



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:13 AM GMT

PDB ID : 2WNR  
Title : The structure of Methanothermobacter thermautotrophicus exosome core assembly  
Authors : Ng, C.L.; Waterman, D.G.; Antson, A.A.; Ortiz-Lombardia, M.  
Deposited on : 2009-07-19  
Resolution : 2.65 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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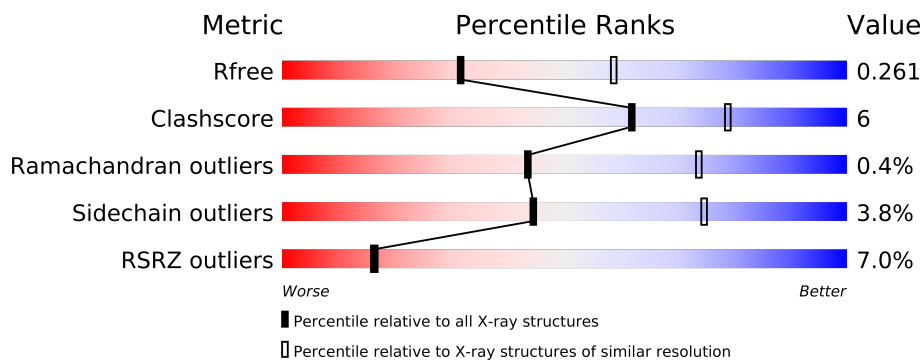
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.65 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))
$R_{free}$	66092	2232 (2.70-2.62)
Clashscore	79885	2700 (2.70-2.62)
Ramachandran outliers	78287	2657 (2.70-2.62)
Sidechain outliers	78261	2657 (2.70-2.62)
RSRZ outliers	66119	2234 (2.70-2.62)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	271	
1	C	271	
1	E	271	
2	B	240	
2	D	240	
2	F	240	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11066 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PROBABLE EXOSOME COMPLEX EXONUCLEASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			2010	1264	338	396	12			
1	C	258	Total	C	N	O	S	0	1	0
			1994	1253	338	391	12			
1	E	250	Total	C	N	O	S	0	1	0
			1929	1212	326	379	12			

- Molecule 2 is a protein called PROBABLE EXOSOME COMPLEX EXONUCLEASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	222	Total	C	N	O	S	0	0	0
			1714	1067	312	328	7			
2	D	210	Total	C	N	O	S	0	0	0
			1612	1006	288	311	7			
2	F	217	Total	C	N	O	S	0	0	0
			1667	1038	301	321	7			

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



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

- Molecule 4 is water.

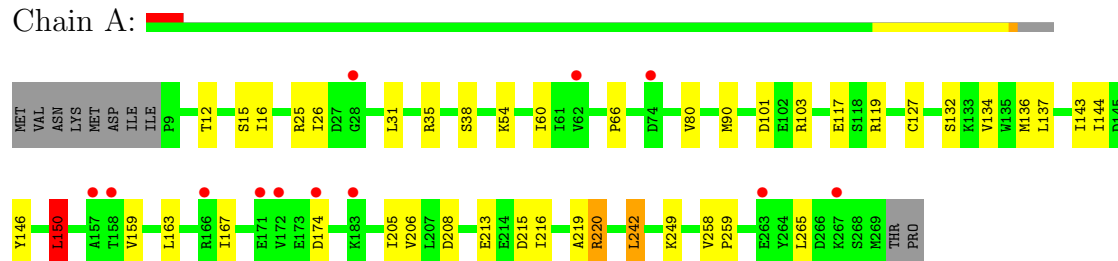
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	19	Total	O	0	0
			19	19		
4	B	25	Total	O	0	0
			25	25		
4	C	21	Total	O	0	0
			21	21		
4	D	16	Total	O	0	0
			16	16		
4	E	17	Total	O	0	0
			17	17		
4	F	27	Total	O	0	0
			27	27		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

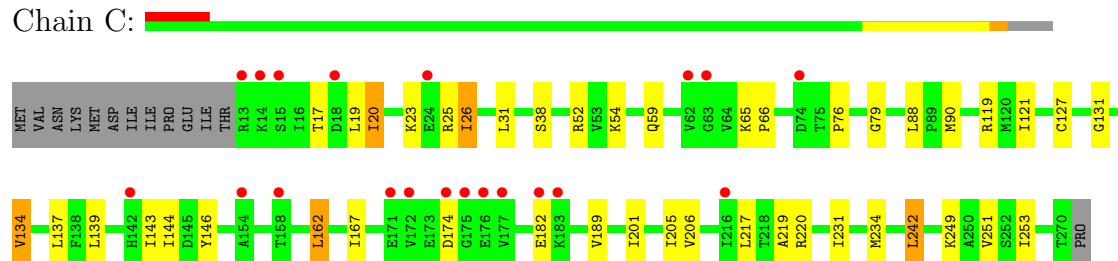
#### • Molecule 1: PROBABLE EXOSOME COMPLEX EXONUCLEASE 2

Chain A:



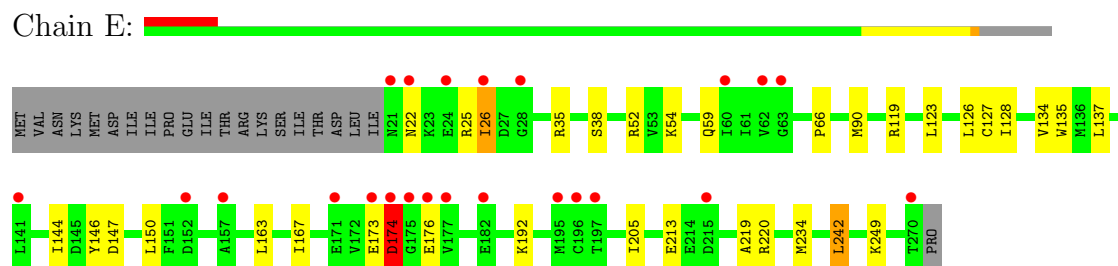
#### • Molecule 1: PROBABLE EXOSOME COMPLEX EXONUCLEASE 2

Chain C:



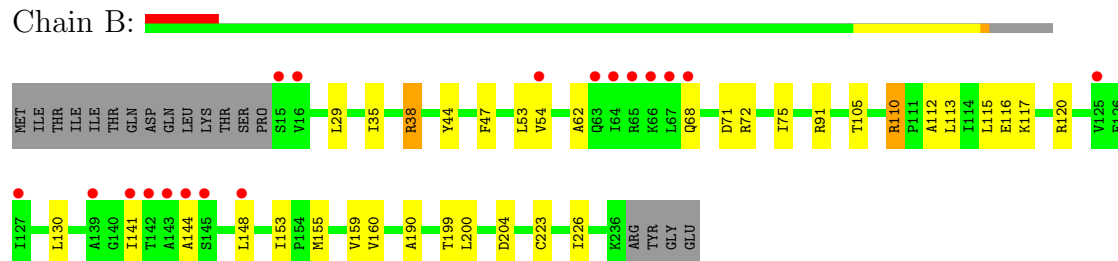
#### • Molecule 1: PROBABLE EXOSOME COMPLEX EXONUCLEASE 2

Chain E:



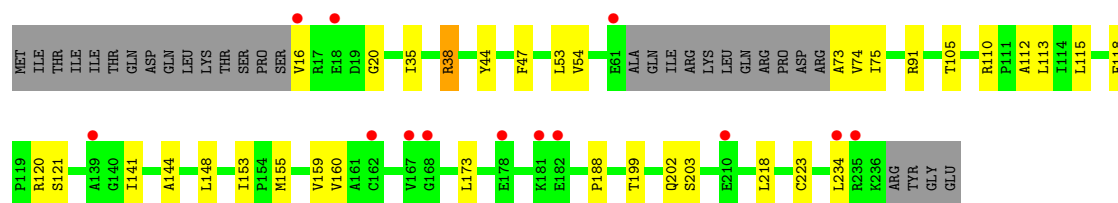
#### • Molecule 2: PROBABLE EXOSOME COMPLEX EXONUCLEASE 1

Chain B:



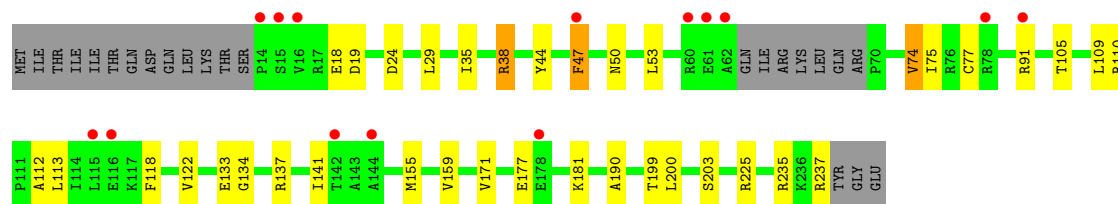
- Molecule 2: PROBABLE EXOSOME COMPLEX EXONUCLEASE 1

Chain D:



- Molecule 2: PROBABLE EXOSOME COMPLEX EXONUCLEASE 1

Chain F:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.26Å 118.23Å 154.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.86 – 2.65 24.86 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.7 (24.86-2.65) 98.7 (24.86-2.65)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 2.64Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.211 , 0.251 0.222 , 0.261	Depositor DCC
$R_{free}$ test set	973 reflections (2.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.2	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 47579 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11066	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0/2037	0.76	6/2757 (0.2%)
1	C	0.42	0/2023	0.69	5/2737 (0.2%)
1	E	0.45	0/1958	0.76	5/2650 (0.2%)
2	B	0.49	0/1735	0.81	7/2340 (0.3%)
2	D	0.41	0/1631	0.77	6/2200 (0.3%)
2	F	0.47	0/1688	0.81	7/2276 (0.3%)
All	All	0.44	0/11072	0.76	36/14960 (0.2%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	38	ARG	NE-CZ-NH1	-14.72	112.94	120.30
2	D	38	ARG	NE-CZ-NH2	14.50	127.55	120.30
2	B	110	ARG	NE-CZ-NH1	-14.41	113.09	120.30
2	B	110	ARG	NE-CZ-NH2	13.85	127.23	120.30
1	A	220	ARG	NE-CZ-NH2	13.57	127.09	120.30
2	F	91	ARG	NE-CZ-NH1	13.56	127.08	120.30
1	A	220	ARG	NE-CZ-NH1	-13.30	113.65	120.30
2	F	91	ARG	NE-CZ-NH2	-13.18	113.71	120.30
1	E	119	ARG	NE-CZ-NH1	-12.63	113.98	120.30
1	E	119	ARG	NE-CZ-NH2	12.38	126.49	120.30
1	E	220	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	E	220	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	C	220	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	C	220	ARG	NE-CZ-NH1	7.37	123.98	120.30
2	D	38	ARG	CD-NE-CZ	7.28	133.78	123.60
2	F	110	ARG	NE-CZ-NH2	-6.75	116.93	120.30
2	B	38	ARG	NE-CZ-NH1	6.66	123.63	120.30
2	B	91	ARG	NE-CZ-NH2	6.58	123.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	110	ARG	CD-NE-CZ	6.58	132.81	123.60
2	B	38	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	A	119	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	A	119	ARG	NE-CZ-NH1	6.48	123.54	120.30
2	F	91	ARG	CD-NE-CZ	6.44	132.62	123.60
2	F	110	ARG	NE-CZ-NH1	6.37	123.49	120.30
2	D	110	ARG	NE-CZ-NH2	-6.37	117.12	120.30
2	B	91	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	A	220	ARG	CD-NE-CZ	6.33	132.46	123.60
2	F	38	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	C	119	ARG	NE-CZ-NH2	-6.04	117.28	120.30
2	F	38	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	C	119	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	150	LEU	CB-CG-CD1	5.82	120.89	111.00
1	C	19	LEU	CA-CB-CG	5.75	128.53	115.30
2	D	110	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	E	119	ARG	CD-NE-CZ	5.61	131.45	123.60
2	D	91	ARG	NE-CZ-NH1	-5.19	117.70	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2010	0	2062	21	0
1	C	1994	0	2050	25	0
1	E	1929	0	1975	18	0
2	B	1714	0	1751	26	0
2	D	1612	0	1639	20	0
2	F	1667	0	1695	21	0
3	B	5	0	0	0	0
3	D	5	0	0	0	0
3	F	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	19	0	0	3	0
4	B	25	0	0	0	0
4	C	21	0	0	0	0
4	D	16	0	0	0	0
4	E	17	0	0	0	0
4	F	27	0	0	2	0
All	All	11066	0	11172	125	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (125) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:120:ARG:HG3	2:B:120:ARG:HH11	1.46	0.80
1:A:146:TYR:CD1	1:A:150:LEU:HD13	2.23	0.72
1:C:127:CYS:HA	1:C:134:VAL:HG22	1.72	0.72
1:C:20:ILE:HG21	1:C:201:ILE:HG22	1.75	0.67
2:F:137:ARG:HG2	4:F:2026:HOH:O	1.95	0.66
1:E:163:LEU:HD11	1:E:192:LYS:HD3	1.79	0.65
1:A:220:ARG:HD2	4:A:2017:HOH:O	1.95	0.64
2:B:35:ILE:HD13	2:B:44:TYR:HB2	1.80	0.64
1:A:146:TYR:HD1	1:A:150:LEU:HD13	1.63	0.64
1:C:31:LEU:HD22	1:C:206:VAL:HG22	1.83	0.61
2:D:35:ILE:HD13	2:D:44:TYR:HB2	1.82	0.60
2:F:35:ILE:HD13	2:F:44:TYR:HB2	1.84	0.59
1:C:79:GLY:HA2	1:C:134:VAL:HG13	1.83	0.59
1:E:128:ILE:HD11	1:E:135:TRP:CD1	2.37	0.58
2:F:35:ILE:CD1	2:F:53:LEU:HD11	2.34	0.58
1:C:121:ILE:HD11	1:C:162:LEU:HG	1.85	0.57
2:D:16:VAL:HG13	2:D:20:GLY:HA2	1.86	0.57
2:D:73:ALA:HB2	2:D:118:PHE:O	2.05	0.56
1:E:66:PRO:HG3	1:E:167:ILE:HG22	1.88	0.56
2:B:116:GLU:H	2:B:116:GLU:CD	2.09	0.55
1:C:90:MET:HE3	1:C:144:ILE:HG23	1.88	0.55
1:A:103:ARG:HD2	4:A:2015:HOH:O	2.05	0.54
1:E:173:GLU:O	1:E:174:ASP:C	2.45	0.54
1:C:66:PRO:HG3	1:C:167:ILE:HG22	1.90	0.54
2:B:115:LEU:C	2:B:117:LYS:H	2.10	0.54
1:A:127:CYS:HA	1:A:134:VAL:HG12	1.89	0.54
1:C:234:MET:HB3	2:D:203:SER:HB3	1.89	0.53
2:D:35:ILE:CD1	2:D:53:LEU:HD11	2.38	0.53
2:B:120:ARG:HH11	2:B:120:ARG:CG	2.20	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:249:LYS:O	1:C:253:ILE:HD12	2.09	0.53
2:B:115:LEU:C	2:B:117:LYS:N	2.62	0.53
2:F:113:LEU:HD23	2:F:155:MET:HG2	1.90	0.53
2:B:38:ARG:HD3	1:E:146:TYR:O	2.09	0.52
2:B:29:LEU:HD21	2:B:226:ILE:HG23	1.91	0.52
1:A:66:PRO:HG3	1:A:167:ILE:HG22	1.91	0.52
2:F:35:ILE:HD11	2:F:53:LEU:CD1	2.39	0.52
1:C:76:PRO:HB3	1:C:131:GLY:HA2	1.92	0.52
1:A:90:MET:HE3	1:A:144:ILE:HG23	1.92	0.52
1:A:25:ARG:HD2	1:A:213:GLU:OE2	2.11	0.51
2:B:160:VAL:HG13	2:B:223:CYS:HB3	1.93	0.51
2:F:75:ILE:HG13	2:F:75:ILE:O	2.11	0.50
2:B:115:LEU:O	2:B:117:LYS:N	2.45	0.50
2:D:75:ILE:HD11	2:D:115:LEU:HD11	1.94	0.50
1:E:35:ARG:NH2	1:E:147:ASP:O	2.44	0.50
1:E:25:ARG:HD2	1:E:213:GLU:OE2	2.11	0.49
2:B:35:ILE:CD1	2:B:53:LEU:HD11	2.43	0.49
2:B:62:ALA:HB3	2:B:68:GLN:HE21	1.78	0.49
1:E:52[B]:ARG:HH11	1:E:59:GLN:HE22	1.60	0.49
1:A:38:SER:HB3	1:A:54:LYS:HB2	1.95	0.48
2:D:188:PRO:HG2	2:D:202:GLN:HB2	1.95	0.48
2:F:190:ALA:HB3	2:F:200:LEU:HB3	1.95	0.48
1:E:234:MET:HB3	2:F:203:SER:HB3	1.95	0.48
2:D:105:THR:HG23	2:D:141:ILE:HG12	1.95	0.48
1:E:127:CYS:HA	1:E:134:VAL:HG12	1.96	0.48
1:A:117:GLU:HG3	2:B:204:ASP:HB2	1.96	0.48
2:F:74:VAL:O	2:F:122:VAL:HA	2.14	0.48
1:E:90:MET:HE3	1:E:144:ILE:HG23	1.95	0.48
1:C:20:ILE:HG21	1:C:201:ILE:CG2	2.44	0.47
2:D:35:ILE:HD11	2:D:53:LEU:CD1	2.44	0.47
1:C:38:SER:HB3	1:C:54:LYS:HB2	1.95	0.47
1:E:52[B]:ARG:HH11	1:E:59:GLN:NE2	2.13	0.47
1:E:38:SER:HB3	1:E:54:LYS:HB2	1.97	0.47
2:F:112:ALA:HB2	2:F:159:VAL:CG2	2.45	0.47
1:C:26:ILE:HG13	1:C:26:ILE:H	1.53	0.46
2:B:71:ASP:OD2	2:B:72:ARG:HG2	2.15	0.46
1:A:219:ALA:HB3	1:A:242:LEU:CD1	2.46	0.46
2:D:112:ALA:HB2	2:D:159:VAL:CG2	2.46	0.46
2:D:113:LEU:HD23	2:D:155:MET:HG2	1.97	0.46
2:D:160:VAL:HG13	2:D:223:CYS:HB3	1.98	0.46
2:D:54:VAL:HG11	2:D:144:ALA:HA	1.97	0.46
2:D:153:ILE:O	2:D:155:MET:HG3	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:60:ILE:HG12	1:A:143:ILE:HG13	1.98	0.45
2:F:235:ARG:O	2:F:237:ARG:HD2	2.16	0.45
1:A:16:ILE:HB	1:A:216:ILE:HD13	1.99	0.45
2:B:112:ALA:HB2	2:B:159:VAL:CG2	2.47	0.45
1:A:159:VAL:HG12	1:A:265:LEU:HD21	1.99	0.45
2:B:105:THR:HG23	2:B:141:ILE:HG12	1.99	0.45
1:C:79:GLY:HA2	1:C:134:VAL:CG1	2.46	0.45
1:C:146:TYR:O	2:F:38:ARG:HD3	2.17	0.45
2:B:113:LEU:HD23	2:B:155:MET:HG2	1.99	0.44
2:B:54:VAL:HG11	2:B:144:ALA:HA	1.98	0.44
1:E:205:ILE:HD11	1:E:249:LYS:HG2	1.99	0.44
2:D:173:LEU:HB2	2:D:218:LEU:HG	2.00	0.44
1:E:146:TYR:CD1	1:E:150:LEU:HD21	2.53	0.44
2:F:24:ASP:O	2:F:225:ARG:NH2	2.44	0.43
2:B:120:ARG:CG	2:B:120:ARG:NH1	2.81	0.43
2:F:19:ASP:HB2	4:F:2001:HOH:O	2.18	0.43
2:F:35:ILE:CD1	2:F:53:LEU:CD1	2.96	0.43
1:A:80:VAL:HB	1:A:136:MET:HG2	1.99	0.43
2:F:29:LEU:HD12	2:F:47:PHE:CG	2.54	0.43
1:A:31:LEU:HD22	1:A:206:VAL:HG12	2.00	0.43
1:C:231:ILE:HD11	1:C:251:VAL:HG13	2.01	0.42
2:B:35:ILE:CD1	2:B:44:TYR:HB2	2.48	0.42
1:E:219:ALA:HB3	1:E:242:LEU:CD1	2.49	0.42
2:B:53:LEU:HD22	2:B:130:LEU:HD11	2.00	0.42
1:C:25:ARG:CZ	1:C:206:VAL:HG13	2.49	0.42
2:B:153:ILE:O	2:B:155:MET:HG3	2.19	0.42
2:B:35:ILE:HD11	2:B:53:LEU:CD1	2.50	0.42
1:C:205:ILE:HD11	1:C:249:LYS:HG2	2.01	0.42
1:A:205:ILE:HD11	1:A:249:LYS:HG2	2.01	0.42
2:F:105:THR:HG23	2:F:141:ILE:HG12	2.01	0.42
2:D:35:ILE:CD1	2:D:44:TYR:HB2	2.48	0.42
2:B:190:ALA:HB3	2:B:200:LEU:HB3	2.02	0.42
1:A:146:TYR:CD1	1:A:150:LEU:CD1	2.99	0.42
1:A:258:VAL:N	1:A:259:PRO:HD2	2.35	0.41
1:C:219:ALA:HB3	1:C:242:LEU:CD1	2.50	0.41
1:E:26:ILE:HG13	1:E:26:ILE:H	1.42	0.41
2:B:120:ARG:HG3	2:B:120:ARG:NH1	2.22	0.41
2:F:141:ILE:CD1	2:F:200:LEU:HD13	2.50	0.41
2:D:73:ALA:HA	2:D:121:SER:O	2.21	0.41
1:C:65:LYS:HA	1:C:66:PRO:HD2	1.96	0.41
1:A:35:ARG:NH2	1:A:208:ASP:OD1	2.50	0.41
1:C:217:LEU:O	1:C:217:LEU:HD12	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:143:ILE:HD12	1:C:143:ILE:N	2.35	0.41
1:C:234:MET:CB	2:D:203:SER:HB3	2.51	0.41
2:F:141:ILE:HD11	2:F:200:LEU:HD13	2.02	0.41
1:A:101:ASP:HB2	4:A:2008:HOH:O	2.20	0.41
2:F:133:GLU:OE2	2:F:177:GLU:HB2	2.21	0.41
1:E:126:LEU:HB3	1:E:135:TRP:HB2	2.02	0.40
1:C:52[B]:ARG:HD2	1:C:59:GLN:NE2	2.36	0.40
2:D:38:ARG:HD2	2:D:38:ARG:HA	1.83	0.40
2:B:75:ILE:HD11	2:B:113:LEU:HD12	2.03	0.40
2:F:50:ASN:OD1	2:F:133:GLU:N	2.48	0.40
2:D:73:ALA:HB3	2:D:115:LEU:HB3	2.03	0.40
1:C:17:THR:O	1:C:20:ILE:HG22	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	259/271 (96%)	250 (96%)	8 (3%)	1 (0%)	43	74
1	C	257/271 (95%)	248 (96%)	8 (3%)	1 (0%)	43	74
1	E	249/271 (92%)	240 (96%)	8 (3%)	1 (0%)	43	74
2	B	220/240 (92%)	211 (96%)	9 (4%)	0	100	100
2	D	206/240 (86%)	198 (96%)	8 (4%)	0	100	100
2	F	213/240 (89%)	205 (96%)	6 (3%)	2 (1%)	25	52
All	All	1404/1533 (92%)	1352 (96%)	47 (3%)	5 (0%)	43	74

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	174	ASP
1	C	174	ASP
1	A	132	SER

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Mol	Chain	Res	Type
2	F	181	LYS
2	F	134	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	229/239 (96%)	220 (96%)	9 (4%)	43	74
1	C	227/239 (95%)	216 (95%)	11 (5%)	35	65
1	E	219/239 (92%)	212 (97%)	7 (3%)	51	81
2	B	181/198 (91%)	177 (98%)	4 (2%)	64	89
2	D	170/198 (86%)	164 (96%)	6 (4%)	48	78
2	F	176/198 (89%)	168 (96%)	8 (4%)	38	68
All	All	1202/1311 (92%)	1157 (96%)	45 (4%)	44	76

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	15	SER
1	A	26	ILE
1	A	137	LEU
1	A	150	LEU
1	A	163	LEU
1	A	174	ASP
1	A	215	ASP
1	A	242	LEU
2	B	47	PHE
2	B	110	ARG
2	B	148	LEU
2	B	199	THR
1	C	20	ILE
1	C	23	LYS
1	C	26	ILE
1	C	88	LEU

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Mol	Chain	Res	Type
1	C	134	VAL
1	C	137	LEU
1	C	139	LEU
1	C	162	LEU
1	C	182	GLU
1	C	189	VAL
1	C	242	LEU
2	D	47	PHE
2	D	74	VAL
2	D	120	ARG
2	D	148	LEU
2	D	199	THR
2	D	234	LEU
1	E	22	ASN
1	E	26	ILE
1	E	123	LEU
1	E	137	LEU
1	E	174	ASP
1	E	176	GLU
1	E	242	LEU
2	F	18	GLU
2	F	47	PHE
2	F	74	VAL
2	F	77	CYS
2	F	109	LEU
2	F	118	PHE
2	F	171	VAL
2	F	199	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	GLN
2	B	68	GLN
2	B	80	ASN
2	B	170	GLN
2	B	227	HIS
2	D	80	ASN
2	D	227	HIS
1	E	22	ASN
1	E	59	GLN
1	E	260	GLN

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Mol	Chain	Res	Type
2	F	227	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

3 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	B	1237	-	4,4,4	0.26	0	6,6,6	0.31	0
3	PO4	D	1237	-	4,4,4	0.24	0	6,6,6	0.31	0
3	PO4	F	1238	-	4,4,4	0.28	0	6,6,6	0.32	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	PO4	B	1237	-	-	0/0/0/0	0/0/0/0
3	PO4	D	1237	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	F	1238	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	261/271 (96%)	0.35	12 (4%)	31 33	5, 24, 34, 50	0
1	C	258/271 (95%)	0.43	20 (7%)	13 13	14, 24, 42, 59	1 (0%)
1	E	250/271 (92%)	0.48	23 (9%)	9 8	6, 23, 32, 52	0
2	B	222/240 (92%)	0.41	18 (8%)	12 12	8, 23, 45, 76	0
2	D	210/240 (87%)	0.51	13 (6%)	20 21	14, 23, 36, 45	1 (0%)
2	F	217/240 (90%)	0.38	14 (6%)	18 19	13, 23, 41, 64	4 (1%)
All	All	1418/1533 (92%)	0.42	100 (7%)	16 16	5, 23, 38, 76	6 (0%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	67	LEU	5.8
1	C	174	ASP	4.9
1	C	13	ARG	4.7
2	B	64	ILE	4.3
2	B	66	LYS	4.3
2	B	16	VAL	4.1
2	F	62	ALA	4.0
1	C	14	LYS	3.9
1	E	175	GLY	3.9
1	E	176	GLU	3.8
1	A	172	VAL	3.8
1	E	174	ASP	3.7
2	D	61	GLU	3.6
1	E	22	ASN	3.5
1	C	183	LYS	3.5
1	A	171	GLU	3.3
2	F	16	VAL	3.2
1	C	15	SER	3.1
1	C	216	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	175	GLY	3.1
2	B	65	ARG	3.1
1	A	174	ASP	3.0
2	F	61	GLU	3.0
1	A	263	GLU	3.0
1	E	182	GLU	3.0
1	A	267	LYS	2.9
2	F	115	LEU	2.9
1	C	24	GLU	2.9
2	D	181	LYS	2.9
2	B	54	VAL	2.8
1	C	177	VAL	2.8
2	B	127	ILE	2.8
2	F	14	PRO	2.8
1	C	172	VAL	2.8
2	B	143	ALA	2.8
1	E	28	GLY	2.8
1	C	18	ASP	2.8
2	D	168	GLY	2.7
2	B	144	ALA	2.7
2	F	78	ARG	2.7
1	E	173	GLU	2.7
1	E	63	GLY	2.7
1	C	63	GLY	2.7
2	B	141	ILE	2.7
1	C	182	GLU	2.6
2	D	18	GLU	2.6
1	C	176	GLU	2.6
2	D	178	GLU	2.6
1	C	62	VAL	2.6
2	F	144	ALA	2.5
2	B	145	SER	2.5
1	A	183	LYS	2.5
1	E	177	VAL	2.5
2	B	15	SER	2.5
2	B	68	GLN	2.5
1	E	195	MET	2.5
2	D	167	VAL	2.5
2	F	60	ARG	2.5
1	E	171	GLU	2.4
2	D	182	GLU	2.4
1	E	62	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	26	ILE	2.4
2	B	125	VAL	2.4
1	C	154	ALA	2.4
2	F	91	ARG	2.4
1	C	171	GLU	2.4
2	F	178	GLU	2.3
2	D	210	GLU	2.3
1	E	197	THR	2.3
2	D	16	VAL	2.3
1	E	21	ASN	2.3
1	C	158	THR	2.3
2	D	139	ALA	2.3
1	A	158	THR	2.3
2	B	142	THR	2.3
2	F	47	PHE	2.3
2	B	63	GLN	2.3
2	F	116	GLU	2.2
2	F	142	THR	2.2
1	E	60	ILE	2.2
2	D	234	LEU	2.2
1	A	28	GLY	2.2
2	D	162	CYS	2.1
1	E	157	ALA	2.1
1	E	215	ASP	2.1
2	B	139	ALA	2.1
1	E	196	CYS	2.1
1	E	152	ASP	2.1
1	E	24	GLU	2.1
2	D	235	ARG	2.1
2	B	148	LEU	2.1
1	A	166	ARG	2.1
1	A	157	ALA	2.1
1	C	142	HIS	2.1
1	A	62	VAL	2.1
1	A	74	ASP	2.1
1	E	270	THR	2.0
2	F	15	SER	2.0
1	E	141	LEU	2.0
1	C	74	ASP	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 carbohydrates in this entry.

## 6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	PO4	D	1237	5/5	0.24	1.80	48,49,56,61	0
3	PO4	B	1237	5/5	0.23	1.39	40,43,49,53	0
3	PO4	F	1238	5/5	0.17	-0.90	68,74,75,76	0

## 6.5 Other polymers

There are no such residues in this entry.