Full wwPDB X-ray Structure Validation Report (i)

Mar 24, 2022 – 03:37 pm GMT

PDB ID	:	6QKY
Title	:	Tryptophan synthase subunit alpha from Streptococcus pneumoniae with 3D domain swap in the core of TIM barrel
Authors	:	Michalska, K.; Kowiel, M.; Bigelow, L.; Endres, M.; Gilski, M.; Jaskolski, M.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2019-01-30
Resolution	:	2.54 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

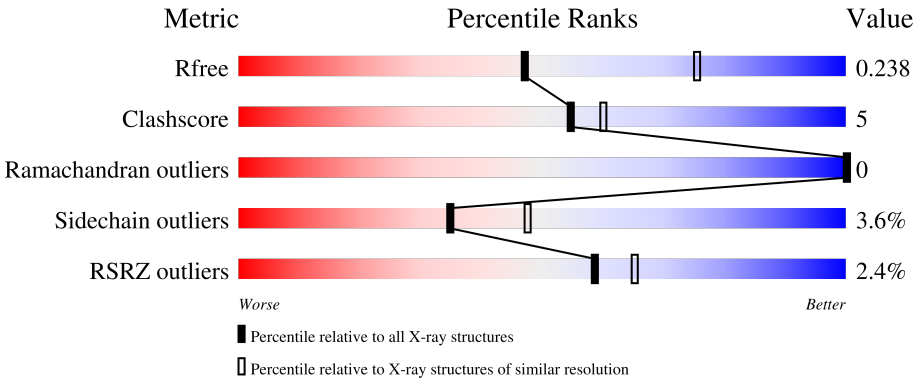
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 2.54 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	261	87% 9%
1	B	261	87% 9%
1	C	261	89% 10%
1	D	261	87% 10%
1	E	261	81% 13% 5%

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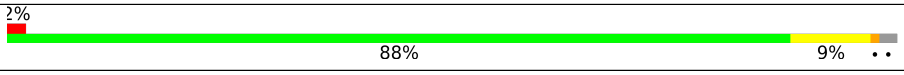
Mol	Chain	Length	Quality of chain
1	F	261	
1	G	261	
1	H	261	
1	I	261	
1	J	261	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19389 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 Tryptophan synthase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	Se	0	1	0
			1912	1232	309	367	4			
1	B	254	Total	C	N	O	Se	0	1	0
			1911	1231	313	363	4			
1	C	258	Total	C	N	O	Se	0	1	0
			1936	1247	316	370	3			
1	D	254	Total	C	N	O	Se	0	1	0
			1903	1228	312	360	3			
1	E	249	Total	C	N	O	Se	0	1	0
			1875	1214	302	355	4			
1	F	247	Total	C	N	O	Se	0	1	0
			1849	1196	298	352	3			
1	G	247	Total	C	N	O	Se	0	2	0
			1846	1197	296	349	4			
1	H	253	Total	C	N	O	Se	0	3	0
			1913	1233	310	367	3			
1	I	252	Total	C	N	O	Se	0	2	0
			1909	1230	311	365	3			
1	J	255	Total	C	N	O	Se	0	1	0
			1924	1239	314	368	3			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q97P33
A	-1	ASN	-	expression tag	UNP Q97P33
A	0	ALA	-	expression tag	UNP Q97P33
B	-2	SER	-	expression tag	UNP Q97P33
B	-1	ASN	-	expression tag	UNP Q97P33
B	0	ALA	-	expression tag	UNP Q97P33
C	-2	SER	-	expression tag	UNP Q97P33
C	-1	ASN	-	expression tag	UNP Q97P33
C	0	ALA	-	expression tag	UNP Q97P33

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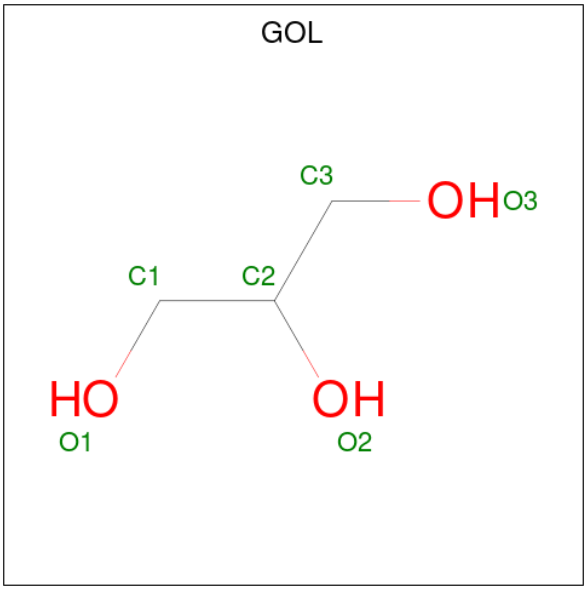
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	SER	-	expression tag	UNP Q97P33
D	-1	ASN	-	expression tag	UNP Q97P33
D	0	ALA	-	expression tag	UNP Q97P33
E	-2	SER	-	expression tag	UNP Q97P33
E	-1	ASN	-	expression tag	UNP Q97P33
E	0	ALA	-	expression tag	UNP Q97P33
F	-2	SER	-	expression tag	UNP Q97P33
F	-1	ASN	-	expression tag	UNP Q97P33
F	0	ALA	-	expression tag	UNP Q97P33
G	-2	SER	-	expression tag	UNP Q97P33
G	-1	ASN	-	expression tag	UNP Q97P33
G	0	ALA	-	expression tag	UNP Q97P33
H	-2	SER	-	expression tag	UNP Q97P33
H	-1	ASN	-	expression tag	UNP Q97P33
H	0	ALA	-	expression tag	UNP Q97P33
I	-2	SER	-	expression tag	UNP Q97P33
I	-1	ASN	-	expression tag	UNP Q97P33
I	0	ALA	-	expression tag	UNP Q97P33
J	-2	SER	-	expression tag	UNP Q97P33
J	-1	ASN	-	expression tag	UNP Q97P33
J	0	ALA	-	expression tag	UNP Q97P33

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	6	3	3	0	0

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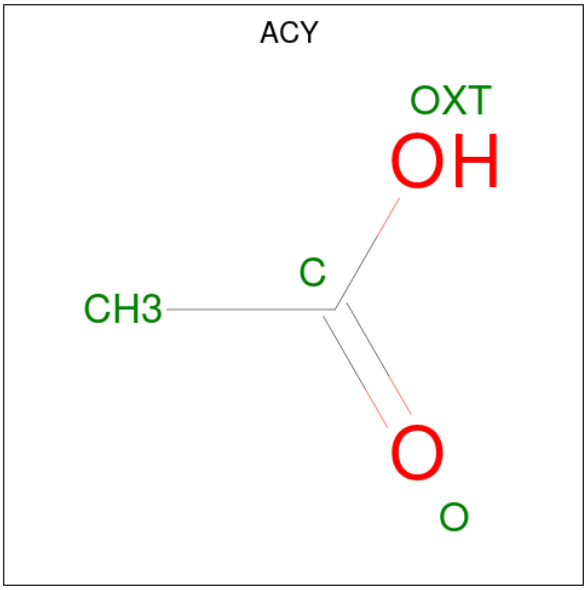
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0

- Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0
3	I	1	Total C O 4 2 2	0	0

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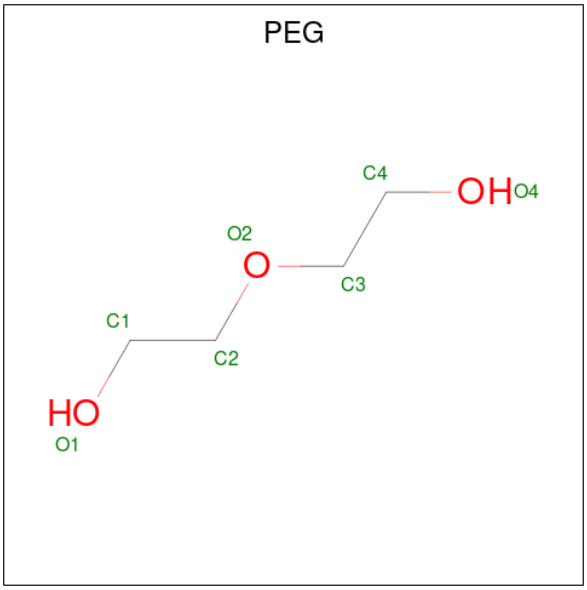
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	1	Total C O 4 2 2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	51	Total O 51 51	0	0
5	B	44	Total O 44 44	0	0
5	C	53	Total O 53 53	0	0
5	D	42	Total O 42 42	0	0
5	E	27	Total O 27 27	0	0
5	F	23	Total O 23 23	0	0

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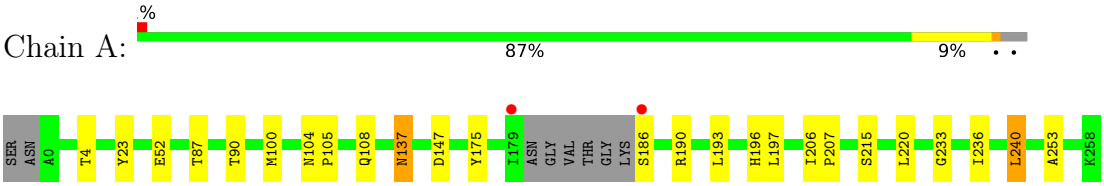
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	17	Total O 17 17	0	0
5	H	15	Total O 15 15	0	0
5	I	34	Total O 34 34	0	0
5	J	33	Total O 33 33	0	0

3 Residue-property plots (i)

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

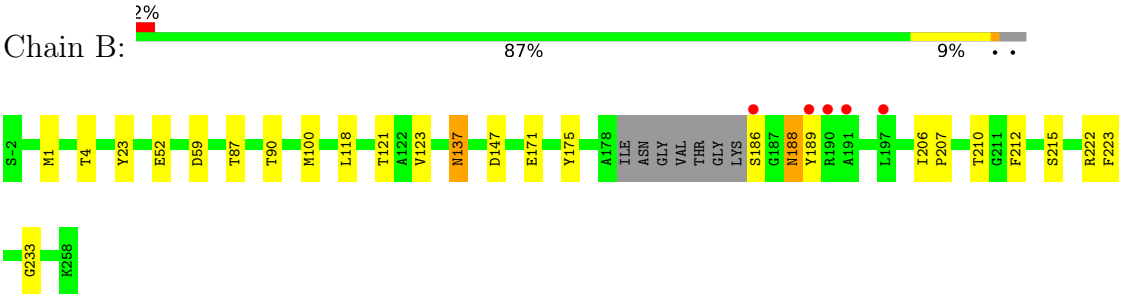
• Molecule 1: Tryptophan synthase alpha chain

Chain A:



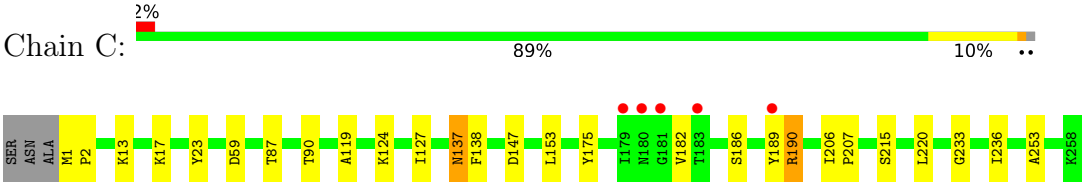
• Molecule 1: Tryptophan synthase alpha chain

Chain B:



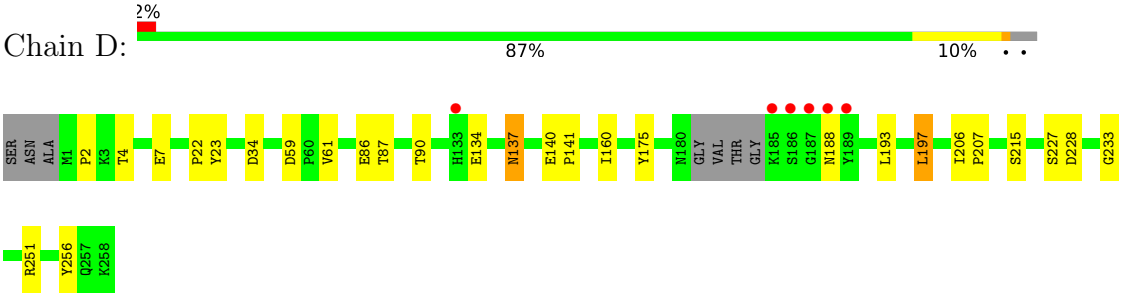
• Molecule 1: Tryptophan synthase alpha chain

Chain C:



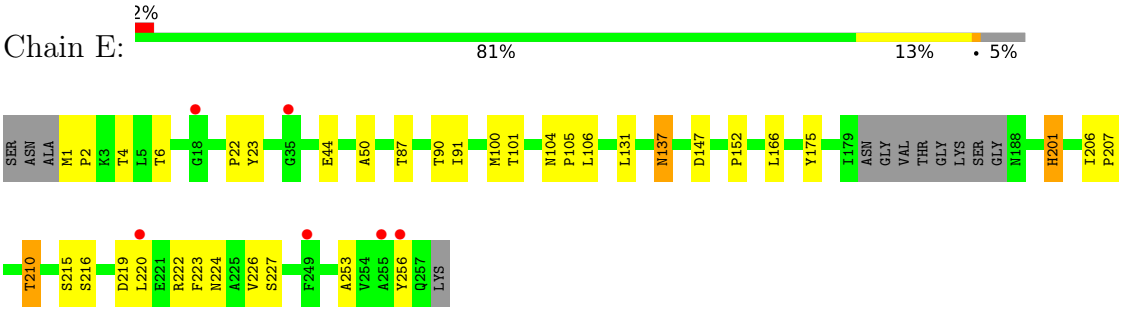
• Molecule 1: Tryptophan synthase alpha chain

Chain D:



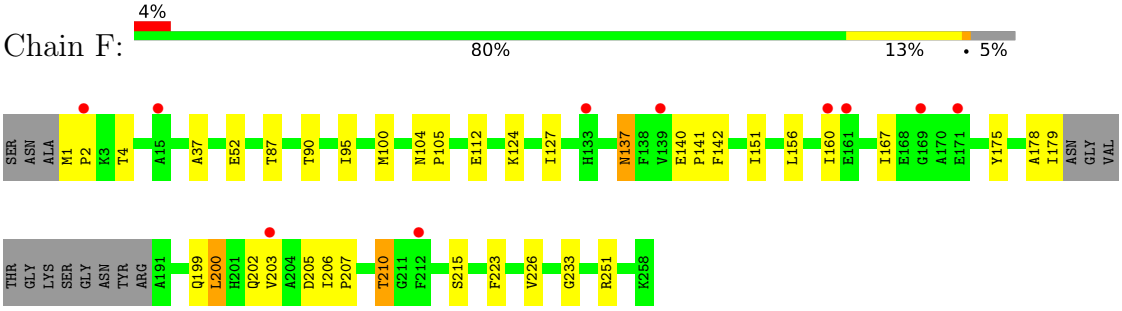
• Molecule 1: Tryptophan synthase alpha chain

Chain E:



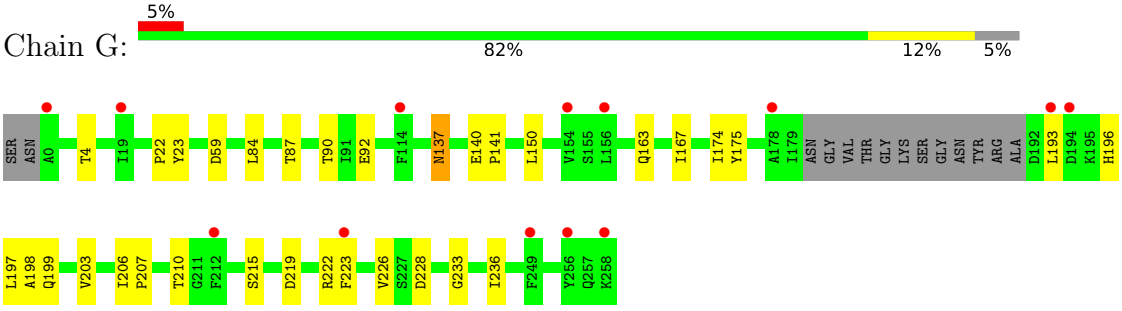
• Molecule 1: Tryptophan synthase alpha chain

Chain F:



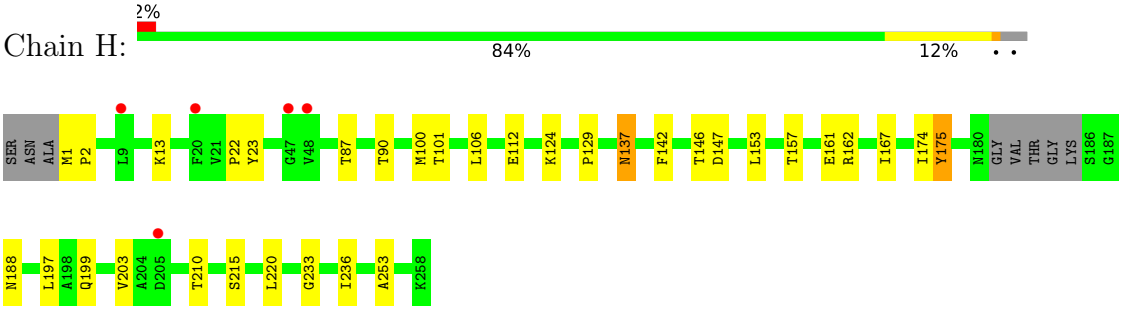
• Molecule 1: Tryptophan synthase alpha chain

Chain G:



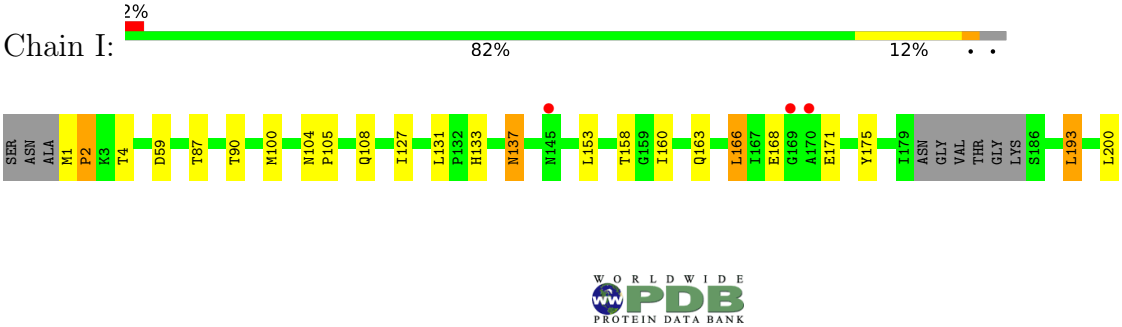
• Molecule 1: Tryptophan synthase alpha chain

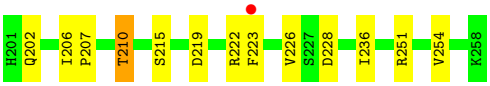
Chain H:



• Molecule 1: Tryptophan synthase alpha chain

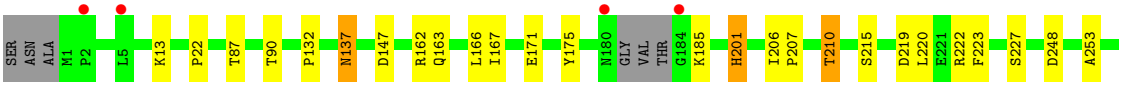
Chain I:





• Molecule 1: Tryptophan synthase alpha chain

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	104.81Å 138.62Å 107.25Å 90.00° 117.21° 90.00°	Depositor
Resolution (Å)	48.99 – 2.54 48.99 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.99-2.54) 99.5 (48.99-2.54)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.193 , 0.234 0.197 , 0.238	Depositor DCC
R_{free} test set	1066 reflections (1.20%)	wwPDB-VP
Wilson B-factor (Å^2)	68.7	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	19389	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.58	0/1949	0.62	0/2649
1	B	0.59	0/1945	0.63	0/2643
1	C	0.57	0/1975	0.63	0/2686
1	D	0.56	0/1938	0.58	0/2638
1	E	0.56	0/1910	0.61	0/2599
1	F	0.55	0/1883	0.60	0/2565
1	G	0.54	0/1885	0.62	0/2566
1	H	0.55	0/1954	0.62	0/2658
1	I	0.55	0/1947	0.62	0/2647
1	J	0.55	0/1959	0.59	0/2662
All	All	0.56	0/19345	0.61	0/26313

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	D	0	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	251	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	F	251	ARG	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	A	1912	0	1906	24	0
1	B	1911	0	1904	23	0
1	C	1936	0	1933	23	0
1	D	1903	0	1887	25	0
1	E	1875	0	1870	29	0
1	F	1849	0	1838	29	0
1	G	1846	0	1845	23	0
1	H	1913	0	1899	27	0
1	I	1909	0	1906	29	0
1	J	1924	0	1917	17	0
2	A	6	0	8	0	0
2	C	12	0	16	0	0
3	A	4	0	3	1	0
3	B	4	0	3	1	0
3	C	4	0	3	1	0
3	D	4	0	3	0	0
3	E	8	0	6	0	0
3	G	4	0	3	0	0
3	H	4	0	3	1	0
3	I	4	0	3	0	0
3	J	4	0	3	0	0
4	B	7	0	10	0	0
4	E	7	0	10	0	0
5	A	51	0	0	0	0
5	B	44	0	0	0	0
5	C	53	0	0	1	0
5	D	42	0	0	2	0
5	E	27	0	0	0	0
5	F	23	0	0	0	0
5	G	17	0	0	0	0
5	H	15	0	0	0	0
5	I	34	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	33	0	0	0	0
All	All	19389	0	18979	199	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 (199) 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:B:118:LEU:O	1:B:121:THR:HG22	1.66	0.95
1:C:182:VAL:HB	1:C:186:SER:HB2	1.57	0.86
1:G:167:ILE:HD12	1:G:174:ILE:HD13	1.63	0.80
1:G:84:LEU:O	1:G:87:THR:HG22	1.86	0.74
1:F:1:MSE:CB	1:F:2:PRO:CD	2.66	0.74
1:B:121:THR:HG23	1:B:123:VAL:H	1.54	0.72
1:C:1:MSE:CB	1:C:2:PRO:CD	2.67	0.71
1:H:233:GLY:HA3	3:H:301:ACY:H2	1.73	0.70
1:D:160:ILE:H	1:D:160:ILE:HD12	1.57	0.70
1:B:188:ASN:O	1:B:188:ASN:ND2	2.24	0.68
1:C:137:ASN:H	1:C:137:ASN:HD22	1.42	0.67
1:D:134:GLU:HG2	5:D:429:HOH:O	1.94	0.67
1:E:210:THR:HG21	1:E:223:PHE:HB3	1.77	0.67
1:G:199:GLN:O	1:G:203:VAL:HG23	1.96	0.66
1:J:201:HIS:HE1	1:J:227:SER:HA	1.62	0.65
1:C:190:ARG:HB2	1:C:190:ARG:HH21	1.62	0.64
1:H:199:GLN:O	1:H:203:VAL:HG23	1.99	0.63
1:A:104:ASN:HD21	1:A:108:GLN:HE21	1.47	0.63
1:A:233:GLY:HA3	3:A:302:ACY:H2	1.81	0.62
1:J:201:HIS:CE1	1:J:227:SER:HA	2.34	0.62
1:F:179:ILE:HD12	1:F:179:ILE:N	2.13	0.62
1:G:137:ASN:ND2	1:G:137:ASN:H	1.98	0.61
1:H:153:LEU:HD23	1:H:175:TYR:HB3	1.82	0.61
1:I:137:ASN:ND2	1:I:137:ASN:H	1.98	0.61
1:J:210:THR:HG21	1:J:223:PHE:HB3	1.82	0.61
1:E:137:ASN:ND2	1:E:137:ASN:H	1.99	0.61
1:I:4:THR:HG22	1:J:147:ASP:OD2	2.01	0.60
1:A:4:THR:HG22	1:B:147:ASP:OD2	2.00	0.60
1:C:1:MSE:CB	1:C:2:PRO:HD3	2.31	0.60
1:J:137:ASN:ND2	1:J:137:ASN:H	1.99	0.60
1:E:201:HIS:HE1	1:E:227:SER:HA	1.67	0.60
1:G:140:GLU:HB2	1:G:141:PRO:HD3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:137:ASN:ND2	1:H:137:ASN:H	1.99	0.60
1:C:13:LYS:HE3	1:D:228:ASP:OD1	2.02	0.59
1:B:137:ASN:ND2	1:B:137:ASN:H	2.00	0.59
1:A:137:ASN:ND2	1:A:137:ASN:H	1.98	0.59
1:H:167:ILE:HG21	1:H:174:ILE:HD13	1.84	0.59
1:F:137:ASN:ND2	1:F:137:ASN:H	2.00	0.58
1:C:137:ASN:H	1:C:137:ASN:ND2	2.01	0.58
1:G:163:GLN:O	1:G:167:ILE:HG12	2.03	0.58
1:A:190:ARG:NH1	1:I:108:GLN:OE1	2.34	0.58
1:H:100[B]:MSE:HE2	1:H:129:PRO:HG2	1.86	0.58
1:D:137:ASN:ND2	1:D:137:ASN:H	2.00	0.57
1:H:197:LEU:HD21	1:H:210:THR:OG1	2.03	0.57
1:A:147:ASP:OD2	1:B:4:THR:CG2	2.53	0.56
1:C:233:GLY:HA3	3:C:303:ACY:H2	1.87	0.56
1:C:17:LYS:HD2	1:D:256:TYR:O	2.06	0.56
1:I:166:LEU:N	1:I:166:LEU:HD23	2.21	0.56
1:E:219:ASP:HA	1:E:222:ARG:HD3	1.87	0.56
1:E:219:ASP:OD1	1:E:222:ARG:NH1	2.39	0.55
1:A:147:ASP:CG	1:B:4:THR:HG22	2.26	0.55
1:I:166:LEU:HD23	1:I:166:LEU:H	1.71	0.55
1:A:147:ASP:OD2	1:B:4:THR:HG22	2.07	0.55
1:I:251:ARG:O	1:I:254:VAL:HG22	2.06	0.55
1:B:233:GLY:HA3	3:B:302:ACY:H2	1.88	0.55
1:C:190:ARG:HH21	1:C:190:ARG:CB	2.20	0.55
1:F:140:GLU:HB3	1:F:141:PRO:HD3	1.89	0.55
1:H:162:ARG:O	1:H:162:ARG:HD2	2.07	0.54
1:G:23:TYR:HB3	1:H:233:GLY:HA2	1.90	0.54
1:F:167:ILE:HD11	1:F:203:VAL:HG12	1.89	0.54
1:F:200:LEU:HD12	1:F:200:LEU:O	2.07	0.54
1:A:4:THR:HG22	1:B:147:ASP:CG	2.28	0.53
1:E:1:MSE:N	1:E:2:PRO:HD2	2.24	0.53
1:D:160:ILE:HD12	1:D:160:ILE:N	2.23	0.52
1:F:1:MSE:CB	1:F:2:PRO:HD3	2.40	0.52
1:H:188:ASN:ND2	1:I:131:LEU:O	2.43	0.51
1:E:224:ASN:HB3	1:E:256:TYR:CE2	2.46	0.51
1:A:4:THR:CG2	1:B:147:ASP:OD2	2.58	0.51
1:D:87:THR:O	1:D:90:THR:HB	2.12	0.50
1:E:201:HIS:CE1	1:E:227:SER:HA	2.46	0.50
1:F:1:MSE:CB	1:F:2:PRO:HD2	2.38	0.50
1:G:198:ALA:HB2	1:G:226:VAL:HG13	1.93	0.50
1:I:87:THR:O	1:I:90:THR:HB	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ARG:NH2	1:D:86:GLU:OE1	2.34	0.50
1:E:147:ASP:CG	1:F:4:THR:HG22	2.31	0.50
1:D:140:GLU:HG2	5:D:436:HOH:O	2.11	0.50
1:C:87:THR:O	1:C:90:THR:HB	2.12	0.50
1:F:87:THR:O	1:F:90:THR:HB	2.12	0.50
1:E:152:PRO:HB2	1:E:166:LEU:HD22	1.94	0.50
1:C:119:ALA:HA	5:C:415:HOH:O	2.11	0.50
1:H:87:THR:O	1:H:90:THR:HB	2.12	0.49
1:I:133:HIS:CG	1:I:166:LEU:HD22	2.47	0.49
1:E:87:THR:O	1:E:90:THR:HB	2.11	0.49
1:B:87:THR:O	1:B:90:THR:HB	2.12	0.49
1:C:124:LYS:HD2	1:D:4:THR:CG2	2.43	0.49
1:I:4:THR:CG2	1:J:147:ASP:OD2	2.60	0.49
1:A:23:TYR:HB3	1:B:233:GLY:HA2	1.94	0.49
1:A:233:GLY:HA2	1:B:23:TYR:HB3	1.93	0.49
1:F:179:ILE:N	1:F:179:ILE:CD1	2.76	0.49
1:G:167:ILE:CD1	1:G:174:ILE:HD13	2.36	0.48
1:G:4:THR:CG2	1:H:124:LYS:HD2	2.43	0.48
1:G:87:THR:O	1:G:90:THR:HB	2.13	0.48
1:G:236:ILE:HD13	1:H:22:PRO:HB3	1.95	0.48
1:H:101:THR:HG21	1:H:106:LEU:HD13	1.95	0.48
1:I:158:THR:HB	1:I:163:GLN:NE2	2.28	0.48
1:I:137:ASN:H	1:I:137:ASN:HD22	1.60	0.48
1:J:87:THR:O	1:J:90:THR:HB	2.13	0.48
1:I:236:ILE:HD13	1:J:22:PRO:HB3	1.96	0.48
1:A:87:THR:O	1:A:90:THR:HB	2.13	0.48
1:E:101:THR:HG21	1:E:106:LEU:HD13	1.95	0.48
1:E:206:ILE:HB	1:E:207:PRO:CD	2.44	0.48
1:E:220:LEU:HD11	1:E:253:ALA:CB	2.43	0.48
1:B:188:ASN:HD22	1:B:188:ASN:C	2.13	0.48
1:F:160:ILE:HG21	1:F:199:GLN:OE1	2.14	0.48
1:I:210:THR:HG21	1:I:223:PHE:HB3	1.94	0.48
1:H:1:MSE:N	1:H:2:PRO:HD2	2.28	0.48
1:A:147:ASP:OD1	1:B:4:THR:HG22	2.14	0.47
1:I:193:LEU:C	1:I:193:LEU:HD13	2.35	0.47
1:C:233:GLY:HA2	1:D:23:TYR:HB3	1.95	0.47
1:E:100[A]:MSE:SE	1:F:52:GLU:OE2	2.82	0.47
1:E:147:ASP:OD1	1:F:4:THR:HG22	2.15	0.47
1:I:226:VAL:HG22	1:I:226:VAL:O	2.15	0.47
1:E:147:ASP:OD2	1:F:4:THR:HG22	2.15	0.47
1:A:137:ASN:H	1:A:137:ASN:HD22	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4:THR:HG22	1:H:147:ASP:CG	2.35	0.46
1:F:156:LEU:HD12	1:F:178:ALA:HB2	1.97	0.46
1:I:127:ILE:HG23	1:I:153:LEU:HD11	1.96	0.46
1:B:210:THR:HG21	1:B:223:PHE:CD2	2.50	0.46
1:E:226:VAL:HG22	1:E:226:VAL:O	2.15	0.46
1:J:137:ASN:H	1:J:137:ASN:HD22	1.63	0.46
1:D:140:GLU:N	1:D:141:PRO:HD2	2.31	0.46
1:G:137:ASN:H	1:G:137:ASN:HD22	1.63	0.46
1:D:2:PRO:HG2	1:D:7:GLU:OE2	2.16	0.45
1:I:4:THR:HG22	1:J:147:ASP:CG	2.36	0.45
1:H:112:GLU:HB2	1:H:142:PHE:CE2	2.51	0.45
1:J:220:LEU:HD11	1:J:253:ALA:HB1	1.98	0.45
1:B:210:THR:HG21	1:B:223:PHE:CG	2.51	0.45
1:F:137:ASN:H	1:F:137:ASN:HD22	1.65	0.45
1:G:22:PRO:HB3	1:H:236:ILE:HD13	1.99	0.45
1:I:160:ILE:HD12	1:I:200:LEU:HB2	1.99	0.45
1:C:147:ASP:OD2	1:D:4:THR:HG22	2.16	0.45
1:D:59:ASP:OD1	1:D:61:VAL:HG23	2.16	0.45
1:E:91:ILE:HG12	1:F:37:ALA:HB2	1.98	0.45
1:F:210:THR:HG21	1:F:223:PHE:HB3	1.98	0.45
1:H:157:THR:HB	1:I:158:THR:HG23	1.98	0.45
1:H:161[B]:GLU:HA	1:H:161[B]:GLU:OE1	2.17	0.45
1:G:233:GLY:HA2	1:H:23:TYR:HB3	1.98	0.45
1:I:1:MSE:N	1:I:2:PRO:HD3	2.32	0.44
1:A:220:LEU:HD11	1:A:253:ALA:HB1	1.99	0.44
1:H:137:ASN:H	1:H:137:ASN:HD22	1.64	0.44
1:C:124:LYS:HE3	1:D:4:THR:HG21	1.99	0.44
1:G:206:ILE:HB	1:G:207:PRO:CD	2.48	0.44
1:J:206:ILE:HB	1:J:207:PRO:CD	2.47	0.44
1:F:226:VAL:HG12	1:F:226:VAL:O	2.17	0.44
1:A:193:LEU:HD23	1:A:193:LEU:HA	1.85	0.44
1:G:226:VAL:O	1:G:226:VAL:HG12	2.17	0.43
1:E:147:ASP:OD2	1:F:4:THR:CG2	2.66	0.43
1:E:220:LEU:HD11	1:E:253:ALA:HB2	2.00	0.43
1:C:236:ILE:HD13	1:D:22:PRO:HB3	2.00	0.43
1:I:1:MSE:N	1:I:2:PRO:CD	2.81	0.43
1:J:163:GLN:O	1:J:167:ILE:HG13	2.18	0.43
1:B:206:ILE:HB	1:B:207:PRO:CD	2.49	0.43
1:D:206:ILE:HB	1:D:207:PRO:CD	2.49	0.43
1:C:206:ILE:HB	1:C:207:PRO:CD	2.49	0.43
1:I:219:ASP:OD1	1:I:222:ARG:NH2	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:GLU:OE2	1:B:100[A]:MSE:SE	2.86	0.43
1:C:220:LEU:HD11	1:C:253:ALA:HB1	2.01	0.43
1:A:100[A]:MSE:SE	1:B:52:GLU:OE2	2.87	0.43
1:H:167:ILE:CG2	1:H:174:ILE:HD13	2.46	0.43
1:B:210:THR:HG23	1:B:212:PHE:CD2	2.54	0.43
1:E:23:TYR:HB3	1:F:233:GLY:HA2	2.01	0.43
1:C:127:ILE:HG23	1:C:153:LEU:HD11	2.01	0.42
1:I:228:ASP:OD1	1:J:13:LYS:HE3	2.19	0.42
1:D:34:ASP:OD2	1:E:216:SER:HA	2.19	0.42
1:D:197:LEU:HD22	1:D:227:SER:HB3	2.01	0.42
1:F:206:ILE:HB	1:F:207:PRO:CD	2.49	0.42
1:G:210:THR:HG21	1:G:223:PHE:HB3	2.01	0.42
1:I:206:ILE:HB	1:I:207:PRO:CD	2.49	0.42
1:C:23:TYR:HB3	1:D:233:GLY:HA2	2.02	0.42
1:E:44:GLU:HG3	1:F:95:ILE:HG12	2.02	0.42
1:E:4:THR:CG2	1:F:124:LYS:HD2	2.50	0.41
1:G:197:LEU:O	1:G:197:LEU:HD23	2.20	0.41
1:I:104:ASN:HB3	1:I:105:PRO:HD3	2.01	0.41
1:A:236:ILE:HG22	1:A:240:LEU:HD22	2.03	0.41
1:H:112:GLU:HB2	1:H:142:PHE:CD2	2.55	0.41
1:A:190:ARG:NH1	1:J:132:PRO:HG3	2.35	0.41
1:F:199:GLN:HA	1:F:202:GLN:HE21	1.86	0.41
1:A:196:HIS:CD2	1:J:162:ARG:NH1	2.89	0.41
1:C:17:LYS:CD	1:D:256:TYR:O	2.67	0.41
1:D:137:ASN:H	1:D:137:ASN:HD22	1.67	0.41
1:G:228:ASP:OD1	1:H:13:LYS:HE3	2.21	0.41
1:G:4:THR:HG22	1:H:147:ASP:OD1	2.20	0.41
1:E:1:MSE:N	1:E:1:MSE:SE	3.04	0.41
1:F:127:ILE:HG12	1:F:151:ILE:HB	2.03	0.41
1:D:193:LEU:HD23	1:D:193:LEU:HA	1.86	0.41
1:F:112:GLU:HB2	1:F:142:PHE:CE2	2.56	0.41
1:J:219:ASP:OD1	1:J:222:ARG:NH2	2.49	0.41
1:I:202:GLN:HA	1:I:202:GLN:OE1	2.21	0.41
1:A:206:ILE:HB	1:A:207:PRO:CD	2.50	0.40
1:C:138:PHE:N	1:C:138:PHE:CD1	2.89	0.40
1:E:104:ASN:HB3	1:E:105:PRO:HD3	2.02	0.40
1:I:133:HIS:CD2	1:I:166:LEU:HD22	2.56	0.40
1:I:166:LEU:N	1:I:166:LEU:CD2	2.84	0.40
1:E:22:PRO:HD2	1:E:50:ALA:O	2.22	0.40
1:H:220:LEU:HD11	1:H:253:ALA:HB1	2.03	0.40
1:A:104:ASN:HB3	1:A:105:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:ASN:ND2	1:E:131:LEU:O	2.53	0.40
1:G:219:ASP:OD1	1:G:222:ARG:NH2	2.53	0.40
1:F:104:ASN:HB3	1:F:105:PRO:HD3	2.04	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	250/261 (96%)	248 (99%)	2 (1%)	0	100	100
1	B	251/261 (96%)	244 (97%)	7 (3%)	0	100	100
1	C	257/261 (98%)	250 (97%)	7 (3%)	0	100	100
1	D	251/261 (96%)	248 (99%)	3 (1%)	0	100	100
1	E	246/261 (94%)	244 (99%)	2 (1%)	0	100	100
1	F	244/261 (94%)	239 (98%)	5 (2%)	0	100	100
1	G	245/261 (94%)	240 (98%)	5 (2%)	0	100	100
1	H	252/261 (97%)	249 (99%)	3 (1%)	0	100	100
1	I	250/261 (96%)	247 (99%)	3 (1%)	0	100	100
1	J	252/261 (97%)	248 (98%)	4 (2%)	0	100	100
All	All	2498/2610 (96%)	2457 (98%)	41 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	201/208 (97%)	195 (97%)	6 (3%)	41	55
1	B	199/208 (96%)	190 (96%)	9 (4%)	27	37
1	C	202/208 (97%)	196 (97%)	6 (3%)	41	55
1	D	196/208 (94%)	192 (98%)	4 (2%)	55	70
1	E	195/208 (94%)	189 (97%)	6 (3%)	40	54
1	F	192/208 (92%)	184 (96%)	8 (4%)	30	40
1	G	192/208 (92%)	183 (95%)	9 (5%)	26	35
1	H	200/208 (96%)	196 (98%)	4 (2%)	55	70
1	I	201/208 (97%)	189 (94%)	12 (6%)	19	25
1	J	201/208 (97%)	192 (96%)	9 (4%)	27	37
All	All	1979/2080 (95%)	1906 (96%)	73 (4%)	35	46

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	175	TYR
1	A	186	SER
1	A	197	LEU
1	A	215	SER
1	A	240	LEU
1	B	1	MSE
1	B	59	ASP
1	B	137	ASN
1	B	171	GLU
1	B	175	TYR
1	B	186	SER
1	B	188	ASN
1	B	189	TYR
1	B	215	SER
1	C	59	ASP
1	C	137	ASN
1	C	175	TYR
1	C	189	TYR
1	C	190	ARG
1	C	215	SER
1	D	137	ASN

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Mol	Chain	Res	Type
1	D	175	TYR
1	D	197	LEU
1	D	215	SER
1	E	6	THR
1	E	137	ASN
1	E	175	TYR
1	E	201	HIS
1	E	210	THR
1	E	215	SER
1	F	100[A]	MSE
1	F	100[B]	MSE
1	F	137	ASN
1	F	175	TYR
1	F	200	LEU
1	F	205	ASP
1	F	210	THR
1	F	215	SER
1	G	59[A]	ASP
1	G	59[B]	ASP
1	G	92	GLU
1	G	137	ASN
1	G	150	LEU
1	G	175	TYR
1	G	193	LEU
1	G	196	HIS
1	G	215	SER
1	H	137	ASN
1	H	146	THR
1	H	175	TYR
1	H	215	SER
1	I	2	PRO
1	I	59	ASP
1	I	100[A]	MSE
1	I	100[B]	MSE
1	I	137	ASN
1	I	166	LEU
1	I	168	GLU
1	I	171	GLU
1	I	175	TYR
1	I	193	LEU
1	I	210	THR
1	I	215	SER

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Mol	Chain	Res	Type
1	J	137	ASN
1	J	166	LEU
1	J	171	GLU
1	J	175	TYR
1	J	185	LYS
1	J	201	HIS
1	J	210	THR
1	J	215	SER
1	J	248	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	137	ASN
1	A	199	GLN
1	B	-1	ASN
1	B	137	ASN
1	B	242	GLN
1	B	257	GLN
1	C	137	ASN
1	C	247	GLN
1	D	137	ASN
1	D	163	GLN
1	D	180	ASN
1	E	108	GLN
1	E	137	ASN
1	F	137	ASN
1	F	202	GLN
1	G	137	ASN
1	H	137	ASN
1	H	145	ASN
1	H	180	ASN
1	I	137	ASN
1	I	188	ASN
1	J	137	ASN
1	J	199	GLN
1	J	201	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

15 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	GOL	C	301	-	5,5,5	0.54	0	5,5,5	0.24	0
3	ACY	B	302	-	1,3,3	0.63	0	0,3,3	-	-
3	ACY	H	301	-	1,3,3	1.30	0	0,3,3	-	-
3	ACY	A	302	-	1,3,3	2.10	1 (100%)	0,3,3	-	-
2	GOL	C	302	-	5,5,5	0.54	0	5,5,5	0.52	0
2	GOL	A	301	-	5,5,5	0.56	0	5,5,5	0.32	0
3	ACY	D	301	-	1,3,3	2.11	1 (100%)	0,3,3	-	-
3	ACY	E	302	-	1,3,3	2.01	1 (100%)	0,3,3	-	-
3	ACY	G	301	-	1,3,3	1.39	0	0,3,3	-	-
4	PEG	E	301	-	6,6,6	0.69	0	5,5,5	0.29	0
3	ACY	E	303	-	1,3,3	1.81	0	0,3,3	-	-
3	ACY	C	303	-	1,3,3	0.77	0	0,3,3	-	-
4	PEG	B	301	-	6,6,6	0.69	0	5,5,5	0.31	0
3	ACY	I	301	-	1,3,3	1.32	0	0,3,3	-	-
3	ACY	J	301	-	1,3,3	1.56	0	0,3,3	-	-

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
2	GOL	C	301	-	-	2/4/4/4	-
2	GOL	C	302	-	-	0/4/4/4	-
2	GOL	A	301	-	-	2/4/4/4	-
4	PEG	B	301	-	-	2/4/4/4	-
4	PEG	E	301	-	-	1/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	301	ACY	CH3-C	2.11	1.51	1.48
3	A	302	ACY	CH3-C	2.10	1.51	1.48
3	E	302	ACY	CH3-C	2.01	1.51	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	GOL	O1-C1-C2-C3
2	C	301	GOL	O1-C1-C2-C3
4	B	301	PEG	O1-C1-C2-O2
2	C	301	GOL	O1-C1-C2-O2
4	E	301	PEG	O2-C3-C4-O4
2	A	301	GOL	O1-C1-C2-O2
4	B	301	PEG	C4-C3-O2-C2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	ACY	1	0
3	H	301	ACY	1	0
3	A	302	ACY	1	0
3	C	303	ACY	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	250/261 (95%)	0.00	2 (0%)	86	89	45, 65, 95, 137	0
1	B	251/261 (96%)	0.05	5 (1%)	65	72	42, 69, 108, 149	0
1	C	255/261 (97%)	0.04	5 (1%)	65	72	48, 68, 105, 158	0
1	D	251/261 (96%)	0.05	6 (2%)	59	65	49, 73, 111, 162	0
1	E	246/261 (94%)	0.16	6 (2%)	59	65	56, 83, 124, 169	0
1	F	244/261 (93%)	0.28	10 (4%)	37	44	58, 85, 133, 173	0
1	G	244/261 (93%)	0.36	13 (5%)	26	31	60, 94, 152, 165	0
1	H	250/261 (95%)	0.20	5 (2%)	65	72	55, 94, 123, 143	0
1	I	249/261 (95%)	0.16	4 (1%)	72	78	54, 87, 122, 142	0
1	J	252/261 (96%)	0.12	5 (1%)	65	72	56, 80, 110, 144	0
All	All	2492/2610 (95%)	0.14	61 (2%)	59	65	42, 79, 124, 173	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	191	ALA	6.1
1	B	186	SER	5.8
1	D	187	GLY	5.0
1	F	160	ILE	4.6
1	G	223	PHE	4.2
1	C	179	ILE	4.1
1	G	193	LEU	4.0
1	I	145[A]	ASN	3.9
1	C	183	THR	3.9
1	F	2	PRO	3.9
1	E	255	ALA	3.9
1	J	184	GLY	3.8
1	G	249	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	179	ILE	3.5
1	B	189	TYR	3.4
1	B	190	ARG	3.4
1	I	169	GLY	3.3
1	H	205	ASP	3.3
1	C	180	ASN	3.2
1	C	181	GLY	3.1
1	E	18	GLY	3.1
1	E	220	LEU	3.1
1	J	5	LEU	3.0
1	D	185	LYS	3.0
1	D	186	SER	2.8
1	F	169	GLY	2.8
1	G	194	ASP	2.8
1	F	212	PHE	2.8
1	G	178	ALA	2.8
1	E	256	TYR	2.8
1	I	170	ALA	2.7
1	F	139	VAL	2.7
1	H	9	LEU	2.6
1	J	180	ASN	2.6
1	G	114	PHE	2.6
1	F	161	GLU	2.5
1	D	189	TYR	2.5
1	C	189	TYR	2.5
1	J	2	PRO	2.5
1	J	256	TYR	2.4
1	F	203	VAL	2.4
1	G	19	ILE	2.4
1	A	186	SER	2.4
1	H	48	VAL	2.4
1	H	20	PHE	2.3
1	F	15	ALA	2.3
1	F	133	HIS	2.3
1	F	171	GLU	2.3
1	B	197	LEU	2.2
1	G	256	TYR	2.2
1	G	154	VAL	2.2
1	E	249	PHE	2.2
1	D	188	ASN	2.2
1	G	156	LEU	2.2
1	D	133	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	47	GLY	2.2
1	G	258	LYS	2.1
1	G	212	PHE	2.1
1	E	35	GLY	2.1
1	G	0	ALA	2.1
1	I	223	PHE	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	A	301	6/6	0.70	0.37	94,106,108,108	0
4	PEG	E	301	7/7	0.72	0.33	90,112,120,120	0
2	GOL	C	301	6/6	0.73	0.21	105,108,108,111	0
4	PEG	B	301	7/7	0.83	0.18	87,88,98,98	0
2	GOL	C	302	6/6	0.84	0.19	81,87,92,95	0
3	ACY	G	301	4/4	0.91	0.12	89,90,92,94	0
3	ACY	B	302	4/4	0.91	0.19	88,92,93,93	0
3	ACY	C	303	4/4	0.91	0.14	68,72,79,80	0
3	ACY	A	302	4/4	0.93	0.17	67,71,73,75	0
3	ACY	J	301	4/4	0.93	0.17	73,73,85,85	0
3	ACY	D	301	4/4	0.94	0.11	76,82,83,88	0
3	ACY	H	301	4/4	0.94	0.16	83,92,92,93	0
3	ACY	I	301	4/4	0.94	0.18	90,94,98,99	0
3	ACY	E	302	4/4	0.97	0.17	86,91,93,96	0
3	ACY	E	303	4/4	0.97	0.15	77,81,84,85	0

6.5 Other polymers (i)

There are no such residues in this entry.