Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2026 – 10:12 AM JST

PDB ID	:	27BN / pdb_000027bn
Title	:	Crystal structure of sulfolactate sulfolyase, SuyAB from Caballeronia jiangsuensis strain McCoy
Authors	:	Lee, M.
Deposited on	:	2026-05-25
Resolution	:	2.81 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:

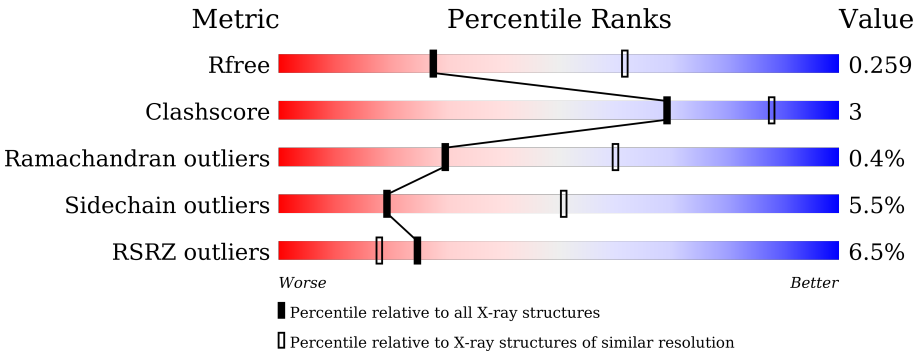
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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.



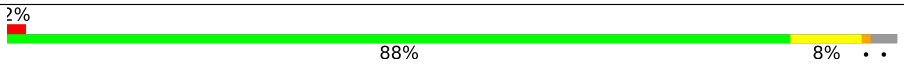
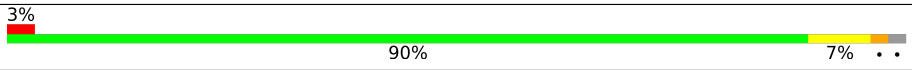
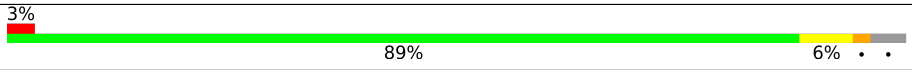
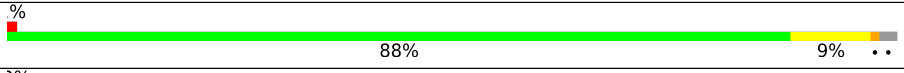
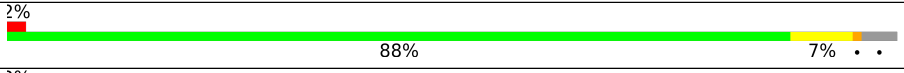
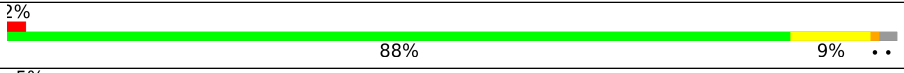
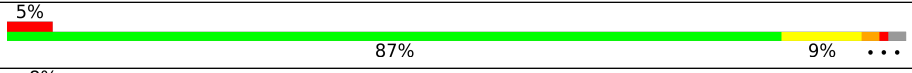
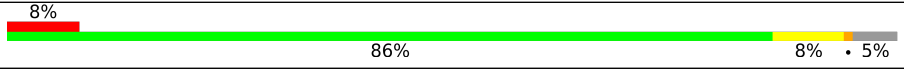
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 <=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	130	18% 58% 12% • 29%
1	C	130	13% 55% 15% • 28%
1	E	130	13% 54% 15% • 28%
1	G	130	8% 53% 17% • 28%
1	I	130	17% 57% 13% • 28%
1	K	130	23% 55% 16% • 28%

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Mol	Chain	Length	Quality of chain
1	M	130	
2	B	391	
2	D	391	
2	F	391	
2	H	391	
2	J	391	
2	L	391	
2	N	391	
2	O	391	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 28138 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 SuyA from Caballeronia jiangsuensis strain McCoy.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	92	Total	C	N	O	S	0	0	0
			699	445	123	129	2			
1	C	93	Total	C	N	O	S	0	0	0
			708	451	125	130	2			
1	E	94	Total	C	N	O	S	0	0	0
			723	462	127	132	2			
1	G	93	Total	C	N	O	S	0	0	0
			708	451	125	130	2			
1	I	93	Total	C	N	O	S	0	0	0
			708	451	125	130	2			
1	K	94	Total	C	N	O	S	0	0	0
			723	462	127	132	2			
1	M	92	Total	C	N	O	S	0	0	0
			699	445	123	129	2			

- Molecule 2 is a protein called SuyB from Caballeronia jiangsuensis strain McCoy.

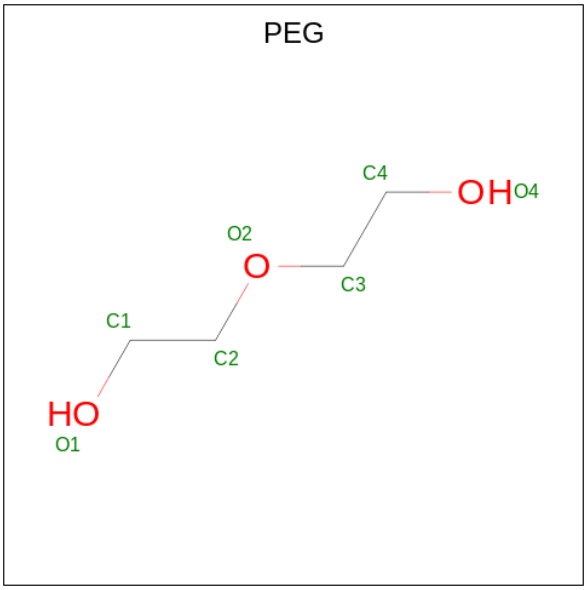
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	381	Total	C	N	O	S	0	0	0
			2880	1799	511	551	19			
2	D	383	Total	C	N	O	S	0	0	0
			2893	1806	513	555	19			
2	F	376	Total	C	N	O	S	0	0	0
			2849	1783	506	542	18			
2	H	383	Total	C	N	O	S	0	0	0
			2893	1806	513	555	19			
2	J	377	Total	C	N	O	S	0	0	0
			2857	1787	507	545	18			
2	L	384	Total	C	N	O	S	0	0	0
			2901	1810	514	558	19			
2	N	384	Total	C	N	O	S	0	0	0
			2901	1810	514	558	19			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	373	Total	C	N	O	S	0	0	0
			2829	1770	503	538	18			

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	1	Total	C	O		0	0
			7	4	3			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O		0	0
			1	1			
4	B	29	Total	O		0	0
			29	29			
4	D	17	Total	O		0	0
			17	17			
4	F	20	Total	O		0	0
			20	20			
4	G	2	Total	O		0	0
			2	2			
4	H	20	Total	O		0	0
			20	20			
4	J	14	Total	O		0	0
			14	14			

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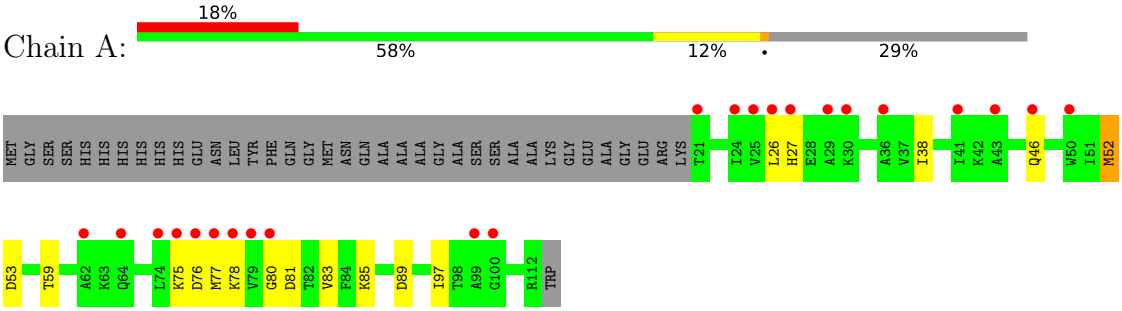
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	26	Total O 26 26	0	0
4	M	2	Total O 2 2	0	0
4	N	19	Total O 19 19	0	0
4	O	10	Total O 10 10	0	0

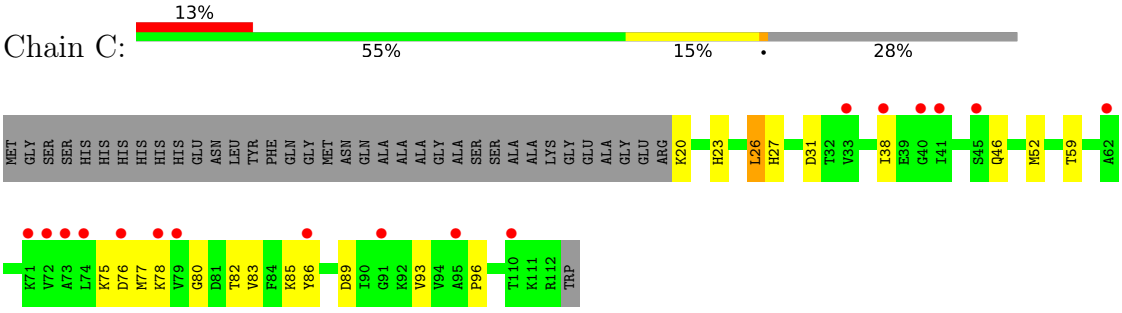
3 Residue-property plots (i)

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.

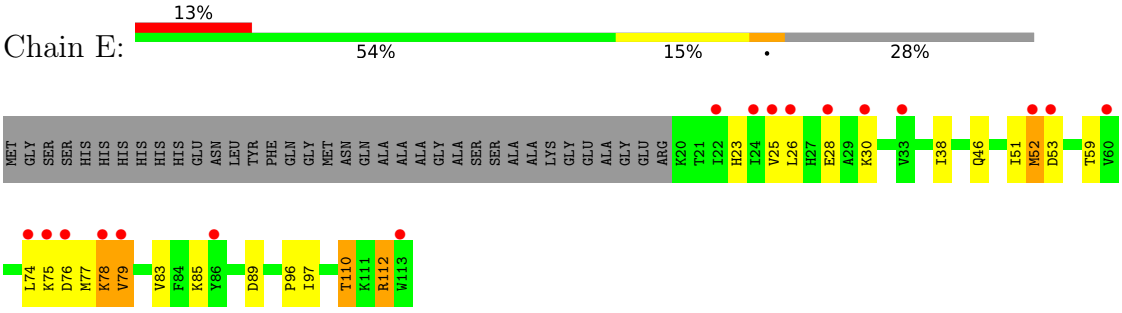
• Molecule 1: SuyA from Caballeronia jiangsuensis strain McCoy



• Molecule 1: SuyA from Caballeronia jiangsuensis strain McCoy

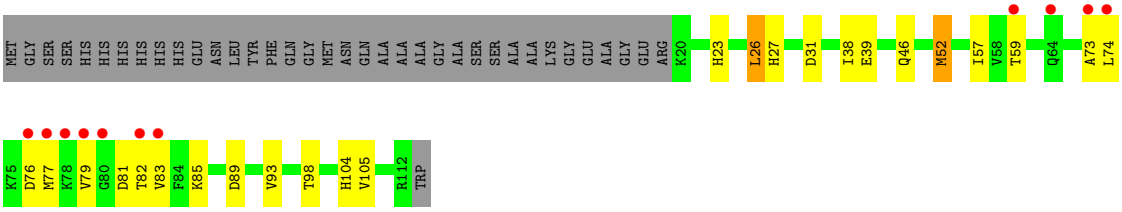


• Molecule 1: SuyA from Caballeronia jiangsuensis strain McCoy



• Molecule 1: SuyA from Caballeronia jiangsuensis strain McCoy

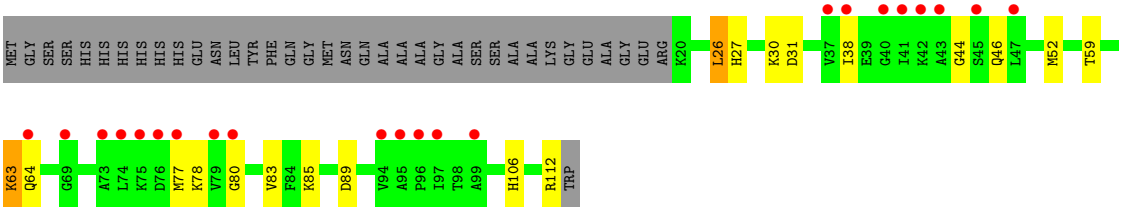




• Molecule 1: SuyA from Caballeronia jiangsuensis strain McCoy

Chain I:

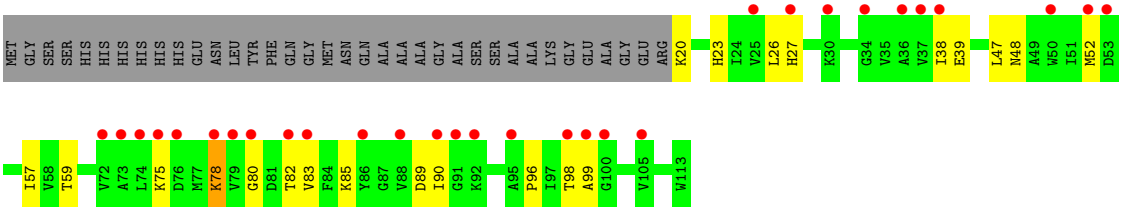




• Molecule 1: SuyA from Caballeronia jiangsuensis strain McCoy

Chain K:

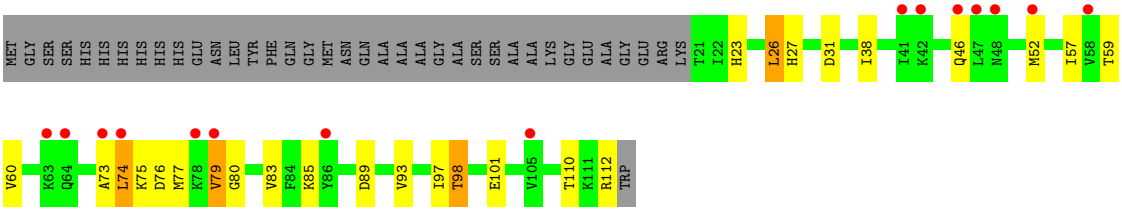




• Molecule 1: SuyA from Caballeronia jiangsuensis strain McCoy

Chain M:

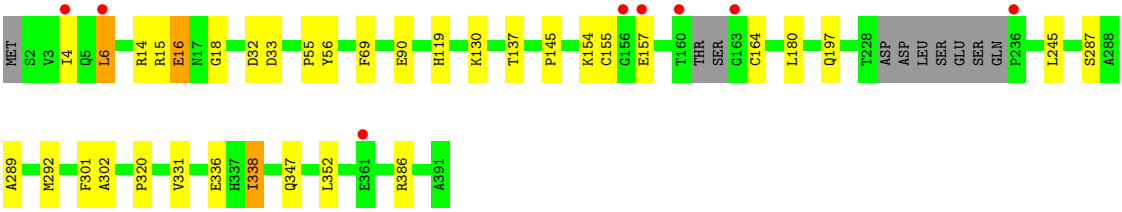




• Molecule 2: SuyB from Caballeronia jiangsuensis strain McCoy

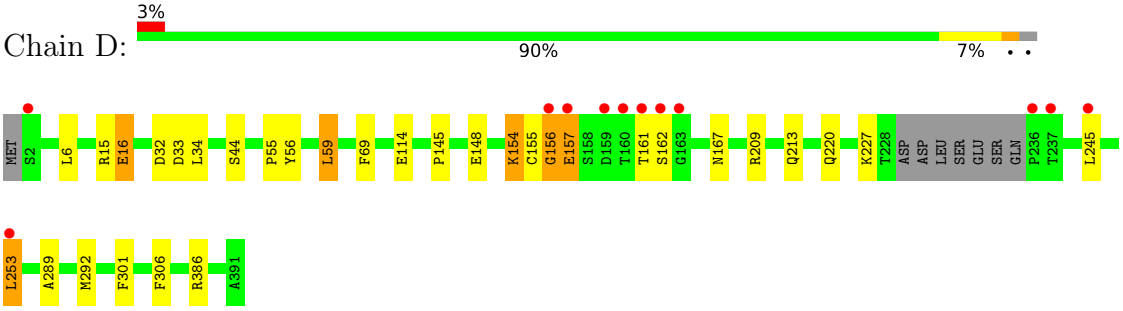
Chain B:





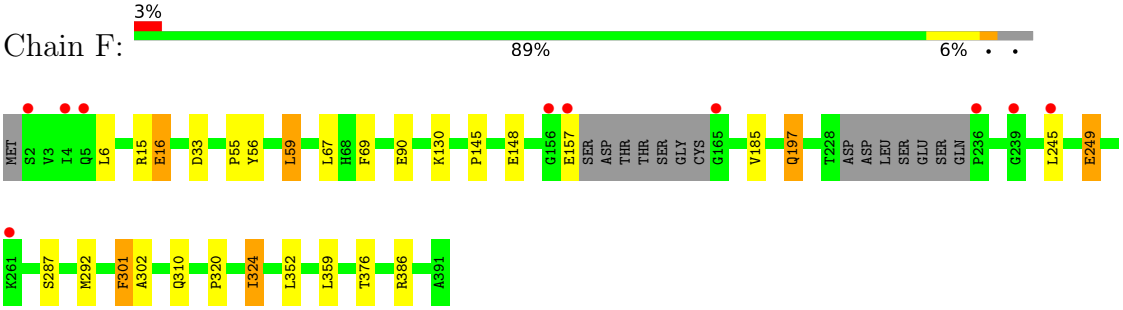
• Molecule 2: SuyB from Caballeronia jiangsuensis strain McCoy

Chain D:



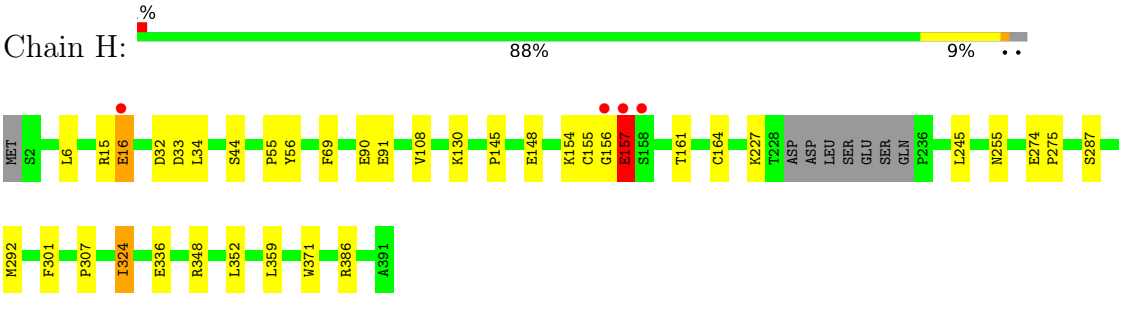
• Molecule 2: SuyB from Caballeronia jiangsuensis strain McCoy

Chain F:



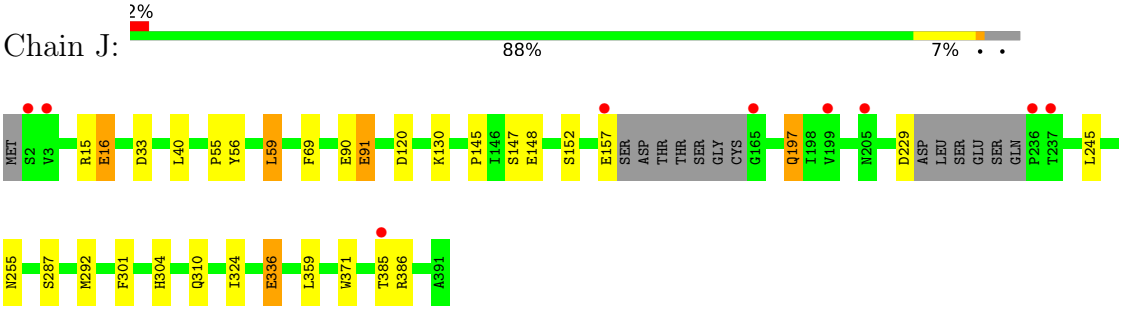
• Molecule 2: SuyB from Caballeronia jiangsuensis strain McCoy

Chain H:



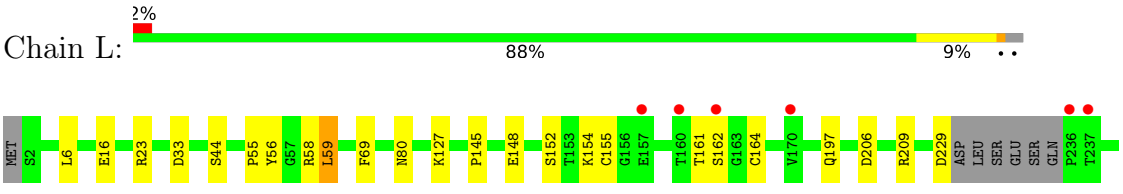
• Molecule 2: SuyB from Caballeronia jiangsuensis strain McCoy

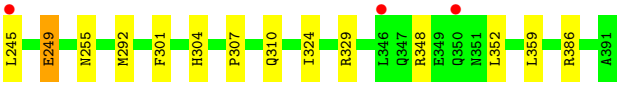
Chain J:



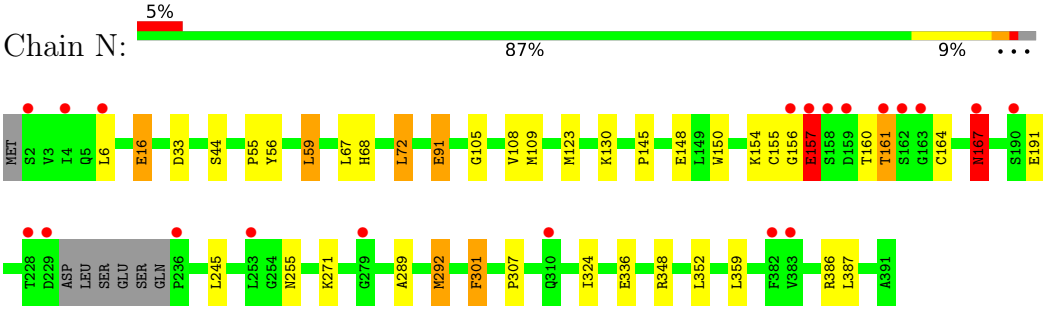
• Molecule 2: SuyB from Caballeronia jiangsuensis strain McCoy

Chain L:

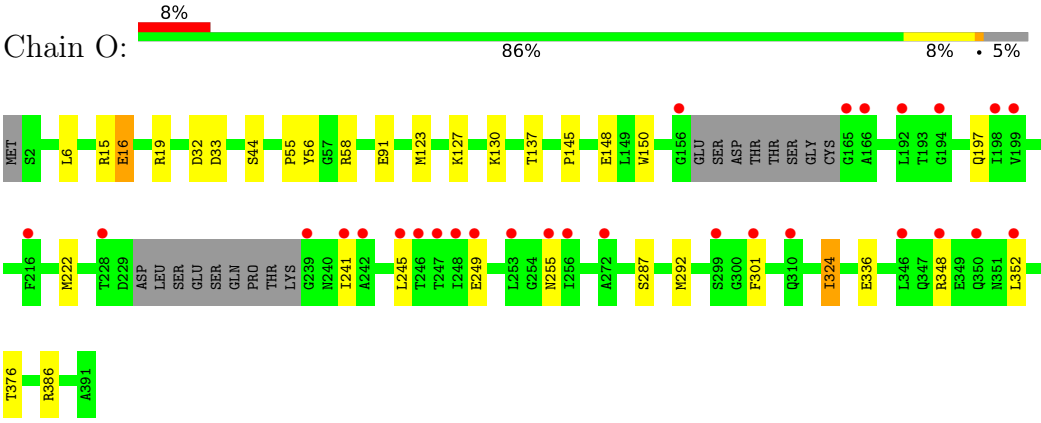




• Molecule 2: SuyB from Caballeronia jiangsuensis strain McCoy



• Molecule 2: SuyB from Caballeronia jiangsuensis strain McCoy



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	95.43Å 104.10Å 125.71Å 86.81° 86.44° 84.20°	Depositor
Resolution (Å)	49.69 – 2.81 49.69 – 2.81	Depositor EDS
% Data completeness (in resolution range)	95.5 (49.69-2.81) 95.5 (49.69-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.246 , 0.268 0.238 , 0.259	Depositor DCC
R_{free} test set	5543 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å^2)	49.7	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 42.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	28138	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.64	0/710	1.08	3/961 (0.3%)
1	C	0.68	0/719	1.08	1/972 (0.1%)
1	E	0.71	0/736	1.14	5/995 (0.5%)
1	G	0.75	0/719	1.18	8/972 (0.8%)
1	I	0.68	0/719	1.07	1/972 (0.1%)
1	K	0.67	0/736	1.08	1/995 (0.1%)
1	M	0.74	0/710	1.09	5/961 (0.5%)
2	B	0.66	1/2928 (0.0%)	1.03	4/3956 (0.1%)
2	D	0.66	0/2942	1.05	6/3977 (0.2%)
2	F	0.62	0/2897	1.02	4/3914 (0.1%)
2	H	0.63	0/2942	1.03	7/3977 (0.2%)
2	J	0.62	0/2905	1.01	5/3925 (0.1%)
2	L	0.62	0/2950	1.02	2/3988 (0.1%)
2	N	0.63	0/2950	1.06	9/3988 (0.2%)
2	O	0.59	0/2876	1.01	3/3885 (0.1%)
All	All	0.64	1/28439 (0.0%)	1.04	64/38438 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	338	ILE	CG1-CD1	-6.89	1.24	1.51

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	81	ASP	CA-CB-CG	8.86	121.46	112.60
2	N	167	ASN	CA-CB-CG	8.33	120.93	112.60
2	N	157	GLU	CB-CG-CD	6.99	124.48	112.60
1	G	89	ASP	CA-CB-CG	6.98	119.58	112.60
1	E	52	MET	CA-C-N	6.69	129.57	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	52	MET	C-N-CA	6.69	129.57	120.54
2	F	301	PHE	CA-CB-CG	-6.53	107.27	113.80
2	L	301	PHE	CA-CB-CG	-6.52	107.28	113.80
2	H	157	GLU	CB-CG-CD	6.46	123.58	112.60
2	D	301	PHE	CA-CB-CG	-6.36	107.44	113.80
2	D	154	LYS	CA-C-N	6.33	130.47	121.42
2	D	154	LYS	C-N-CA	6.33	130.47	121.42
1	I	89	ASP	CA-CB-CG	6.31	118.91	112.60
2	J	301	PHE	CA-CB-CG	-6.21	107.59	113.80
2	N	301	PHE	CA-CB-CG	-6.19	107.61	113.80
1	C	89	ASP	CA-CB-CG	6.16	118.76	112.60
2	B	69	PHE	CA-CB-CG	-6.13	107.67	113.80
2	N	16	GLU	CA-C-N	6.12	130.39	120.60
2	N	16	GLU	C-N-CA	6.12	130.39	120.60
1	G	73	ALA	CA-C-N	6.07	130.81	121.83
1	G	73	ALA	C-N-CA	6.07	130.81	121.83
2	F	15	ARG	CA-C-N	6.06	128.40	120.28
2	F	15	ARG	C-N-CA	6.06	128.40	120.28
2	J	15	ARG	CA-C-N	6.04	128.65	120.38
2	J	15	ARG	C-N-CA	6.04	128.65	120.38
2	O	15	ARG	CA-C-N	6.01	128.62	120.38
2	O	15	ARG	C-N-CA	6.01	128.62	120.38
1	K	89	ASP	CA-CB-CG	5.99	118.59	112.60
2	B	301	PHE	CA-CB-CG	-5.99	107.81	113.80
2	H	301	PHE	CA-CB-CG	-5.98	107.82	113.80
1	A	89	ASP	CA-CB-CG	5.97	118.57	112.60
2	L	69	PHE	CA-CB-CG	-5.95	107.85	113.80
1	M	89	ASP	CA-CB-CG	5.93	118.53	112.60
1	G	81	ASP	N-CA-CB	5.93	119.02	110.06
2	D	15	ARG	CA-C-N	5.80	128.32	120.38
2	D	15	ARG	C-N-CA	5.80	128.32	120.38
2	N	156	GLY	CA-C-N	5.77	132.56	121.54
2	N	156	GLY	C-N-CA	5.77	132.56	121.54
1	A	52	MET	CA-C-N	5.76	128.32	120.54
1	A	52	MET	C-N-CA	5.76	128.32	120.54
1	E	89	ASP	CA-CB-CG	5.75	118.35	112.60
2	D	69	PHE	CA-CB-CG	-5.66	108.14	113.80
2	B	15	ARG	CA-C-N	5.55	128.49	120.38
2	B	15	ARG	C-N-CA	5.55	128.49	120.38
2	H	156	GLY	CA-C-N	5.52	132.08	121.54
2	H	156	GLY	C-N-CA	5.52	132.08	121.54
2	O	301	PHE	CA-CB-CG	-5.50	108.30	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	15	ARG	CA-C-N	5.50	127.91	120.38
2	H	15	ARG	C-N-CA	5.50	127.91	120.38
2	J	91	GLU	N-CA-C	-5.44	102.83	110.50
2	F	69	PHE	CA-CB-CG	-5.41	108.39	113.80
1	E	74	LEU	CA-C-N	5.41	131.87	121.54
1	E	74	LEU	C-N-CA	5.41	131.87	121.54
1	G	74	LEU	CA-C-N	5.38	131.82	121.54
1	G	74	LEU	C-N-CA	5.38	131.82	121.54
2	J	69	PHE	CA-CB-CG	-5.27	108.53	113.80
2	N	161	THR	CA-C-N	5.25	131.63	122.81
2	N	161	THR	C-N-CA	5.25	131.63	122.81
1	M	73	ALA	CA-C-N	5.09	130.16	122.67
1	M	73	ALA	C-N-CA	5.09	130.16	122.67
1	G	52	MET	N-CA-C	5.04	116.46	111.07
2	H	69	PHE	CA-CB-CG	-5.02	108.78	113.80
1	M	74	LEU	CA-C-N	5.01	131.10	121.54
1	M	74	LEU	C-N-CA	5.01	131.10	121.54

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	699	0	723	6	0
1	C	708	0	736	10	0
1	E	723	0	746	14	0
1	G	708	0	736	13	0
1	I	708	0	736	11	0
1	K	723	0	746	14	0
1	M	699	0	723	16	0
2	B	2880	0	2845	22	0
2	D	2893	0	2858	13	0
2	F	2849	0	2821	15	0
2	H	2893	0	2858	17	0
2	J	2857	0	2825	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	2901	0	2862	20	0
2	N	2901	0	2862	25	0
2	O	2829	0	2802	16	0
3	F	7	0	10	2	0
4	A	1	0	0	0	0
4	B	29	0	0	0	0
4	D	17	0	0	0	0
4	F	20	0	0	0	0
4	G	2	0	0	0	0
4	H	20	0	0	0	0
4	J	14	0	0	0	0
4	L	26	0	0	0	0
4	M	2	0	0	0	0
4	N	19	0	0	0	0
4	O	10	0	0	0	0
All	All	28138	0	27889	194	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 (194) 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)
2:N:154:LYS:HD3	2:N:292:MET:HG2	1.46	0.96
2:B:145:PRO:HG3	1:I:64:GLN:HG2	1.64	0.79
2:N:91:GLU:H	2:N:91:GLU:CD	1.92	0.77
2:D:145:PRO:HG2	2:D:148:GLU:HG3	1.68	0.76
2:H:145:PRO:HG2	2:H:148:GLU:HG3	1.68	0.76
2:N:154:LYS:HD3	2:N:292:MET:CG	2.17	0.75
2:N:145:PRO:HG2	2:N:148:GLU:HG3	1.70	0.73
2:L:145:PRO:HG2	2:L:148:GLU:HG3	1.70	0.72
2:O:145:PRO:HG2	2:O:148:GLU:HG3	1.70	0.72
2:F:287:SER:HB2	2:J:59:LEU:HD22	1.70	0.72
1:K:23:HIS:HD2	1:K:38:ILE:CD1	2.03	0.71
2:J:145:PRO:HG2	2:J:148:GLU:HG3	1.72	0.71
1:G:23:HIS:HD2	1:G:38:ILE:CD1	2.03	0.70
1:G:23:HIS:HD2	1:G:38:ILE:HD11	1.56	0.70
2:F:145:PRO:HG2	2:F:148:GLU:HG3	1.73	0.69
2:N:157:GLU:HG3	2:O:58:ARG:HH21	1.56	0.69
1:E:25:VAL:HG21	1:E:52:MET:HE3	1.74	0.68
1:M:23:HIS:HD2	1:M:38:ILE:CD1	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:160:THR:HG22	2:N:161:THR:H	1.59	0.67
1:K:20:LYS:HZ1	1:K:48:ASN:HD21	1.42	0.67
1:E:23:HIS:HD2	1:E:38:ILE:CD1	2.06	0.67
1:K:20:LYS:NZ	1:K:48:ASN:HD21	1.91	0.67
1:C:23:HIS:HD2	1:C:38:ILE:CD1	2.07	0.67
2:B:155:CYS:HB2	2:B:164:CYS:SG	2.35	0.66
2:B:287:SER:HB2	2:D:59:LEU:HD22	1.78	0.65
2:L:155:CYS:HB2	2:L:164:CYS:SG	2.37	0.65
2:H:287:SER:HB2	2:L:59:LEU:HD22	1.79	0.64
2:J:157:GLU:HG3	2:J:310:GLN:HB2	1.79	0.63
2:N:155:CYS:SG	2:N:167:ASN:ND2	2.72	0.61
1:C:23:HIS:HD2	1:C:38:ILE:HD13	1.65	0.60
1:K:23:HIS:HD2	1:K:38:ILE:HD13	1.66	0.60
2:N:59:LEU:HD22	2:O:287:SER:HB2	1.83	0.60
1:A:27:HIS:CD2	1:A:52:MET:HE2	2.37	0.59
2:H:155:CYS:HB2	2:H:164:CYS:SG	2.42	0.59
2:H:157:GLU:CG	2:L:58:ARG:HH21	2.16	0.58
2:D:209:ARG:O	2:D:213:GLN:HG3	2.03	0.58
1:G:27:HIS:CD2	1:G:52:MET:HE2	2.38	0.58
1:M:98:THR:HG23	1:M:101:GLU:HG3	1.85	0.57
2:H:157:GLU:HG3	2:L:58:ARG:HH21	1.68	0.57
2:L:206:ASP:OD2	2:L:209:ARG:NH1	2.38	0.57
2:F:130:LYS:HE3	2:N:336:GLU:O	2.03	0.57
2:F:59:LEU:HD22	2:J:287:SER:HB2	1.87	0.57
1:E:110:THR:HB	2:F:249:GLU:OE1	2.05	0.57
1:M:23:HIS:HD2	1:M:38:ILE:HD11	1.68	0.57
1:M:27:HIS:CD2	1:M:52:MET:HE2	2.40	0.56
1:E:23:HIS:HD2	1:E:38:ILE:HD11	1.69	0.56
1:M:57:ILE:HD11	2:N:348:ARG:HD2	1.87	0.56
1:G:57:ILE:HD11	2:H:348:ARG:HD2	1.88	0.56
1:E:112:ARG:NH1	2:F:197:GLN:HE21	2.03	0.56
3:F:401:PEG:H32	2:J:40:LEU:HD12	1.87	0.56
2:B:331:VAL:HA	2:B:338:ILE:HD13	1.88	0.55
1:E:26:LEU:HD23	1:E:51:ILE:HG12	1.87	0.55
1:K:75:LYS:HG2	1:K:99:ALA:HB2	1.88	0.55
1:K:23:HIS:HD2	1:K:38:ILE:HD11	1.70	0.54
1:G:23:HIS:CD2	1:G:38:ILE:HD11	2.40	0.54
1:E:23:HIS:HD2	1:E:38:ILE:HD13	1.73	0.54
2:B:6:LEU:HD23	1:I:106:HIS:CD2	2.43	0.53
2:D:156:GLY:HA2	2:D:306:PHE:CE1	2.44	0.53
2:D:155:CYS:SG	2:D:167:ASN:ND2	2.81	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:120:ASP:HA	2:N:123:MET:HE3	1.90	0.53
2:N:157:GLU:CG	2:O:58:ARG:HH21	2.20	0.53
2:F:157:GLU:HG3	2:F:310:GLN:HB2	1.92	0.52
1:M:23:HIS:HD2	1:M:38:ILE:HD13	1.74	0.52
2:F:376:THR:HG21	2:N:130:LYS:HG3	1.91	0.52
2:B:336:GLU:O	2:H:130:LYS:HE3	2.10	0.52
2:N:154:LYS:HE3	2:N:289:ALA:HA	1.92	0.51
1:K:78:LYS:HG2	1:K:96:PRO:HG3	1.92	0.51
2:J:90:GLU:OE1	2:J:91:GLU:O	2.29	0.51
1:M:77:MET:HB3	1:M:79:VAL:HG12	1.92	0.51
2:B:6:LEU:HB3	1:I:106:HIS:HB3	1.94	0.50
1:C:26:LEU:HD12	1:C:31:ASP:HB2	1.94	0.50
1:E:23:HIS:HA	1:E:38:ILE:HG12	1.93	0.50
2:J:336:GLU:O	2:O:130:LYS:HE3	2.12	0.49
2:L:33:ASP:HB3	2:L:55:PRO:HA	1.95	0.49
2:O:16:GLU:H	2:O:16:GLU:CD	2.19	0.49
2:N:164:CYS:O	2:N:167:ASN:OD1	2.30	0.49
2:O:19:ARG:NH2	2:O:150:TRP:CE2	2.80	0.49
2:F:33:ASP:HB3	2:F:55:PRO:HA	1.94	0.49
2:B:119:HIS:CD2	2:L:127:LYS:HG2	2.49	0.48
1:E:78:LYS:NZ	1:E:79:VAL:HB	2.28	0.48
2:H:16:GLU:H	2:H:16:GLU:CD	2.20	0.48
1:K:90:ILE:O	2:L:249:GLU:HG3	2.12	0.48
1:C:78:LYS:HG2	1:C:96:PRO:HG3	1.95	0.48
2:O:33:ASP:HB3	2:O:55:PRO:HA	1.96	0.48
1:A:27:HIS:HD2	1:A:52:MET:CE	2.27	0.48
1:M:23:HIS:CD2	1:M:38:ILE:HD11	2.49	0.48
2:N:271:LYS:HE3	2:N:387:LEU:HD21	1.94	0.48
1:E:23:HIS:CD2	1:E:38:ILE:HD11	2.49	0.48
1:I:112:ARG:NH1	2:J:197:GLN:HE21	2.12	0.48
1:K:57:ILE:HD11	2:L:348:ARG:HD2	1.96	0.48
2:J:130:LYS:HE3	2:O:336:GLU:O	2.15	0.47
2:N:324:ILE:HG12	2:N:359:LEU:HD13	1.95	0.47
2:B:14:ARG:NH1	1:I:63:LYS:O	2.48	0.47
1:K:23:HIS:CD2	1:K:38:ILE:HD11	2.49	0.47
2:B:137:THR:HG21	2:H:371:TRP:CD1	2.49	0.47
2:H:33:ASP:HB3	2:H:55:PRO:HA	1.97	0.47
1:M:60:VAL:HG11	1:M:74:LEU:HD11	1.97	0.47
2:J:16:GLU:H	2:J:16:GLU:CD	2.21	0.46
1:K:90:ILE:C	2:L:249:GLU:HG3	2.40	0.46
2:B:130:LYS:HE3	2:H:336:GLU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:324:ILE:HG12	2:H:359:LEU:HD13	1.97	0.46
2:L:152:SER:HG	2:L:304:HIS:HD1	1.63	0.46
2:F:16:GLU:H	2:F:16:GLU:CD	2.21	0.46
1:C:23:HIS:HD2	1:C:38:ILE:HD11	1.78	0.46
2:F:56:TYR:CD1	2:F:386:ARG:NH1	2.84	0.46
2:D:16:GLU:H	2:D:16:GLU:CD	2.23	0.46
2:B:16:GLU:CD	2:B:16:GLU:H	2.22	0.46
1:G:27:HIS:HD2	1:G:52:MET:CE	2.29	0.46
2:O:56:TYR:CD1	2:O:386:ARG:NH1	2.84	0.46
2:N:56:TYR:CD1	2:N:386:ARG:NH1	2.85	0.45
1:K:27:HIS:ND1	1:K:52:MET:HE2	2.32	0.45
2:B:18:GLY:HA3	1:I:44:GLY:HA3	1.97	0.45
2:B:137:THR:HG21	2:H:371:TRP:CG	2.52	0.45
2:N:33:ASP:HB3	2:N:55:PRO:HA	1.98	0.45
2:N:91:GLU:CD	2:N:91:GLU:N	2.70	0.45
2:B:157:GLU:OE1	2:D:114:GLU:OE1	2.35	0.45
2:L:55:PRO:HG2	2:L:56:TYR:CE2	2.52	0.45
1:K:23:HIS:HA	1:K:38:ILE:HG12	1.99	0.44
1:M:60:VAL:HG11	1:M:74:LEU:CD1	2.47	0.44
2:J:56:TYR:CD1	2:J:386:ARG:NH1	2.86	0.44
1:M:26:LEU:HD12	1:M:31:ASP:HB2	1.99	0.44
1:M:98:THR:CG2	1:M:101:GLU:HG3	2.47	0.44
2:N:68:HIS:NE2	2:N:72:LEU:HD21	2.33	0.44
2:L:249:GLU:H	2:L:249:GLU:HG2	1.63	0.44
1:A:27:HIS:CD2	1:A:52:MET:CE	3.01	0.44
2:O:324:ILE:HG12	2:O:359:LEU:HD13	2.00	0.44
1:E:78:LYS:HZ2	1:E:79:VAL:HB	1.83	0.44
1:G:77:MET:HB3	1:G:79:VAL:HG12	2.00	0.44
1:G:23:HIS:HA	1:G:38:ILE:HG12	1.99	0.44
2:L:324:ILE:HG12	2:L:359:LEU:HD13	2.00	0.43
2:N:55:PRO:HG2	2:N:56:TYR:CE2	2.53	0.43
2:O:123:MET:HE3	2:O:127:LYS:HE3	2.00	0.43
2:B:56:TYR:CD1	2:B:386:ARG:NH1	2.86	0.43
1:G:27:HIS:CD2	1:G:52:MET:CE	3.01	0.43
2:J:371:TRP:CD1	2:O:137:THR:HG21	2.53	0.43
2:O:55:PRO:HG2	2:O:56:TYR:CE2	2.53	0.43
2:D:33:ASP:HB3	2:D:55:PRO:HA	2.01	0.43
2:D:56:TYR:CD1	2:D:386:ARG:NH1	2.87	0.43
1:I:112:ARG:HH11	2:J:197:GLN:HE21	1.64	0.43
2:J:324:ILE:HG12	2:J:359:LEU:HD13	2.00	0.43
1:M:27:HIS:HD2	1:M:52:MET:CE	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:33:ASP:HB3	2:J:55:PRO:HA	1.99	0.43
2:F:302:ALA:O	2:F:320:PRO:HD2	2.19	0.43
2:F:55:PRO:HG2	2:F:56:TYR:CE2	2.54	0.42
2:H:56:TYR:CD1	2:H:386:ARG:NH1	2.88	0.42
2:N:16:GLU:HG2	2:N:105:GLY:HA3	2.01	0.42
2:D:55:PRO:HG2	2:D:56:TYR:CE2	2.55	0.42
2:L:162:SER:HB3	2:L:310:GLN:HG2	2.01	0.42
1:C:76:ASP:HB3	1:C:93:VAL:HG21	2.01	0.42
1:E:76:ASP:HB2	1:E:97:ILE:HB	2.02	0.42
1:G:23:HIS:HD2	1:G:38:ILE:HD13	1.79	0.42
1:I:27:HIS:ND1	1:I:52:MET:HE2	2.33	0.42
1:G:104:HIS:CG	1:G:105:VAL:H	2.38	0.42
2:H:154:LYS:O	2:H:307:PRO:HD2	2.20	0.42
2:B:33:ASP:HB3	2:B:55:PRO:HA	2.02	0.42
2:B:302:ALA:O	2:B:320:PRO:HD2	2.20	0.42
3:F:401:PEG:H21	2:J:40:LEU:HD12	2.01	0.42
2:J:130:LYS:HG3	2:O:376:THR:HG21	2.00	0.42
2:D:157:GLU:O	2:D:162:SER:HB2	2.20	0.41
2:L:56:TYR:CD1	2:L:386:ARG:NH1	2.88	0.41
2:L:310:GLN:HE22	2:L:329:ARG:NH2	2.18	0.41
2:B:145:PRO:HG3	1:I:64:GLN:CG	2.41	0.41
1:C:86:TYR:HD2	2:D:253:LEU:HD12	1.85	0.41
1:E:78:LYS:HB3	1:E:96:PRO:HD3	2.03	0.41
2:D:154:LYS:HE3	2:D:289:ALA:HA	2.02	0.41
1:A:76:ASP:HB2	1:A:97:ILE:HB	2.02	0.41
2:B:4:ILE:HD12	2:B:180:LEU:HD12	2.02	0.41
1:G:26:LEU:HD12	1:G:31:ASP:HB2	2.01	0.41
1:I:26:LEU:HD12	1:I:31:ASP:HB2	2.01	0.41
1:M:76:ASP:HB3	1:M:93:VAL:HG21	2.03	0.41
1:M:76:ASP:HB2	1:M:97:ILE:HB	2.02	0.41
1:C:23:HIS:CD2	1:C:38:ILE:HD11	2.55	0.41
2:F:324:ILE:HG12	2:F:359:LEU:HD13	2.02	0.41
2:J:152:SER:HG	2:J:304:HIS:HD1	1.65	0.41
1:K:23:HIS:CD2	1:K:38:ILE:CD1	2.94	0.41
1:A:38:ILE:HD13	1:A:38:ILE:HA	1.97	0.41
2:B:6:LEU:HB3	1:I:106:HIS:CB	2.51	0.41
2:B:154:LYS:HE3	2:B:289:ALA:HA	2.03	0.41
2:H:55:PRO:HG2	2:H:56:TYR:CE2	2.56	0.41
1:E:26:LEU:HG	1:E:28:GLU:O	2.21	0.41
1:M:79:VAL:HG22	1:M:80:GLY:H	1.85	0.41
2:N:150:TRP:HB3	2:N:301:PHE:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:274:GLU:HA	2:H:275:PRO:HD3	2.00	0.41
2:L:23:ARG:HB2	2:L:80:ASN:HB3	2.03	0.41
2:O:222:MET:HE3	2:O:222:MET:HB3	1.99	0.41
1:C:23:HIS:HA	1:C:38:ILE:HG12	2.03	0.40
2:F:185:VAL:HB	2:F:301:PHE:CZ	2.56	0.40
2:J:55:PRO:HG2	2:J:56:TYR:CE2	2.55	0.40
2:J:336:GLU:H	2:J:336:GLU:HG3	1.54	0.40
2:L:154:LYS:O	2:L:307:PRO:HD2	2.22	0.40
2:N:154:LYS:O	2:N:307:PRO:HD2	2.21	0.40
1:A:27:HIS:HD2	1:A:52:MET:HE2	1.83	0.40
1:C:27:HIS:HA	1:C:52:MET:HE2	2.03	0.40
1:G:76:ASP:HB3	1:G:93:VAL:HG21	2.03	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	90/130 (69%)	83 (92%)	5 (6%)	2 (2%)	5 19
1	C	91/130 (70%)	84 (92%)	5 (6%)	2 (2%)	5 19
1	E	92/130 (71%)	84 (91%)	6 (6%)	2 (2%)	5 19
1	G	91/130 (70%)	84 (92%)	7 (8%)	0	100 100
1	I	91/130 (70%)	84 (92%)	6 (7%)	1 (1%)	11 36
1	K	92/130 (71%)	85 (92%)	6 (6%)	1 (1%)	11 36
1	M	90/130 (69%)	82 (91%)	6 (7%)	2 (2%)	5 19
2	B	375/391 (96%)	364 (97%)	11 (3%)	0	100 100
2	D	379/391 (97%)	366 (97%)	11 (3%)	2 (0%)	24 55
2	F	370/391 (95%)	359 (97%)	11 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	H	379/391 (97%)	365 (96%)	12 (3%)	2 (0%)	24 55
2	J	371/391 (95%)	359 (97%)	12 (3%)	0	100 100
2	L	380/391 (97%)	367 (97%)	12 (3%)	1 (0%)	36 66
2	N	380/391 (97%)	364 (96%)	15 (4%)	1 (0%)	36 66
2	O	367/391 (94%)	357 (97%)	10 (3%)	0	100 100
All	All	3638/4038 (90%)	3487 (96%)	135 (4%)	16 (0%)	30 60

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	157	GLU
2	N	157	GLU
2	D	156	GLY
2	D	161	THR
2	H	161	THR
2	L	161	THR
1	A	80	GLY
1	C	80	GLY
1	I	80	GLY
1	K	80	GLY
1	M	75	LYS
1	A	75	LYS
1	E	75	LYS
1	C	75	LYS
1	M	79	VAL
1	E	79	VAL

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	75/101 (74%)	66 (88%)	9 (12%)	5 17
1	C	76/101 (75%)	68 (90%)	8 (10%)	6 22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	77/101 (76%)	67 (87%)	10 (13%)	4 14
1	G	76/101 (75%)	68 (90%)	8 (10%)	6 22
1	I	76/101 (75%)	66 (87%)	10 (13%)	4 14
1	K	77/101 (76%)	68 (88%)	9 (12%)	5 18
1	M	75/101 (74%)	67 (89%)	8 (11%)	6 21
2	B	302/313 (96%)	293 (97%)	9 (3%)	36 72
2	D	304/313 (97%)	292 (96%)	12 (4%)	28 64
2	F	298/313 (95%)	287 (96%)	11 (4%)	30 65
2	H	304/313 (97%)	289 (95%)	15 (5%)	22 55
2	J	299/313 (96%)	289 (97%)	10 (3%)	33 69
2	L	305/313 (97%)	294 (96%)	11 (4%)	31 66
2	N	305/313 (97%)	289 (95%)	16 (5%)	21 53
2	O	296/313 (95%)	281 (95%)	15 (5%)	21 54
All	All	2945/3211 (92%)	2784 (94%)	161 (6%)	19 51

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	46	GLN
1	A	53	ASP
1	A	59	THR
1	A	77	MET
1	A	78	LYS
1	A	81	ASP
1	A	83	VAL
1	A	85	LYS
2	B	6	LEU
2	B	16	GLU
2	B	32	ASP
2	B	90	GLU
2	B	197	GLN
2	B	245	LEU
2	B	292	MET
2	B	347	GLN
2	B	352	LEU
1	C	20	LYS

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Mol	Chain	Res	Type
1	C	26	LEU
1	C	46	GLN
1	C	59	THR
1	C	77	MET
1	C	82	THR
1	C	83	VAL
1	C	85	LYS
2	D	6	LEU
2	D	16	GLU
2	D	32	ASP
2	D	34	LEU
2	D	44	SER
2	D	59	LEU
2	D	157	GLU
2	D	220	GLN
2	D	227	LYS
2	D	245	LEU
2	D	253	LEU
2	D	292	MET
1	E	30	LYS
1	E	46	GLN
1	E	53	ASP
1	E	59	THR
1	E	77	MET
1	E	78	LYS
1	E	83	VAL
1	E	85	LYS
1	E	110	THR
1	E	112	ARG
2	F	6	LEU
2	F	16	GLU
2	F	59	LEU
2	F	67	LEU
2	F	90	GLU
2	F	197	GLN
2	F	245	LEU
2	F	249	GLU
2	F	292	MET
2	F	324	ILE
2	F	352	LEU
1	G	26	LEU
1	G	39	GLU

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Mol	Chain	Res	Type
1	G	46	GLN
1	G	59	THR
1	G	82	THR
1	G	83	VAL
1	G	85	LYS
1	G	98	THR
2	H	6	LEU
2	H	16	GLU
2	H	32	ASP
2	H	34	LEU
2	H	44	SER
2	H	90	GLU
2	H	91	GLU
2	H	108	VAL
2	H	157	GLU
2	H	227	LYS
2	H	245	LEU
2	H	255	ASN
2	H	292	MET
2	H	324	ILE
2	H	352	LEU
1	I	26	LEU
1	I	30	LYS
1	I	38	ILE
1	I	46	GLN
1	I	59	THR
1	I	63	LYS
1	I	77	MET
1	I	78	LYS
1	I	83	VAL
1	I	85	LYS
2	J	16	GLU
2	J	59	LEU
2	J	147	SER
2	J	197	GLN
2	J	229	ASP
2	J	245	LEU
2	J	255	ASN
2	J	292	MET
2	J	336	GLU
2	J	385	THR
1	K	26	LEU

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Mol	Chain	Res	Type
1	K	39	GLU
1	K	47	LEU
1	K	59	THR
1	K	78	LYS
1	K	82	THR
1	K	83	VAL
1	K	85	LYS
1	K	98	THR
2	L	6	LEU
2	L	16	GLU
2	L	44	SER
2	L	59	LEU
2	L	197	GLN
2	L	229	ASP
2	L	245	LEU
2	L	249	GLU
2	L	255	ASN
2	L	292	MET
2	L	352	LEU
1	M	26	LEU
1	M	46	GLN
1	M	59	THR
1	M	83	VAL
1	M	85	LYS
1	M	98	THR
1	M	110	THR
1	M	112	ARG
2	N	6	LEU
2	N	44	SER
2	N	59	LEU
2	N	67	LEU
2	N	72	LEU
2	N	91	GLU
2	N	108	VAL
2	N	109	MET
2	N	157	GLU
2	N	167	ASN
2	N	191	GLU
2	N	197	GLN
2	N	245	LEU
2	N	255	ASN
2	N	292	MET

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Mol	Chain	Res	Type
2	N	352	LEU
2	O	6	LEU
2	O	16	GLU
2	O	32	ASP
2	O	44	SER
2	O	91	GLU
2	O	197	GLN
2	O	241	ILE
2	O	245	LEU
2	O	249	GLU
2	O	255	ASN
2	O	292	MET
2	O	324	ILE
2	O	348	ARG
2	O	352	LEU
2	O	370	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	106	HIS
2	B	25	HIS
1	C	23	HIS
2	D	25	HIS
2	D	257	GLN
2	D	312	ASN
1	E	23	HIS
1	E	106	HIS
2	F	197	GLN
1	G	27	HIS
1	G	106	HIS
2	H	25	HIS
1	I	106	HIS
2	J	25	HIS
2	J	119	HIS
2	J	197	GLN
2	J	220	GLN
1	K	23	HIS
1	K	48	ASN
2	L	25	HIS
2	L	310	GLN

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Mol	Chain	Res	Type
1	M	23	HIS
1	M	27	HIS
2	N	25	HIS
2	N	197	GLN
2	N	220	GLN
2	N	310	GLN
2	O	25	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PEG	F	401	-	6,6,6	0.44	0	5,5,5	0.40	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	F	401	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	401	PEG	O1-C1-C2-O2
3	F	401	PEG	C1-C2-O2-C3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	401	PEG	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^{th} 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	92/130 (70%)	1.32	23 (25%)	2	1	55, 82, 104, 113	0
1	C	93/130 (71%)	1.33	17 (18%)	3	2	65, 81, 94, 98	0
1	E	94/130 (72%)	1.08	17 (18%)	3	3	43, 68, 93, 103	0
1	G	93/130 (71%)	0.93	11 (11%)	9	7	50, 64, 79, 85	0
1	I	93/130 (71%)	1.43	22 (23%)	2	1	65, 83, 104, 108	0
1	K	94/130 (72%)	1.76	30 (31%)	1	1	75, 107, 121, 125	0
1	M	92/130 (70%)	1.29	15 (16%)	4	4	54, 74, 87, 92	0
2	B	381/391 (97%)	0.18	8 (2%)	63	54	33, 46, 70, 84	0
2	D	383/391 (97%)	0.20	12 (3%)	51	41	31, 44, 68, 85	0
2	F	376/391 (96%)	0.34	10 (2%)	56	46	37, 48, 66, 79	0
2	H	383/391 (97%)	0.29	4 (1%)	79	72	33, 52, 67, 81	0
2	J	377/391 (96%)	0.44	9 (2%)	59	49	37, 55, 76, 89	0
2	L	384/391 (98%)	0.41	9 (2%)	61	51	34, 54, 85, 107	0
2	N	384/391 (98%)	0.57	21 (5%)	30	23	37, 57, 77, 93	0
2	O	373/391 (95%)	0.82	31 (8%)	17	12	42, 65, 100, 130	0
All	All	3692/4038 (91%)	0.56	239 (6%)	25	18	31, 55, 95, 130	0

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	79	VAL	5.8
1	I	45	SER	4.7
1	C	79	VAL	4.5
1	G	78	LYS	4.4
2	J	165	GLY	4.4
1	M	79	VAL	4.3
1	K	37	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	G	79	VAL	4.3
2	J	236	PRO	4.3
2	F	2	SER	4.2
1	I	79	VAL	4.0
1	K	79	VAL	4.0
2	O	346	LEU	4.0
1	K	74	LEU	3.9
1	C	72	VAL	3.9
1	I	41	ILE	3.9
1	G	74	LEU	3.8
1	E	79	VAL	3.8
2	L	236	PRO	3.8
2	L	346	LEU	3.8
1	K	73	ALA	3.8
2	L	160	THR	3.8
1	E	74	LEU	3.7
1	E	86	TYR	3.6
1	K	72	VAL	3.6
1	E	75	LYS	3.6
1	C	41	ILE	3.5
1	K	38	ILE	3.5
1	G	80	GLY	3.5
2	L	245	LEU	3.4
2	N	157	GLU	3.4
2	O	247	THR	3.4
1	M	78	LYS	3.4
1	A	76	ASP	3.4
1	I	40	GLY	3.4
1	M	64	GLN	3.4
1	I	42	LYS	3.3
1	C	45	SER	3.3
2	D	160	THR	3.3
1	M	74	LEU	3.3
2	O	248	ILE	3.3
2	D	157	GLU	3.2
2	D	2	SER	3.2
1	A	25	VAL	3.2
2	O	165	GLY	3.1
1	C	74	LEU	3.1
1	K	99	ALA	3.1
1	K	91	GLY	3.1
2	B	160	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	73	ALA	3.1
1	G	76	ASP	3.1
2	H	156	GLY	3.0
1	K	105	VAL	3.0
1	K	52	MET	3.0
1	K	78	LYS	3.0
1	G	73	ALA	3.0
2	O	245	LEU	2.9
1	I	76	ASP	2.9
1	C	38	ILE	2.9
2	F	165	GLY	2.9
1	K	92	LYS	2.9
2	O	166	ALA	2.9
2	N	158	SER	2.9
2	O	241	ILE	2.8
1	M	63	LYS	2.8
2	F	157	GLU	2.8
1	I	99	ALA	2.8
2	O	204	ALA	2.8
1	E	78	LYS	2.8
2	N	163	GLY	2.8
1	K	76	ASP	2.8
1	K	80	GLY	2.8
2	B	236	PRO	2.8
2	B	6	LEU	2.7
2	N	167	ASN	2.7
2	D	161	THR	2.7
1	A	74	LEU	2.7
2	N	156	GLY	2.7
2	N	159	ASP	2.7
2	D	236	PRO	2.7
1	A	29	ALA	2.7
1	I	74	LEU	2.7
2	D	163	GLY	2.7
2	O	299	SER	2.7
1	G	82	THR	2.7
2	B	156	GLY	2.7
2	O	255	ASN	2.7
1	I	75	LYS	2.6
1	K	100	GLY	2.6
1	A	21	THR	2.6
1	K	25	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	L	157	GLU	2.6
2	O	192	LEU	2.6
1	M	73	ALA	2.6
1	A	50	TRP	2.6
2	D	237	THR	2.6
1	I	47	LEU	2.6
2	J	205	ASN	2.6
1	E	53	ASP	2.6
1	I	95	ALA	2.6
2	F	236	PRO	2.6
1	I	80	GLY	2.6
2	F	156	GLY	2.6
2	N	236	PRO	2.6
1	M	46	GLN	2.6
2	O	212	PHE	2.6
2	O	156	GLY	2.5
1	I	64	GLN	2.5
2	O	348	ARG	2.5
2	D	162	SER	2.5
2	B	157	GLU	2.5
2	L	350	GLN	2.5
2	N	228	THR	2.5
2	O	228	THR	2.5
1	K	30	LYS	2.5
2	N	162	SER	2.5
1	E	22	ILE	2.5
1	K	90	ILE	2.5
2	N	310	GLN	2.5
1	A	27	HIS	2.5
1	A	80	GLY	2.5
2	O	194	GLY	2.5
2	L	170	VAL	2.5
1	C	86	TYR	2.5
2	O	246	THR	2.5
1	A	24	ILE	2.4
1	M	41	ILE	2.4
1	C	78	LYS	2.4
2	L	237	THR	2.4
2	N	253	LEU	2.4
1	I	96	PRO	2.4
2	B	163	GLY	2.4
2	H	158	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	J	157	GLU	2.4
1	K	82	THR	2.4
2	F	245	LEU	2.4
2	N	382	PHE	2.4
1	I	43	ALA	2.4
1	I	73	ALA	2.4
1	G	64	GLN	2.4
1	E	33	VAL	2.4
1	I	94	VAL	2.4
2	F	239	GLY	2.4
2	N	2	SER	2.4
2	O	352	LEU	2.4
1	K	53	ASP	2.3
2	D	159	ASP	2.3
2	B	361	GLU	2.3
1	K	36	ALA	2.3
1	G	77	MET	2.3
2	F	261	LYS	2.3
2	O	242	ALA	2.3
1	C	76	ASP	2.3
2	B	4	ILE	2.3
2	N	190	SER	2.3
2	O	256	ILE	2.3
1	K	86	TYR	2.3
1	A	43	ALA	2.3
1	C	95	ALA	2.3
2	H	157	GLU	2.3
1	A	26	LEU	2.3
2	J	237	THR	2.3
1	I	37	VAL	2.3
1	C	40	GLY	2.3
1	A	99	ALA	2.2
1	M	48	ASN	2.2
1	M	47	LEU	2.2
2	D	245	LEU	2.2
1	C	71	LYS	2.2
1	I	38	ILE	2.2
1	K	83	VAL	2.2
2	J	2	SER	2.2
1	K	34	GLY	2.2
2	O	239	GLY	2.2
2	O	301	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	O	272	ALA	2.2
1	E	24	ILE	2.2
2	O	198	ILE	2.2
1	E	25	VAL	2.2
1	A	36	ALA	2.2
1	E	52	MET	2.2
1	M	52	MET	2.2
2	D	253	LEU	2.2
2	O	253	LEU	2.2
1	E	28	GLU	2.2
1	M	105	VAL	2.2
1	K	98	THR	2.2
2	L	162	SER	2.2
1	C	62	ALA	2.2
2	O	249	GLU	2.2
1	I	97	ILE	2.1
2	F	4	ILE	2.1
1	A	46	GLN	2.1
1	E	76	ASP	2.1
1	K	95	ALA	2.1
1	K	27	HIS	2.1
1	K	88	VAL	2.1
2	N	383	VAL	2.1
1	E	30	LYS	2.1
1	K	75	LYS	2.1
1	C	91	GLY	2.1
1	C	110	THR	2.1
1	G	59	THR	2.1
2	N	212	PHE	2.1
1	A	62	ALA	2.1
2	F	5	GLN	2.1
1	A	30	LYS	2.1
1	A	75	LYS	2.1
1	A	77	MET	2.1
1	M	58	VAL	2.1
1	E	26	LEU	2.1
2	J	385	THR	2.1
2	N	161	THR	2.1
1	E	113	TRP	2.1
1	K	50	TRP	2.1
2	N	4	ILE	2.1
1	A	64	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	33	VAL	2.1
1	E	60	VAL	2.1
2	J	199	VAL	2.1
2	O	205	ASN	2.1
2	O	216	PHE	2.1
2	N	229	ASP	2.1
1	A	41	ILE	2.1
2	H	16	GLU	2.1
1	M	86	TYR	2.1
2	J	3	VAL	2.0
1	A	100	GLY	2.0
2	D	156	GLY	2.0
1	A	78	LYS	2.0
2	O	310	GLN	2.0
2	O	350	GLN	2.0
2	N	6	LEU	2.0
1	I	69	GLY	2.0
2	N	279	GLY	2.0
1	M	42	LYS	2.0
1	I	77	MET	2.0
1	G	83	VAL	2.0
2	O	199	VAL	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, 95^{th} 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
3	PEG	F	401	7/7	0.82	0.24	40,41,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.