wwPDB X-ray Structure Validation Summary Report (i)

Aug 21, 2023 – 02:55 PM EDT

PDB ID	:	2Q4P
Title	:	Ensemble refinement of the crystal structure of protein from Mus musculus Mm.29898
Authors	:	Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on	:	2007-05-31
Resolution	:	2.32 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

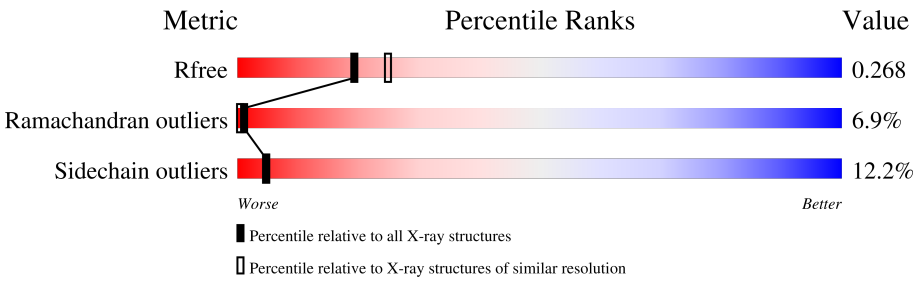
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.32 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5974 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)

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%

Mol	Chain	Length	Quality of chain
1	1-A	170	55% 11% • 34%
1	1-B	170	56% 8% 36%
1	10-A	170	55% 9% • 34%
1	10-B	170	54% 10% 36%
1	11-A	170	49% 16% • 34%
1	11-B	170	57% 6% • 36%
1	12-A	170	54% 11% • 34%
1	12-B	170	50% 14% • 36%

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Mol	Chain	Length	Quality of chain
1	13-A	170	52% 14% • 34%
1	13-B	170	46% 15% • 36%
1	14-A	170	49% 16% • 34%
1	14-B	170	45% 16% • 36%
1	15-A	170	52% 14% • 34%
1	15-B	170	46% 16% • 36%
1	16-A	170	46% 15% 5% 34%
1	16-B	170	41% 21% • 36%
1	2-A	170	55% 11% • 34%
1	2-B	170	54% 9% • 36%
1	3-A	170	59% 6% • 34%
1	3-B	170	58% 6% 36%
1	4-A	170	58% 8% 34%
1	4-B	170	53% 10% • 36%
1	5-A	170	58% 8% 34%
1	5-B	170	54% 9% • 36%
1	6-A	170	58% 8% • 34%
1	6-B	170	53% 11% • 36%
1	7-A	170	58% 7% • 34%
1	7-B	170	53% 10% • 36%
1	8-A	170	59% 8% 34%
1	8-B	170	52% 11% • 36%
1	9-A	170	54% 11% • 34%
1	9-B	170	57% 6% • 36%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 29392 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 Protein RS21-C6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	1-A	113	922	589	163	168	1	1	0	0	0
1	2-A	113	922	589	163	168	1	1	0	0	0
1	3-A	113	922	589	163	168	1	1	0	0	0
1	4-A	113	922	589	163	168	1	1	0	0	0
1	5-A	113	922	589	163	168	1	1	0	0	0
1	6-A	113	922	589	163	168	1	1	0	0	0
1	7-A	113	922	589	163	168	1	1	0	0	0
1	8-A	113	922	589	163	168	1	1	0	0	0
1	9-A	113	922	589	163	168	1	1	0	0	0
1	10-A	113	922	589	163	168	1	1	0	0	0
1	11-A	113	922	589	163	168	1	1	0	0	0
1	12-A	113	922	589	163	168	1	1	0	0	0
1	13-A	113	922	589	163	168	1	1	0	0	0
1	14-A	113	922	589	163	168	1	1	0	0	0
1	15-A	113	922	589	163	168	1	1	0	0	0
1	16-A	113	922	589	163	168	1	1	0	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	1-B	109	891	569	157	163	1	1	0	0	0
1	2-B	109	891	569	157	163	1	1	0	0	0
1	3-B	109	891	569	157	163	1	1	0	0	0
1	4-B	109	891	569	157	163	1	1	0	0	0
1	5-B	109	891	569	157	163	1	1	0	0	0
1	6-B	109	891	569	157	163	1	1	0	0	0
1	7-B	109	891	569	157	163	1	1	0	0	0
1	8-B	109	891	569	157	163	1	1	0	0	0
1	9-B	109	891	569	157	163	1	1	0	0	0
1	10-B	109	891	569	157	163	1	1	0	0	0
1	11-B	109	891	569	157	163	1	1	0	0	0
1	12-B	109	891	569	157	163	1	1	0	0	0
1	13-B	109	891	569	157	163	1	1	0	0	0
1	14-B	109	891	569	157	163	1	1	0	0	0
1	15-B	109	891	569	157	163	1	1	0	0	0
1	16-B	109	891	569	157	163	1	1	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q9QY93
A	122	MSE	MET	modified residue	UNP Q9QY93
B	1	MSE	MET	modified residue	UNP Q9QY93
B	122	MSE	MET	modified residue	UNP Q9QY93

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	1-A	12	12	12	0	0
2	2-A	11	11	11	0	0
2	3-A	12	12	12	0	0
2	4-A	11	11	11	0	0
2	5-A	12	12	12	0	0
2	6-A	11	11	11	0	0
2	7-A	12	12	12	0	0
2	8-A	13	13	13	0	0
2	9-A	11	11	11	0	0
2	10-A	10	10	10	0	0
2	11-A	12	12	12	0	0
2	12-A	12	12	12	0	0
2	13-A	13	13	13	0	0
2	14-A	12	12	12	0	0
2	15-A	12	12	12	0	0
2	16-A	13	13	13	0	0
2	1-B	12	12	12	0	0
2	2-B	13	13	13	0	0
2	3-B	12	12	12	0	0
2	4-B	13	13	13	0	0
2	5-B	12	12	12	0	0
2	6-B	13	13	13	0	0

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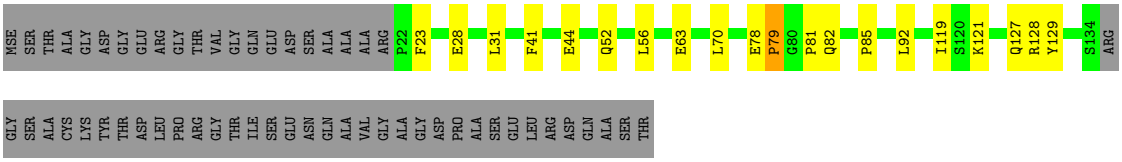
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	7-B	12	12	12	0	0
			Total	O		
2	8-B	11	11	11	0	0
			Total	O		
2	9-B	13	13	13	0	0
			Total	O		
2	10-B	14	14	14	0	0
			Total	O		
2	11-B	12	12	12	0	0
			Total	O		
2	12-B	12	12	12	0	0
			Total	O		
2	13-B	11	11	11	0	0
			Total	O		
2	14-B	12	12	12	0	0
			Total	O		
2	15-B	12	12	12	0	0
			Total	O		
2	16-B	11	11	11	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. 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. 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.

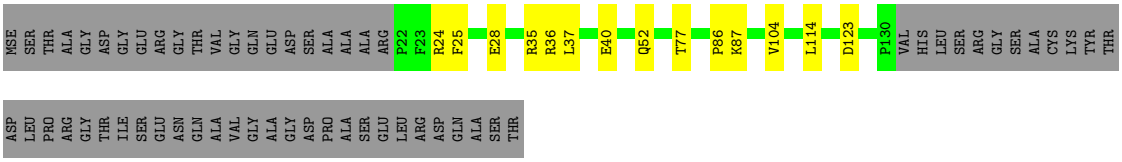
• Molecule 1: Protein RS21-C6

Chain 1-A:



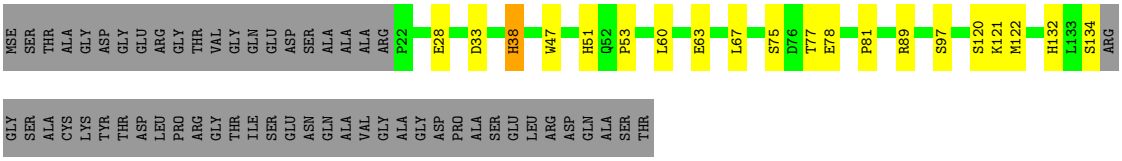
• Molecule 1: Protein RS21-C6

Chain 1-B:



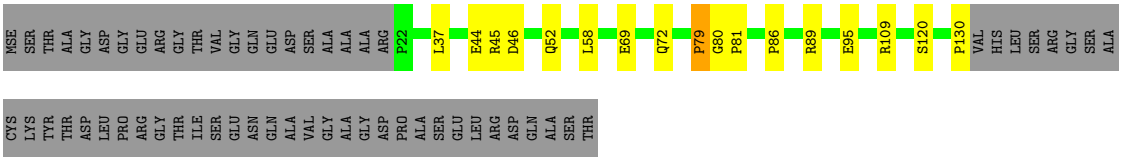
• Molecule 1: Protein RS21-C6

Chain 2-A:



• Molecule 1: Protein RS21-C6

Chain 2-B:



• Molecule 1: Protein RS21-C6

Chain 3-A: 59% 6% • 34%

MSE SER THR ALA GLY ASP GLY GLU ARG GLY THR VAL GLY GLN GLU ASP SER ALA ALA ALA ARG P22 E40 F41 A42 E48 Q52 P53 R54 E63 L67 D76 T77 Q82 Y129 S134 ARG GLY SER ALA CYS LYS TYR THR ASP LEU PRO ARG GLY THR ILE SER GLU ASN GLN ALA VAL GLY ALA GLY ASP PRO ALA SER GLU LEU ARG ASP GLN ALA SER THR

• Molecule 1: Protein RS21-C6

Chain 3-B: 58% 6% 36%

MSE SER THR ALA GLY ASP GLY GLU ARG GLY THR VAL GLY GLN GLU ASP SER ALA ALA ALA ARG P22 F23 R24 H38 T77 E78 P79 W84 P85 P86 R89 E94 V104 I119 P130 VAL HIS LEU SER ARG GLY SER ALA CYS LYS TYR THR ASP LEU PRO ARG GLY THR ILE SER GLU ASN GLN ALA VAL GLY ALA GLY ASP PRO ALA SER GLU LEU ARG ASP GLN ALA SER THR

• Molecule 1: Protein RS21-C6

Chain 4-A: 58% 8% 34%

MSE SER THR ALA GLY ASP GLY GLU ARG GLY THR VAL GLY GLN GLU ASP SER ALA ALA ALA ARG P22 W47 R54 E63 V64 L67 T77 P81 W84 P85 P86 Y102 R109 M122 R126 Y129 S134 ARG GLY SER ALA CYS LYS TYR THR ASP LEU PRO ARG GLY THR ILE SER GLU ASN GLN ALA VAL GLY ALA GLY ASP PRO ALA SER GLU LEU ARG ASP GLN ALA SER THR

• Molecule 1: Protein RS21-C6

Chain 4-B: 53% 10% • 36%

MSE SER THR ALA GLY ASP GLY GLU ARG GLY THR VAL GLY GLN GLU ASP SER ALA ALA ALA ARG P22 F23 R24 L31 D46 Q49 R54 E63 Q72 T77 E78 P79 G80 P81 Q82 A83 R89 V104 R109 D113 I119 M122 P130 VAL HIS LEU SER ARG GLY SER ALA CYS LYS TYR THR ASP LEU PRO ARG GLY THR ILE SER GLU ASN GLN ALA VAL GLY ALA GLY ASP PRO ALA SER GLU LEU ARG ASP GLN ALA SER THR

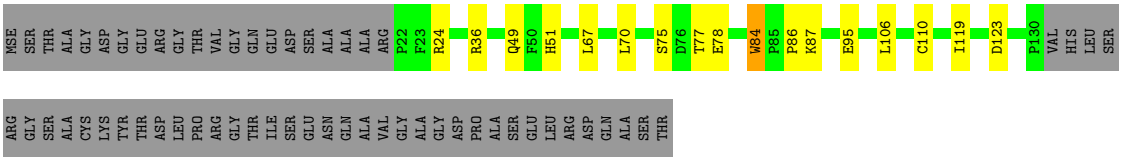
• Molecule 1: Protein RS21-C6

Chain 5-A: 58% 8% 34%

MSE SER THR ALA GLY ASP GLY GLU ARG GLY THR VAL GLY GLN GLU ASP SER ALA ALA ALA ARG P22 S26 P27 D33 E48 L67 Q72 P79 G80 P81 Q82 R89 I119 R128 Y129 H132 L133 S134 ARG GLY SER ALA CYS LYS TYR THR ASP LEU PRO ARG GLY THR ILE SER GLU ASN GLN ALA VAL GLY ALA GLY ASP PRO ALA SER GLU LEU ARG ASP GLN ALA SER THR

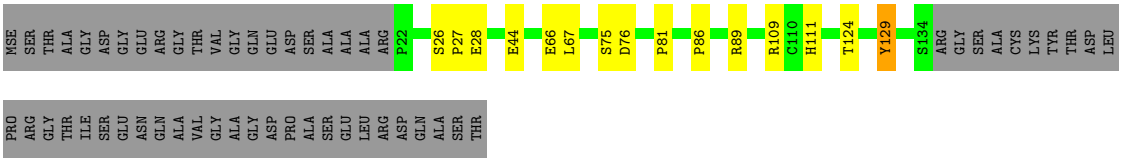
• Molecule 1: Protein RS21-C6

Chain 5-B: 54% 9% • 36%



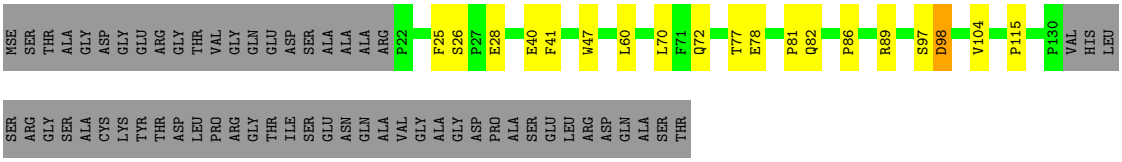
- Molecule 1: Protein RS21-C6

Chain 6-A:



- Molecule 1: Protein RS21-C6

Chain 6-B:

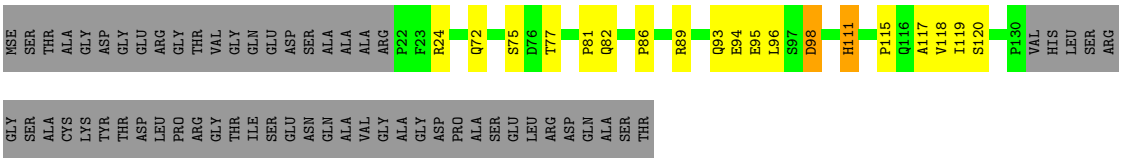


- Molecule 1: Protein RS21-C6

Chain 7-A:

- Molecule 1: Protein RS21-C6

Chain 7-B:



- Molecule 1: Protein RS21-C6

Chain 8-A:

GLY THR ILE SER GLU ASN GLN ALA VAL GLY ALA GLY ASP PRO ALA SER GLU LEU ARG ASP GLN ALA SER THR

• Molecule 1: Protein RS21-C6

Chain 8-B: 52% 11% • 36%

MSE SER THR ALA GLY ASP GLY GLU ARG GLY THR VAL GLY GLN GLU ASP SER ALA ALA ALA ARG P22 D33 R36 L37 R45 F50 L56 L60 E63 L67 A68 E69 Q72 P85 P86 K87 Q93 E94 E95 H111 V112 D113 L114 D123 Q127

P130 VAL HIS LEU SER ARG GLY SER ALA CYS LYS TYR THR ASP LEU PRO ARG GLY THR ILE SER GLU ASN GLN ALA VAL GLY ALA GLY ASP PRO ALA SER GLU LEU ARG ASP GLN ALA SER THR

• Molecule 1: Protein RS21-C6

Chain 9-A: 54% 11% • 34%

MSE SER THR ALA GLY ASP GLY GLU ARG GLY THR VAL GLY GLN GLU ASP SER ALA ALA ALA ARG P22 F23 D46 W47 E48 F71 Q72 E78 Q82 P86 K87 E88 Q93 E94 E95 D98 V99 L100 P115 I119 M122 D123 Y129 S134 ARG GLY SER

ALA CYS LYS TYR THR ASP LEU PRO ARG GLY THR ILE SER GLU ASN GLN ALA VAL GLY ALA GLY ASP PRO ALA SER GLU LEU ARG ASP GLN ALA SER THR

• Molecule 1: Protein RS21-C6

Chain 9-B: 57% 6% • 36%

MSE SER THR ALA GLY ASP GLY GLU ARG GLY THR VAL GLY GLN GLU ASP SER ALA ALA ALA ARG P22 R36 D46 Q49 L67 Q72 S75 E78 P85 R89 A90 Q93 Y129 P130 VAL HIS LEU SER ARG GLY SER ALA CYS LYS TYR THR ASP LEU

PRO ARG GLY THR ILE SER GLU ASN GLN ALA VAL GLY ALA GLY ASP PRO ALA SER GLU LEU ARG ASP GLN ALA SER THR

• Molecule 1: Protein RS21-C6

Chain 10-A: 55% 9% • 34%

MSE SER THR ALA GLY ASP GLY GLU ARG GLY THR VAL GLY GLN GLU ASP SER ALA ALA ALA ARG P22 F23 R24 E28 L37 D46 W47 E48 V64 Q72 S75 E78 P81 Q82 A83 W84 P85 P86 Q93 E94 E95 Y102 Y129 H132 L133 S134 ARG

GLY SER ALA CYS LYS TYR THR ASP LEU PRO ARG GLY THR ILE SER GLU ASN GLN ALA ALA VAL GLY ALA GLY ASP PRO ALA SER GLU LEU ARG ASP GLN ALA SER THR

• Molecule 1: Protein RS21-C6

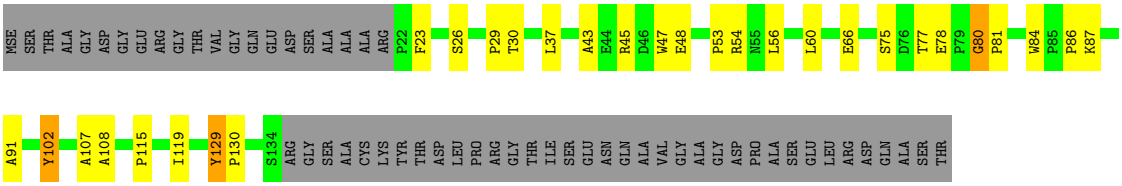
Chain 10-B: 54% 10% 36%

MSE SER THR ALA GLY ASP GLY GLU ARG GLY THR VAL GLY GLN GLU ASP SER ALA ALA ALA ARG P22 F25 S26 P27 E28 P29 T30 D33 W73 K74 S75 D76 T77 E78 P86 D98 V104 Q116 M122 D123 T124 N125 R126 P130 VAL HIS LEU SER ARG GLY

SER ALA CYS LYS TYR THR ASP LEU PRO ARG GLY THR ILE SER GLU ASN GLN ALA VAL GLY ALA GLY ASP PRO ALA SER GLU LEU ARG ASP GLN ALA SER THR

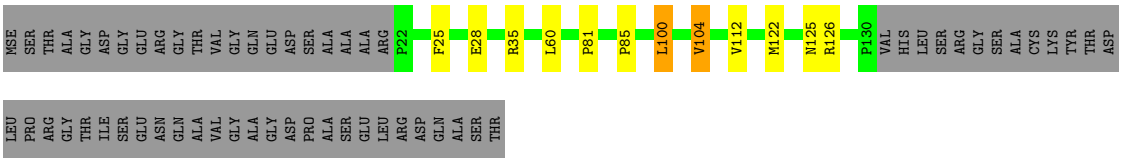
- Molecule 1: Protein RS21-C6

Chain 11-A:



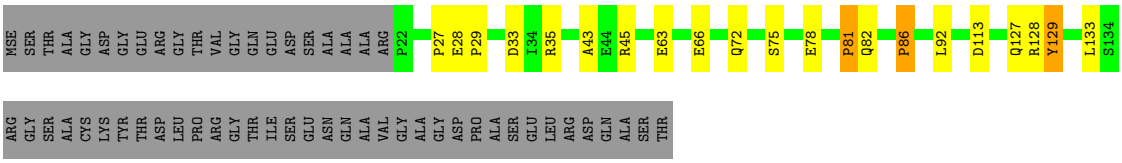
- Molecule 1: Protein RS21-C6

Chain 11-B:



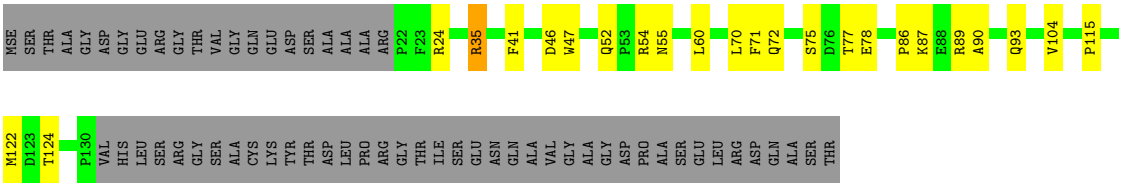
- Molecule 1: Protein RS21-C6

Chain 12-A:



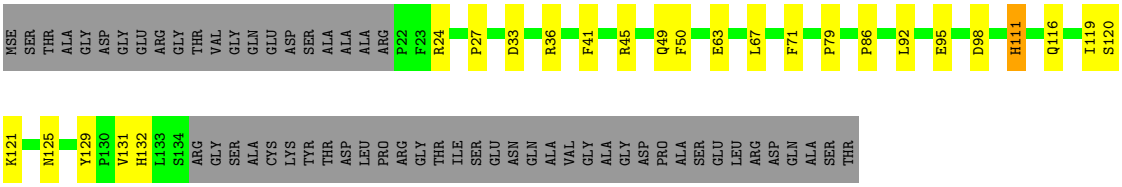
- Molecule 1: Protein RS21-C6

Chain 12-B:



- Molecule 1: Protein RS21-C6

Chain 13-A:



- Molecule 1: Protein RS21-C6

Chain 13-B: 46% 15% • 36%

MSE SER THR ALA GLY ASP GLY GLU ARG GLY THR VAL GLY GLN GLU ASP SER ALA ALA ALA ARG P22 S26 P27 E28 E32 D33 L37 H38 A39 E40 F41 E44 R45 D46 Q49 Q52 P53 R54 S75 D76 T77 A83 W84 P85 P86 K87 E88 R89 E95

Y102 L103 C110 V118 M122 Q127 R128 Y129 P130 VAL HIS LEU SER ARG GLY SER ALA CYS LYS TYR THR ASP LEU PRO ARG GLY THR ILE SER GLU ASN GLN ALA VAL GLY ALA GLY ASP PRO ALA SER GLU LEU ARG ASP GLN ALA SER THR

- Molecule 1: Protein RS21-C6

Chain 14-A: 49% 16% • 34%

MSE SER THR ALA GLY ASP GLY GLU ARG GLY THR VAL GLY GLN GLU ASP SER ALA ALA ALA ARG P22 P27 E28 P29 T30 L31 D46 Q49 Q52 L56 L60 E63 S75 D76 T77 E78 P79 G80 P81 P85 R89 A90 Q93 E94 E95 L96 S97 D98

V112 M122 Q127 R128 Y129 P130 V131 H132 L133 S134 ARG GLY SER ALA CYS LYS TYR THR ASP LEU PRO ARG GLY THR ILE SER GLU ASN GLN ALA VAL GLY ALA GLY ASP PRO ALA SER GLU LEU ARG ASP GLN ALA SER THR

- Molecule 1: Protein RS21-C6

Chain 14-B: 45% 16% • 36%

MSE SER THR ALA GLY ASP GLY GLU ARG GLY THR VAL GLY GLN GLU ASP SER ALA ALA ALA ARG P22 F23 R24 E32 D33 R36 L37 E40 F41 A42 A43 E44 R45 D46 W47 E48 Q49 R54 E63 L70 F71 Q72 W73 T77 P86 K87 E88 R109 D113

L114 P115 S120 K121 M122 R126 Q127 R128 Y129 P130 VAL HIS LEU SER ARG GLY SER ALA CYS LYS TYR THR ASP LEU PRO ARG GLY THR ILE SER GLU ASN GLN ALA VAL GLY ALA GLY ASP PRO ALA SER GLU LEU ARG ASP GLN ALA SER THR

- Molecule 1: Protein RS21-C6

Chain 15-A: 52% 14% • 34%

MSE SER THR ALA GLY ASP GLY GLU ARG GLY THR VAL GLY GLN GLU ASP SER ALA ALA ALA ARG P22 F23 R24 E28 I34 E44 W47 E48 Q49 Q52 P53 R54 E63 E66 Q72 S75 D76 P81 Q82 A90 E95 L96 S97 R109 D123

Q127 R128 Y129 S134 ARG GLY SER ALA CYS LYS TYR THR ASP LEU PRO ARG GLY THR ILE SER GLU ASN GLN ALA VAL GLY ALA GLY ASP PRO ALA SER GLU LEU ARG ASP GLN ALA SER THR

- Molecule 1: Protein RS21-C6

Chain 15-B: 46% 16% • 36%

MSE SER THR ALA GLY ASP GLY GLU ARG GLY THR VAL GLY GLN GLU ASP SER ALA ALA ALA ARG P22 E28 H38 D46 W47 E48 Q49 F50 H51 Q52 L56 L60 L70 F71 D76 T77 E78 P79 G80 A83 W84 P85 P86 K87 E88 R89 Q93 E94 E95

L100 V112 S120 K121 M122 N125 R126 Q127 R128 Y129 P130 VAL HIS LEU SER ARG GLY SER ALA CYS LYS TYR THR ASP LEU PRO ARG GLY THR ILE SER GLU ASN GLN ALA VAL GLY ALA GLY ASP PRO ALA SER GLU LEU ARG ASP GLN ALA SER THR

- Molecule 1: Protein RS21-C6

Chain 16-A: 46% 15% 5% 34%

MSE SER THR ALA GLY ASP GLY GLU ARG GLY THR VAL GLY GLN GLU ASP SER ALA ALA ALA ARG P22 E28 E32 R35 R36 L37 R45 D46 W47 E48 Q49 F50 P53 R54 N55 L56 L57 L60 E66 L67 A68 E69 T77 E78 P79 G80 P81 Q82 A83 W84 P85

P86 Y102 L103 L106 H111 V112 D113 S120 T124 N125 R126 S134 ARG GLY SER ALA CYS LYS TYR THR ASP LEU PRO ARG GLY THR ILE SER GLU ASN GLN ALA VAL GLY ALA ALA GLY ASP PRO ALA SER GLU LEU ARG ASP GLN ALA SER THR

- Molecule 1: Protein RS21-C6

Chain 16-B: 41% 21% • 36%

MSE SER THR ALA GLY ASP GLY GLU ARG GLY THR VAL GLY GLN GLU ASP SER ALA ALA ALA ARG P22 F23 R24 F25 E28 P29 T30 L31 E32 R36 L37 H38 A39 E40 F41 A42 A43 E44 Q49 P53 R54 L67 A68 E69 L70 F71 Q72 W73 K74 S75 D76 T77 E78

K87 E88 R89 A90 A91 L92 Q93 E94 E95 L96 V104 C110 D113 Q116 M122 D123 T124 N125 R126 Y129 P130 VAL HIS LEU SER ARG GLY SER ALA CYS LYS TYR THR ASP LEU PRO ARG GLY THR ILE SER GLU ASN GLN ALA VAL GLY ALA GLY ASP PRO ALA SER GLU

LEU ARG ASP GLN ALA SER THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	73.54Å 73.54Å 236.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.93 – 2.32 43.29 – 2.32	Depositor EDS
% Data completeness (in resolution range)	98.3 (37.93-2.32) 98.5 (43.29-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.69 (at 2.32Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.138 , 0.233 0.192 , 0.268	Depositor DCC
R_{free} test set	858 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	55.5	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 652.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	29392	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% 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 (i)

5.1 Standard geometry (i)

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	1-A	0.83	0/947	1.09	1/1288 (0.1%)
1	1-B	0.93	0/915	1.02	2/1244 (0.2%)
1	2-A	0.92	0/947	1.08	2/1288 (0.2%)
1	2-B	0.94	1/915 (0.1%)	1.01	1/1244 (0.1%)
1	3-A	0.87	0/947	0.94	0/1288
1	3-B	0.99	0/915	0.95	0/1244
1	4-A	0.94	0/947	0.98	0/1288
1	4-B	1.01	0/915	1.11	3/1244 (0.2%)
1	5-A	0.89	0/947	0.91	0/1288
1	5-B	0.93	1/915 (0.1%)	0.98	3/1244 (0.2%)
1	6-A	0.87	0/947	0.98	0/1288
1	6-B	1.05	2/915 (0.2%)	1.11	4/1244 (0.3%)
1	7-A	0.90	0/947	0.99	2/1288 (0.2%)
1	7-B	0.92	0/915	0.98	1/1244 (0.1%)
1	8-A	0.86	0/947	0.99	1/1288 (0.1%)
1	8-B	0.99	2/915 (0.2%)	1.09	2/1244 (0.2%)
1	9-A	0.94	2/947 (0.2%)	0.98	0/1288
1	9-B	0.90	0/915	0.94	1/1244 (0.1%)
1	10-A	0.93	1/947 (0.1%)	1.01	2/1288 (0.2%)
1	10-B	0.98	0/915	1.04	4/1244 (0.3%)
1	11-A	0.95	1/947 (0.1%)	1.12	7/1288 (0.5%)
1	11-B	0.99	1/915 (0.1%)	1.22	4/1244 (0.3%)
1	12-A	0.96	1/947 (0.1%)	1.02	2/1288 (0.2%)
1	12-B	0.91	1/915 (0.1%)	1.07	3/1244 (0.2%)
1	13-A	1.05	0/947	1.15	2/1288 (0.2%)
1	13-B	1.28	5/915 (0.5%)	1.26	7/1244 (0.6%)
1	14-A	1.05	1/947 (0.1%)	1.23	4/1288 (0.3%)
1	14-B	1.10	2/915 (0.2%)	1.13	3/1244 (0.2%)
1	15-A	0.98	1/947 (0.1%)	1.10	2/1288 (0.2%)
1	15-B	1.16	2/915 (0.2%)	1.16	4/1244 (0.3%)
1	16-A	1.11	2/947 (0.2%)	1.31	10/1288 (0.8%)
1	16-B	1.39	9/915 (1.0%)	1.41	13/1244 (1.0%)
All	All	0.99	35/29792 (0.1%)	1.08	90/40512 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	5-B	0	1
1	9-A	0	1
1	11-A	0	1
1	12-A	0	1
1	13-B	0	2
1	16-A	0	1
1	16-B	0	1
All	All	0	8

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16-B	42	ALA	CA-CB	13.50	1.80	1.52
1	16-B	28	GLU	CD-OE1	-8.05	1.16	1.25
1	16-B	28	GLU	CG-CD	7.98	1.64	1.51
1	13-B	39	ALA	CA-CB	-7.26	1.37	1.52
1	14-A	94	GLU	CG-CD	7.26	1.62	1.51

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	11-B	35	ARG	NE-CZ-NH1	15.25	127.92	120.30
1	11-B	35	ARG	NE-CZ-NH2	-14.82	112.89	120.30
1	12-B	35	ARG	NE-CZ-NH2	-10.14	115.23	120.30
1	6-B	89	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	5-B	36	ARG	NE-CZ-NH1	8.12	124.36	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	11-A	102	TYR	Sidechain
1	12-A	129	TYR	Sidechain
1	13-B	41	PHE	Sidechain
1	5-B	51	HIS	Sidechain
1	9-A	71	PHE	Sidechain

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	1-A	922	0	901	0	0
1	1-B	891	0	869	0	0
1	2-A	922	0	901	0	0
1	2-B	891	0	869	0	0
1	3-A	922	0	901	0	0
1	3-B	891	0	869	0	0
1	4-A	922	0	901	0	0
1	4-B	891	0	869	0	0
1	5-A	922	0	901	0	0
1	5-B	891	0	869	0	0
1	6-A	922	0	901	0	0
1	6-B	891	0	869	0	0
1	7-A	922	0	901	0	0
1	7-B	891	0	869	0	0
1	8-A	922	0	901	0	0
1	8-B	891	0	869	0	0
1	9-A	922	0	901	0	0
1	9-B	891	0	869	0	0
1	10-A	922	0	901	0	0
1	10-B	891	0	869	0	0
1	11-A	922	0	901	0	0
1	11-B	891	0	869	0	0
1	12-A	922	0	901	0	0
1	12-B	891	0	869	0	0
1	13-A	922	0	901	0	0
1	13-B	891	0	869	0	0
1	14-A	922	0	901	0	0
1	14-B	891	0	869	0	0
1	15-A	922	0	901	0	0
1	15-B	891	0	869	0	0
1	16-A	922	0	901	0	0
1	16-B	891	0	869	0	0
2	1-A	12	0	0	0	0
2	1-B	12	0	0	0	0
2	2-A	11	0	0	0	0
2	2-B	13	0	0	0	0
2	3-A	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	3-B	12	0	0	0	0
2	4-A	11	0	0	0	0
2	4-B	13	0	0	0	0
2	5-A	12	0	0	0	0
2	5-B	12	0	0	0	0
2	6-A	11	0	0	0	0
2	6-B	13	0	0	0	0
2	7-A	12	0	0	0	0
2	7-B	12	0	0	0	0
2	8-A	13	0	0	0	0
2	8-B	11	0	0	0	0
2	9-A	11	0	0	0	0
2	9-B	13	0	0	0	0
2	10-A	10	0	0	0	0
2	10-B	14	0	0	0	0
2	11-A	12	0	0	0	0
2	11-B	12	0	0	0	0
2	12-A	12	0	0	0	0
2	12-B	12	0	0	0	0
2	13-A	13	0	0	0	0
2	13-B	11	0	0	0	0
2	14-A	12	0	0	0	0
2	14-B	12	0	0	0	0
2	15-A	12	0	0	0	0
2	15-B	12	0	0	0	0
2	16-A	13	0	0	0	0
2	16-B	11	0	0	0	0
All	All	29392	0	28320	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	1-A	111/170 (65%)	83 (75%)	23 (21%)	5 (4%)	2	1
1	1-B	107/170 (63%)	83 (78%)	22 (21%)	2 (2%)	8	6
1	2-A	111/170 (65%)	89 (80%)	18 (16%)	4 (4%)	3	2
1	2-B	107/170 (63%)	90 (84%)	10 (9%)	7 (6%)	1	0
1	3-A	111/170 (65%)	97 (87%)	9 (8%)	5 (4%)	2	1
1	3-B	107/170 (63%)	98 (92%)	6 (6%)	3 (3%)	5	3
1	4-A	111/170 (65%)	92 (83%)	14 (13%)	5 (4%)	2	1
1	4-B	107/170 (63%)	85 (79%)	14 (13%)	8 (8%)	1	0
1	5-A	111/170 (65%)	95 (86%)	12 (11%)	4 (4%)	3	2
1	5-B	107/170 (63%)	98 (92%)	6 (6%)	3 (3%)	5	3
1	6-A	111/170 (65%)	91 (82%)	13 (12%)	7 (6%)	1	0
1	6-B	107/170 (63%)	85 (79%)	16 (15%)	6 (6%)	2	0
1	7-A	111/170 (65%)	85 (77%)	18 (16%)	8 (7%)	1	0
1	7-B	107/170 (63%)	85 (79%)	10 (9%)	12 (11%)	0	0
1	8-A	111/170 (65%)	96 (86%)	12 (11%)	3 (3%)	5	3
1	8-B	107/170 (63%)	80 (75%)	18 (17%)	9 (8%)	1	0
1	9-A	111/170 (65%)	80 (72%)	22 (20%)	9 (8%)	1	0
1	9-B	107/170 (63%)	92 (86%)	11 (10%)	4 (4%)	3	1
1	10-A	111/170 (65%)	90 (81%)	16 (14%)	5 (4%)	2	1
1	10-B	107/170 (63%)	85 (79%)	15 (14%)	7 (6%)	1	0
1	11-A	111/170 (65%)	79 (71%)	17 (15%)	15 (14%)	0	0
1	11-B	107/170 (63%)	87 (81%)	14 (13%)	6 (6%)	2	0
1	12-A	111/170 (65%)	82 (74%)	19 (17%)	10 (9%)	1	0
1	12-B	107/170 (63%)	75 (70%)	22 (21%)	10 (9%)	0	0
1	13-A	111/170 (65%)	85 (77%)	19 (17%)	7 (6%)	1	0
1	13-B	107/170 (63%)	82 (77%)	16 (15%)	9 (8%)	1	0
1	14-A	111/170 (65%)	77 (69%)	21 (19%)	13 (12%)	0	0
1	14-B	107/170 (63%)	81 (76%)	14 (13%)	12 (11%)	0	0
1	15-A	111/170 (65%)	80 (72%)	20 (18%)	11 (10%)	0	0
1	15-B	107/170 (63%)	84 (78%)	16 (15%)	7 (6%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	16-A	111/170 (65%)	75 (68%)	23 (21%)	13 (12%)	0	0
1	16-B	107/170 (63%)	76 (71%)	19 (18%)	12 (11%)	0	0
All	All	3488/5440 (64%)	2742 (79%)	505 (14%)	241 (7%)	1	0

5 of 241 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	78	GLU
1	1-A	128	ARG
1	1-B	86	PRO
1	2-A	81	PRO
1	2-B	72	GLN

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	1-A	98/136 (72%)	83 (85%)	15 (15%)	2	2
1	1-B	94/136 (69%)	84 (89%)	10 (11%)	6	7
1	2-A	98/136 (72%)	83 (85%)	15 (15%)	2	2
1	2-B	94/136 (69%)	85 (90%)	9 (10%)	8	9
1	3-A	98/136 (72%)	88 (90%)	10 (10%)	7	8
1	3-B	94/136 (69%)	86 (92%)	8 (8%)	10	12
1	4-A	98/136 (72%)	89 (91%)	9 (9%)	9	10
1	4-B	94/136 (69%)	84 (89%)	10 (11%)	6	7
1	5-A	98/136 (72%)	88 (90%)	10 (10%)	7	8
1	5-B	94/136 (69%)	82 (87%)	12 (13%)	4	4
1	6-A	98/136 (72%)	89 (91%)	9 (9%)	9	10
1	6-B	94/136 (69%)	85 (90%)	9 (10%)	8	9
1	7-A	98/136 (72%)	89 (91%)	9 (9%)	9	10
1	7-B	94/136 (69%)	86 (92%)	8 (8%)	10	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	8-A	98/136 (72%)	89 (91%)	9 (9%)	9	10
1	8-B	94/136 (69%)	84 (89%)	10 (11%)	6	7
1	9-A	98/136 (72%)	87 (89%)	11 (11%)	6	6
1	9-B	94/136 (69%)	86 (92%)	8 (8%)	10	12
1	10-A	98/136 (72%)	84 (86%)	14 (14%)	3	3
1	10-B	94/136 (69%)	86 (92%)	8 (8%)	10	12
1	11-A	98/136 (72%)	88 (90%)	10 (10%)	7	8
1	11-B	94/136 (69%)	90 (96%)	4 (4%)	29	40
1	12-A	98/136 (72%)	87 (89%)	11 (11%)	6	6
1	12-B	94/136 (69%)	82 (87%)	12 (13%)	4	4
1	13-A	98/136 (72%)	80 (82%)	18 (18%)	1	1
1	13-B	94/136 (69%)	79 (84%)	15 (16%)	2	2
1	14-A	98/136 (72%)	85 (87%)	13 (13%)	4	4
1	14-B	94/136 (69%)	74 (79%)	20 (21%)	1	1
1	15-A	98/136 (72%)	86 (88%)	12 (12%)	5	5
1	15-B	94/136 (69%)	75 (80%)	19 (20%)	1	1
1	16-A	98/136 (72%)	79 (81%)	19 (19%)	1	1
1	16-B	94/136 (69%)	76 (81%)	18 (19%)	1	1
All	All	3072/4352 (71%)	2698 (88%)	374 (12%)	5	5

5 of 374 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	12-B	54	ARG
1	14-B	24	ARG
1	12-B	104	VAL
1	13-B	37	LEU
1	14-B	113	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 114 such sidechains are listed below:

Mol	Chain	Res	Type
1	9-B	52	GLN
1	16-A	52	GLN
1	11-B	111	HIS

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Mol	Chain	Res	Type
1	16-A	51	HIS
1	14-B	52	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.