



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:33 PM UTC

PDB ID : 3QNK / pdb_00003qnk
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

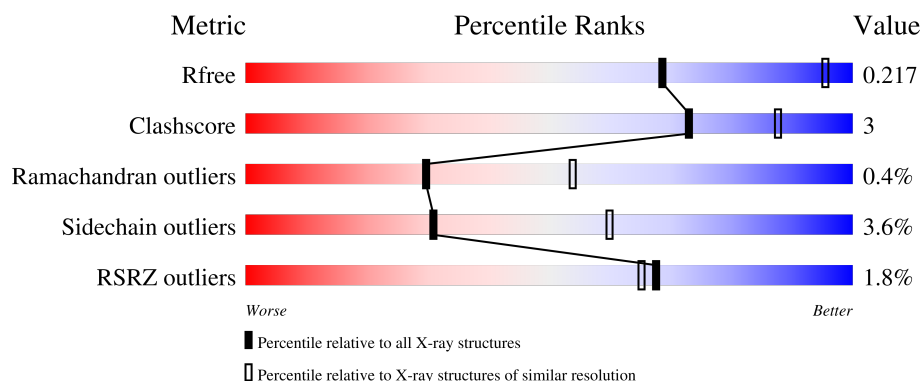
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

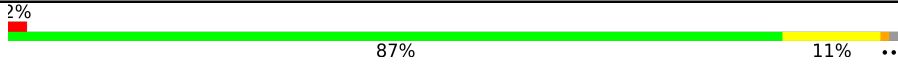
The reported resolution of this entry is 2.70 Å.

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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	 2% 87% 11% ..
1	B	517	 2% 86% 12% ..
1	C	517	 % 85% 12% ..
1	D	517	 2% 87% 11% ..

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
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	-	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 (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: 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 (CCD ID: ACT) (formula: C₂H₃O₂).



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		

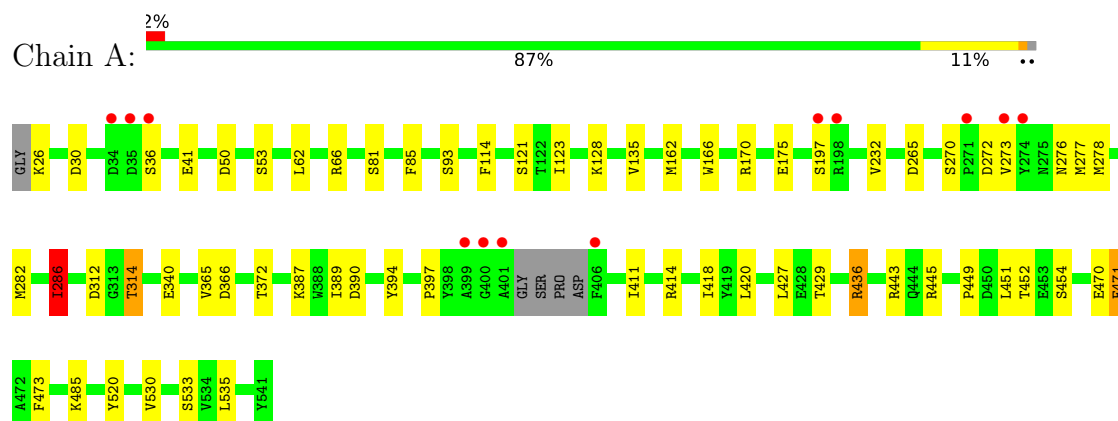
- Molecule 5 is water.

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		

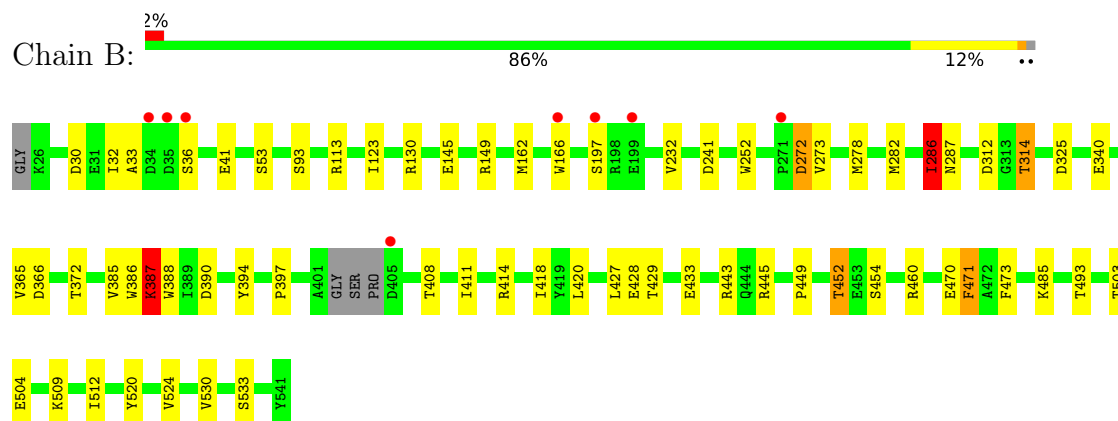
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

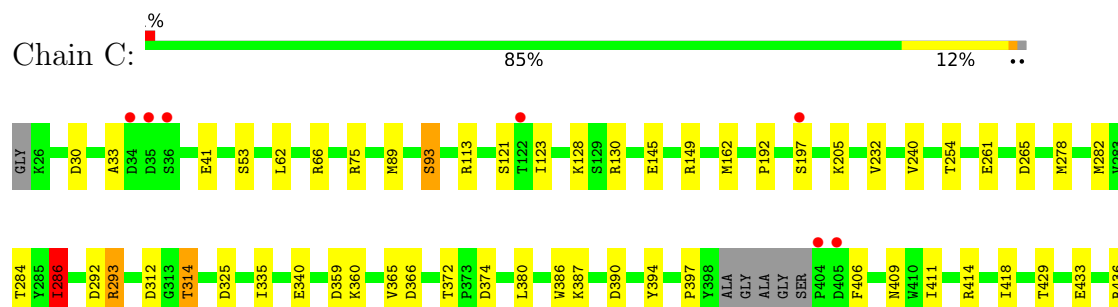
• Molecule 1: Putative lipoprotein



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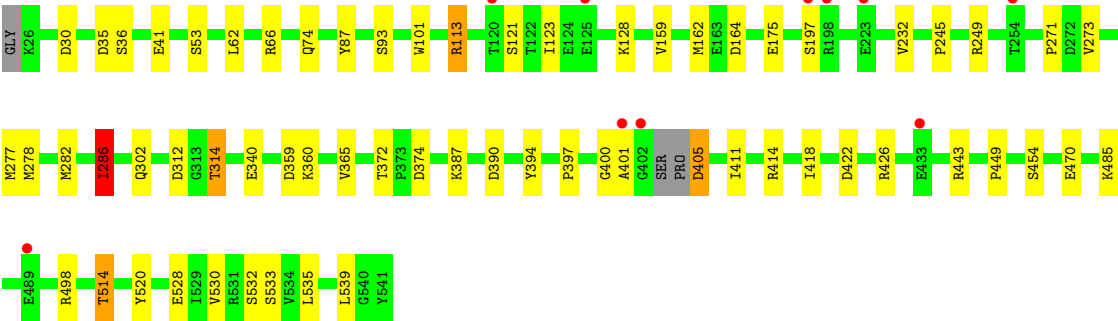
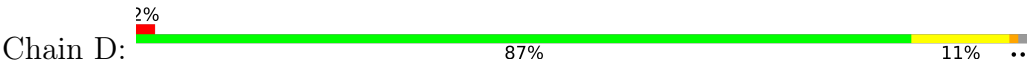


• Molecule 1: Putative lipoprotein





● Molecule 1: Putative lipoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, 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)	Xtriage
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	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 75.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
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

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.*

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: CL, PO4, 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	0.81	1/4180 (0.0%)	1.28	12/5669 (0.2%)
1	B	0.87	2/4250 (0.0%)	1.27	19/5749 (0.3%)
1	C	0.85	1/4252 (0.0%)	1.29	17/5749 (0.3%)
1	D	0.81	2/4163 (0.0%)	1.28	13/5650 (0.2%)
All	All	0.84	6/16845 (0.0%)	1.28	61/22817 (0.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	386	TRP	CA-C	13.30	1.59	1.52
1	D	277	MSE	SE-CE	-5.57	1.78	1.95
1	B	385	VAL	CA-C	5.53	1.59	1.52
1	A	277	MSE	SE-CE	-5.41	1.79	1.95
1	D	401	ALA	CA-C	5.04	1.58	1.52
1	C	386	TRP	CA-C	5.01	1.54	1.52

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	405	ASP	CA-C-N	7.43	134.07	122.78
1	D	405	ASP	C-N-CA	7.43	134.07	122.78
1	A	473	PHE	CA-CB-CG	-7.36	106.44	113.80
1	C	433	GLU	CB-CG-CD	6.76	124.09	112.60
1	B	286	ILE	CA-CB-CG2	6.45	121.46	110.50
1	D	286	ILE	CA-CB-CG2	6.41	121.39	110.50
1	A	286	ILE	CA-CB-CG2	6.33	121.26	110.50
1	B	433	GLU	CB-CG-CD	6.21	123.16	112.60
1	D	30	ASP	CA-CB-CG	5.90	118.50	112.60
1	B	471	PHE	CA-CB-CG	-5.90	107.90	113.80
1	A	530	VAL	CA-C-N	5.87	128.74	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	530	VAL	C-N-CA	5.87	128.74	120.28
1	C	473	PHE	CA-CB-CG	-5.81	107.99	113.80
1	C	33	ALA	CA-C-N	5.78	129.48	120.75
1	C	33	ALA	C-N-CA	5.78	129.48	120.75
1	B	325	ASP	CA-CB-CG	5.70	118.30	112.60
1	B	366	ASP	CA-CB-CG	5.69	118.29	112.60
1	B	524	VAL	N-CA-C	-5.65	103.77	108.63
1	A	30	ASP	CA-CB-CG	5.60	118.20	112.60
1	C	286	ILE	N-CA-CB	-5.59	102.00	111.23
1	B	33	ALA	CA-C-N	5.55	130.25	120.87
1	B	33	ALA	C-N-CA	5.55	130.25	120.87
1	C	286	ILE	CA-CB-CG2	5.52	119.89	110.50
1	A	471	PHE	CA-CB-CG	-5.51	108.29	113.80
1	C	530	VAL	CA-C-N	5.45	128.60	120.31
1	C	530	VAL	C-N-CA	5.45	128.60	120.31
1	A	366	ASP	CA-CB-CG	5.45	118.05	112.60
1	B	530	VAL	CA-C-N	5.44	128.11	120.28
1	B	530	VAL	C-N-CA	5.44	128.11	120.28
1	B	452	THR	N-CA-CB	-5.43	103.12	110.67
1	B	241	ASP	CA-CB-CG	5.43	118.03	112.60
1	D	74	GLN	CA-C-N	5.36	127.78	120.54
1	D	74	GLN	C-N-CA	5.36	127.78	120.54
1	C	205	LYS	CA-C-N	5.32	125.85	119.94
1	C	205	LYS	C-N-CA	5.32	125.85	119.94
1	C	366	ASP	CA-CB-CG	5.28	117.88	112.60
1	D	302	GLN	CA-C-N	5.28	127.35	120.28
1	D	302	GLN	C-N-CA	5.28	127.35	120.28
1	B	286	ILE	N-CA-CB	-5.27	102.54	111.23
1	A	389	ILE	N-CA-CB	5.25	116.99	111.00
1	D	530	VAL	CA-C-N	5.20	128.22	120.31
1	D	530	VAL	C-N-CA	5.20	128.22	120.31
1	A	265	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	197	SER	CA-C-N	5.12	127.10	120.44
1	A	197	SER	C-N-CA	5.12	127.10	120.44
1	D	197	SER	CA-C-N	5.10	127.08	120.44
1	D	197	SER	C-N-CA	5.10	127.08	120.44
1	B	287	ASN	CA-CB-CG	5.10	117.70	112.60
1	C	30	ASP	CA-CB-CG	5.08	117.67	112.60
1	C	325	ASP	CA-CB-CG	5.07	117.67	112.60
1	B	197	SER	CA-C-N	5.07	127.03	120.44
1	B	197	SER	C-N-CA	5.07	127.03	120.44
1	B	473	PHE	CA-CB-CG	-5.06	108.74	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	452	THR	N-CA-CB	-5.05	103.64	110.67
1	B	272	ASP	CA-CB-CG	5.05	117.65	112.60
1	B	30	ASP	CA-CB-CG	5.05	117.65	112.60
1	D	286	ILE	N-CA-CB	-5.05	102.90	111.23
1	C	197	SER	CA-C-N	5.04	127.00	120.44
1	C	197	SER	C-N-CA	5.04	127.00	120.44
1	C	265	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	286	ILE	N-CA-CB	-5.00	102.98	111.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4090	0	3779	27	0
1	B	4157	0	3906	27	0
1	C	4156	0	3917	34	0
1	D	4073	0	3725	27	0
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	102	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 (102) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:261:GLU:CD	1:C:445:ARG:HH12	2.27	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:D:422:ASP:CG	1:D:426:ARG:HE	2.29	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%)	30	54
1	B	510/517 (99%)	495 (97%)	13 (2%)	2 (0%)	30	54
1	C	509/517 (98%)	497 (98%)	10 (2%)	2 (0%)	30	54
1	D	510/517 (99%)	492 (96%)	15 (3%)	3 (1%)	21	44
All	All	2037/2068 (98%)	1974 (97%)	54 (3%)	9 (0%)	30	54

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%)	404 (96%)	16 (4%)	29	58
1	B	434/445 (98%)	418 (96%)	16 (4%)	30	59
1	C	436/445 (98%)	420 (96%)	16 (4%)	30	59
1	D	415/445 (93%)	401 (97%)	14 (3%)	32	62
All	All	1705/1780 (96%)	1643 (96%)	62 (4%)	31	60

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LYS
1	A	53	SER
1	A	81	SER
1	A	93	SER
1	A	175	GLU
1	A	286	ILE
1	A	314	THR
1	A	340	GLU
1	A	372	THR
1	A	427	LEU
1	A	429	THR

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Mol	Chain	Res	Type
1	A	436	ARG
1	A	445	ARG
1	A	452	THR
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	314	THR
1	B	340	GLU
1	B	372	THR
1	B	387	LYS
1	B	408	THR
1	B	427	LEU
1	B	429	THR
1	B	445	ARG
1	B	452	THR
1	B	454	SER
1	B	533	SER
1	C	53	SER
1	C	89	MSE
1	C	93	SER
1	C	113	ARG
1	C	286	ILE
1	C	293	ARG
1	C	314	THR
1	C	340	GLU
1	C	372	THR
1	C	374	ASP
1	C	429	THR
1	C	436	ARG
1	C	452	THR
1	C	454	SER
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	175	GLU

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Mol	Chain	Res	Type
1	D	286	ILE
1	D	314	THR
1	D	340	GLU
1	D	372	THR
1	D	405	ASP
1	D	454	SER
1	D	514	THR
1	D	533	SER
1	D	539	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	B	49	ASN
1	C	49	ASN
1	C	61	GLN
1	C	287	ASN
1	D	49	ASN

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 oligosaccharides 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	3.32	3 (75%)	6,6,6	1.65	1 (16%)
4	ACT	B	607	-	3,3,3	1.08	0	3,3,3	2.53	2 (66%)
4	ACT	C	609	-	3,3,3	2.11	1 (33%)	3,3,3	1.75	2 (66%)
4	ACT	B	608	-	3,3,3	2.45	2 (66%)	3,3,3	1.67	1 (33%)
3	PO4	C	605	-	4,4,4	2.64	4 (100%)	6,6,6	2.12	3 (50%)
3	PO4	B	602	-	4,4,4	5.87	3 (75%)	6,6,6	2.36	4 (66%)
4	ACT	C	611	-	3,3,3	1.95	1 (33%)	3,3,3	2.32	2 (66%)
3	PO4	C	603	-	4,4,4	4.96	4 (100%)	6,6,6	2.74	3 (50%)
3	PO4	B	604	-	4,4,4	2.08	2 (50%)	6,6,6	0.83	0
3	PO4	C	606	-	4,4,4	2.41	2 (50%)	6,6,6	1.52	1 (16%)
4	ACT	C	610	-	3,3,3	1.57	1 (33%)	3,3,3	2.67	2 (66%)
4	ACT	D	613	-	3,3,3	2.10	2 (66%)	3,3,3	3.12	2 (66%)
4	ACT	C	612	-	3,3,3	1.26	0	3,3,3	0.78	0

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	PO4	P-O1	8.52	1.70	1.50
3	B	602	PO4	P-O2	7.15	1.75	1.54
3	C	603	PO4	P-O4	6.48	1.73	1.54
3	C	603	PO4	P-O3	4.90	1.68	1.54
3	B	601	PO4	P-O1	4.83	1.61	1.50
3	C	603	PO4	P-O2	4.53	1.67	1.54
3	B	602	PO4	P-O4	3.60	1.65	1.54
3	B	604	PO4	P-O1	3.51	1.58	1.50
3	C	603	PO4	P-O1	3.45	1.58	1.50
4	B	608	ACT	O-C	3.26	1.36	1.22
4	C	609	ACT	O-C	3.20	1.36	1.22
3	B	601	PO4	P-O2	3.18	1.63	1.54
3	C	606	PO4	P-O3	3.18	1.63	1.54
3	C	605	PO4	P-O1	3.01	1.57	1.50
3	B	601	PO4	P-O3	3.01	1.63	1.54
3	C	606	PO4	P-O1	2.95	1.57	1.50
3	C	605	PO4	P-O4	2.89	1.63	1.54
4	C	611	ACT	CH3-C	2.85	1.60	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	610	ACT	CH3-C	2.54	1.59	1.49
4	B	608	ACT	CH3-C	2.46	1.58	1.49
4	D	613	ACT	OXT-C	2.39	1.42	1.30
3	C	605	PO4	P-O3	2.38	1.61	1.54
3	B	604	PO4	P-O2	2.22	1.61	1.54
3	C	605	PO4	P-O2	2.19	1.61	1.54
4	D	613	ACT	CH3-C	2.08	1.57	1.49

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	603	PO4	O3-P-O1	-4.50	95.03	110.95
4	D	613	ACT	O-C-CH3	-4.29	104.94	122.53
3	C	605	PO4	O3-P-O1	-3.81	97.48	110.95
4	C	610	ACT	OXT-C-CH3	3.65	130.37	115.05
3	C	603	PO4	O3-P-O2	3.37	118.39	107.91
3	B	602	PO4	O4-P-O3	-3.35	97.49	107.91
3	B	601	PO4	O3-P-O2	3.35	118.32	107.91
4	B	607	ACT	O-C-CH3	-3.18	109.48	122.53
4	C	611	ACT	OXT-C-CH3	3.15	128.25	115.05
3	B	602	PO4	O3-P-O1	-3.06	100.12	110.95
4	B	607	ACT	OXT-C-CH3	3.00	127.65	115.05
4	D	613	ACT	OXT-C-CH3	2.86	127.06	115.05
3	C	603	PO4	O2-P-O1	-2.66	101.55	110.95
3	C	605	PO4	O4-P-O3	2.63	116.10	107.91
3	C	606	PO4	O3-P-O2	2.60	116.00	107.91
4	C	610	ACT	OXT-C-O	-2.47	112.88	122.03
3	B	602	PO4	O4-P-O2	2.40	115.39	107.91
4	C	611	ACT	O-C-CH3	-2.33	112.96	122.53
4	B	608	ACT	O-C-CH3	2.27	131.82	122.53
3	C	605	PO4	O3-P-O2	2.23	114.85	107.91
4	C	609	ACT	OXT-C-CH3	-2.15	106.02	115.05
4	C	609	ACT	O-C-CH3	2.12	131.20	122.53
3	B	602	PO4	O3-P-O2	2.11	114.48	107.91

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%)	-0.11	12 (2%) 59 56	45, 75, 109, 145	0
1	B	502/517 (97%)	-0.37	8 (1%) 70 68	39, 58, 94, 121	1 (0%)
1	C	500/517 (96%)	-0.39	7 (1%) 73 72	32, 57, 86, 116	2 (0%)
1	D	503/517 (97%)	0.11	10 (1%) 65 62	57, 89, 120, 147	0
All	All	2006/2068 (97%)	-0.19	37 (1%) 67 65	32, 69, 109, 147	3 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	402	GLY	4.9
1	A	34	ASP	4.8
1	B	34	ASP	4.4
1	A	401	ALA	4.1
1	A	35	ASP	4.1
1	A	271	PRO	4.0
1	B	271	PRO	3.9
1	D	401	ALA	3.8
1	C	404	PRO	3.4
1	D	223	GLU	3.4
1	A	273	VAL	3.2
1	C	34	ASP	3.1
1	C	35	ASP	2.9
1	B	36	SER	2.8
1	A	399	ALA	2.7
1	B	35	ASP	2.7
1	A	406	PHE	2.6
1	A	36	SER	2.5
1	C	197	SER	2.5
1	D	125	GLU	2.5
1	C	405	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	197	SER	2.4
1	A	198	ARG	2.4
1	D	198	ARG	2.4
1	B	199	GLU	2.3
1	B	405	ASP	2.3
1	C	122	THR	2.3
1	C	36	SER	2.2
1	D	254	THR	2.2
1	D	433	GLU	2.1
1	A	400	GLY	2.1
1	A	274	TYR	2.1
1	D	197	SER	2.1
1	B	166	TRP	2.1
1	A	197	SER	2.1
1	D	489	GLU	2.0
1	D	120	THR	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 oligosaccharides 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	D	613	4/4	0.54	0.22	67,70,70,70	0
4	ACT	C	612	4/4	0.67	0.27	86,87,88,88	0
4	ACT	C	611	4/4	0.67	0.16	57,61,62,63	0
3	PO4	C	605	5/5	0.78	0.23	128,131,133,135	0
3	PO4	B	601	5/5	0.79	0.19	107,111,113,115	0
4	ACT	B	608	4/4	0.81	0.26	58,59,62,63	0
4	ACT	C	609	4/4	0.82	0.14	55,56,58,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACT	B	607	4/4	0.84	0.16	62,65,66,66	0
3	PO4	C	603	5/5	0.84	0.25	81,81,85,88	0
3	PO4	B	602	5/5	0.84	0.24	81,83,89,92	0
4	ACT	C	610	4/4	0.85	0.17	54,59,61,64	0
2	CL	B	600	1/1	0.92	0.08	88,88,88,88	0
3	PO4	C	606	5/5	0.96	0.06	78,81,86,86	0
3	PO4	B	604	5/5	0.97	0.07	70,75,78,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.