



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 02:17 PM JST

PDB ID : 5ZFR  
Title : Crystal structure of PilB, an extension ATPase motor of Type IV pilus, from *Geobacter sulfurreducens*  
Authors : Thakur, K.G.; Solanki, V.; Kapoor, S.  
Deposited on : 2018-03-06  
Resolution : 3.10 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) : 1.13  
EDS : 2.36  
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) : 2.36

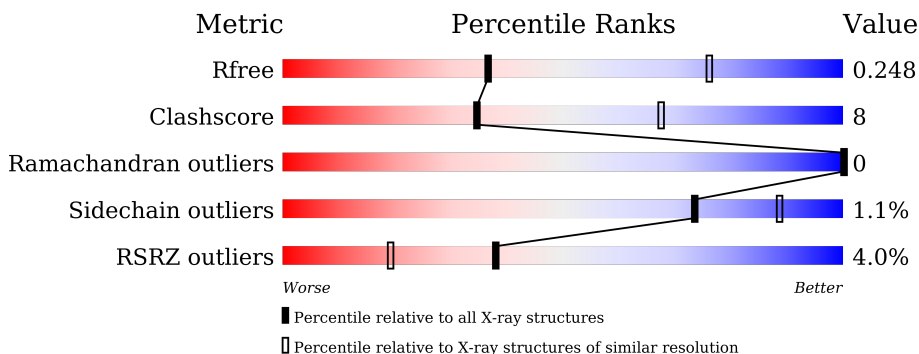
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	582	
1	B	582	
1	C	582	

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	PO4	B	602	-	-	X	-

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 9055 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 Type IV pilus biogenesis ATPase PilB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	383	2984	1896	514	556	18	0	0	0
1	B	385	3001	1904	516	564	17	0	0	0
1	C	386	3004	1906	517	563	18	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP Q74D28
A	-12	GLY	-	expression tag	UNP Q74D28
A	-11	SER	-	expression tag	UNP Q74D28
A	-10	SER	-	expression tag	UNP Q74D28
A	-9	HIS	-	expression tag	UNP Q74D28
A	-8	HIS	-	expression tag	UNP Q74D28
A	-7	HIS	-	expression tag	UNP Q74D28
A	-6	HIS	-	expression tag	UNP Q74D28
A	-5	HIS	-	expression tag	UNP Q74D28
A	-4	HIS	-	expression tag	UNP Q74D28
A	-3	SER	-	expression tag	UNP Q74D28
A	-2	GLN	-	expression tag	UNP Q74D28
A	-1	ASP	-	expression tag	UNP Q74D28
A	0	PRO	-	expression tag	UNP Q74D28
B	-13	MET	-	initiating methionine	UNP Q74D28
B	-12	GLY	-	expression tag	UNP Q74D28
B	-11	SER	-	expression tag	UNP Q74D28
B	-10	SER	-	expression tag	UNP Q74D28
B	-9	HIS	-	expression tag	UNP Q74D28
B	-8	HIS	-	expression tag	UNP Q74D28
B	-7	HIS	-	expression tag	UNP Q74D28
B	-6	HIS	-	expression tag	UNP Q74D28
B	-5	HIS	-	expression tag	UNP Q74D28

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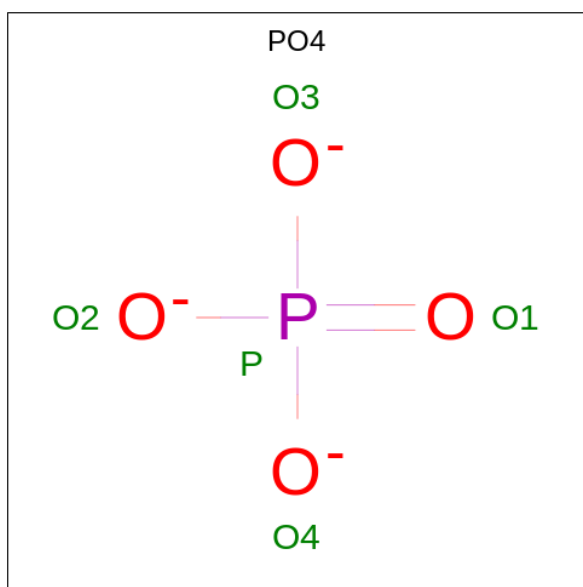
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	expression tag	UNP Q74D28
B	-3	SER	-	expression tag	UNP Q74D28
B	-2	GLN	-	expression tag	UNP Q74D28
B	-1	ASP	-	expression tag	UNP Q74D28
B	0	PRO	-	expression tag	UNP Q74D28
C	-13	MET	-	initiating methionine	UNP Q74D28
C	-12	GLY	-	expression tag	UNP Q74D28
C	-11	SER	-	expression tag	UNP Q74D28
C	-10	SER	-	expression tag	UNP Q74D28
C	-9	HIS	-	expression tag	UNP Q74D28
C	-8	HIS	-	expression tag	UNP Q74D28
C	-7	HIS	-	expression tag	UNP Q74D28
C	-6	HIS	-	expression tag	UNP Q74D28
C	-5	HIS	-	expression tag	UNP Q74D28
C	-4	HIS	-	expression tag	UNP Q74D28
C	-3	SER	-	expression tag	UNP Q74D28
C	-2	GLN	-	expression tag	UNP Q74D28
C	-1	ASP	-	expression tag	UNP Q74D28
C	0	PRO	-	expression tag	UNP Q74D28

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

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



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

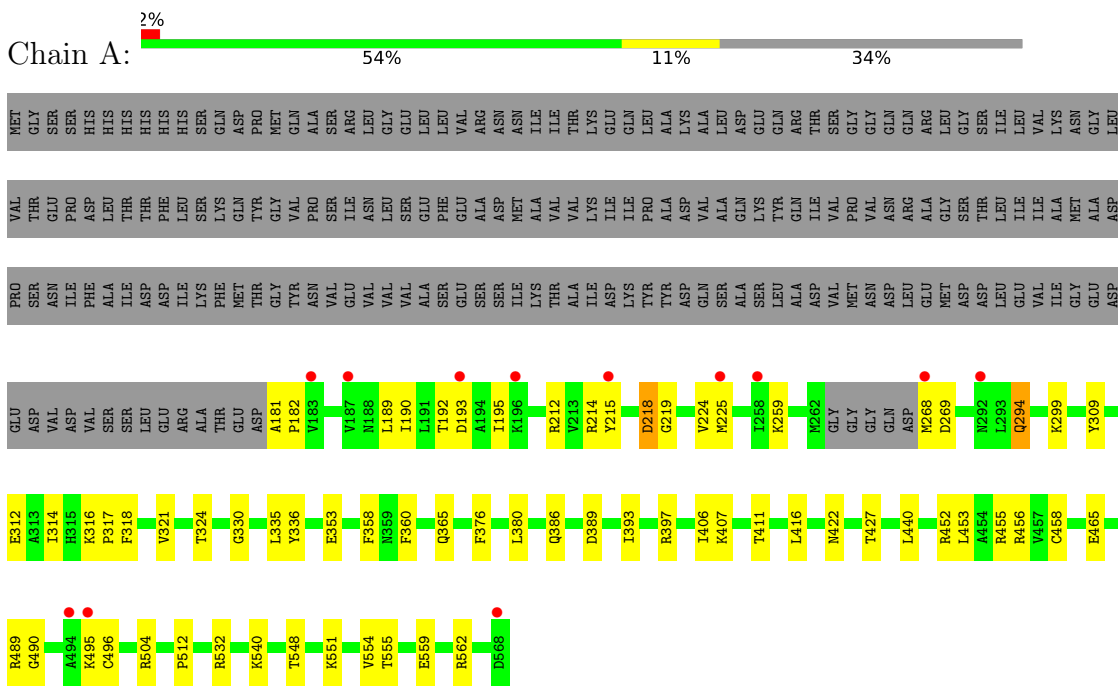
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total	O	0	0
			16	16		
4	B	14	Total	O	0	0
			14	14		
4	C	18	Total	O	0	0
			18	18		

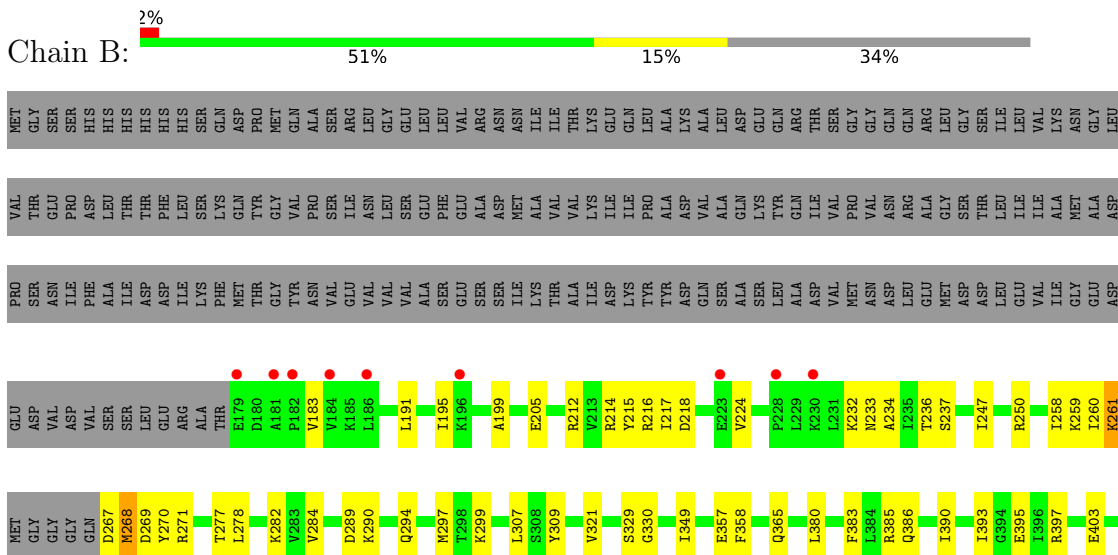
### 3 Residue-property plots [i](#)

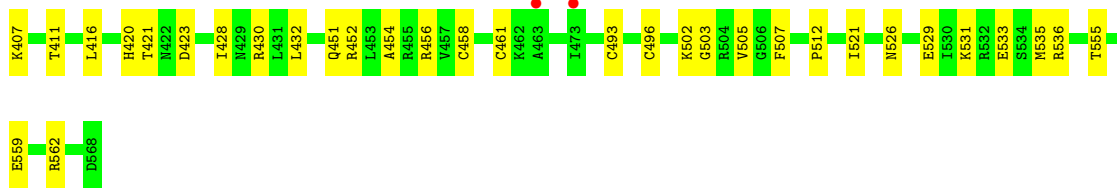
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Type IV pilus biogenesis ATPase PilB



- Molecule 1: Type IV pilus biogenesis ATPase PilB





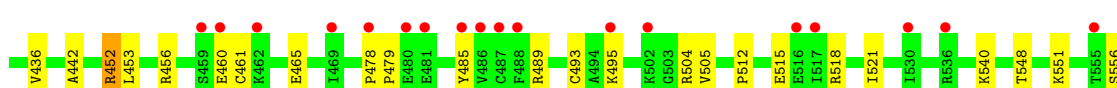
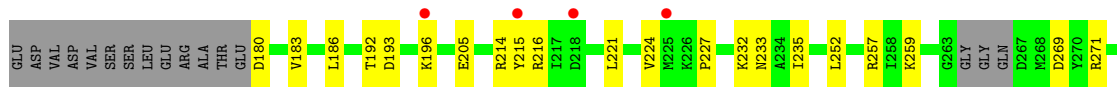
● Molecule 1: Type IV pilus biogenesis ATPase PilB



MET GLY SER HIS HIS HIS HIS HIS HIS HIS HIS ASP PRO MET MET GLN PRO ASP ARG ARG ARG ASN ASN ASN ILE ILE ILE THR LYS LYS ILE ILE ILE THR SER GLY GLY GLN GLN ARG ARG LEU LEU SER ASP

VAL THR GLU PRO ASP PHE ALA ILE ASP PHE ASP LYS SER LYS MET TYR GLY VAL PRO ASN ILE ASN LEU SER GLU PHE LEU VAL ARG ALA ASP MET ILE LYS VAL VAL VAL VAL VAL VAL VAL ILE ILE ILE PRO TYR ALA GLN LYS TYR GLN ASP VAL PRO VAL ASP ASP ASP MET ASP MET ASP THR THR THR ILE ILE ILE ALA ALA ASP

PRO SER ASN ILE PHE ALA ILE ASP ASP ASP LYS PHE THR MET THR GLY TYR ASN VAL VAL VAL VAL VAL VAL SER GLU SER ILE MET LYS THR VAL VAL VAL ILE ASP LYS ILE ILE ILE TYR TYR TYR ASP GLN SER ALA ALA LYS SER ALA GLN TYR GLN ASP ASP ASP ASP GLN MET ASN ASP ASP ASP ASP MET VAL VAL VAL VAL VAL VAL VAL MET ASP





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	176.30Å 176.30Å 138.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.34 – 3.10 46.34 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.0 (46.34-3.10) 98.0 (46.34-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 3.12Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.218 , 0.247 0.219 , 0.248	Depositor DCC
$R_{free}$ test set	1989 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	101.8	Xtrriage
Anisotropy	0.078	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 85.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9055	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	102.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.27	0/3028	0.51	0/4091
1	B	0.28	0/3045	0.49	0/4115
1	C	0.28	0/3048	0.51	0/4118
All	All	0.27	0/9121	0.50	0/12324

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2984	0	3093	44	0
1	B	3001	0	3098	60	0
1	C	3004	0	3104	55	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	5	0	0	1	0
3	B	5	0	0	2	0
3	C	5	0	0	0	0
4	A	16	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	14	0	0	0	0
4	C	18	0	0	0	0
All	All	9055	0	9295	151	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 8.

All (151) 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:452:ARG:HD3	1:C:453:LEU:H	1.43	0.83
1:A:540:LYS:NZ	1:A:548:THR:OG1	2.20	0.75
1:A:224:VAL:HG12	1:A:225:MET:HG3	1.69	0.72
1:B:259:LYS:C	1:B:260:ILE:HD13	2.10	0.72
1:C:460:GLU:HG3	1:C:495:LYS:HG3	1.73	0.71
1:B:267:ASP:N	1:B:267:ASP:OD1	2.24	0.70
1:B:380:LEU:HD13	1:B:393:ILE:HD11	1.73	0.69
1:B:259:LYS:O	1:B:260:ILE:HD13	1.92	0.69
1:C:461:CYS:HB3	1:C:493:CYS:HB3	1.73	0.69
1:B:260:ILE:HG22	1:B:261:LYS:N	2.08	0.69
1:B:321:VAL:HB	1:B:416:LEU:HD23	1.77	0.67
1:C:515:GLU:OE1	1:C:518:ARG:NH2	2.27	0.67
1:A:559:GLU:OE2	1:A:562:ARG:NH1	2.28	0.65
1:B:205:GLU:OE2	1:B:282:LYS:NZ	2.29	0.65
1:C:428:ILE:HD13	1:C:521:ILE:HD11	1.79	0.65
1:B:199:ALA:HA	1:B:217:ILE:HG22	1.79	0.64
1:B:330:GLY:N	3:B:602:PO4:O3	2.30	0.64
1:A:465:GLU:OE2	1:A:489:ARG:NH1	2.31	0.63
1:C:452:ARG:HD3	1:C:453:LEU:N	2.11	0.63
1:A:380:LEU:HD13	1:A:393:ILE:HD11	1.81	0.62
1:C:186:LEU:HD21	1:C:227:PRO:HB3	1.82	0.62
1:C:257:ARG:NH1	1:C:357:GLU:OE1	2.35	0.60
1:A:422:ASN:O	1:A:452:ARG:NH1	2.34	0.60
1:C:335:LEU:HD11	1:C:416:LEU:HB3	1.83	0.60
1:A:407:LYS:HD3	1:B:397:ARG:HD3	1.84	0.60
1:B:386:GLN:HG3	1:C:284:VAL:HG21	1.82	0.60
1:A:259:LYS:HZ2	1:A:268:MET:N	1.99	0.60
1:A:555:THR:HG22	1:A:559:GLU:HB3	1.83	0.59
1:C:456:ARG:HB2	1:C:505:VAL:HG23	1.85	0.59
1:C:540:LYS:NZ	1:C:548:THR:OG1	2.30	0.58
1:B:533:GLU:OE2	1:B:536:ARG:NH1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:VAL:HG13	1:C:418:THR:HG22	1.85	0.57
1:C:358:PHE:O	1:C:365:GLN:NE2	2.34	0.56
1:A:218:ASP:HB3	1:A:455:ARG:HG2	1.86	0.56
1:C:180:ASP:HA	1:C:183:VAL:HG22	1.87	0.56
1:C:380:LEU:HD13	1:C:393:ILE:HD11	1.86	0.56
1:B:233:ASN:OD1	1:B:250:ARG:NH2	2.39	0.56
1:C:215:TYR:CD2	1:C:224:VAL:HG21	2.39	0.56
1:A:386:GLN:HB2	1:B:284:VAL:HG21	1.88	0.56
1:B:269:ASP:OD1	1:B:269:ASP:N	2.37	0.55
1:A:495:LYS:H	1:A:495:LYS:HD2	1.72	0.54
1:B:259:LYS:HA	1:B:269:ASP:HA	1.89	0.54
1:A:336:TYR:OH	1:A:353:GLU:OE1	2.21	0.53
1:C:349:ILE:HG12	1:C:390:ILE:HB	1.91	0.53
1:C:453:LEU:HD23	1:C:504:ARG:HD2	1.90	0.53
1:B:212:ARG:NE	1:B:214:ARG:HD2	2.23	0.53
1:C:452:ARG:CD	1:C:453:LEU:H	2.19	0.53
1:B:559:GLU:OE1	1:B:562:ARG:NH2	2.39	0.52
1:C:293:LEU:HD22	1:C:358:PHE:CE1	2.45	0.52
1:B:420:HIS:O	1:B:430:ARG:NH2	2.43	0.52
1:C:380:LEU:O	1:C:384:LEU:HD22	2.09	0.51
1:A:532:ARG:NH2	4:A:701:HOH:O	2.43	0.51
1:B:461:CYS:HB3	1:B:493:CYS:HB3	1.90	0.51
1:B:261:LYS:HA	1:B:267:ASP:N	2.26	0.51
1:A:411:THR:HG23	1:B:395:GLU:OE1	2.11	0.51
1:B:260:ILE:CG2	1:B:261:LYS:N	2.73	0.51
1:A:219:GLY:N	1:A:504:ARG:HH21	2.08	0.51
1:A:406:ILE:HG21	1:A:440:LEU:HB3	1.92	0.50
1:B:232:LYS:O	1:B:236:THR:HG22	2.11	0.50
1:A:389:ASP:OD2	1:B:216:ARG:NH2	2.23	0.49
1:A:219:GLY:H	1:A:504:ARG:HH21	1.59	0.49
1:B:403:GLU:HG3	1:B:407:LYS:HE3	1.94	0.49
1:B:385:ARG:O	1:C:286:ARG:NH1	2.46	0.49
1:A:309:TYR:CD1	1:A:512:PRO:HG3	2.48	0.49
1:C:186:LEU:HD23	1:C:235:ILE:HD11	1.95	0.48
1:C:205:GLU:OE2	1:C:214:ARG:NH2	2.45	0.48
1:C:465:GLU:OE2	1:C:489:ARG:NH2	2.41	0.48
1:B:232:LYS:HG3	1:B:233:ASN:N	2.29	0.48
1:B:458:CYS:HB2	1:B:496:CYS:HB3	1.96	0.48
1:B:268:MET:HG3	1:B:270:TYR:HE1	1.79	0.48
1:A:317:PRO:HG2	1:A:318:PHE:CE2	2.49	0.47
1:B:383:PHE:HE1	1:C:275:LEU:HD21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ILE:HG22	1:A:225:MET:SD	2.54	0.47
1:C:403:GLU:O	1:C:407:LYS:HG2	2.14	0.47
1:B:526:ASN:OD1	1:B:529:GLU:HB2	2.14	0.47
1:C:295:LEU:HD12	1:C:340:SER:HB2	1.97	0.47
1:A:358:PHE:O	1:A:365:GLN:NE2	2.46	0.47
1:C:290:LYS:HD3	1:C:358:PHE:CZ	2.49	0.47
1:A:192:THR:HA	1:A:195:ILE:HD12	1.97	0.47
1:B:271:ARG:NE	1:B:357:GLU:OE1	2.47	0.47
1:C:295:LEU:HD13	1:C:337:SER:HA	1.97	0.47
1:C:309:TYR:CD1	1:C:512:PRO:HG3	2.50	0.47
1:B:329:SER:N	3:B:602:PO4:O3	2.48	0.46
1:B:428:ILE:HG21	1:B:521:ILE:HG12	1.96	0.46
1:C:216:ARG:NH2	1:C:221:LEU:HD11	2.30	0.46
1:B:260:ILE:HG22	1:B:261:LYS:H	1.79	0.46
1:A:212:ARG:NE	1:A:214:ARG:HD2	2.31	0.46
1:C:396:ILE:HG13	1:C:417:SER:OG	2.16	0.46
1:C:232:LYS:HG3	1:C:233:ASN:N	2.30	0.46
1:C:485:TYR:CE1	1:C:551:LYS:HE2	2.51	0.45
1:A:269:ASP:OD1	1:A:269:ASP:N	2.41	0.44
1:B:555:THR:HG22	1:B:559:GLU:HB3	1.98	0.44
1:B:309:TYR:CD1	1:B:512:PRO:HG3	2.52	0.44
1:C:478:PRO:HA	1:C:479:PRO:HD3	1.91	0.44
1:A:407:LYS:O	1:A:411:THR:OG1	2.35	0.44
1:C:257:ARG:HH12	1:C:357:GLU:CD	2.21	0.44
1:C:407:LYS:O	1:C:411:THR:HG23	2.17	0.44
1:B:183:VAL:HG21	1:B:234:ALA:HB1	1.99	0.44
1:B:277:THR:HG22	1:B:278:LEU:H	1.83	0.44
1:A:215:TYR:CD2	1:A:224:VAL:HG21	2.53	0.44
1:C:559:GLU:OE1	1:C:562:ARG:NH1	2.51	0.44
1:A:330:GLY:N	3:A:602:PO4:O1	2.45	0.44
1:B:358:PHE:O	1:B:365:GLN:NE2	2.46	0.44
1:B:423:ASP:OD1	1:B:423:ASP:N	2.50	0.43
1:C:259:LYS:HG2	1:C:269:ASP:HB3	1.99	0.43
1:A:314:ILE:HD12	1:A:321:VAL:HG21	2.01	0.43
1:B:258:ILE:CG2	1:B:260:ILE:HD11	2.49	0.43
1:C:540:LYS:HZ1	1:C:548:THR:HG1	1.60	0.43
1:A:335:LEU:HD11	1:A:416:LEU:HB3	2.00	0.43
1:A:489:ARG:HG3	1:A:490:GLY:N	2.34	0.43
1:A:551:LYS:HE2	1:A:551:LYS:HB3	1.60	0.43
1:B:215:TYR:CD2	1:B:224:VAL:HG21	2.53	0.43
1:A:189:LEU:HA	1:A:192:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:THR:HG21	1:A:427:THR:OG1	2.19	0.43
1:B:349:ILE:HG12	1:B:390:ILE:HB	2.00	0.43
1:C:257:ARG:HG2	1:C:271:ARG:HD2	2.01	0.43
1:A:376:PHE:HE2	1:A:397:ARG:NH2	2.16	0.43
1:B:294:GLN:NE2	1:B:299:LYS:HD2	2.34	0.43
1:B:421:THR:O	1:B:452:ARG:NH2	2.52	0.43
1:B:531:LYS:HG2	1:B:535:MET:HE2	2.00	0.43
1:C:452:ARG:CD	1:C:453:LEU:N	2.79	0.43
1:B:237:SER:HB3	1:B:247:ILE:HD13	2.01	0.42
1:C:269:ASP:OD1	1:C:269:ASP:N	2.44	0.42
1:C:485:TYR:CZ	1:C:551:LYS:HE2	2.55	0.42
1:A:458:CYS:HB2	1:A:496:CYS:HB3	2.01	0.42
1:B:195:ILE:HG12	1:B:268:MET:CE	2.49	0.42
1:A:294:GLN:HB3	1:A:299:LYS:HD2	2.02	0.42
1:A:453:LEU:HD13	1:A:504:ARG:HD2	2.00	0.42
1:C:489:ARG:HG2	1:C:556:SER:CB	2.50	0.42
1:C:344:LYS:HA	1:C:344:LYS:HD3	1.59	0.42
1:C:192:THR:HG22	1:C:196:LYS:HE3	2.02	0.42
1:C:406:ILE:HD13	1:C:436:VAL:HG11	2.02	0.42
1:B:297:MET:HB3	1:B:307:LEU:HD11	2.01	0.41
1:B:289:ASP:OD1	1:B:289:ASP:N	2.39	0.41
1:B:454:ALA:O	1:B:505:VAL:N	2.45	0.41
1:B:428:ILE:O	1:B:432:LEU:HD13	2.20	0.41
1:A:259:LYS:HD3	1:A:269:ASP:HB3	2.03	0.41
1:B:411:THR:HG23	1:C:562:ARG:HH22	1.86	0.41
1:B:458:CYS:HA	1:B:502:LYS:HG2	2.01	0.41
1:A:456:ARG:HG3	1:A:554:VAL:HG12	2.02	0.41
1:A:336:TYR:CE2	1:A:358:PHE:HB3	2.55	0.41
1:B:456:ARG:HD3	1:B:502:LYS:HE3	2.02	0.41
1:A:181:ALA:HA	1:A:182:PRO:HD3	1.94	0.41
1:B:218:ASP:OD2	1:B:503:GLY:HA2	2.21	0.41
1:C:274:VAL:HG13	1:C:281:GLU:HB3	2.03	0.41
1:A:312:GLU:O	1:A:316:LYS:HG3	2.21	0.41
1:C:274:VAL:HG22	1:C:283:VAL:HG22	2.03	0.41
1:C:442:ALA:O	1:C:518:ARG:HD3	2.21	0.41
1:C:289:ASP:OD1	1:C:289:ASP:N	2.54	0.40
1:B:451:GLN:HA	1:B:507:PHE:O	2.22	0.40
1:B:191:LEU:HB3	1:B:270:TYR:OH	2.22	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	379/582 (65%)	369 (97%)	10 (3%)	0	100	100
1	B	381/582 (66%)	368 (97%)	13 (3%)	0	100	100
1	C	382/582 (66%)	370 (97%)	12 (3%)	0	100	100
All	All	1142/1746 (65%)	1107 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	328/498 (66%)	324 (99%)	4 (1%)	71	88
1	B	330/498 (66%)	327 (99%)	3 (1%)	78	91
1	C	330/498 (66%)	326 (99%)	4 (1%)	71	88
All	All	988/1494 (66%)	977 (99%)	11 (1%)	73	89

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	ASP
1	A	218	ASP
1	A	294	GLN
1	A	360	PHE
1	B	261	LYS

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Mol	Chain	Res	Type
1	B	268	MET
1	B	290	LYS
1	C	193	ASP
1	C	252	LEU
1	C	422	ASN
1	C	452	ARG

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\# Z  > 2$
3	PO4	B	602	-	4,4,4	0.99	0	6,6,6	0.48	0
3	PO4	C	602	-	4,4,4	0.89	0	6,6,6	0.45	0
3	PO4	A	602	-	4,4,4	0.92	0	6,6,6	0.45	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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	PO4	2	0
3	A	602	PO4	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	383/582 (65%)	0.26	12 (3%)	49 26	66, 93, 138, 198	0
1	B	385/582 (66%)	0.26	11 (2%)	51 28	65, 98, 135, 191	0
1	C	386/582 (66%)	0.46	23 (5%)	21 10	70, 102, 150, 212	0
All	All	1154/1746 (66%)	0.33	46 (3%)	38 19	65, 98, 145, 212	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	495	LYS	4.1
1	C	487	CYS	4.1
1	A	268	MET	3.2
1	A	196	LYS	3.2
1	C	459	SER	3.1
1	C	480	GLU	2.9
1	B	182	PRO	2.9
1	C	218	ASP	2.9
1	C	289	ASP	2.9
1	B	179	GLU	2.9
1	B	181	ALA	2.7
1	A	495	LYS	2.7
1	A	215	TYR	2.7
1	B	463	ALA	2.7
1	B	230	LYS	2.6
1	C	478	PRO	2.6
1	C	486	VAL	2.6
1	C	516	GLU	2.6
1	C	481	GLU	2.5
1	C	196	LYS	2.5
1	A	187	VAL	2.4
1	B	186	LEU	2.4
1	B	473	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	258	ILE	2.4
1	C	502	LYS	2.4
1	A	568	ASP	2.3
1	C	462	LYS	2.3
1	A	193	ASP	2.3
1	B	228	PRO	2.3
1	C	460	GLU	2.3
1	A	225	MET	2.3
1	C	485	TYR	2.2
1	B	196	LYS	2.2
1	C	225	MET	2.2
1	C	215	TYR	2.1
1	B	184	VAL	2.1
1	C	530	ILE	2.1
1	C	469	ILE	2.1
1	C	536	ARG	2.1
1	C	488	PHE	2.1
1	A	183	VAL	2.1
1	A	292	ASN	2.0
1	C	555	THR	2.0
1	B	223	GLU	2.0
1	A	494	ALA	2.0
1	C	517	ILE	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 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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3	PO4	B	602	5/5	0.85	0.35	154,159,161,168	0
3	PO4	C	602	5/5	0.88	0.19	135,138,142,143	0
3	PO4	A	602	5/5	0.93	0.28	140,145,148,149	0
2	ZN	B	601	1/1	0.94	0.08	167,167,167,167	0
2	ZN	A	601	1/1	0.96	0.11	132,132,132,132	0
2	ZN	C	601	1/1	0.97	0.04	166,166,166,166	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.