wwPDB X-ray Structure Validation Summary Report (i)

May 29, 2024 – 06:52 PM EDT

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)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

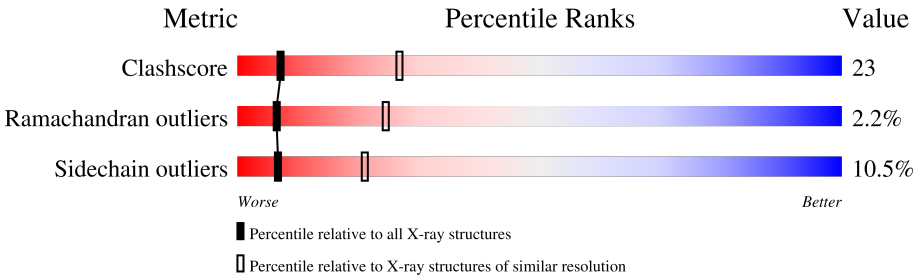
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (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 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%

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%
4	E	110	54% 40% 5%

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Mol	Chain	Length	Quality of chain
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			

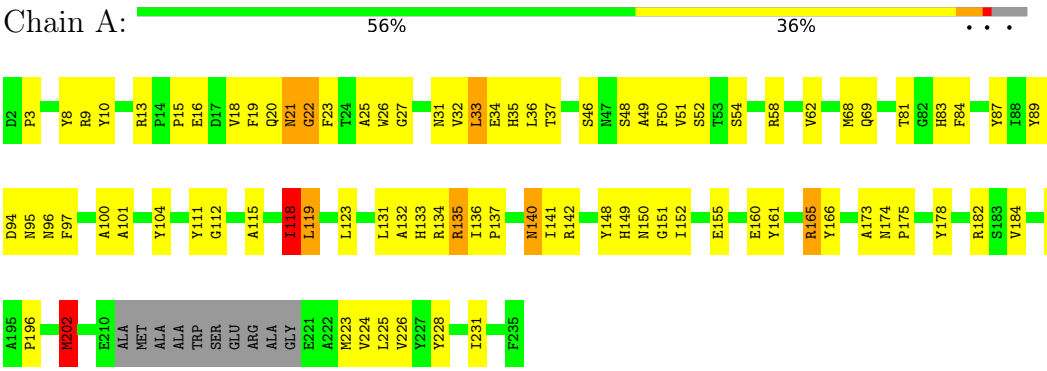
3 Residue-property plots (i)

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

Note EDS was not executed.

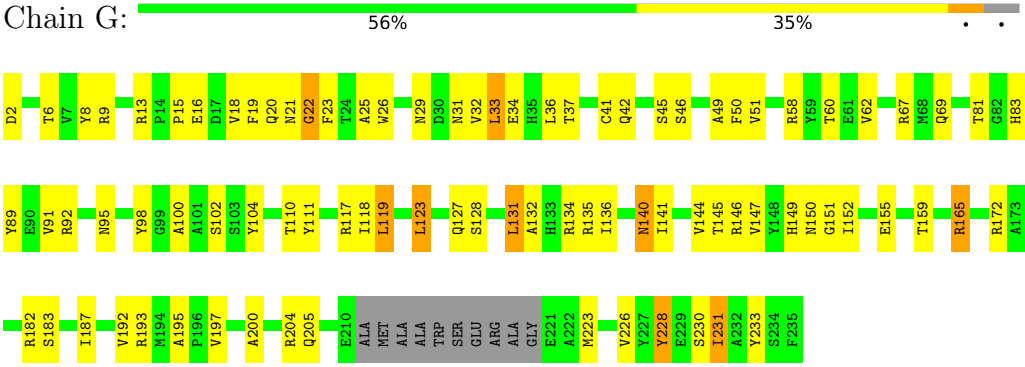
• Molecule 1: PERTUSSIS TOXIN (SUBUNIT S1)

Chain A:



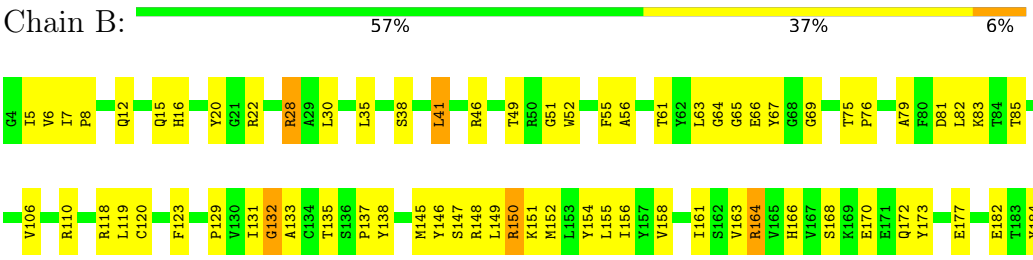
• Molecule 1: PERTUSSIS TOXIN (SUBUNIT S1)

Chain G:



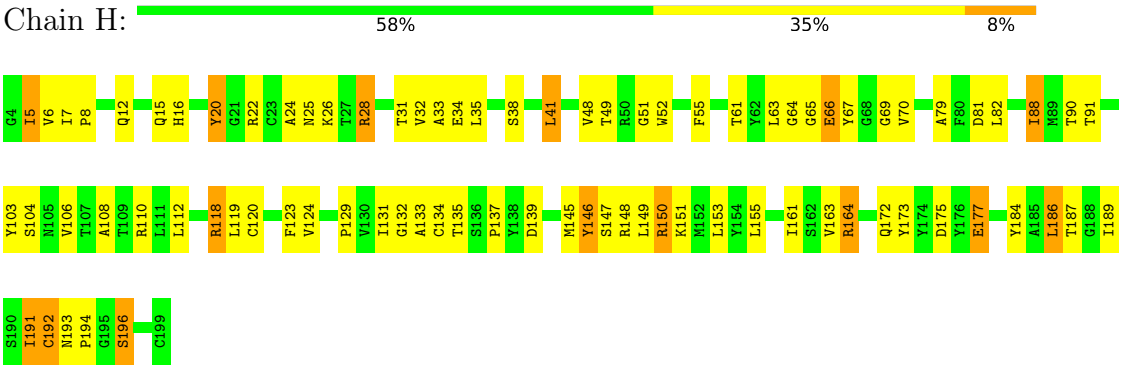
• Molecule 2: PERTUSSIS TOXIN (SUBUNIT S2)

Chain B:



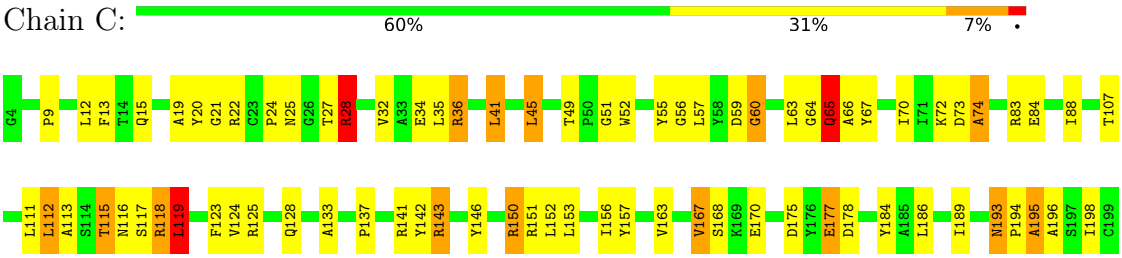
• Molecule 2: PERTUSSIS TOXIN (SUBUNIT S2)

Chain H:



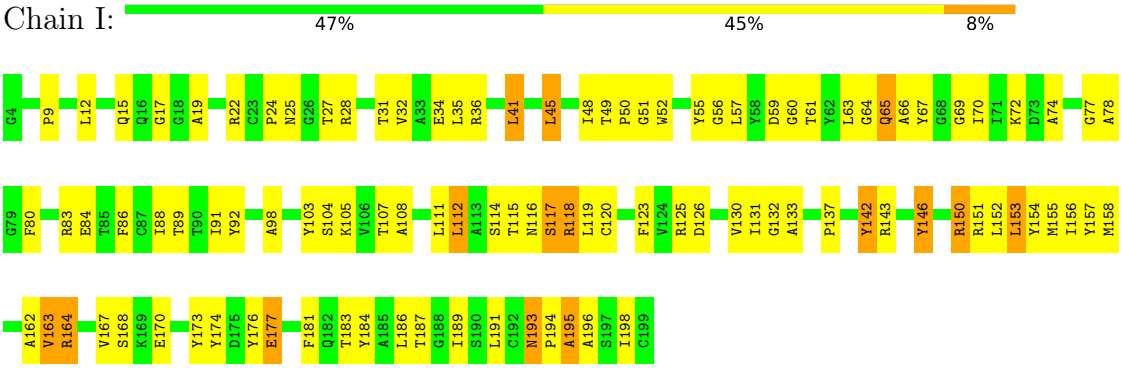
• Molecule 3: PERTUSSIS TOXIN (SUBUNIT S3)

Chain C:



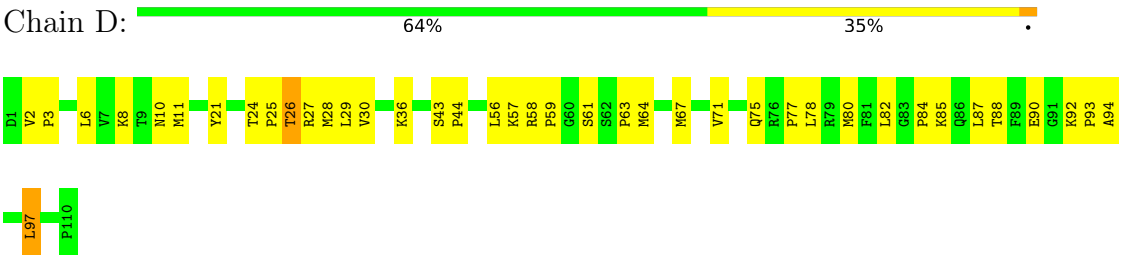
• Molecule 3: PERTUSSIS TOXIN (SUBUNIT S3)

Chain I:



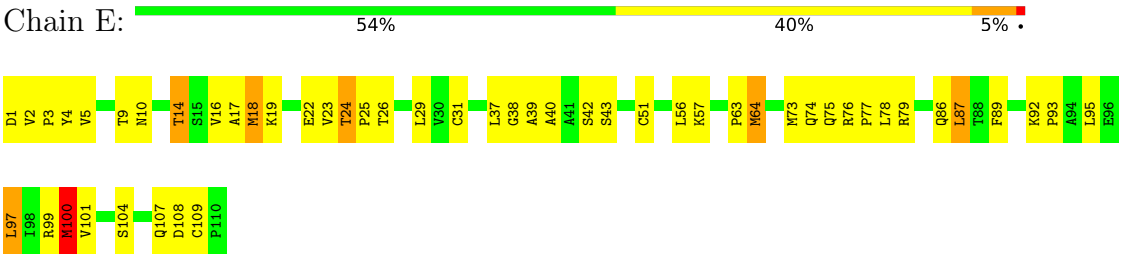
• Molecule 4: PERTUSSIS TOXIN (SUBUNIT S4)

Chain D:



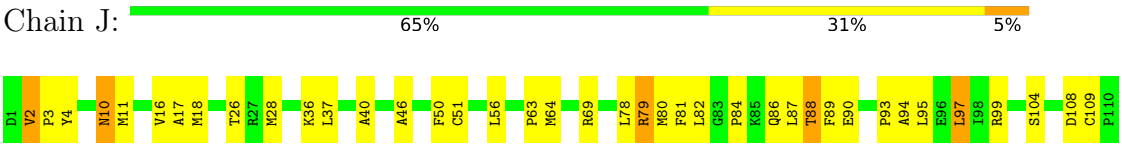
• Molecule 4: PERTUSSIS TOXIN (SUBUNIT S4)

Chain E:



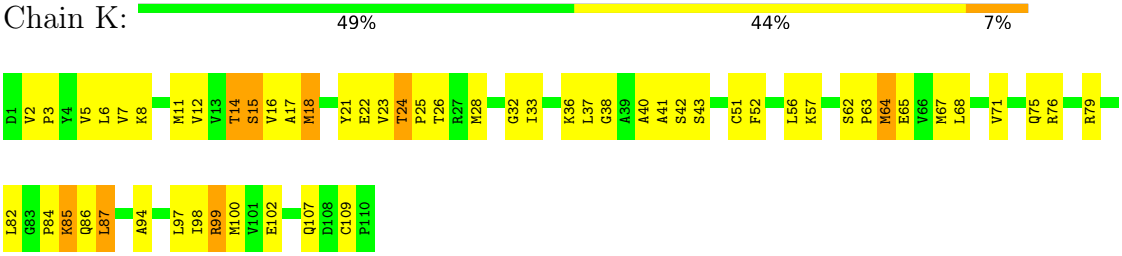
• Molecule 4: PERTUSSIS TOXIN (SUBUNIT S4)

Chain J:



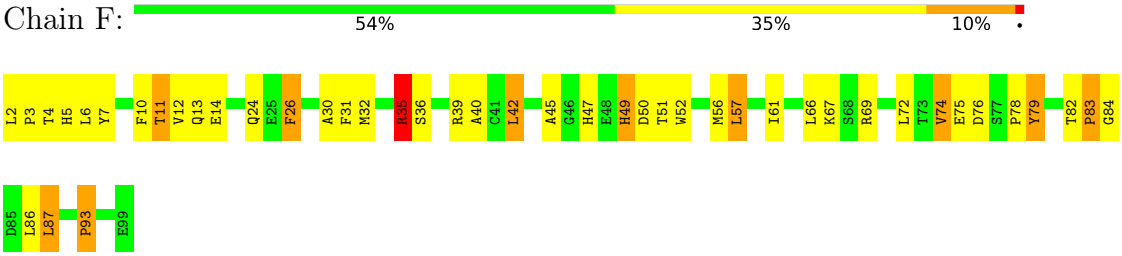
• Molecule 4: PERTUSSIS TOXIN (SUBUNIT S4)

Chain K:



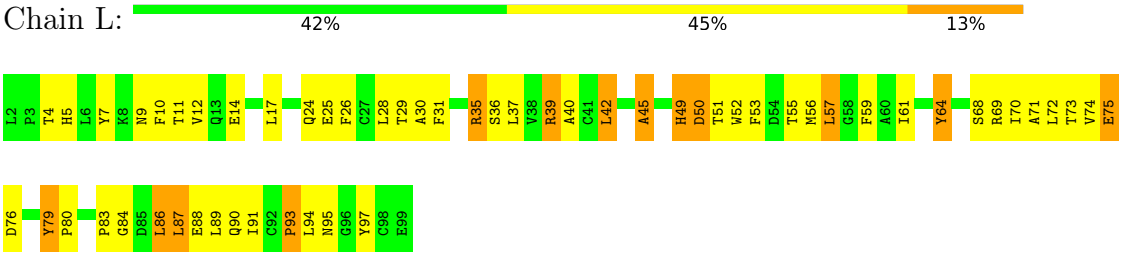
• Molecule 5: PERTUSSIS TOXIN (SUBUNIT S5)

Chain F:



• Molecule 5: PERTUSSIS TOXIN (SUBUNIT S5)

Chain L:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore 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

5.1 Standard geometry

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(^{o})	Ideal(^{o})
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%)	11 36
1	G	220/234 (94%)	194 (88%)	24 (11%)	2 (1%)	17 48
2	B	194/196 (99%)	176 (91%)	15 (8%)	3 (2%)	10 34
2	H	194/196 (99%)	173 (89%)	17 (9%)	4 (2%)	7 26
3	C	194/196 (99%)	168 (87%)	21 (11%)	5 (3%)	5 20
3	I	194/196 (99%)	171 (88%)	18 (9%)	5 (3%)	5 20
4	D	108/110 (98%)	99 (92%)	9 (8%)	0	100 100
4	E	108/110 (98%)	95 (88%)	9 (8%)	4 (4%)	3 13

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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 5
5	F	96/98 (98%)	83 (86%)	8 (8%)	5 (5%)	2 6
5	L	96/98 (98%)	81 (84%)	11 (12%)	4 (4%)	3 10
All	All	1840/1888 (98%)	1632 (89%)	167 (9%)	41 (2%)	6 24

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%)	8 25
1	G	185/190 (97%)	170 (92%)	15 (8%)	11 33
2	B	163/163 (100%)	144 (88%)	19 (12%)	5 16
2	H	163/163 (100%)	140 (86%)	23 (14%)	3 10
3	C	155/155 (100%)	136 (88%)	19 (12%)	4 14
3	I	155/155 (100%)	139 (90%)	16 (10%)	7 22
4	D	94/94 (100%)	87 (93%)	7 (7%)	13 38
4	E	94/94 (100%)	85 (90%)	9 (10%)	8 25
4	J	94/94 (100%)	88 (94%)	6 (6%)	17 45
4	K	94/94 (100%)	86 (92%)	8 (8%)	10 31
5	F	83/83 (100%)	70 (84%)	13 (16%)	2 8
5	L	83/83 (100%)	73 (88%)	10 (12%)	5 15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1548/1558 (99%)	1385 (90%)	163 (10%)	7 21

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

Mol	Chain	Res	Type
2	H	164	ARG
4	J	88	THR
2	H	187	THR
3	I	117	SER
4	K	64	MET

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

Mol	Chain	Res	Type
1	G	31	ASN
4	J	10	ASN
1	G	83	HIS
5	L	24	GLN
2	H	172	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	100:MET	C	101:VAL	N	1.70

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.