



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:29 PM GMT

PDB ID : 4S17  
Title : The crystal structure of glutamine synthetase from Bifidobacterium adolescentis ATCC 15703  
Authors : Cuff, M.; Tan, K.; Mack, J.; Clancy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2015-01-08  
Resolution : 2.30 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

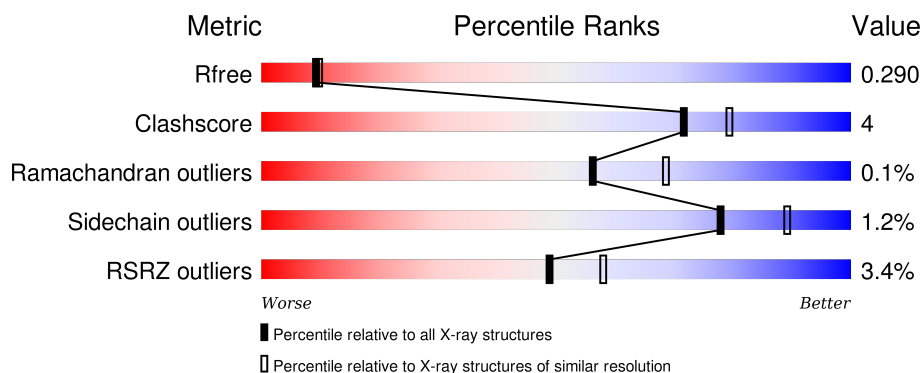
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	481	<div> <div>3%</div> <div>83% 11% 6%</div> </div>
1	B	481	<div> <div>3%</div> <div>83% 11% 6%</div> </div>
1	C	481	<div> <div>4%</div> <div>81% 12% 7%</div> </div>
1	D	481	<div> <div>3%</div> <div>80% 14% 6%</div> </div>
1	E	481	<div> <div>3%</div> <div>80% 13% 6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	481	<div><div></div><div>3%</div><div>82%</div><div>12%</div><div>7%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21259 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 Glutamine synthetase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	Se	0	0	0
			3500	2236	586	667	2	9			
1	B	451	Total	C	N	O	S	Se	0	0	0
			3482	2223	583	665	2	9			
1	C	447	Total	C	N	O	S	Se	0	0	0
			3450	2206	576	657	2	9			
1	D	450	Total	C	N	O	S	Se	0	0	0
			3471	2217	583	660	2	9			
1	E	450	Total	C	N	O	S	Se	0	0	0
			3457	2210	577	659	2	9			
1	F	449	Total	C	N	O	S	Se	0	0	0
			3473	2221	582	659	2	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP A1A1Z1
A	-1	ASN	-	EXPRESSION TAG	UNP A1A1Z1
A	0	ALA	-	EXPRESSION TAG	UNP A1A1Z1
B	-2	SER	-	EXPRESSION TAG	UNP A1A1Z1
B	-1	ASN	-	EXPRESSION TAG	UNP A1A1Z1
B	0	ALA	-	EXPRESSION TAG	UNP A1A1Z1
C	-2	SER	-	EXPRESSION TAG	UNP A1A1Z1
C	-1	ASN	-	EXPRESSION TAG	UNP A1A1Z1
C	0	ALA	-	EXPRESSION TAG	UNP A1A1Z1
D	-2	SER	-	EXPRESSION TAG	UNP A1A1Z1
D	-1	ASN	-	EXPRESSION TAG	UNP A1A1Z1
D	0	ALA	-	EXPRESSION TAG	UNP A1A1Z1
E	-2	SER	-	EXPRESSION TAG	UNP A1A1Z1
E	-1	ASN	-	EXPRESSION TAG	UNP A1A1Z1
E	0	ALA	-	EXPRESSION TAG	UNP A1A1Z1
F	-2	SER	-	EXPRESSION TAG	UNP A1A1Z1
F	-1	ASN	-	EXPRESSION TAG	UNP A1A1Z1

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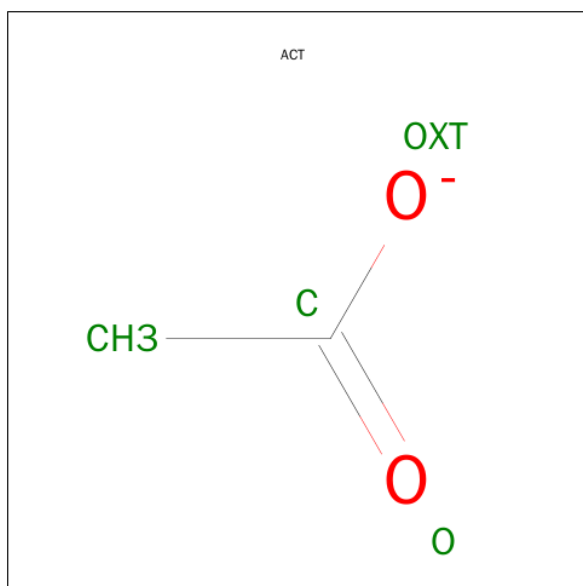
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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	ALA	-	EXPRESSION TAG	UNP A1A1Z1

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).

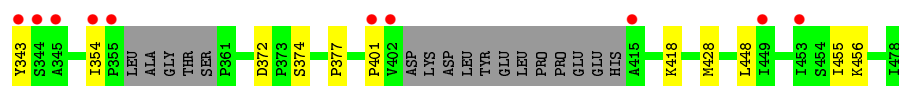


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0

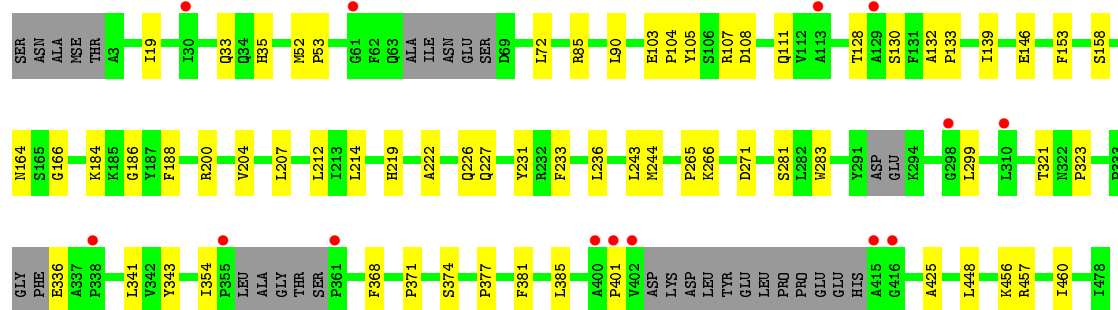
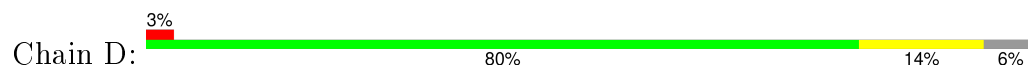
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	63	Total 63	O 63	0	0
4	B	64	Total 64	O 64	0	0
4	C	67	Total 67	O 67	0	0
4	D	59	Total 59	O 59	0	0
4	E	68	Total 68	O 68	0	0
4	F	91	Total 91	O 91	0	0

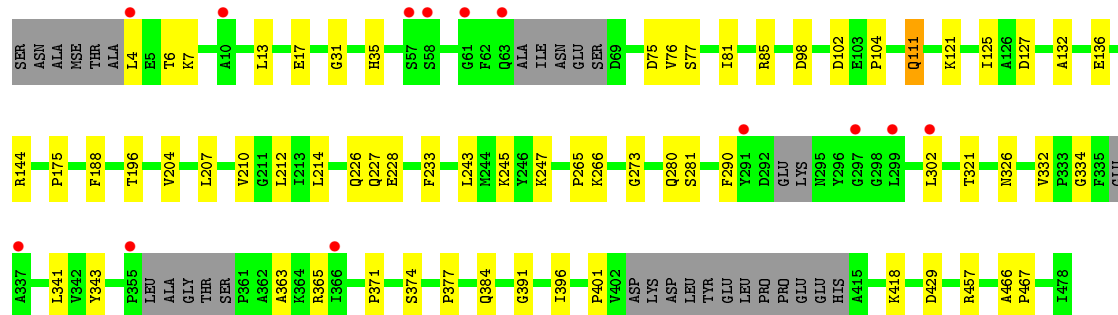
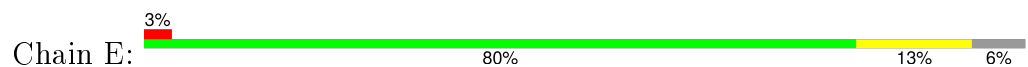




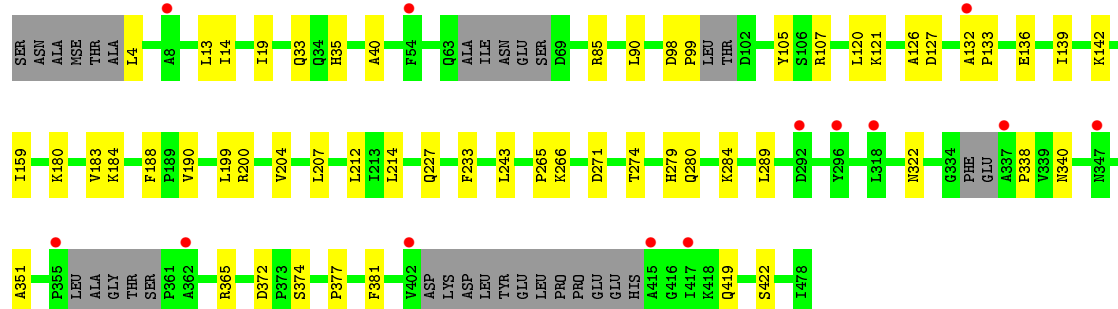
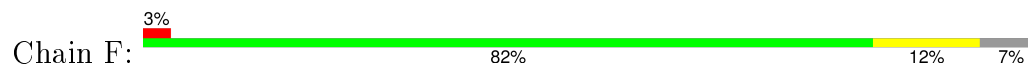
• Molecule 1: Glutamine synthetase



• Molecule 1: Glutamine synthetase



• Molecule 1: Glutamine synthetase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.05Å 134.05Å 298.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.78 – 2.30 45.84 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.7 (45.78-2.30) 98.7 (45.84-2.30)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.69 (at 2.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.238 , 0.287 0.242 , 0.290	Depositor DCC
$R_{free}$ test set	6714 reflections (5.19%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.9	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.078 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 136069 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	21259	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.21	0/3580	0.38	0/4845
1	B	0.21	0/3561	0.38	0/4821
1	C	0.22	0/3528	0.39	0/4777
1	D	0.21	0/3548	0.38	0/4802
1	E	0.21	0/3535	0.38	0/4785
1	F	0.21	0/3552	0.38	0/4805
All	All	0.21	0/21304	0.38	0/28835

There are no bond length outliers.

There are no bond angle outliers.

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	3500	0	3356	30	0
1	B	3482	0	3327	28	0
1	C	3450	0	3299	31	0
1	D	3471	0	3330	34	0
1	E	3457	0	3298	32	0
1	F	3473	0	3336	27	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	B	4	0	3	0	0
3	C	4	0	3	0	0
4	A	63	0	0	1	0
4	B	64	0	0	0	0
4	C	67	0	0	3	0
4	D	59	0	0	0	0
4	E	68	0	0	0	0
4	F	91	0	0	0	0
All	All	21259	0	19952	175	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 4.

All (175) 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:F:243:LEU:HD23	1:F:377:PRO:HB3	1.68	0.76
1:E:243:LEU:HD23	1:E:377:PRO:HB3	1.69	0.74
1:E:104:PRO:HB3	1:E:111:GLN:HG2	1.69	0.74
1:A:243:LEU:HD23	1:A:377:PRO:HB3	1.69	0.73
1:D:243:LEU:HD23	1:D:377:PRO:HB3	1.70	0.72
1:D:200:ARG:HE	1:D:227:GLN:HG3	1.54	0.72
1:B:243:LEU:HD23	1:B:377:PRO:HB3	1.73	0.71
1:C:243:LEU:HD23	1:C:377:PRO:HB3	1.73	0.69
1:F:183:VAL:HG12	1:F:184:LYS:HG3	1.75	0.69
1:B:200:ARG:HE	1:B:227:GLN:HG2	1.58	0.68
1:E:204:VAL:HG13	1:E:214:LEU:HD22	1.75	0.67
1:D:204:VAL:HG13	1:D:214:LEU:HD22	1.77	0.67
1:B:339:VAL:HG13	1:B:420:VAL:HG22	1.78	0.65
1:B:204:VAL:HG13	1:B:214:LEU:HD22	1.79	0.65
1:C:322:ASN:ND2	1:C:372:ASP:OD2	2.29	0.65
1:C:216:ARG:NH2	1:D:53:PRO:O	2.32	0.62
1:D:107:ARG:HA	1:D:448:LEU:HD12	1.82	0.62
1:A:429:ASP:OD1	1:A:457:ARG:NH2	2.33	0.61
1:C:107:ARG:HA	1:C:448:LEU:HD12	1.84	0.60
1:C:111:GLN:NE2	4:C:665:HOH:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:VAL:HG13	1:A:214:LEU:HG	1.85	0.59
1:B:19:ILE:HD13	1:B:90:LEU:HB2	1.83	0.59
1:E:429:ASP:OD1	1:E:457:ARG:NH2	2.32	0.59
1:A:136:GLU:HB2	1:A:274:THR:HG23	1.84	0.58
1:A:14:ILE:HG23	1:A:19:ILE:HB	1.85	0.58
1:A:107:ARG:HA	1:A:448:LEU:HD12	1.84	0.58
1:C:136:GLU:HB2	1:C:274:THR:HG23	1.85	0.58
1:F:14:ILE:HD13	1:F:40:ALA:HB1	1.86	0.58
1:B:143:VAL:HG22	1:B:156:VAL:HG12	1.85	0.57
1:D:128:THR:HB	1:D:283:TRP:HB2	1.87	0.57
1:B:14:ILE:HD13	1:B:40:ALA:HB1	1.87	0.57
1:B:313:HIS:NE2	1:B:390:ASP:OD2	2.34	0.57
1:A:322:ASN:ND2	1:A:372:ASP:OD2	2.38	0.57
1:D:457:ARG:HA	1:D:460:ILE:HD12	1.86	0.57
1:B:104:PRO:HB3	1:B:111:GLN:HG2	1.87	0.57
1:A:207:LEU:HD22	1:A:212:LEU:HD12	1.87	0.56
1:B:216:ARG:NH2	1:C:53:PRO:O	2.34	0.56
1:D:299:LEU:HD11	1:D:354:ILE:HG13	1.87	0.56
1:F:204:VAL:HG13	1:F:214:LEU:HD22	1.88	0.56
1:B:130:SER:OG	1:B:281:SER:OG	2.23	0.56
1:F:19:ILE:HD13	1:F:90:LEU:HB2	1.88	0.55
1:D:323:PRO:HB2	1:D:456:LYS:HE3	1.88	0.55
1:F:136:GLU:HB2	1:F:274:THR:HG23	1.89	0.55
1:A:216:ARG:NH2	1:B:53:PRO:O	2.34	0.54
1:A:197:GLN:OE1	1:A:200:ARG:NH2	2.41	0.54
1:B:197:GLN:OE1	1:B:200:ARG:NH2	2.39	0.54
1:E:136:GLU:HG2	1:E:228:GLU:HB2	1.89	0.53
1:D:266:LYS:NZ	1:D:271:ASP:O	2.37	0.53
1:E:280:GLN:NE2	1:E:384:GLN:OE1	2.42	0.53
1:F:132:ALA:HB2	1:F:233:PHE:HB3	1.92	0.52
1:D:158:SER:O	1:D:164:ASN:ND2	2.43	0.52
1:D:265:PRO:HD3	1:D:374:SER:HB3	1.92	0.51
1:F:338:PRO:HB2	1:F:351:ALA:HA	1.91	0.51
1:C:311:ILE:O	1:C:418:LYS:NZ	2.44	0.51
1:B:136:GLU:HB2	1:B:274:THR:HG23	1.91	0.51
1:F:207:LEU:HD22	1:F:212:LEU:HD12	1.93	0.51
1:D:343:TYR:CZ	1:D:401:PRO:HG3	2.46	0.51
1:B:207:LEU:HD22	1:B:212:LEU:HD12	1.93	0.50
1:E:125:ILE:HG23	1:E:302:LEU:HD11	1.93	0.50
1:C:299:LEU:HD11	1:C:354:ILE:HG13	1.94	0.50
1:A:19:ILE:HD13	1:A:88:LYS:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:LEU:HD22	1:E:212:LEU:HD12	1.93	0.50
1:C:204:VAL:HG13	1:C:214:LEU:HD22	1.94	0.49
1:A:299:LEU:HD11	1:A:354:ILE:HG13	1.95	0.49
1:C:343:TYR:CZ	1:C:401:PRO:HG3	2.48	0.49
1:E:343:TYR:CZ	1:E:401:PRO:HG3	2.47	0.49
1:F:279:HIS:HB3	1:F:365:ARG:HD2	1.95	0.48
1:A:343:TYR:CZ	1:A:401:PRO:HG3	2.48	0.48
1:E:4:LEU:HD11	1:E:13:LEU:HD22	1.94	0.48
1:E:363:ALA:O	1:E:365:ARG:NH1	2.44	0.48
1:C:132:ALA:HB2	1:C:233:PHE:HB3	1.95	0.48
1:A:279:HIS:HB3	1:A:365:ARG:HD2	1.95	0.48
1:D:222:ALA:HB3	1:D:226:GLN:HB2	1.95	0.48
1:C:190:VAL:HG22	1:C:191:PRO:HD2	1.94	0.48
1:A:391:GLY:HA2	1:A:396:ILE:HD12	1.96	0.48
1:F:132:ALA:HB3	1:F:279:HIS:HB2	1.96	0.47
1:A:312:LYS:HD3	1:A:396:ILE:HD13	1.95	0.47
1:D:236:LEU:HD13	1:D:385:LEU:HD22	1.96	0.47
1:A:264:MSE:HB2	1:A:267:PRO:HG3	1.96	0.47
1:A:340:ASN:HB3	1:A:417:ILE:HG21	1.97	0.47
1:A:265:PRO:HD3	1:A:374:SER:HB3	1.96	0.47
1:D:132:ALA:HB2	1:D:233:PHE:HB3	1.96	0.47
1:E:75:ASP:OD1	1:E:77:SER:OG	2.29	0.47
1:B:264:MSE:HB2	1:B:267:PRO:HG3	1.97	0.47
1:C:120:LEU:HD11	1:C:126:ALA:HB3	1.96	0.47
1:A:35:HIS:CG	1:F:190:VAL:HG12	2.51	0.47
1:C:222:ALA:HB3	1:C:226:GLN:HB2	1.97	0.47
1:C:264:MSE:HB2	1:C:267:PRO:HG3	1.98	0.46
1:C:19:ILE:HD13	1:C:90:LEU:HB2	1.97	0.46
1:E:265:PRO:HD3	1:E:374:SER:HB3	1.97	0.46
1:E:391:GLY:HA2	1:E:396:ILE:HD12	1.97	0.46
1:D:207:LEU:HD22	1:D:212:LEU:HD12	1.98	0.46
1:A:132:ALA:HB2	1:A:233:PHE:HB3	1.97	0.46
1:C:54:PHE:CZ	1:C:70:MSE:HE3	2.51	0.46
1:D:52:MSE:HB2	1:D:72:LEU:HB2	1.98	0.46
1:F:322:ASN:ND2	1:F:372:ASP:OD2	2.49	0.46
1:B:210:VAL:HB	1:B:245:LYS:HD2	1.97	0.46
1:B:166:GLY:O	1:C:144:ARG:NH1	2.48	0.46
1:C:14:ILE:HD13	1:C:40:ALA:HB1	1.97	0.45
1:D:186:GLY:O	1:D:219:HIS:ND1	2.48	0.45
1:C:132:ALA:HB3	1:C:279:HIS:HB2	1.99	0.45
1:E:17:GLU:HG3	1:E:81:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:SER:HA	1:A:290:PHE:CE2	2.51	0.45
1:C:225:GLY:O	1:C:227:GLN:NE2	2.50	0.45
1:D:166:GLY:O	1:E:144:ARG:NH1	2.50	0.45
1:F:266:LYS:NZ	1:F:271:ASP:O	2.38	0.45
1:A:105:TYR:CE2	1:A:107:ARG:HB2	2.52	0.44
1:C:298:GLY:N	4:C:663:HOH:O	2.49	0.44
1:E:121:LYS:HG2	1:E:127:ASP:HA	2.00	0.44
1:F:120:LEU:HD11	1:F:126:ALA:HB3	2.00	0.44
1:B:132:ALA:HB3	1:B:279:HIS:HB2	1.99	0.44
1:F:121:LYS:HG2	1:F:127:ASP:HA	2.00	0.44
1:E:175:PRO:HB3	1:F:142:LYS:HD3	1.98	0.44
1:F:159:ILE:O	1:F:180:LYS:NZ	2.43	0.44
1:B:372:ASP:OD1	1:B:374:SER:OG	2.28	0.44
1:E:321:THR:HB	1:E:371:PRO:HB3	2.00	0.43
1:F:284:LYS:HB2	1:F:289:LEU:HD11	2.00	0.43
1:E:210:VAL:HB	1:E:245:LYS:HD2	2.00	0.43
1:E:132:ALA:HB2	1:E:233:PHE:HB3	2.01	0.43
1:E:332:VAL:HG12	1:E:334:GLY:H	1.82	0.43
1:E:98:ASP:O	1:E:102:ASP:N	2.49	0.43
1:D:341:LEU:HD13	1:D:341:LEU:HA	1.89	0.43
1:C:103:GLU:HA	1:C:104:PRO:HD2	1.74	0.43
1:E:266:LYS:N	1:E:326:ASN:OD1	2.51	0.43
1:A:197:GLN:NE2	1:A:201:ASP:OD1	2.51	0.43
1:D:146:GLU:HB3	1:D:153:PHE:CE2	2.54	0.43
1:C:61:GLY:HA2	1:C:455:ILE:HD11	2.01	0.43
1:B:196:THR:OG1	1:B:227:GLN:NE2	2.52	0.43
1:E:226:GLN:NE2	1:E:273:GLY:O	2.45	0.43
1:D:214:LEU:HA	1:D:231:TYR:HA	2.01	0.42
1:C:151:ARG:NH2	4:C:646:HOH:O	2.47	0.42
1:D:139:ILE:HD12	1:D:227:GLN:HE21	1.84	0.42
1:B:208:GLN:HG3	1:B:214:LEU:HD13	2.01	0.42
1:B:391:GLY:HA2	1:B:396:ILE:HD12	2.00	0.42
1:F:98:ASP:HA	1:F:99:PRO:HD3	1.85	0.42
1:D:105:TYR:CE2	1:D:107:ARG:HB2	2.54	0.42
1:A:183:VAL:HG12	1:A:184:LYS:HG3	2.01	0.42
1:D:19:ILE:HD13	1:D:90:LEU:HB2	2.02	0.42
1:F:200:ARG:NH1	1:F:227:GLN:OE1	2.46	0.42
1:D:103:GLU:HA	1:D:104:PRO:HD2	1.80	0.42
1:F:4:LEU:HD11	1:F:13:LEU:HD22	2.00	0.42
1:B:146:GLU:HB3	1:B:153:PHE:CE1	2.54	0.42
1:C:265:PRO:HD3	1:C:374:SER:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:ALA:HA	1:A:401:PRO:HD3	1.91	0.42
1:B:281:SER:HA	1:B:290:PHE:CE2	2.55	0.42
1:B:332:VAL:O	1:B:334:GLY:N	2.52	0.42
1:C:38:VAL:HG11	1:C:52:MSE:HE2	2.02	0.41
1:A:338:PRO:HB2	1:A:351:ALA:HA	2.01	0.41
1:D:130:SER:OG	1:D:281:SER:OG	2.37	0.41
1:E:281:SER:HA	1:E:290:PHE:CE2	2.55	0.41
1:D:108:ASP:HB3	1:D:111:GLN:HB2	2.01	0.41
1:C:318:LEU:HA	1:C:321:THR:OG1	2.20	0.41
1:D:133:PRO:HG3	1:D:381:PHE:HZ	1.85	0.41
1:B:105:TYR:CE2	1:B:107:ARG:HB2	2.55	0.41
1:E:6:THR:OG1	1:E:7:LYS:N	2.52	0.41
1:F:265:PRO:HD3	1:F:374:SER:HB3	2.02	0.41
1:B:132:ALA:HB2	1:B:233:PHE:HB3	2.03	0.41
1:E:243:LEU:O	1:E:247:LYS:HG3	2.20	0.41
1:E:4:LEU:HB3	1:E:76:VAL:HG12	2.02	0.41
1:E:341:LEU:HB2	1:E:418:LYS:HB3	2.01	0.41
1:E:196:THR:OG1	1:E:227:GLN:NE2	2.54	0.41
1:C:323:PRO:HB2	1:C:456:LYS:HE3	2.02	0.41
1:F:133:PRO:HG3	1:F:381:PHE:CZ	2.56	0.41
1:A:457:ARG:NE	4:A:631:HOH:O	2.40	0.41
1:C:428:MSE:HE3	1:C:456:LYS:HG3	2.03	0.41
1:F:105:TYR:CE2	1:F:107:ARG:HB2	2.56	0.40
1:F:340:ASN:OD1	1:F:419:GLN:NE2	2.41	0.40
1:A:146:GLU:HB3	1:A:153:PHE:CE2	2.56	0.40
1:D:425:ALA:HB2	1:D:460:ILE:HD13	2.03	0.40
1:D:33:GLN:HG3	1:D:244:MSE:HE2	2.03	0.40
1:D:321:THR:HB	1:D:371:PRO:HB3	2.04	0.40
1:E:466:ALA:HA	1:E:467:PRO:HD3	1.94	0.40
1:F:139:ILE:HD13	1:F:199:LEU:HD23	2.03	0.40
1:D:184:LYS:HE3	1:D:184:LYS:HB2	1.88	0.40
1:A:323:PRO:HB2	1:A:456:LYS:HE3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	442/481 (92%)	416 (94%)	26 (6%)	0	100	100
1	B	441/481 (92%)	424 (96%)	16 (4%)	1 (0%)	52	64
1	C	435/481 (90%)	417 (96%)	17 (4%)	1 (0%)	52	64
1	D	438/481 (91%)	420 (96%)	18 (4%)	0	100	100
1	E	438/481 (91%)	416 (95%)	21 (5%)	1 (0%)	52	64
1	F	437/481 (91%)	417 (95%)	20 (5%)	0	100	100
All	All	2631/2886 (91%)	2510 (95%)	118 (4%)	3 (0%)	56	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	333	PRO
1	C	338	PRO
1	E	31	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	366/391 (94%)	363 (99%)	3 (1%)	86	94
1	B	363/391 (93%)	359 (99%)	4 (1%)	80	90
1	C	359/391 (92%)	354 (99%)	5 (1%)	74	86
1	D	362/391 (93%)	357 (99%)	5 (1%)	74	86
1	E	358/391 (92%)	354 (99%)	4 (1%)	80	90
1	F	363/391 (93%)	357 (98%)	6 (2%)	68	83
All	All	2171/2346 (92%)	2144 (99%)	27 (1%)	78	89

All (27) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	35	HIS
1	A	188	PHE
1	A	368	PHE
1	B	35	HIS
1	B	188	PHE
1	B	280	GLN
1	B	368	PHE
1	C	35	HIS
1	C	130	SER
1	C	188	PHE
1	C	190	VAL
1	C	227	GLN
1	D	35	HIS
1	D	85	ARG
1	D	188	PHE
1	D	336	GLU
1	D	368	PHE
1	E	35	HIS
1	E	85	ARG
1	E	111	GLN
1	E	188	PHE
1	F	33	GLN
1	F	35	HIS
1	F	85	ARG
1	F	188	PHE
1	F	280	GLN
1	F	422	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	111	GLN
1	E	111	GLN
1	E	227	GLN
1	F	347	ASN

### 5.3.3 RNA ⓘ

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](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ACT	B	501	-	1,3,3	1.17	0	0,3,3	0.00	-
3	ACT	C	501	-	1,3,3	1.20	0	0,3,3	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACT	B	501	-	-	0/0/0/0	0/0/0/0
3	ACT	C	501	-	-	0/0/0/0	0/0/0/0

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	443/481 (92%)	0.31	16 (3%) 46 55	17, 34, 66, 89	0
1	B	442/481 (91%)	0.31	15 (3%) 49 58	17, 35, 68, 95	0
1	C	438/481 (91%)	0.44	20 (4%) 36 45	20, 37, 71, 93	0
1	D	441/481 (91%)	0.35	14 (3%) 51 60	19, 37, 71, 98	0
1	E	441/481 (91%)	0.27	13 (2%) 55 64	18, 33, 65, 91	0
1	F	440/481 (91%)	0.23	13 (2%) 54 63	17, 33, 67, 97	0
All	All	2645/2886 (91%)	0.32	91 (3%) 49 58	17, 35, 68, 98	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	355	PRO	6.6
1	A	297	GLY	6.2
1	A	296	TYR	5.7
1	E	291	TYR	5.2
1	B	343	TYR	4.8
1	A	63	GLN	4.6
1	C	402	VAL	4.6
1	F	355	PRO	4.4
1	F	296	TYR	4.4
1	B	291	TYR	3.9
1	C	343	TYR	3.9
1	C	345	ALA	3.9
1	F	402	VAL	3.8
1	D	129	ALA	3.8
1	A	341	LEU	3.8
1	F	415	ALA	3.7
1	A	354	ILE	3.6
1	D	402	VAL	3.5
1	A	333	PRO	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	291	TYR	3.3
1	B	337	ALA	3.3
1	E	299	LEU	3.1
1	B	341	LEU	3.1
1	E	366	ILE	3.0
1	C	58	SER	3.0
1	A	332	VAL	3.0
1	B	347	ASN	2.9
1	D	361	PRO	2.9
1	B	297	GLY	2.9
1	C	57	SER	2.9
1	D	61	GLY	2.9
1	C	449	ILE	2.9
1	D	415	ALA	2.8
1	D	338	PRO	2.8
1	C	62	PHE	2.8
1	D	30	ILE	2.7
1	C	401	PRO	2.7
1	A	307	ILE	2.7
1	D	400	ALA	2.7
1	E	58	SER	2.7
1	E	61	GLY	2.7
1	B	125	ILE	2.6
1	A	343	TYR	2.6
1	E	10	ALA	2.6
1	B	43	PHE	2.6
1	B	299	LEU	2.6
1	F	292	ASP	2.6
1	E	297	GLY	2.5
1	E	63	GLN	2.5
1	C	14	ILE	2.5
1	D	355	PRO	2.5
1	F	347	ASN	2.5
1	C	415	ALA	2.4
1	D	416	GLY	2.4
1	A	339	VAL	2.4
1	C	354	ILE	2.4
1	B	355	PRO	2.4
1	E	4	LEU	2.3
1	C	288	PRO	2.3
1	D	401	PRO	2.3
1	D	298	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	362	ALA	2.3
1	F	417	ILE	2.2
1	C	318	LEU	2.2
1	E	57	SER	2.2
1	F	337	ALA	2.2
1	C	100	LEU	2.2
1	B	420	VAL	2.1
1	E	302	LEU	2.1
1	B	290	PHE	2.1
1	A	342	VAL	2.1
1	D	310	LEU	2.1
1	F	54	PHE	2.1
1	F	318	LEU	2.1
1	B	345	ALA	2.1
1	F	8	ALA	2.1
1	F	132	ALA	2.1
1	A	361	PRO	2.1
1	E	355	PRO	2.1
1	A	347	ASN	2.0
1	B	44	LEU	2.0
1	E	337	ALA	2.0
1	C	344	SER	2.0
1	C	453	ILE	2.0
1	A	441	GLY	2.0
1	C	310	LEU	2.0
1	C	56	GLY	2.0
1	A	62	PHE	2.0
1	C	43	PHE	2.0
1	D	113	ALA	2.0
1	B	349	SER	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

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<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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ACT	C	501	4/4	0.89	0.14	-1.27	38,38,42,46	0
3	ACT	B	501	4/4	0.96	0.11	-1.67	44,51,53,54	0
2	MG	E	501	1/1	0.95	0.06	-	43,43,43,43	0
2	MG	A	501	1/1	0.96	0.06	-	42,42,42,42	0
2	MG	B	502	1/1	0.69	0.09	-	57,57,57,57	0
2	MG	F	501	1/1	0.90	0.09	-	35,35,35,35	0
2	MG	D	501	1/1	0.92	0.10	-	36,36,36,36	0
2	MG	C	502	1/1	0.93	0.07	-	38,38,38,38	0

## 6.5 Other polymers

There are no such residues in this entry.