



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 25, 2023 – 06:45 AM EST

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

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>.

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 : 2.31.2
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) : 2.31.2

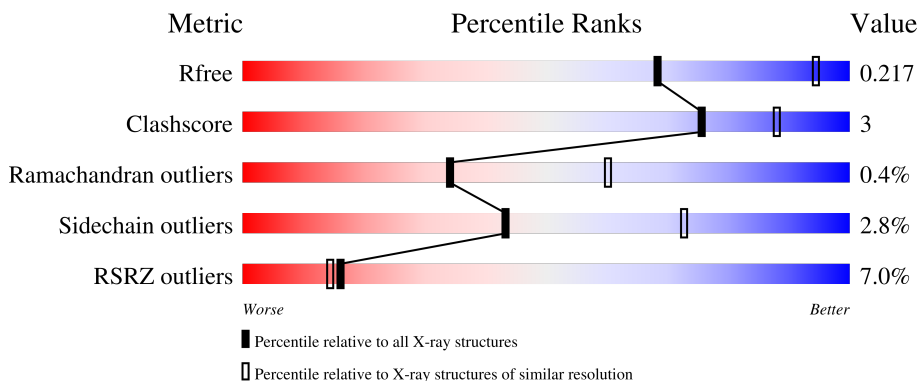
1 Overall quality at a glance

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	517	 7% 89% 9% .
1	B	517	 4% 90% 9% .
1	C	517	 2% 88% 10% ..
1	D	517	 14% 89% 10% .

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	601	-	X	-	-
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	D	613	-	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
			Total	C	N	O	S	Se			
1	A	512	4090	2600	680	794	5	11	0	0	0
1	B	513	4157	2642	697	802	5	11	0	1	0
1	C	511	4156	2642	696	802	5	11	0	2	0
1	D	514	4073	2585	676	796	5	11	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q5L904
B	0	GLY	-	expression tag	UNP Q5L904
C	0	GLY	-	expression tag	UNP Q5L904
D	0	GLY	-	expression tag	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: O₄P).



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: C₂H₃O₂).



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

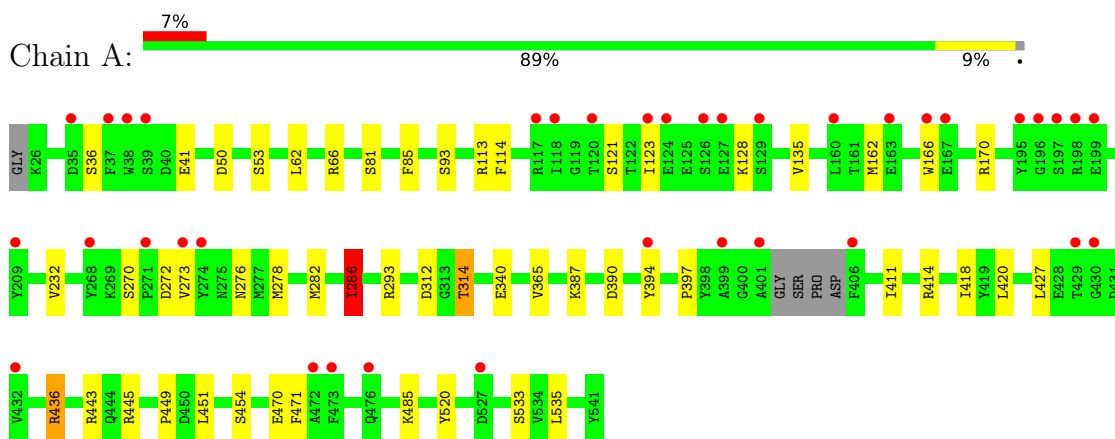
- Molecule 5 is water.

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

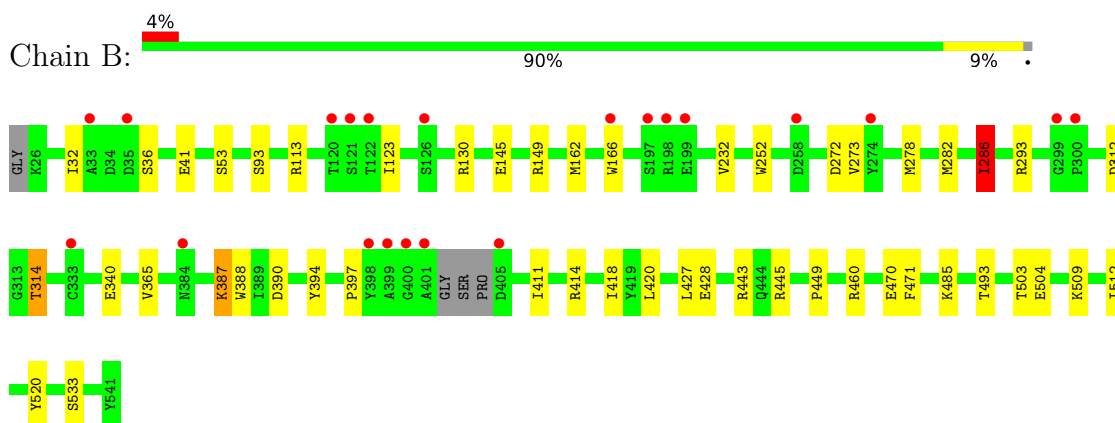
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

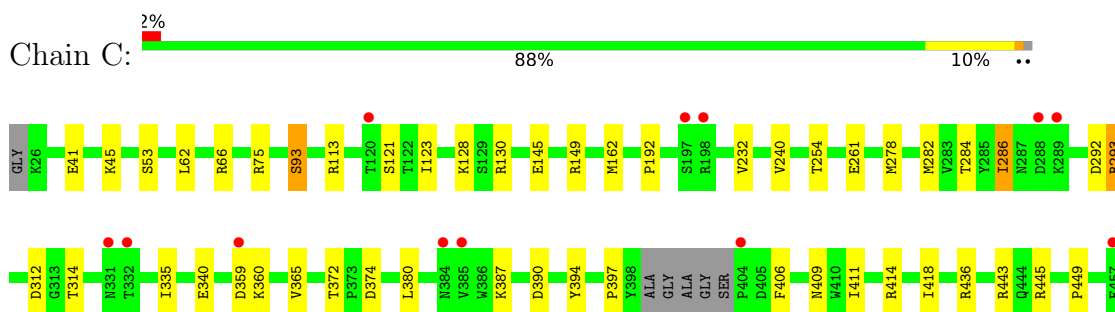
- Molecule 1: Putative lipoprotein



- Molecule 1: Putative lipoprotein



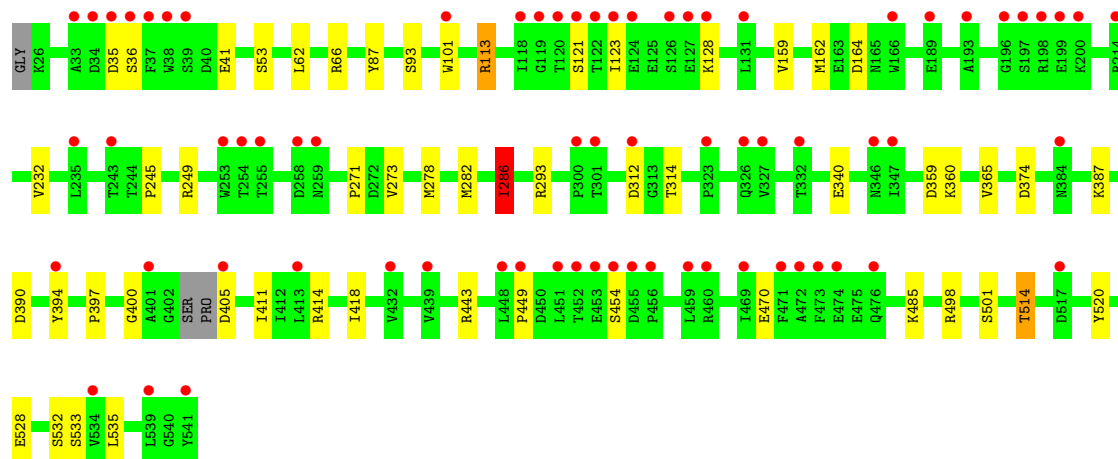
- Molecule 1: Putative lipoprotein





● Molecule 1: Putative lipoprotein

Chain D: 14% 89% 10%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.68Å)	Xtrriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.183 , 0.211 0.190 , 0.217	Depositor DCC
R_{free} test set	3910 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	61.5	Xtrriage
Anisotropy	0.402	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16607	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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, 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:A:443:ARG:NH1	1:A:449:PRO:O	2.36	0.57
1:C:282:MSE:HE1	1:C:397:PRO:HG3	1.86	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: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:121:SER:HB3	1:D:128:LYS:HD2	1.96	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:A:66:ARG:HD2	1:A:85:PHE:HB3	1.98	0.46
1:B:145:GLU:OE1	1:B:149:ARG:NH1	2.49	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:62:LEU:O	1:A:66:ARG:HG3	2.17	0.45
1:A:272:ASP:HA	1:B:166:TRP:CZ2	2.52	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:A:121:SER:HB3	1:A:128:LYS:HD2	2.00	0.44
1:D:312:ASP:OD1	1:D:314:THR:HB	2.17	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:B:390:ASP:O	1:B:394:TYR:HB2	2.19	0.43
1:C:232:VAL:HG11	1:C:418:ILE:HG13	2.00	0.43
1:C:284:THR:O	1:C:292:ASP:HA	2.18	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:C:411:ILE:CG2	1:C:414:ARG:HG3	2.49	0.43
1:A:390:ASP:O	1:A:394:TYR:HB2	2.19	0.42
1:A:170:ARG:HG3	1:A:535:LEU:HD12	2.02	0.42
1:C:445:ARG:O	1:C:445:ARG:CG	2.65	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:A:114:PHE:CD1	1:A:135:VAL:HG21	2.55	0.42
1:C:75:ARG:CZ	1:C:380:LEU:HD13	2.49	0.42
1:D:359:ASP:O	1:D:360:LYS:HB2	2.20	0.42
1:B:252:TRP:CH2	1:B:387:LYS:HE3	2.55	0.42
1:B:411:ILE:CG2	1:B:414:ARG:HG3	2.50	0.42
1:D:390:ASP:O	1:D:394:TYR:HB2	2.19	0.42
1:C:485:LYS:HA	1:C:520:TYR:CE1	2.55	0.41
1:D:411:ILE:CG2	1:D:414:ARG:HG3	2.50	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 [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	508/517 (98%)	490 (96%)	16 (3%)	2 (0%)	34	60
1	B	510/517 (99%)	495 (97%)	13 (2%)	2 (0%)	34	60
1	C	509/517 (98%)	497 (98%)	10 (2%)	2 (0%)	34	60
1	D	510/517 (99%)	492 (96%)	15 (3%)	3 (1%)	25	50
All	All	2037/2068 (98%)	1974 (97%)	54 (3%)	9 (0%)	34	60

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 [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	420/445 (94%)	407 (97%)	13 (3%)	40	69
1	B	434/445 (98%)	423 (98%)	11 (2%)	47	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	436/445 (98%)	424 (97%)	12 (3%)	43	73
1	D	415/445 (93%)	403 (97%)	12 (3%)	42	71
All	All	1705/1780 (96%)	1657 (97%)	48 (3%)	43	73

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

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 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
4	ACT	D	613	-	3,3,3	2.01	1 (33%)	3,3,3	3.21	2 (66%)
4	ACT	C	610	-	3,3,3	1.47	1 (33%)	3,3,3	2.69	2 (66%)
4	ACT	B	608	-	3,3,3	2.31	2 (66%)	3,3,3	1.77	1 (33%)
3	PO4	C	605	-	4,4,4	2.56	4 (100%)	6,6,6	2.04	3 (50%)
4	ACT	C	611	-	3,3,3	1.84	1 (33%)	3,3,3	2.35	2 (66%)
4	ACT	C	612	-	3,3,3	1.20	0	3,3,3	0.79	0
3	PO4	B	604	-	4,4,4	2.01	2 (50%)	6,6,6	0.81	0
4	ACT	C	609	-	3,3,3	2.00	1 (33%)	3,3,3	1.84	2 (66%)
3	PO4	B	601	-	4,4,4	3.22	3 (75%)	6,6,6	1.60	1 (16%)
3	PO4	C	606	-	4,4,4	2.33	2 (50%)	6,6,6	1.47	1 (16%)
3	PO4	C	603	-	4,4,4	4.81	4 (100%)	6,6,6	2.63	3 (50%)
4	ACT	B	607	-	3,3,3	1.03	0	3,3,3	2.58	2 (66%)
3	PO4	B	602	-	4,4,4	5.70	3 (75%)	6,6,6	2.28	4 (66%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	PO4	P-O1	8.28	1.70	1.50
3	B	602	PO4	P-O2	6.94	1.75	1.54
3	C	603	PO4	P-O4	6.29	1.73	1.54
3	C	603	PO4	P-O3	4.76	1.68	1.54
3	B	601	PO4	P-O1	4.67	1.61	1.50
3	C	603	PO4	P-O2	4.40	1.67	1.54
3	B	602	PO4	P-O4	3.50	1.65	1.54
3	B	604	PO4	P-O1	3.37	1.58	1.50
3	C	603	PO4	P-O1	3.31	1.58	1.50
3	B	601	PO4	P-O2	3.09	1.63	1.54
3	C	606	PO4	P-O3	3.09	1.63	1.54
4	B	608	ACT	O-C	3.09	1.36	1.22
4	C	609	ACT	O-C	3.03	1.36	1.22
3	B	601	PO4	P-O3	2.92	1.63	1.54
3	C	605	PO4	P-O1	2.88	1.57	1.50
3	C	606	PO4	P-O1	2.82	1.57	1.50
3	C	605	PO4	P-O4	2.81	1.63	1.54
4	C	611	ACT	CH3-C	2.67	1.60	1.49
4	C	610	ACT	CH3-C	2.38	1.59	1.49
4	D	613	ACT	OXT-C	2.34	1.42	1.30
3	C	605	PO4	P-O3	2.32	1.61	1.54
4	B	608	ACT	CH3-C	2.31	1.58	1.49
3	B	604	PO4	P-O2	2.16	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	605	PO4	P-O2	2.14	1.61	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	613	ACT	O-C-CH3	-4.47	104.94	122.33
3	C	603	PO4	O3-P-O1	-4.34	95.03	110.89
4	C	610	ACT	OXT-C-CH3	3.68	130.37	115.18
3	C	605	PO4	O3-P-O1	-3.66	97.48	110.89
4	B	607	ACT	O-C-CH3	-3.30	109.48	122.33
3	B	602	PO4	O4-P-O3	-3.26	97.49	107.97
3	C	603	PO4	O3-P-O2	3.25	118.39	107.97
3	B	601	PO4	O3-P-O2	3.23	118.32	107.97
4	C	611	ACT	OXT-C-CH3	3.16	128.25	115.18
4	B	607	ACT	OXT-C-CH3	3.02	127.65	115.18
3	B	602	PO4	O3-P-O1	-2.95	100.12	110.89
4	D	613	ACT	OXT-C-CH3	2.88	127.06	115.18
3	C	603	PO4	O2-P-O1	-2.55	101.55	110.89
3	C	605	PO4	O4-P-O3	2.53	116.10	107.97
3	C	606	PO4	O3-P-O2	2.50	116.00	107.97
4	C	610	ACT	OXT-C-O	-2.49	112.88	122.05
4	B	608	ACT	O-C-CH3	2.44	131.82	122.33
4	C	611	ACT	O-C-CH3	-2.41	112.96	122.33
3	B	602	PO4	O4-P-O2	2.31	115.39	107.97
4	C	609	ACT	O-C-CH3	2.28	131.20	122.33
4	C	609	ACT	OXT-C-CH3	-2.22	106.02	115.18
3	C	605	PO4	O3-P-O2	2.14	114.85	107.97
3	B	602	PO4	O3-P-O2	2.03	114.48	107.97

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
4	C	609	ACT	2	0
3	C	606	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, 95th 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 ²)	Q<0.9
1	A	501/517 (96%)	0.20	37 (7%) 14 12	45, 75, 109, 145	0
1	B	502/517 (97%)	0.06	21 (4%) 36 35	39, 58, 94, 121	0
1	C	500/517 (96%)	-0.09	12 (2%) 59 60	39, 57, 86, 116	0
1	D	503/517 (97%)	0.64	71 (14%) 2 1	57, 89, 120, 147	0
All	All	2006/2068 (97%)	0.20	141 (7%) 16 14	39, 69, 109, 147	0

All (141) 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	5.4
1	D	120	THR	5.1
1	D	452	THR	5.0
1	D	255	THR	4.9
1	D	472	ALA	4.9
1	D	198	ARG	4.8
1	D	119	GLY	4.8
1	A	271	PRO	4.7
1	B	401	ALA	4.5
1	D	35	ASP	4.4
1	D	124	GLU	4.3
1	A	199	GLU	4.3
1	D	37	PHE	4.1
1	D	123	ILE	4.1
1	B	197	SER	4.1
1	D	121	SER	4.0
1	D	199	GLU	3.9
1	D	453	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	122	THR	3.9
1	D	456	PRO	3.8
1	A	196	GLY	3.7
1	D	449	PRO	3.7
1	B	198	ARG	3.7
1	A	39	SER	3.6
1	C	289	LYS	3.6
1	B	400	GLY	3.5
1	C	197	SER	3.4
1	A	123	ILE	3.4
1	A	35	ASP	3.4
1	A	274	TYR	3.4
1	D	118	ILE	3.4
1	A	197	SER	3.4
1	D	300	PRO	3.3
1	D	451	LEU	3.3
1	D	254	THR	3.3
1	D	473	PHE	3.3
1	B	199	GLU	3.3
1	D	469	ILE	3.2
1	A	198	ARG	3.2
1	D	405	ASP	3.2
1	A	472	ALA	3.2
1	D	323	PRO	3.2
1	A	120	THR	3.2
1	A	401	ALA	3.2
1	D	346	ASN	3.2
1	D	258	ASP	3.1
1	D	455	ASP	3.1
1	D	196	GLY	3.1
1	B	120	THR	3.1
1	C	120	THR	3.1
1	D	401	ALA	3.1
1	D	474	GLU	3.1
1	D	193	ALA	3.1
1	A	166	TRP	3.0
1	A	429	THR	3.0
1	D	454	SER	3.0
1	D	34	ASP	3.0
1	C	359	ASP	2.9
1	B	398	TYR	2.9
1	D	432	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	332	THR	2.9
1	D	200	LYS	2.9
1	D	39	SER	2.9
1	B	166	TRP	2.9
1	D	38	TRP	2.9
1	D	476	GLN	2.8
1	D	36	SER	2.8
1	A	126	SER	2.8
1	A	406	PHE	2.8
1	C	331	ASN	2.8
1	A	195	TYR	2.8
1	A	432	VAL	2.8
1	B	33	ALA	2.8
1	D	235	LEU	2.8
1	D	332	THR	2.8
1	A	273	VAL	2.7
1	D	517	ASP	2.6
1	A	118	ILE	2.6
1	A	37	PHE	2.6
1	D	131	LEU	2.6
1	D	459	LEU	2.6
1	D	539	LEU	2.5
1	D	127	GLU	2.5
1	D	448	LEU	2.5
1	D	166	TRP	2.5
1	B	274	TYR	2.5
1	A	399	ALA	2.5
1	D	347	ILE	2.5
1	D	126	SER	2.5
1	A	167	GLU	2.4
1	D	541	TYR	2.4
1	D	460	ARG	2.4
1	D	327	VAL	2.4
1	D	394	TYR	2.4
1	D	413	LEU	2.4
1	D	214	ARG	2.4
1	A	38	TRP	2.4
1	D	189	GLU	2.4
1	D	326	GLN	2.3
1	B	35	ASP	2.3
1	C	288	ASP	2.3
1	D	33	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	534	VAL	2.3
1	B	300	PRO	2.3
1	D	259	ASN	2.3
1	A	268	TYR	2.3
1	C	404	PRO	2.2
1	A	476	GLN	2.2
1	D	101	TRP	2.2
1	A	394	TYR	2.2
1	D	439	VAL	2.2
1	B	121	SER	2.2
1	A	124	GLU	2.2
1	A	163	GLU	2.1
1	C	385	VAL	2.1
1	B	405	ASP	2.1
1	D	312	ASP	2.1
1	D	128	LYS	2.1
1	A	430	GLY	2.1
1	B	126	SER	2.1
1	D	301	THR	2.1
1	D	384	ASN	2.1
1	A	160	LEU	2.1
1	A	527	ASP	2.1
1	A	127	GLU	2.1
1	A	209	TYR	2.1
1	C	457	GLU	2.1
1	C	198	ARG	2.1
1	D	243	THR	2.1
1	B	384	ASN	2.0
1	B	299	GLY	2.0
1	A	129	SER	2.0
1	A	473	PHE	2.0
1	A	117	ARG	2.0
1	C	384	ASN	2.0
1	B	258	ASP	2.0
1	B	333	CYS	2.0
1	D	253	TRP	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 [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, 95th 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(Å ²)	Q<0.9
4	ACT	C	612	4/4	0.69	0.33	86,87,88,88	0
2	CL	B	600	1/1	0.74	0.23	88,88,88,88	0
3	PO4	C	605	5/5	0.76	0.32	128,131,133,135	0
4	ACT	D	613	4/4	0.78	0.20	67,70,70,70	0
3	PO4	B	602	5/5	0.84	0.29	81,83,89,92	0
4	ACT	C	611	4/4	0.84	0.24	57,61,62,63	0
3	PO4	B	601	5/5	0.88	0.23	107,111,113,115	0
3	PO4	C	603	5/5	0.89	0.24	81,81,85,88	0
4	ACT	C	610	4/4	0.90	0.35	54,59,61,64	0
4	ACT	B	607	4/4	0.91	0.21	62,65,66,66	0
4	ACT	C	609	4/4	0.91	0.26	55,56,58,60	0
4	ACT	B	608	4/4	0.94	0.42	58,59,62,63	0
3	PO4	C	606	5/5	0.96	0.13	78,81,86,86	0
3	PO4	B	604	5/5	0.98	0.13	70,75,78,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.