W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:37 PM GMT

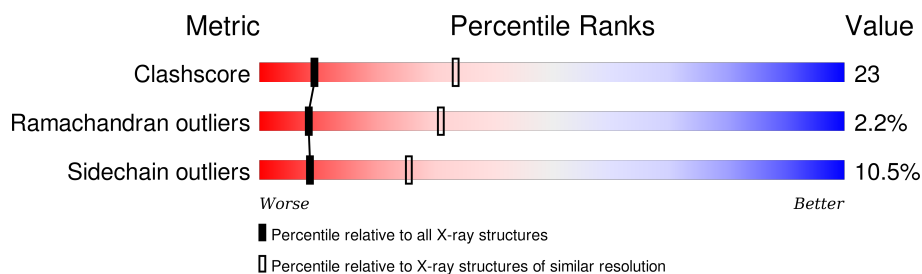|		
PDB ID	:	1PRT
Title	:	THE CRYSTAL STRUCTURE OF PERTUSSIS TOXIN
Authors	:	Stein, P.E.; Read, R.J.
Deposited on	:	1993-11-22
Resolution	:	2.90 Å(reported)

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 2.90 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	Percentile Ranks	Value
Clashscore		23
Ramachandran outliers		2.2%
Sidechain outliers		10.5%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
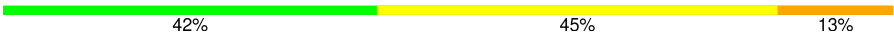
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	234	56% 36% · · ·
1	G	234	56% 35% · ·
2	B	196	57% 37% 6%
2	H	196	58% 35% 8%
3	C	196	60% 31% 7% ·
3	I	196	47% 45% 8%
4	D	110	64% 35% ·

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Mol	Chain	Length	Quality of chain
4	E	110	54% 40% 5%
4	J	110	65% 31% 5%
4	K	110	49% 44% 7%
5	F	98	54% 35% 10%
5	L	98	42% 45% 13%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14504 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 PERTUSSIS TOXIN (SUBUNIT S1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1769	1095	318	350	6			
1	G	224	Total	C	N	O	S	0	0	0
			1769	1095	318	350	6			

- Molecule 2 is a protein called PERTUSSIS TOXIN (SUBUNIT S2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	196	Total	C	N	O	S	0	0	0
			1522	961	260	292	9			
2	H	196	Total	C	N	O	S	0	0	0
			1522	961	260	292	9			

- Molecule 3 is a protein called PERTUSSIS TOXIN (SUBUNIT S3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	196	Total	C	N	O	S	0	0	0
			1521	969	258	285	9			
3	I	196	Total	C	N	O	S	0	0	0
			1521	969	258	285	9			

- Molecule 4 is a protein called PERTUSSIS TOXIN (SUBUNIT S4).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	110	Total	C	N	O	S	0	0	0
			838	536	143	147	12			
4	E	110	Total	C	N	O	S	0	0	0
			838	536	143	147	12			
4	J	110	Total	C	N	O	S	0	0	0
			838	536	143	147	12			
4	K	110	Total	C	N	O	S	0	0	0
			838	536	143	147	12			

• Molecule 5 is a protein called PERTUSSIS TOXIN (SUBUNIT S5).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	98	Total	C	N	O	S	0	0	0
			764	489	125	144	6			
5	L	98	Total	C	N	O	S	0	0	0
			764	489	125	144	6			

3 Residue-property plots (i)

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

Note EDS was not executed.

- Molecule 1: PERTUSSIS TOXIN (SUBUNIT S1)

- Molecule 1: PERTUSSIS TOXIN (SUBUNIT S1)

- Molecule 2: PERTUSSIS TOXIN (SUBUNIT S2)

• Molecule 2: PERTUSSIS TOXIN (SUBUNIT S2)

Chain H: 58%   35%   8%

G4 I5 V6 I7 P8 Q12 Q15 H16 Y20 G21 R22 C23 A24 N25 K26 T27 R28 T31 V32 A33 E34 L35 S38 L41 V48 T49 R50 G51 W52 F55 T61 Y62 L63 G64 G65 E66 Y67 G68 G69 V70 A79 F80 D81 L82 I88 M89 T90 T91

Y103 S104 N105 V106 T107 A108 T109 R110 L111 L112 R118 L119 C120 F123 V124 P129 V130 I131 G132 A133 C134 T135 S136 P137 Y138 D139 M145 Y146 S147 R148 L149 R150 K151 M152 L153 Y154 L155 I161 S162 V163 R164 Q172 Y173 Y174 D175 Y176 E177 Y184 A185 L186 T187 G188 I189

S190 I191 C192 N193 P194 G195 S196 C199
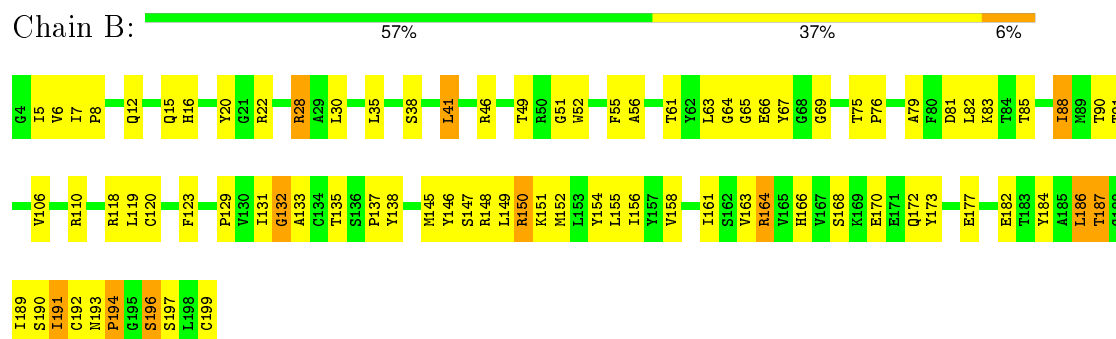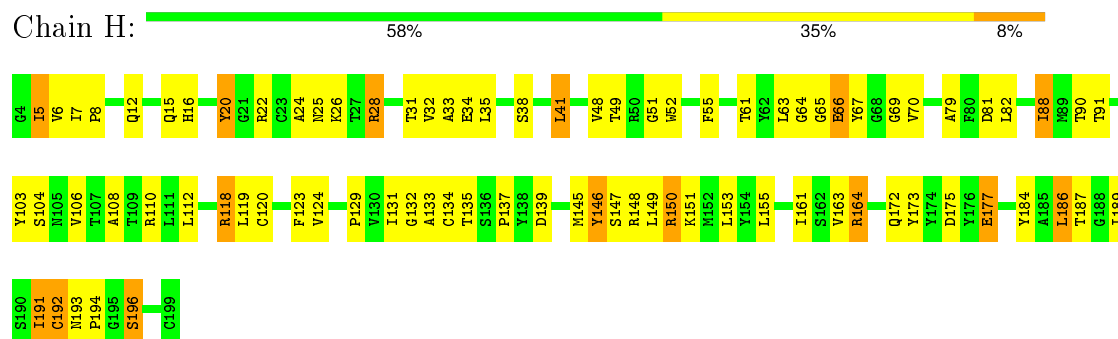
• Molecule 3: PERTUSSIS TOXIN (SUBUNIT S3)

Chain C: 60%   31%   7% •

G4 P9 L12 F13 T14 Q15 A19 Y20 G21 R22 C23 P24 N25 G26 T27 R28 V32 A33 E34 L35 R36 L41 L45 T49 P50 G51 W52 Y55 G56 L57 Y58 D59 G60 L63 G64 Q65 A66 Y67 I70 I71 K72 D73 A74 R83 E84 I88 T107

L111 L112 A113 S114 T115 N116 S117 R118 L119 F123 V124 R125 Q128 A133 P137 R141 Y142 R143 Y146 R150 R151 L152 L153 I156 Y157 V163 V167 S168 K169 E170 D175 Y176 E177 D178 Y184 A185 L186 I189 N193 P194 A195 A196 S197 I198 C199

• Molecule 3: PERTUSSIS TOXIN (SUBUNIT S3)

Chain I: 47%   45%   8%

G4 P9 L12 Q15 Q16 G17 G18 A19 R22 C23 P24 N25 G26 T27 R28 T31 V32 A33 E34 L35 R36 L41 L45 I48 T49 P50 G51 W52 Y55 G56 L57 Y58 D59 G60 T61 Y62 L63 G64 Q65 A66 Y67 G68 G69 I70 I71 K72 D73 A74 G77 A78

G79 F80 R83 E84 T85 F86 C87 I88 T89 T90 I91 Y92 A98 Y103 S104 K105 V106 T107 A108 L111 L112 A113 S114 T115 N116 S117 R118 L119 C120 F123 V124 R125 D126 V130 I131 G132 A133 P137 Y142 R143 Y146 R150 R151 L152 L153 Y154 M155 I156 Y157 M158

A162 V163 R164 V167 S168 K169 E170 Y173 Y174 D175 Y176 E177 F181 Q182 T183 Y184 A185 L186 T187 G188 I189 S190 L191 C192 N193 P194 A195 A196 S197 I198 C199

• Molecule 4: PERTUSSIS TOXIN (SUBUNIT S4)

Chain D: 64%   35% •

D1 V2 P3 L6 V7 K8 T9 N10 M11 Y21 T24 P25 T26 R27 M28 L29 V30 K36 S43 P44 L56 K57 R58 P59 G60 S61 S62 P63 M64 M67 V71 Q75 R76 P77 L78 R79 M80 F81 L82 G83 P84 K85 Q86 L87 T88 F89 E90 G91 K92 P93 A94

L97 P110

• Molecule 4: PERTUSSIS TOXIN (SUBUNIT S4)

Chain E: 54%   40%   5% •

D1 V2 P3 Y4 V5 T9 N10 T14 S15 V16 A17 M18 K19 E22 V23 T24 P25 T26 L29 V30 C31 L37 G38 A39 A40 A41 S42 S43 C51 L56 K57 P63 M64 M73 Q74 Q75 R76 P77 L78 R79 Q86 L87 T88 F89 K92 P93 A94 L95 E96

L97 I98 R99 M100 V101 S104 Q107 D108 C109 P110

● Molecule 4: PERTUSSIS TOXIN (SUBUNIT S4)

Chain J:

65% | 31% | 5%

D1 V2 P3 Y4 N10 M11 V16 A17 M18 T26 R27 M28 K36 L37 A40 A46 F50 C51 L56 P63 M64 R69 L78 R79 M80 F81 L82 G83 P84 K85 Q86 L87 T88 F89 E90 P93 A94 L95 E96 L97 I98 R99 S104 D108 C109 P110

● Molecule 4: PERTUSSIS TOXIN (SUBUNIT S4)

Chain K:

49% | 44% | 7%

D1 V2 P3 Y4 V5 L6 V7 K8 M11 V12 V13 T14 S15 V16 A17 M18 Y21 E22 V23 T24 P25 T26 R27 M28 G32 I33 K36 L37 G38 A39 A40 A41 S42 S43 C51 F52 L56 K57 S62 P63 M64 E65 V66 M67 L68 V71 Q75 R76 R79

L82 G83 P84 K85 Q86 L87 A94 L97 I98 R99 M100 V101 E102 Q107 D108 C109 P110

● Molecule 5: PERTUSSIS TOXIN (SUBUNIT S5)

Chain F:

54% | 35% | 10% | ·

L2 P3 T4 H5 L6 Y7 F10 T11 V12 Q13 E14 Q24 E25 F26 A30 F31 M32 R35 S36 R39 A40 C41 L42 A45 G46 H47 E48 H49 D50 T51 W52 M56 L57 I61 L66 K67 S68 R69 L72 T73 V74 E75 D76 S77 P78 Y79 T82 P83 G84

D85 L86 L87 P93 E99

● Molecule 5: PERTUSSIS TOXIN (SUBUNIT S5)

Chain L:

42% | 45% | 13%

L2 P3 T4 H5 L6 Y7 K8 N9 F10 T11 V12 Q13 E14 L17 Q24 E25 F26 C27 L28 T29 A30 F31 R35 S36 L37 V38 R39 A40 C41 L42 A45 H49 D50 T51 W52 F53 D54 T55 M56 L57 G58 F59 A60 I61 Y64 S68 R69 I70 A71 L72 T73 V74 E75

D76 Y79 P80 P83 G84 D85 L86 L87 E88 L89 Q90 I91 C92 P93 L94 N95 G96 Y97 C98 E99

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	163.80Å 98.20Å 194.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.195 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14504	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	0.72	2/1809 (0.1%)	0.88	3/2457 (0.1%)
1	G	0.55	1/1809 (0.1%)	0.78	3/2457 (0.1%)
2	B	0.68	0/1558	0.90	2/2115 (0.1%)
2	H	0.65	0/1558	0.89	2/2115 (0.1%)
3	C	0.68	0/1557	0.87	1/2115 (0.0%)
3	I	0.64	0/1557	0.84	1/2115 (0.0%)
4	D	0.72	0/856	0.93	1/1155 (0.1%)
4	E	0.88	1/856 (0.1%)	0.98	3/1155 (0.3%)
4	J	0.66	0/856	0.89	2/1155 (0.2%)
4	K	0.62	0/856	0.87	1/1155 (0.1%)
5	F	0.69	0/782	0.91	1/1059 (0.1%)
5	L	0.61	0/782	0.88	0/1059
All	All	0.67	4/14836 (0.0%)	0.88	20/20112 (0.1%)

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	G	0	1
2	B	0	1
2	H	0	1
3	C	0	1
3	I	0	2
5	L	0	1
All	All	0	7

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	100	MET	C-N	15.84	1.70	1.34
1	A	202	MET	C-N	5.89	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	135	ARG	N-CA	5.03	1.56	1.46
1	G	134	ARG	C-O	5.00	1.32	1.23

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	100	MET	O-C-N	11.77	141.53	122.70
1	A	135	ARG	N-CA-CB	9.61	127.89	110.60
4	E	100	MET	CA-C-N	-9.22	96.92	117.20
1	G	135	ARG	NE-CZ-NH2	8.11	124.36	120.30
1	G	134	ARG	NE-CZ-NH2	8.03	124.31	120.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	138	TYR	Sidechain
3	C	28	ARG	Sidechain
1	G	87	TYR	Sidechain
2	H	146	TYR	Sidechain
3	I	103	TYR	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	1769	0	1655	71	0
1	G	1769	0	1655	83	0
2	B	1522	0	1473	72	0
2	H	1522	0	1473	68	0
3	C	1521	0	1484	68	0
3	I	1521	0	1484	92	0
4	D	838	0	874	27	0
4	E	838	0	873	47	0
4	J	838	0	874	34	0
4	K	838	0	874	48	0
5	F	764	0	747	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	764	0	747	65	0
All	All	14504	0	14213	652	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 23.

The worst 5 of 652 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)
4:E:100:MET:C	4:E:101:VAL:N	1.70	1.44
4:D:2:VAL:HG22	4:D:3:PRO:HD2	1.35	1.07
4:J:2:VAL:HG22	4:J:3:PRO:HD2	1.40	0.99
1:A:69:GLN:HG3	4:E:37:LEU:HD23	1.45	0.97
2:B:163:VAL:HG21	2:B:189:ILE:HG23	1.49	0.95

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	220/234 (94%)	197 (90%)	20 (9%)	3 (1%)	14	44
1	G	220/234 (94%)	194 (88%)	24 (11%)	2 (1%)	21	57
2	B	194/196 (99%)	176 (91%)	15 (8%)	3 (2%)	13	42
2	H	194/196 (99%)	173 (89%)	17 (9%)	4 (2%)	9	32
3	C	194/196 (99%)	168 (87%)	21 (11%)	5 (3%)	7	26
3	I	194/196 (99%)	171 (88%)	18 (9%)	5 (3%)	7	26
4	D	108/110 (98%)	99 (92%)	9 (8%)	0	100	100
4	E	108/110 (98%)	95 (88%)	9 (8%)	4 (4%)	4	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	J	108/110 (98%)	98 (91%)	10 (9%)	0	100	100
4	K	108/110 (98%)	97 (90%)	5 (5%)	6 (6%)	2	7
5	F	96/98 (98%)	83 (86%)	8 (8%)	5 (5%)	2	8
5	L	96/98 (98%)	81 (84%)	11 (12%)	4 (4%)	3	13
All	All	1840/1888 (98%)	1632 (89%)	167 (9%)	41 (2%)	8	31

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	45	ALA
5	F	49	HIS
5	L	49	HIS
5	L	50	ASP
2	B	110	ARG

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	185/190 (97%)	167 (90%)	18 (10%)	10	30
1	G	185/190 (97%)	170 (92%)	15 (8%)	15	39
2	B	163/163 (100%)	144 (88%)	19 (12%)	7	19
2	H	163/163 (100%)	140 (86%)	23 (14%)	4	12
3	C	155/155 (100%)	136 (88%)	19 (12%)	6	17
3	I	155/155 (100%)	139 (90%)	16 (10%)	9	26
4	D	94/94 (100%)	87 (93%)	7 (7%)	17	44
4	E	94/94 (100%)	85 (90%)	9 (10%)	10	31
4	J	94/94 (100%)	88 (94%)	6 (6%)	22	53
4	K	94/94 (100%)	86 (92%)	8 (8%)	13	37
5	F	83/83 (100%)	70 (84%)	13 (16%)	3	9
5	L	83/83 (100%)	73 (88%)	10 (12%)	6	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1548/1558 (99%)	1385 (90%)	163 (10%)	8 25

5 of 163 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	12	VAL
1	G	123	LEU
4	K	64	MET
5	F	26	PHE
5	F	83	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	24	GLN
1	G	66	HIS
4	J	10	ASN
1	G	42	GLN
1	G	83	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.