



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:32 am BST

PDB ID : 5JNF  
Title : Crystal structure of the LgrA initiation module excluding the Asub domain:  
F-A-delta-sub  
Authors : Reimer, J.M.; Aloise, M.N.; Schmeing, T.M.  
Deposited on : 2016-04-29  
Resolution : 2.75 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](mailto: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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

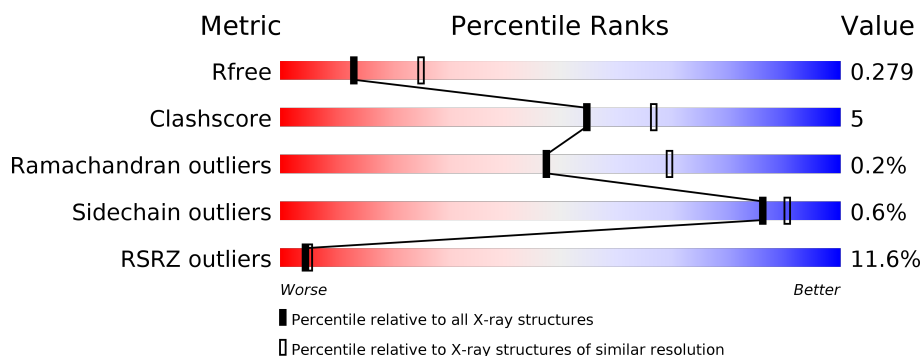
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	587	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>
1	B	587	<div> <div>23%</div> <div> <div></div> <div>80%</div> <div>18%</div> <div>.</div> </div> </div>
1	C	587	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div>.</div> </div> </div>
1	D	587	<div> <div>21%</div> <div> <div></div> <div>84%</div> <div>15%</div> <div>.</div> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 36748 atoms, of which 18083 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 Linear gramicidin synthase subunit A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	583	Total	C	H	N	O	S	0	0	0
			9221	2957	4577	796	869	22			
1	A	585	Total	C	H	N	O	S	0	0	0
			9239	2962	4585	798	872	22			
1	B	580	Total	C	H	N	O	S	0	0	0
			9033	2918	4452	777	864	22			
1	D	581	Total	C	H	N	O	S	0	0	0
			9050	2920	4459	783	866	22			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP Q70LM7
C	0	ALA	-	expression tag	UNP Q70LM7
C	1	MET	-	expression tag	UNP Q70LM7
C	2	GLY	-	expression tag	UNP Q70LM7
A	-1	GLY	-	expression tag	UNP Q70LM7
A	0	ALA	-	expression tag	UNP Q70LM7
A	1	MET	-	expression tag	UNP Q70LM7
A	2	GLY	-	expression tag	UNP Q70LM7
B	-1	GLY	-	expression tag	UNP Q70LM7
B	0	ALA	-	expression tag	UNP Q70LM7
B	1	MET	-	expression tag	UNP Q70LM7
B	2	GLY	-	expression tag	UNP Q70LM7
D	-1	GLY	-	expression tag	UNP Q70LM7
D	0	ALA	-	expression tag	UNP Q70LM7
D	1	MET	-	expression tag	UNP Q70LM7
D	2	GLY	-	expression tag	UNP Q70LM7

- Molecule 2 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	H	O	0	0
			5	1	2	2		
2	C	1	Total	C	H	O	0	0
			5	1	2	2		
2	C	1	Total	C	H	O	0	0
			5	1	2	2		
2	C	1	Total	C	H	O	0	0
			5	1	2	2		
2	A	1	Total	C	H	O	0	0
			5	1	2	2		

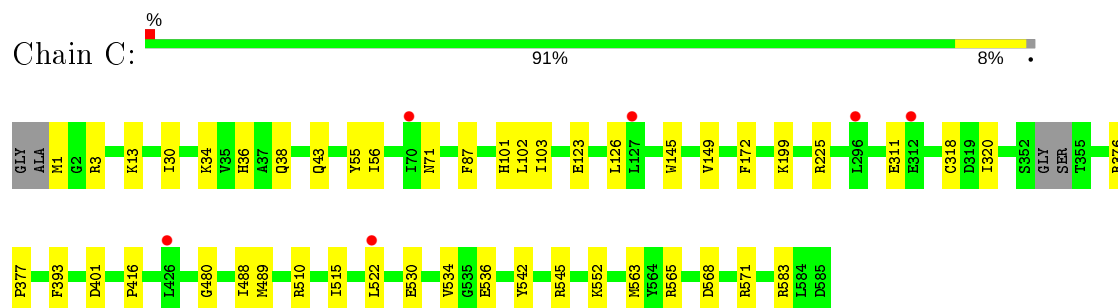
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	83	Total	O	0	0
			83	83		
3	A	73	Total	O	0	0
			73	73		
3	B	10	Total	O	0	0
			10	10		
3	D	14	Total	O	0	0
			14	14		

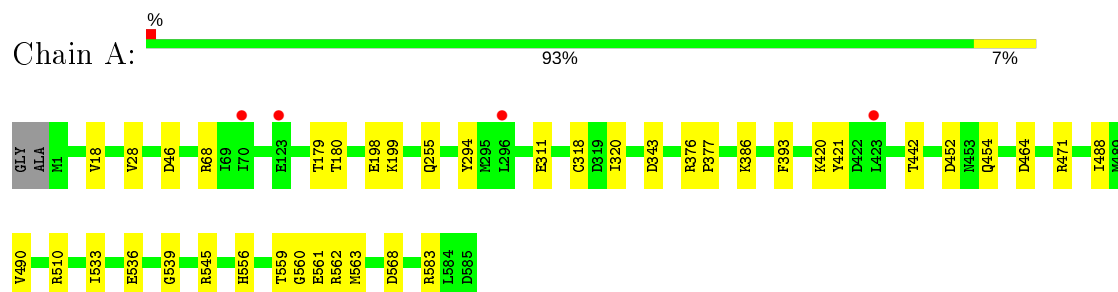
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

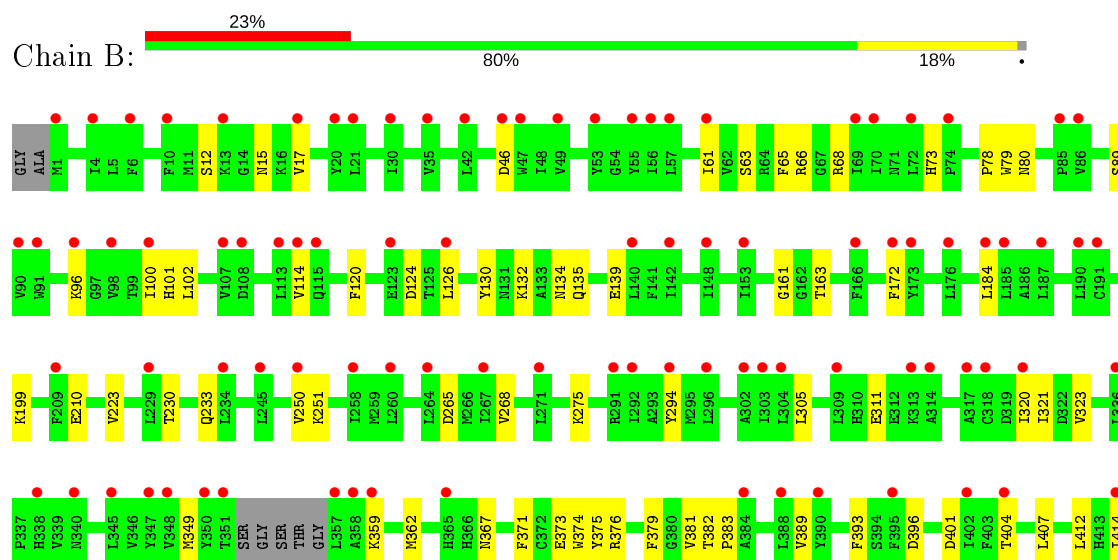
- Molecule 1: Linear gramicidin synthase subunit A

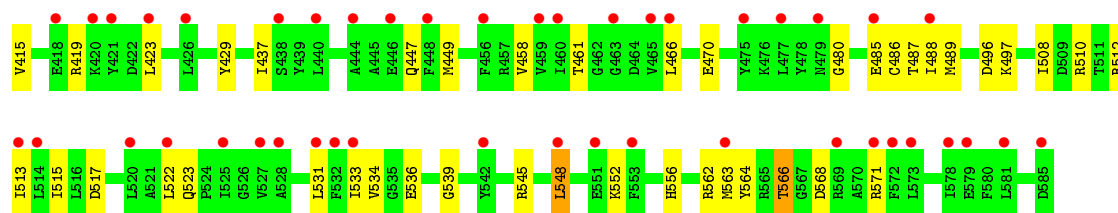


- Molecule 1: Linear gramicidin synthase subunit A

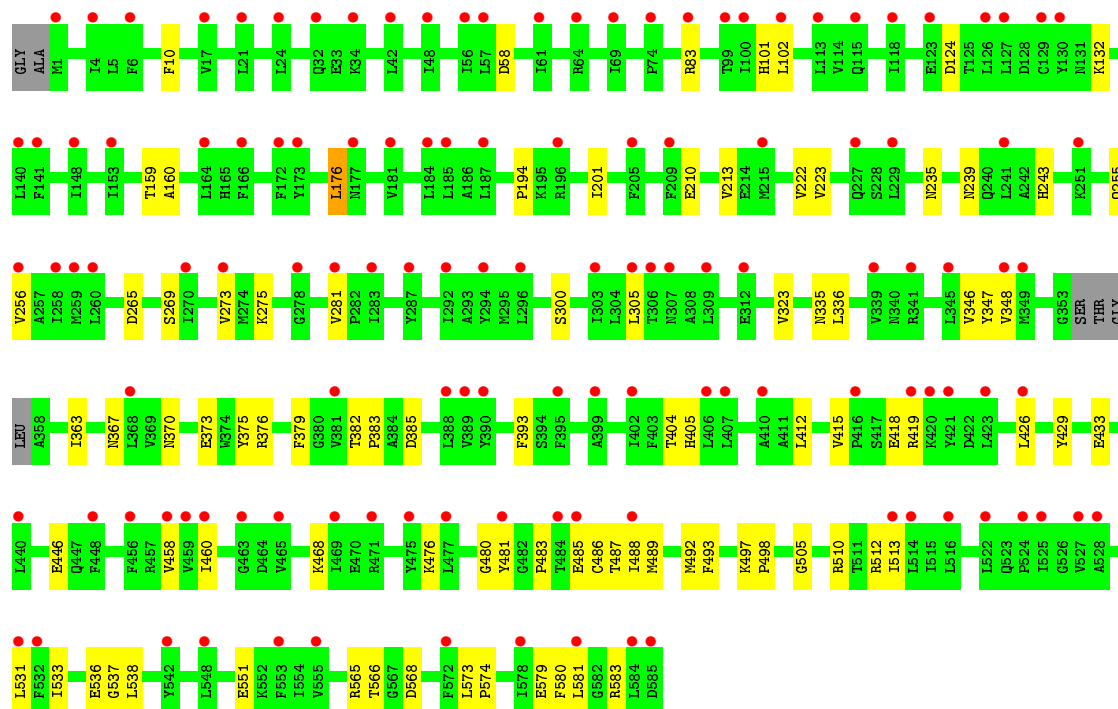
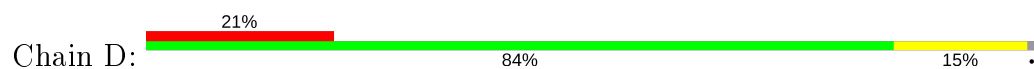


- Molecule 1: Linear gramicidin synthase subunit A





● Molecule 1: Linear gramicidin synthase subunit A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.31Å 161.31Å 139.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.79 – 2.75 88.40 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.79-2.75) 99.9 (88.40-2.55)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.247 , 0.275 0.251 , 0.279	Depositor DCC
$R_{free}$ test set	5817 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.0	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 45.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.478 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	36748	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.19 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4522e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.27	0/4760	0.46	0/6459
1	B	0.31	1/4686 (0.0%)	0.48	1/6371 (0.0%)
1	C	0.27	0/4749	0.45	0/6443
1	D	0.29	0/4696	0.48	0/6383
All	All	0.28	1/18891 (0.0%)	0.47	1/25656 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	HIS	C-N	6.22	1.46	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	548	LEU	CB-CG-CD2	-5.22	102.13	111.00

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	4654	4585	4586	23	0
1	B	4581	4452	4452	83	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4644	4577	4577	30	0
1	D	4591	4459	4460	60	0
2	A	3	2	1	0	0
2	C	12	8	4	0	0
3	A	73	0	0	2	0
3	B	10	0	0	1	0
3	C	83	0	0	3	0
3	D	14	0	0	0	0
All	All	18665	18083	18080	191	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 5.

All (191) 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:D:210:GLU:OE2	1:D:275:LYS:NZ	1.64	1.27
1:B:210:GLU:OE2	1:B:275:LYS:NZ	1.74	1.20
1:C:510:ARG:NH1	1:C:536:GLU:OE1	2.09	0.85
1:C:123:GLU:OE2	1:D:574:PRO:O	1.98	0.80
1:A:199:LYS:O	1:A:510:ARG:NH2	2.15	0.79
1:C:199:LYS:O	1:C:510:ARG:NH2	2.18	0.77
1:D:481:TYR:OH	1:D:568:ASP:OD2	2.02	0.76
1:B:531:LEU:O	1:B:566:THR:HG23	1.85	0.76
1:B:367:ASN:HB3	1:B:487:THR:HG21	1.67	0.76
1:D:551:GLU:O	1:D:565:ARG:NH2	2.20	0.75
1:B:486:CYS:O	1:B:487:THR:OG1	2.06	0.73
1:D:375:TYR:CD2	1:D:404:THR:HG21	2.27	0.69
1:D:222:VAL:HG12	1:D:412:LEU:HB2	1.74	0.68
1:C:568:ASP:OD1	1:C:583:ARG:NH1	2.27	0.67
1:B:100:ILE:HB	1:B:114:VAL:HG12	1.78	0.66
1:B:79:TRP:HE3	1:B:163:THR:HG23	1.62	0.65
1:B:375:TYR:CD2	1:B:404:THR:CG2	2.81	0.63
1:A:568:ASP:OD1	1:A:583:ARG:NH1	2.29	0.63
1:B:556:HIS:HB2	1:B:563:MET:CE	2.27	0.63
1:B:61:ILE:O	1:B:65:PHE:HD1	1.82	0.63
1:B:311:GLU:HG3	1:B:320:ILE:HD13	1.82	0.62
1:B:15:ASN:HB3	1:B:17:VAL:HG12	1.82	0.61
1:B:199:LYS:O	1:B:510:ARG:NH2	2.33	0.61
1:B:359:LYS:HG2	1:B:545:ARG:NH1	2.16	0.60
1:B:359:LYS:CE	1:B:548:LEU:HD21	2.31	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:ASP:OD1	1:B:132:LYS:NZ	2.31	0.59
1:B:230:THR:HG23	1:B:233:GLN:H	1.68	0.59
1:C:3:ARG:NH2	1:A:343:ASP:OD2	2.35	0.59
1:B:130:TYR:O	1:B:134:ASN:ND2	2.34	0.59
1:D:235:ASN:ND2	1:D:335:ASN:OD1	2.36	0.59
1:B:80:ASN:H	1:B:163:THR:HG1	1.49	0.58
1:A:452:ASP:OD1	1:A:454:GLN:NE2	2.36	0.58
1:C:34:LYS:NZ	1:C:56:ILE:O	2.36	0.58
1:D:243:HIS:CD2	1:D:336:LEU:HD11	2.38	0.58
1:C:401:ASP:OD1	3:C:701:HOH:O	2.17	0.57
1:A:539:GLY:O	1:A:562:ARG:NH2	2.32	0.57
1:D:375:TYR:CG	1:D:404:THR:HG21	2.40	0.57
1:A:386:LYS:NZ	3:A:704:HOH:O	2.38	0.57
1:B:552:LYS:HB3	1:B:564:TYR:CE1	2.39	0.56
1:B:294:TYR:OH	1:B:545:ARG:NH2	2.38	0.56
1:B:101:HIS:ND1	1:B:102:LEU:O	2.37	0.56
1:B:311:GLU:CG	1:B:320:ILE:HD13	2.36	0.55
1:D:210:GLU:CD	1:D:275:LYS:NZ	2.51	0.55
1:B:172:PHE:CZ	1:B:522:LEU:CD1	2.89	0.55
1:D:373:GLU:OE1	1:D:376:ARG:NH2	2.34	0.55
1:D:367:ASN:HB3	1:D:487:THR:HG21	1.89	0.54
1:B:375:TYR:CD2	1:B:404:THR:HG21	2.43	0.54
1:B:539:GLY:O	1:B:562:ARG:NH2	2.38	0.54
1:B:480:GLY:HA3	1:B:489:MET:CE	2.39	0.53
1:D:210:GLU:CD	1:D:275:LYS:HZ1	2.09	0.53
1:D:347:TYR:O	1:D:363:ILE:HG22	2.09	0.53
1:D:201:ILE:HD11	1:D:536:GLU:HG2	1.91	0.52
1:A:510:ARG:NH1	1:A:536:GLU:OE2	2.41	0.52
1:B:389:VAL:HG11	1:B:414:ILE:HD13	1.92	0.52
1:D:255:GLN:OE1	1:D:300:SER:N	2.37	0.52
1:D:281:VAL:HG22	1:D:348:VAL:HB	1.91	0.51
1:D:101:HIS:ND1	1:D:102:LEU:O	2.43	0.51
1:D:458:VAL:HG22	1:D:476:LYS:HD2	1.91	0.51
1:D:480:GLY:HA3	1:D:489:MET:CE	2.40	0.51
1:B:375:TYR:CE2	1:B:381:VAL:HG21	2.46	0.51
1:B:423:LEU:HD12	1:B:447:GLN:HB3	1.92	0.51
1:A:559:THR:HG21	1:A:561:GLU:OE2	2.11	0.50
1:B:79:TRP:CE3	1:B:163:THR:HG23	2.42	0.50
1:C:3:ARG:NH1	1:C:43:GLN:O	2.44	0.50
1:C:515:ILE:HD13	1:C:571:ARG:HA	1.94	0.50
1:D:194:PRO:HD3	1:D:512:ARG:NH1	2.27	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ASP:HA	1:B:268:VAL:HG12	1.94	0.50
1:B:265:ASP:HA	1:B:268:VAL:CG1	2.41	0.50
1:A:311:GLU:HG3	1:A:320:ILE:HD13	1.93	0.50
1:D:513:ILE:CD1	1:D:533:ILE:HG12	2.42	0.50
1:B:12:SER:O	1:B:15:ASN:ND2	2.45	0.49
1:C:172:PHE:CZ	1:C:522:LEU:CD1	2.95	0.49
1:B:375:TYR:CD2	1:B:404:THR:HG22	2.47	0.49
1:B:46:ASP:O	1:B:68:ARG:HD2	2.12	0.49
1:B:172:PHE:CZ	1:B:522:LEU:HD11	2.48	0.49
1:B:61:ILE:O	1:B:65:PHE:CD1	2.64	0.49
1:B:552:LYS:O	1:B:564:TYR:HA	2.12	0.49
1:B:250:VAL:C	1:B:251:LYS:HD2	2.33	0.49
1:C:311:GLU:HG3	1:C:320:ILE:HD13	1.94	0.49
1:A:18:VAL:HG13	1:A:28:VAL:HG11	1.94	0.48
1:D:446:GLU:HB3	1:D:468:LYS:HD2	1.95	0.48
1:B:487:THR:O	1:B:489:MET:N	2.46	0.48
1:B:531:LEU:HD22	1:B:566:THR:HG21	1.96	0.48
1:D:487:THR:HG23	1:D:537:GLY:O	2.13	0.48
1:A:442:THR:HG21	1:A:464:ASP:HB2	1.95	0.48
1:D:486:CYS:O	1:D:487:THR:OG1	2.32	0.47
1:B:415:VAL:O	1:B:415:VAL:HG23	2.15	0.47
1:B:512:ARG:O	1:B:534:VAL:HG12	2.15	0.47
1:C:38:GLN:NE2	1:A:198:GLU:OE1	2.46	0.47
1:C:534:VAL:HG12	1:C:563:MET:HG2	1.96	0.46
1:D:176:LEU:N	1:D:176:LEU:HD12	2.29	0.46
1:B:96:LYS:HD3	1:B:120:PHE:CD1	2.50	0.46
1:B:371:PHE:CE2	1:B:374:TRP:HZ3	2.34	0.46
1:B:389:VAL:HA	1:B:401:ASP:HB3	1.97	0.46
1:D:375:TYR:CD2	1:D:404:THR:CG2	2.97	0.46
1:D:513:ILE:HD13	1:D:533:ILE:HA	1.97	0.46
1:D:483:PRO:HB2	1:D:485:GLU:OE1	2.15	0.46
1:C:36:HIS:NE2	1:A:561:GLU:OE1	2.47	0.46
1:C:71:ASN:HB2	1:C:103:ILE:HD11	1.98	0.46
1:C:123:GLU:O	1:C:123:GLU:HG2	2.15	0.46
1:B:63:SER:HA	1:B:66:ARG:HG3	1.96	0.46
1:C:225:ARG:NH1	1:C:416:PRO:CB	2.79	0.46
1:D:239:ASN:OD1	1:D:275:LYS:HE2	2.16	0.46
1:B:265:ASP:HB3	1:B:323:VAL:HG11	1.97	0.46
1:B:449:MET:HB3	1:B:470:GLU:O	2.16	0.46
1:A:376:ARG:HB3	1:A:377:PRO:HD3	1.98	0.46
1:D:382:THR:OG1	1:D:383:PRO:HD2	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:TYR:OH	1:A:545:ARG:NH2	2.50	0.45
1:B:349:MET:HE1	1:B:396:ASP:N	2.30	0.45
1:C:87:PHE:HD1	1:C:126:LEU:HD13	1.80	0.45
1:D:458:VAL:HG22	1:D:476:LYS:HB2	1.97	0.45
1:B:359:LYS:HD3	1:B:548:LEU:HD21	1.98	0.45
1:C:13:LYS:HG2	1:C:30:ILE:CD1	2.47	0.45
1:B:496:ASP:OD2	1:B:497:LYS:HE3	2.17	0.45
1:B:359:LYS:HE2	1:B:548:LEU:HD21	1.98	0.45
1:D:159:THR:HG22	1:D:160:ALA:O	2.17	0.45
1:D:370:ASN:OD1	1:D:510:ARG:HD2	2.17	0.45
1:B:515:ILE:HD13	1:B:571:ARG:HA	1.97	0.45
1:D:222:VAL:HG12	1:D:412:LEU:HD12	1.99	0.45
1:B:480:GLY:HA3	1:B:489:MET:HE1	1.99	0.45
1:D:265:ASP:HB3	1:D:323:VAL:HG11	1.99	0.45
1:B:80:ASN:N	1:B:163:THR:OG1	2.35	0.44
1:D:566:THR:O	1:D:583:ARG:NH1	2.48	0.44
1:B:485:GLU:HG3	1:B:564:TYR:OH	2.16	0.44
1:C:480:GLY:HA3	1:C:489:MET:CE	2.47	0.44
1:B:517:ASP:OD1	1:B:523:GLN:NE2	2.51	0.44
1:B:512:ARG:HB2	1:B:534:VAL:HG13	1.98	0.44
1:C:145:TRP:CE2	1:C:149:VAL:CG2	3.01	0.44
1:D:487:THR:O	1:D:489:MET:N	2.51	0.44
1:C:376:ARG:HB3	1:C:377:PRO:HD3	2.00	0.44
1:B:135:GLN:O	1:B:139:GLU:HG3	2.17	0.43
1:B:126:LEU:HD11	1:B:184:LEU:HD22	1.99	0.43
1:B:362:MET:HE1	3:B:609:HOH:O	2.18	0.43
1:D:573:LEU:HD21	1:D:579:GLU:OE2	2.18	0.43
1:C:552:LYS:HD3	3:C:729:HOH:O	2.18	0.43
1:B:389:VAL:HG11	1:B:414:ILE:CD1	2.48	0.43
1:D:379:PHE:CZ	1:D:460:ILE:HD11	2.53	0.43
1:B:382:THR:OG1	1:B:383:PRO:HD2	2.19	0.43
1:B:15:ASN:CB	1:B:17:VAL:HG12	2.47	0.43
1:B:61:ILE:HG23	1:B:65:PHE:CE1	2.54	0.43
1:D:243:HIS:NE2	1:D:336:LEU:HD11	2.32	0.43
1:A:46:ASP:O	1:A:68:ARG:HD2	2.19	0.43
1:B:437:ILE:HA	1:B:458:VAL:O	2.17	0.43
1:D:256:VAL:HB	1:D:273:VAL:HG11	2.01	0.43
1:D:269:SER:HB3	1:D:305:LEU:HD13	2.01	0.43
1:B:367:ASN:ND2	1:B:536:GLU:O	2.51	0.42
1:B:223:VAL:N	1:B:412:LEU:O	2.51	0.42
1:C:55:TYR:CE1	1:A:560:GLY:HA3	2.54	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:VAL:N	1:D:412:LEU:O	2.47	0.42
1:D:493:PHE:HB2	1:D:505:GLY:CA	2.49	0.42
1:B:373:GLU:OE1	1:B:376:ARG:NH2	2.42	0.42
1:B:461:THR:HG21	1:B:466:LEU:HD13	2.01	0.42
1:D:580:PHE:C	1:D:581:LEU:HD12	2.39	0.42
1:B:89:SER:HB3	1:B:96:LYS:HG2	2.00	0.42
1:C:13:LYS:HG2	1:C:30:ILE:HD12	2.01	0.42
1:A:490:VAL:HG21	1:A:533:ILE:CD1	2.50	0.42
1:B:512:ARG:HB2	1:B:534:VAL:CG1	2.49	0.42
1:D:124:ASP:OD1	1:D:132:LYS:NZ	2.52	0.42
1:A:420:LYS:HE3	1:A:421:TYR:CE2	2.55	0.42
1:B:419:ARG:HH11	1:B:429:TYR:HB2	1.85	0.42
1:C:1:MET:HE3	3:C:731:HOH:O	2.20	0.42
1:C:542:TYR:HB2	1:C:545:ARG:HB2	2.02	0.41
1:B:78:PRO:CG	1:B:161:GLY:O	2.68	0.41
1:D:10:PHE:CZ	1:D:83:ARG:NH2	2.88	0.41
1:C:145:TRP:CZ2	1:C:149:VAL:HG22	2.55	0.41
1:D:531:LEU:O	1:D:566:THR:OG1	2.20	0.41
1:B:359:LYS:CD	1:B:548:LEU:HD21	2.50	0.41
1:C:101:HIS:ND1	1:C:102:LEU:O	2.52	0.41
1:D:210:GLU:C	1:D:213:VAL:HG22	2.41	0.41
1:B:513:ILE:HD13	1:B:533:ILE:HA	2.02	0.41
1:C:530:GLU:OE2	1:C:565:ARG:HG2	2.20	0.41
1:D:429:TYR:CE2	1:D:433:GLU:HG3	2.56	0.41
1:D:405:HIS:HB2	1:D:412:LEU:HD21	2.03	0.41
1:D:497:LYS:HB3	1:D:498:PRO:HD2	2.02	0.41
1:D:367:ASN:ND2	1:D:538:LEU:O	2.51	0.41
1:B:376:ARG:HH11	1:B:407:LEU:HB3	1.86	0.41
1:A:179:THR:HG22	1:A:180:THR:N	2.36	0.41
1:B:379:PHE:HD2	1:B:458:VAL:HG11	1.84	0.41
1:D:210:GLU:O	1:D:213:VAL:HG22	2.21	0.41
1:D:415:VAL:HG23	1:D:415:VAL:O	2.21	0.41
1:B:371:PHE:CE2	1:B:374:TRP:CZ3	3.08	0.41
1:A:454:GLN:OE1	1:A:454:GLN:N	2.54	0.41
1:B:566:THR:OG1	1:B:568:ASP:N	2.50	0.41
1:D:419:ARG:NH1	1:D:429:TYR:HB2	2.36	0.41
1:A:471:ARG:O	3:A:701:HOH:O	2.22	0.40
1:B:305:LEU:HD23	1:B:321:ILE:HB	2.02	0.40
1:D:382:THR:HG22	1:D:385:ASP:OD2	2.20	0.40
1:A:556:HIS:HD2	1:A:563:MET:HE1	1.87	0.40
1:B:531:LEU:CD2	1:B:566:THR:HG21	2.50	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:346:VAL:CG1	1:D:363:ILE:HG23	2.51	0.40
1:D:492:MET:HA	1:D:492:MET:HE3	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	583/587 (99%)	565 (97%)	17 (3%)	1 (0%)	47	69
1	B	576/587 (98%)	560 (97%)	14 (2%)	2 (0%)	41	60
1	C	579/587 (99%)	564 (97%)	14 (2%)	1 (0%)	47	69
1	D	577/587 (98%)	560 (97%)	16 (3%)	1 (0%)	47	69
All	All	2315/2348 (99%)	2249 (97%)	61 (3%)	5 (0%)	47	69

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	488	ILE
1	A	488	ILE
1	C	488	ILE
1	D	488	ILE
1	B	508	ILE

### 5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	501/501 (100%)	498 (99%)	3 (1%)	86	90
1	B	488/501 (97%)	486 (100%)	2 (0%)	91	93
1	C	500/501 (100%)	498 (100%)	2 (0%)	91	93
1	D	489/501 (98%)	484 (99%)	5 (1%)	76	85
All	All	1978/2004 (99%)	1966 (99%)	12 (1%)	86	90

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	318	CYS
1	C	393	PHE
1	A	255	GLN
1	A	318	CYS
1	A	393	PHE
1	B	393	PHE
1	B	566	THR
1	D	58	ASP
1	D	176	LEU
1	D	393	PHE
1	D	418	GLU
1	D	426	LEU

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

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

5 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	$\# Z  > 2$
2	FMT	C	604	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	C	603	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	A	601	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	C	602	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	C	601	-	0,2,2	0.00	-	0,1,1	0.00	-

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.

No monomer is involved in short contacts.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	585/587 (99%)	0.37	4 (0%)  	39, 60, 96, 186	0
1	B	580/587 (98%)	1.13	136 (23%)  	96, 130, 147, 164	0
1	C	583/587 (99%)	0.37	6 (1%)  	39, 60, 93, 116	0
1	D	581/587 (98%)	1.08	125 (21%)  	100, 130, 148, 158	0
All	All	2329/2348 (99%)	0.74	271 (11%)  	39, 110, 144, 186	0

All (271) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	514	LEU	6.4
1	D	532	PHE	6.1
1	B	173	TYR	5.7
1	D	531	LEU	5.4
1	D	514	LEU	5.4
1	D	229	LEU	5.2
1	B	466	LEU	5.1
1	B	390	TYR	5.1
1	B	531	LEU	5.0
1	B	358	ALA	4.9
1	B	72	LEU	4.8
1	B	525	ILE	4.8
1	B	98	VAL	4.7
1	D	296	LEU	4.7
1	B	395	PHE	4.7
1	B	49	VAL	4.6
1	B	357	LEU	4.6
1	D	525	ILE	4.5
1	B	317	ALA	4.5
1	B	296	LEU	4.5
1	D	407	LEU	4.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	345	LEU	4.5
1	D	389	VAL	4.4
1	D	123	GLU	4.4
1	B	513	ILE	4.4
1	B	271	LEU	4.4
1	D	513	ILE	4.3
1	B	318	CYS	4.3
1	D	305	LEU	4.2
1	D	209	PHE	4.2
1	D	585	ASP	4.2
1	B	421	TYR	4.1
1	D	196	ARG	4.0
1	B	572	PHE	4.0
1	D	578	ILE	4.0
1	B	292	ILE	3.9
1	B	585	ASP	3.9
1	D	256	VAL	3.9
1	B	91	TRP	3.8
1	B	359	LYS	3.8
1	B	86	VAL	3.8
1	D	426	LEU	3.8
1	D	423	LEU	3.8
1	B	70	ILE	3.8
1	D	420	LYS	3.8
1	B	42	LEU	3.8
1	B	573	LEU	3.8
1	B	90	VAL	3.7
1	B	459	VAL	3.7
1	D	294	TYR	3.7
1	B	166	PHE	3.7
1	B	388	LEU	3.7
1	D	419	ARG	3.6
1	D	390	TYR	3.6
1	D	126	LEU	3.6
1	D	83	ARG	3.6
1	D	463	GLY	3.6
1	D	475	TYR	3.6
1	B	187	LEU	3.6
1	B	61	ILE	3.5
1	B	176	LEU	3.5
1	D	421	TYR	3.5
1	D	572	PHE	3.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	448	PHE	3.4
1	D	522	LEU	3.4
1	B	303	ILE	3.4
1	D	345	LEU	3.4
1	D	100	ILE	3.4
1	B	17	VAL	3.4
1	B	475	TYR	3.4
1	B	126	LEU	3.4
1	B	250	VAL	3.4
1	D	127	LEU	3.4
1	D	278	GLY	3.3
1	D	1	MET	3.3
1	B	414	ILE	3.3
1	B	579	GLU	3.3
1	D	57	LEU	3.3
1	B	351	THR	3.3
1	B	465	VAL	3.3
1	B	6	PHE	3.3
1	D	287	TYR	3.3
1	D	61	ILE	3.3
1	D	303	ILE	3.3
1	B	548	LEU	3.3
1	B	172	PHE	3.2
1	B	113	LEU	3.2
1	D	113	LEU	3.2
1	D	368	LEU	3.2
1	B	551	GLU	3.2
1	D	251	LYS	3.2
1	B	267	ILE	3.2
1	D	102	LEU	3.2
1	D	516	LEU	3.2
1	B	47	TRP	3.2
1	B	10	PHE	3.2
1	D	395	PHE	3.2
1	D	460	ILE	3.2
1	D	153	ILE	3.1
1	B	96	LYS	3.1
1	B	309	LEU	3.1
1	B	520	LEU	3.1
1	D	166	PHE	3.1
1	B	423	LEU	3.1
1	D	34	LYS	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	21	LEU	3.0
1	D	341	ARG	3.0
1	D	21	LEU	3.0
1	D	458	VAL	3.0
1	D	4	ILE	3.0
1	B	314	ALA	3.0
1	B	100	ILE	2.9
1	B	313	LYS	2.9
1	D	456	PHE	2.9
1	B	426	LEU	2.9
1	D	459	VAL	2.9
1	D	227	GLN	2.9
1	B	522	LEU	2.9
1	D	260	LEU	2.9
1	D	306	THR	2.9
1	B	440	LEU	2.9
1	B	571	ARG	2.9
1	B	402	ILE	2.9
1	D	281	VAL	2.9
1	D	349	MET	2.9
1	D	528	ALA	2.9
1	D	581	LEU	2.8
1	D	465	VAL	2.8
1	D	184	LEU	2.8
1	B	55	TYR	2.8
1	B	140	LEU	2.8
1	B	418	GLU	2.8
1	B	479	ASN	2.8
1	B	46	ASP	2.8
1	D	440	LEU	2.8
1	D	469	ILE	2.8
1	B	108	ASP	2.7
1	B	350	TYR	2.7
1	D	553	PHE	2.7
1	B	229	LEU	2.7
1	D	185	LEU	2.7
1	D	485	GLU	2.7
1	B	115	GLN	2.7
1	D	24	LEU	2.7
1	B	258	ILE	2.7
1	B	348	VAL	2.7
1	D	187	LEU	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	30	ILE	2.7
1	B	578	ILE	2.7
1	B	336	LEU	2.7
1	C	426	LEU	2.7
1	B	20	TYR	2.7
1	D	292	ILE	2.7
1	B	448	PHE	2.6
1	B	209	PHE	2.6
1	B	69	ILE	2.6
1	B	153	ILE	2.6
1	D	56	ILE	2.6
1	B	35	VAL	2.6
1	D	17	VAL	2.6
1	D	141	PHE	2.6
1	D	48	ILE	2.6
1	D	555	VAL	2.6
1	B	581	LEU	2.6
1	A	296	LEU	2.5
1	D	416	PRO	2.5
1	D	42	LEU	2.5
1	D	542	TYR	2.5
1	B	114	VAL	2.5
1	B	245	LEU	2.5
1	B	304	LEU	2.5
1	D	99	THR	2.5
1	D	241	LEU	2.5
1	B	563	MET	2.5
1	A	70	ILE	2.5
1	D	406	LEU	2.5
1	D	527	VAL	2.5
1	B	553	PHE	2.4
1	B	446	GLU	2.4
1	C	296	LEU	2.4
1	B	533	ILE	2.4
1	B	532	PHE	2.4
1	D	118	ILE	2.4
1	D	181	VAL	2.4
1	B	384	ALA	2.4
1	D	399	ALA	2.4
1	B	107	VAL	2.4
1	D	348	VAL	2.4
1	B	456	PHE	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	74	PRO	2.4
1	D	129	CYS	2.4
1	D	410	ALA	2.4
1	D	32	GLN	2.4
1	B	1	MET	2.4
1	B	185	LEU	2.4
1	B	463	GLY	2.4
1	B	420	LYS	2.4
1	B	291	ARG	2.4
1	B	85	PRO	2.3
1	B	477	LEU	2.3
1	A	123	GLU	2.3
1	D	115	GLN	2.3
1	B	53	TYR	2.3
1	B	294	TYR	2.3
1	A	423	LEU	2.3
1	B	184	LEU	2.3
1	B	260	LEU	2.3
1	D	584	LEU	2.3
1	D	484	THR	2.3
1	B	302	ALA	2.3
1	C	70	ILE	2.3
1	B	56	ILE	2.3
1	D	205	PHE	2.3
1	D	273	VAL	2.3
1	D	283	ILE	2.3
1	B	148	ILE	2.3
1	C	522	LEU	2.3
1	B	264	LEU	2.3
1	D	548	LEU	2.3
1	D	173	TYR	2.3
1	D	6	PHE	2.2
1	D	312	GLU	2.2
1	B	234	LEU	2.2
1	D	130	TYR	2.2
1	B	340	ASN	2.2
1	B	365	HIS	2.2
1	D	388	LEU	2.2
1	D	259	MET	2.2
1	B	13	LYS	2.2
1	B	320	ILE	2.2
1	D	471	ARG	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	485	GLU	2.2
1	D	481	TYR	2.2
1	B	4	ILE	2.2
1	B	142	ILE	2.2
1	D	488	ILE	2.2
1	B	438	SER	2.1
1	B	542	TYR	2.1
1	B	460	ILE	2.1
1	D	69	ILE	2.1
1	B	444	ALA	2.1
1	B	569	ARG	2.1
1	B	347	TYR	2.1
1	B	404	THR	2.1
1	B	338	HIS	2.1
1	D	270	ILE	2.1
1	D	381	VAL	2.1
1	D	177	ASN	2.1
1	B	527	VAL	2.1
1	D	258	ILE	2.1
1	D	402	ILE	2.1
1	D	477	LEU	2.1
1	D	172	PHE	2.1
1	B	57	LEU	2.1
1	D	164	LEU	2.1
1	B	488	ILE	2.1
1	B	528	ALA	2.1
1	D	307	ASN	2.1
1	D	339	VAL	2.1
1	D	74	PRO	2.1
1	D	309	LEU	2.0
1	D	148	ILE	2.0
1	B	123	GLU	2.0
1	B	191	CYS	2.0
1	D	215	MET	2.0
1	B	190	LEU	2.0
1	D	140	LEU	2.0
1	D	64	ARG	2.0
1	D	524	PRO	2.0
1	C	127	LEU	2.0
1	C	312	GLU	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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	FMT	A	601	3/3	0.85	0.18	62,66,74,80	0
2	FMT	C	603	3/3	0.87	0.20	59,65,78,79	0
2	FMT	C	601	3/3	0.91	0.15	76,77,91,96	0
2	FMT	C	604	3/3	0.93	0.24	64,65,78,84	0
2	FMT	C	602	3/3	0.94	0.19	69,69,82,82	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.