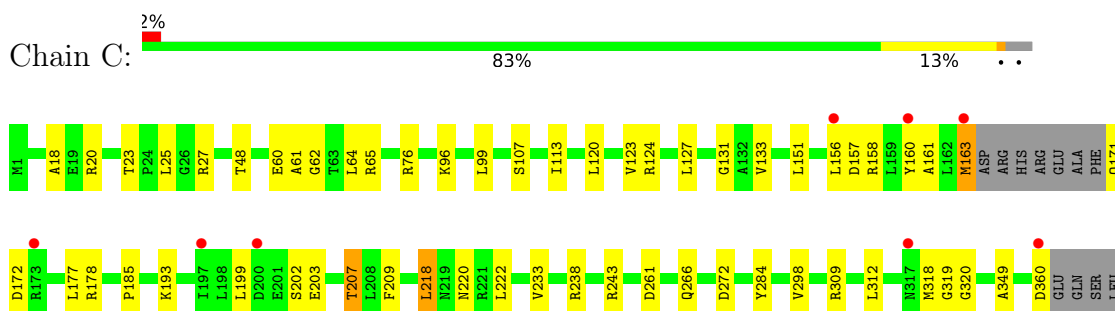
#### • Molecule 1: Endonuclease MutS2



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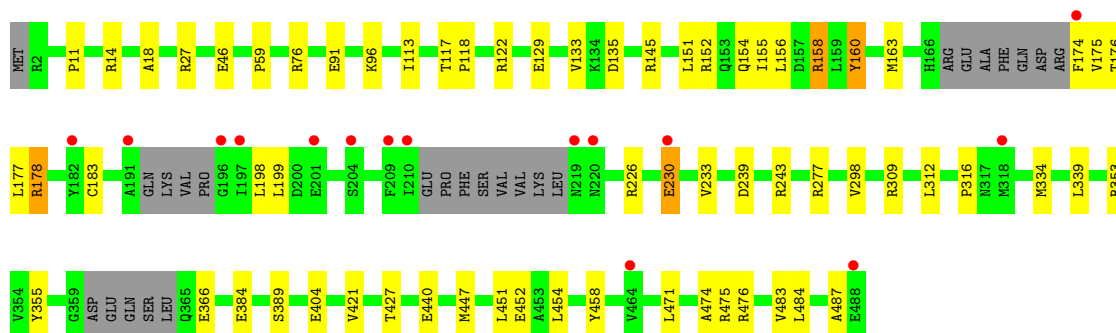
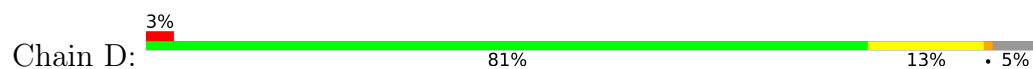


#### • Molecule 1: Endonuclease MutS2





● Molecule 1: Endonuclease MutS2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.48Å 114.21Å 292.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.89 – 3.11 40.89 – 3.11	Depositor EDS
% Data completeness (in resolution range)	94.0 (40.89-3.11) 94.0 (40.89-3.11)	Depositor EDS
$R_{merge}$	0.27	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.77 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.19.2	Depositor
R, $R_{free}$	0.225 , 0.279 0.226 , 0.278	Depositor DCC
$R_{free}$ test set	2767 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.1	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 34.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	14442	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, PEG

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	0.24	0/3591	0.52	0/4854
1	B	0.24	0/3633	0.49	0/4915
1	C	0.24	0/3675	0.51	0/4966
1	D	0.24	0/3584	0.52	0/4837
All	All	0.24	0/14483	0.51	0/19572

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10
1	B	0	5
1	C	0	14
1	D	0	11
All	All	0	40

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (40) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	LEU	Peptide
1	A	157	ASP	Peptide
1	A	160	TYR	Peptide
1	A	181	ARG	Peptide
1	A	198	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	A	200	ASP	Peptide
1	A	201	GLU	Peptide
1	A	208	LEU	Peptide
1	A	215	VAL	Peptide
1	A	469	TYR	Peptide
1	B	315	GLY	Peptide
1	B	316	PRO	Peptide
1	B	318	MET	Peptide
1	B	77	LEU	Peptide
1	B	80	PRO	Peptide
1	C	157	ASP	Peptide
1	C	172	ASP	Peptide
1	C	193	LYS	Peptide
1	C	199	LEU	Peptide
1	C	207	THR	Peptide
1	C	218	LEU	Peptide
1	C	220	ASN	Peptide
1	C	319	GLY	Peptide
1	C	367	ASN	Peptide
1	C	457	THR	Peptide
1	C	458	TYR	Peptide
1	C	485	LYS	Peptide
1	C	60	GLU	Peptide
1	C	62	GLY	Peptide
1	D	129	GLU	Peptide
1	D	158	ARG	Peptide
1	D	160	TYR	Peptide
1	D	163	MET	Peptide
1	D	174	PHE	Peptide
1	D	175	VAL	Peptide
1	D	198	LEU	Peptide
1	D	230	GLU	Peptide
1	D	316	PRO	Peptide
1	D	366	GLU	Peptide
1	D	474	ALA	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	3541	0	3625	38	0
1	B	3584	0	3641	33	0
1	C	3624	0	3714	35	0
1	D	3536	0	3592	36	0
2	A	14	0	20	1	0
2	B	28	0	40	0	0
2	C	7	0	10	2	0
3	C	1	0	0	0	0
4	A	35	0	0	1	0
4	B	22	0	0	1	0
4	C	31	0	0	1	0
4	D	19	0	0	1	0
All	All	14442	0	14642	138	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (138) 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:156:LEU:HA	1:A:158:ARG:H	1.47	0.79
1:B:318:MET:H	1:B:321:LYS:HE2	1.48	0.78
1:A:427:THR:HG22	1:A:429:LEU:H	1.47	0.77
1:A:321:LYS:HE2	1:A:426:THR:HB	1.72	0.72
1:D:152:ARG:HH21	1:D:226:ARG:HH21	1.41	0.68
1:C:202:SER:HB3	1:C:207:THR:HA	1.77	0.67
1:B:318:MET:HG2	1:B:320:GLY:H	1.62	0.64
1:B:160:TYR:HA	1:B:162:LEU:N	2.13	0.64
1:D:230:GLU:HA	1:D:233:VAL:HB	1.80	0.64
1:C:151:LEU:HD11	1:C:218:LEU:HB2	1.79	0.64
1:A:353:ARG:NH2	1:A:380:GLU:OE2	2.31	0.62
1:B:382:LEU:O	1:B:419:ARG:NH2	2.31	0.62
1:A:353:ARG:NH1	1:A:384:GLU:OE1	2.34	0.61
1:B:12:ARG:HD2	1:B:293:LEU:HD13	1.81	0.61
1:A:155:ILE:HG12	1:A:218:LEU:HD13	1.83	0.60
1:A:320:GLY:H	2:A:502:PEG:H31	1.66	0.60
1:A:404:GLU:HG2	1:D:471:LEU:HD23	1.84	0.60
1:C:298:VAL:HG21	1:C:458:TYR:HB2	1.84	0.59
1:D:353:ARG:NH2	1:D:384:GLU:O	2.36	0.58
1:C:309:ARG:NH1	1:C:417:LEU:O	2.36	0.58
1:D:155:ILE:HA	1:D:158:ARG:HB2	1.84	0.58
1:D:309:ARG:NH2	1:D:440:GLU:OE2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ALA:HA	1:B:208:LEU:HD12	1.87	0.56
1:A:96:LYS:HD2	1:A:113:ILE:HB	1.86	0.56
1:C:61:ALA:HA	1:C:64:LEU:HB3	1.86	0.56
1:D:46:GLU:HA	1:D:277:ARG:HH22	1.70	0.56
1:B:181:ARG:NH2	1:B:211:GLU:OE2	2.38	0.56
1:B:448:ARG:NH2	1:B:459:GLU:OE1	2.38	0.56
1:A:470:ALA:HB3	1:D:404:GLU:HG2	1.88	0.55
1:D:353:ARG:NE	1:D:355:TYR:OH	2.38	0.55
1:A:18:ALA:HB1	1:A:27:ARG:HG3	1.89	0.54
1:C:20:ARG:NH1	1:C:272:ASP:OD2	2.41	0.54
1:D:452:GLU:O	1:D:476:ARG:NH2	2.33	0.54
1:B:297:ALA:O	1:B:299:ARG:NH1	2.40	0.54
1:D:176:THR:OG1	1:D:177:LEU:N	2.41	0.53
1:A:382:LEU:HD13	1:D:483:VAL:HG21	1.90	0.52
1:A:76:ARG:NH2	4:A:603:HOH:O	2.42	0.52
1:D:298:VAL:HG21	1:D:458:TYR:HB2	1.93	0.51
1:C:96:LYS:HD2	1:C:113:ILE:HB	1.93	0.51
1:C:320:GLY:H	2:C:501:PEG:H22	1.75	0.51
1:B:8:LEU:HD12	1:B:333:LEU:HD22	1.93	0.51
1:D:239:ASP:OD2	1:D:243:ARG:NH1	2.44	0.51
1:B:127:LEU:HD13	1:B:131:GLY:HA2	1.93	0.51
1:A:159:LEU:HB3	1:A:161:ALA:H	1.77	0.50
1:B:433:LYS:O	1:B:444:ASN:ND2	2.41	0.50
1:C:18:ALA:HB1	1:C:27:ARG:HG3	1.93	0.50
1:C:99:LEU:O	1:C:107:SER:OG	2.28	0.50
1:A:391:VAL:HG13	1:A:421:VAL:HG11	1.93	0.50
1:C:163:MET:HA	1:C:171:GLN:HE21	1.77	0.49
1:A:427:THR:HG21	1:A:432:LEU:HD12	1.95	0.49
1:A:481:GLU:C	1:A:483:VAL:H	2.16	0.49
1:B:133:VAL:HG21	1:B:233:VAL:HG13	1.95	0.48
1:D:475:ARG:HG3	1:D:484:LEU:HD13	1.95	0.48
1:B:96:LYS:HE2	1:B:100:LEU:HD11	1.96	0.48
1:B:318:MET:HA	1:B:321:LYS:HG3	1.95	0.48
1:D:451:LEU:O	1:D:476:ARG:NH1	2.46	0.48
1:B:207:THR:HG22	1:B:208:LEU:HG	1.96	0.48
1:C:76:ARG:HG3	1:C:238:ARG:HB2	1.96	0.48
1:B:152:ARG:NH1	4:B:603:HOH:O	2.38	0.48
1:B:382:LEU:HD21	1:B:412:ILE:HG23	1.96	0.48
1:A:76:ARG:HG3	1:A:238:ARG:HB2	1.96	0.48
1:D:243:ARG:NH2	4:D:503:HOH:O	2.46	0.47
1:C:185:PRO:HB3	1:C:209:PHE:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:ARG:NH2	1:D:226:ARG:HH21	2.11	0.47
1:A:177:LEU:HD12	1:A:182:TYR:HA	1.97	0.47
1:A:284:TYR:CZ	1:A:349:ALA:HB3	2.49	0.47
1:A:313:ILE:HG22	1:A:321:LYS:HE3	1.97	0.47
1:C:48:THR:OG1	1:C:266:GLN:NE2	2.48	0.47
1:D:183:CYS:HB2	1:D:199:LEU:HA	1.96	0.47
1:D:389:SER:HB2	1:D:421:VAL:HG23	1.97	0.47
1:D:96:LYS:HD2	1:D:113:ILE:HB	1.96	0.47
1:C:185:PRO:HB3	1:C:209:PHE:HE1	1.79	0.46
1:A:96:LYS:HE3	1:A:111:GLU:HA	1.96	0.46
1:C:367:ASN:O	1:C:370:THR:N	2.48	0.46
1:D:151:LEU:O	1:D:155:ILE:HG23	2.16	0.46
1:C:127:LEU:HD12	1:C:131:GLY:HA2	1.97	0.46
1:C:318:MET:O	1:C:320:GLY:N	2.49	0.46
1:C:360:ASP:N	1:C:360:ASP:OD1	2.49	0.46
1:A:407:ALA:HB1	1:D:487:ALA:HB1	1.98	0.45
1:C:218:LEU:HD23	1:C:218:LEU:H	1.82	0.45
1:C:452:GLU:O	1:C:476:ARG:NH2	2.43	0.45
1:B:430:SER:O	1:B:433:LYS:HG2	2.16	0.45
1:C:177:LEU:O	1:C:178:ARG:NH1	2.46	0.45
1:D:18:ALA:HB1	1:D:27:ARG:HG3	1.98	0.45
1:C:123:VAL:HG13	1:C:127:LEU:HD21	1.98	0.45
1:D:152:ARG:O	1:D:156:LEU:HD23	2.17	0.45
1:B:72:LEU:HD23	1:B:245:ALA:HB1	1.98	0.44
1:B:312:LEU:HB2	1:B:442:ILE:HD11	2.00	0.44
1:D:454:LEU:HG	1:D:476:ARG:NH1	2.32	0.44
1:C:120:LEU:O	1:C:124:ARG:HG2	2.18	0.44
1:C:23:THR:OG1	1:C:261:ASP:OD2	2.29	0.44
1:A:314:SER:HB2	1:A:433:LYS:HB3	1.99	0.44
1:C:312:LEU:O	1:C:445:ALA:N	2.50	0.44
1:B:430:SER:HA	1:B:433:LYS:HE3	2.00	0.43
1:A:203:GLU:CB	1:A:213:PHE:HB2	2.47	0.43
1:D:312:LEU:HD11	1:D:427:THR:HG22	2.00	0.43
1:B:317:ASN:ND2	1:B:395:GLU:OE2	2.52	0.43
1:A:181:ARG:HD3	1:A:213:PHE:CZ	2.53	0.43
1:B:18:ALA:O	1:B:27:ARG:NH1	2.51	0.43
1:B:239:ASP:O	1:B:243:ARG:HG2	2.18	0.43
1:B:298:VAL:HG11	1:B:458:TYR:HB2	2.01	0.43
1:B:96:LYS:HD2	1:B:113:ILE:HB	2.00	0.43
1:C:133:VAL:HG21	1:C:233:VAL:HG13	2.00	0.43
1:D:176:THR:HG21	1:D:178:ARG:HH21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:ARG:NH2	4:C:605:HOH:O	2.51	0.42
1:D:59:PRO:HB3	1:D:91:GLU:HB2	2.00	0.42
1:B:160:TYR:N	1:B:161:ALA:HB3	2.35	0.42
1:A:4:VAL:HA	1:A:7:VAL:HG12	2.01	0.42
1:A:151:LEU:HD11	1:A:218:LEU:HB2	2.01	0.42
1:A:316:PRO:O	1:A:318:MET:HG2	2.19	0.42
1:C:284:TYR:CZ	1:C:349:ALA:HB3	2.55	0.42
1:A:476:ARG:O	1:A:476:ARG:NH1	2.52	0.42
1:B:227:LEU:HD23	1:B:227:LEU:HA	1.86	0.42
1:D:135:ASP:OD1	1:D:145:ARG:NH1	2.51	0.42
1:A:419:ARG:HB3	1:A:421:VAL:HG23	2.02	0.42
1:D:11:PRO:HA	1:D:14:ARG:HD2	2.02	0.41
1:D:117:THR:N	1:D:118:PRO:HD2	2.35	0.41
1:B:76:ARG:HB2	1:B:238:ARG:NH2	2.35	0.41
1:A:160:TYR:CG	1:A:160:TYR:O	2.73	0.41
1:C:222:LEU:HD13	1:C:222:LEU:O	2.19	0.41
1:D:334:MET:HB3	1:D:339:LEU:HB2	2.02	0.41
1:B:352:ASP:OD1	1:B:353:ARG:N	2.53	0.41
1:C:25:LEU:HD21	1:C:65:ARG:HD3	2.01	0.41
1:D:178:ARG:HA	1:D:178:ARG:HD3	1.92	0.41
1:B:5:LEU:HD13	1:B:14:ARG:HH22	1.85	0.41
1:D:133:VAL:HG21	1:D:233:VAL:HG13	2.02	0.41
1:A:424:MET:HB3	1:A:424:MET:HE2	1.81	0.41
1:A:22:LYS:HE2	1:A:264:GLN:NE2	2.35	0.41
1:A:321:LYS:NZ	1:A:427:THR:O	2.53	0.41
1:C:156:LEU:HB3	1:C:158:ARG:H	1.86	0.41
1:C:320:GLY:HA2	2:C:501:PEG:H12	2.03	0.41
1:C:160:TYR:HA	1:C:161:ALA:C	2.42	0.40
1:A:16:LEU:O	1:A:20:ARG:NH1	2.55	0.40
1:A:1:MET:HG3	1:A:2:ARG:H	1.87	0.40
1:D:118:PRO:O	1:D:122:ARG:HD2	2.21	0.40
1:B:160:TYR:HA	1:B:162:LEU:H	1.85	0.40
1:A:10:PHE:N	1:A:11:PRO:HD2	2.37	0.40
1:C:202:SER:OG	1:C:203:GLU:N	2.54	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	454/488 (93%)	435 (96%)	16 (4%)	3 (1%)	19	49
1	B	461/488 (94%)	450 (98%)	8 (2%)	3 (1%)	19	49
1	C	465/488 (95%)	441 (95%)	24 (5%)	0	100	100
1	D	453/488 (93%)	434 (96%)	19 (4%)	0	100	100
All	All	1833/1952 (94%)	1760 (96%)	67 (4%)	6 (0%)	37	67

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	81	GLU
1	A	176	THR
1	A	210	ILE
1	A	214	SER
1	B	470	ALA
1	B	161	ALA

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	355/392 (91%)	350 (99%)	5 (1%)	62	79
1	B	357/392 (91%)	355 (99%)	2 (1%)	84	91
1	C	366/392 (93%)	364 (100%)	2 (0%)	86	92
1	D	349/392 (89%)	344 (99%)	5 (1%)	62	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1427/1568 (91%)	1413 (99%)	14 (1%)	73 85

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	264	GLN
1	B	419	ARG
1	A	122	ARG
1	A	156	LEU
1	A	184	VAL
1	A	213	PHE
1	A	305	ASP
1	C	163	MET
1	C	460	LEU
1	D	76	ARG
1	D	154	GLN
1	D	160	TYR
1	D	178	ARG
1	D	447	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	266	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 oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	$\# Z  > 2$
2	PEG	B	502	-	6,6,6	0.10	0	5,5,5	0.10	0
2	PEG	C	501	-	6,6,6	0.10	0	5,5,5	0.09	0
2	PEG	A	502	-	6,6,6	0.11	0	5,5,5	0.09	0
2	PEG	A	501	-	6,6,6	0.11	0	5,5,5	0.12	0
2	PEG	B	504	-	6,6,6	0.10	0	5,5,5	0.14	0
2	PEG	B	503	-	6,6,6	0.10	0	5,5,5	0.10	0
2	PEG	B	501	-	6,6,6	0.10	0	5,5,5	0.10	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
2	PEG	B	502	-	-	1/4/4/4	-
2	PEG	C	501	-	-	0/4/4/4	-
2	PEG	A	502	-	-	3/4/4/4	-
2	PEG	A	501	-	-	2/4/4/4	-
2	PEG	B	504	-	-	2/4/4/4	-
2	PEG	B	503	-	-	2/4/4/4	-
2	PEG	B	501	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	502	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	B	504	PEG	O1-C1-C2-O2
2	B	504	PEG	O2-C3-C4-O4
2	A	502	PEG	C1-C2-O2-C3
2	A	501	PEG	C1-C2-O2-C3
2	A	501	PEG	C4-C3-O2-C2
2	B	503	PEG	C1-C2-O2-C3
2	B	503	PEG	C4-C3-O2-C2
2	A	502	PEG	O2-C3-C4-O4
2	A	502	PEG	C4-C3-O2-C2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	PEG	2	0
2	A	502	PEG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	462/488 (94%)	-0.31	15 (3%)	50	33	30, 43, 75, 137	0
1	B	471/488 (96%)	-0.31	9 (1%)	66	48	32, 51, 82, 145	0
1	C	473/488 (96%)	-0.20	12 (2%)	58	40	30, 50, 84, 134	0
1	D	463/488 (94%)	-0.16	15 (3%)	50	33	35, 50, 79, 121	0
All	All	1869/1952 (95%)	-0.25	51 (2%)	56	38	30, 49, 80, 145	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	468	SER	4.2
1	A	160	TYR	4.2
1	C	197	ILE	4.2
1	D	197	ILE	4.1
1	D	488	GLU	4.0
1	A	360	ASP	3.9
1	A	467	ARG	3.9
1	A	215	VAL	3.7
1	C	160	TYR	3.6
1	B	203	GLU	3.3
1	B	207	THR	3.3
1	B	80	PRO	3.1
1	A	159	LEU	3.1
1	C	163	MET	2.9
1	C	156	LEU	2.9
1	A	464	VAL	2.9
1	B	464	VAL	2.8
1	D	174	PHE	2.8
1	C	465	PRO	2.7
1	D	318	MET	2.7
1	B	318	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	79	GLY	2.6
1	B	468	SER	2.6
1	D	201	GLU	2.6
1	D	209	PHE	2.6
1	C	360	ASP	2.6
1	D	196	GLY	2.6
1	D	191	ALA	2.6
1	D	182	TYR	2.4
1	A	204	SER	2.4
1	A	482	GLU	2.4
1	D	204	SER	2.3
1	D	464	VAL	2.3
1	D	230	GLU	2.3
1	D	220	ASN	2.3
1	C	464	VAL	2.2
1	D	210	ILE	2.2
1	C	200	ASP	2.2
1	A	463	GLY	2.2
1	A	157	ASP	2.2
1	D	219	ASN	2.2
1	A	202	SER	2.2
1	C	317	ASN	2.2
1	B	202	SER	2.2
1	C	173	ARG	2.1
1	A	156	LEU	2.1
1	C	453	ALA	2.1
1	B	128	ASP	2.1
1	A	209	PHE	2.0
1	A	213	PHE	2.0
1	A	183	CYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	PEG	B	504	7/7	0.69	0.26	55,60,81,85	0
2	PEG	A	501	7/7	0.70	0.25	45,55,77,78	0
2	PEG	B	503	7/7	0.82	0.17	62,62,75,83	0
2	PEG	A	502	7/7	0.82	0.17	39,59,68,86	0
2	PEG	C	501	7/7	0.85	0.14	40,54,68,70	0
2	PEG	B	501	7/7	0.87	0.13	44,56,64,72	0
2	PEG	B	502	7/7	0.93	0.10	46,53,60,61	0
3	MG	C	502	1/1	0.97	0.31	40,40,40,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.