Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:02 PM GMT

PDB ID	:	4WJV
Title	:	Crystal structure of Rsa4 in complex with the Nsa2 binding peptide
Authors	:	Holdermann, I.; Paternoga, H.; Bassler, J.; Hurt, E.; Sinning, I.
Deposited on	:	2014-10-01
Resolution	:	3.20 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

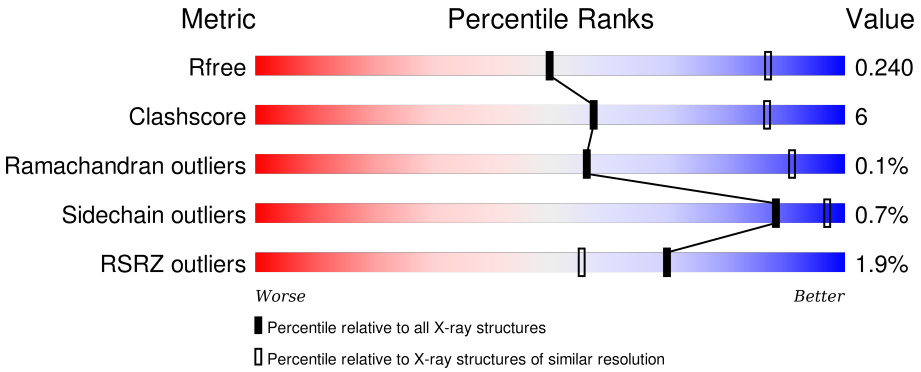
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	381	6% 78% 21%
1	B	381	% 78% 21%
1	C	381	3% 79% 20%
1	D	381	2% 80% 19%
2	E	381	86% 10%

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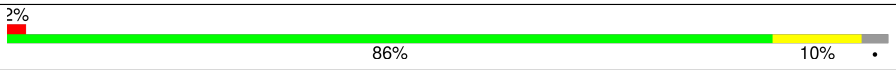
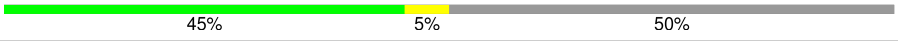
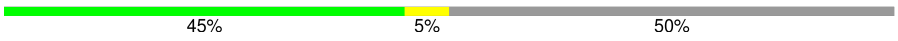
Mol	Chain	Length	Quality of chain
2	F	381	
2	G	381	
2	H	381	
3	I	22	
3	J	22	
3	K	22	
3	L	22	

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
4	SO4	C	602	-	-	-	X
4	SO4	D	602	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23675 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 Ribosome assembly protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	0	0
			2958	1854	534	550	20			
1	B	378	Total	C	N	O	S	0	0	0
			2958	1854	534	550	20			
1	C	378	Total	C	N	O	S	0	0	0
			2958	1854	534	550	20			
1	D	378	Total	C	N	O	S	0	0	0
			2958	1854	534	550	20			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	135	MET	-	initiating methionine	UNP P25382
A	136	GLY	-	expression tag	UNP P25382
B	135	MET	-	initiating methionine	UNP P25382
B	136	GLY	-	expression tag	UNP P25382
C	135	MET	-	initiating methionine	UNP P25382
C	136	GLY	-	expression tag	UNP P25382
D	135	MET	-	initiating methionine	UNP P25382
D	136	GLY	-	expression tag	UNP P25382

- Molecule 2 is a protein called Maltose-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	369	Total	C	N	O	S	0	0	0
			2834	1825	461	542	6			
2	F	368	Total	C	N	O	S	0	0	0
			2826	1819	460	541	6			
2	G	369	Total	C	N	O	S	0	0	0
			2834	1825	461	542	6			
2	H	369	Total	C	N	O	S	0	0	0
			2834	1825	461	542	6			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	MET	-	initiating methionine	UNP P0AEX9
E	2	LYS	-	expression tag	UNP P0AEX9
E	3	HIS	-	expression tag	UNP P0AEX9
E	4	HIS	-	expression tag	UNP P0AEX9
E	5	HIS	-	expression tag	UNP P0AEX9
E	6	HIS	-	expression tag	UNP P0AEX9
E	7	HIS	-	expression tag	UNP P0AEX9
E	8	HIS	-	expression tag	UNP P0AEX9
E	9	PRO	-	expression tag	UNP P0AEX9
E	10	MET	-	expression tag	UNP P0AEX9
E	92	ALA	ASP	engineered mutation	UNP P0AEX9
E	93	ALA	LYS	engineered mutation	UNP P0AEX9
E	249	ALA	LYS	engineered mutation	UNP P0AEX9
E	369	ALA	GLU	engineered mutation	UNP P0AEX9
E	372	ALA	LYS	engineered mutation	UNP P0AEX9
E	373	ALA	ASP	engineered mutation	UNP P0AEX9
E	377	ASN	ARG	engineered mutation	UNP P0AEX9
E	378	ALA	-	expression tag	UNP P0AEX9
E	379	ALA	-	expression tag	UNP P0AEX9
E	380	ALA	-	expression tag	UNP P0AEX9
E	381	ALA	-	expression tag	UNP P0AEX9
F	1	MET	-	initiating methionine	UNP P0AEX9
F	2	LYS	-	expression tag	UNP P0AEX9
F	3	HIS	-	expression tag	UNP P0AEX9
F	4	HIS	-	expression tag	UNP P0AEX9
F	5	HIS	-	expression tag	UNP P0AEX9
F	6	HIS	-	expression tag	UNP P0AEX9
F	7	HIS	-	expression tag	UNP P0AEX9
F	8	HIS	-	expression tag	UNP P0AEX9
F	9	PRO	-	expression tag	UNP P0AEX9
F	10	MET	-	expression tag	UNP P0AEX9
F	92	ALA	ASP	engineered mutation	UNP P0AEX9
F	93	ALA	LYS	engineered mutation	UNP P0AEX9
F	249	ALA	LYS	engineered mutation	UNP P0AEX9
F	369	ALA	GLU	engineered mutation	UNP P0AEX9
F	372	ALA	LYS	engineered mutation	UNP P0AEX9
F	373	ALA	ASP	engineered mutation	UNP P0AEX9
F	377	ASN	ARG	engineered mutation	UNP P0AEX9
F	378	ALA	-	expression tag	UNP P0AEX9
F	379	ALA	-	expression tag	UNP P0AEX9
F	380	ALA	-	expression tag	UNP P0AEX9
F	381	ALA	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1	MET	-	initiating methionine	UNP P0AEX9
G	2	LYS	-	expression tag	UNP P0AEX9
G	3	HIS	-	expression tag	UNP P0AEX9
G	4	HIS	-	expression tag	UNP P0AEX9
G	5	HIS	-	expression tag	UNP P0AEX9
G	6	HIS	-	expression tag	UNP P0AEX9
G	7	HIS	-	expression tag	UNP P0AEX9
G	8	HIS	-	expression tag	UNP P0AEX9
G	9	PRO	-	expression tag	UNP P0AEX9
G	10	MET	-	expression tag	UNP P0AEX9
G	92	ALA	ASP	engineered mutation	UNP P0AEX9
G	93	ALA	LYS	engineered mutation	UNP P0AEX9
G	249	ALA	LYS	engineered mutation	UNP P0AEX9
G	369	ALA	GLU	engineered mutation	UNP P0AEX9
G	372	ALA	LYS	engineered mutation	UNP P0AEX9
G	373	ALA	ASP	engineered mutation	UNP P0AEX9
G	377	ASN	ARG	engineered mutation	UNP P0AEX9
G	378	ALA	-	expression tag	UNP P0AEX9
G	379	ALA	-	expression tag	UNP P0AEX9
G	380	ALA	-	expression tag	UNP P0AEX9
G	381	ALA	-	expression tag	UNP P0AEX9
H	1	MET	-	initiating methionine	UNP P0AEX9
H	2	LYS	-	expression tag	UNP P0AEX9
H	3	HIS	-	expression tag	UNP P0AEX9
H	4	HIS	-	expression tag	UNP P0AEX9
H	5	HIS	-	expression tag	UNP P0AEX9
H	6	HIS	-	expression tag	UNP P0AEX9
H	7	HIS	-	expression tag	UNP P0AEX9
H	8	HIS	-	expression tag	UNP P0AEX9
H	9	PRO	-	expression tag	UNP P0AEX9
H	10	MET	-	expression tag	UNP P0AEX9
H	92	ALA	ASP	engineered mutation	UNP P0AEX9
H	93	ALA	LYS	engineered mutation	UNP P0AEX9
H	249	ALA	LYS	engineered mutation	UNP P0AEX9
H	369	ALA	GLU	engineered mutation	UNP P0AEX9
H	372	ALA	LYS	engineered mutation	UNP P0AEX9
H	373	ALA	ASP	engineered mutation	UNP P0AEX9
H	377	ASN	ARG	engineered mutation	UNP P0AEX9
H	378	ALA	-	expression tag	UNP P0AEX9
H	379	ALA	-	expression tag	UNP P0AEX9
H	380	ALA	-	expression tag	UNP P0AEX9
H	381	ALA	-	expression tag	UNP P0AEX9

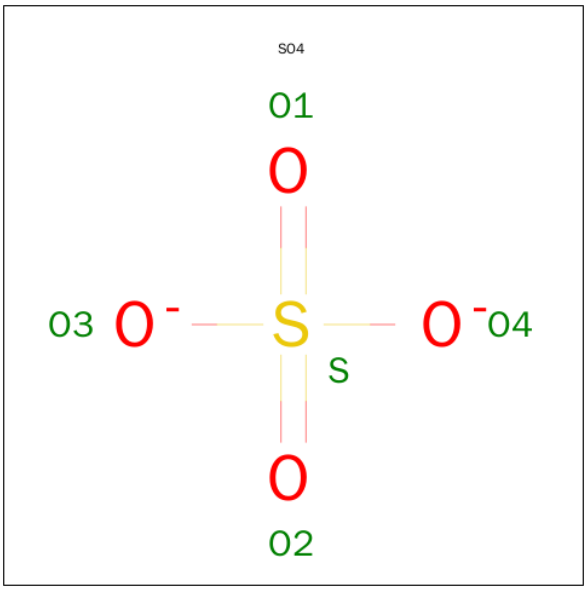
- Molecule 3 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	11	Total	C	N	O	0	0	0
			91	58	14	19			
3	J	11	Total	C	N	O	0	0	0
			91	58	14	19			
3	K	12	Total	C	N	O	0	0	0
			100	63	16	21			
3	L	11	Total	C	N	O	0	0	0
			91	58	14	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	80	MET	LEU	conflict	UNP P40078
J	80	MET	LEU	conflict	UNP P40078
K	80	MET	LEU	conflict	UNP P40078
L	80	MET	LEU	conflict	UNP P40078

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

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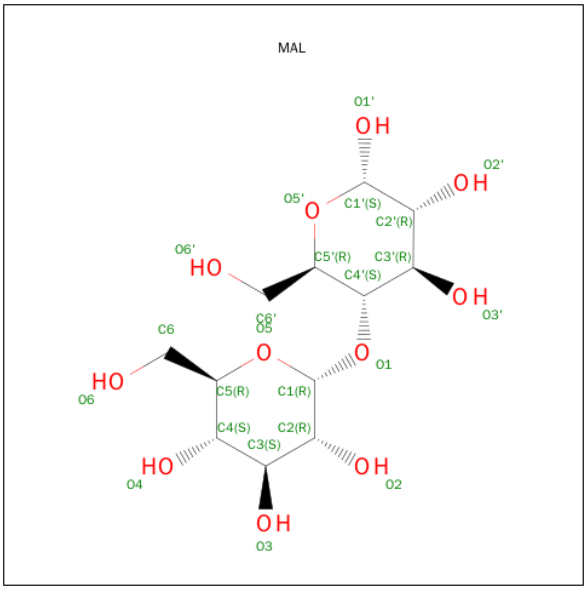
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

- Molecule 5 is SUGAR (MALTOSE) (three-letter code: MAL) (formula: $C_{12}H_{22}O_{11}$).



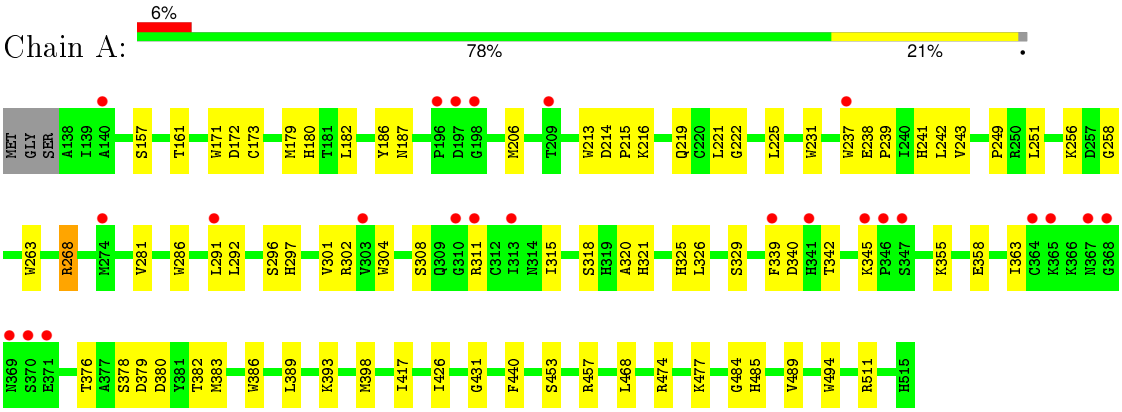
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C O 23 12 11	0	0
5	F	1	Total C O 23 12 11	0	0
5	G	1	Total C O 23 12 11	0	0
5	H	1	Total C O 23 12 11	0	0

3 Residue-property plots (i)

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

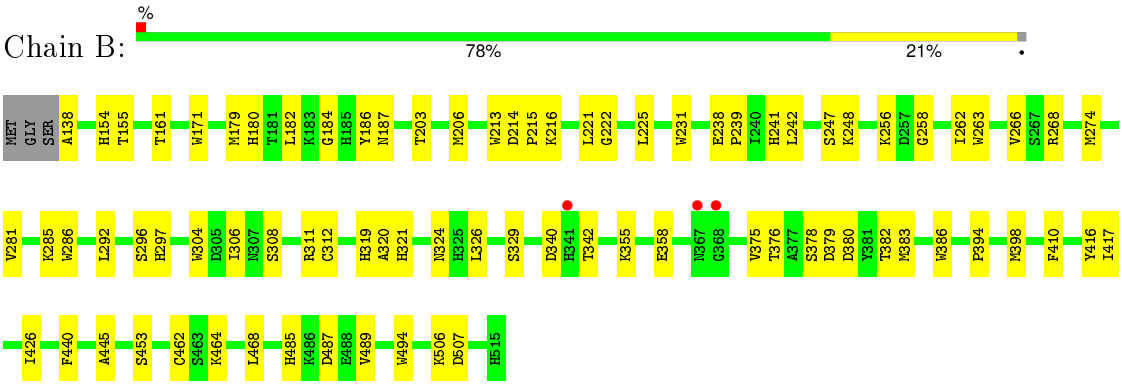
- Molecule 1: Ribosome assembly protein 4

Chain A:



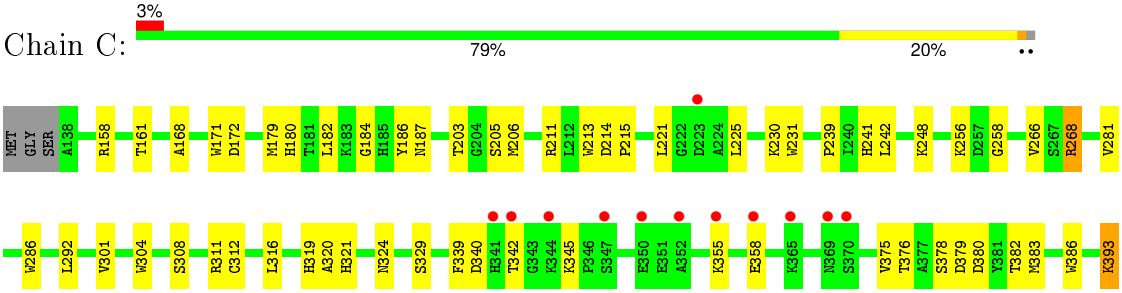
- Molecule 1: Ribosome assembly protein 4

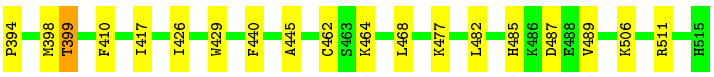
Chain B:



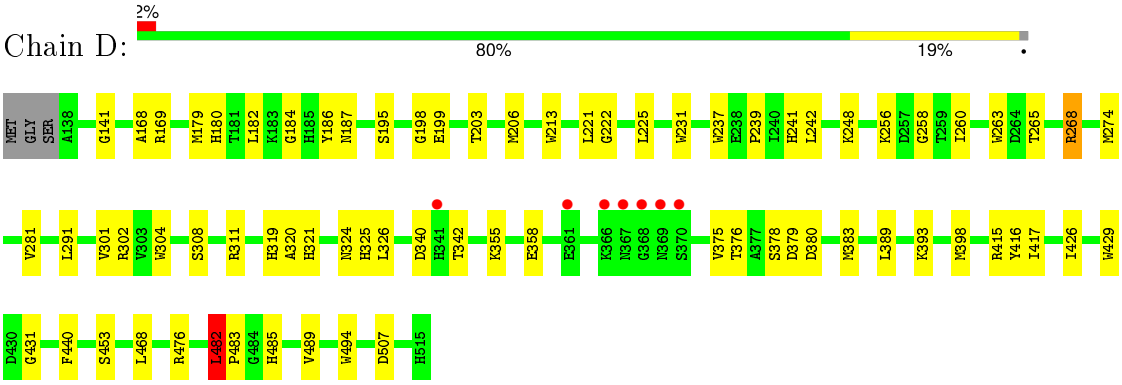
- Molecule 1: Ribosome assembly protein 4

Chain C:

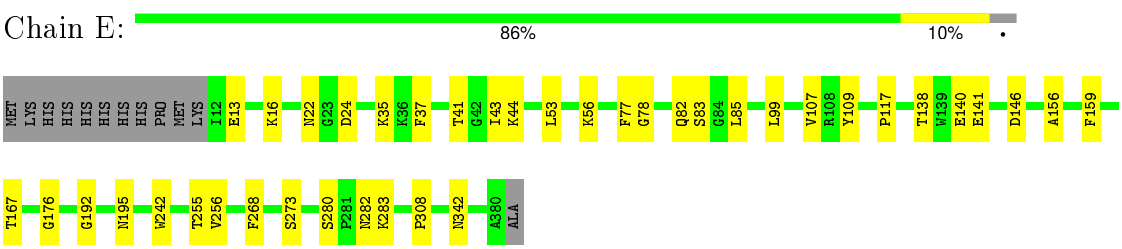




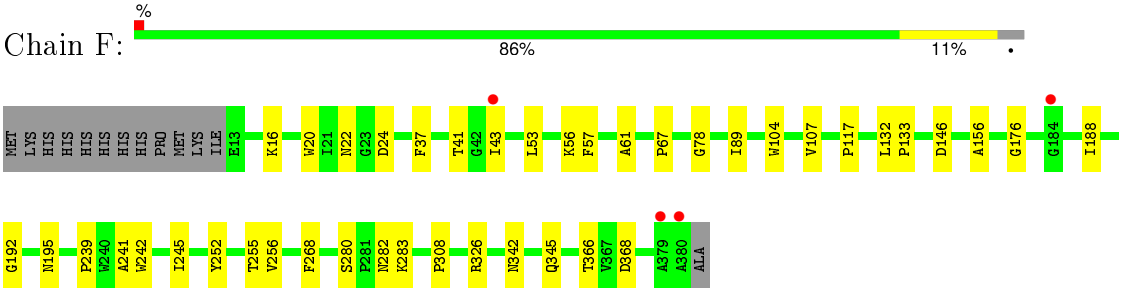
• Molecule 1: Ribosome assembly protein 4



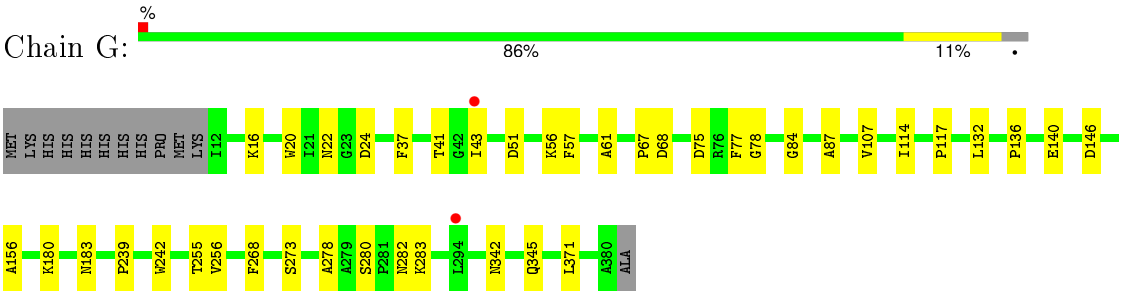
• Molecule 2: Maltose-binding periplasmic protein



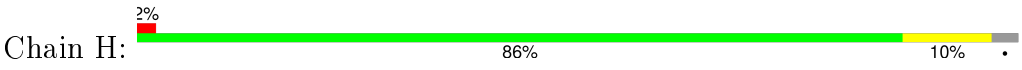
• Molecule 2: Maltose-binding periplasmic protein

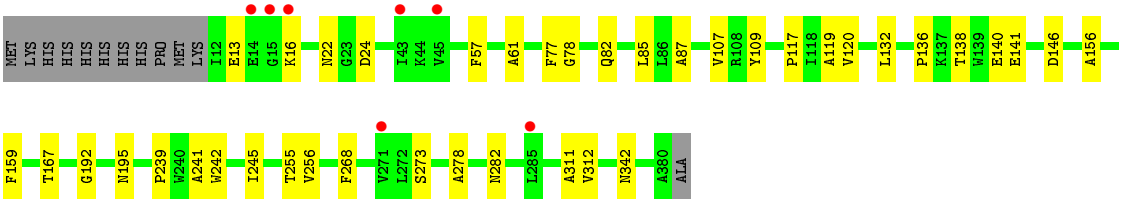


• Molecule 2: Maltose-binding periplasmic protein



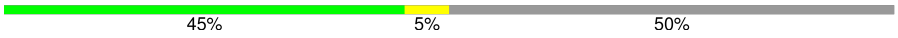
• Molecule 2: Maltose-binding periplasmic protein

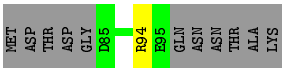




- Molecule 3: Ribosome biogenesis protein NSA2

Chain I:



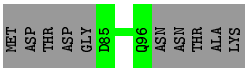


- Molecule 3: Ribosome biogenesis protein NSA2

Chain J:

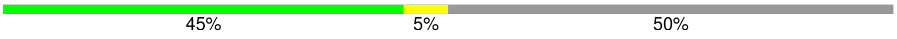
- Molecule 3: Ribosome biogenesis protein NSA2

Chain K:



- Molecule 3: Ribosome biogenesis protein NSA2

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	198.58Å 96.49Å 196.44Å 90.00° 115.45° 90.00°	Depositor
Resolution (Å)	48.98 – 3.20 48.98 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.98-3.20) 96.6 (48.98-3.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.95 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.192 , 0.244 0.192 , 0.240	Depositor DCC
R_{free} test set	2720 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	65.3	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 42.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 55662 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	23675	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MAL, SO4

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	0.22	0/3035	0.42	0/4116
1	B	0.22	0/3035	0.42	0/4116
1	C	0.22	0/3035	0.41	0/4116
1	D	0.23	0/3035	0.43	1/4116 (0.0%)
2	E	0.23	0/2903	0.40	0/3948
2	F	0.23	0/2895	0.39	0/3937
2	G	0.23	0/2903	0.39	0/3948
2	H	0.22	0/2903	0.39	0/3948
3	I	0.21	0/92	0.53	0/125
3	J	0.21	0/92	0.40	0/125
3	K	0.21	0/101	0.45	0/137
3	L	0.21	0/92	0.46	0/125
All	All	0.23	0/24121	0.41	1/32757 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	482	LEU	CA-CB-CG	5.97	129.02	115.30

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	2958	0	2896	50	0
1	B	2958	0	2896	50	1
1	C	2958	0	2896	54	0
1	D	2958	0	2896	46	0
2	E	2834	0	2797	25	0
2	F	2826	0	2786	22	0
2	G	2834	0	2797	22	0
2	H	2834	0	2797	22	0
3	I	91	0	87	1	0
3	J	91	0	87	1	0
3	K	100	0	95	0	0
3	L	91	0	87	0	0
4	A	15	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
4	D	15	0	0	1	1
5	E	23	0	22	0	0
5	F	23	0	22	0	0
5	G	23	0	22	1	0
5	H	23	0	22	0	0
All	All	23675	0	23205	283	1

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 6.

All (283) 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:382:THR:HG22	1:C:399:THR:HG23	1.72	0.72
1:A:221:LEU:O	1:A:268:ARG:NH1	2.24	0.71
1:A:302:ARG:HG2	1:A:315:ILE:HG12	1.76	0.68
1:D:378:SER:OG	1:D:380:ASP:OD1	2.10	0.68
1:A:378:SER:OG	1:A:380:ASP:OD1	2.09	0.68
1:C:378:SER:OG	1:C:380:ASP:OD1	2.13	0.66
1:B:378:SER:OG	1:B:380:ASP:OD1	2.13	0.66
1:A:383:MET:HB2	1:A:398:MET:HG3	1.78	0.66
1:B:383:MET:HB2	1:B:398:MET:HG3	1.78	0.65
1:A:308:SER:HB3	1:A:311:ARG:HD2	1.79	0.65
1:D:324:ASN:ND2	1:D:379:ASP:OD1	2.26	0.64
1:D:308:SER:HB3	1:D:311:ARG:HD2	1.78	0.64
1:B:221:LEU:O	1:B:268:ARG:NH1	2.31	0.64
1:D:221:LEU:O	1:D:268:ARG:NH1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:LEU:HD11	1:D:268:ARG:HE	1.62	0.64
1:D:320:ALA:O	1:D:321:HIS:ND1	2.32	0.63
2:G:280:SER:O	2:G:283:LYS:NZ	2.33	0.62
1:A:222:GLY:HA3	1:A:268:ARG:HH12	1.63	0.61
1:B:355:LYS:HA	1:B:358:GLU:HB3	1.83	0.61
1:C:383:MET:HB2	1:C:398:MET:HG3	1.82	0.61
1:B:320:ALA:O	1:B:321:HIS:ND1	2.34	0.61
1:D:383:MET:HB2	1:D:398:MET:HG3	1.83	0.60
1:C:355:LYS:HA	1:C:358:GLU:HB3	1.83	0.60
1:A:320:ALA:O	1:A:321:HIS:ND1	2.34	0.60
2:F:16:LYS:O	2:F:282:ASN:ND2	2.35	0.60
1:A:457:ARG:HH21	1:A:474:ARG:HD2	1.67	0.60
1:C:320:ALA:O	1:C:321:HIS:ND1	2.35	0.59
1:B:222:GLY:HA3	1:B:268:ARG:HH12	1.67	0.59
2:E:280:SER:O	2:E:283:LYS:NZ	2.36	0.59
1:D:187:ASN:HB3	1:D:206:MET:HB3	1.85	0.58
1:D:468:LEU:HD21	1:D:489:VAL:HG11	1.84	0.58
2:E:176:GLY:HA2	2:E:195:ASN:HD21	1.69	0.58
1:C:301:VAL:HG21	1:C:376:THR:HG21	1.85	0.57
1:C:225:LEU:HD11	1:C:268:ARG:HE	1.69	0.56
1:A:186:TYR:HE1	1:C:186:TYR:HE1	1.53	0.56
1:A:355:LYS:HA	1:A:358:GLU:HB3	1.87	0.56
2:G:57:PHE:O	2:G:61:ALA:N	2.38	0.56
2:E:22:ASN:ND2	2:E:24:ASP:OD1	2.38	0.56
1:C:158:ARG:NH1	1:C:172:ASP:OD1	2.39	0.56
1:C:324:ASN:ND2	1:C:379:ASP:OD1	2.25	0.56
1:A:225:LEU:HD11	1:A:268:ARG:HE	1.70	0.55
1:B:187:ASN:HB3	1:B:206:MET:HB3	1.88	0.55
1:C:231:TRP:CZ2	1:C:256:LYS:HG3	2.42	0.55
1:B:324:ASN:ND2	1:B:379:ASP:OD1	2.28	0.55
2:E:16:LYS:O	2:E:282:ASN:ND2	2.39	0.54
1:B:340:ASP:OD1	1:B:342:THR:OG1	2.22	0.54
1:D:222:GLY:HA3	1:D:268:ARG:HH12	1.73	0.54
2:G:16:LYS:O	2:G:282:ASN:ND2	2.41	0.53
2:F:22:ASN:ND2	2:F:24:ASP:OD1	2.42	0.53
1:B:426:ILE:HB	1:B:440:PHE:HB2	1.90	0.53
1:C:375:VAL:HG11	1:C:417:ILE:HD13	1.91	0.53
1:A:180:HIS:NE2	1:A:216:LYS:O	2.36	0.53
1:C:179:MET:O	1:C:180:HIS:ND1	2.41	0.53
1:A:340:ASP:OD1	1:A:342:THR:OG1	2.22	0.52
1:C:172:ASP:HB2	1:C:179:MET:HE3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:82:GLN:OE1	2:E:109:TYR:OH	2.23	0.52
2:E:192:GLY:O	2:E:195:ASN:ND2	2.42	0.52
2:E:107:VAL:HG21	2:E:117:PRO:HD3	1.91	0.52
1:A:301:VAL:HG21	1:A:376:THR:HG21	1.91	0.52
1:A:172:ASP:HB2	1:A:179:MET:HE3	1.92	0.52
2:E:159:PHE:HE1	2:E:167:THR:HG22	1.75	0.52
1:B:308:SER:HB3	1:B:311:ARG:HD2	1.92	0.52
1:D:355:LYS:HA	1:D:358:GLU:HB3	1.91	0.52
2:H:120:VAL:N	2:H:311:ALA:O	2.33	0.52
2:H:61:ALA:HB3	2:H:85:LEU:HD13	1.92	0.51
1:A:339:PHE:HE1	1:A:345:LYS:HG2	1.76	0.51
1:C:308:SER:HB3	1:C:311:ARG:HD2	1.93	0.51
1:C:203:THR:HG22	1:C:213:TRP:HE1	1.75	0.51
1:A:225:LEU:HD23	1:A:263:TRP:CD2	2.45	0.51
1:B:184:GLY:HA2	1:D:186:TYR:CZ	2.46	0.51
2:H:107:VAL:HG21	2:H:117:PRO:HD3	1.91	0.51
1:C:258:GLY:HA2	1:C:281:VAL:HG23	1.93	0.51
2:H:22:ASN:ND2	2:H:24:ASP:OD1	2.44	0.51
1:C:340:ASP:OD1	1:C:342:THR:OG1	2.23	0.51
1:D:340:ASP:OD1	1:D:342:THR:OG1	2.22	0.51
1:B:180:HIS:NE2	1:B:216:LYS:O	2.41	0.50
2:H:82:GLN:OE1	2:H:109:TYR:OH	2.28	0.50
2:F:107:VAL:HG21	2:F:117:PRO:HD3	1.92	0.50
1:B:225:LEU:HD11	1:B:268:ARG:HE	1.76	0.49
2:G:239:PRO:HA	2:G:242:TRP:CE2	2.47	0.49
1:A:239:PRO:HB2	1:A:241:HIS:CE1	2.47	0.49
2:F:252:TYR:OH	2:F:326:ARG:NH1	2.46	0.49
1:D:203:THR:HG22	1:D:213:TRP:HE1	1.78	0.49
1:D:225:LEU:HD23	1:D:263:TRP:CD2	2.48	0.49
1:B:186:TYR:HE1	1:D:186:TYR:HE1	1.61	0.49
1:B:241:HIS:CE1	1:B:242:LEU:HG	2.48	0.49
1:B:179:MET:O	1:B:180:HIS:ND1	2.45	0.49
2:H:119:ALA:HA	2:H:312:VAL:HA	1.96	0.48
1:C:221:LEU:O	1:C:268:ARG:NH1	2.44	0.48
1:C:426:ILE:HB	1:C:440:PHE:HB2	1.95	0.48
1:A:417:ILE:HG13	1:A:431:GLY:HA2	1.94	0.48
2:F:280:SER:O	2:F:283:LYS:NZ	2.46	0.48
1:D:241:HIS:CE1	1:D:242:LEU:HG	2.47	0.48
1:B:161:THR:HG22	1:B:171:TRP:HE1	1.78	0.48
2:H:16:LYS:O	2:H:282:ASN:ND2	2.47	0.48
1:D:301:VAL:HG21	1:D:376:THR:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:255:THR:OG1	2:G:256:VAL:N	2.46	0.47
1:B:203:THR:HG22	1:B:213:TRP:HE1	1.79	0.47
2:H:239:PRO:HA	2:H:242:TRP:CE2	2.49	0.47
2:H:146:ASP:HA	2:H:156:ALA:HB2	1.96	0.47
2:F:57:PHE:O	2:F:61:ALA:N	2.46	0.47
1:C:239:PRO:HB2	1:C:241:HIS:CE1	2.49	0.47
1:C:241:HIS:CE1	1:C:242:LEU:HG	2.50	0.47
1:A:241:HIS:CE1	1:A:242:LEU:HG	2.49	0.47
1:B:138:ALA:O	2:G:84:GLY:HA3	2.14	0.47
2:F:188:ILE:HG21	2:F:345:GLN:HG3	1.95	0.47
2:G:68:ASP:OD2	2:G:280:SER:OG	2.26	0.47
1:B:182:LEU:HD23	1:B:213:TRP:CD2	2.50	0.47
1:D:485:HIS:HB3	1:D:507:ASP:OD2	2.15	0.47
1:B:285:LYS:HE3	1:B:326:LEU:O	2.15	0.47
1:C:487:ASP:HB3	1:C:506:LYS:HB3	1.95	0.47
1:A:258:GLY:HA2	1:A:281:VAL:HG23	1.96	0.47
1:A:426:ILE:HB	1:A:440:PHE:HB2	1.97	0.47
1:A:231:TRP:CZ2	1:A:256:LYS:HG3	2.50	0.47
1:B:258:GLY:HA2	1:B:281:VAL:HG23	1.97	0.47
2:F:53:LEU:HA	2:F:56:LYS:HB2	1.97	0.47
2:H:132:LEU:HD21	2:H:136:PRO:HD3	1.96	0.47
1:B:225:LEU:HD23	1:B:263:TRP:CD2	2.50	0.47
2:F:192:GLY:O	2:F:195:ASN:ND2	2.48	0.47
1:C:161:THR:CG2	1:C:171:TRP:HE1	2.29	0.46
1:B:239:PRO:HB2	1:B:241:HIS:CE1	2.51	0.46
1:B:231:TRP:CZ2	1:B:256:LYS:HG3	2.50	0.46
1:D:476:ARG:NH2	4:D:602:SO4:O2	2.43	0.46
1:A:286:TRP:HA	1:A:292:LEU:HG	1.97	0.46
2:G:107:VAL:O	2:G:114:ILE:HG12	2.15	0.46
1:C:214:ASP:HB2	1:C:221:LEU:HD21	1.98	0.46
2:G:20:TRP:CD2	2:G:67:PRO:HG3	2.50	0.46
2:E:78:GLY:HA3	2:E:342:ASN:O	2.15	0.46
1:D:231:TRP:CZ2	1:D:256:LYS:HG3	2.50	0.46
1:D:482:LEU:H	1:D:482:LEU:HD23	1.80	0.46
1:D:417:ILE:HG13	1:D:431:GLY:HA2	1.97	0.46
1:D:179:MET:O	1:D:180:HIS:ND1	2.49	0.46
1:C:375:VAL:HG22	1:C:410:PHE:CE2	2.50	0.46
1:C:445:ALA:HB1	1:C:464:LYS:HB3	1.97	0.46
2:E:13:GLU:HB3	2:E:16:LYS:HD3	1.97	0.46
2:H:120:VAL:HB	2:H:311:ALA:HB3	1.97	0.46
2:G:77:PHE:HE2	2:G:273:SER:HB2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:140:GLU:N	2:G:140:GLU:OE1	2.46	0.45
2:F:41:THR:HG23	2:F:43:ILE:H	1.82	0.45
2:G:107:VAL:HG21	2:G:117:PRO:HD3	1.97	0.45
2:G:75:ASP:OD2	5:G:700:MAL:O3	2.27	0.45
2:H:77:PHE:HE2	2:H:273:SER:HB2	1.82	0.45
1:D:239:PRO:HB2	1:D:241:HIS:CE1	2.52	0.45
2:G:22:ASN:ND2	2:G:24:ASP:OD1	2.50	0.45
1:C:187:ASN:HB3	1:C:206:MET:HB3	1.99	0.45
1:A:237:TRP:CE2	1:A:251:LEU:HD13	2.52	0.45
1:C:319:HIS:CD2	1:C:376:THR:HG1	2.30	0.45
1:B:487:ASP:HB3	1:B:506:LYS:HB3	1.99	0.45
1:A:243:VAL:HG21	1:A:249:PRO:HB3	1.99	0.45
1:B:186:TYR:OH	1:D:184:GLY:HA2	2.17	0.44
2:E:146:ASP:HA	2:E:156:ALA:HB2	1.98	0.44
1:A:318:SER:HG	1:A:386:TRP:HH2	1.63	0.44
2:F:78:GLY:HA3	2:F:342:ASN:O	2.17	0.44
2:F:242:TRP:HB2	2:F:308:PRO:HG2	1.99	0.44
1:A:157:SER:HA	1:A:173:CYS:HB2	1.99	0.44
2:H:78:GLY:HA3	2:H:342:ASN:O	2.18	0.44
1:C:286:TRP:HA	1:C:292:LEU:HG	2.00	0.44
1:D:482:LEU:HB2	1:D:483:PRO:HD2	1.99	0.44
2:H:255:THR:OG1	2:H:256:VAL:N	2.50	0.44
1:B:445:ALA:HB1	1:B:464:LYS:HB3	1.99	0.44
1:A:485:HIS:CD2	1:A:511:ARG:HD2	2.51	0.44
1:C:301:VAL:HB	1:C:316:LEU:HB2	1.99	0.44
1:C:203:THR:CG2	1:C:213:TRP:HE1	2.31	0.44
1:D:375:VAL:HG11	1:D:417:ILE:HD13	2.00	0.44
2:G:87:ALA:HB2	2:G:278:ALA:HA	2.00	0.44
2:G:78:GLY:HA3	2:G:342:ASN:O	2.18	0.44
2:F:89:ILE:HD11	2:F:104:TRP:HZ3	1.83	0.43
1:B:248:LYS:HD2	1:B:266:VAL:HG22	2.00	0.43
1:B:329:SER:HA	1:B:410:PHE:CG	2.53	0.43
1:B:286:TRP:HA	1:B:292:LEU:HG	2.01	0.43
1:D:415:ARG:HD3	1:D:416:TYR:CZ	2.53	0.43
2:E:255:THR:OG1	2:E:256:VAL:N	2.52	0.43
1:B:386:TRP:CH2	1:B:394:PRO:HG3	2.53	0.43
1:D:258:GLY:HA2	1:D:281:VAL:HG23	2.01	0.43
1:D:199:GLU:OE1	1:D:248:LYS:NZ	2.35	0.43
1:A:161:THR:HG22	1:A:171:TRP:HE1	1.84	0.43
1:D:426:ILE:HB	1:D:440:PHE:HB2	2.01	0.43
1:A:219:GLN:HG2	2:E:44:LYS:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:99:LEU:HD22	2:E:117:PRO:HG2	1.99	0.43
2:F:239:PRO:HA	2:F:242:TRP:CE2	2.54	0.43
1:B:262:ILE:HD11	1:B:274:MET:HE1	2.01	0.43
1:B:453:SER:HB2	1:B:494:TRP:CE2	2.53	0.43
1:B:286:TRP:CE2	1:B:292:LEU:HD11	2.53	0.43
2:H:138:THR:OG1	2:H:141:GLU:HG3	2.18	0.43
2:F:20:TRP:CD2	2:F:67:PRO:HG3	2.54	0.43
1:C:182:LEU:HD23	1:C:213:TRP:CD2	2.54	0.43
1:C:379:ASP:OD2	3:I:94:ARG:NH1	2.46	0.43
2:G:51:ASP:O	2:G:56:LYS:HE2	2.19	0.43
2:E:37:PHE:O	2:E:41:THR:HG22	2.19	0.43
2:E:41:THR:HG23	2:E:43:ILE:H	1.84	0.42
1:B:485:HIS:HB3	1:B:507:ASP:OD2	2.18	0.42
1:D:141:GLY:O	1:D:169:ARG:NE	2.52	0.42
1:A:325:HIS:CG	1:A:326:LEU:H	2.37	0.42
2:G:146:ASP:HA	2:G:156:ALA:HB2	2.01	0.42
2:F:176:GLY:HA2	2:F:195:ASN:HD21	1.84	0.42
2:F:37:PHE:O	2:F:41:THR:HG22	2.19	0.42
1:A:219:GLN:NE2	2:E:44:LYS:HG2	2.34	0.42
1:A:182:LEU:HD23	1:A:213:TRP:CG	2.54	0.42
3:J:88:PRO:HD2	3:J:91:LEU:HD12	2.00	0.42
2:G:41:THR:HG23	2:G:43:ILE:H	1.85	0.42
1:A:468:LEU:HD21	1:A:489:VAL:HG11	2.00	0.42
1:C:485:HIS:N	1:C:485:HIS:CD2	2.88	0.42
1:D:453:SER:HB2	1:D:494:TRP:CE2	2.55	0.42
1:D:398:MET:HG2	1:D:398:MET:H	1.70	0.42
2:H:192:GLY:O	2:H:195:ASN:ND2	2.51	0.42
1:B:214:ASP:HA	1:B:215:PRO:HD2	1.86	0.42
1:A:238:GLU:HA	1:A:239:PRO:HD3	1.86	0.42
2:E:242:TRP:HB2	2:E:308:PRO:HG2	2.02	0.42
1:C:468:LEU:HB2	1:C:482:LEU:HB2	2.01	0.42
1:B:186:TYR:HE1	1:D:186:TYR:CE1	2.38	0.42
1:C:161:THR:HG22	1:C:171:TRP:HE1	1.84	0.42
1:A:182:LEU:HD23	1:A:213:TRP:CD2	2.54	0.42
1:B:468:LEU:HD21	1:B:489:VAL:HG11	2.02	0.42
2:E:83:SER:HB2	2:E:85:LEU:HG	2.02	0.42
1:C:386:TRP:CH2	1:C:394:PRO:HG3	2.55	0.42
1:A:214:ASP:HA	1:A:215:PRO:HD2	1.86	0.42
1:A:380:ASP:O	1:A:382:THR:HG23	2.19	0.42
1:B:154:HIS:CD2	1:B:155:THR:HG22	2.54	0.42
2:H:140:GLU:N	2:H:140:GLU:OE1	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:LYS:HB3	1:A:477:LYS:HE2	1.81	0.42
1:C:214:ASP:HA	1:C:215:PRO:HD2	1.85	0.42
1:D:325:HIS:CG	1:D:326:LEU:H	2.37	0.42
2:H:57:PHE:O	2:H:61:ALA:N	2.52	0.42
2:G:37:PHE:O	2:G:41:THR:HG22	2.20	0.42
1:C:339:PHE:HE1	1:C:345:LYS:HG2	1.85	0.42
1:B:319:HIS:NE2	1:B:376:THR:OG1	2.42	0.42
1:C:184:GLY:O	1:C:211:ARG:NE	2.53	0.42
1:A:187:ASN:HB3	1:A:206:MET:HB3	2.01	0.42
1:C:230:LYS:HB3	1:C:256:LYS:HB3	2.02	0.41
1:B:238:GLU:HA	1:B:239:PRO:HD3	1.92	0.41
1:C:468:LEU:HD21	1:C:489:VAL:HG11	2.02	0.41
1:A:329:SER:O	1:A:363:ILE:HD11	2.21	0.41
1:C:329:SER:HA	1:C:410:PHE:CG	2.55	0.41
1:C:168:ALA:HB3	1:C:182:LEU:HB2	2.02	0.41
2:F:241:ALA:O	2:F:245:ILE:HG13	2.21	0.41
2:F:255:THR:OG1	2:F:256:VAL:N	2.52	0.41
1:B:380:ASP:O	1:B:382:THR:HG23	2.21	0.41
1:B:161:THR:CG2	1:B:171:TRP:HE1	2.31	0.41
2:H:13:GLU:HB3	2:H:16:LYS:HD3	2.01	0.41
1:C:462:CYS:HB2	1:C:489:VAL:HB	2.02	0.41
2:E:140:GLU:N	2:E:140:GLU:OE1	2.52	0.41
1:A:214:ASP:HB2	1:A:221:LEU:HD21	2.03	0.41
1:A:180:HIS:CE1	2:E:35:LYS:HE3	2.56	0.41
1:C:485:HIS:CD2	1:C:511:ARG:HD2	2.56	0.41
1:C:477:LYS:HB3	1:C:477:LYS:HE2	1.81	0.41
1:D:291:LEU:HD11	1:D:389:LEU:HD12	2.03	0.41
1:D:195:SER:O	1:D:198:GLY:N	2.52	0.41
1:C:304:TRP:CZ3	1:C:312:CYS:HB2	2.55	0.41
2:H:241:ALA:O	2:H:245:ILE:HG13	2.21	0.41
1:D:398:MET:HB2	1:D:429:TRP:CZ3	2.56	0.41
1:D:179:MET:HE3	1:D:179:MET:HB2	1.89	0.41
1:A:291:LEU:HD11	1:A:389:LEU:HD12	2.02	0.41
1:B:375:VAL:HG11	1:B:417:ILE:HD13	2.01	0.41
1:D:260:ILE:HB	1:D:274:MET:HE2	2.03	0.41
1:B:304:TRP:CZ3	1:B:312:CYS:HB2	2.55	0.41
1:B:286:TRP:CZ2	1:B:306:ILE:HG12	2.55	0.41
1:C:393:LYS:HA	1:C:394:PRO:HD3	1.94	0.41
1:D:302:ARG:HD3	1:D:304:TRP:CZ2	2.56	0.41
1:C:248:LYS:HD3	1:C:266:VAL:HG22	2.02	0.41
1:D:237:TRP:CZ3	1:D:265:THR:HG21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:159:PHE:HE1	2:H:167:THR:HG22	1.85	0.41
1:D:168:ALA:HB3	1:D:182:LEU:HB2	2.02	0.41
1:A:179:MET:O	1:A:180:HIS:ND1	2.54	0.41
1:B:462:CYS:HB2	1:B:489:VAL:HB	2.03	0.41
2:H:87:ALA:HB2	2:H:278:ALA:HA	2.03	0.41
2:E:77:PHE:CE2	2:E:273:SER:HB2	2.56	0.41
2:E:53:LEU:HA	2:E:56:LYS:HB2	2.03	0.41
1:C:398:MET:HB2	1:C:429:TRP:CZ3	2.56	0.40
1:A:296:SER:OG	1:A:297:HIS:N	2.54	0.40
2:G:132:LEU:HD21	2:G:136:PRO:HD3	2.01	0.40
1:C:205:SER:OG	1:C:206:MET:N	2.54	0.40
2:E:77:PHE:HE2	2:E:273:SER:HB2	1.86	0.40
1:A:453:SER:HB2	1:A:494:TRP:CE2	2.57	0.40
2:F:366:THR:HG22	2:F:368:ASP:H	1.86	0.40
1:C:380:ASP:O	1:C:382:THR:HG23	2.21	0.40
1:A:321:HIS:HB3	1:A:379:ASP:HB2	2.02	0.40
2:G:371:LEU:HD23	2:G:371:LEU:HA	1.92	0.40
1:A:302:ARG:HD3	1:A:304:TRP:CZ2	2.57	0.40
2:E:138:THR:OG1	2:E:141:GLU:HG3	2.22	0.40
2:F:146:ASP:HA	2:F:156:ALA:HB2	2.04	0.40
1:D:319:HIS:NE2	1:D:376:THR:OG1	2.44	0.40
2:F:132:LEU:HA	2:F:133:PRO:HD2	1.96	0.40
1:B:296:SER:OG	1:B:297:HIS:N	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:TYR:OH	4:D:602:SO4:O3[1_565]	2.17	0.03

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	376/381 (99%)	357 (95%)	18 (5%)	1 (0%)	46 85
1	B	376/381 (99%)	358 (95%)	18 (5%)	0	100 100
1	C	376/381 (99%)	358 (95%)	18 (5%)	0	100 100
1	D	376/381 (99%)	358 (95%)	18 (5%)	0	100 100
2	E	367/381 (96%)	356 (97%)	11 (3%)	0	100 100
2	F	366/381 (96%)	354 (97%)	12 (3%)	0	100 100
2	G	367/381 (96%)	355 (97%)	11 (3%)	1 (0%)	46 85
2	H	367/381 (96%)	355 (97%)	12 (3%)	0	100 100
3	I	9/22 (41%)	8 (89%)	1 (11%)	0	100 100
3	J	9/22 (41%)	8 (89%)	1 (11%)	0	100 100
3	K	10/22 (46%)	9 (90%)	1 (10%)	0	100 100
3	L	9/22 (41%)	8 (89%)	1 (11%)	0	100 100
All	All	3008/3136 (96%)	2884 (96%)	122 (4%)	2 (0%)	56 91

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	484	GLY
2	G	183	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	328/330 (99%)	326 (99%)	2 (1%)	90 97
1	B	328/330 (99%)	327 (100%)	1 (0%)	94 98
1	C	328/330 (99%)	325 (99%)	3 (1%)	84 95
1	D	328/330 (99%)	325 (99%)	3 (1%)	84 95
2	E	287/298 (96%)	286 (100%)	1 (0%)	94 98
2	F	286/298 (96%)	285 (100%)	1 (0%)	94 98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	G	287/298 (96%)	284 (99%)	3 (1%)	82 95
2	H	287/298 (96%)	286 (100%)	1 (0%)	94 98
3	I	10/19 (53%)	10 (100%)	0	100 100
3	J	10/19 (53%)	9 (90%)	1 (10%)	9 37
3	K	11/19 (58%)	11 (100%)	0	100 100
3	L	10/19 (53%)	9 (90%)	1 (10%)	9 37
All	All	2500/2588 (97%)	2483 (99%)	17 (1%)	88 97

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	268	ARG
1	A	393	LYS
1	B	247	SER
1	C	268	ARG
1	C	393	LYS
1	C	399	THR
1	D	268	ARG
1	D	393	LYS
1	D	482	LEU
2	E	268	PHE
2	F	268	PHE
2	G	180	LYS
2	G	268	PHE
2	G	345	GLN
2	H	268	PHE
3	J	93	ASP
3	L	95	GLU

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

14 ligands are 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	$\#\|Z\| > 2$
4	SO4	A	601	-	4,4,4	0.25	0	6,6,6	0.06	0
4	SO4	A	602	-	4,4,4	0.24	0	6,6,6	0.13	0
4	SO4	A	603	-	4,4,4	0.24	0	6,6,6	0.14	0
4	SO4	B	601	-	4,4,4	0.25	0	6,6,6	0.08	0
4	SO4	B	602	-	4,4,4	0.25	0	6,6,6	0.11	0
4	SO4	C	601	-	4,4,4	0.25	0	6,6,6	0.07	0
4	SO4	C	602	-	4,4,4	0.26	0	6,6,6	0.15	0
4	SO4	D	601	-	4,4,4	0.26	0	6,6,6	0.08	0
4	SO4	D	602	-	4,4,4	0.28	0	6,6,6	0.07	0
4	SO4	D	603	-	4,4,4	0.24	0	6,6,6	0.08	0
5	MAL	E	700	-	24,24,24	0.55	0	35,35,35	0.57	0
5	MAL	F	700	-	24,24,24	0.54	0	35,35,35	0.58	0
5	MAL	G	700	-	24,24,24	0.54	0	35,35,35	0.58	0
5	MAL	H	700	-	24,24,24	0.54	0	35,35,35	0.53	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
4	SO4	A	601	-	-	0/0/0/0	0/0/0/0
4	SO4	A	602	-	-	0/0/0/0	0/0/0/0
4	SO4	A	603	-	-	0/0/0/0	0/0/0/0
4	SO4	B	601	-	-	0/0/0/0	0/0/0/0
4	SO4	B	602	-	-	0/0/0/0	0/0/0/0
4	SO4	C	601	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	C	602	-	-	0/0/0/0	0/0/0/0
4	SO4	D	601	-	-	0/0/0/0	0/0/0/0
4	SO4	D	602	-	-	0/0/0/0	0/0/0/0
4	SO4	D	603	-	-	0/0/0/0	0/0/0/0
5	MAL	E	700	-	-	0/8/48/48	0/2/2/2
5	MAL	F	700	-	-	0/8/48/48	0/2/2/2
5	MAL	G	700	-	-	0/8/48/48	0/2/2/2
5	MAL	H	700	-	-	0/8/48/48	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	602	SO4	1	1
5	G	700	MAL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	378/381 (99%)	0.37	24 (6%) 23 13	45, 83, 146, 187	0
1	B	378/381 (99%)	-0.08	3 (0%) 87 80	39, 57, 113, 168	0
1	C	378/381 (99%)	0.18	12 (3%) 51 36	41, 69, 133, 168	0
1	D	378/381 (99%)	0.07	7 (1%) 70 55	38, 61, 123, 190	0
2	E	369/381 (96%)	-0.22	0 100 100	34, 51, 80, 113	0
2	F	368/381 (96%)	0.00	4 (1%) 82 72	36, 59, 106, 147	0
2	G	369/381 (96%)	-0.12	2 (0%) 91 87	29, 56, 110, 145	0
2	H	369/381 (96%)	0.10	7 (1%) 70 55	37, 74, 132, 156	0
3	I	11/22 (50%)	0.05	0 100 100	58, 64, 110, 112	0
3	J	11/22 (50%)	-0.00	0 100 100	51, 60, 119, 126	0
3	K	12/22 (54%)	0.12	0 100 100	61, 64, 126, 142	0
3	L	11/22 (50%)	-0.01	0 100 100	50, 53, 84, 112	0
All	All	3032/3136 (96%)	0.04	59 (1%) 70 55	29, 62, 124, 190	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	370	SER	4.9
1	C	341	HIS	4.9
1	A	345	LYS	4.6
2	H	15	GLY	4.3
1	B	367	ASN	4.3
1	C	344	LYS	4.1
1	D	369	ASN	4.0
1	A	237	TRP	3.9
1	A	368	GLY	3.7
1	D	368	GLY	3.7
2	F	379	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	366	LYS	3.4
1	A	303	VAL	3.4
1	D	367	ASN	3.4
1	A	365	LYS	3.3
1	C	223	ASP	3.1
2	F	184	GLY	3.1
2	H	16	LYS	3.1
1	A	313	ILE	3.1
1	D	341	HIS	3.0
1	A	367	ASN	2.9
1	B	341	HIS	2.9
1	C	365	LYS	2.9
1	A	364	CYS	2.9
1	C	369	ASN	2.8
1	A	341	HIS	2.7
1	A	346	PRO	2.7
1	B	368	GLY	2.6
1	D	361	GLU	2.6
1	D	370	SER	2.6
1	A	197	ASP	2.6
1	A	274	MET	2.5
1	C	342	THR	2.5
1	C	370	SER	2.5
1	A	140	ALA	2.5
2	H	43	ILE	2.5
2	H	45	VAL	2.5
1	C	352	ALA	2.4
1	C	355	LYS	2.4
1	C	347	SER	2.3
1	A	347	SER	2.3
1	A	209	THR	2.3
1	A	196	PRO	2.3
1	A	371	GLU	2.3
1	A	310	GLY	2.3
1	A	291	LEU	2.3
2	F	380	ALA	2.2
2	H	285	LEU	2.2
2	G	294	LEU	2.2
2	H	271	VAL	2.2
1	A	311	ARG	2.2
2	H	14	GLU	2.2
2	F	43	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	369	ASN	2.1
1	C	350	GLU	2.1
1	A	339	PHE	2.1
2	G	43	ILE	2.0
1	C	358	GLU	2.0
1	A	198	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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	LLDF	B-factors(Å^2)	Q<0.9
4	SO4	C	602	5/5	0.95	0.24	3.44	64,65,69,70	0
4	SO4	A	603	5/5	0.94	0.24	1.53	105,106,107,115	0
4	SO4	A	602	5/5	0.80	0.27	0.94	69,78,85,92	0
4	SO4	B	602	5/5	0.95	0.20	0.42	77,79,80,84	0
4	SO4	A	601	5/5	0.96	0.16	-0.13	80,80,83,85	0
4	SO4	D	603	5/5	0.97	0.19	-0.69	62,63,66,70	0
5	MAL	H	700	23/23	0.95	0.17	-0.79	41,52,66,73	0
5	MAL	E	700	23/23	0.97	0.17	-1.05	20,35,48,50	0
5	MAL	F	700	23/23	0.97	0.17	-1.27	40,48,52,60	0
5	MAL	G	700	23/23	0.96	0.17	-1.35	22,31,45,68	0
4	SO4	D	602	5/5	0.98	0.14	-2.26	42,43,45,52	0
4	SO4	B	601	5/5	0.97	0.11	-	70,70,74,77	0
4	SO4	C	601	5/5	0.89	0.15	-	83,84,87,92	0
4	SO4	D	601	5/5	0.98	0.14	-	65,68,69,73	0

6.5 Other polymers (i)

There are no such residues in this entry.