



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:02 PM GMT

PDB ID : 3QNK  
Title : Crystal structure of a SusD-like protein (BF3747) from Bacteroides fragilis  
NCTC 9343 at 2.70 Å resolution  
Authors : Joint Center for Structural Genomics (JCSG)  
Deposited on : 2011-02-08  
Resolution : 2.70 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

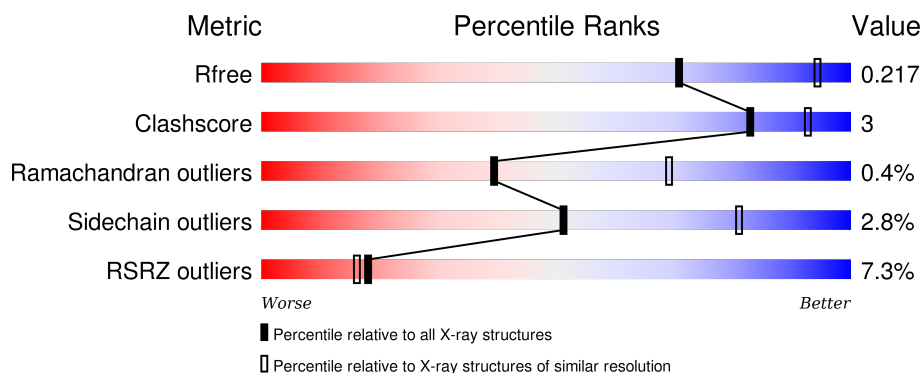
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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. 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	517	<div> <div>7%</div> <div>89%</div> <div>9%</div> <div>.</div> </div>
1	B	517	<div> <div>4%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
1	C	517	<div> <div>2%</div> <div>88%</div> <div>10%</div> <div>..</div> </div>
1	D	517	<div> <div>14%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	B	602	-	-	-	X
3	PO4	C	603	-	-	-	X
3	PO4	C	605	-	-	-	X
4	ACT	B	608	-	-	-	X
4	ACT	C	609	-	-	X	X
4	ACT	C	610	-	-	-	X
4	ACT	C	611	-	-	-	X
4	ACT	C	612	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16607 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 Putative lipoprotein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	512	Total	C	N	O	S	Se	0	0	0
			4090	2600	680	794	5	11			
1	B	513	Total	C	N	O	S	Se	0	1	0
			4157	2642	697	802	5	11			
1	C	511	Total	C	N	O	S	Se	0	2	0
			4156	2642	696	802	5	11			
1	D	514	Total	C	N	O	S	Se	0	0	0
			4073	2585	676	796	5	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	leader sequence	UNP Q5L904
B	0	GLY	-	leader sequence	UNP Q5L904
C	0	GLY	-	leader sequence	UNP Q5L904
D	0	GLY	-	leader sequence	UNP Q5L904

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

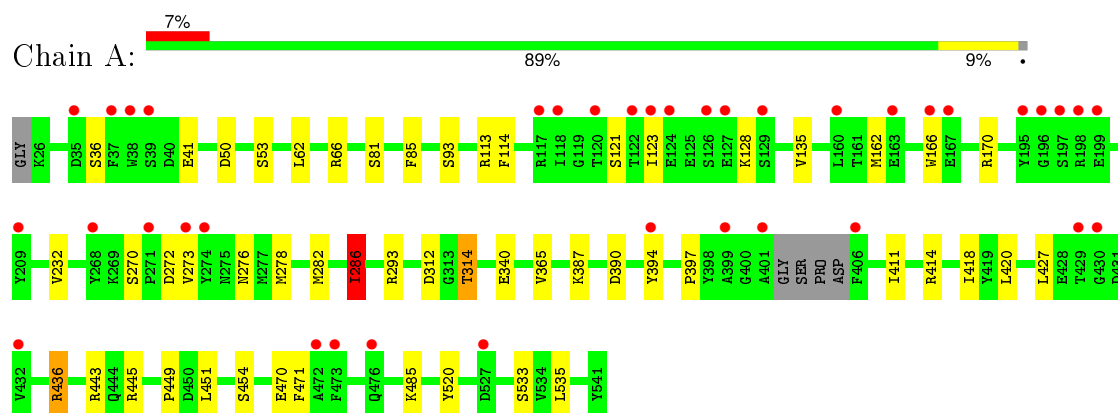
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	O	0	0
			11	11		
5	B	25	Total	O	0	0
			25	25		
5	C	28	Total	O	0	0
			28	28		
5	D	8	Total	O	0	0
			8	8		

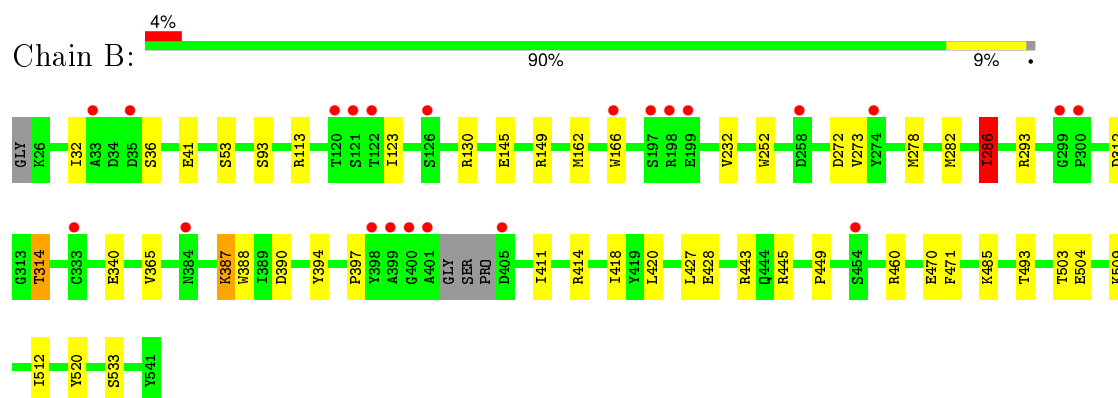
### 3 Residue-property plots

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.

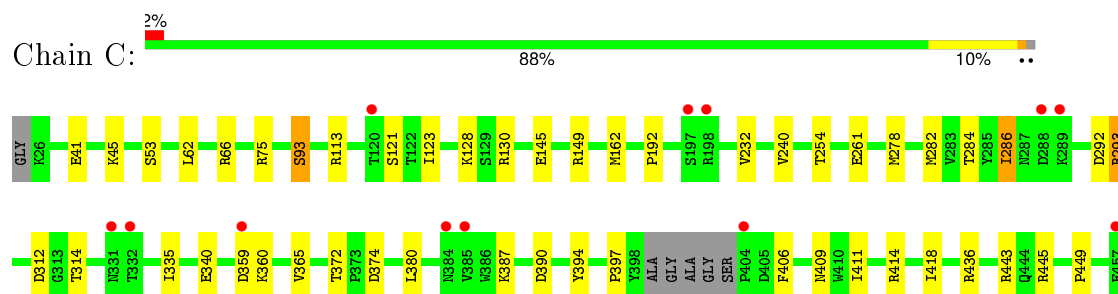
#### • Molecule 1: Putative lipoprotein



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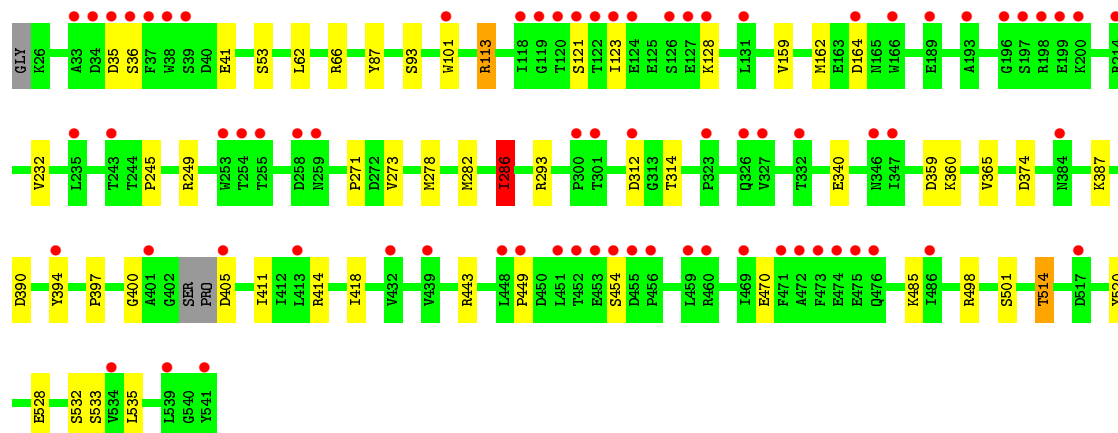
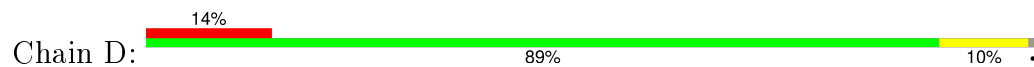


#### • Molecule 1: Putative lipoprotein





● Molecule 1: Putative lipoprotein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.65Å 146.65Å 226.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.90 – 2.70 29.90 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.90-2.70) 99.8 (29.90-2.70)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 2.68Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, $R_{free}$	0.183 , 0.211 0.190 , 0.217	Depositor DCC
$R_{free}$ test set	3910 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.5	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 58.5	EDS
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 77869 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16607	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, CL, ACT

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	0.50	0/4180	0.67	1/5669 (0.0%)
1	B	0.53	0/4250	0.69	1/5749 (0.0%)
1	C	0.54	0/4252	0.70	0/5749
1	D	0.48	0/4163	0.65	1/5650 (0.0%)
All	All	0.51	0/16845	0.68	3/22817 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	286	ILE	CA-CB-CG2	5.28	121.46	110.90
1	D	286	ILE	CA-CB-CG2	5.25	121.39	110.90
1	A	286	ILE	CA-CB-CG2	5.18	121.26	110.90

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	4090	0	3779	27	0
1	B	4157	0	3906	27	0
1	C	4156	0	3917	33	0
1	D	4073	0	3725	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
3	B	15	0	0	0	0
3	C	15	0	0	1	0
4	B	8	0	6	0	0
4	C	16	0	12	2	0
4	D	4	0	3	0	0
5	A	11	0	0	0	0
5	B	25	0	0	0	0
5	C	28	0	0	0	0
5	D	8	0	0	0	0
All	All	16607	0	15348	100	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 3.

All (100) 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:145:GLU:HG2	4:C:609:ACT:H3	1.58	0.84
1:C:162:MSE:HE1	1:D:273:VAL:HA	1.59	0.84
1:C:162:MSE:HE2	1:D:271:PRO:O	1.91	0.71
1:C:145:GLU:CG	4:C:609:ACT:H3	2.23	0.68
1:C:278:MSE:HE2	1:C:282:MSE:HE2	1.76	0.68
1:A:273:VAL:HA	1:B:162:MSE:HE1	1.78	0.65
1:B:282:MSE:HE1	1:B:397:PRO:HG3	1.81	0.63
1:C:406:PHE:HD2	1:D:162:MSE:HG3	1.64	0.62
1:C:130[B]:ARG:HG3	1:C:192:PRO:HD3	1.82	0.61
1:C:406:PHE:CD2	1:D:162:MSE:HG3	2.34	0.61
1:C:93:SER:OG	3:C:606:PO4:O2	2.20	0.60
1:D:278:MSE:HE2	1:D:282:MSE:HE2	1.84	0.59
1:A:282:MSE:HE1	1:A:397:PRO:HG3	1.85	0.59
1:C:443:ARG:NH1	1:C:449:PRO:O	2.35	0.59
1:D:282:MSE:HE1	1:D:397:PRO:HG3	1.85	0.58
1:D:443:ARG:NH1	1:D:449:PRO:O	2.35	0.58
1:D:62:LEU:O	1:D:66:ARG:HG3	2.03	0.58
1:C:240:VAL:O	1:C:445:ARG:HD2	2.04	0.57
1:B:278:MSE:HE2	1:B:282:MSE:HE2	1.87	0.57
1:C:282:MSE:HE1	1:C:397:PRO:HG3	1.86	0.57
1:A:443:ARG:NH1	1:A:449:PRO:O	2.36	0.57
1:B:443:ARG:NH1	1:B:449:PRO:O	2.38	0.56
1:B:312:ASP:OD1	1:B:314:THR:HB	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:MSE:HE2	1:A:282:MSE:HE2	1.85	0.56
1:A:272:ASP:HA	1:B:166:TRP:CH2	2.41	0.56
1:D:113:ARG:HG2	1:D:159:VAL:HG21	1.88	0.55
1:B:512:ILE:HG21	1:C:514:THR:HB	1.90	0.54
1:C:261:GLU:OE1	1:C:445:ARG:NH1	2.42	0.53
1:D:87:TYR:HA	1:D:514:THR:HG23	1.92	0.52
1:C:414:ARG:NH2	1:C:470:GLU:OE2	2.39	0.52
1:C:254:THR:HG22	1:C:409[B]:ASN:OD1	2.10	0.51
1:A:286:ILE:HD11	1:A:365:VAL:HG22	1.92	0.51
1:A:41:GLU:HA	1:A:123:ILE:HD11	1.92	0.51
1:A:166:TRP:CH2	1:B:272:ASP:HA	2.46	0.50
1:D:414:ARG:NH2	1:D:470:GLU:OE2	2.41	0.50
1:B:503:THR:HG23	1:B:504:GLU:HG3	1.94	0.50
1:D:41:GLU:HA	1:D:123:ILE:HD11	1.93	0.50
1:D:374:ASP:OD1	1:D:498:ARG:NH2	2.44	0.49
1:C:411:ILE:HG21	1:C:414:ARG:HG3	1.94	0.49
1:C:62:LEU:O	1:C:66:ARG:HG3	2.12	0.49
1:C:414:ARG:HH21	1:C:445:ARG:HH22	1.60	0.49
1:C:41:GLU:HA	1:C:123:ILE:HD11	1.95	0.48
1:B:41:GLU:HA	1:B:123:ILE:HD11	1.95	0.48
1:D:121:SER:HB3	1:D:128:LYS:HD2	1.96	0.48
1:B:411:ILE:HG21	1:B:414:ARG:HG3	1.94	0.48
1:B:414:ARG:NH2	1:B:470:GLU:OE2	2.47	0.48
1:D:286:ILE:HD11	1:D:365:VAL:HG22	1.96	0.48
1:A:162:MSE:HE1	1:B:273:VAL:HA	1.95	0.47
1:A:312:ASP:OD1	1:A:314:THR:HB	2.15	0.47
1:D:101:TRP:NE1	1:D:528:GLU:HG2	2.30	0.47
1:A:414:ARG:NH2	1:A:470:GLU:OE2	2.45	0.47
1:B:145:GLU:OE1	1:B:149:ARG:NH1	2.49	0.46
1:A:66:ARG:HD2	1:A:85:PHE:HB3	1.98	0.46
1:D:411:ILE:HG21	1:D:414:ARG:HG3	1.97	0.46
1:B:387:LYS:HB3	1:B:388:TRP:H	1.66	0.46
1:C:145:GLU:OE1	1:C:149:ARG:NH1	2.49	0.46
1:C:390:ASP:O	1:C:394:TYR:HB2	2.15	0.46
1:C:293:ARG:NH2	1:D:164:ASP:O	2.48	0.46
1:C:121:SER:HB3	1:C:128:LYS:HD2	1.97	0.45
1:A:411:ILE:HG21	1:A:414:ARG:HG3	1.96	0.45
1:A:272:ASP:HA	1:B:166:TRP:CZ2	2.52	0.45
1:A:62:LEU:O	1:A:66:ARG:HG3	2.17	0.45
1:A:420:LEU:HD12	1:A:471:PHE:HE2	1.83	0.44
1:B:493:THR:HG21	1:B:509:LYS:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:SER:HB3	1:A:276:ASN:HA	2.00	0.44
1:D:312:ASP:OD1	1:D:314:THR:HB	2.17	0.44
1:A:121:SER:HB3	1:A:128:LYS:HD2	2.00	0.44
1:A:485:LYS:HA	1:A:520:TYR:CE1	2.52	0.44
1:B:286:ILE:HD11	1:B:365:VAL:HG22	1.99	0.44
1:B:428:GLU:OE2	1:B:460:ARG:HD3	2.18	0.44
1:D:245:PRO:O	1:D:249:ARG:HG3	2.17	0.44
1:C:312:ASP:OD1	1:C:314:THR:HB	2.18	0.43
1:D:532:SER:HB3	1:D:535:LEU:HB2	2.00	0.43
1:A:50:ASP:HA	1:B:32:ILE:HD12	2.01	0.43
1:A:232:VAL:HG11	1:A:418:ILE:HG13	2.00	0.43
1:C:232:VAL:HG11	1:C:418:ILE:HG13	2.00	0.43
1:B:390:ASP:O	1:B:394:TYR:HB2	2.19	0.43
1:C:284:THR:O	1:C:292:ASP:HA	2.18	0.43
1:C:411:ILE:CG2	1:C:414:ARG:HG3	2.49	0.43
1:A:436:ARG:HD2	1:A:451:LEU:O	2.18	0.43
1:C:286:ILE:HD11	1:C:365:VAL:HG22	2.00	0.43
1:A:390:ASP:O	1:A:394:TYR:HB2	2.19	0.42
1:C:445:ARG:CG	1:C:445:ARG:O	2.65	0.42
1:A:170:ARG:HG3	1:A:535:LEU:HD12	2.02	0.42
1:C:359:ASP:O	1:C:360:LYS:HB2	2.19	0.42
1:A:443:ARG:HD2	1:A:451:LEU:HG	2.01	0.42
1:C:75:ARG:CZ	1:C:380:LEU:HD13	2.49	0.42
1:A:114:PHE:CD1	1:A:135:VAL:HG21	2.55	0.42
1:D:359:ASP:O	1:D:360:LYS:HB2	2.20	0.42
1:B:411:ILE:CG2	1:B:414:ARG:HG3	2.50	0.42
1:B:252:TRP:CH2	1:B:387:LYS:HE3	2.55	0.42
1:D:390:ASP:O	1:D:394:TYR:HB2	2.19	0.42
1:D:411:ILE:CG2	1:D:414:ARG:HG3	2.50	0.41
1:C:485:LYS:HA	1:C:520:TYR:CE1	2.55	0.41
1:D:485:LYS:HA	1:D:520:TYR:CE1	2.55	0.41
1:B:485:LYS:HA	1:B:520:TYR:CE1	2.55	0.41
1:D:232:VAL:HG11	1:D:418:ILE:HG13	2.02	0.41
1:A:272:ASP:HB3	1:B:166:TRP:CZ3	2.56	0.40
1:B:232:VAL:HG11	1:B:418:ILE:HG13	2.02	0.40
1:B:420:LEU:HD12	1:B:471:PHE:HE2	1.87	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	508/517 (98%)	490 (96%)	16 (3%)	2 (0%)	39	69
1	B	510/517 (99%)	495 (97%)	13 (2%)	2 (0%)	39	69
1	C	509/517 (98%)	497 (98%)	10 (2%)	2 (0%)	39	69
1	D	510/517 (99%)	492 (96%)	15 (3%)	3 (1%)	30	59
All	All	2037/2068 (98%)	1974 (97%)	54 (3%)	9 (0%)	39	69

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	36	SER
1	D	387	LYS
1	A	36	SER
1	A	387	LYS
1	B	387	LYS
1	D	36	SER
1	C	387	LYS
1	D	400	GLY
1	C	335	ILE

### 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	420/445 (94%)	407 (97%)	13 (3%)	47	78
1	B	434/445 (98%)	423 (98%)	11 (2%)	55	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	436/445 (98%)	424 (97%)	12 (3%)	51	81
1	D	415/445 (93%)	403 (97%)	12 (3%)	50	80
All	All	1705/1780 (96%)	1657 (97%)	48 (3%)	51	81

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	SER
1	A	81	SER
1	A	93	SER
1	A	113	ARG
1	A	286	ILE
1	A	293	ARG
1	A	314	THR
1	A	340	GLU
1	A	427	LEU
1	A	436	ARG
1	A	445	ARG
1	A	454	SER
1	A	533	SER
1	B	53	SER
1	B	93	SER
1	B	113	ARG
1	B	130	ARG
1	B	286	ILE
1	B	293	ARG
1	B	314	THR
1	B	340	GLU
1	B	427	LEU
1	B	445	ARG
1	B	533	SER
1	C	45	LYS
1	C	53	SER
1	C	93	SER
1	C	113	ARG
1	C	286	ILE
1	C	293	ARG
1	C	340	GLU
1	C	372	THR
1	C	374	ASP
1	C	436	ARG

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Mol	Chain	Res	Type
1	C	533	SER
1	C	539	LEU
1	D	35	ASP
1	D	53	SER
1	D	93	SER
1	D	113	ARG
1	D	286	ILE
1	D	293	ARG
1	D	340	GLU
1	D	405	ASP
1	D	454	SER
1	D	501	SER
1	D	514	THR
1	D	533	SER

Some 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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	601	-	4,4,4	2.39	3 (75%)	6,6,6	0.33	0
3	PO4	B	602	-	4,4,4	4.08	3 (75%)	6,6,6	0.41	0
3	PO4	B	604	-	4,4,4	1.35	1 (25%)	6,6,6	0.25	0
4	ACT	B	607	-	1,3,3	3.65	1 (100%)	0,3,3	0.00	-
4	ACT	B	608	-	1,3,3	7.21	1 (100%)	0,3,3	0.00	-
3	PO4	C	603	-	4,4,4	4.13	3 (75%)	6,6,6	0.49	0
3	PO4	C	605	-	4,4,4	2.14	3 (75%)	6,6,6	0.42	0
3	PO4	C	606	-	4,4,4	1.92	1 (25%)	6,6,6	0.32	0
4	ACT	C	609	-	1,3,3	3.61	1 (100%)	0,3,3	0.00	-
4	ACT	C	610	-	1,3,3	7.42	1 (100%)	0,3,3	0.00	-
4	ACT	C	611	-	1,3,3	8.31	1 (100%)	0,3,3	0.00	-
4	ACT	C	612	-	1,3,3	2.92	1 (100%)	0,3,3	0.00	-
4	ACT	D	613	-	1,3,3	6.13	1 (100%)	0,3,3	0.00	-

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	601	-	-	0/0/0/0	0/0/0/0
3	PO4	B	602	-	-	0/0/0/0	0/0/0/0
3	PO4	B	604	-	-	0/0/0/0	0/0/0/0
4	ACT	B	607	-	-	0/0/0/0	0/0/0/0
4	ACT	B	608	-	-	0/0/0/0	0/0/0/0
3	PO4	C	603	-	-	0/0/0/0	0/0/0/0
3	PO4	C	605	-	-	0/0/0/0	0/0/0/0
3	PO4	C	606	-	-	0/0/0/0	0/0/0/0
4	ACT	C	609	-	-	0/0/0/0	0/0/0/0
4	ACT	C	610	-	-	0/0/0/0	0/0/0/0
4	ACT	C	611	-	-	0/0/0/0	0/0/0/0
4	ACT	C	612	-	-	0/0/0/0	0/0/0/0
4	ACT	D	613	-	-	0/0/0/0	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	605	PO4	P-O2	2.12	1.61	1.53
3	B	604	PO4	P-O2	2.14	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	PO4	P-O1	2.15	1.61	1.52
3	C	605	PO4	P-O3	2.28	1.61	1.53
3	C	605	PO4	P-O4	2.69	1.63	1.53
3	B	601	PO4	P-O3	2.78	1.63	1.53
3	C	606	PO4	P-O3	2.92	1.63	1.53
3	B	601	PO4	P-O2	2.92	1.63	1.53
4	C	612	ACT	CH3-C	2.92	1.52	1.48
3	B	602	PO4	P-O4	3.26	1.65	1.53
4	C	609	ACT	CH3-C	3.61	1.53	1.48
4	B	607	ACT	CH3-C	3.65	1.53	1.48
3	C	603	PO4	P-O2	4.01	1.67	1.53
3	B	602	PO4	P-O1	4.09	1.70	1.52
3	C	603	PO4	P-O3	4.32	1.68	1.53
3	C	603	PO4	P-O4	5.60	1.73	1.53
4	D	613	ACT	CH3-C	6.13	1.57	1.48
3	B	602	PO4	P-O2	6.14	1.75	1.53
4	B	608	ACT	CH3-C	7.21	1.58	1.48
4	C	610	ACT	CH3-C	7.42	1.59	1.48
4	C	611	ACT	CH3-C	8.31	1.60	1.48

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	C	606	PO4	1	0
4	C	609	ACT	2	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	501/517 (96%)	0.24	38 (7%) 17 15	45, 75, 109, 145	0
1	B	502/517 (97%)	0.10	22 (4%) 38 37	39, 58, 94, 121	0
1	C	500/517 (96%)	-0.05	12 (2%) 62 62	39, 57, 86, 116	0
1	D	503/517 (97%)	0.68	74 (14%) 3 2	57, 89, 120, 147	0
All	All	2006/2068 (97%)	0.24	146 (7%) 18 16	39, 69, 109, 147	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	197	SER	7.6
1	B	122	THR	6.3
1	B	399	ALA	5.5
1	D	471	PHE	5.5
1	D	120	THR	5.2
1	D	255	THR	5.1
1	D	452	THR	5.1
1	D	472	ALA	5.0
1	D	198	ARG	4.9
1	D	119	GLY	4.8
1	A	271	PRO	4.7
1	B	401	ALA	4.5
1	D	35	ASP	4.5
1	A	199	GLU	4.4
1	D	124	GLU	4.4
1	D	37	PHE	4.2
1	D	123	ILE	4.2
1	B	197	SER	4.1
1	D	121	SER	4.1
1	D	453	GLU	4.0
1	D	199	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	122	THR	3.9
1	D	456	PRO	3.9
1	A	196	GLY	3.8
1	B	198	ARG	3.8
1	D	449	PRO	3.7
1	A	39	SER	3.7
1	C	289	LYS	3.7
1	B	400	GLY	3.6
1	A	35	ASP	3.6
1	A	274	TYR	3.5
1	C	197	SER	3.4
1	A	123	ILE	3.4
1	D	300	PRO	3.4
1	D	118	ILE	3.4
1	A	197	SER	3.4
1	D	405	ASP	3.4
1	B	199	GLU	3.4
1	D	254	THR	3.3
1	D	451	LEU	3.3
1	D	473	PHE	3.3
1	A	401	ALA	3.3
1	D	258	ASP	3.3
1	D	455	ASP	3.3
1	A	472	ALA	3.3
1	A	120	THR	3.2
1	A	198	ARG	3.2
1	D	469	ILE	3.2
1	D	323	PRO	3.2
1	D	346	ASN	3.2
1	D	193	ALA	3.2
1	B	120	THR	3.2
1	D	196	GLY	3.2
1	D	401	ALA	3.2
1	D	474	GLU	3.1
1	C	120	THR	3.1
1	D	454	SER	3.1
1	D	34	ASP	3.1
1	A	166	TRP	3.1
1	C	359	ASP	3.1
1	A	429	THR	3.0
1	D	200	LYS	3.0
1	B	398	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	332	THR	3.0
1	D	476	GLN	3.0
1	B	166	TRP	2.9
1	D	39	SER	2.9
1	D	432	VAL	2.9
1	D	38	TRP	2.9
1	D	36	SER	2.9
1	A	195	TYR	2.9
1	C	331	ASN	2.9
1	A	406	PHE	2.9
1	A	126	SER	2.8
1	A	432	VAL	2.8
1	D	332	THR	2.8
1	D	235	LEU	2.8
1	B	33	ALA	2.7
1	D	517	ASP	2.7
1	A	273	VAL	2.7
1	A	118	ILE	2.7
1	D	459	LEU	2.6
1	A	37	PHE	2.6
1	D	127	GLU	2.6
1	D	539	LEU	2.6
1	D	131	LEU	2.6
1	A	399	ALA	2.5
1	D	448	LEU	2.5
1	B	274	TYR	2.5
1	A	167	GLU	2.5
1	D	347	ILE	2.5
1	D	541	TYR	2.5
1	D	327	VAL	2.5
1	D	126	SER	2.5
1	D	394	TYR	2.5
1	D	166	TRP	2.5
1	D	460	ARG	2.5
1	D	214	ARG	2.5
1	D	189	GLU	2.4
1	B	35	ASP	2.4
1	D	413	LEU	2.4
1	D	326	GLN	2.4
1	A	38	TRP	2.4
1	C	288	ASP	2.4
1	B	300	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	534	VAL	2.4
1	D	33	ALA	2.3
1	D	259	ASN	2.3
1	A	268	TYR	2.3
1	C	404	PRO	2.3
1	A	476	GLN	2.3
1	A	394	TYR	2.3
1	D	312	ASP	2.3
1	A	163	GLU	2.2
1	A	124	GLU	2.2
1	D	101	TRP	2.2
1	B	405	ASP	2.2
1	B	121	SER	2.2
1	D	439	VAL	2.2
1	D	128	LYS	2.2
1	C	385	VAL	2.2
1	A	527	ASP	2.2
1	A	430	GLY	2.2
1	D	384	ASN	2.2
1	B	258	ASP	2.2
1	A	160	LEU	2.1
1	D	301	THR	2.2
1	B	126	SER	2.1
1	A	209	TYR	2.1
1	C	457	GLU	2.1
1	D	243	THR	2.1
1	B	384	ASN	2.1
1	A	127	GLU	2.1
1	A	129	SER	2.1
1	B	299	GLY	2.1
1	A	117	ARG	2.1
1	C	198	ARG	2.1
1	C	384	ASN	2.1
1	B	333	CYS	2.1
1	D	475	GLU	2.1
1	D	253	TRP	2.1
1	D	164	ASP	2.1
1	B	454	SER	2.1
1	A	473	PHE	2.1
1	A	122	THR	2.0
1	D	486	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	PO4	B	602	5/5	0.84	0.29	9.35	81,83,89,92	0
4	ACT	C	612	4/4	0.69	0.34	9.32	86,87,88,88	0
3	PO4	C	605	5/5	0.76	0.32	8.89	128,131,133,135	0
3	PO4	C	603	5/5	0.89	0.24	7.09	81,81,85,88	0
4	ACT	B	608	4/4	0.94	0.43	6.93	58,59,62,63	0
4	ACT	C	610	4/4	0.90	0.35	6.78	54,59,61,64	0
4	ACT	C	609	4/4	0.91	0.27	5.58	55,56,58,60	0
4	ACT	C	611	4/4	0.84	0.25	2.72	57,61,62,63	0
3	PO4	B	601	5/5	0.88	0.23	1.46	107,111,113,115	0
4	ACT	D	613	4/4	0.78	0.20	0.79	67,70,70,70	0
4	ACT	B	607	4/4	0.91	0.21	0.76	62,65,66,66	0
3	PO4	B	604	5/5	0.98	0.13	-0.27	70,75,78,79	0
2	CL	B	600	1/1	0.75	0.23	-0.36	88,88,88,88	0
3	PO4	C	606	5/5	0.96	0.13	-0.91	78,81,86,86	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.