



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2021 – 02:07 PM EDT

PDB ID : 7R66  
Title : Structure of Pfp1 protease from *Thermococcus thio-reducens*: large unit cell at 1.44 Å resolution  
Authors : McPherson, A.  
Deposited on : 2021-06-22  
Resolution : 1.44 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 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 : 2.23.1  
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) : 2.23.1

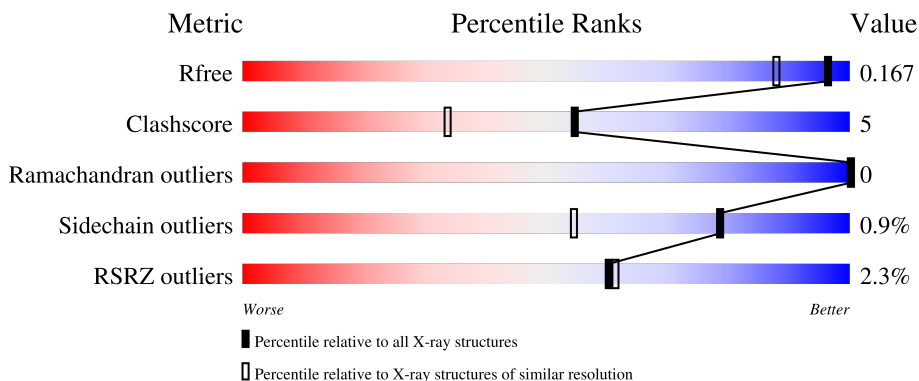
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.44 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	2021 (1.46-1.42)
Clashscore	141614	2086 (1.46-1.42)
Ramachandran outliers	138981	2047 (1.46-1.42)
Sidechain outliers	138945	2047 (1.46-1.42)
RSRZ outliers	127900	1993 (1.46-1.42)

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	166	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>11%</div> </div> </div>
1	B	166	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
1	C	166	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>12%</div> </div> </div>
1	D	166	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>15%</div> </div> </div>

## 2 Entry composition [i](#)

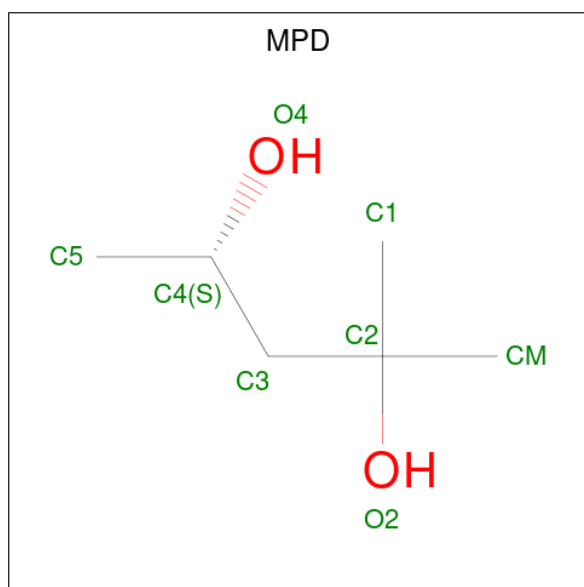
There are 4 unique types of molecules in this entry. The entry contains 11582 atoms, of which 5548 are hydrogens and 0 are deuteriums.

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 Peptidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	166	Total	C	H	N	O	S	0	9	0
			2699	858	1361	224	251	5			
1	B	166	Total	C	H	N	O	S	0	12	0
			2742	868	1389	230	250	5			
1	C	166	Total	C	H	N	O	S	0	14	0
			2737	872	1371	230	259	5			
1	D	166	Total	C	H	N	O	S	0	9	0
			2704	857	1371	225	246	5			

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



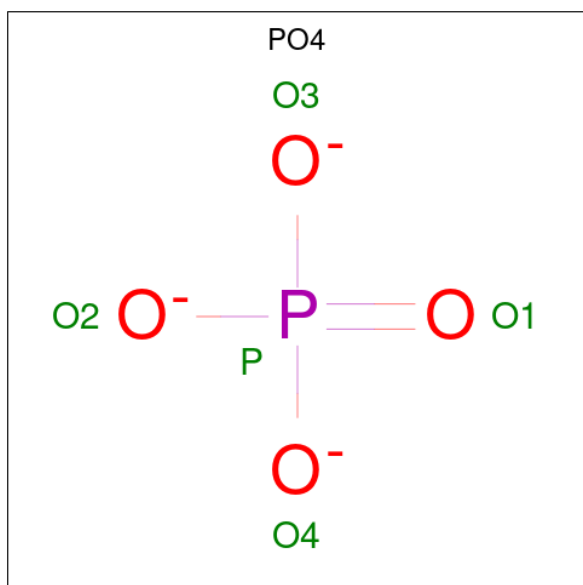
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			22	6	14	2		
2	A	1	Total	C	H	O	0	0
			22	6	14	2		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	H	O	0	0
			22	6	14	2		
2	D	1	Total	C	H	O	0	0
			22	6	14	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

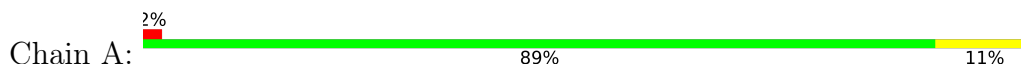
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	150	Total	O	0	6
			151	151		
4	B	173	Total	O	0	8
			175	175		
4	C	154	Total	O	0	4
			155	155		
4	D	121	Total	O	0	5
			121	121		

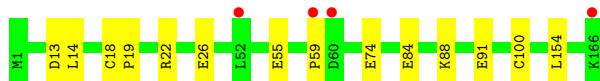
### 3 Residue-property plots [i](#)

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.

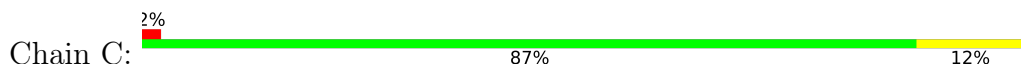
- Molecule 1: Peptidase



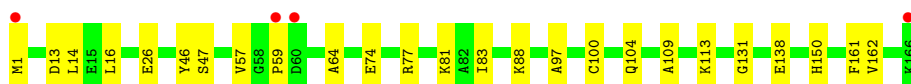
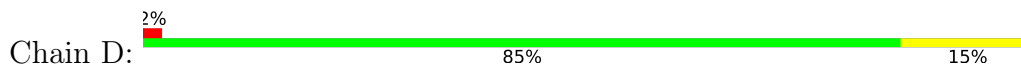
- Molecule 1: Peptidase



- Molecule 1: Peptidase



- Molecule 1: Peptidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.03Å 151.03Å 80.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	68.69 – 1.44 75.52 – 1.44	Depositor EDS
% Data completeness (in resolution range)	100.0 (68.69-1.44) 100.0 (75.52-1.44)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	0.21	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 1.44Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, $R_{free}$	0.134 , 0.166 0.135 , 0.167	Depositor DCC
$R_{free}$ test set	6118 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.5	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 49.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	11582	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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: PO4, OCS, MPD

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	0.54	0/1389	0.71	0/1874
1	B	0.49	0/1417	0.71	0/1910
1	C	0.56	2/1437 (0.1%)	0.71	0/1937
1	D	0.53	0/1390	0.70	0/1875
All	All	0.53	2/5633 (0.0%)	0.71	0/7596

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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	26[A]	GLU	CB-CG	5.50	1.62	1.52
1	C	26[B]	GLU	CB-CG	5.50	1.62	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	37	ARG	Sidechain

## 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	1338	1361	1352	16	0
1	B	1353	1389	1369	11	0
1	C	1366	1371	1360	19	0
1	D	1333	1371	1354	14	0
2	A	16	28	28	1	0
2	B	8	14	14	0	0
2	D	8	14	14	1	0
3	C	5	0	0	1	0
3	D	5	0	0	0	0
4	A	151	0	0	5	3
4	B	175	0	0	5	3
4	C	155	0	0	6	0
4	D	121	0	0	1	4
All	All	6034	5548	5491	57	5

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 (57) 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:26[B]:GLU:OE1	4:C:501:HOH:O	1.72	1.06
1:B:74:GLU:OE2	4:B:301:HOH:O	1.77	0.99
1:B:26:GLU:OE1	4:B:302[A]:HOH:O	1.85	0.93
1:A:83:ILE:HG23	1:A:109:ALA:HA	1.70	0.74
1:C:150:HIS:ND1	3:C:401:PO4:O3	2.21	0.74
1:B:91[A]:GLU:OE1	4:B:303:HOH:O	2.06	0.73
1:C:83:ILE:HG23	1:C:109:ALA:HA	1.72	0.69
1:A:137[B]:GLU:OE1	4:A:302:HOH:O	2.12	0.68
1:A:137[B]:GLU:OE2	4:A:301:HOH:O	2.11	0.67
1:A:91[B]:GLU:OE1	4:A:303:HOH:O	2.14	0.66
1:D:83[A]:ILE:HG23	1:D:109:ALA:HA	1.76	0.66
1:A:163:LYS:HA	1:A:166:LYS:HE3	1.79	0.64
1:A:88[B]:LYS:HG2	4:A:359:HOH:O	1.99	0.61
1:A:88[B]:LYS:HA	1:A:88[B]:LYS:HE2	1.83	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:PRO:HB2	1:B:88:LYS:HD3	1.85	0.59
1:B:55:GLU:HG3	4:B:433[B]:HOH:O	2.04	0.56
1:C:77:ARG:HA	1:C:83:ILE:HD11	1.87	0.56
1:C:87[B]:ARG:NE	4:C:504:HOH:O	2.41	0.54
1:A:88[B]:LYS:HE3	4:A:359:HOH:O	2.06	0.53
1:D:138:GLU:OE2	4:D:301:HOH:O	2.19	0.53
1:A:148[B]:SER:OG	1:A:153:ASP:CB	2.58	0.52
1:D:77:ARG:HA	1:D:83[A]:ILE:HD11	1.94	0.50
1:C:83:ILE:CG2	1:C:109:ALA:HA	2.42	0.48
1:B:22:ARG:NH1	1:B:26:GLU:HG2	2.28	0.48
1:D:59:PRO:CB	1:D:88:LYS:HD2	2.44	0.47
1:C:22:ARG:HH12	1:C:26[B]:GLU:CD	2.18	0.47
1:B:59:PRO:HB2	1:B:88:LYS:CD	2.45	0.47
1:C:1:MET:HE3	1:C:63:ASP:HB3	1.97	0.47
1:C:80:GLU:HG2	4:C:608:HOH:O	2.16	0.46
1:C:87[B]:ARG:NH2	4:C:506:HOH:O	2.49	0.46
1:A:88[B]:LYS:HA	1:A:88[B]:LYS:CE	2.46	0.45
1:C:14:LEU:HG	1:D:46:TYR:CZ	2.52	0.45
1:C:57:VAL:O	1:C:81:LYS:NZ	2.47	0.45
1:C:74[B]:GLU:HG3	1:C:104:GLN:OE1	2.17	0.45
1:D:26:GLU:OE2	1:D:162[A]:VAL:HG13	2.17	0.45
1:A:46:TYR:CZ	1:B:14:LEU:HG	2.52	0.45
1:A:29:GLU:OE1	1:A:31:TYR:OH	2.30	0.44
1:D:74[A]:GLU:HG3	1:D:104:GLN:OE1	2.17	0.44
1:C:81:LYS:NZ	4:C:508:HOH:O	2.50	0.44
1:A:155:TYR:HE2	2:A:202:MPD:H32	1.84	0.43
1:C:166:LYS:HE3	4:C:611:HOH:O	2.17	0.43
1:D:1:MET:HE1	1:D:64:ALA:HB2	2.00	0.43
1:A:148[B]:SER:OG	1:A:153:ASP:HB3	2.19	0.43
1:D:57:VAL:O	1:D:81[A]:LYS:NZ	2.51	0.42
1:D:113[B]:LYS:HD3	1:D:131:GLY:HA3	2.00	0.42
1:C:18:CYS:HB2	1:C:19[A]:PRO:HD3	2.01	0.42
1:B:84:GLU:HG3	4:B:387:HOH:O	2.19	0.41
1:D:97:ALA:HB2	1:D:161:PHE:CD1	2.55	0.41
1:A:113:LYS:HE2	1:A:113:LYS:HB2	1.86	0.41
1:C:46:TYR:CZ	1:D:14:LEU:HG	2.56	0.41
1:B:18:CYS:CB	1:B:154[B]:LEU:HD21	2.51	0.41
1:C:83:ILE:HG23	1:C:109:ALA:CA	2.45	0.41
1:A:77:ARG:HA	1:A:83:ILE:HD11	2.01	0.41
1:D:47:SER:O	2:D:201:MPD:HM3	2.21	0.41
1:C:22:ARG:NH2	1:C:26[B]:GLU:OE2	2.54	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:CYS:HB2	1:B:19[A]:PRO:HD3	2.03	0.40

All (5) 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)
4:A:370:HOH:O	4:B:317:HOH:O[2_665]	1.72	0.48
4:A:424:HOH:O	4:D:349:HOH:O[9_555]	1.94	0.26
4:B:413:HOH:O	4:D:405:HOH:O[1_556]	2.12	0.08
4:B:462:HOH:O	4:D:420:HOH:O[1_556]	2.15	0.05
4:A:303:HOH:O	4:D:324:HOH:O[9_555]	2.19	0.01

## 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	172/166 (104%)	171 (99%)	1 (1%)	0	100	100
1	B	175/166 (105%)	174 (99%)	1 (1%)	0	100	100
1	C	177/166 (107%)	174 (98%)	3 (2%)	0	100	100
1	D	172/166 (104%)	170 (99%)	2 (1%)	0	100	100
All	All	696/664 (105%)	689 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	146/137 (107%)	145 (99%)	1 (1%)	84	64
1	B	149/137 (109%)	148 (99%)	1 (1%)	84	64
1	C	151/137 (110%)	150 (99%)	1 (1%)	84	64
1	D	146/137 (107%)	144 (99%)	2 (1%)	67	37
All	All	592/548 (108%)	587 (99%)	5 (1%)	78	61

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASP
1	B	13	ASP
1	C	13	ASP
1	D	13	ASP
1	D	150	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	OCS	B	100	1	7,8,9	1.00	0	6,11,13	1.45	1 (16%)
1	OCS	C	100	1	7,8,9	0.53	0	6,11,13	1.54	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	OCS	D	100	1	7,8,9	1.11	0	6,11,13	3.48	3 (50%)
1	OCS	A	100	1	7,8,9	1.63	2 (28%)	6,11,13	1.81	2 (33%)

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
1	OCS	B	100	1	-	4/4/7/9	-
1	OCS	C	100	1	-	4/4/7/9	-
1	OCS	D	100	1	-	4/4/7/9	-
1	OCS	A	100	1	-	4/4/7/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	100	OCS	CB-CA	2.80	1.56	1.53
1	A	100	OCS	CB-SG	2.31	1.85	1.77

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	100	OCS	OD1-SG-CB	4.90	112.77	106.94
1	D	100	OCS	OD3-SG-CB	4.82	112.66	106.94
1	D	100	OCS	OD3-SG-OD1	-3.98	100.16	113.95
1	A	100	OCS	OD2-SG-CB	3.17	110.78	105.74
1	A	100	OCS	OD3-SG-CB	2.39	109.78	106.94
1	C	100	OCS	OD2-SG-CB	2.24	109.31	105.74
1	B	100	OCS	OD3-SG-OD1	-2.11	106.64	113.95

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	100	OCS	N-CA-CB-SG
1	A	100	OCS	CA-CB-SG-OD1
1	A	100	OCS	CA-CB-SG-OD2
1	B	100	OCS	N-CA-CB-SG
1	B	100	OCS	CA-CB-SG-OD2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
1	B	100	OCS	CA-CB-SG-OD3
1	C	100	OCS	N-CA-CB-SG
1	C	100	OCS	CA-CB-SG-OD1
1	C	100	OCS	CA-CB-SG-OD2
1	C	100	OCS	CA-CB-SG-OD3
1	D	100	OCS	N-CA-CB-SG
1	D	100	OCS	CA-CB-SG-OD1
1	D	100	OCS	CA-CB-SG-OD2
1	D	100	OCS	CA-CB-SG-OD3
1	A	100	OCS	CA-CB-SG-OD3
1	B	100	OCS	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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	PO4	C	401	-	4,4,4	1.24	0	6,6,6	0.52	0
2	MPD	A	201	-	7,7,7	0.29	0	9,10,10	0.60	0
2	MPD	A	202	-	7,7,7	0.25	0	9,10,10	0.50	0
2	MPD	D	201	-	7,7,7	0.27	0	9,10,10	0.79	0
2	MPD	B	201	-	7,7,7	0.24	0	9,10,10	0.51	0
3	PO4	D	202	-	4,4,4	0.93	0	6,6,6	1.07	1 (16%)

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	MPD	D	201	-	-	0/5/5/5	-
2	MPD	A	201	-	-	1/5/5/5	-
2	MPD	B	201	-	-	0/5/5/5	-
2	MPD	A	202	-	-	0/5/5/5	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	202	PO4	O4-P-O2	2.01	114.44	107.97

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	MPD	C1-C2-C3-C4

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	PO4	1	0
2	A	202	MPD	1	0
2	D	201	MPD	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	165/166 (99%)	0.14	3 (1%) 68 68	16, 23, 38, 59	0
1	B	165/166 (99%)	0.13	4 (2%) 59 60	16, 22, 38, 59	0
1	C	165/166 (99%)	0.11	4 (2%) 59 60	18, 24, 38, 59	0
1	D	165/166 (99%)	0.09	4 (2%) 59 60	17, 24, 40, 63	0
All	All	660/664 (99%)	0.12	15 (2%) 60 61	16, 23, 40, 63	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	166	LYS	3.9
1	C	60	ASP	3.7
1	B	60	ASP	3.5
1	C	166	LYS	3.4
1	A	1	MET	3.3
1	D	1	MET	3.3
1	D	166	LYS	3.2
1	A	166	LYS	2.9
1	C	1	MET	2.5
1	B	59	PRO	2.5
1	B	52	LEU	2.3
1	D	60	ASP	2.2
1	D	59	PRO	2.1
1	A	150	HIS	2.1
1	C	20[A]	LEU	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	OCS	A	100	9/10	0.86	0.15	19,28,39,43	3
1	OCS	D	100	9/10	0.88	0.15	13,26,34,39	5
1	OCS	B	100	9/10	0.89	0.14	19,27,35,39	3
1	OCS	C	100	9/10	0.91	0.11	19,28,36,38	3

### 6.3 Carbohydrates [i](#)

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	MPD	A	202	8/8	0.81	0.27	60,72,74,74	0
2	MPD	B	201	8/8	0.84	0.24	69,83,83,83	0
3	PO4	C	401	5/5	0.89	0.25	22,46,62,64	5
2	MPD	A	201	8/8	0.91	0.19	36,45,53,53	0
2	MPD	D	201	8/8	0.93	0.15	36,43,52,52	0
3	PO4	D	202	5/5	0.94	0.20	25,32,43,57	5

### 6.5 Other polymers [i](#)

There are no such residues in this entry.